



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2022 – 10:19 AM EDT

PDB ID : 7TIH
Title : Structure of oxidized bovine cytochrome c oxidase with reduced metal centers induced by synchrotron X-ray exposure
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.; Russi, S.; Cohen, A.
Deposited on : 2022-01-13
Resolution : 2.35 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.29
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) : 2.29

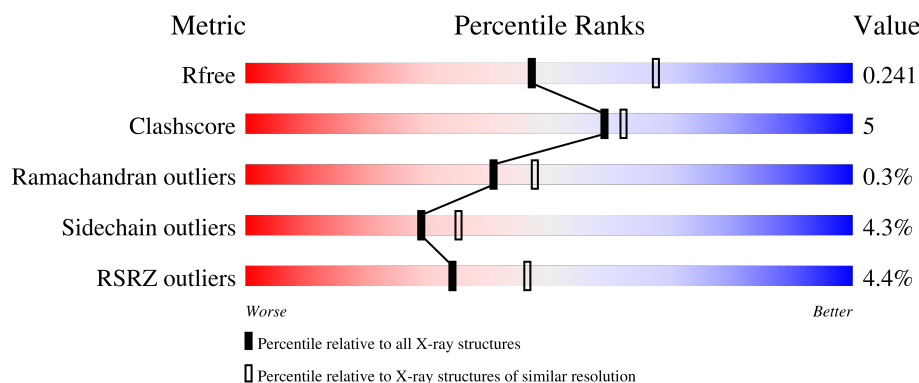
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.

















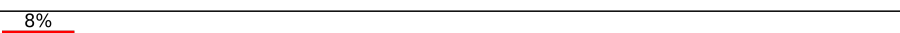
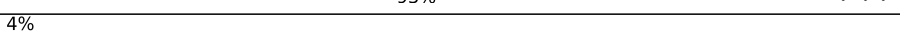





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 $\leq 5\%$. 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	<div> <div>89%</div> <div>11%</div> </div>
1	N	514	<div> <div>86%</div> <div>13%</div> </div>
2	B	227	<div> <div>82%</div> <div>17%</div> </div>
2	O	227	<div> <div>84%</div> <div>16%</div> </div>
3	C	261	<div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	 90% 9% .
4	D	147	 90% 7% ..
4	Q	147	 10% 86% 11% ..
5	E	109	 3% 87% 9% .
5	R	109	 4% 85% 11% .
6	F	98	 6% 87% 12% .
6	S	98	 6% 72% 23% .
7	G	85	 18% 80% 18% ..
7	T	85	 25% 78% 13% 8% .
8	H	85	 12% 76% 14% .. 7%
8	U	85	 11% 79% 13% . 7%
9	I	73	 16% 92% 7% .
9	V	73	 14% 90% 7% ..
10	J	59	 8% 90% 7% ..
10	W	59	 8% 93% . . .
11	K	56	 4% 80% 7% 12%
11	X	56	 11% 80% 7% 12%
12	L	47	 87% 11% .
12	Y	47	 4% 70% 23% . .
13	M	46	 4% 80% 11% . 7%
13	Z	46	 13% 70% 24% 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
18	HEA	A	606	X	-	-	-
18	HEA	A	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	605	X	-	-	-
18	HEA	N	606	X	-	-	-
19	EDO	A	617	-	-	-	X
19	EDO	D	205	-	-	-	X
19	EDO	N	608	-	-	-	X
19	EDO	N	614	-	-	-	X
23	PSC	R	201	X	-	-	-
26	DMU	G	101	-	-	-	X
29	SAC	I	101	-	-	-	X
29	SAC	V	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Cu	0	0
			1	1		
14	N	1	Total	Cu	0	0
			1	1		

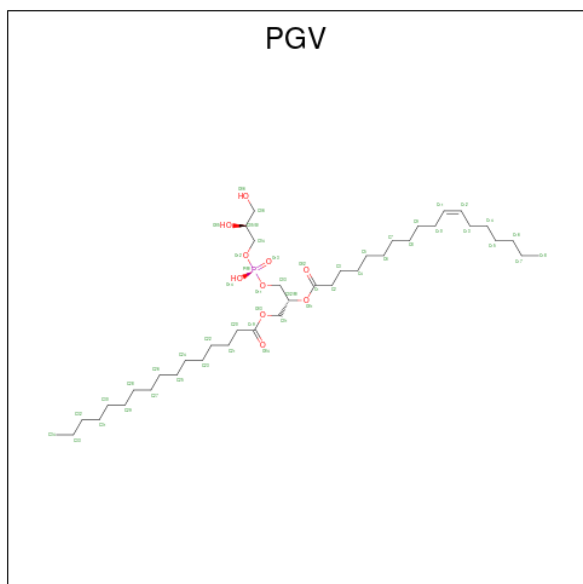
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

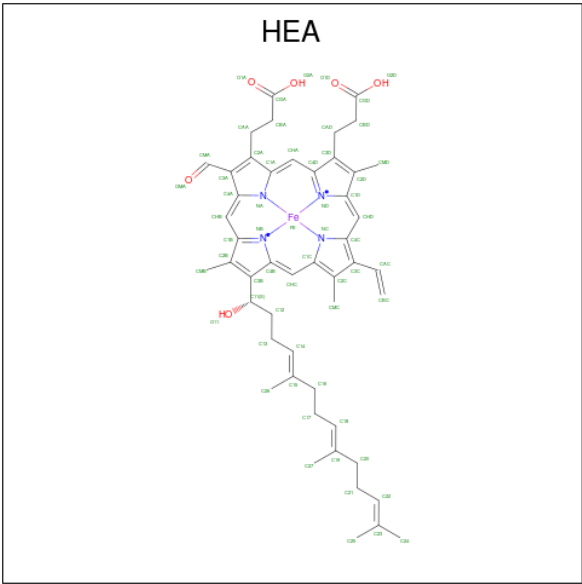
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



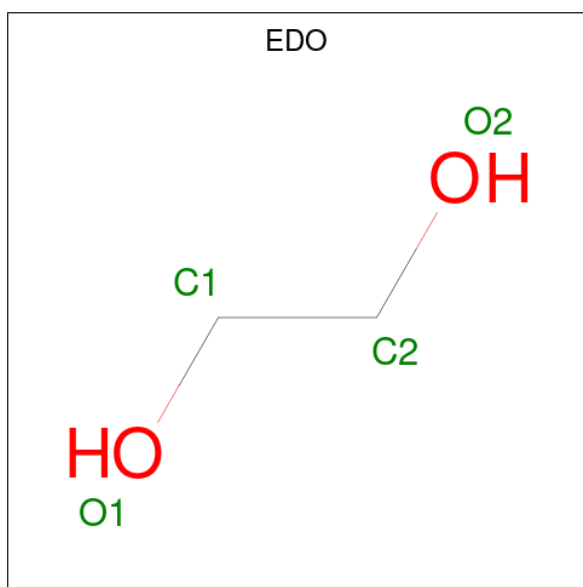
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	B	1	Total	C	O	0	0
			4	2	2		
19	B	1	Total	C	O	0	0
			4	2	2		
19	B	1	Total	C	O	0	0
			4	2	2		
19	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total 4	C 2	O 2	0	0
19	B	1	Total 4	C 2	O 2	0	0
19	B	1	Total 4	C 2	O 2	0	0
19	B	1	Total 4	C 2	O 2	0	0
19	C	1	Total 4	C 2	O 2	0	0
19	C	1	Total 4	C 2	O 2	0	0
19	C	1	Total 4	C 2	O 2	0	0
19	C	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	D	1	Total 4	C 2	O 2	0	0
19	E	1	Total 4	C 2	O 2	0	0
19	E	1	Total 4	C 2	O 2	0	0
19	E	1	Total 4	C 2	O 2	0	0
19	E	1	Total 4	C 2	O 2	0	0
19	E	1	Total 4	C 2	O 2	0	0
19	F	1	Total 4	C 2	O 2	0	0
19	F	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	M	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0

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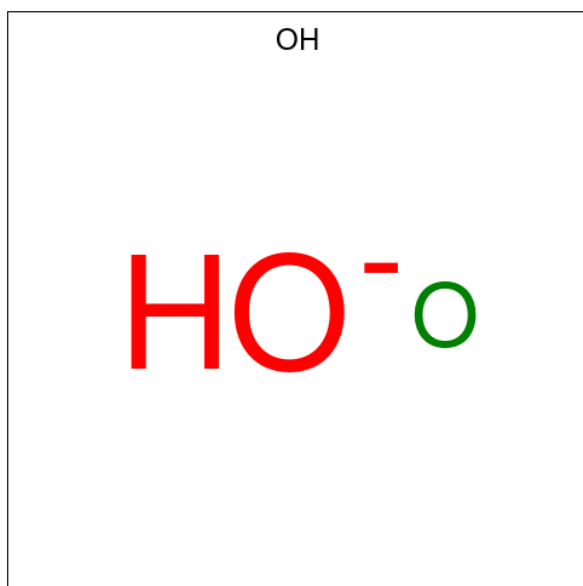
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	O	1	Total C O 4 2 2	0	0
19	O	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4 2 2	0	0
19	Q	1	Total C O 4 2 2	0	0
19	Q	1	Total C O 4 2 2	0	0
19	Q	1	Total C O 4 2 2	0	0
19	Q	1	Total C O 4 2 2	0	0
19	R	1	Total C O 4 2 2	0	0
19	R	1	Total C O 4 2 2	0	0
19	S	1	Total C O 4 2 2	0	0
19	S	1	Total C O 4 2 2	0	0
19	S	1	Total C O 4 2 2	0	0

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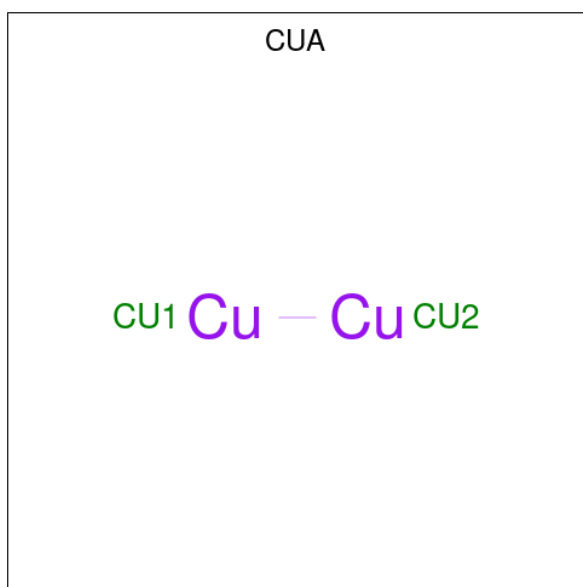
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	S	1	Total C O 4 2 2	0	0
19	T	1	Total C O 4 2 2	0	0
19	V	1	Total C O 4 2 2	0	0
19	V	1	Total C O 4 2 2	0	0
19	W	1	Total C O 4 2 2	0	0
19	W	1	Total C O 4 2 2	0	0
19	Z	1	Total C O 4 2 2	0	0

- Molecule 20 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



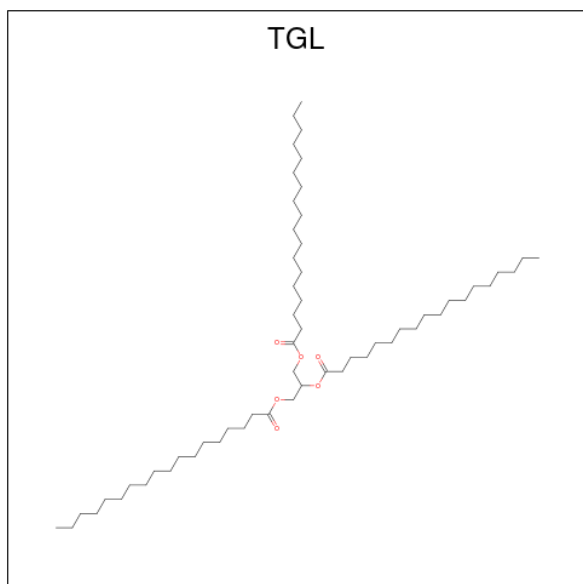
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total O 1 1	0	0
20	N	1	Total O 1 1	0	0

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$) (labeled as "Ligand of Interest" by depositor).



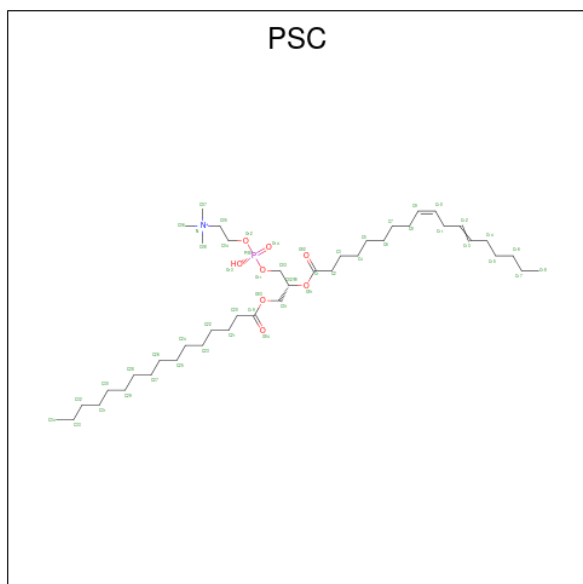
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		

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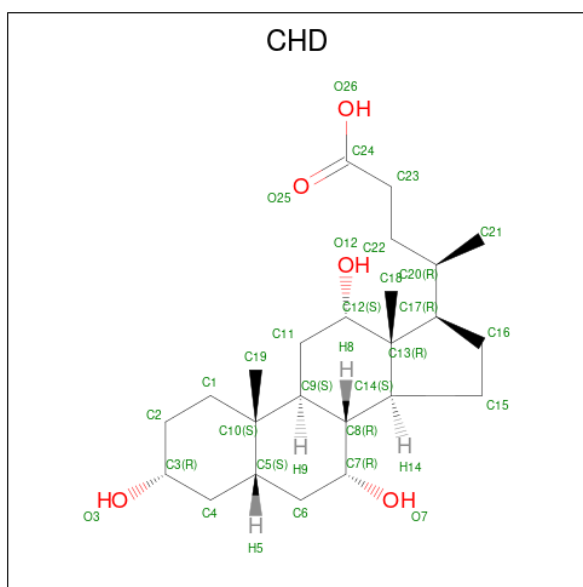
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	D	1	Total	C	O	0	0
			63	57	6		
22	L	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	Q	1	Total	C	O	0	0
			63	57	6		
22	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 23 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: C₄₂H₈₁NO₈P).



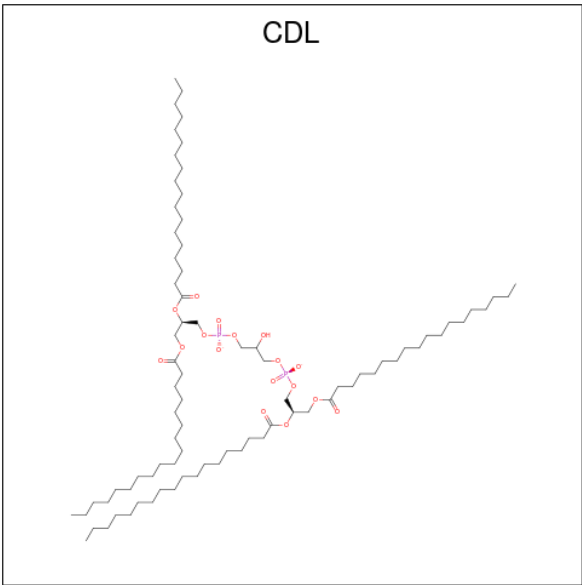
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



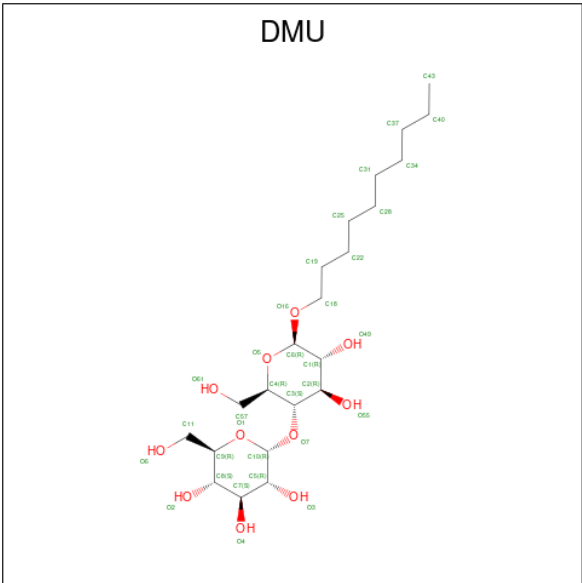
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	G	1	Total C O 29 24 5	0	0
24	J	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	W	1	Total C O 29 24 5	0	0
24	Y	1	Total C O 29 24 5	0	0

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



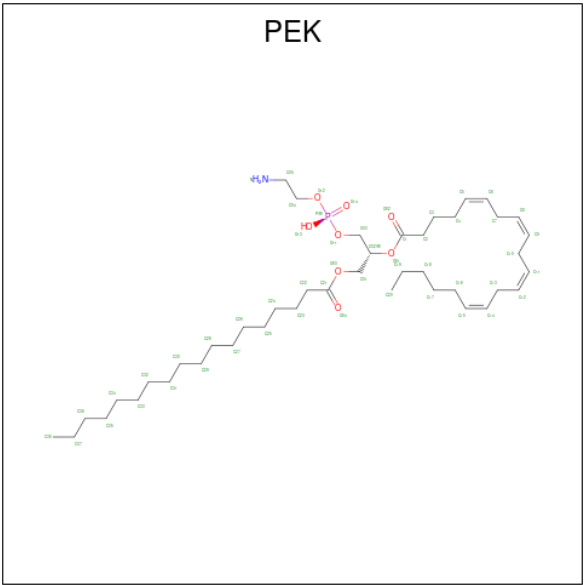
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	C	1	Total	C	O	0	0
			33	22	11		
26	D	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	Q	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 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: C₄₃H₇₈NO₈P).



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

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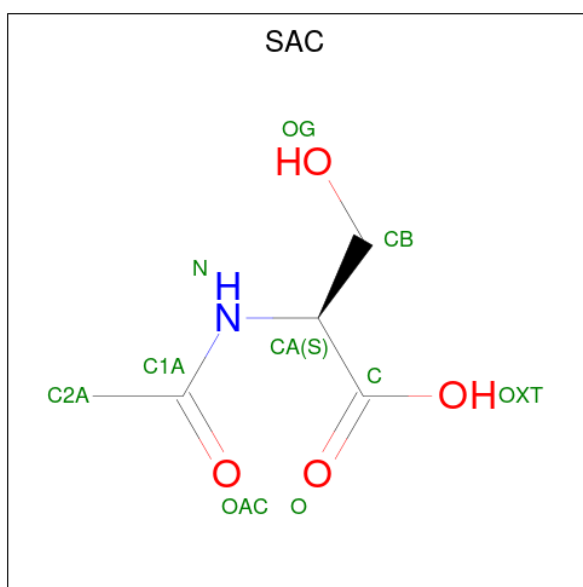
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	F	1	Total	Zn	0	0
			1	1		
28	S	1	Total	Zn	0	0
			1	1		

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	I	1	Total	C	N	O	0	0
			9	5	1	3		
29	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	188	Total	O	0	0
			188	188		
30	B	107	Total	O	0	0
			107	107		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	C	107	Total 107	O 107	0	0
30	D	89	Total 89	O 89	0	0
30	E	71	Total 71	O 71	0	0
30	F	68	Total 68	O 68	0	0
30	G	32	Total 32	O 32	0	0
30	H	41	Total 41	O 41	0	0
30	I	31	Total 31	O 31	0	0
30	J	23	Total 23	O 23	0	0
30	K	19	Total 19	O 19	0	0
30	L	25	Total 25	O 25	0	0
30	M	18	Total 18	O 18	0	0
30	N	167	Total 167	O 167	0	0
30	O	90	Total 90	O 90	0	0
30	P	105	Total 105	O 105	0	0
30	Q	69	Total 69	O 69	0	0
30	R	52	Total 52	O 52	0	0
30	S	81	Total 81	O 81	0	0
30	T	43	Total 43	O 43	0	0
30	U	34	Total 34	O 34	0	0
30	V	17	Total 17	O 17	0	0
30	W	26	Total 26	O 26	0	0

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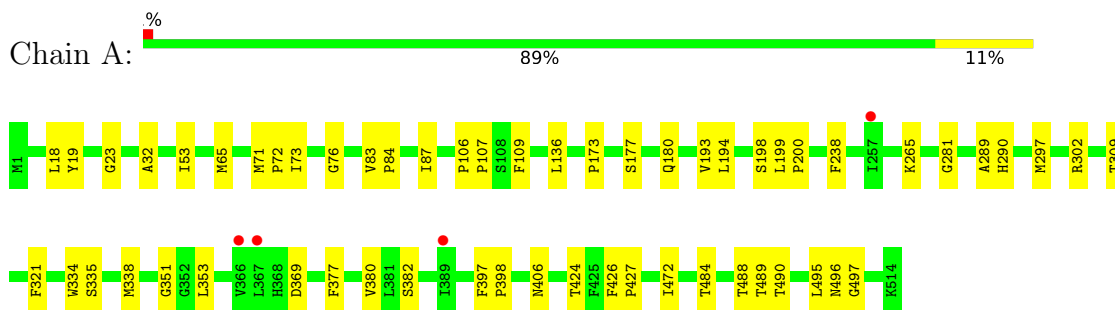
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	14	Total 14	O 14	0	0
30	Y	4	Total 4	O 4	0	0
30	Z	8	Total 8	O 8	0	0

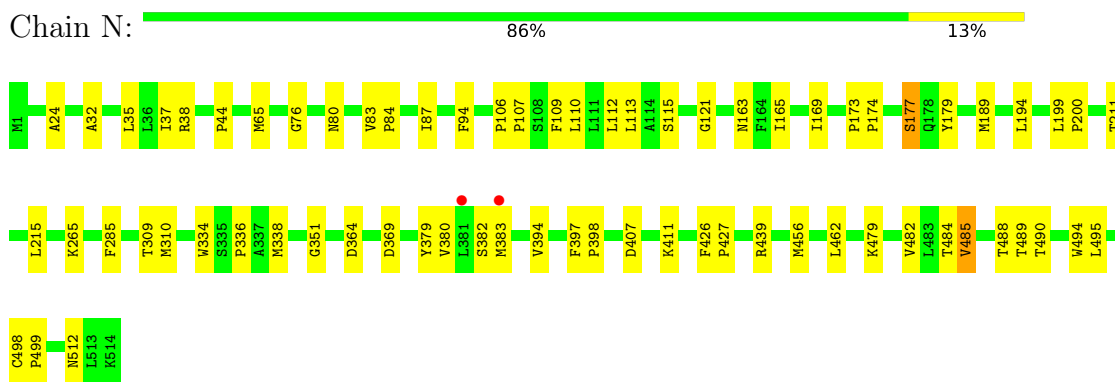
3 Residue-property plots

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

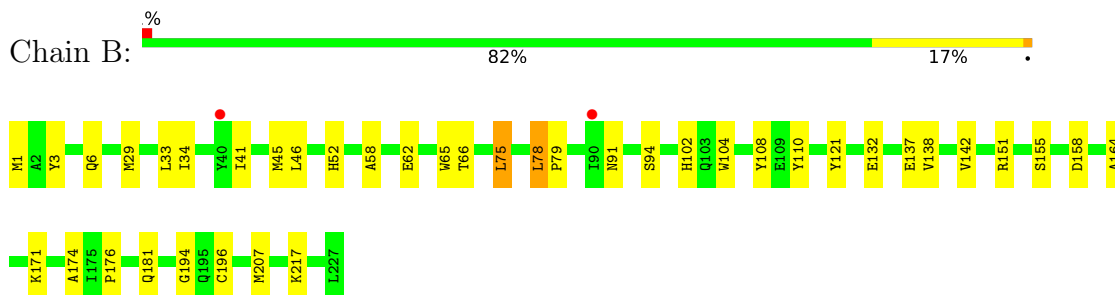
- Molecule 1: Cytochrome c oxidase subunit 1



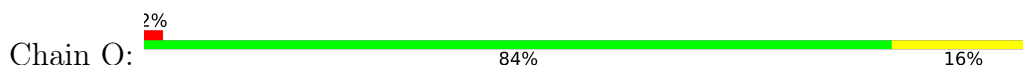
- Molecule 1: Cytochrome c oxidase subunit 1

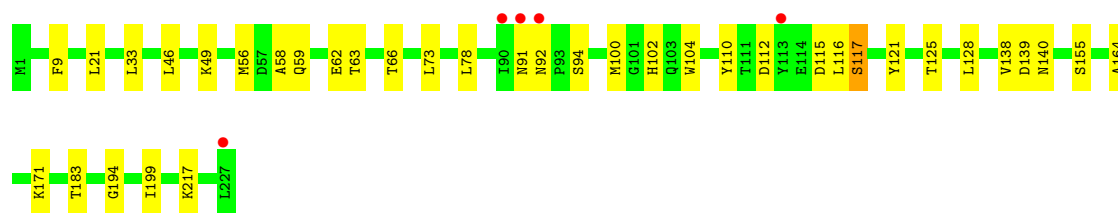


- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 92% 8% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 90% 9% .



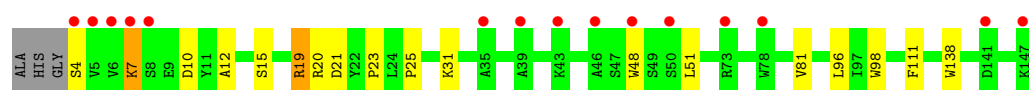
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 90% 7% ..



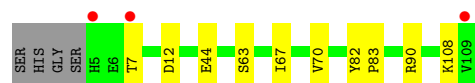
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 86% 11% ..



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

Chain E: 87% 9% .

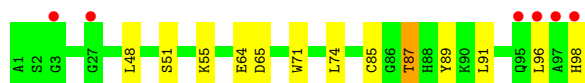
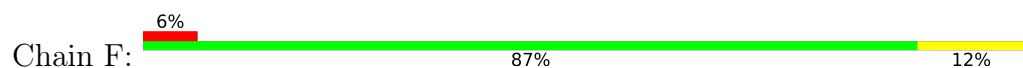


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

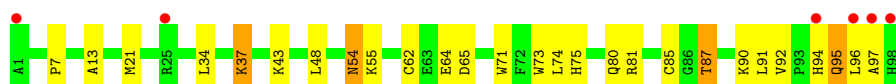
Chain R: 85% 11% .



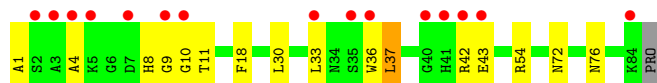
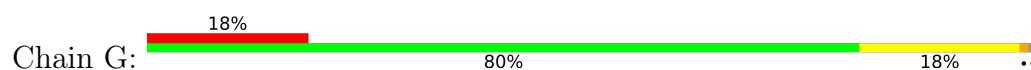
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



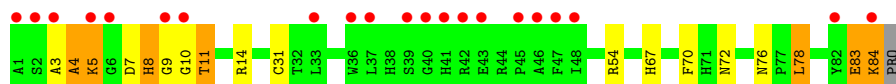
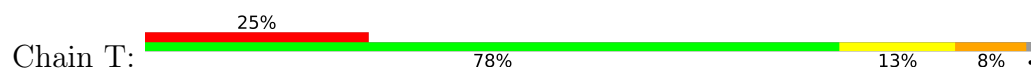
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



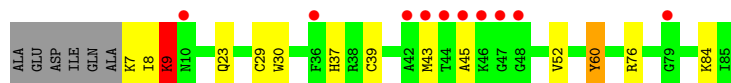
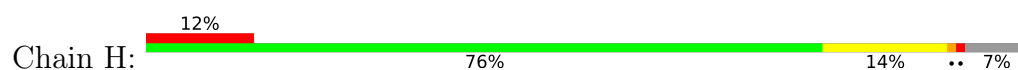
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



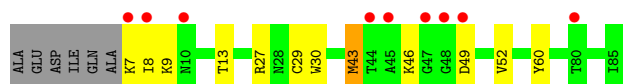
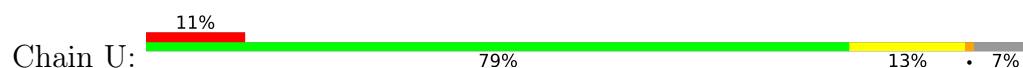
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



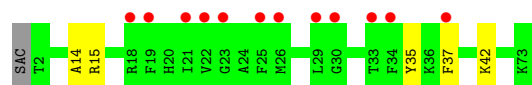
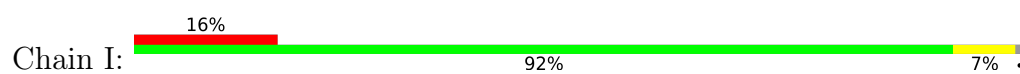
- Molecule 8: Cytochrome c oxidase subunit 6B1



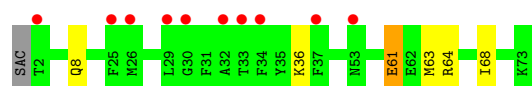
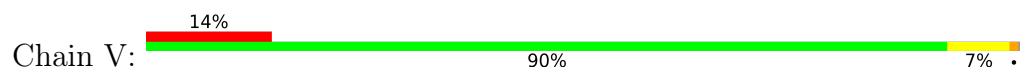
- Molecule 8: Cytochrome c oxidase subunit 6B1



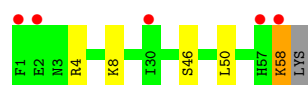
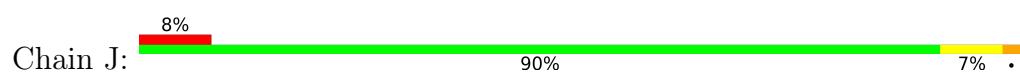
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 9: Cytochrome c oxidase subunit 6C



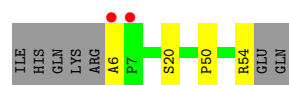
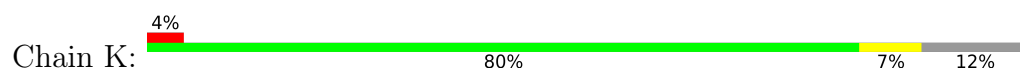
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



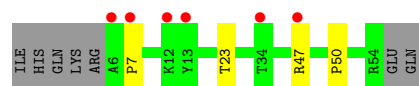
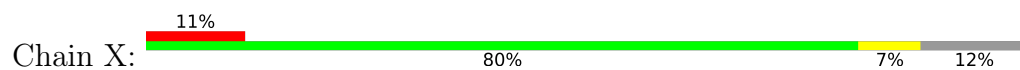
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



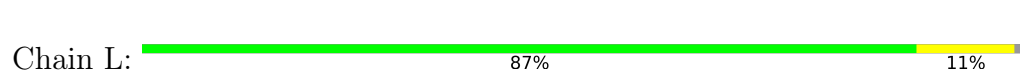
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



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




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

Chain Y:  4% 70% 23% . .



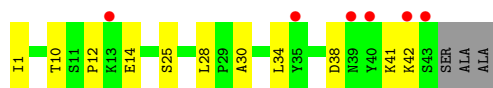
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  4% 80% 11% • 7%



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

Chain Z:  13% 70% 24% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.04Å 182.70Å 205.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.35 39.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.34-2.35) 99.9 (39.31-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.235 0.203 , 0.241	Depositor DCC
R_{free} test set	13603 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32721	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.66	0/4156	0.78	0/5678
1	N	0.66	0/4156	0.77	0/5678
2	B	0.68	0/1860	0.85	0/2534
2	O	0.67	0/1860	0.84	0/2534
3	C	0.63	0/2197	0.75	0/3005
3	P	0.66	0/2197	0.77	0/3005
4	D	0.69	0/1229	0.77	0/1658
4	Q	0.68	0/1229	0.78	0/1658
5	E	0.67	0/871	0.78	0/1182
5	R	0.67	0/871	0.78	0/1182
6	F	0.70	0/765	0.85	0/1038
6	S	0.71	0/765	0.83	0/1038
7	G	0.65	0/690	0.85	0/937
7	T	0.64	0/690	0.84	0/937
8	H	0.66	0/682	0.81	0/921
8	U	0.67	0/682	0.87	0/921
9	I	0.66	0/605	0.83	0/802
9	V	0.65	0/605	0.82	0/802
10	J	0.66	0/471	0.78	0/636
10	W	0.67	0/471	0.74	0/636
11	K	0.68	0/398	0.80	0/546
11	X	0.67	0/398	0.81	0/546
12	L	0.60	0/393	0.74	0/526
12	Y	0.63	0/393	0.77	0/526
13	M	0.65	0/345	0.79	0/470
13	Z	0.64	0/345	0.75	0/470
All	All	0.66	0/29324	0.79	0/39866

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	T	0	1
8	H	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	9	LYS	Peptide
7	T	83	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	41	0
1	N	4027	0	4001	43	0
2	B	1824	0	1833	21	0
2	O	1824	0	1833	19	0
3	C	2110	0	2027	11	0
3	P	2110	0	2027	18	0
4	D	1195	0	1183	8	0
4	Q	1195	0	1183	12	0
5	E	852	0	845	5	0
5	R	852	0	845	4	0
6	F	748	0	728	6	0
6	S	748	0	728	16	0
7	G	675	0	643	10	0
7	T	675	0	644	20	0
8	H	662	0	623	7	0
8	U	662	0	623	7	0
9	I	592	0	604	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	592	0	604	2	0
10	J	460	0	459	2	0
10	W	460	0	459	1	0
11	K	384	0	366	2	0
11	X	384	0	366	1	0
12	L	380	0	380	5	0
12	Y	380	0	380	10	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	102	0	152	1	0
17	C	102	0	152	3	0
17	N	51	0	76	4	0
17	P	153	0	228	3	0
18	A	120	0	108	6	0
18	N	120	0	108	12	0
19	A	40	0	60	3	0
19	B	32	0	48	1	0
19	C	16	0	24	1	0
19	D	24	0	36	0	0
19	E	20	0	30	0	0
19	F	12	0	18	0	0
19	G	20	0	30	0	0
19	I	8	0	12	0	0
19	J	16	0	24	0	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	40	0	60	4	0
19	O	8	0	12	0	0
19	P	20	0	30	0	0
19	Q	16	0	24	2	0
19	R	8	0	12	0	0
19	S	16	0	24	1	0
19	T	4	0	6	0	0
19	V	8	0	12	0	0
19	W	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z	4	0	6	0	0
20	A	1	0	0	1	0
20	N	1	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	0	0
22	D	63	0	110	3	0
22	L	63	0	110	2	0
22	N	63	0	110	0	0
22	Q	63	0	110	1	0
22	Y	63	0	110	2	0
23	B	52	0	80	3	0
23	R	52	0	80	2	0
24	C	58	0	78	1	0
24	G	29	0	39	0	0
24	J	29	0	39	1	0
24	P	58	0	78	1	0
24	T	58	0	78	12	0
24	W	29	0	39	1	0
24	Y	29	0	39	3	0
25	C	200	0	312	4	0
25	P	100	0	156	2	0
25	T	100	0	156	6	0
26	C	66	0	84	2	0
26	D	33	0	42	3	0
26	G	33	0	42	0	0
26	P	33	0	42	0	0
26	Q	33	0	42	2	0
27	C	53	0	77	1	0
27	G	106	0	154	5	0
27	P	106	0	154	4	0
27	T	53	0	77	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	0	0
29	V	9	0	8	2	0
30	A	188	0	0	6	0
30	B	107	0	0	0	0
30	C	107	0	0	1	0
30	D	89	0	0	2	0
30	E	71	0	0	0	0
30	F	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	G	32	0	0	0	0
30	H	41	0	0	1	0
30	I	31	0	0	1	0
30	J	23	0	0	1	0
30	K	19	0	0	1	0
30	L	25	0	0	1	0
30	M	18	0	0	0	0
30	N	167	0	0	6	0
30	O	90	0	0	0	0
30	P	105	0	0	5	0
30	Q	69	0	0	1	0
30	R	52	0	0	0	0
30	S	81	0	0	1	0
30	T	43	0	0	3	0
30	U	34	0	0	1	0
30	V	17	0	0	0	0
30	W	26	0	0	0	0
30	X	14	0	0	0	0
30	Y	4	0	0	1	0
30	Z	8	0	0	1	0
All	All	32721	0	31981	295	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (295) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:24:MET:SD	22:Y:101:TGL:HC42	2.14	0.87
27:P:305:PEK:H381	25:T:103:CDL:H271	1.56	0.85
7:G:76:ASN:HD21	27:G:102:PEK:HN2	1.21	0.85
20:A:618:OH:O	30:A:701:HOH:O	1.99	0.81
20:N:618:OH:O	30:N:701:HOH:O	1.98	0.81
24:T:105:CHD:H183	24:T:105:CHD:H231	1.64	0.79
25:C:304:CDL:H1	25:C:304:CDL:OA5	1.82	0.78
3:C:246:ASP:HB2	30:C:476:HOH:O	1.85	0.77
7:T:72:ASN:H	7:T:76:ASN:HD22	1.30	0.76
7:G:72:ASN:H	7:G:76:ASN:HD22	1.31	0.75
18:N:606:HEA:HMC1	18:N:606:HEA:HBC1	1.67	0.75
8:U:43:MET:HE1	8:U:52:VAL:HG21	1.68	0.74
18:N:605:HEA:HMC1	18:N:605:HEA:HBC1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLY:HA2	19:A:608:EDO:H21	1.72	0.71
1:A:297:MET:HG3	1:A:302:ARG:HG3	1.73	0.70
27:P:305:PEK:H381	25:T:103:CDL:C27	2.20	0.70
3:P:149:HIS:CE1	24:T:105:CHD:H182	2.28	0.69
19:N:611:EDO:O2	30:N:702:HOH:O	2.10	0.69
7:T:8:HIS:O	24:T:105:CHD:H42	1.93	0.69
7:T:76:ASN:HD21	27:T:102:PEK:HN2	1.39	0.68
7:G:8:HIS:HB3	1:N:179:TYR:OH	1.94	0.67
2:O:58:ALA:O	2:O:62:GLU:HG3	1.95	0.66
7:T:31:CYS:SG	25:T:103:CDL:C54	2.84	0.66
27:G:102:PEK:C12	27:G:102:PEK:H161	2.27	0.64
17:N:617:PGV:C5	17:N:617:PGV:C1	2.77	0.63
18:A:607:HEA:HBC1	18:A:607:HEA:HMC1	1.80	0.63
1:A:472:ILE:HG21	22:L:101:TGL:H202	1.80	0.63
17:C:303:PGV:H11	17:C:303:PGV:H42	1.79	0.63
7:T:31:CYS:SG	25:T:103:CDL:H542	2.39	0.63
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.82	0.62
3:C:103:HIS:ND1	24:C:301:CHD:O26	2.29	0.62
1:N:336:PRO:HB2	1:N:394:VAL:HG11	1.81	0.62
12:L:28:PHE:CD1	22:L:101:TGL:HA32	2.35	0.62
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.81	0.62
3:P:246:ASP:HB2	30:P:477:HOH:O	2.00	0.61
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.83	0.61
1:A:497:GLY:HA2	19:A:608:EDO:C2	2.31	0.61
3:P:149:HIS:NE2	24:T:105:CHD:C18	2.64	0.60
3:C:149:HIS:NE2	26:C:311:DMU:H2	2.17	0.60
6:F:87:THR:HG22	6:F:89:TYR:CE1	2.36	0.60
2:O:121:TYR:O	2:O:138:VAL:HA	2.01	0.60
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.60
29:V:101:SAC:C	29:V:101:SAC:H2A1	2.32	0.60
12:Y:24:MET:SD	22:Y:101:TGL:CC4	2.89	0.59
18:A:606:HEA:HBC1	18:A:606:HEA:HMC1	1.85	0.59
7:T:9:GLY:N	30:T:201:HOH:O	2.36	0.58
8:U:27:ARG:NH1	30:U:101:HOH:O	2.36	0.58
25:P:308:CDL:OA2	30:P:401:HOH:O	2.17	0.57
2:B:58:ALA:O	2:B:62:GLU:HG3	2.05	0.57
1:A:281:GLY:C	7:T:4:ALA:HB3	2.24	0.57
3:P:116:TRP:HA	3:P:117:PRO:C	2.24	0.57
1:A:193:VAL:HG21	7:T:5:LYS:O	2.06	0.56
1:A:496:ASN:O	30:A:702:HOH:O	2.17	0.56
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:MET:HA	23:R:201:PSC:H202	1.88	0.56
2:O:116:LEU:HD12	2:O:117:SER:N	2.20	0.56
6:F:55:LYS:HA	6:F:74:LEU:O	2.07	0.55
1:A:309:THR:HG22	18:A:606:HEA:HMB2	1.89	0.55
12:L:46:LYS:HA	30:L:213:HOH:O	2.07	0.55
3:P:3:HIS:HB2	30:P:479:HOH:O	2.07	0.55
6:S:92:VAL:O	6:S:92:VAL:HG23	2.07	0.55
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.88	0.55
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.41	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.88	0.54
25:T:103:CDL:H531	25:T:103:CDL:H211	1.90	0.54
1:A:194:LEU:CD2	7:T:4:ALA:HB1	2.37	0.54
10:J:58:LYS:HA	30:J:216:HOH:O	2.07	0.54
24:T:105:CHD:C18	24:T:105:CHD:H222	2.37	0.54
3:C:58:TRP:HB3	17:C:302:PGV:H31	1.88	0.54
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.91	0.53
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.08	0.53
19:N:614:EDO:H12	30:N:732:HOH:O	2.09	0.53
1:N:87:ILE:O	1:N:173:PRO:HD3	2.09	0.52
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.90	0.52
19:N:612:EDO:H11	30:N:771:HOH:O	2.09	0.52
1:A:87:ILE:O	1:A:173:PRO:HD3	2.08	0.52
2:B:78:LEU:CB	2:B:79:PRO:CD	2.87	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.91	0.52
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.36	0.52
17:N:617:PGV:H282	13:Z:12:PRO:HG3	1.91	0.52
24:T:105:CHD:H183	24:T:105:CHD:C23	2.37	0.52
25:C:310:CDL:H452	7:G:37:LEU:HD23	1.92	0.52
7:T:70:PHE:O	27:T:102:PEK:N	2.43	0.51
27:G:103:PEK:H231	2:O:59:GLN:HE22	1.75	0.51
6:S:75:HIS:H	6:S:80:GLN:HE22	1.57	0.51
13:Z:30:ALA:N	30:Z:1701:HOH:O	2.40	0.51
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.45	0.51
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.51
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.51
7:T:5:LYS:NZ	30:T:204:HOH:O	2.44	0.51
2:B:121:TYR:O	2:B:138:VAL:HA	2.10	0.51
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.76	0.51
1:N:364:ASP:OD1	18:N:605:HEA:O2A	2.29	0.51
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.93	0.51
12:Y:2:HIS:N	30:Y:201:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:479:LYS:HD3	30:N:759:HOH:O	2.12	0.50
24:T:105:CHD:H222	24:T:105:CHD:H181	1.93	0.50
1:N:397:PHE:N	1:N:398:PRO:CD	2.74	0.50
1:A:484:THR:HG22	30:A:813:HOH:O	2.11	0.50
3:P:124:LEU:HD13	3:P:180:GLU:OE1	2.12	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.11	0.50
1:N:407:ASP:O	1:N:411:LYS:HG3	2.11	0.50
3:P:95:THR:HG21	17:P:307:PGV:H302	1.92	0.50
1:A:65:MET:HB3	18:A:607:HEA:CAC	2.42	0.49
17:N:617:PGV:H241	17:N:617:PGV:H202	1.93	0.49
23:R:201:PSC:H341	23:R:201:PSC:H142	1.94	0.49
1:N:174:PRO:HD2	19:N:612:EDO:H11	1.92	0.49
27:P:301:PEK:O02	27:P:301:PEK:H031	2.12	0.49
29:V:101:SAC:C	29:V:101:SAC:C2A	2.89	0.49
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.95	0.49
8:U:43:MET:CE	8:U:52:VAL:HG21	2.40	0.49
24:Y:102:CHD:H192	24:Y:102:CHD:H3	1.95	0.48
1:N:489:THR:HA	6:S:71:TRP:O	2.13	0.48
8:H:9:LYS:HG3	30:H:113:HOH:O	2.12	0.48
24:T:105:CHD:C18	24:T:105:CHD:C22	2.91	0.48
4:D:98:TRP:CE2	26:D:208:DMU:H8	2.49	0.48
1:N:24:ALA:HB2	18:N:606:HEA:H253	1.94	0.48
3:P:3:HIS:CB	30:P:479:HOH:O	2.62	0.48
3:P:103:HIS:HA	17:P:307:PGV:O04	2.12	0.48
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.96	0.48
4:D:78:TRP:HA	22:D:201:TGL:HB52	1.94	0.48
2:B:155:SER:O	2:B:174:ALA:HB1	2.14	0.48
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.96	0.48
3:P:149:HIS:NE2	24:T:105:CHD:H182	2.27	0.48
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.96	0.47
1:A:489:THR:HA	6:F:71:TRP:O	2.13	0.47
1:N:199:LEU:N	1:N:200:PRO:CD	2.77	0.47
19:A:608:EDO:H12	30:A:735:HOH:O	2.14	0.47
12:Y:41:ARG:HH22	24:Y:102:CHD:H191	1.80	0.47
7:T:31:CYS:SG	25:T:103:CDL:H541	2.54	0.47
11:K:6:ALA:N	30:K:204:HOH:O	2.48	0.47
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.49	0.47
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.96	0.47
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.97	0.47
1:A:194:LEU:HD21	7:T:4:ALA:HB1	1.95	0.47
7:G:4:ALA:HB1	1:N:194:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.15	0.47
7:T:67:HIS:NE2	7:T:84:LYS:HB3	2.30	0.47
25:P:308:CDL:CA2	30:P:401:HOH:O	2.63	0.47
1:A:353:LEU:HD11	2:B:34:ILE:HG22	1.97	0.47
3:C:129:VAL:N	3:C:130:PRO:CD	2.78	0.47
26:C:312:DMU:H26	26:C:312:DMU:H18	1.73	0.47
2:B:29:MET:HG3	9:I:35:TYR:CD1	2.50	0.46
4:Q:7:LYS:HA	4:Q:10:ASP:HB2	1.98	0.46
1:A:377:PHE:HB2	18:A:606:HEA:HMD3	1.97	0.46
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.50	0.46
3:C:116:TRP:HA	3:C:117:PRO:C	2.34	0.46
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.97	0.46
1:A:406:ASN:HD21	17:A:604:PGV:H31	1.81	0.46
7:G:76:ASN:ND2	27:G:102:PEK:HN2	2.01	0.46
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.97	0.46
1:A:424:THR:HG21	18:A:607:HEA:HMB2	1.98	0.46
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.51	0.46
2:O:102:HIS:O	2:O:104:TRP:HA	2.15	0.46
7:G:4:ALA:CB	1:N:285:PHE:CE2	2.99	0.46
1:N:379:TYR:O	1:N:383:MET:HB2	2.15	0.46
18:N:606:HEA:H122	18:N:606:HEA:HHC	1.98	0.46
3:P:149:HIS:CE1	24:T:105:CHD:C18	2.98	0.46
24:P:309:CHD:H212	24:P:309:CHD:H183	1.98	0.46
6:S:94:HIS:O	30:S:201:HOH:O	2.21	0.46
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.45	0.46
3:P:228:THR:HA	6:S:7:PRO:O	2.15	0.46
6:S:54:ASN:HD22	6:S:54:ASN:C	2.19	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.15	0.45
2:O:116:LEU:HD12	2:O:117:SER:H	1.80	0.45
2:O:125:THR:HA	2:O:128:LEU:HD12	1.98	0.45
1:A:302:ARG:NH2	8:H:23:GLN:HE21	2.13	0.45
27:T:102:PEK:H32	27:T:102:PEK:H101	1.98	0.45
2:B:158:ASP:HB2	19:B:305:EDO:H22	1.97	0.45
17:C:303:PGV:H22	17:C:303:PGV:H141	1.97	0.45
26:D:208:DMU:C11	30:D:301:HOH:O	2.65	0.45
1:N:112:LEU:HD23	1:N:112:LEU:C	2.37	0.45
27:T:102:PEK:H32	27:T:102:PEK:H71	1.99	0.45
1:A:488:THR:HB	1:A:495:LEU:HD13	1.98	0.45
3:C:55:TYR:HA	25:C:304:CDL:H551	1.98	0.45
12:Y:45:LEU:HD12	24:Y:102:CHD:H7	1.99	0.45
23:B:303:PSC:O03	23:B:303:PSC:H232	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:64:GLU:O	6:S:65:ASP:HB2	2.18	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.44
4:D:127:LYS:HD2	30:I:226:HOH:O	2.17	0.44
7:T:9:GLY:CA	30:T:201:HOH:O	2.64	0.44
1:N:115:SER:O	1:N:121:GLY:HA2	2.17	0.44
24:T:101:CHD:O7	24:T:101:CHD:H41	2.17	0.44
5:E:12:ASP:OD2	5:E:44:GLU:HG3	2.16	0.44
1:N:309:THR:HG22	18:N:605:HEA:HMB2	2.00	0.44
1:A:335:SER:HB2	30:A:839:HOH:O	2.18	0.44
2:B:158:ASP:O	2:B:176:PRO:HG3	2.18	0.44
1:N:83:VAL:HB	1:N:84:PRO:HD3	1.99	0.44
2:B:75:LEU:HD12	2:B:75:LEU:HA	1.88	0.44
5:R:67:ILE:O	5:R:71:VAL:HG23	2.17	0.44
2:B:78:LEU:CB	2:B:79:PRO:HD3	2.48	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.00	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.17	0.43
7:T:67:HIS:NE2	7:T:84:LYS:HG2	2.32	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.00	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
5:E:63:SER:O	5:E:67:ILE:HG13	2.19	0.43
1:N:37:ILE:HG21	18:N:606:HEA:CMA	2.49	0.43
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	2.01	0.43
3:P:22:LEU:O	3:P:25:LEU:HB3	2.19	0.43
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.00	0.43
2:B:52:HIS:CE1	23:B:303:PSC:H02	2.54	0.43
6:F:64:GLU:O	6:F:65:ASP:HB2	2.19	0.43
18:N:605:HEA:HBC1	18:N:605:HEA:CMC	2.45	0.43
18:N:605:HEA:HMD1	18:N:605:HEA:HBD2	2.01	0.43
26:Q:206:DMU:H6	13:Z:28:LEU:HD23	2.00	0.43
24:T:105:CHD:H183	24:T:105:CHD:C22	2.48	0.43
7:G:1:ALA:HB2	27:P:301:PEK:C37	2.49	0.43
8:H:60:TYR:CD1	8:H:60:TYR:C	2.92	0.43
8:H:52:VAL:HG12	8:U:46:LYS:HB3	1.99	0.43
2:B:108:TYR:CE2	2:B:142:VAL:HG21	2.54	0.43
1:A:289:ALA:HB1	1:A:297:MET:HE1	2.01	0.42
24:J:101:CHD:H17	24:J:101:CHD:H232	1.88	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.42
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.18	0.42
4:Q:81:VAL:HG11	22:Q:201:TGL:HB82	2.01	0.42
1:N:110:LEU:HD12	1:N:113:LEU:HD23	2.02	0.42
30:N:745:HOH:O	6:S:37:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:199:ILE:HG23	2:O:199:ILE:O	2.18	0.42
1:A:397:PHE:N	1:A:398:PRO:CD	2.83	0.42
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.55	0.42
1:N:65:MET:HB3	18:N:606:HEA:CAC	2.49	0.42
2:O:139:ASP:OD1	2:O:140:ASN:N	2.52	0.42
1:N:94:PHE:HB2	1:N:163:ASN:ND2	2.34	0.42
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.01	0.42
3:P:129:VAL:N	3:P:130:PRO:CD	2.83	0.42
8:H:37:HIS:CD2	8:H:76:ARG:CZ	3.02	0.42
3:P:192:VAL:HA	3:P:195:SER:HB2	2.02	0.42
1:A:351:GLY:HA3	1:A:380:VAL:HG13	2.00	0.42
1:A:426:PHE:N	1:A:427:PRO:CD	2.83	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.18	0.42
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.01	0.42
4:Q:7:LYS:HD2	19:Q:204:EDO:O2	2.19	0.42
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.49	0.42
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.02	0.42
27:C:313:PEK:H302	7:T:3:ALA:HB3	2.02	0.42
10:J:8:LYS:HD3	10:J:8:LYS:HA	1.85	0.42
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.02	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
7:T:78:LEU:HD22	7:T:84:LYS:HB2	2.02	0.42
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.02	0.42
1:A:302:ARG:HD2	30:A:879:HOH:O	2.20	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.42
3:C:158:HIS:CB	19:C:306:EDO:H11	2.50	0.42
12:Y:45:LEU:O	12:Y:46:LYS:C	2.57	0.42
7:G:10:GLY:CA	1:N:177:SER:HB2	2.50	0.42
8:H:39:CYS:O	8:H:43:MET:HG2	2.19	0.42
6:S:34:LEU:O	19:S:105:EDO:H21	2.19	0.42
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.02	0.41
7:G:1:ALA:HA	17:P:307:PGV:H312	2.02	0.41
18:N:605:HEA:HMC1	18:N:605:HEA:CBC	2.47	0.41
4:Q:98:TRP:CE2	26:Q:206:DMU:H11	2.55	0.41
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.56	0.41
13:M:34:LEU:HD12	13:M:34:LEU:HA	1.88	0.41
1:N:165:ILE:O	1:N:169:ILE:HG12	2.20	0.41
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.55	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.88	0.41
2:O:112:ASP:OD1	8:U:13:THR:OG1	2.27	0.41
19:Q:205:EDO:H11	30:Q:365:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:81:ARG:HA	6:S:87:THR:O	2.20	0.41
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	2.01	0.41
3:C:62:ILE:HD12	25:C:304:CDL:H511	2.02	0.41
4:D:98:TRP:CE3	26:D:208:DMU:H13	2.56	0.41
18:N:606:HEA:H172	18:N:606:HEA:H261	1.79	0.41
6:S:13:ALA:CB	6:S:21:MET:HE1	2.50	0.41
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.55	0.41
1:N:310:MET:HE3	2:O:73:LEU:HD22	2.02	0.41
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.02	0.41
1:N:485:VAL:HG21	1:N:494:TRP:CE3	2.55	0.41
10:W:36:MET:HE3	10:W:36:MET:HA	2.03	0.41
4:D:77:GLU:HB3	22:D:201:TGL:HB32	2.02	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.93	0.41
1:A:199:LEU:N	1:A:200:PRO:CD	2.84	0.41
30:D:345:HOH:O	13:M:4:LYS:HE2	2.20	0.41
5:E:90:ARG:HD3	5:E:90:ARG:HA	1.98	0.41
6:F:85:CYS:SG	6:F:87:THR:HB	2.61	0.41
23:B:303:PSC:H32	9:I:14:ALA:CB	2.50	0.41
1:N:426:PHE:N	1:N:427:PRO:CD	2.83	0.41
17:N:617:PGV:H241	17:N:617:PGV:H012	2.03	0.41
2:O:100:MET:SD	2:O:155:SER:HB3	2.60	0.40
1:A:198:SER:HB2	1:A:238:PHE:HA	2.03	0.40
1:A:297:MET:O	1:A:302:ARG:NH2	2.54	0.40
27:G:102:PEK:C12	27:G:102:PEK:C16	2.96	0.40
24:W:302:CHD:H161	24:W:302:CHD:O25	2.20	0.40
5:R:52:LEU:O	5:R:55:CYS:HB2	2.21	0.40
7:T:11:TPO:HG23	7:T:14:ARG:HB2	2.02	0.40
3:C:16:TRP:N	3:C:17:PRO:CD	2.84	0.40
4:D:78:TRP:N	22:D:201:TGL:HB32	2.35	0.40
3:P:31:LEU:HD23	3:P:31:LEU:HA	1.91	0.40
8:U:49:ASP:O	8:U:52:VAL:HG22	2.21	0.40
1:A:321:PHE:HB3	2:B:65:TRP:CE2	2.56	0.40
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.87	0.40
5:E:82:TYR:N	5:E:83:PRO:CD	2.84	0.40
1:N:35:LEU:HD13	1:N:462:LEU:HD22	2.03	0.40
6:S:92:VAL:O	6:S:92:VAL:CG2	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	498 (97%)	14 (3%)	0	100	100
1	N	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
2	B	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
2	O	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	131 (92%)	11 (8%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
6	S	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7	4
7	G	81/85 (95%)	69 (85%)	10 (12%)	2 (2%)	5	3
7	T	81/85 (95%)	66 (82%)	13 (16%)	2 (2%)	5	3
8	H	77/85 (91%)	68 (88%)	7 (9%)	2 (3%)	5	3
8	U	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	12	10
9	I	70/73 (96%)	70 (100%)	0	0	100	100
9	V	70/73 (96%)	66 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	44 (94%)	2 (4%)	1 (2%)	7	4
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	6	4
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3502/3614 (97%)	3351 (96%)	140 (4%)	11 (0%)	41	47

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	8	ILE
8	H	45	ALA
7	G	43	GLU
12	Y	46	LYS
6	S	95	GLN
6	S	97	ALA
7	T	8	HIS
11	X	7	PRO
7	T	4	ALA
7	G	9	GLY
8	U	8	ILE

5.3.2 Protein sidechains ⓘ

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%)	419 (98%)	7 (2%)	62	75
1	N	426/426 (100%)	416 (98%)	10 (2%)	50	61
2	B	210/210 (100%)	201 (96%)	9 (4%)	29	35
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	19
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	55
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	55
4	D	128/129 (99%)	122 (95%)	6 (5%)	26	31
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	40
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	46
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	29
6	S	81/81 (100%)	73 (90%)	8 (10%)	8	7
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	6
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	8
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	15
8	U	71/75 (95%)	66 (93%)	5 (7%)	15	15
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	26
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	26
10	J	49/50 (98%)	45 (92%)	4 (8%)	11	11
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	20
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	27
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	27
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	6
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	11
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	6
All	All	3040/3082 (99%)	2908 (96%)	132 (4%)	29	35

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	136	LEU
1	A	180	GLN
1	A	290	HIS
1	A	338	MET
1	A	369	ASP
1	A	382	SER
2	B	33	LEU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	110	TYR
2	B	171	LYS

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Mol	Chain	Res	Type
2	B	217	LYS
3	C	42	LEU
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	223	LEU
3	C	230	ASN
4	D	4	SER
4	D	36	SER
4	D	45	LYS
4	D	51	LEU
4	D	121	LYS
4	D	147	LYS
5	E	7	THR
5	E	70	VAL
5	E	108	LYS
6	F	48	LEU
6	F	87	THR
6	F	96	LEU
6	F	98	HIS
7	G	18	PHE
7	G	30	LEU
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	54	ARG
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
8	H	84	LYS
9	I	15	ARG
9	I	37	PHE
9	I	42	LYS
10	J	4	ARG
10	J	46	SER
10	J	50	LEU
10	J	58	LYS
11	K	20	SER
11	K	54	ARG
13	M	13	LYS

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Mol	Chain	Res	Type
13	M	34	LEU
13	M	38	ASP
1	N	38	ARG
1	N	109	PHE
1	N	177	SER
1	N	189	MET
1	N	338	MET
1	N	369	ASP
1	N	382	SER
1	N	484	THR
1	N	485	VAL
1	N	512	ASN
2	O	33	LEU
2	O	63	THR
2	O	66	THR
2	O	78	LEU
2	O	91	ASN
2	O	92	ASN
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	117	SER
2	O	171	LYS
2	O	183	THR
2	O	217	LYS
3	P	3	HIS
3	P	33	MET
3	P	127	LEU
3	P	159	MET
3	P	223	LEU
3	P	230	ASN
4	Q	4	SER
4	Q	7	LYS
4	Q	15	SER
4	Q	19	ARG
4	Q	31	LYS
5	R	5	HIS
5	R	7	THR
5	R	70	VAL
5	R	79	LYS
6	S	37	LYS
6	S	43	LYS

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Mol	Chain	Res	Type
6	S	48	LEU
6	S	54	ASN
6	S	87	THR
6	S	90	LYS
6	S	91	LEU
6	S	95	GLN
7	T	5	LYS
7	T	7	ASP
7	T	54	ARG
7	T	78	LEU
7	T	83	GLU
7	T	84	LYS
8	U	7	LYS
8	U	9	LYS
8	U	29	CYS
8	U	43	MET
8	U	60	TYR
9	V	8	GLN
9	V	36	LYS
9	V	61	GLU
10	W	36	MET
10	W	50	LEU
10	W	58	LYS
11	X	23	THR
11	X	47	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	27	LEU
12	Y	47	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	41	LYS
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	22	HIS
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN

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Mol	Chain	Res	Type
3	C	68	GLN
5	E	94	ASN
7	G	76	ASN
8	H	10	ASN
10	J	29	ASN
1	N	178	GLN
1	N	232	GLN
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
3	P	76	GLN
3	P	243	HIS
4	Q	32	ASN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
9	V	70	GLN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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
2	FME	O	1	2	8,9,10	0.51	0	7,9,11	0.78	0
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	0.95	0
2	FME	B	1	2	8,9,10	0.59	0	7,9,11	0.99	1 (14%)
1	FME	A	1	1	8,9,10	0.69	0	7,9,11	0.82	0
7	TPO	T	11	7	8,10,11	0.95	1 (12%)	10,14,16	0.80	0
7	TPO	G	11	7	8,10,11	0.94	1 (12%)	10,14,16	0.72	0

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
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	4/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	7/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	2.14	1.63	1.59
7	T	11	TPO	P-OG1	2.04	1.63	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	2.18	113.66	109.73

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
2	B	1	FME	CA-CB-CG-SD
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	O-C-CA-CB
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	O-C-CA-CB
7	T	11	TPO	CA-CB-OG1-P
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	C-CA-CB-CG
2	B	1	FME	CB-CG-SD-CE
1	N	1	FME	C-CA-CB-CG
2	B	1	FME	N-CA-CB-CG
7	G	11	TPO	CB-OG1-P-O1P
7	T	11	TPO	CB-OG1-P-O1P
7	T	11	TPO	CB-OG1-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 134 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	$\# Z > 2$
19	EDO	A	608	-	3,3,3	0.71	0	2,2,2	0.93	0
19	EDO	A	614	-	3,3,3	0.08	0	2,2,2	0.18	0
19	EDO	Q	202	-	3,3,3	0.09	0	2,2,2	0.23	0
19	EDO	E	205	-	3,3,3	0.06	0	2,2,2	0.11	0
19	EDO	V	103	-	3,3,3	0.19	0	2,2,2	0.34	0
19	EDO	G	106	-	3,3,3	0.12	0	2,2,2	0.30	0
24	CHD	C	301	-	32,32,32	0.53	0	51,51,51	0.70	1 (1%)
24	CHD	G	108	-	32,32,32	0.61	0	51,51,51	0.83	0
23	PSC	B	303	-	51,51,51	0.33	0	57,59,59	0.39	0
19	EDO	P	314	-	3,3,3	0.09	0	2,2,2	0.22	0
19	EDO	J	104	-	3,3,3	0.17	0	2,2,2	0.28	0
19	EDO	B	307	-	3,3,3	0.07	0	2,2,2	0.18	0
19	EDO	P	313	-	3,3,3	0.13	0	2,2,2	0.04	0
26	DMU	C	311	-	34,34,34	2.09	8 (23%)	45,45,45	1.76	9 (20%)
19	EDO	F	704	-	3,3,3	0.25	0	2,2,2	0.35	0
22	TGL	Y	101	-	62,62,62	0.28	0	65,65,65	0.40	1 (1%)
19	EDO	D	206	-	3,3,3	0.24	0	2,2,2	0.44	0
17	PGV	C	302	-	50,50,50	0.39	0	53,56,56	0.51	0
27	PEK	G	102	-	52,52,52	0.32	0	55,57,57	0.57	0
24	CHD	T	101	-	32,32,32	0.65	0	51,51,51	1.06	2 (3%)
19	EDO	G	105	-	3,3,3	0.20	0	2,2,2	0.30	0
19	EDO	L	102	-	3,3,3	0.24	0	2,2,2	0.39	0
19	EDO	D	203	-	3,3,3	0.08	0	2,2,2	0.06	0
19	EDO	O	303	-	3,3,3	0.22	0	2,2,2	0.50	0
19	EDO	E	203	-	3,3,3	0.17	0	2,2,2	0.33	0
27	PEK	C	313	-	52,52,52	0.40	0	55,57,57	0.54	1 (1%)
26	DMU	D	208	-	34,34,34	1.07	3 (8%)	45,45,45	2.75	8 (17%)
26	DMU	C	312	-	34,34,34	1.19	3 (8%)	45,45,45	1.31	6 (13%)
25	CDL	T	103	-	99,99,99	0.41	0	105,111,111	0.48	1 (0%)
19	EDO	C	306	-	3,3,3	0.73	0	2,2,2	0.85	0
19	EDO	T	104	-	3,3,3	0.16	0	2,2,2	0.23	0
19	EDO	K	101	-	3,3,3	0.10	0	2,2,2	0.16	0
19	EDO	D	207	-	3,3,3	0.24	0	2,2,2	0.29	0
19	EDO	A	615	-	3,3,3	0.11	0	2,2,2	0.23	0
19	EDO	N	608	-	3,3,3	0.73	0	2,2,2	0.67	0
19	EDO	B	304	-	3,3,3	0.05	0	2,2,2	0.07	0
19	EDO	C	308	-	3,3,3	0.14	0	2,2,2	0.28	0
22	TGL	L	101	-	62,62,62	0.32	0	65,65,65	0.37	0
27	PEK	P	301	-	52,52,52	0.37	0	55,57,57	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	K	102	-	3,3,3	0.18	0	2,2,2	0.27	0
22	TGL	N	604	-	62,62,62	0.32	0	65,65,65	0.53	1 (1%)
27	PEK	G	103	-	52,52,52	0.36	0	55,57,57	0.50	0
18	HEA	A	607	1	57,67,67	2.06	13 (22%)	61,103,103	2.46	24 (39%)
19	EDO	A	612	-	3,3,3	0.36	0	2,2,2	0.39	0
19	EDO	G	107	-	3,3,3	0.05	0	2,2,2	0.15	0
19	EDO	I	102	-	3,3,3	0.08	0	2,2,2	0.16	0
19	EDO	E	201	-	3,3,3	0.13	0	2,2,2	0.26	0
19	EDO	N	615	-	3,3,3	0.14	0	2,2,2	0.20	0
19	EDO	E	202	-	3,3,3	0.15	0	2,2,2	0.18	0
29	SAC	V	101	-	7,8,9	0.50	0	8,9,11	1.39	1 (12%)
26	DMU	P	303	-	34,34,34	1.70	8 (23%)	45,45,45	1.53	9 (20%)
19	EDO	N	616	-	3,3,3	0.04	0	2,2,2	0.35	0
19	EDO	G	104	-	3,3,3	0.27	0	2,2,2	0.40	0
17	PGV	N	617	-	50,50,50	0.36	0	53,56,56	0.46	0
19	EDO	N	611	-	3,3,3	0.16	0	2,2,2	0.18	0
19	EDO	P	312	-	3,3,3	0.11	0	2,2,2	0.32	0
24	CHD	C	305	-	32,32,32	0.62	0	51,51,51	0.92	1 (1%)
23	PSC	R	201	-	51,51,51	0.34	0	57,59,59	0.49	0
19	EDO	B	309	-	3,3,3	0.38	0	2,2,2	0.50	0
21	CUA	B	301	2	0,1,1	-	-	-	-	-
17	PGV	A	605	-	50,50,50	0.40	0	53,56,56	0.56	0
19	EDO	W	301	-	3,3,3	0.09	0	2,2,2	0.18	0
19	EDO	C	307	-	3,3,3	0.15	0	2,2,2	0.17	0
24	CHD	P	304	-	32,32,32	0.57	0	51,51,51	0.68	0
24	CHD	Y	102	-	32,32,32	0.68	0	51,51,51	1.21	7 (13%)
19	EDO	S	104	-	3,3,3	0.07	0	2,2,2	0.07	0
19	EDO	A	609	-	3,3,3	0.24	0	2,2,2	0.27	0
21	CUA	O	301	2	0,1,1	-	-	-	-	-
17	PGV	C	303	-	50,50,50	0.42	0	53,56,56	0.55	1 (1%)
19	EDO	J	102	-	3,3,3	0.12	0	2,2,2	0.13	0
19	EDO	A	611	-	3,3,3	0.33	0	2,2,2	0.45	0
26	DMU	G	101	-	34,34,34	2.39	9 (26%)	45,45,45	2.03	10 (22%)
19	EDO	D	204	-	3,3,3	0.13	0	2,2,2	0.13	0
19	EDO	S	102	-	3,3,3	0.35	0	2,2,2	0.43	0
19	EDO	F	703	-	3,3,3	0.13	0	2,2,2	0.11	0
19	EDO	M	701	-	3,3,3	0.09	0	2,2,2	0.19	0
19	EDO	N	614	-	3,3,3	0.61	0	2,2,2	0.83	0
19	EDO	O	302	-	3,3,3	0.23	0	2,2,2	0.42	0
19	EDO	E	204	-	3,3,3	0.25	0	2,2,2	0.29	0
19	EDO	N	609	-	3,3,3	0.18	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	A	613	-	3,3,3	0.09	0	2,2,2	0.16	0
19	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.48	0
19	EDO	Q	205	-	3,3,3	0.16	0	2,2,2	0.33	0
19	EDO	W	303	-	3,3,3	0.11	0	2,2,2	0.14	0
19	EDO	I	103	-	3,3,3	0.13	0	2,2,2	0.14	0
25	CDL	C	310	-	99,99,99	0.37	0	105,111,111	0.44	0
26	DMU	Q	206	-	34,34,34	1.02	1 (2%)	45,45,45	1.19	6 (13%)
19	EDO	F	701	-	3,3,3	0.11	0	2,2,2	0.55	0
24	CHD	P	309	-	32,32,32	0.53	0	51,51,51	0.86	1 (1%)
19	EDO	B	306	-	3,3,3	0.11	0	2,2,2	0.11	0
19	EDO	B	310	-	3,3,3	0.20	0	2,2,2	0.33	0
19	EDO	P	311	-	3,3,3	0.15	0	2,2,2	0.43	0
24	CHD	T	105	-	32,32,32	0.68	0	51,51,51	1.28	5 (9%)
29	SAC	I	101	-	7,8,9	0.54	0	8,9,11	1.21	1 (12%)
19	EDO	G	109	-	3,3,3	0.10	0	2,2,2	0.31	0
17	PGV	A	604	-	50,50,50	0.38	0	53,56,56	0.51	0
19	EDO	D	205	-	3,3,3	0.11	0	2,2,2	0.22	0
17	PGV	P	302	-	50,50,50	0.36	0	53,56,56	0.61	0
19	EDO	A	616	-	3,3,3	0.09	0	2,2,2	0.37	0
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.23	0
19	EDO	B	308	-	3,3,3	0.25	0	2,2,2	0.33	0
19	EDO	B	311	-	3,3,3	0.11	0	2,2,2	0.12	0
19	EDO	A	617	-	3,3,3	0.17	0	2,2,2	0.32	0
27	PEK	P	305	-	52,52,52	0.36	0	55,57,57	0.57	0
19	EDO	J	105	-	3,3,3	0.05	0	2,2,2	0.25	0
25	CDL	P	308	-	99,99,99	0.38	0	105,111,111	0.52	1 (0%)
19	EDO	N	607	-	3,3,3	0.14	0	2,2,2	0.26	0
25	CDL	C	304	-	99,99,99	0.35	0	105,111,111	0.51	0
18	HEA	A	606	1	57,67,67	1.94	14 (24%)	61,103,103	2.39	22 (36%)
18	HEA	N	605	1	57,67,67	1.90	14 (24%)	61,103,103	2.32	25 (40%)
19	EDO	R	203	-	3,3,3	0.12	0	2,2,2	0.16	0
22	TGL	B	302	-	62,62,62	0.38	0	65,65,65	0.41	1 (1%)
17	PGV	P	307	-	50,50,50	0.33	0	53,56,56	0.42	0
19	EDO	Q	204	-	3,3,3	0.26	0	2,2,2	0.40	0
24	CHD	J	101	-	32,32,32	0.65	1 (3%)	51,51,51	0.78	1 (1%)
27	PEK	T	102	-	52,52,52	0.31	0	55,57,57	0.58	1 (1%)
24	CHD	W	302	-	32,32,32	0.63	0	51,51,51	0.86	0
19	EDO	N	612	-	3,3,3	0.27	0	2,2,2	0.58	0
19	EDO	D	202	-	3,3,3	0.27	0	2,2,2	0.51	0
19	EDO	Q	203	-	3,3,3	0.20	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	HEA	N	606	1	57,67,67	1.98	16 (28%)	61,103,103	2.54	25 (40%)
19	EDO	A	610	-	3,3,3	0.19	0	2,2,2	0.25	0
17	PGV	P	306	-	50,50,50	0.34	0	53,56,56	0.50	0
22	TGL	Q	201	-	62,62,62	0.34	0	65,65,65	0.38	0
19	EDO	J	103	-	3,3,3	0.79	0	2,2,2	0.88	0
19	EDO	P	310	-	3,3,3	0.12	0	2,2,2	0.23	0
22	TGL	D	201	-	62,62,62	0.34	0	65,65,65	0.32	0
19	EDO	S	103	-	3,3,3	0.09	0	2,2,2	0.06	0
19	EDO	S	105	-	3,3,3	0.19	0	2,2,2	0.36	0
19	EDO	Z	1601	-	3,3,3	0.19	0	2,2,2	0.34	0
19	EDO	R	202	-	3,3,3	0.14	0	2,2,2	0.28	0
19	EDO	C	309	-	3,3,3	0.10	0	2,2,2	0.15	0
19	EDO	N	610	-	3,3,3	0.25	0	2,2,2	0.26	0
19	EDO	N	613	-	3,3,3	0.15	0	2,2,2	0.27	0

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
19	EDO	A	608	-	-	0/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
19	EDO	Q	202	-	-	1/1/1/1	-
19	EDO	E	205	-	-	0/1/1/1	-
19	EDO	V	103	-	-	1/1/1/1	-
19	EDO	G	106	-	-	0/1/1/1	-
24	CHD	C	301	-	-	0/9/74/74	0/4/4/4
24	CHD	G	108	-	-	2/9/74/74	0/4/4/4
23	PSC	B	303	-	-	30/55/55/55	-
19	EDO	P	314	-	-	1/1/1/1	-
19	EDO	J	104	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
19	EDO	P	313	-	-	1/1/1/1	-
26	DMU	C	311	-	-	9/19/59/59	0/2/2/2
19	EDO	F	704	-	-	0/1/1/1	-
22	TGL	Y	101	-	-	36/65/65/65	-
19	EDO	D	206	-	-	1/1/1/1	-
17	PGV	C	302	-	-	17/55/55/55	-
27	PEK	G	102	-	-	22/56/56/56	-
24	CHD	T	101	-	-	3/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	G	105	-	-	1/1/1/1	-
19	EDO	L	102	-	-	0/1/1/1	-
19	EDO	D	203	-	-	1/1/1/1	-
19	EDO	O	303	-	-	1/1/1/1	-
19	EDO	E	203	-	-	0/1/1/1	-
27	PEK	C	313	-	-	25/56/56/56	-
26	DMU	D	208	-	-	10/19/59/59	0/2/2/2
26	DMU	C	312	-	-	9/19/59/59	0/2/2/2
25	CDL	T	103	-	-	55/110/110/110	-
19	EDO	C	306	-	-	0/1/1/1	-
19	EDO	T	104	-	-	0/1/1/1	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	D	207	-	-	0/1/1/1	-
19	EDO	A	615	-	-	0/1/1/1	-
19	EDO	N	608	-	-	0/1/1/1	-
19	EDO	B	304	-	-	0/1/1/1	-
19	EDO	C	308	-	-	1/1/1/1	-
22	TGL	L	101	-	-	29/65/65/65	-
27	PEK	P	301	-	-	26/56/56/56	-
19	EDO	K	102	-	-	1/1/1/1	-
22	TGL	N	604	-	-	31/65/65/65	-
27	PEK	G	103	-	-	27/56/56/56	-
18	HEA	A	607	1	3/3/7/16	4/32/76/76	-
19	EDO	A	612	-	-	1/1/1/1	-
19	EDO	G	107	-	-	1/1/1/1	-
19	EDO	I	102	-	-	0/1/1/1	-
19	EDO	E	201	-	-	0/1/1/1	-
19	EDO	N	615	-	-	1/1/1/1	-
19	EDO	E	202	-	-	1/1/1/1	-
29	SAC	V	101	-	-	6/7/8/10	-
26	DMU	P	303	-	-	9/19/59/59	0/2/2/2
19	EDO	N	616	-	-	0/1/1/1	-
19	EDO	G	104	-	-	1/1/1/1	-
17	PGV	N	617	-	-	30/55/55/55	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	P	312	-	-	1/1/1/1	-
24	CHD	C	305	-	-	2/9/74/74	0/4/4/4
23	PSC	R	201	-	1/1/5/9	30/55/55/55	-
19	EDO	B	309	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	A	605	-	-	15/55/55/55	-
19	EDO	W	301	-	-	1/1/1/1	-
19	EDO	C	307	-	-	1/1/1/1	-
24	CHD	P	304	-	-	1/9/74/74	0/4/4/4
24	CHD	Y	102	-	-	4/9/74/74	2/4/4/4
19	EDO	S	104	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
17	PGV	C	303	-	-	33/55/55/55	-
19	EDO	J	102	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
26	DMU	G	101	-	-	6/19/59/59	0/2/2/2
19	EDO	D	204	-	-	0/1/1/1	-
19	EDO	S	102	-	-	0/1/1/1	-
19	EDO	F	703	-	-	1/1/1/1	-
19	EDO	M	701	-	-	0/1/1/1	-
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	O	302	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
19	EDO	N	609	-	-	0/1/1/1	-
19	EDO	A	613	-	-	1/1/1/1	-
19	EDO	B	305	-	-	1/1/1/1	-
19	EDO	Q	205	-	-	1/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	I	103	-	-	1/1/1/1	-
25	CDL	C	310	-	-	56/110/110/110	-
26	DMU	Q	206	-	-	10/19/59/59	0/2/2/2
19	EDO	F	701	-	-	0/1/1/1	-
24	CHD	P	309	-	-	3/9/74/74	1/4/4/4
19	EDO	B	306	-	-	0/1/1/1	-
19	EDO	B	310	-	-	1/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
24	CHD	T	105	-	-	7/9/74/74	1/4/4/4
29	SAC	I	101	-	-	4/7/8/10	-
19	EDO	G	109	-	-	1/1/1/1	-
17	PGV	A	604	-	-	31/55/55/55	-
19	EDO	D	205	-	-	1/1/1/1	-
17	PGV	P	302	-	-	15/55/55/55	-
19	EDO	A	616	-	-	0/1/1/1	-
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	B	311	-	-	1/1/1/1	-
19	EDO	A	617	-	-	0/1/1/1	-
27	PEK	P	305	-	-	28/56/56/56	-
19	EDO	J	105	-	-	1/1/1/1	-
25	CDL	P	308	-	-	54/110/110/110	-
19	EDO	N	607	-	-	1/1/1/1	-
25	CDL	C	304	-	-	53/110/110/110	-
18	HEA	N	605	1	3/3/7/16	6/32/76/76	-
18	HEA	A	606	1	3/3/7/16	6/32/76/76	-
19	EDO	R	203	-	-	1/1/1/1	-
22	TGL	B	302	-	-	34/65/65/65	-
17	PGV	P	307	-	-	27/55/55/55	-
19	EDO	Q	204	-	-	1/1/1/1	-
24	CHD	J	101	-	-	1/9/74/74	0/4/4/4
27	PEK	T	102	-	-	16/56/56/56	-
24	CHD	W	302	-	-	2/9/74/74	0/4/4/4
19	EDO	N	612	-	-	0/1/1/1	-
19	EDO	D	202	-	-	1/1/1/1	-
19	EDO	Q	203	-	-	0/1/1/1	-
18	HEA	N	606	1	3/3/7/16	5/32/76/76	-
19	EDO	A	610	-	-	0/1/1/1	-
17	PGV	P	306	-	-	11/55/55/55	-
22	TGL	Q	201	-	-	38/65/65/65	-
19	EDO	J	103	-	-	0/1/1/1	-
19	EDO	P	310	-	-	0/1/1/1	-
22	TGL	D	201	-	-	41/65/65/65	-
19	EDO	S	103	-	-	0/1/1/1	-
19	EDO	S	105	-	-	1/1/1/1	-
19	EDO	Z	1601	-	-	1/1/1/1	-
19	EDO	R	202	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	610	-	-	1/1/1/1	-
19	EDO	N	613	-	-	1/1/1/1	-

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	311	DMU	O16-C6	7.82	1.53	1.40
26	G	101	DMU	O16-C6	7.82	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	607	HEA	C3C-C2C	5.36	1.47	1.40
18	N	606	HEA	C3B-C2B	5.33	1.46	1.34
18	N	605	HEA	C3D-C2D	5.01	1.47	1.36
26	G	101	DMU	O5-C6	4.96	1.54	1.41
26	G	101	DMU	O7-C10	4.89	1.55	1.41
18	N	605	HEA	C3B-C2B	4.86	1.45	1.34
18	N	606	HEA	C3D-C2D	4.79	1.46	1.36
18	A	607	HEA	C3A-C2A	4.70	1.46	1.40
18	A	606	HEA	C3D-C2D	4.68	1.46	1.36
18	A	607	HEA	CHD-C1D	4.57	1.46	1.35
18	A	607	HEA	C1D-ND	-4.49	1.32	1.40
18	A	607	HEA	C3B-C2B	4.47	1.44	1.34
18	N	606	HEA	C3A-C2A	4.47	1.46	1.40
18	N	606	HEA	CHC-C4B	4.47	1.46	1.35
18	A	606	HEA	C3B-C2B	4.42	1.44	1.34
18	A	607	HEA	C3D-C2D	4.38	1.46	1.36
18	A	606	HEA	CHD-C1D	4.33	1.46	1.35
18	A	606	HEA	CHC-C4B	4.27	1.45	1.35
18	A	607	HEA	CHC-C4B	4.26	1.45	1.35
26	G	101	DMU	O1-C10	4.25	1.52	1.41
18	N	605	HEA	CHD-C1D	4.25	1.45	1.35
26	C	311	DMU	O7-C10	4.25	1.53	1.41
18	A	606	HEA	C1B-NB	-4.12	1.30	1.38
18	N	606	HEA	CHD-C1D	4.08	1.45	1.35
26	P	303	DMU	O7-C10	3.98	1.53	1.41
18	A	606	HEA	C1D-ND	-3.97	1.33	1.40
18	N	605	HEA	CHC-C4B	3.80	1.44	1.35
18	A	607	HEA	C4B-C3B	3.79	1.51	1.44
18	A	606	HEA	C4B-NB	-3.77	1.33	1.40
26	C	312	DMU	O16-C6	3.74	1.46	1.40
18	N	605	HEA	C3C-C2C	3.70	1.45	1.40
26	G	101	DMU	O5-C4	3.68	1.53	1.44
26	C	311	DMU	O7-C3	3.66	1.53	1.43
26	P	303	DMU	C8-C9	3.65	1.60	1.53
18	N	606	HEA	C4D-ND	-3.64	1.31	1.38
18	A	607	HEA	C4B-NB	-3.64	1.34	1.40
26	P	303	DMU	O1-C10	3.57	1.50	1.41
18	N	606	HEA	C3C-C2C	3.55	1.45	1.40
26	P	303	DMU	O16-C6	3.49	1.46	1.40
18	A	606	HEA	C3C-C2C	3.48	1.45	1.40
18	A	606	HEA	C3A-C2A	3.45	1.45	1.40
26	Q	206	DMU	O16-C6	3.41	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	101	DMU	O7-C3	3.40	1.52	1.43
18	N	606	HEA	C1D-ND	-3.38	1.34	1.40
18	N	605	HEA	C3A-C2A	3.38	1.45	1.40
18	N	606	HEA	C4B-C3B	3.32	1.50	1.44
18	N	605	HEA	C4B-NB	-3.31	1.34	1.40
18	N	605	HEA	C1B-NB	-3.31	1.32	1.38
18	A	606	HEA	C2A-C1A	3.17	1.49	1.42
26	P	303	DMU	O1-C9	3.11	1.51	1.44
18	N	606	HEA	C2A-C1A	3.11	1.49	1.42
26	P	303	DMU	O7-C3	2.91	1.51	1.43
26	D	208	DMU	O5-C4	2.88	1.51	1.44
18	N	606	HEA	C1B-NB	-2.76	1.33	1.38
18	N	605	HEA	C1B-C2B	2.74	1.49	1.44
18	N	605	HEA	C2A-C1A	2.73	1.48	1.42
26	C	311	DMU	C3-C4	2.69	1.60	1.52
18	A	607	HEA	C4D-ND	-2.67	1.33	1.38
18	N	605	HEA	C4D-ND	-2.66	1.33	1.38
18	A	607	HEA	C1B-NB	-2.63	1.33	1.38
26	G	101	DMU	C6-C1	2.57	1.59	1.52
18	N	605	HEA	C4B-C3B	2.56	1.48	1.44
18	N	605	HEA	C1D-ND	-2.54	1.35	1.40
18	A	607	HEA	C2A-C1A	2.40	1.48	1.42
18	A	606	HEA	C4D-ND	-2.39	1.33	1.38
26	C	311	DMU	C10-C5	2.35	1.59	1.52
18	N	606	HEA	C4C-CHD	2.34	1.47	1.41
18	A	606	HEA	C4B-C3B	2.34	1.48	1.44
26	C	311	DMU	C2-C3	2.32	1.58	1.52
18	N	606	HEA	FE-ND	2.31	2.08	1.96
18	N	606	HEA	C1C-CHC	2.30	1.47	1.41
18	N	606	HEA	FE-NB	2.28	2.08	1.96
18	A	607	HEA	FE-NB	2.26	2.08	1.96
26	C	312	DMU	O1-C10	2.25	1.47	1.41
26	C	311	DMU	O5-C4	2.22	1.49	1.44
26	C	312	DMU	O49-C1	2.20	1.48	1.43
26	P	303	DMU	C2-C1	2.20	1.57	1.52
18	N	605	HEA	C4C-CHD	2.20	1.47	1.41
18	A	606	HEA	C1B-C2B	2.10	1.48	1.44
26	C	311	DMU	O1-C10	2.09	1.47	1.41
18	A	606	HEA	FE-ND	2.09	2.07	1.96
24	J	101	CHD	O26-C24	-2.08	1.23	1.30
18	N	606	HEA	C4B-NB	-2.07	1.36	1.40
26	G	101	DMU	O1-C9	2.07	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	208	DMU	O1-C10	2.05	1.47	1.41
26	P	303	DMU	C11-C9	2.05	1.58	1.51
26	G	101	DMU	C7-C5	2.04	1.57	1.52
26	D	208	DMU	C3-C4	2.00	1.58	1.52

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	208	DMU	C18-O16-C6	15.73	139.93	113.84
18	N	605	HEA	C3B-C4B-NB	6.09	117.05	109.84
18	N	606	HEA	C3D-C4D-ND	5.99	116.16	110.36
18	N	606	HEA	C1D-C2D-C3D	-5.97	100.68	106.96
26	G	101	DMU	O5-C4-C57	5.70	120.62	106.44
18	N	606	HEA	C2D-C1D-ND	5.58	116.45	109.84
18	A	606	HEA	C2B-C1B-NB	5.48	116.44	109.88
18	A	607	HEA	C2B-C1B-NB	5.44	116.40	109.88
18	A	607	HEA	C2D-C1D-ND	5.39	116.23	109.84
26	D	208	DMU	O5-C6-O16	5.33	122.59	109.97
26	C	311	DMU	C18-O16-C6	5.20	122.46	113.84
18	N	605	HEA	C2B-C1B-NB	5.16	116.06	109.88
18	A	607	HEA	C3D-C4D-ND	5.15	115.34	110.36
18	A	606	HEA	C3B-C4B-NB	5.09	115.87	109.84
18	N	605	HEA	C3D-C4D-ND	5.08	115.28	110.36
18	A	607	HEA	C3B-C4B-NB	4.89	115.63	109.84
18	A	606	HEA	C4A-CHB-C1B	4.86	128.98	122.56
18	A	607	HEA	C1D-C2D-C3D	-4.76	101.95	106.96
18	A	606	HEA	C3D-C4D-ND	4.75	114.96	110.36
18	A	606	HEA	CMB-C2B-C1B	4.74	132.26	125.04
18	N	606	HEA	C3B-C4B-NB	4.69	115.40	109.84
18	N	606	HEA	C2B-C1B-NB	4.59	115.38	109.88
18	A	606	HEA	CAD-CBD-CGD	-4.54	103.84	113.60
18	N	606	HEA	C4D-CHA-C1A	4.51	128.50	122.56
26	G	101	DMU	C6-O5-C4	4.42	122.36	113.69
18	A	606	HEA	C1D-C2D-C3D	-4.39	102.34	106.96
18	N	605	HEA	C2D-C1D-ND	4.31	114.95	109.84
18	N	606	HEA	C17-C18-C19	-4.27	117.37	127.66
26	G	101	DMU	C2-C3-C4	-4.23	101.22	110.93
18	A	606	HEA	C2D-C1D-ND	4.09	114.69	109.84
18	A	607	HEA	C3C-C4C-NC	4.08	114.48	109.21
18	N	605	HEA	C1D-C2D-C3D	-4.07	102.68	106.96
26	G	101	DMU	C18-O16-C6	4.04	120.53	113.84
26	P	303	DMU	C18-O16-C6	4.02	120.51	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	605	HEA	C3C-C4C-NC	4.01	114.39	109.21
18	N	606	HEA	C4A-CHB-C1B	3.88	127.68	122.56
26	C	311	DMU	C1-C2-C3	3.87	118.52	109.68
18	N	606	HEA	C4B-C3B-C2B	-3.82	100.89	107.41
26	G	101	DMU	C10-O1-C9	3.81	121.16	113.69
26	C	311	DMU	C10-O7-C3	3.80	127.36	117.96
18	A	607	HEA	CHB-C1B-C2B	-3.77	119.09	124.98
18	A	607	HEA	C4A-CHB-C1B	3.74	127.49	122.56
18	N	605	HEA	C4B-C3B-C2B	-3.70	101.09	107.41
26	C	312	DMU	O1-C9-C11	3.68	115.59	106.44
18	N	606	HEA	C3C-C4C-NC	3.68	113.97	109.21
18	A	607	HEA	OMA-CMA-C3A	-3.67	116.91	124.91
18	A	607	HEA	CMC-C2C-C3C	3.62	131.46	124.68
26	P	303	DMU	O7-C10-O1	3.61	120.75	110.67
18	N	605	HEA	C4D-CHA-C1A	3.60	127.31	122.56
26	G	101	DMU	O7-C10-O1	3.56	120.63	110.67
18	A	606	HEA	C1B-C2B-C3B	-3.54	102.56	106.80
18	N	606	HEA	C26-C15-C16	3.44	121.06	115.27
18	A	607	HEA	C4B-C3B-C2B	-3.43	101.56	107.41
26	P	303	DMU	C10-O1-C9	3.41	120.38	113.69
18	N	605	HEA	CHA-C4D-C3D	-3.35	119.92	124.84
26	C	311	DMU	O5-C6-O16	3.34	117.89	109.97
18	A	606	HEA	C4B-C3B-C2B	-3.34	101.70	107.41
18	N	606	HEA	C27-C19-C20	3.34	120.89	115.27
18	A	606	HEA	C3C-C4C-NC	3.33	113.52	109.21
18	A	606	HEA	CMC-C2C-C3C	3.33	130.90	124.68
18	N	605	HEA	CAD-CBD-CGD	-3.32	106.45	113.60
18	A	607	HEA	CAA-CBA-CGA	-3.32	104.45	113.76
18	N	606	HEA	OMA-CMA-C3A	-3.32	117.68	124.91
18	A	606	HEA	C4D-CHA-C1A	3.30	126.92	122.56
18	A	606	HEA	CHA-C4D-C3D	-3.29	120.00	124.84
22	N	604	TGL	OG2-CB1-CB2	3.27	118.55	111.50
26	G	101	DMU	O7-C3-C4	3.25	118.36	109.45
18	N	605	HEA	C4A-CHB-C1B	3.17	126.75	122.56
18	A	606	HEA	C13-C12-C11	-3.16	109.60	114.35
18	A	607	HEA	C13-C12-C11	-3.15	109.61	114.35
24	Y	102	CHD	C5-C6-C7	-3.15	110.98	114.46
26	C	311	DMU	O5-C4-C3	3.14	116.38	109.75
18	N	605	HEA	C1B-C2B-C3B	-3.13	103.06	106.80
18	N	606	HEA	C16-C15-C14	-3.10	114.84	121.12
18	N	605	HEA	C27-C19-C20	3.10	120.49	115.27
24	T	105	CHD	C14-C8-C7	3.08	115.89	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	607	HEA	CHA-C4D-C3D	-3.07	120.33	124.84
26	G	101	DMU	O7-C3-C2	3.06	115.43	107.28
18	N	605	HEA	CHB-C1B-C2B	-3.04	120.24	124.98
18	N	605	HEA	C20-C19-C18	-3.01	115.02	121.12
26	P	303	DMU	C7-C8-C9	2.99	115.56	110.24
26	Q	206	DMU	C18-O16-C6	2.92	118.68	113.84
18	N	606	HEA	CHA-C4D-C3D	-2.92	120.55	124.84
18	A	607	HEA	CMB-C2B-C1B	2.91	129.47	125.04
18	N	606	HEA	C13-C12-C11	-2.87	110.03	114.35
18	A	607	HEA	C1B-C2B-C3B	-2.87	103.37	106.80
29	V	101	SAC	O-C-CA	-2.87	117.26	124.78
25	P	308	CDL	OB6-CB5-C51	2.86	117.67	111.50
29	I	101	SAC	O-C-CA	-2.84	117.34	124.78
18	A	607	HEA	C4D-C3D-C2D	-2.83	102.77	106.90
24	T	105	CHD	C5-C6-C7	-2.81	111.36	114.46
18	A	606	HEA	CHB-C1B-C2B	-2.80	120.60	124.98
26	D	208	DMU	O1-C9-C11	2.80	113.39	106.44
18	N	605	HEA	C4D-C3D-C2D	-2.76	102.88	106.90
18	N	606	HEA	CHD-C1D-C2D	-2.73	119.18	126.72
18	N	606	HEA	C12-C13-C14	-2.72	105.05	112.23
18	N	605	HEA	CMB-C2B-C1B	2.72	129.18	125.04
18	A	606	HEA	CMB-C2B-C3B	-2.71	125.18	130.34
26	C	311	DMU	O7-C10-O1	2.68	118.17	110.67
18	N	605	HEA	OMA-CMA-C3A	-2.67	119.09	124.91
26	D	208	DMU	O16-C6-C1	-2.67	104.13	108.30
18	A	607	HEA	C27-C19-C20	2.65	119.73	115.27
18	N	606	HEA	CHB-C1B-C2B	-2.62	120.88	124.98
18	A	607	HEA	C4D-CHA-C1A	2.61	126.01	122.56
24	Y	102	CHD	C13-C14-C8	2.61	118.07	114.74
26	D	208	DMU	C22-C19-C18	-2.60	101.96	113.49
18	N	606	HEA	CMC-C2C-C3C	2.59	129.52	124.68
24	Y	102	CHD	C14-C8-C9	2.57	113.24	109.71
26	G	101	DMU	O5-C6-O16	2.57	116.06	109.97
25	T	103	CDL	OB6-CB5-C51	2.57	117.03	111.50
26	P	303	DMU	O1-C9-C11	2.57	112.82	106.44
18	A	607	HEA	C16-C17-C18	-2.56	103.45	111.88
18	N	605	HEA	CMC-C2C-C3C	2.56	129.47	124.68
18	A	607	HEA	CHD-C1D-C2D	-2.55	119.66	126.72
18	A	606	HEA	CMD-C2D-C1D	2.55	128.93	125.04
26	D	208	DMU	O5-C4-C57	2.55	112.77	106.44
18	A	606	HEA	CHC-C4B-C3B	-2.54	119.27	125.80
22	Y	101	TGL	OG2-CB1-CB2	2.52	116.94	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	605	HEA	CHC-C4B-C3B	-2.52	119.31	125.80
26	C	312	DMU	C6-C1-C2	2.52	115.24	110.00
24	T	105	CHD	C9-C11-C12	2.49	117.59	114.30
18	A	606	HEA	C4D-C3D-C2D	-2.49	103.27	106.90
18	N	605	HEA	C13-C12-C11	-2.43	110.69	114.35
26	C	311	DMU	O5-C6-C1	-2.42	105.23	110.35
26	C	312	DMU	O4-C7-C5	-2.41	104.77	110.35
18	N	606	HEA	C21-C22-C23	-2.40	119.53	127.75
24	P	309	CHD	C10-C9-C8	2.40	114.39	111.82
26	P	303	DMU	C1-C2-C3	2.39	115.13	109.68
24	Y	102	CHD	C17-C13-C14	-2.38	97.69	100.09
26	P	303	DMU	O7-C3-C2	2.38	113.60	107.28
18	N	606	HEA	C4D-C3D-C2D	-2.37	103.44	106.90
18	N	605	HEA	CHD-C1D-C2D	-2.37	120.17	126.72
18	N	606	HEA	CMD-C2D-C3D	2.36	132.52	126.12
26	Q	206	DMU	O49-C1-C2	-2.35	104.92	110.35
27	C	313	PEK	O01-C1-C2	2.34	116.55	111.50
26	D	208	DMU	C6-O5-C4	-2.34	109.09	113.69
18	A	606	HEA	OMA-CMA-C3A	-2.34	119.82	124.91
26	G	101	DMU	O5-C4-C3	-2.32	104.86	109.75
26	C	312	DMU	C28-C25-C22	-2.31	102.72	114.42
18	A	607	HEA	C16-C15-C14	-2.29	116.48	121.12
18	N	605	HEA	C4B-NB-C1B	-2.28	102.72	105.07
26	C	311	DMU	C25-C22-C19	-2.26	102.93	114.42
24	Y	102	CHD	C13-C17-C20	2.26	122.19	119.50
26	C	312	DMU	C1-C2-C3	2.26	114.83	109.68
18	A	606	HEA	CAA-CBA-CGA	-2.25	107.45	113.76
18	N	605	HEA	CAD-C3D-C2D	2.25	132.07	127.88
26	P	303	DMU	O1-C10-C5	-2.24	105.62	110.35
26	Q	206	DMU	C10-O1-C9	2.22	118.04	113.69
24	T	101	CHD	C18-C13-C14	2.21	114.67	111.21
24	T	101	CHD	C4-C3-C2	2.20	113.18	110.55
18	A	607	HEA	CHC-C4B-NB	-2.17	121.69	124.38
26	C	311	DMU	O16-C6-C1	2.15	111.65	108.30
24	T	105	CHD	C10-C9-C8	2.15	114.12	111.82
26	Q	206	DMU	O16-C6-C1	2.12	111.62	108.30
17	C	303	PGV	O01-C1-C2	2.11	116.04	111.50
24	Y	102	CHD	C17-C13-C12	2.10	119.58	117.67
24	J	101	CHD	C5-C4-C3	2.10	115.84	112.76
26	D	208	DMU	C25-C22-C19	-2.10	103.79	114.42
18	N	606	HEA	C21-C20-C19	-2.09	106.09	112.98
26	C	312	DMU	C22-C19-C18	-2.09	104.25	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	305	CHD	C4-C5-C10	2.08	114.87	112.66
26	Q	206	DMU	O5-C6-O16	-2.08	105.05	109.97
26	Q	206	DMU	O7-C10-C5	2.06	113.45	108.10
18	N	606	HEA	CAA-CBA-CGA	-2.06	107.97	113.76
18	A	607	HEA	C25-C23-C24	2.06	119.14	114.60
27	T	102	PEK	O13-P-O14	2.05	122.39	112.24
22	B	302	TGL	OG2-CB1-CB2	2.05	115.92	111.50
26	P	303	DMU	O2-C8-C7	-2.03	105.65	110.35
24	Y	102	CHD	C16-C17-C13	-2.03	101.57	103.55
24	C	301	CHD	O25-C24-C23	-2.02	116.58	123.08
18	N	605	HEA	O2D-CGD-CBD	2.01	120.48	114.03
24	T	105	CHD	C17-C13-C14	2.01	102.11	100.09

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	606	HEA	NB
18	A	606	HEA	NA
18	A	606	HEA	ND
18	A	607	HEA	NB
18	A	607	HEA	NA
18	A	607	HEA	ND
18	N	605	HEA	NB
18	N	605	HEA	NA
18	N	605	HEA	ND
18	N	606	HEA	NB
18	N	606	HEA	NA
18	N	606	HEA	ND
23	R	201	PSC	C02

All (970) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	O12-C04-C05-O05
17	C	303	PGV	C03-O11-P-O14
17	C	303	PGV	O01-C02-C03-O11
17	C	303	PGV	O12-C04-C05-C06
17	C	303	PGV	C04-C05-C06-O06
17	N	617	PGV	C03-O11-P-O14
17	N	617	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
17	N	617	PGV	C2-C1-O01-C02
17	P	307	PGV	C03-O11-P-O13
17	P	307	PGV	C04-C05-C06-O06
18	A	607	HEA	C14-C15-C16-C17
18	A	607	HEA	C26-C15-C16-C17
18	A	607	HEA	C19-C20-C21-C22
18	N	605	HEA	C2D-C3D-CAD-CBD
22	D	201	TGL	CB2-CB1-OG2-CG2
22	L	101	TGL	CB2-CB1-OG2-CG2
22	Q	201	TGL	OG2-CG2-CG3-OG3
22	Y	101	TGL	CB2-CB1-OG2-CG2
22	Y	101	TGL	OB1-CB1-OG2-CG2
23	B	303	PSC	C03-O11-P-O12
23	B	303	PSC	C03-O11-P-O14
23	B	303	PSC	C04-O12-P-O13
23	R	201	PSC	C03-O11-P-O12
23	R	201	PSC	C03-O11-P-O14
23	R	201	PSC	C04-O12-P-O11
23	R	201	PSC	C04-O12-P-O14
23	R	201	PSC	O12-C04-C05-N
23	R	201	PSC	C2-C1-O01-C02
25	C	304	CDL	C1-CA2-OA2-PA1
25	C	304	CDL	CA3-OA5-PA1-OA2
25	C	304	CDL	CA3-OA5-PA1-OA3
25	C	304	CDL	OA7-CA5-OA6-CA4
25	C	304	CDL	C11-CA5-OA6-CA4
25	C	310	CDL	CA2-C1-CB2-OB2
25	C	310	CDL	CA2-OA2-PA1-OA3
25	C	310	CDL	CA2-OA2-PA1-OA5
25	C	310	CDL	C11-CA5-OA6-CA4
25	P	308	CDL	C1-CA2-OA2-PA1
25	P	308	CDL	CA3-OA5-PA1-OA2
25	P	308	CDL	CA3-OA5-PA1-OA3
25	P	308	CDL	CA3-OA5-PA1-OA4
25	P	308	CDL	CB2-OB2-PB2-OB3
25	T	103	CDL	O1-C1-CA2-OA2
25	T	103	CDL	CB2-OB2-PB2-OB3
25	T	103	CDL	CB2-OB2-PB2-OB4
25	T	103	CDL	CB2-OB2-PB2-OB5
26	C	311	DMU	C1-C6-O16-C18
26	C	311	DMU	O5-C6-O16-C18
26	C	312	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
26	C	312	DMU	O5-C6-O16-C18
26	D	208	DMU	C19-C18-O16-C6
26	Q	206	DMU	C1-C6-O16-C18
26	Q	206	DMU	O5-C6-O16-C18
27	C	313	PEK	O12-C04-C05-N
27	G	102	PEK	C6-C7-C8-C9
27	G	102	PEK	C12-C13-C14-C15
27	G	103	PEK	O02-C1-O01-C02
27	G	103	PEK	C11-C10-C9-C8
27	P	301	PEK	C04-O12-P-O13
27	P	301	PEK	O12-C04-C05-N
27	P	301	PEK	C11-C12-C13-C14
27	P	305	PEK	C04-O12-P-O14
27	P	305	PEK	O12-C04-C05-N
27	P	305	PEK	O02-C1-O01-C02
27	T	102	PEK	O12-C04-C05-N
27	T	102	PEK	C9-C10-C11-C12
29	I	101	SAC	C2A-C1A-N-CA
29	I	101	SAC	N-CA-CB-OG
29	I	101	SAC	C-CA-CB-OG
29	V	101	SAC	C2A-C1A-N-CA
29	V	101	SAC	C-CA-N-C1A
29	V	101	SAC	O-C-CA-CB
29	V	101	SAC	C-CA-CB-OG
17	N	617	PGV	O04-C19-O03-C01
22	Q	201	TGL	OC1-CC1-OG3-CG3
23	B	303	PSC	O04-C19-O03-C01
26	P	303	DMU	O1-C10-O7-C3
22	Q	201	TGL	CC2-CC1-OG3-CG3
23	B	303	PSC	C20-C19-O03-C01
25	T	103	CDL	OA9-CA7-OA8-CA6
27	G	103	PEK	O04-C21-O03-C01
26	C	311	DMU	O1-C10-O7-C3
17	A	604	PGV	O02-C1-O01-C02
22	D	201	TGL	OB1-CB1-OG2-CG2
22	L	101	TGL	OB1-CB1-OG2-CG2
23	R	201	PSC	O02-C1-O01-C02
25	C	310	CDL	OA7-CA5-OA6-CA4
29	V	101	SAC	OAC-C1A-N-CA
17	N	617	PGV	C20-C19-O03-C01
25	P	308	CDL	C31-CA7-OA8-CA6
25	T	103	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
27	G	103	PEK	C22-C21-O03-C01
17	A	604	PGV	C2-C1-O01-C02
27	G	103	PEK	C2-C1-O01-C02
27	P	305	PEK	C2-C1-O01-C02
22	D	201	TGL	OC1-CC1-OG3-CG3
24	W	302	CHD	C20-C22-C23-C24
17	P	307	PGV	C20-C19-O03-C01
22	D	201	TGL	CC2-CC1-OG3-CG3
18	N	605	HEA	C4D-C3D-CAD-CBD
25	C	310	CDL	OA9-CA7-OA8-CA6
25	P	308	CDL	OA9-CA7-OA8-CA6
27	P	305	PEK	O04-C21-O03-C01
26	D	208	DMU	O6-C11-C9-O1
29	I	101	SAC	OAC-C1A-N-CA
25	P	308	CDL	O1-C1-CB2-OB2
17	A	604	PGV	C20-C19-O03-C01
26	C	311	DMU	O5-C4-C57-O61
25	P	308	CDL	C51-CB5-OB6-CB4
26	G	101	DMU	O6-C11-C9-O1
22	N	604	TGL	C21-C22-C23-C24
22	Y	101	TGL	C11-C12-C13-C14
17	N	617	PGV	C1-C2-C3-C4
17	A	604	PGV	C23-C24-C25-C26
25	C	310	CDL	C31-CA7-OA8-CA6
27	P	305	PEK	C22-C21-O03-C01
26	D	208	DMU	O6-C11-C9-C8
17	A	604	PGV	C05-C04-O12-P
17	P	307	PGV	O04-C19-O03-C01
18	N	606	HEA	C26-C15-C16-C17
18	N	606	HEA	C14-C15-C16-C17
26	D	208	DMU	O5-C6-O16-C18
17	C	303	PGV	C20-C19-O03-C01
22	Y	101	TGL	CA2-CA1-OG1-CG1
22	L	101	TGL	CA3-CA4-CA5-CA6
23	B	303	PSC	C19-C20-C21-C22
26	P	303	DMU	O6-C11-C9-C8
24	Y	102	CHD	C17-C20-C22-C23
17	A	604	PGV	O12-C04-C05-C06
25	P	308	CDL	CA2-C1-CB2-OB2
25	P	308	CDL	OB7-CB5-OB6-CB4
24	Y	102	CHD	C21-C20-C22-C23
17	A	604	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
22	Y	101	TGL	OA1-CA1-OG1-CG1
27	P	301	PEK	O04-C21-O03-C01
25	C	310	CDL	C71-CB7-OB8-CB6
27	P	301	PEK	C22-C21-O03-C01
24	T	105	CHD	C17-C20-C22-C23
27	P	301	PEK	C25-C26-C27-C28
22	D	201	TGL	C14-C29-C30-C31
17	C	303	PGV	O12-C04-C05-O05
25	C	310	CDL	O1-C1-CB2-OB2
25	T	103	CDL	OB6-CB4-CB6-OB8
22	Y	101	TGL	CC9-C15-C16-C17
17	C	303	PGV	C13-C14-C15-C16
17	N	617	PGV	C25-C26-C27-C28
24	T	105	CHD	C13-C17-C20-C22
22	N	604	TGL	CC1-CC2-CC3-CC4
26	C	312	DMU	O5-C4-C57-O61
26	G	101	DMU	O5-C4-C57-O61
26	C	311	DMU	C3-C4-C57-O61
23	B	303	PSC	C21-C22-C23-C24
24	T	105	CHD	C13-C17-C20-C21
17	C	303	PGV	O04-C19-O03-C01
17	A	604	PGV	C1-C2-C3-C4
17	C	303	PGV	C19-C20-C21-C22
22	Y	101	TGL	CA1-CA2-CA3-CA4
25	P	308	CDL	CA7-C31-C32-C33
25	T	103	CDL	CB7-C71-C72-C73
27	C	313	PEK	C1-C2-C3-C4
27	T	102	PEK	C1-C2-C3-C4
17	A	604	PGV	C21-C22-C23-C24
22	Y	101	TGL	CC6-CC7-CC8-CC9
24	T	105	CHD	C21-C20-C22-C23
25	C	310	CDL	CB5-C51-C52-C53
27	G	102	PEK	C1-C2-C3-C4
27	G	103	PEK	C1-C2-C3-C4
19	C	308	EDO	O1-C1-C2-O2
19	Q	202	EDO	O1-C1-C2-O2
25	C	310	CDL	OB9-CB7-OB8-CB6
22	D	201	TGL	CC1-CC2-CC3-CC4
17	P	307	PGV	O12-C04-C05-O05
25	C	304	CDL	O1-C1-CA2-OA2
17	C	302	PGV	C12-C13-C14-C15
22	B	302	TGL	CC1-CC2-CC3-CC4

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Mol	Chain	Res	Type	Atoms
22	N	604	TGL	CB1-CB2-CB3-CB4
25	C	304	CDL	CB7-C71-C72-C73
27	P	301	PEK	C13-C14-C15-C16
17	A	604	PGV	C03-O11-P-O12
17	C	303	PGV	C03-O11-P-O12
17	P	307	PGV	C03-O11-P-O12
23	B	303	PSC	C04-O12-P-O11
25	C	304	CDL	CB2-OB2-PB2-OB5
25	C	310	CDL	CB3-OB5-PB2-OB2
25	P	308	CDL	CB2-OB2-PB2-OB5
27	C	313	PEK	C03-O11-P-O12
27	G	103	PEK	C03-O11-P-O12
17	P	307	PGV	O12-C04-C05-C06
25	C	304	CDL	CB2-C1-CA2-OA2
25	T	103	CDL	CB2-C1-CA2-OA2
27	C	313	PEK	O02-C1-O01-C02
18	N	606	HEA	C27-C19-C20-C21
24	T	105	CHD	C16-C17-C20-C21
25	C	310	CDL	CB7-C71-C72-C73
17	P	302	PGV	C5-C6-C7-C8
22	N	604	TGL	CB9-C10-C11-C12
25	C	310	CDL	C15-C16-C17-C18
27	C	313	PEK	C2-C1-O01-C02
17	C	303	PGV	C6-C7-C8-C9
17	C	303	PGV	C28-C29-C30-C31
17	P	302	PGV	C30-C31-C32-C33
22	B	302	TGL	CA3-CA4-CA5-CA6
22	D	201	TGL	CC5-CC6-CC7-CC8
22	L	101	TGL	CB6-CB7-CB8-CB9
22	N	604	TGL	C11-C12-C13-C14
22	Q	201	TGL	C21-C20-CA9-CA8
25	C	304	CDL	C37-C38-C39-C40
25	C	310	CDL	C57-C58-C59-C60
27	G	102	PEK	C27-C28-C29-C30
27	T	102	PEK	C33-C34-C35-C36
17	A	604	PGV	C4-C5-C6-C7
22	L	101	TGL	C12-C13-C14-C29
22	L	101	TGL	C16-C17-C18-C19
22	Y	101	TGL	CB6-CB7-CB8-CB9
22	Y	101	TGL	CC2-CC3-CC4-CC5
25	C	304	CDL	C17-C18-C19-C20
25	C	304	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	C15-C16-C17-C18
25	T	103	CDL	C81-C82-C83-C84
17	P	307	PGV	C3-C4-C5-C6
22	B	302	TGL	CA6-CA7-CA8-CA9
22	B	302	TGL	CC3-CC4-CC5-CC6
22	Q	201	TGL	C20-C21-C22-C23
25	C	304	CDL	C19-C20-C21-C22
25	P	308	CDL	C20-C21-C22-C23
25	P	308	CDL	C36-C37-C38-C39
27	G	102	PEK	C28-C29-C30-C31
17	C	303	PGV	C10-C11-C12-C13
22	Y	101	TGL	C23-C24-C25-C26
26	G	101	DMU	C31-C34-C37-C40
27	C	313	PEK	C30-C31-C32-C33
25	P	308	CDL	O1-C1-CA2-OA2
22	Q	201	TGL	CA5-CA6-CA7-CA8
22	Q	201	TGL	CC1-CC2-CC3-CC4
22	D	201	TGL	C17-C18-C19-C33
23	B	303	PSC	C25-C26-C27-C28
23	R	201	PSC	C28-C29-C30-C31
26	D	208	DMU	C25-C28-C31-C34
27	C	313	PEK	C29-C30-C31-C32
27	P	301	PEK	C28-C29-C30-C31
27	P	305	PEK	C28-C29-C30-C31
17	C	303	PGV	C4-C5-C6-C7
25	C	304	CDL	C13-C14-C15-C16
25	P	308	CDL	C13-C14-C15-C16
25	T	103	CDL	C33-C34-C35-C36
22	B	302	TGL	CC4-CC5-CC6-CC7
22	B	302	TGL	C18-C19-C33-C34
22	D	201	TGL	CB4-CB5-CB6-CB7
22	D	201	TGL	CC7-CC8-CC9-C15
22	Q	201	TGL	CC5-CC6-CC7-CC8
25	C	310	CDL	C33-C34-C35-C36
25	P	308	CDL	C82-C83-C84-C85
27	C	313	PEK	C28-C29-C30-C31
27	G	103	PEK	C16-C17-C18-C19
24	Y	102	CHD	C20-C22-C23-C24
22	D	201	TGL	CA6-CA7-CA8-CA9
22	N	604	TGL	CC5-CC6-CC7-CC8
25	T	103	CDL	C51-C52-C53-C54
26	D	208	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
22	B	302	TGL	CA9-C20-C21-C22
26	C	312	DMU	C3-C4-C57-O61
17	A	604	PGV	C20-C21-C22-C23
17	A	605	PGV	C5-C6-C7-C8
17	A	605	PGV	C7-C8-C9-C10
17	P	306	PGV	C6-C7-C8-C9
22	D	201	TGL	C23-C24-C25-C26
25	C	304	CDL	C81-C82-C83-C84
25	C	310	CDL	C40-C41-C42-C43
25	C	310	CDL	C75-C76-C77-C78
25	P	308	CDL	C17-C18-C19-C20
26	C	312	DMU	C22-C25-C28-C31
26	C	312	DMU	C25-C28-C31-C34
26	D	208	DMU	C31-C34-C37-C40
26	Q	206	DMU	O16-C18-C19-C22
17	P	307	PGV	C14-C15-C16-C17
22	D	201	TGL	CA9-C20-C21-C22
22	L	101	TGL	CC2-CC3-CC4-CC5
22	N	604	TGL	C16-C15-CC9-CC8
22	Y	101	TGL	CA3-CA4-CA5-CA6
22	Y	101	TGL	CA6-CA7-CA8-CA9
23	R	201	PSC	C20-C21-C22-C23
25	C	304	CDL	C31-C32-C33-C34
25	C	304	CDL	C59-C60-C61-C62
25	P	308	CDL	C58-C59-C60-C61
25	T	103	CDL	C17-C18-C19-C20
27	P	305	PEK	C27-C28-C29-C30
22	B	302	TGL	CB5-CB6-CB7-CB8
22	D	201	TGL	CB2-CB3-CB4-CB5
25	C	304	CDL	C54-C55-C56-C57
25	C	304	CDL	C83-C84-C85-C86
25	C	310	CDL	C16-C17-C18-C19
25	P	308	CDL	C59-C60-C61-C62
25	P	308	CDL	C81-C82-C83-C84
17	C	302	PGV	C1-C2-C3-C4
17	N	617	PGV	C3-C4-C5-C6
17	P	302	PGV	C6-C7-C8-C9
17	P	302	PGV	C7-C8-C9-C10
25	C	304	CDL	C55-C56-C57-C58
25	C	310	CDL	C72-C73-C74-C75
25	C	310	CDL	C79-C80-C81-C82
22	B	302	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
27	C	313	PEK	C34-C35-C36-C37
26	C	312	DMU	C19-C18-O16-C6
26	Q	206	DMU	C19-C18-O16-C6
22	L	101	TGL	C21-C20-CA9-CA8
25	C	310	CDL	C81-C82-C83-C84
26	Q	206	DMU	C28-C31-C34-C37
27	T	102	PEK	C24-C25-C26-C27
17	A	605	PGV	C19-C20-C21-C22
17	N	617	PGV	C6-C7-C8-C9
25	T	103	CDL	C35-C36-C37-C38
25	T	103	CDL	C78-C79-C80-C81
22	N	604	TGL	CA4-CA5-CA6-CA7
25	C	304	CDL	C18-C19-C20-C21
25	P	308	CDL	C31-C32-C33-C34
27	G	102	PEK	C30-C31-C32-C33
22	B	302	TGL	CC7-CC8-CC9-C15
23	B	303	PSC	C2-C1-O01-C02
27	P	301	PEK	C2-C1-O01-C02
17	A	604	PGV	C02-C01-O03-C19
17	P	307	PGV	C28-C29-C30-C31
26	Q	206	DMU	C22-C25-C28-C31
26	P	303	DMU	O6-C11-C9-O1
17	C	303	PGV	O05-C05-C06-O06
17	P	307	PGV	O05-C05-C06-O06
25	P	308	CDL	C78-C79-C80-C81
27	G	102	PEK	C15-C16-C17-C18
25	C	304	CDL	C22-C23-C24-C25
25	T	103	CDL	C58-C59-C60-C61
17	A	604	PGV	C3-C4-C5-C6
22	Y	101	TGL	C16-C17-C18-C19
27	G	103	PEK	C31-C32-C33-C34
25	P	308	CDL	CB2-C1-CA2-OA2
27	P	301	PEK	C34-C35-C36-C37
27	P	301	PEK	O02-C1-O01-C02
22	N	604	TGL	C14-C29-C30-C31
25	C	310	CDL	C80-C81-C82-C83
27	T	102	PEK	C32-C33-C34-C35
17	A	604	PGV	C22-C23-C24-C25
17	P	306	PGV	C20-C21-C22-C23
22	N	604	TGL	CA7-CA8-CA9-C20
22	N	604	TGL	CA9-C20-C21-C22
25	C	304	CDL	C61-C62-C63-C64

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Mol	Chain	Res	Type	Atoms
25	C	310	CDL	C32-C33-C34-C35
25	P	308	CDL	C22-C23-C24-C25
25	P	308	CDL	C56-C57-C58-C59
25	T	103	CDL	C61-C62-C63-C64
29	V	101	SAC	N-CA-CB-OG
19	A	611	EDO	O1-C1-C2-O2
19	A	614	EDO	O1-C1-C2-O2
19	B	305	EDO	O1-C1-C2-O2
19	B	307	EDO	O1-C1-C2-O2
19	C	307	EDO	O1-C1-C2-O2
19	D	206	EDO	O1-C1-C2-O2
19	E	204	EDO	O1-C1-C2-O2
19	F	703	EDO	O1-C1-C2-O2
19	G	105	EDO	O1-C1-C2-O2
19	J	102	EDO	O1-C1-C2-O2
19	J	104	EDO	O1-C1-C2-O2
19	K	101	EDO	O1-C1-C2-O2
19	K	102	EDO	O1-C1-C2-O2
19	O	303	EDO	O1-C1-C2-O2
19	P	313	EDO	O1-C1-C2-O2
19	Q	204	EDO	O1-C1-C2-O2
19	Q	205	EDO	O1-C1-C2-O2
19	R	203	EDO	O1-C1-C2-O2
19	Z	1601	EDO	O1-C1-C2-O2
22	D	201	TGL	C16-C17-C18-C19
22	N	604	TGL	CB6-CB7-CB8-CB9
22	Q	201	TGL	CC4-CC5-CC6-CC7
27	G	102	PEK	C24-C25-C26-C27
22	Y	101	TGL	CC2-CC1-OG3-CG3
17	C	303	PGV	C2-C1-O01-C02
17	C	303	PGV	C7-C8-C9-C10
17	P	302	PGV	C29-C30-C31-C32
25	P	308	CDL	C52-C53-C54-C55
26	P	303	DMU	C28-C31-C34-C37
25	T	103	CDL	C38-C39-C40-C41
26	P	303	DMU	C19-C22-C25-C28
26	P	303	DMU	C31-C34-C37-C40
17	P	307	PGV	C7-C8-C9-C10
17	P	307	PGV	C27-C28-C29-C30
25	T	103	CDL	C34-C35-C36-C37
17	A	605	PGV	C6-C7-C8-C9
25	C	304	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
27	P	305	PEK	C15-C16-C17-C18
23	B	303	PSC	O02-C1-O01-C02
17	N	617	PGV	C19-C20-C21-C22
23	B	303	PSC	C1-C2-C3-C4
22	B	302	TGL	CC2-CC1-OG3-CG3
17	P	307	PGV	C25-C26-C27-C28
22	L	101	TGL	CC9-C15-C16-C17
22	Q	201	TGL	C19-C33-C34-C35
17	P	302	PGV	C23-C24-C25-C26
22	N	604	TGL	CC6-CC7-CC8-CC9
25	C	304	CDL	C76-C77-C78-C79
17	C	302	PGV	C5-C6-C7-C8
22	B	302	TGL	C21-C20-CA9-CA8
22	Y	101	TGL	C16-C15-CC9-CC8
22	Y	101	TGL	OC1-CC1-OG3-CG3
17	C	302	PGV	C6-C7-C8-C9
22	Y	101	TGL	C10-C11-C12-C13
25	T	103	CDL	C31-C32-C33-C34
27	C	313	PEK	C22-C23-C24-C25
22	B	302	TGL	CB2-CB1-OG2-CG2
25	C	304	CDL	C51-CB5-OB6-CB4
25	C	310	CDL	C51-CB5-OB6-CB4
25	T	103	CDL	C51-CB5-OB6-CB4
22	N	604	TGL	CA6-CA7-CA8-CA9
27	P	305	PEK	C23-C24-C25-C26
27	P	301	PEK	C14-C15-C16-C17
27	P	301	PEK	C27-C28-C29-C30
27	P	305	PEK	C32-C33-C34-C35
22	B	302	TGL	OB1-CB1-OG2-CG2
25	T	103	CDL	OB7-CB5-OB6-CB4
17	P	307	PGV	C2-C3-C4-C5
25	C	310	CDL	C59-C60-C61-C62
22	B	302	TGL	OG1-CG1-CG2-OG2
22	Q	201	TGL	C16-C17-C18-C19
25	P	308	CDL	C42-C43-C44-C45
22	N	604	TGL	CB5-CB6-CB7-CB8
25	T	103	CDL	C77-C78-C79-C80
23	B	303	PSC	C13-C14-C15-C16
27	G	103	PEK	C2-C3-C4-C5
27	T	102	PEK	C15-C16-C17-C18
18	N	606	HEA	C18-C19-C20-C21
22	Y	101	TGL	CB2-CB3-CB4-CB5

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Mol	Chain	Res	Type	Atoms
25	C	304	CDL	C77-C78-C79-C80
22	L	101	TGL	CB7-CB8-CB9-C10
23	R	201	PSC	C23-C24-C25-C26
17	C	303	PGV	O02-C1-O01-C02
22	N	604	TGL	OB1-CB1-OG2-CG2
25	C	304	CDL	OB7-CB5-OB6-CB4
25	C	310	CDL	OB7-CB5-OB6-CB4
22	N	604	TGL	CB2-CB1-OG2-CG2
25	T	103	CDL	C76-C77-C78-C79
27	C	313	PEK	C33-C34-C35-C36
17	N	617	PGV	C03-O11-P-O12
17	N	617	PGV	C7-C8-C9-C10
25	T	103	CDL	C72-C73-C74-C75
27	P	301	PEK	C22-C23-C24-C25
23	R	201	PSC	C2-C3-C4-C5
17	C	303	PGV	C01-C02-C03-O11
25	C	304	CDL	OA5-CA3-CA4-CA6
25	T	103	CDL	OA5-CA3-CA4-CA6
27	C	313	PEK	C01-C02-C03-O11
17	C	303	PGV	C2-C3-C4-C5
22	N	604	TGL	CA2-CA3-CA4-CA5
23	B	303	PSC	C4-C5-C6-C7
17	P	307	PGV	C5-C6-C7-C8
22	D	201	TGL	CC9-C15-C16-C17
26	C	311	DMU	O6-C11-C9-O1
25	C	310	CDL	C35-C36-C37-C38
17	P	307	PGV	C11-C10-C9-C8
27	P	301	PEK	C15-C16-C17-C18
27	G	103	PEK	C26-C27-C28-C29
25	C	304	CDL	CA2-C1-CB2-OB2
17	N	617	PGV	C28-C29-C30-C31
22	D	201	TGL	C10-C11-C12-C13
22	L	101	TGL	C11-C12-C13-C14
17	N	617	PGV	C2-C3-C4-C5
25	C	310	CDL	C20-C21-C22-C23
25	T	103	CDL	C59-C60-C61-C62
17	A	604	PGV	O03-C01-C02-C03
22	B	302	TGL	OG1-CG1-CG2-CG3
22	D	201	TGL	CG1-CG2-CG3-OG3
22	D	201	TGL	CC2-CC3-CC4-CC5
22	L	101	TGL	CG1-CG2-CG3-OG3
22	Q	201	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
25	P	308	CDL	CB3-CB4-CB6-OB8
25	T	103	CDL	CB3-CB4-CB6-OB8
27	T	102	PEK	C7-C8-C9-C10
25	C	304	CDL	C24-C25-C26-C27
22	B	302	TGL	C11-C12-C13-C14
22	L	101	TGL	CC7-CC8-CC9-C15
22	B	302	TGL	CB3-CB4-CB5-CB6
22	L	101	TGL	C29-C30-C31-C32
27	P	305	PEK	C17-C18-C19-C20
22	D	201	TGL	C16-C15-CC9-CC8
25	C	310	CDL	C60-C61-C62-C63
25	C	310	CDL	C37-C38-C39-C40
27	G	102	PEK	C17-C18-C19-C20
27	P	305	PEK	C31-C32-C33-C34
22	B	302	TGL	CB4-CB5-CB6-CB7
22	Y	101	TGL	CC4-CC5-CC6-CC7
25	C	304	CDL	C41-C42-C43-C44
25	T	103	CDL	C43-C44-C45-C46
26	D	208	DMU	C19-C22-C25-C28
26	G	101	DMU	C3-C4-C57-O61
25	T	103	CDL	C11-CA5-OA6-CA4
22	D	201	TGL	CC4-CC5-CC6-CC7
17	N	617	PGV	C21-C22-C23-C24
22	Y	101	TGL	CC1-CC2-CC3-CC4
22	Q	201	TGL	CA2-CA1-OG1-CG1
17	N	617	PGV	C15-C16-C17-C18
26	D	208	DMU	C18-C19-C22-C25
17	C	303	PGV	C31-C32-C33-C34
25	C	310	CDL	C78-C79-C80-C81
26	G	101	DMU	O6-C11-C9-C8
17	N	617	PGV	C4-C5-C6-C7
22	L	101	TGL	C21-C22-C23-C24
23	R	201	PSC	C26-C27-C28-C29
25	C	310	CDL	C22-C23-C24-C25
25	T	103	CDL	C55-C56-C57-C58
17	N	617	PGV	C02-C03-O11-P
17	P	307	PGV	C26-C27-C28-C29
26	C	312	DMU	C28-C31-C34-C37
22	D	201	TGL	CB1-CB2-CB3-CB4
22	Q	201	TGL	C12-C13-C14-C29
19	A	612	EDO	O1-C1-C2-O2
19	G	107	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	S	105	EDO	O1-C1-C2-O2
22	B	302	TGL	OC1-CC1-OG3-CG3
25	T	103	CDL	OA7-CA5-OA6-CA4
17	A	604	PGV	C27-C28-C29-C30
22	L	101	TGL	CA6-CA7-CA8-CA9
22	L	101	TGL	C19-C33-C34-C35
26	Q	206	DMU	C25-C28-C31-C34
17	C	302	PGV	C25-C26-C27-C28
22	B	302	TGL	CB9-C10-C11-C12
25	P	308	CDL	C75-C76-C77-C78
22	Q	201	TGL	C22-C23-C24-C25
25	P	308	CDL	C15-C16-C17-C18
25	T	103	CDL	C82-C83-C84-C85
25	T	103	CDL	C12-C13-C14-C15
27	P	305	PEK	C16-C17-C18-C19
25	P	308	CDL	C71-CB7-OB8-CB6
17	C	302	PGV	C15-C16-C17-C18
22	B	302	TGL	C33-C34-C35-C36
22	N	604	TGL	CC3-CC4-CC5-CC6
22	Q	201	TGL	C29-C30-C31-C32
25	P	308	CDL	C54-C55-C56-C57
17	P	307	PGV	C30-C31-C32-C33
25	C	310	CDL	OA5-CA3-CA4-CA6
25	P	308	CDL	OA5-CA3-CA4-CA6
22	B	302	TGL	C20-C21-C22-C23
25	C	310	CDL	C39-C40-C41-C42
25	T	103	CDL	C22-C23-C24-C25
22	Y	101	TGL	CC5-CC6-CC7-CC8
26	Q	206	DMU	C34-C37-C40-C43
23	B	303	PSC	C3-C4-C5-C6
25	P	308	CDL	C44-C45-C46-C47
26	P	303	DMU	C25-C28-C31-C34
22	B	302	TGL	C23-C24-C25-C26
23	B	303	PSC	C15-C16-C17-C18
25	C	310	CDL	C41-C42-C43-C44
27	P	301	PEK	C02-C03-O11-P
27	T	102	PEK	C26-C27-C28-C29
26	C	311	DMU	C19-C18-O16-C6
26	P	303	DMU	C19-C18-O16-C6
17	A	604	PGV	C25-C26-C27-C28
27	C	313	PEK	C16-C17-C18-C19
27	G	102	PEK	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	C71-CB7-OB8-CB6
22	L	101	TGL	C15-C16-C17-C18
23	R	201	PSC	C14-C15-C16-C17
23	B	303	PSC	O03-C01-C02-C03
25	C	310	CDL	CB3-CB4-CB6-OB8
22	L	101	TGL	C13-C14-C29-C30
22	Q	201	TGL	C18-C19-C33-C34
27	P	305	PEK	C13-C14-C15-C16
25	P	308	CDL	C61-C62-C63-C64
17	N	617	PGV	C26-C27-C28-C29
22	Q	201	TGL	CC9-C15-C16-C17
25	C	304	CDL	C71-C72-C73-C74
25	P	308	CDL	C37-C38-C39-C40
22	B	302	TGL	CC6-CC7-CC8-CC9
22	L	101	TGL	CB2-CB3-CB4-CB5
23	B	303	PSC	C9-C10-C11-C12
23	B	303	PSC	C10-C11-C12-C13
23	R	201	PSC	C9-C10-C11-C12
23	R	201	PSC	C10-C11-C12-C13
27	C	313	PEK	C6-C7-C8-C9
27	C	313	PEK	C11-C12-C13-C14
27	C	313	PEK	C12-C13-C14-C15
27	G	103	PEK	C6-C7-C8-C9
27	G	103	PEK	C12-C13-C14-C15
27	P	301	PEK	C5-C6-C7-C8
27	P	301	PEK	C6-C7-C8-C9
27	P	301	PEK	C11-C10-C9-C8
27	P	305	PEK	C5-C6-C7-C8
27	P	305	PEK	C6-C7-C8-C9
27	P	305	PEK	C11-C10-C9-C8
27	P	305	PEK	C9-C10-C11-C12
22	Q	201	TGL	OA1-CA1-OG1-CG1
22	Q	201	TGL	C10-C11-C12-C13
27	C	313	PEK	C15-C16-C17-C18
17	C	303	PGV	C5-C6-C7-C8
23	B	303	PSC	C5-C6-C7-C8
22	Q	201	TGL	C33-C34-C35-C36
22	N	604	TGL	C25-C26-C27-C28
22	Y	101	TGL	CB7-CB8-CB9-C10
27	C	313	PEK	C17-C18-C19-C20
25	C	310	CDL	OB6-CB4-CB6-OB8
25	P	308	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C6-C7-C8-C9
22	D	201	TGL	C19-C33-C34-C35
27	G	103	PEK	C32-C33-C34-C35
17	N	617	PGV	C29-C30-C31-C32
17	C	302	PGV	C02-C03-O11-P
25	C	304	CDL	CA4-CA3-OA5-PA1
25	T	103	CDL	C1-CA2-OA2-PA1
26	C	312	DMU	O6-C11-C9-C8
23	R	201	PSC	C13-C14-C15-C16
27	P	305	PEK	C14-C15-C16-C17
19	D	205	EDO	O1-C1-C2-O2
19	J	105	EDO	O1-C1-C2-O2
19	N	614	EDO	O1-C1-C2-O2
19	P	314	EDO	O1-C1-C2-O2
19	V	102	EDO	O1-C1-C2-O2
25	P	308	CDL	C72-C73-C74-C75
25	C	304	CDL	C57-C58-C59-C60
22	B	302	TGL	CB1-CB2-CB3-CB4
25	C	304	CDL	C44-C45-C46-C47
27	P	305	PEK	C35-C36-C37-C38
22	Y	101	TGL	CA9-C20-C21-C22
23	B	303	PSC	C28-C29-C30-C31
27	T	102	PEK	C29-C30-C31-C32
25	P	308	CDL	C55-C56-C57-C58
23	R	201	PSC	C01-C02-C03-O11
25	C	304	CDL	OB5-CB3-CB4-CB6
25	T	103	CDL	OB5-CB3-CB4-CB6
22	N	604	TGL	CC9-C15-C16-C17
26	Q	206	DMU	C18-C19-C22-C25
17	P	306	PGV	C9-C10-C11-C12
22	Y	101	TGL	C24-C25-C26-C27
26	G	101	DMU	C25-C28-C31-C34
22	B	302	TGL	C19-C33-C34-C35
27	G	103	PEK	C35-C36-C37-C38
25	C	310	CDL	C74-C75-C76-C77
24	T	101	CHD	C17-C20-C22-C23
17	A	604	PGV	C2-C3-C4-C5
22	B	302	TGL	CA4-CA5-CA6-CA7
17	P	302	PGV	C13-C14-C15-C16
22	N	604	TGL	CG1-CG2-CG3-OG3
23	R	201	PSC	O03-C01-C02-C03
25	C	304	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
23	R	201	PSC	O01-C02-C03-O11
25	P	308	CDL	OA5-CA3-CA4-OA6
25	P	308	CDL	OB5-CB3-CB4-OB6
17	C	302	PGV	C3-C4-C5-C6
25	T	103	CDL	C54-C55-C56-C57
25	T	103	CDL	OB9-CB7-OB8-CB6
17	A	604	PGV	O03-C01-C02-O01
22	L	101	TGL	OG2-CG2-CG3-OG3
23	B	303	PSC	O03-C01-C02-O01
17	C	302	PGV	C24-C25-C26-C27
23	B	303	PSC	C29-C30-C31-C32
25	P	308	CDL	OB9-CB7-OB8-CB6
17	N	617	PGV	C30-C31-C32-C33
22	Y	101	TGL	CA4-CA5-CA6-CA7
22	D	201	TGL	CA2-CA3-CA4-CA5
17	C	303	PGV	C11-C10-C9-C8
25	T	103	CDL	C52-C53-C54-C55
17	P	306	PGV	O04-C19-O03-C01
22	L	101	TGL	C14-C29-C30-C31
22	Y	101	TGL	C17-C18-C19-C33
22	D	201	TGL	OA1-CA1-OG1-CG1
23	R	201	PSC	C31-C32-C33-C34
25	C	304	CDL	C38-C39-C40-C41
22	Q	201	TGL	CB4-CB5-CB6-CB7
25	C	304	CDL	C23-C24-C25-C26
22	Y	101	TGL	CA2-CA3-CA4-CA5
17	A	604	PGV	C12-C13-C14-C15
27	P	305	PEK	C04-O12-P-O11
17	C	303	PGV	C20-C21-C22-C23
27	T	102	PEK	C31-C32-C33-C34
25	C	310	CDL	O1-C1-CA2-OA2
22	D	201	TGL	C20-C21-C22-C23
22	L	101	TGL	CC6-CC7-CC8-CC9
22	Y	101	TGL	C19-C33-C34-C35
17	A	604	PGV	C02-C03-O11-P
17	P	306	PGV	C02-C03-O11-P
25	T	103	CDL	CA4-CA3-OA5-PA1
17	P	302	PGV	C14-C15-C16-C17
22	D	201	TGL	C21-C20-CA9-CA8
17	A	604	PGV	C03-O11-P-O14
17	A	604	PGV	C04-O12-P-O14
17	N	617	PGV	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
17	P	307	PGV	C03-O11-P-O14
25	C	304	CDL	CB2-OB2-PB2-OB3
25	C	304	CDL	CB2-OB2-PB2-OB4
25	C	310	CDL	CB3-OB5-PB2-OB3
25	P	308	CDL	CA2-OA2-PA1-OA3
25	P	308	CDL	CB2-OB2-PB2-OB4
27	C	313	PEK	C03-O11-P-O14
27	G	103	PEK	C03-O11-P-O14
25	P	308	CDL	OB5-CB3-CB4-CB6
19	B	310	EDO	O1-C1-C2-O2
27	T	102	PEK	C3-C4-C5-C6
27	G	103	PEK	C10-C11-C12-C13
26	P	303	DMU	O16-C18-C19-C22
18	N	605	HEA	C3B-C11-C12-C13
27	P	301	PEK	C05-C04-O12-P
26	C	311	DMU	C31-C34-C37-C40
27	P	301	PEK	C2-C3-C4-C5
17	A	605	PGV	C31-C32-C33-C34
22	N	604	TGL	C10-C11-C12-C13
25	P	308	CDL	C23-C24-C25-C26
25	C	304	CDL	OA5-CA3-CA4-OA6
25	C	304	CDL	OB5-CB3-CB4-OB6
25	T	103	CDL	OA5-CA3-CA4-OA6
25	T	103	CDL	OB5-CB3-CB4-OB6
27	C	313	PEK	O01-C02-C03-O11
27	P	305	PEK	O01-C02-C03-O11
17	A	605	PGV	C30-C31-C32-C33
22	L	101	TGL	C10-C11-C12-C13
22	Q	201	TGL	CB7-CB8-CB9-C10
25	C	310	CDL	C62-C63-C64-C65
17	C	302	PGV	C4-C5-C6-C7
22	D	201	TGL	C22-C23-C24-C25
22	D	201	TGL	CA1-CA2-CA3-CA4
25	C	304	CDL	CB3-CB4-CB6-OB8
25	C	304	CDL	C72-C73-C74-C75
22	D	201	TGL	OG2-CG2-CG3-OG3
22	N	604	TGL	OG2-CG2-CG3-OG3
25	C	304	CDL	OB6-CB4-CB6-OB8
17	P	302	PGV	C4-C5-C6-C7
25	C	304	CDL	C82-C83-C84-C85
27	G	102	PEK	C7-C8-C9-C10
18	A	606	HEA	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
17	P	306	PGV	C11-C12-C13-C14
22	N	604	TGL	C29-C30-C31-C32
17	P	306	PGV	C20-C19-O03-C01
17	C	303	PGV	C14-C15-C16-C17
25	P	308	CDL	C51-C52-C53-C54
27	T	102	PEK	C23-C24-C25-C26
24	P	309	CHD	C20-C22-C23-C24
27	P	305	PEK	C25-C26-C27-C28
17	P	306	PGV	C19-C20-C21-C22
25	C	310	CDL	C63-C64-C65-C66
22	N	604	TGL	CA3-CA4-CA5-CA6
22	B	302	TGL	C13-C14-C29-C30
22	Q	201	TGL	C11-C10-CB9-CB8
17	C	303	PGV	C22-C23-C24-C25
22	Q	201	TGL	CA3-CA4-CA5-CA6
17	A	605	PGV	C02-C01-O03-C19
22	Q	201	TGL	CB3-CB4-CB5-CB6
22	Y	101	TGL	C18-C19-C33-C34
25	T	103	CDL	C63-C64-C65-C66
25	C	310	CDL	CB6-CB4-OB6-CB5
27	P	305	PEK	C1-C2-C3-C4
17	N	617	PGV	C20-C21-C22-C23
25	C	310	CDL	C21-C22-C23-C24
25	C	310	CDL	OA5-CA3-CA4-OA6
19	B	308	EDO	O1-C1-C2-O2
19	B	311	EDO	O1-C1-C2-O2
19	D	202	EDO	O1-C1-C2-O2
19	V	103	EDO	O1-C1-C2-O2
26	D	208	DMU	O16-C18-C19-C22
25	P	308	CDL	C18-C19-C20-C21
25	C	310	CDL	CB2-OB2-PB2-OB5
25	T	103	CDL	CB3-OB5-PB2-OB2
27	C	313	PEK	C04-O12-P-O11
22	Q	201	TGL	CA4-CA5-CA6-CA7
17	A	605	PGV	C27-C28-C29-C30
17	P	307	PGV	C11-C12-C13-C14
22	Y	101	TGL	C13-C14-C29-C30
25	C	310	CDL	C77-C78-C79-C80
25	T	103	CDL	C20-C21-C22-C23
22	Y	101	TGL	C11-C10-CB9-CB8
17	C	303	PGV	C25-C26-C27-C28
17	P	306	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
17	C	303	PGV	C05-C04-O12-P
17	P	307	PGV	C21-C22-C23-C24
22	D	201	TGL	C21-C22-C23-C24
22	D	201	TGL	CA2-CA1-OG1-CG1
17	P	307	PGV	C12-C13-C14-C15
25	C	304	CDL	C63-C64-C65-C66
17	A	605	PGV	O03-C19-C20-C21
27	C	313	PEK	O04-C21-O03-C01
22	D	201	TGL	CB5-CB6-CB7-CB8
26	Q	206	DMU	C19-C22-C25-C28
24	G	108	CHD	C22-C23-C24-O25
24	T	101	CHD	C22-C23-C24-O25
23	R	201	PSC	O03-C19-C20-C21
27	G	103	PEK	C4-C5-C6-C7
22	Y	101	TGL	C33-C34-C35-C36
18	A	606	HEA	CAA-CBA-CGA-O1A
22	L	101	TGL	C11-C10-CB9-CB8
23	R	201	PSC	C3-C4-C5-C6
24	T	101	CHD	C22-C23-C24-O26
24	T	105	CHD	C22-C23-C24-O25
19	G	104	EDO	O1-C1-C2-O2
19	P	312	EDO	O1-C1-C2-O2
19	S	104	EDO	O1-C1-C2-O2
19	W	301	EDO	O1-C1-C2-O2
25	C	304	CDL	C80-C81-C82-C83
22	Q	201	TGL	CC2-CC3-CC4-CC5
23	B	303	PSC	C27-C28-C29-C30
25	C	310	CDL	C19-C20-C21-C22
17	P	302	PGV	C15-C16-C17-C18
22	D	201	TGL	OG1-CG1-CG2-CG3
18	N	605	HEA	CAD-CBD-CGD-O1D
25	C	304	CDL	C15-C16-C17-C18
17	C	303	PGV	C12-C13-C14-C15
25	P	308	CDL	C43-C44-C45-C46
25	C	310	CDL	CA3-CA4-OA6-CA5
25	T	103	CDL	CA6-CA4-OA6-CA5
27	P	301	PEK	C03-C02-O01-C1
22	N	604	TGL	CC2-CC3-CC4-CC5
25	C	310	CDL	C11-C12-C13-C14
25	C	310	CDL	C61-C62-C63-C64
17	P	302	PGV	C9-C10-C11-C12
27	G	103	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	C	305	CHD	C22-C23-C24-O25
24	P	309	CHD	C22-C23-C24-O25
17	P	302	PGV	C27-C28-C29-C30
27	G	102	PEK	C11-C10-C9-C8
27	G	103	PEK	C5-C6-C7-C8
27	P	305	PEK	C11-C12-C13-C14
22	N	604	TGL	CC4-CC5-CC6-CC7
22	L	101	TGL	CA4-CA5-CA6-CA7
24	J	101	CHD	C20-C22-C23-C24
17	P	307	PGV	C10-C11-C12-C13
18	A	606	HEA	CAA-CBA-CGA-O2A
18	A	606	HEA	CAD-CBD-CGD-O1D
22	Q	201	TGL	OB1-CB1-OG2-CG2
27	G	102	PEK	O02-C1-O01-C02
27	P	305	PEK	C30-C31-C32-C33
26	C	311	DMU	C22-C25-C28-C31
18	A	606	HEA	C2D-C3D-CAD-CBD
27	G	102	PEK	C32-C33-C34-C35
18	N	605	HEA	CAD-CBD-CGD-O2D
18	A	606	HEA	CAD-CBD-CGD-O2D
17	C	302	PGV	C20-C21-C22-C23
22	D	201	TGL	OG2-CB1-CB2-CB3
17	C	302	PGV	C13-C14-C15-C16
22	D	201	TGL	C29-C30-C31-C32
22	L	101	TGL	C20-C21-C22-C23
25	P	308	CDL	C57-C58-C59-C60
22	Y	101	TGL	C20-C21-C22-C23
23	R	201	PSC	C7-C8-C9-C10
27	G	102	PEK	C3-C4-C5-C6
19	N	613	EDO	O1-C1-C2-O2
19	P	311	EDO	O1-C1-C2-O2
22	D	201	TGL	CA3-CA4-CA5-CA6
24	P	309	CHD	C22-C23-C24-O26
22	N	604	TGL	C21-C20-CA9-CA8
27	G	102	PEK	C2-C1-O01-C02
22	Q	201	TGL	C11-C12-C13-C14
27	P	301	PEK	C35-C36-C37-C38
27	C	313	PEK	C22-C21-O03-C01
22	L	101	TGL	CA5-CA6-CA7-CA8
17	C	302	PGV	C11-C12-C13-C14
24	G	108	CHD	C22-C23-C24-O26
22	D	201	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
17	A	605	PGV	C15-C16-C17-C18
25	P	308	CDL	C62-C63-C64-C65
17	N	617	PGV	C23-C24-C25-C26
25	T	103	CDL	C37-C38-C39-C40
17	A	604	PGV	O03-C19-C20-C21
22	B	302	TGL	C24-C25-C26-C27
25	T	103	CDL	C18-C19-C20-C21
24	T	105	CHD	C22-C23-C24-O26
23	R	201	PSC	C30-C31-C32-C33
22	Y	101	TGL	C15-C16-C17-C18
27	G	103	PEK	C17-C18-C19-C20
27	G	102	PEK	C25-C26-C27-C28
27	T	102	PEK	O01-C1-C2-C3
17	C	302	PGV	C31-C32-C33-C34
22	Y	101	TGL	CB5-CB6-CB7-CB8
17	P	306	PGV	C7-C8-C9-C10
17	P	302	PGV	O03-C19-C20-C21
22	D	201	TGL	OG1-CA1-CA2-CA3
22	Q	201	TGL	OG3-CC1-CC2-CC3
17	N	617	PGV	C9-C10-C11-C12
17	P	302	PGV	C11-C12-C13-C14
23	B	303	PSC	C7-C8-C9-C10
23	B	303	PSC	C12-C13-C14-C15
23	R	201	PSC	C12-C13-C14-C15
27	C	313	PEK	C3-C4-C5-C6
27	C	313	PEK	C14-C15-C16-C17
23	B	303	PSC	C31-C32-C33-C34
23	B	303	PSC	O03-C19-C20-C21
17	C	303	PGV	C27-C28-C29-C30
17	A	605	PGV	C12-C13-C14-C15
18	N	606	HEA	C12-C11-C3B-C2B
27	G	102	PEK	O01-C1-C2-C3
22	N	604	TGL	CB4-CB5-CB6-CB7
22	D	201	TGL	C11-C10-CB9-CB8
25	C	310	CDL	C64-C65-C66-C67
17	N	617	PGV	O03-C19-C20-C21
19	A	613	EDO	O1-C1-C2-O2
19	C	309	EDO	O1-C1-C2-O2
19	E	202	EDO	O1-C1-C2-O2
19	I	103	EDO	O1-C1-C2-O2
19	N	615	EDO	O1-C1-C2-O2
19	O	302	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	W	303	EDO	O1-C1-C2-O2
23	R	201	PSC	O04-C19-O03-C01
17	P	307	PGV	C24-C25-C26-C27
17	N	617	PGV	C11-C12-C13-C14
27	T	102	PEK	C14-C15-C16-C17
24	W	302	CHD	C22-C23-C24-O25
27	P	305	PEK	C01-C02-C03-O11
27	G	103	PEK	O03-C01-C02-O01
23	R	201	PSC	C21-C22-C23-C24
27	G	103	PEK	C27-C28-C29-C30
22	Q	201	TGL	OG2-CB1-CB2-CB3
22	L	101	TGL	CC4-CC5-CC6-CC7
22	Q	201	TGL	CC7-CC8-CC9-C15
25	C	310	CDL	C55-C56-C57-C58
17	A	605	PGV	C9-C10-C11-C12
22	B	302	TGL	CB6-CB7-CB8-CB9
24	C	305	CHD	C22-C23-C24-O26
23	R	201	PSC	C20-C19-O03-C01
22	B	302	TGL	OG3-CC1-CC2-CC3
22	Q	201	TGL	CB2-CB1-OG2-CG2
18	A	607	HEA	CAA-CBA-CGA-O2A
25	C	310	CDL	C13-C14-C15-C16
27	G	103	PEK	C29-C30-C31-C32
17	C	302	PGV	C9-C10-C11-C12
17	P	307	PGV	C9-C10-C11-C12
27	P	301	PEK	C3-C4-C5-C6
22	D	201	TGL	OA1-CA1-CA2-CA3
22	Q	201	TGL	OC1-CC1-CC2-CC3
27	G	102	PEK	O02-C1-C2-C3
27	T	102	PEK	O02-C1-C2-C3
22	B	302	TGL	CC9-C15-C16-C17
27	G	103	PEK	O03-C01-C02-C03
17	C	303	PGV	C26-C27-C28-C29
22	N	604	TGL	C24-C25-C26-C27
27	P	301	PEK	C26-C27-C28-C29
17	C	303	PGV	C04-O12-P-O11
17	A	605	PGV	C24-C25-C26-C27
25	C	304	CDL	C34-C35-C36-C37
25	C	304	CDL	O1-C1-CB2-OB2
22	B	302	TGL	OC1-CC1-CC2-CC3
22	Q	201	TGL	CB2-CB3-CB4-CB5
25	T	103	CDL	C83-C84-C85-C86

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Mol	Chain	Res	Type	Atoms
17	C	302	PGV	O01-C1-C2-C3
27	G	103	PEK	C02-C03-O11-P
17	N	617	PGV	O04-C19-C20-C21
22	Q	201	TGL	OB1-CB1-CB2-CB3
17	C	303	PGV	C23-C24-C25-C26
17	P	302	PGV	C04-O12-P-O13
25	C	310	CDL	CB2-OB2-PB2-OB3
25	T	103	CDL	CA2-OA2-PA1-OA3
25	T	103	CDL	CB3-OB5-PB2-OB3
27	P	301	PEK	C04-O12-P-O14
17	A	604	PGV	O04-C19-C20-C21
23	B	303	PSC	O04-C19-C20-C21
19	D	203	EDO	O1-C1-C2-O2
19	G	109	EDO	O1-C1-C2-O2
19	N	607	EDO	O1-C1-C2-O2
19	N	610	EDO	O1-C1-C2-O2
18	N	605	HEA	O11-C11-C12-C13
23	B	303	PSC	C05-C04-O12-P
27	G	103	PEK	C05-C04-O12-P
25	P	308	CDL	C64-C65-C66-C67
24	P	304	CHD	C22-C23-C24-O26
24	Y	102	CHD	C22-C23-C24-O26
17	A	604	PGV	C19-C20-C21-C22
17	A	605	PGV	C26-C27-C28-C29
27	G	102	PEK	O03-C21-C22-C23
22	Q	201	TGL	C17-C18-C19-C33
17	P	306	PGV	C1-C2-C3-C4
17	A	605	PGV	C13-C14-C15-C16
17	N	617	PGV	O01-C02-C03-O11
23	R	201	PSC	O02-C1-C2-C3
25	T	103	CDL	C19-C20-C21-C22
17	N	617	PGV	O01-C1-C2-C3
23	R	201	PSC	O01-C1-C2-C3
17	P	307	PGV	C31-C32-C33-C34
17	C	302	PGV	O02-C1-C2-C3
27	G	102	PEK	C23-C24-C25-C26
27	G	102	PEK	C33-C34-C35-C36

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	P	309	CHD	C1-C10-C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
24	Y	102	CHD	C10-C5-C6-C7-C8-C9
24	Y	102	CHD	C1-C10-C2-C3-C4-C5
24	T	105	CHD	C1-C10-C2-C3-C4-C5

46 monomers are involved in 106 short contacts:

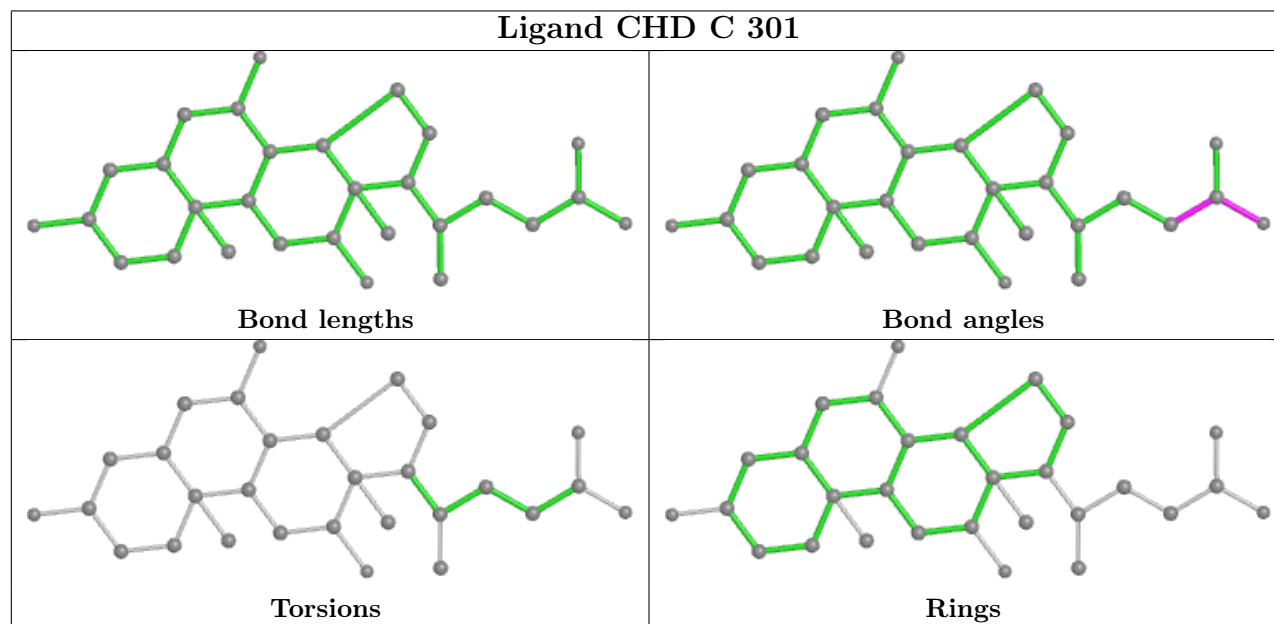
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	608	EDO	3	0
24	C	301	CHD	1	0
23	B	303	PSC	3	0
26	C	311	DMU	1	0
22	Y	101	TGL	2	0
17	C	302	PGV	1	0
27	G	102	PEK	4	0
24	T	101	CHD	1	0
27	C	313	PEK	1	0
26	D	208	DMU	3	0
26	C	312	DMU	1	0
25	T	103	CDL	6	0
19	C	306	EDO	1	0
22	L	101	TGL	2	0
27	P	301	PEK	2	0
27	G	103	PEK	1	0
18	A	607	HEA	3	0
29	V	101	SAC	2	0
17	N	617	PGV	4	0
19	N	611	EDO	1	0
23	R	201	PSC	2	0
24	Y	102	CHD	3	0
17	C	303	PGV	2	0
19	N	614	EDO	1	0
19	B	305	EDO	1	0
19	Q	205	EDO	1	0
25	C	310	CDL	1	0
26	Q	206	DMU	2	0
24	P	309	CHD	1	0
24	T	105	CHD	11	0
17	A	604	PGV	1	0
27	P	305	PEK	2	0
25	P	308	CDL	2	0
25	C	304	CDL	3	0
18	A	606	HEA	3	0
18	N	605	HEA	6	0

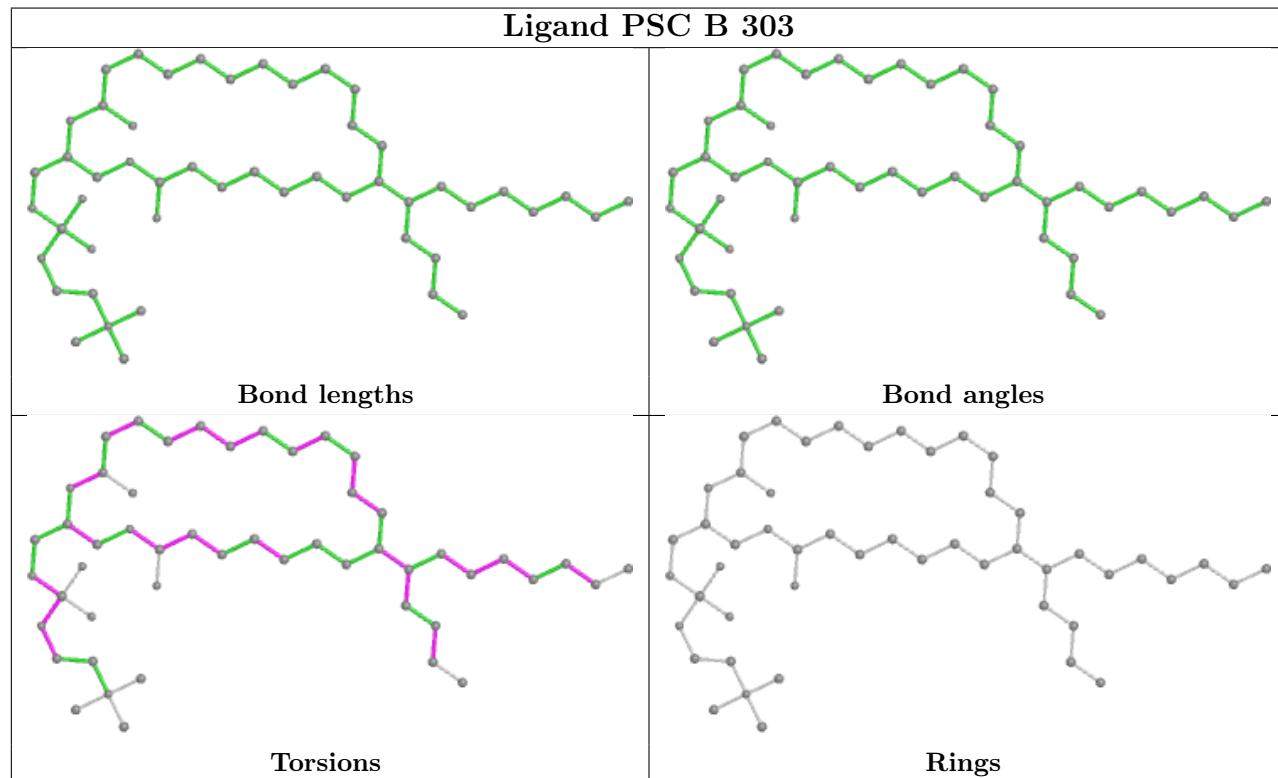
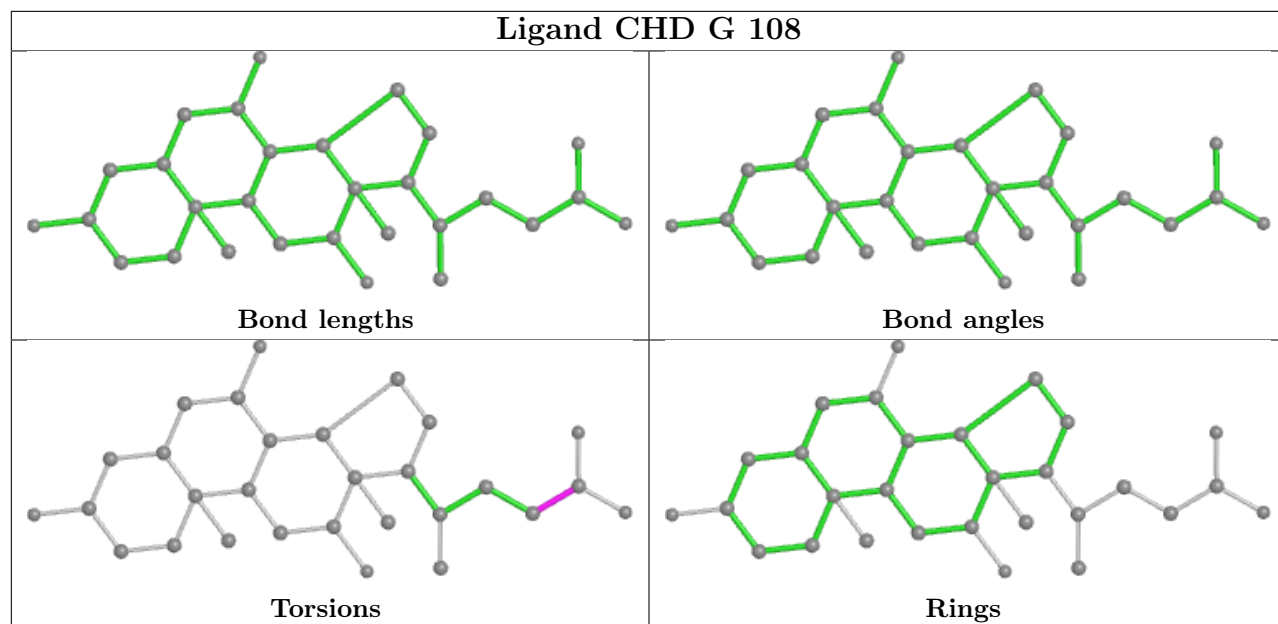
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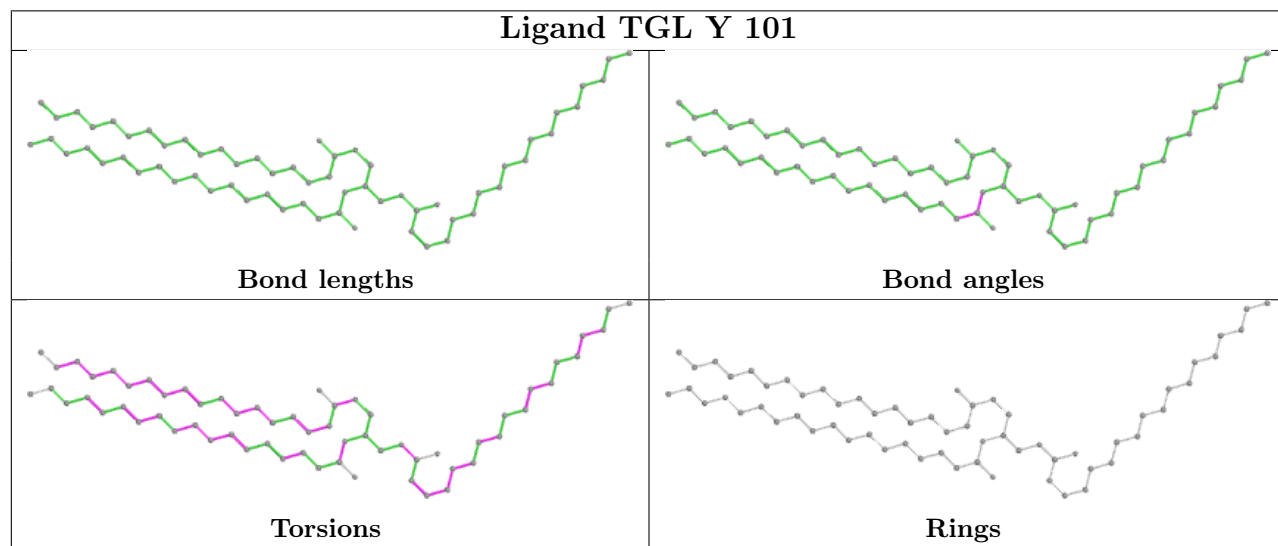
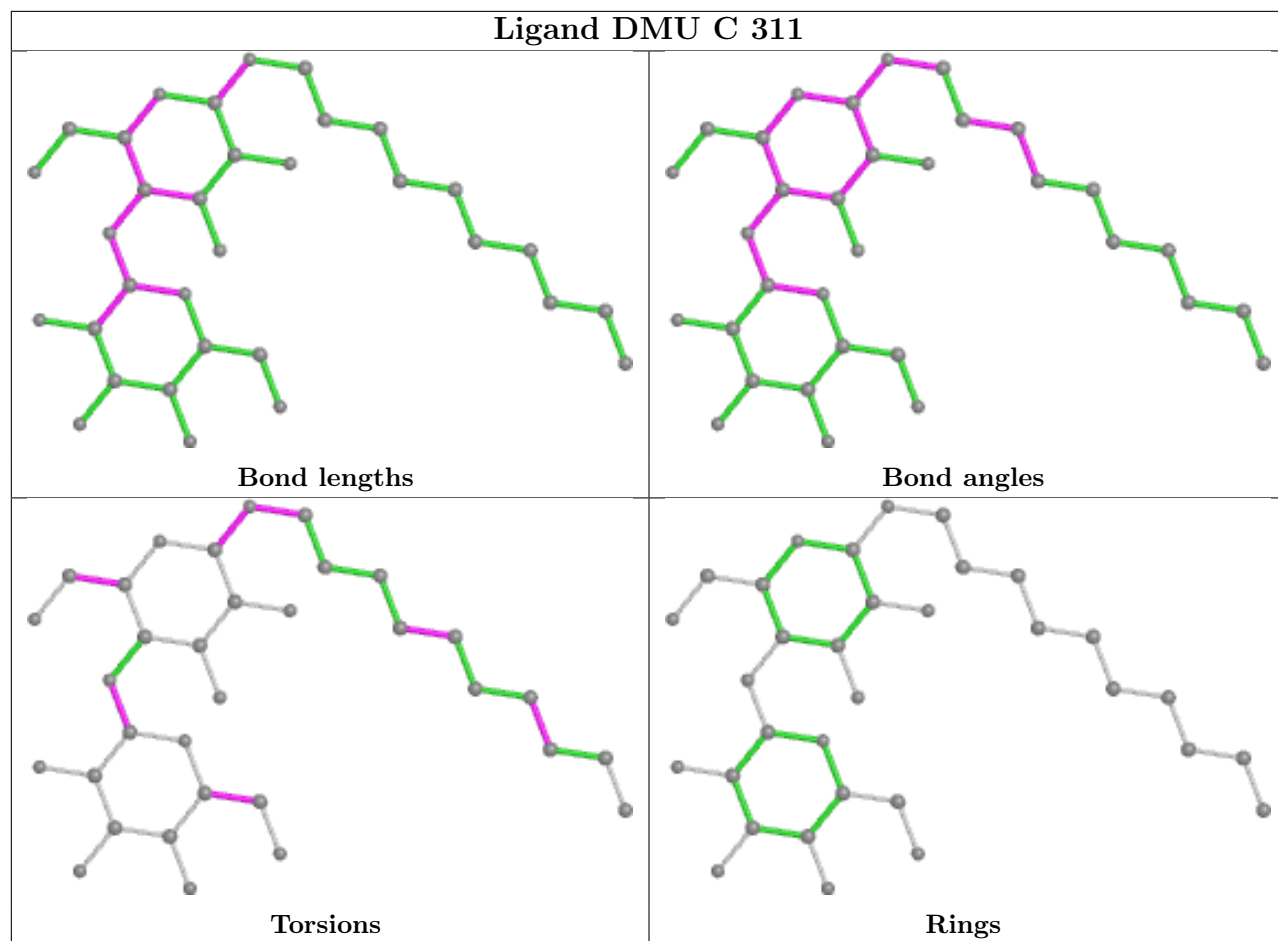
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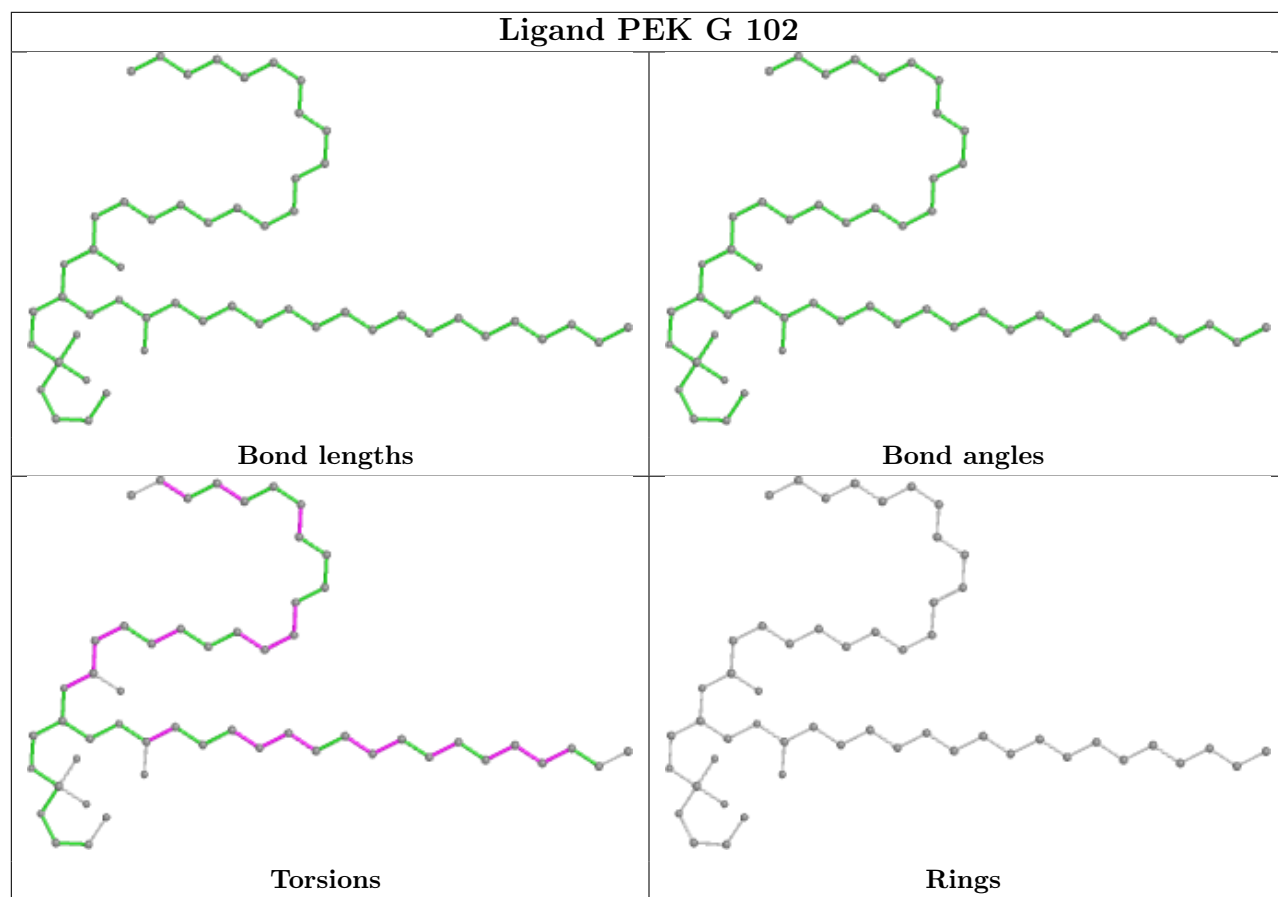
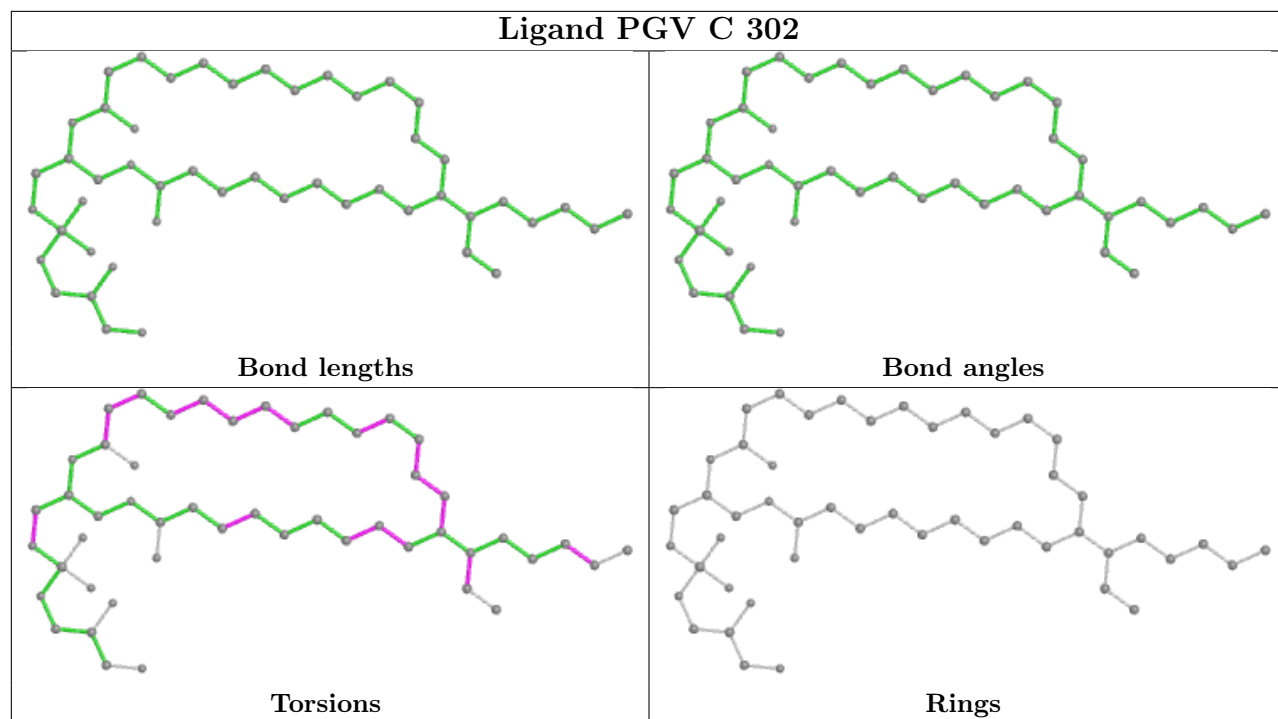
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	P	307	PGV	3	0
19	Q	204	EDO	1	0
24	J	101	CHD	1	0
27	T	102	PEK	4	0
24	W	302	CHD	1	0
19	N	612	EDO	2	0
18	N	606	HEA	6	0
22	Q	201	TGL	1	0
22	D	201	TGL	3	0
19	S	105	EDO	1	0

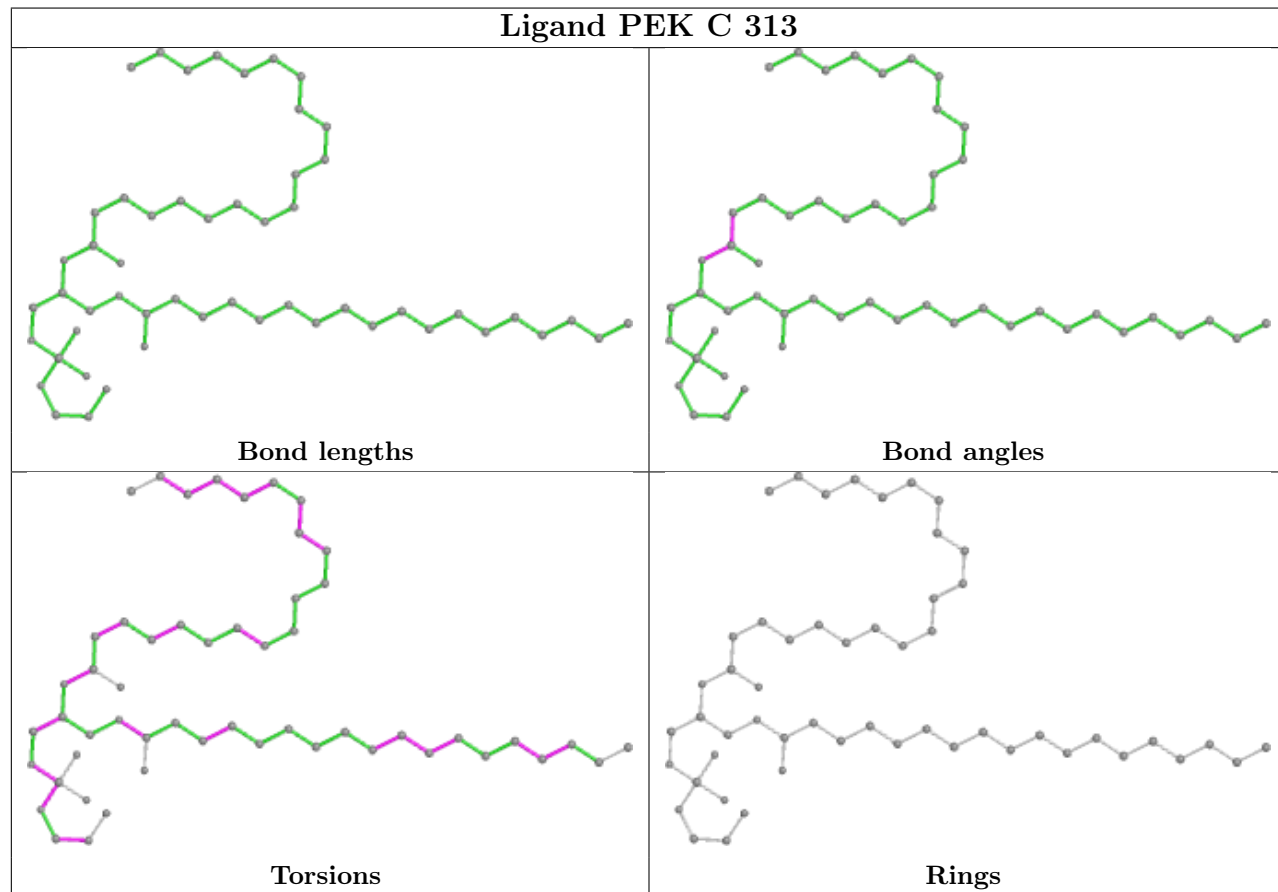
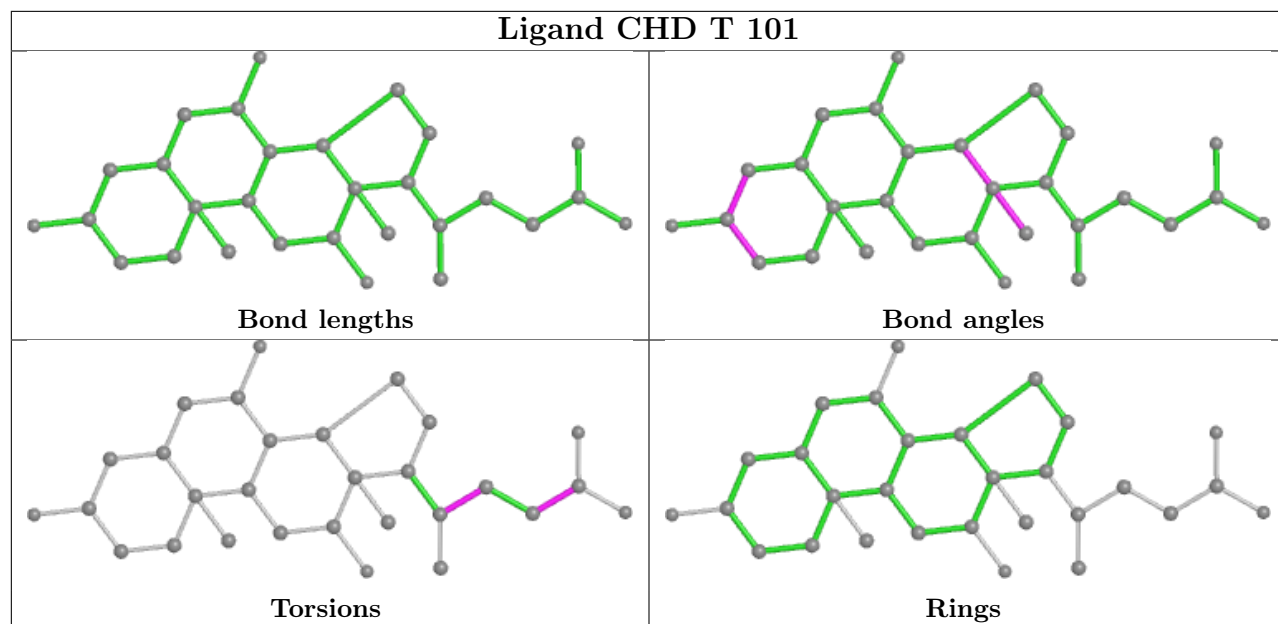
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

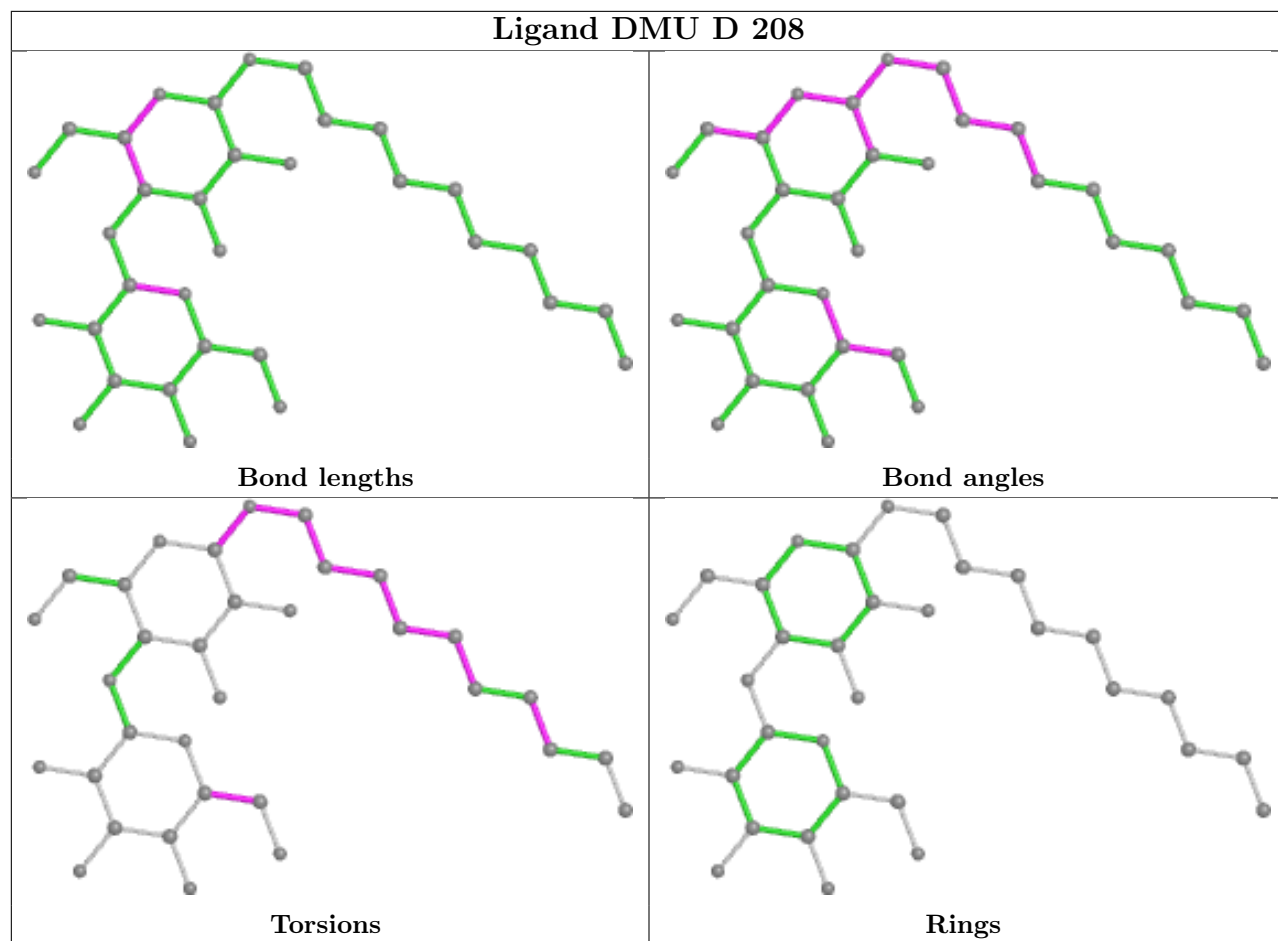


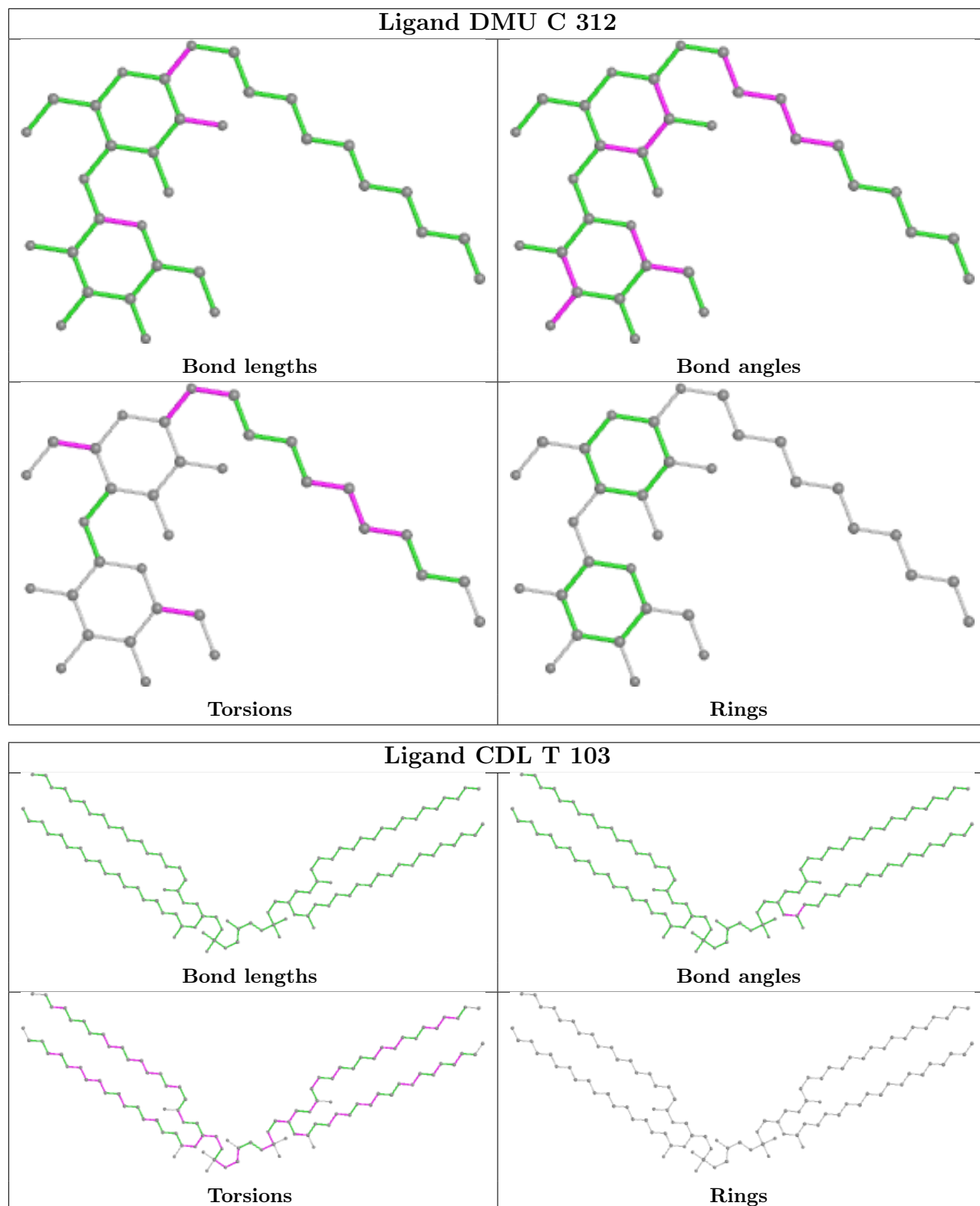


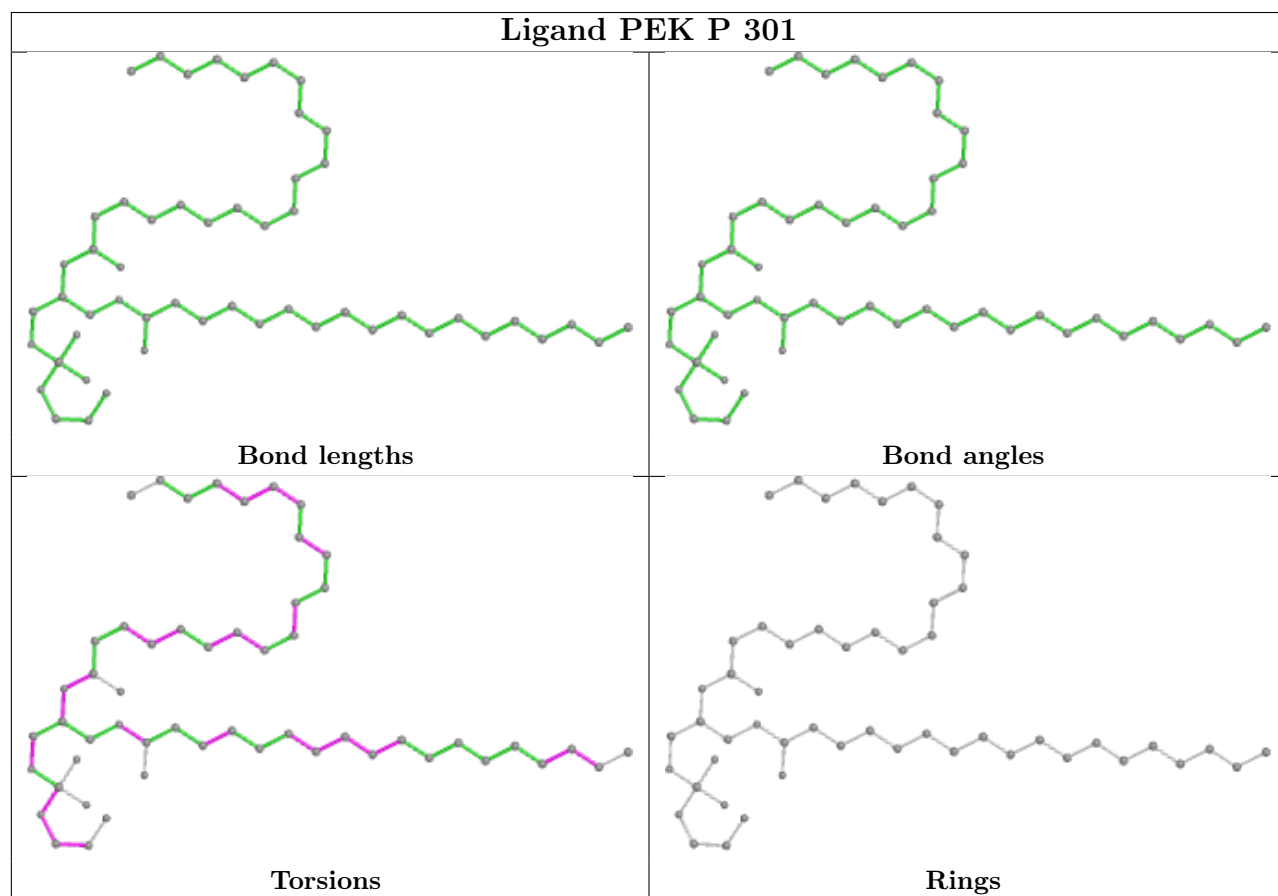
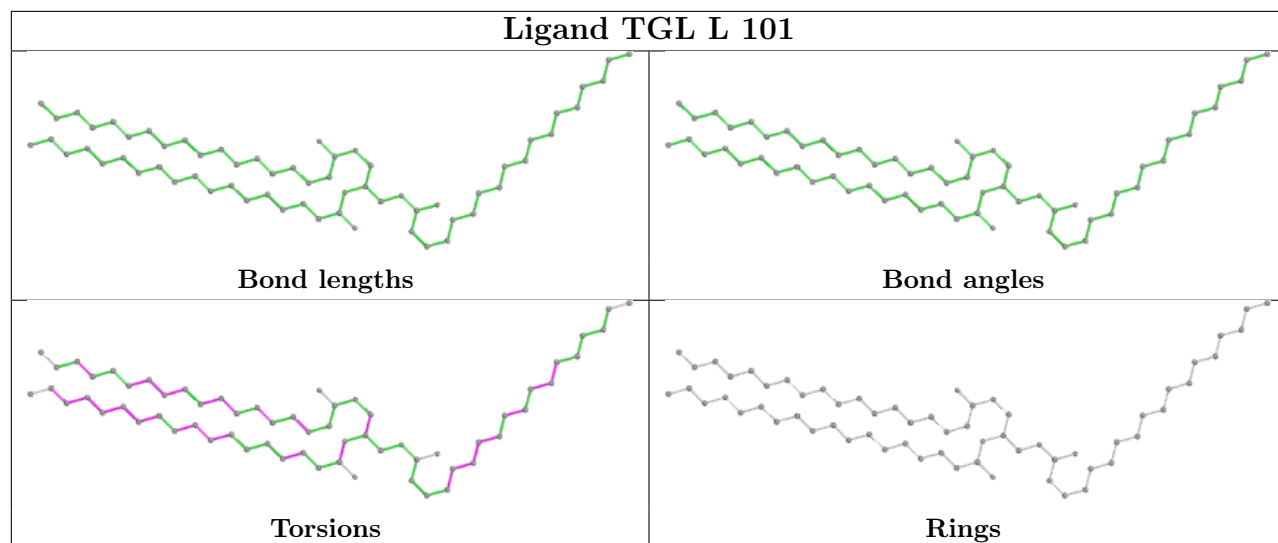


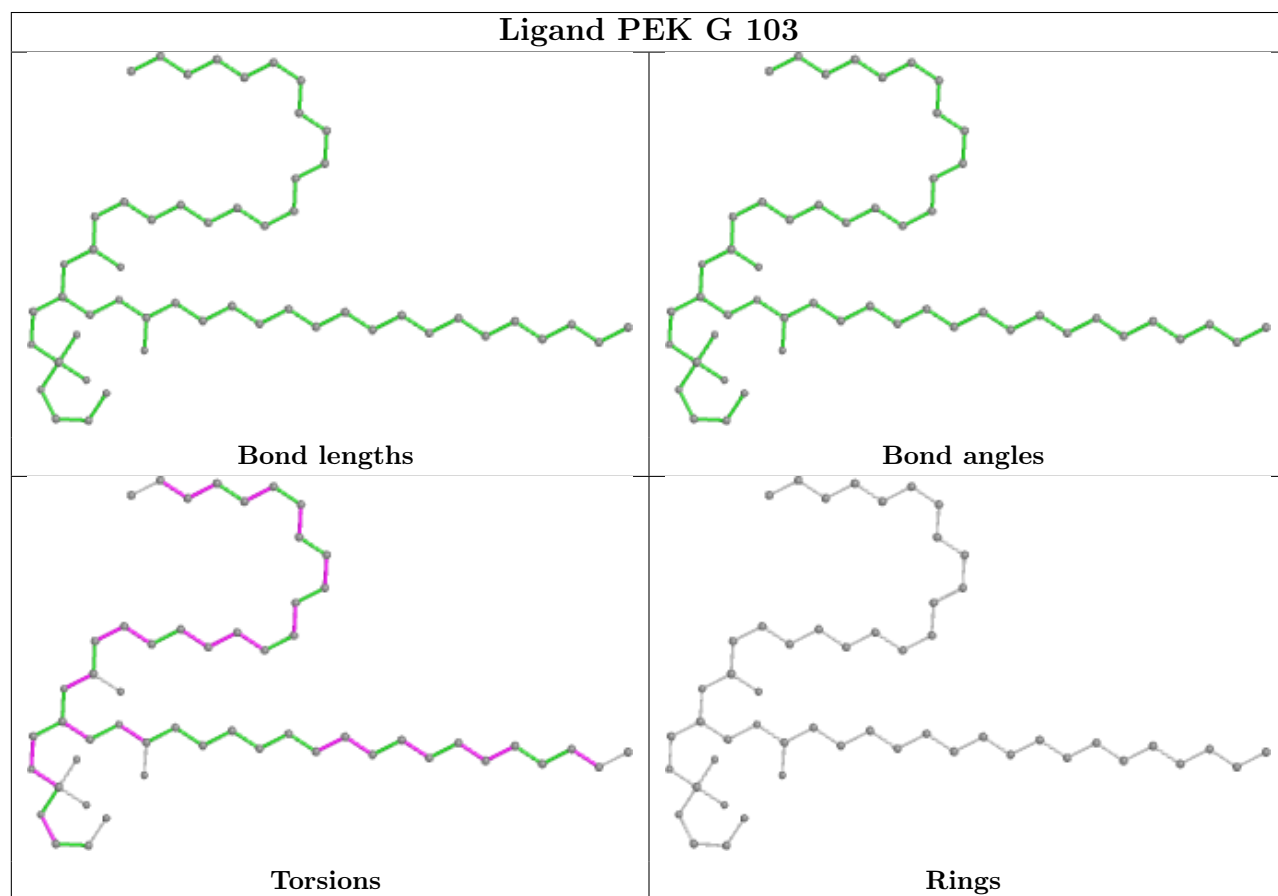
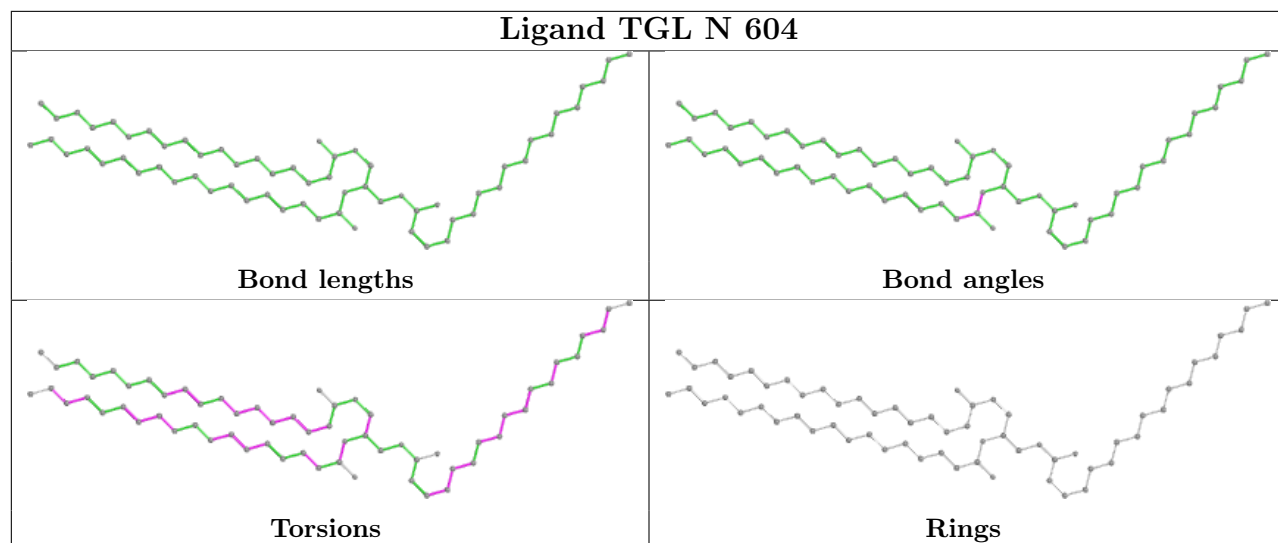


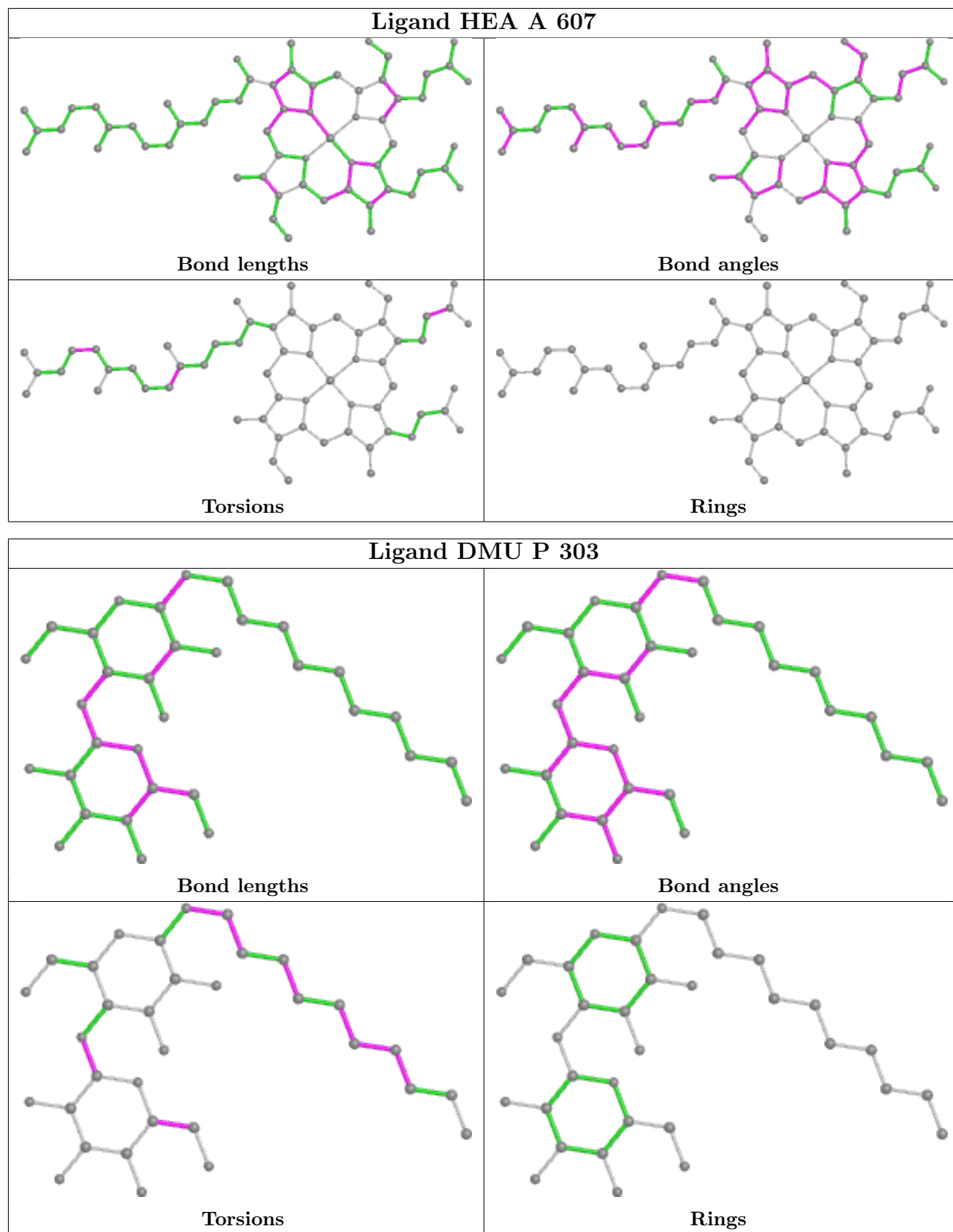


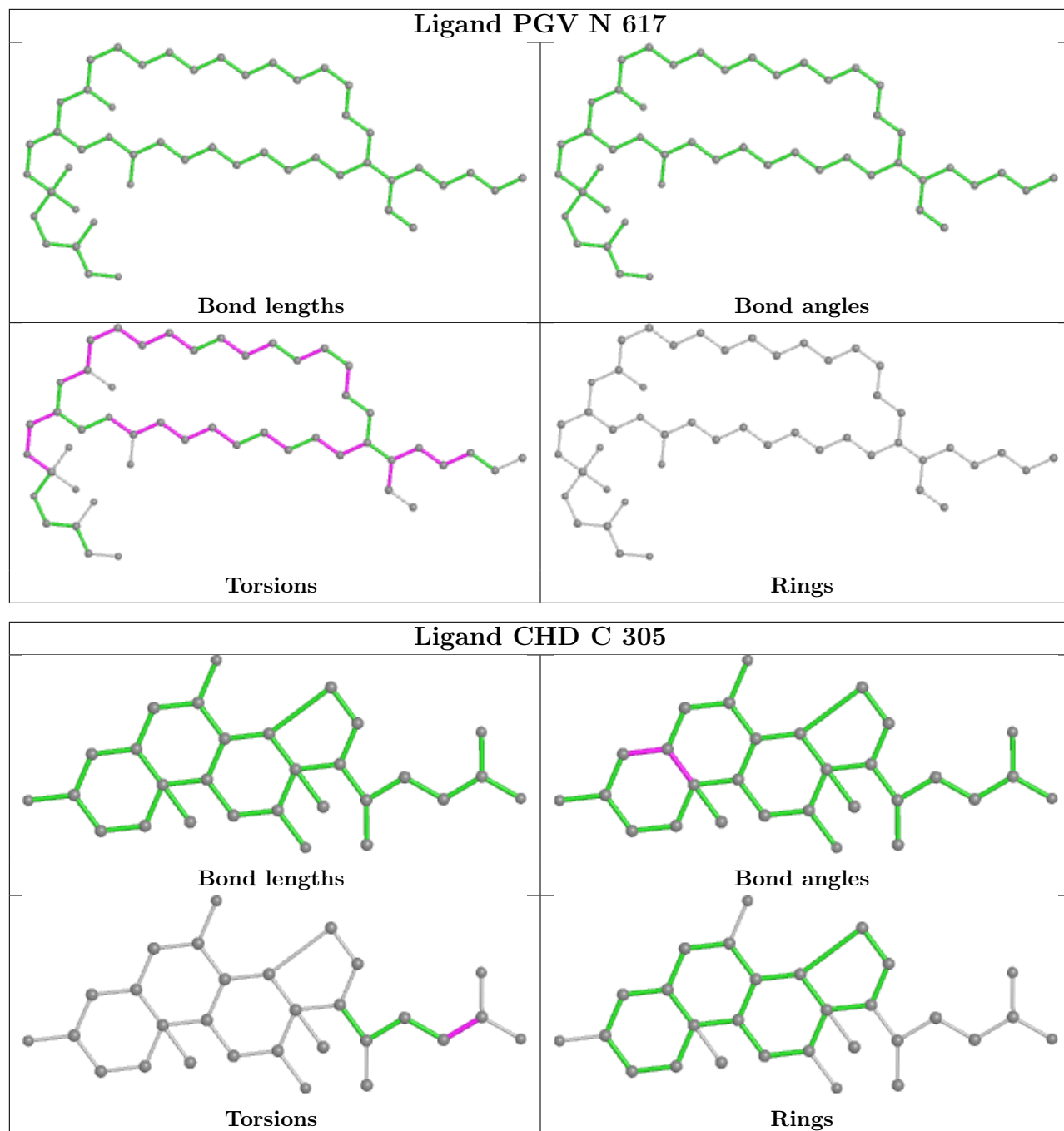




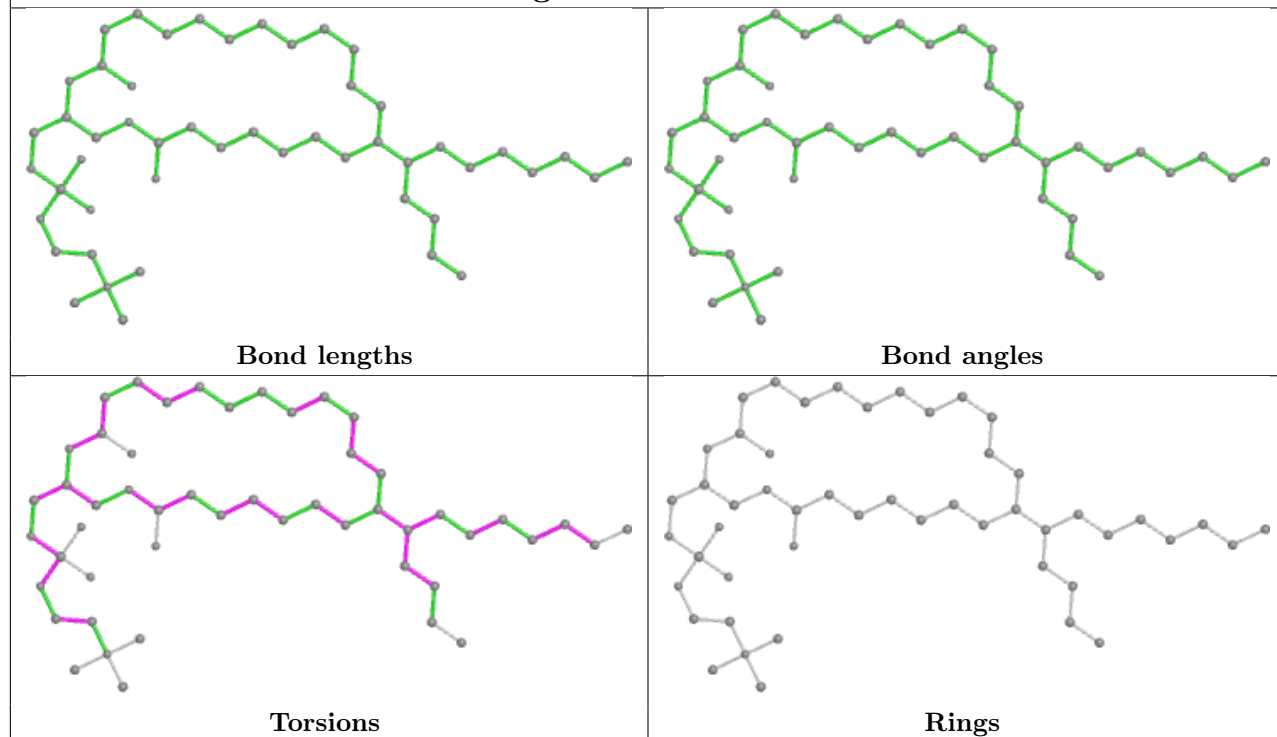




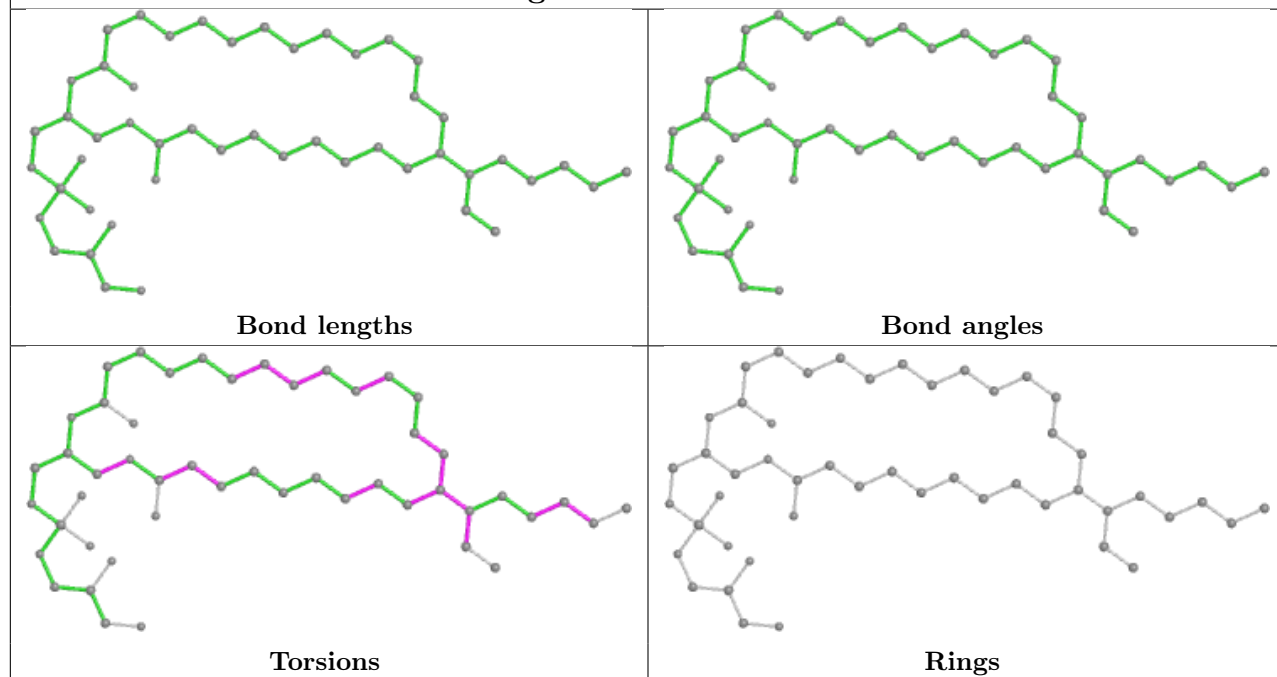


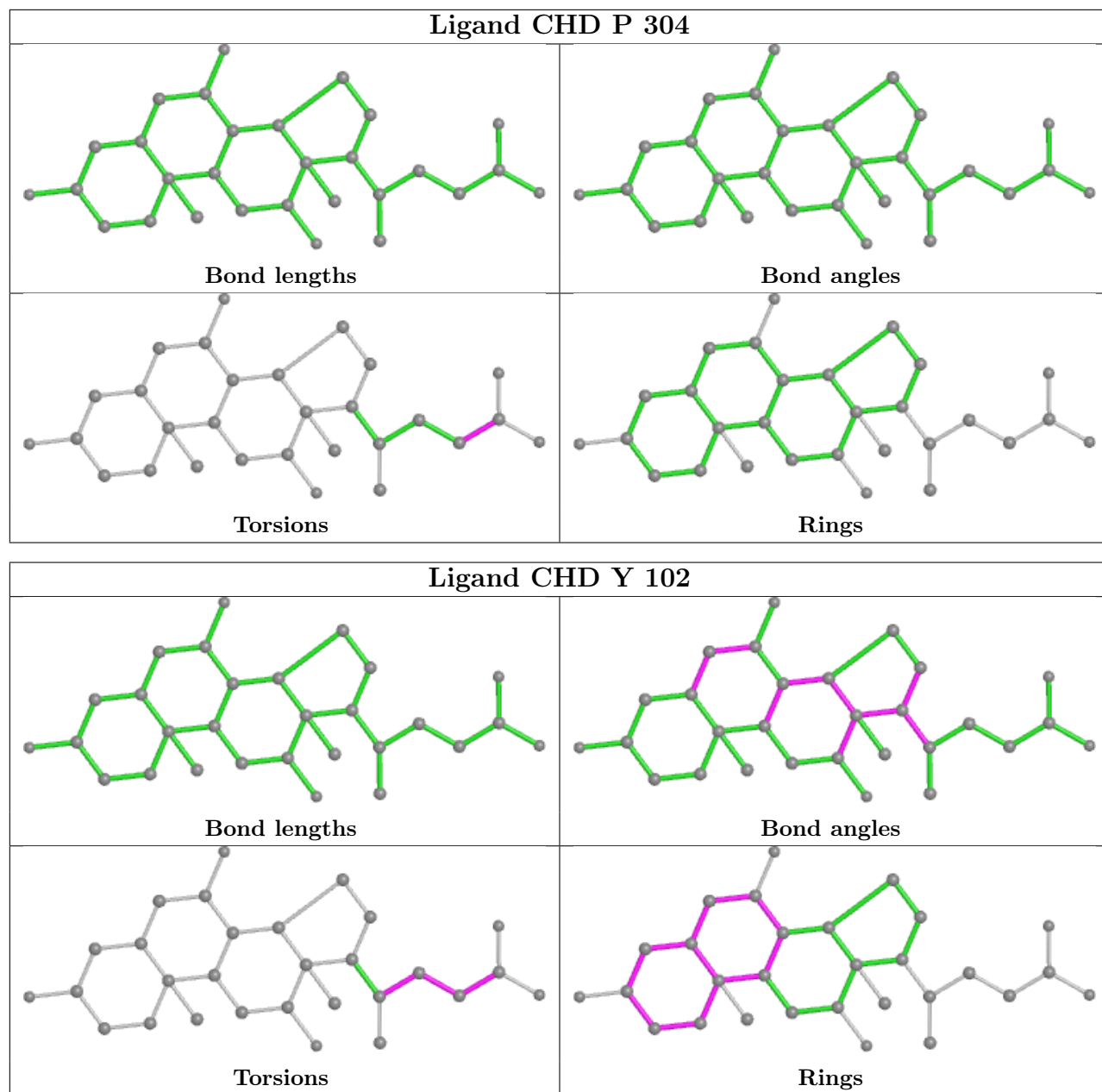


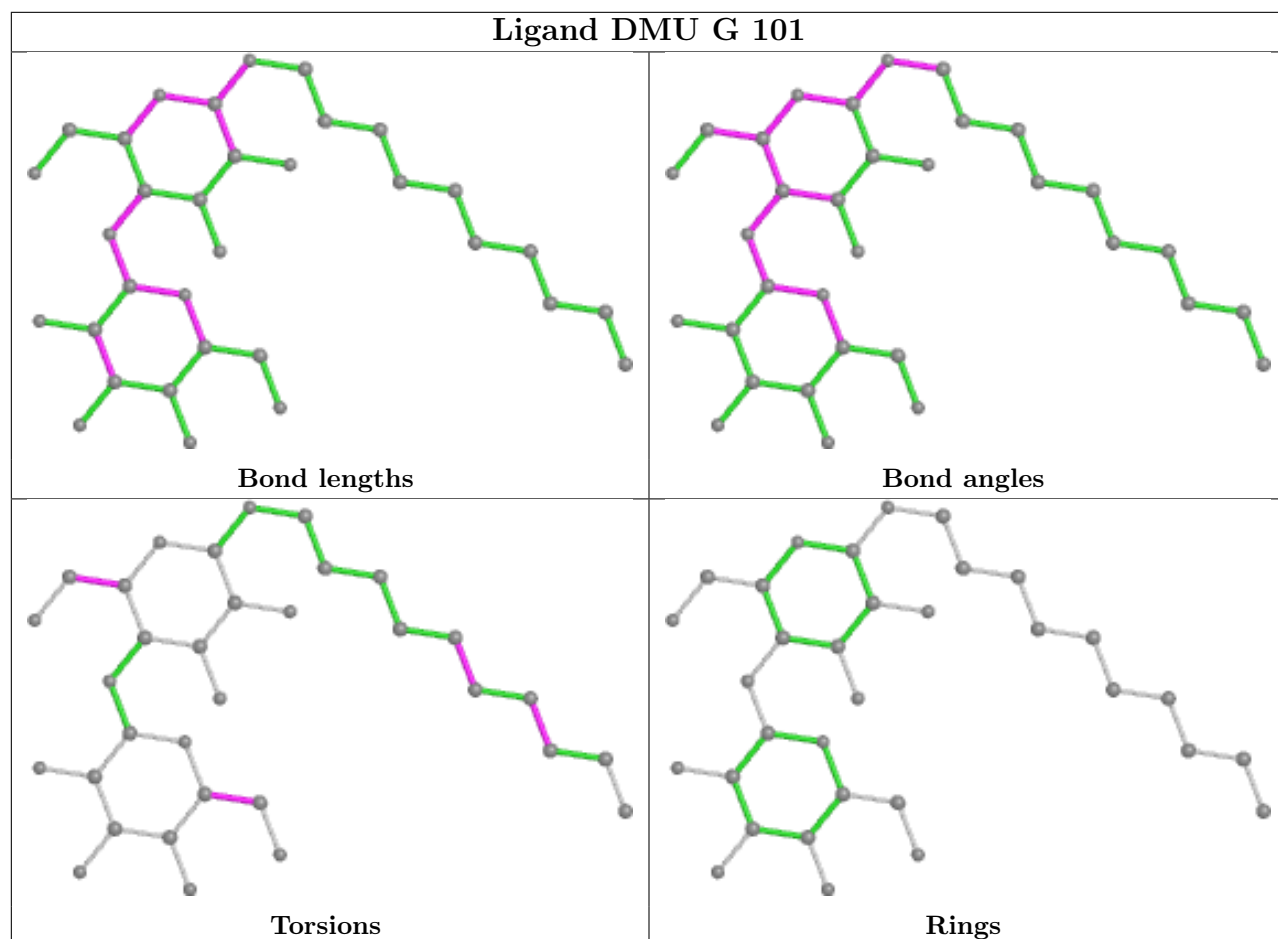
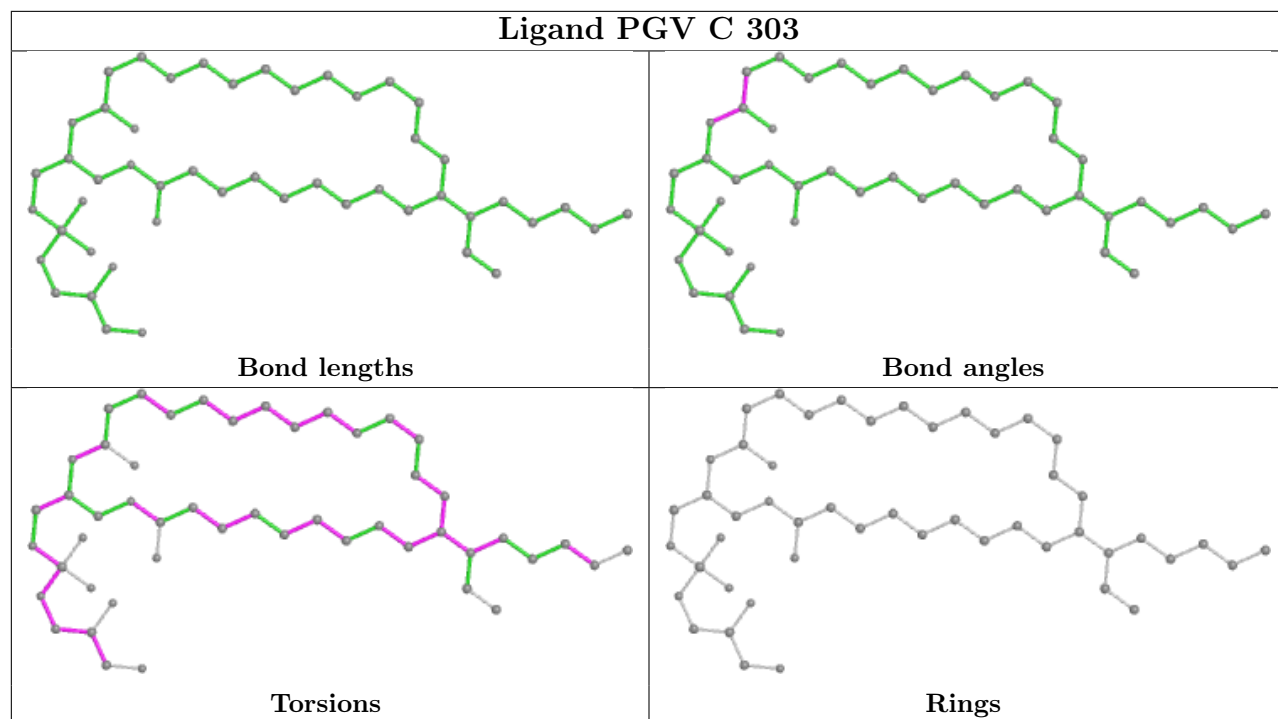
Ligand PSC R 201

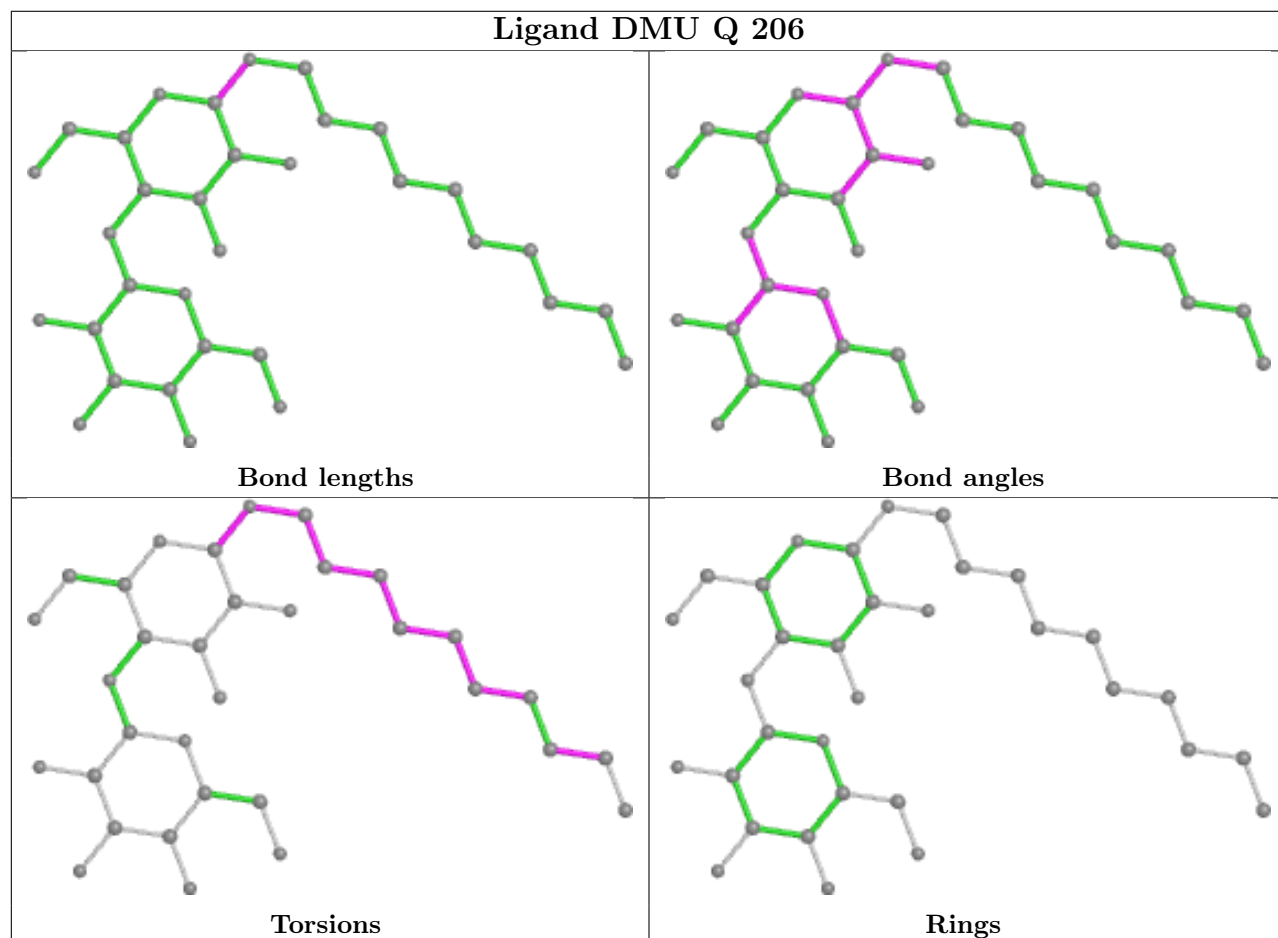
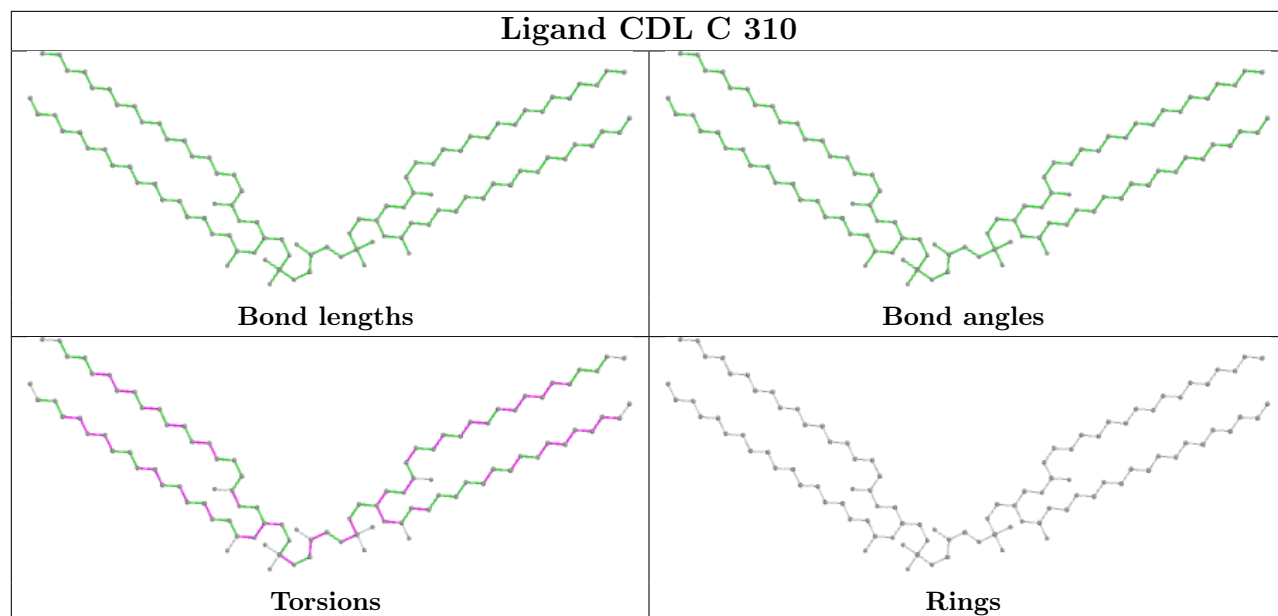


Ligand PGV A 605

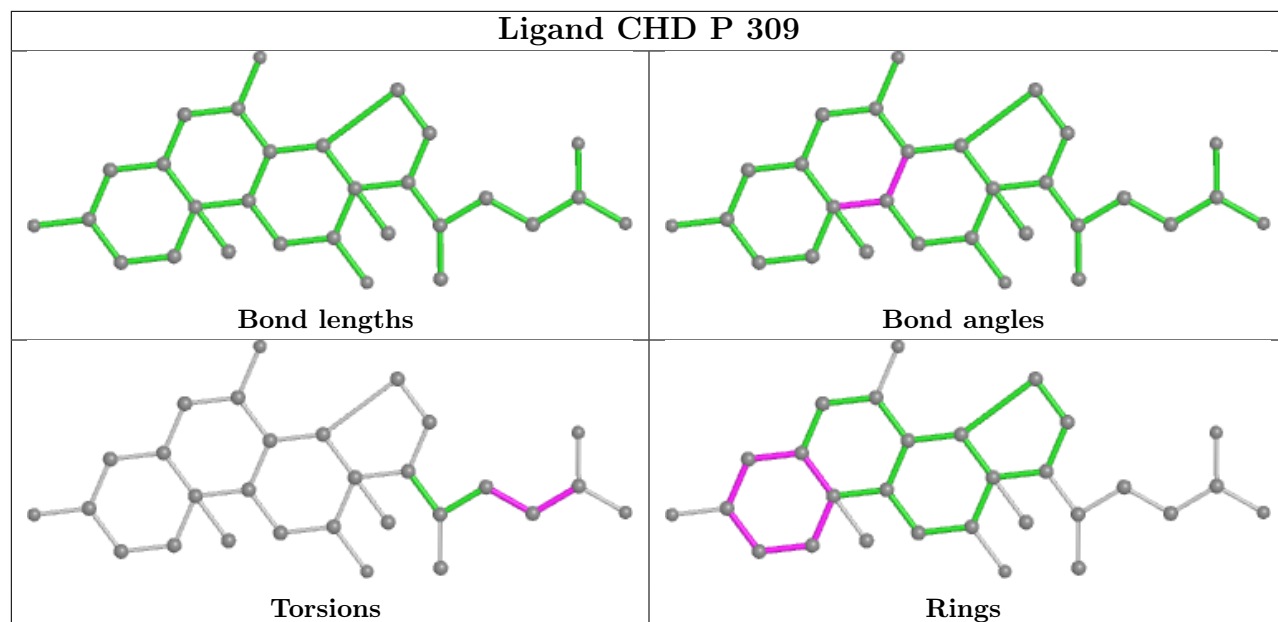




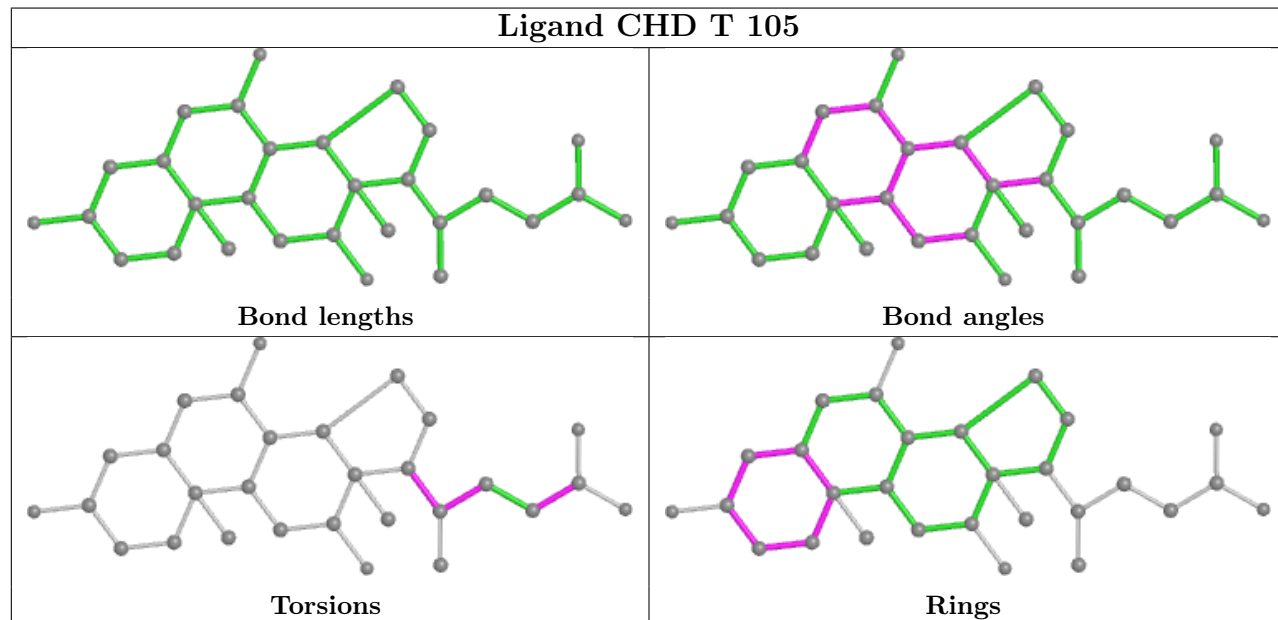


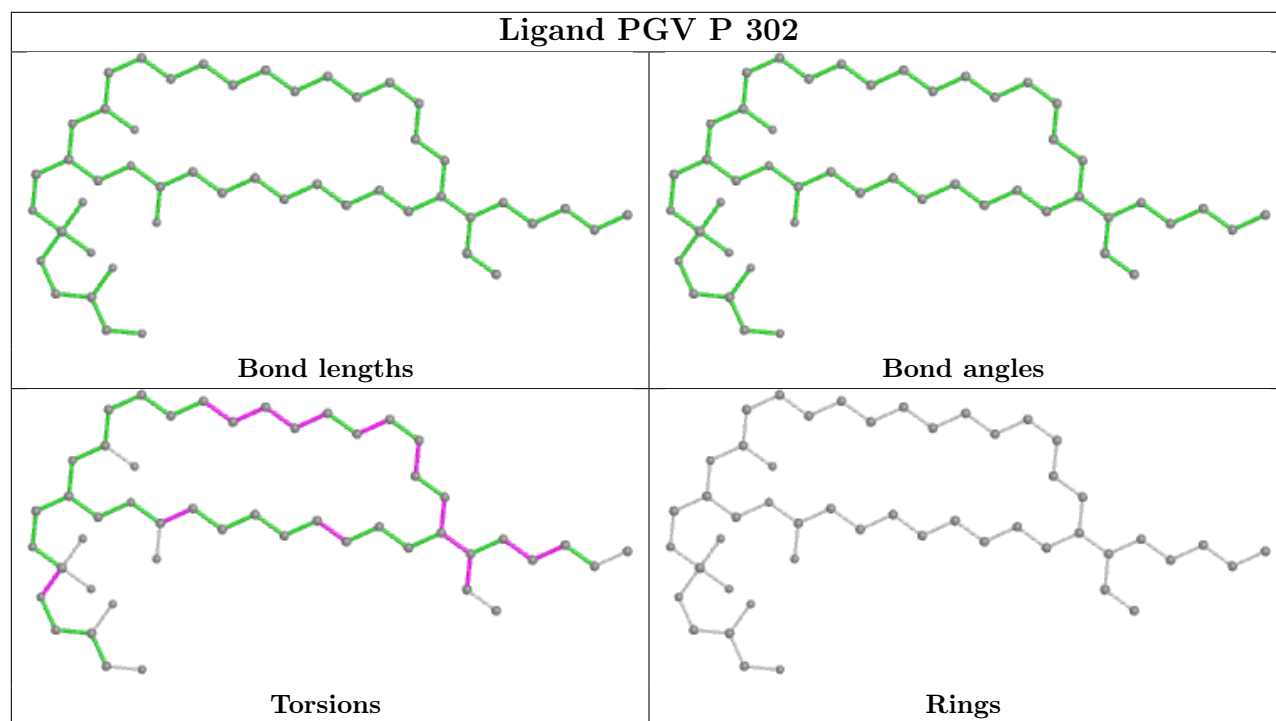
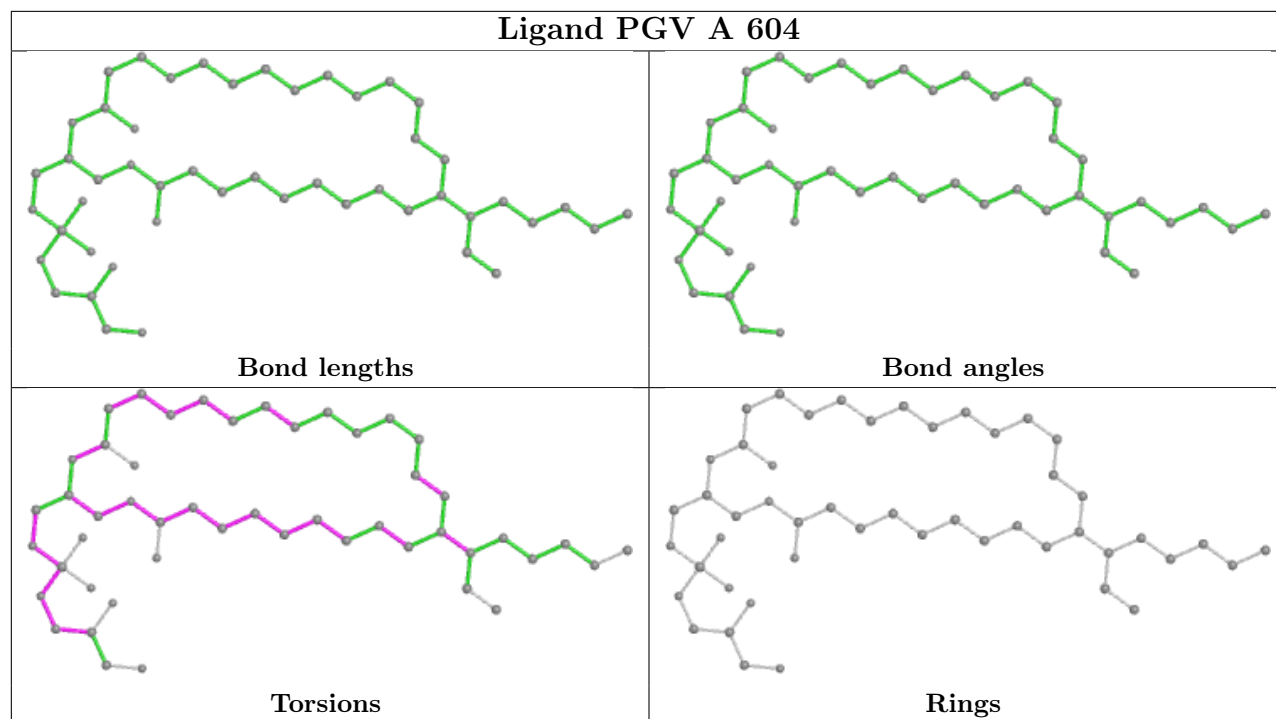


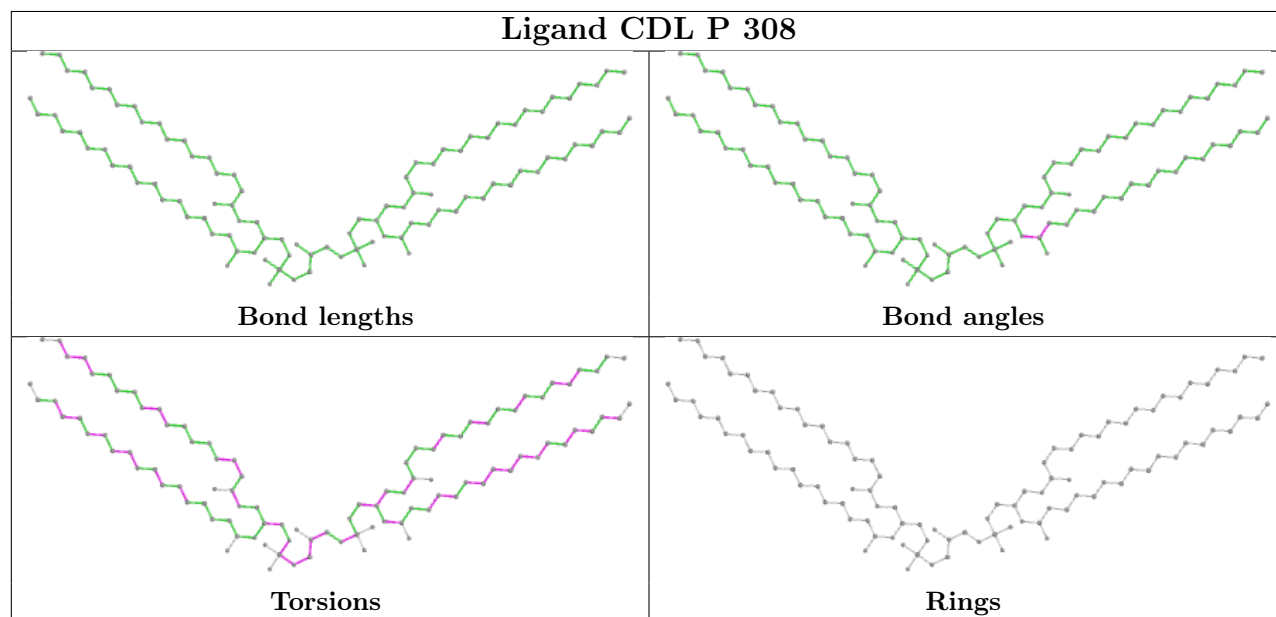
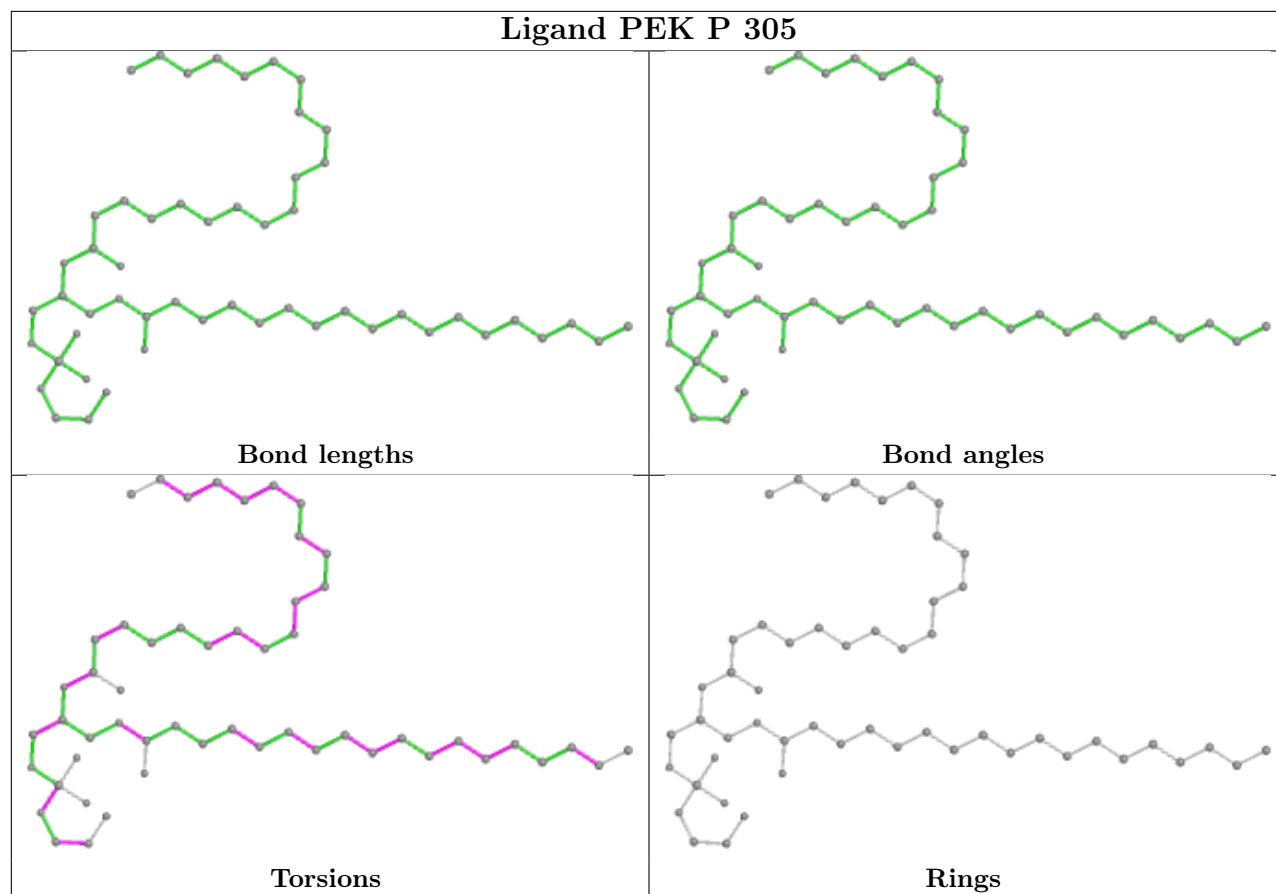
Ligand CHD P 309

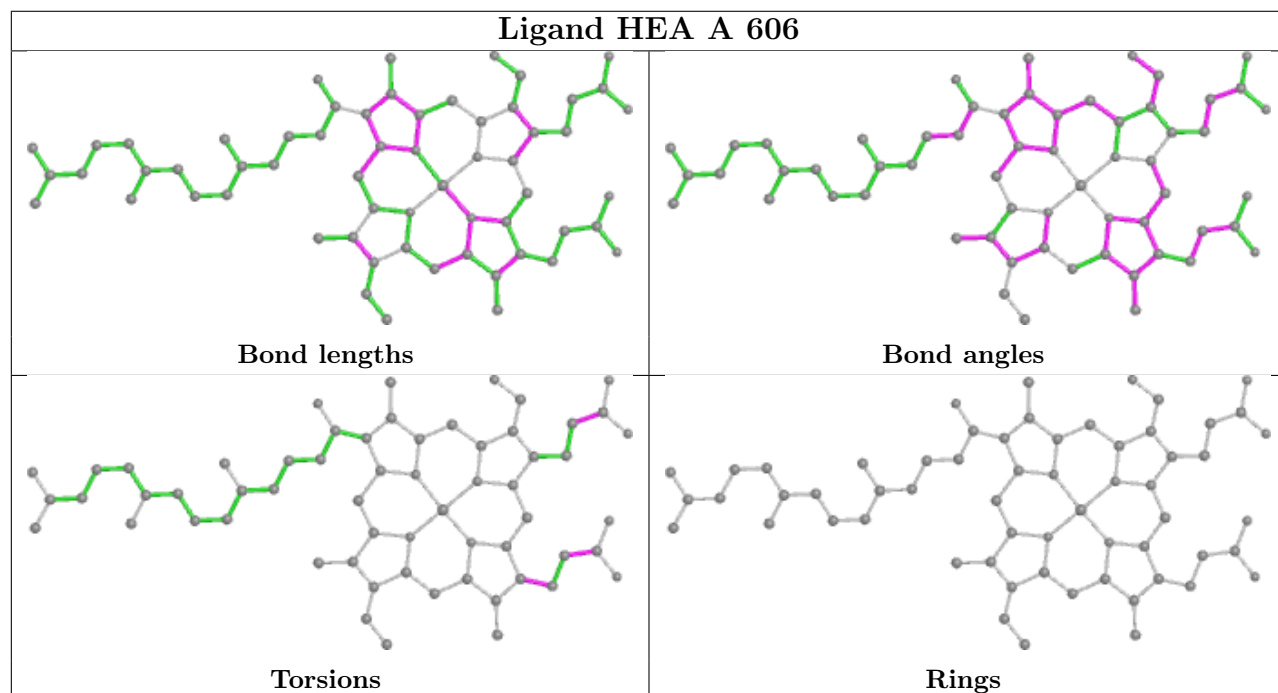
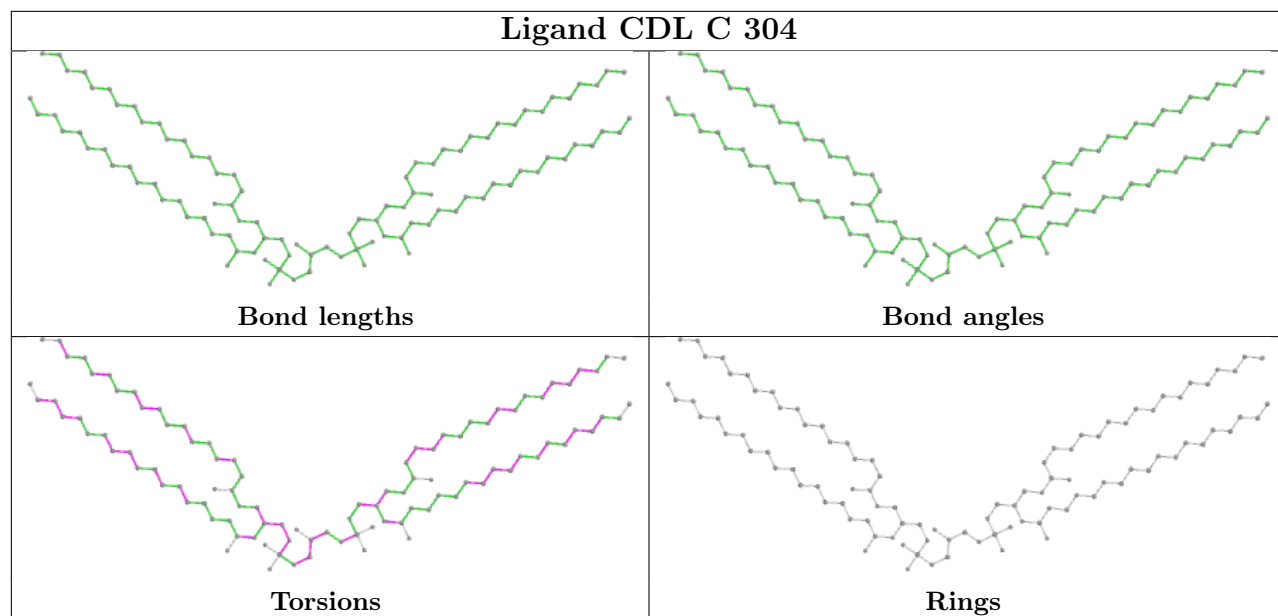


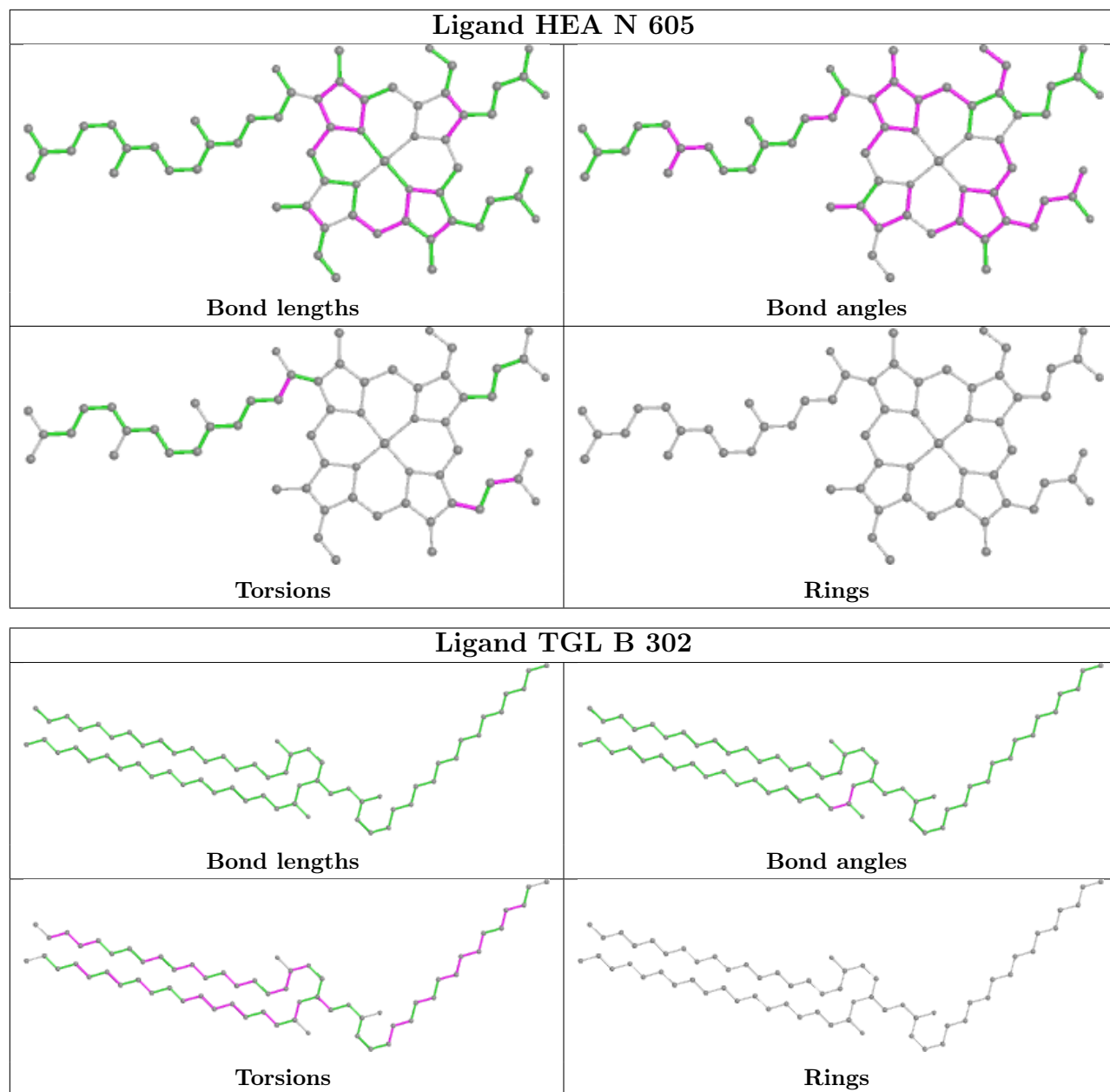
Ligand CHD T 105



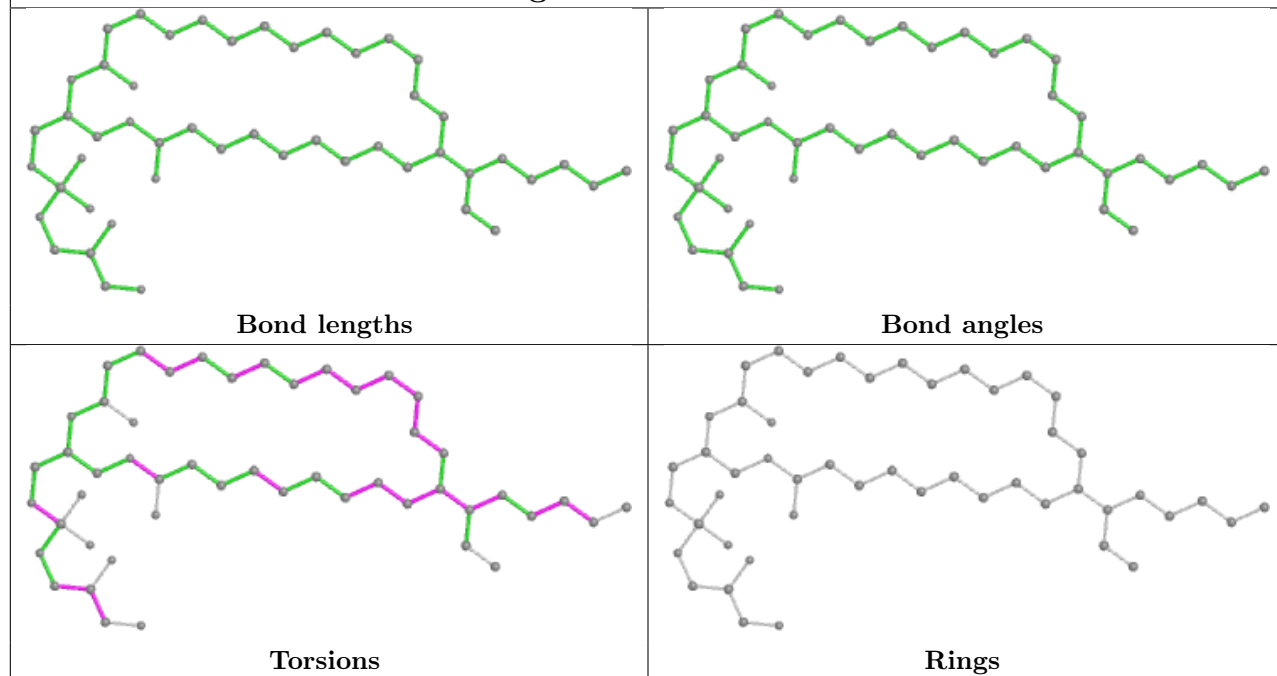




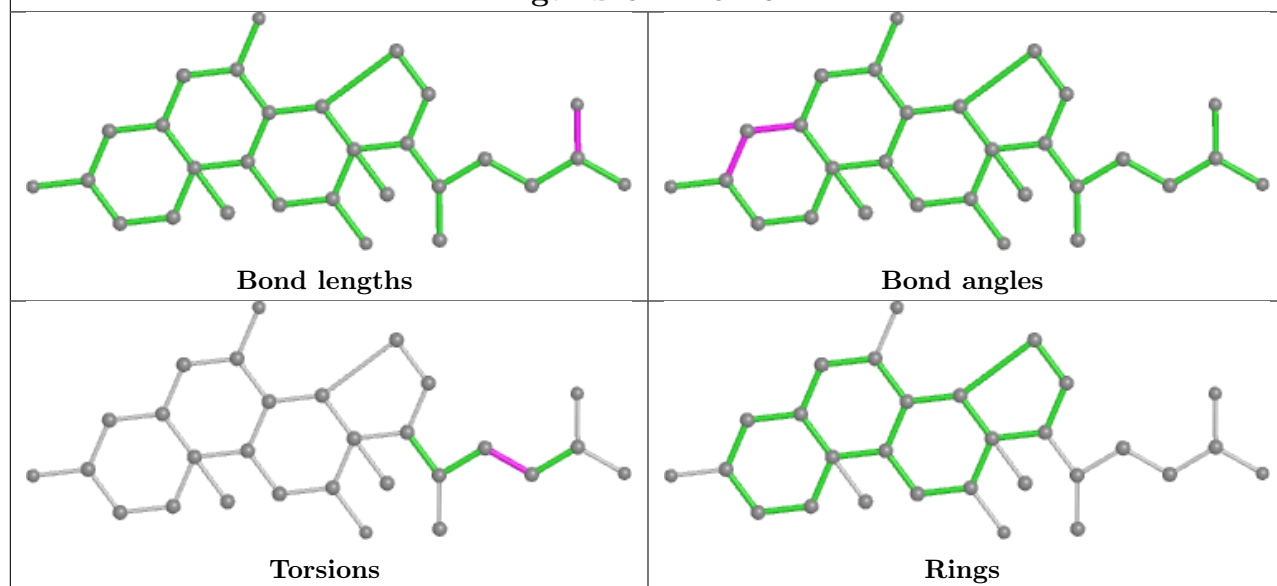




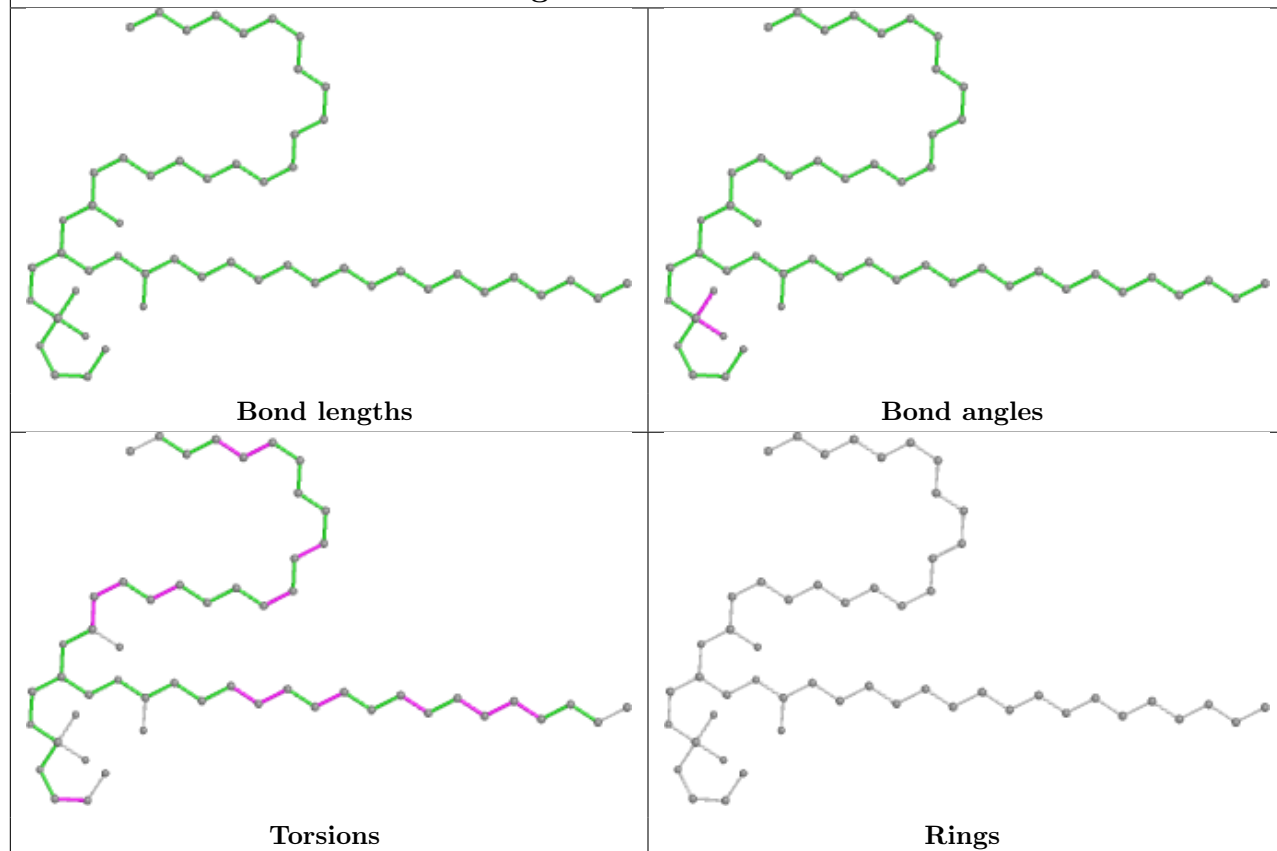
Ligand PGV P 307



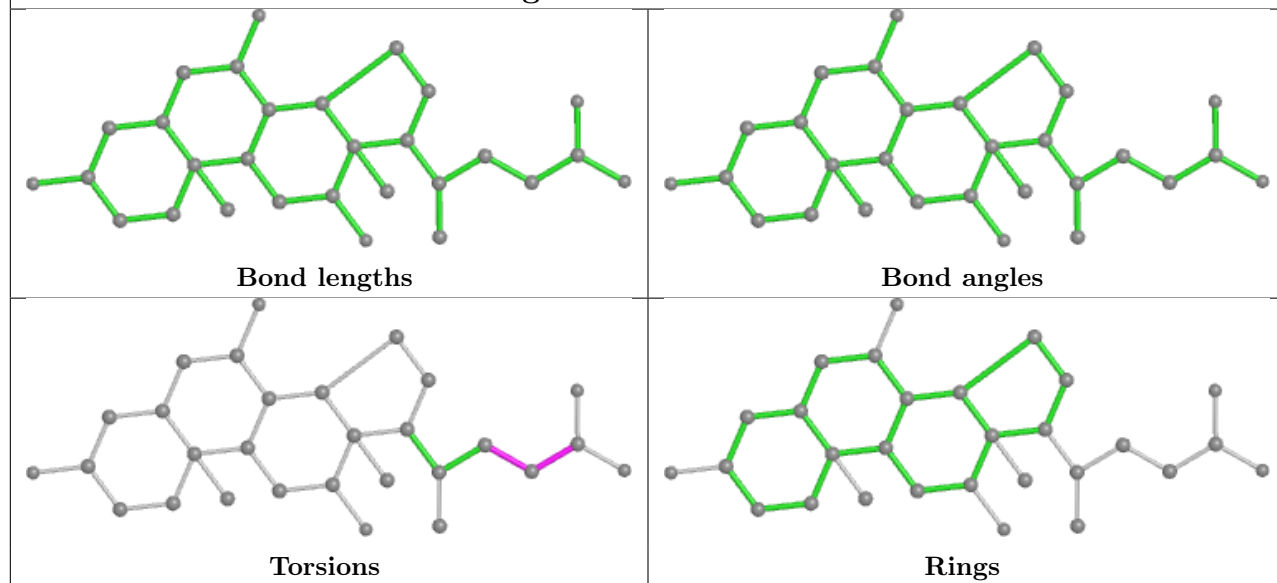
Ligand CHD J 101

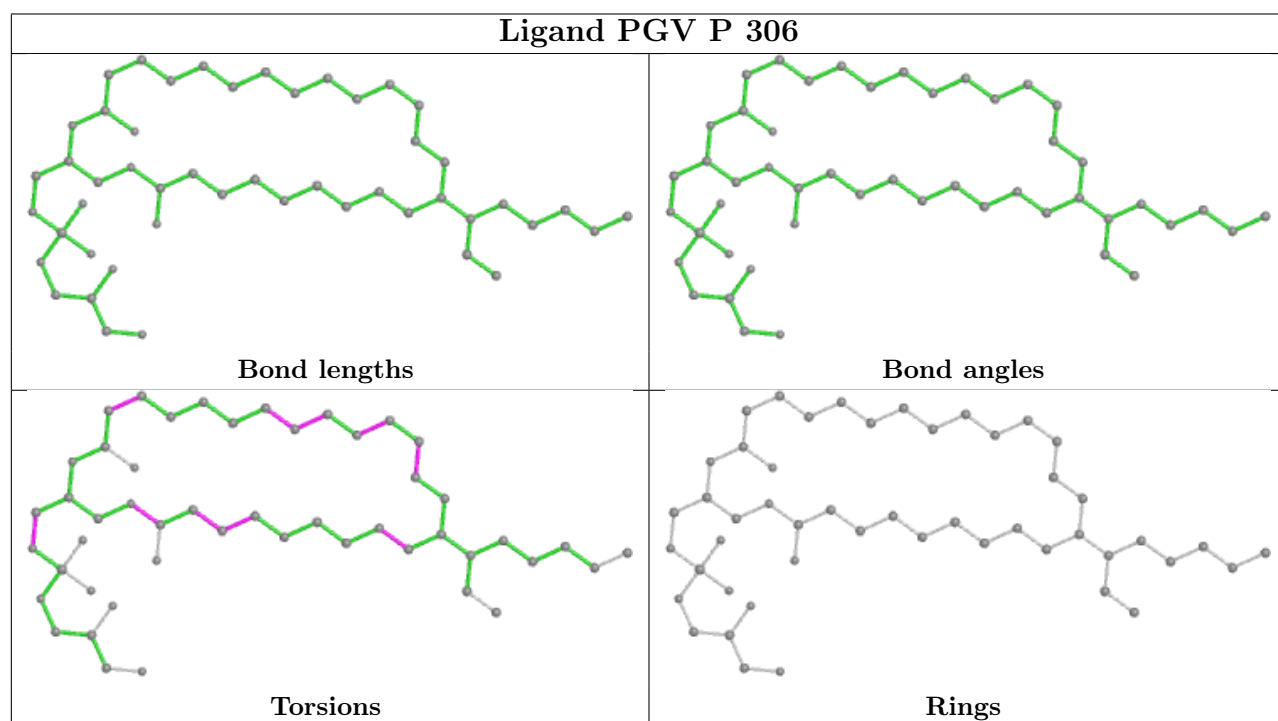
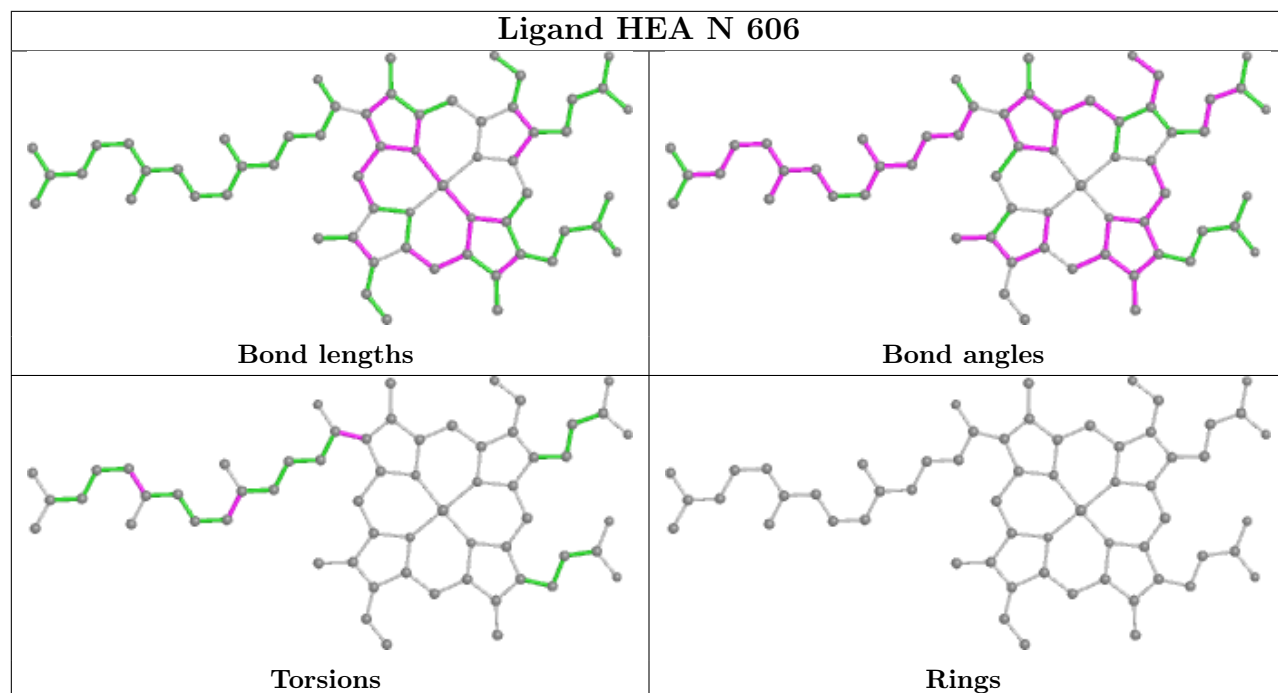


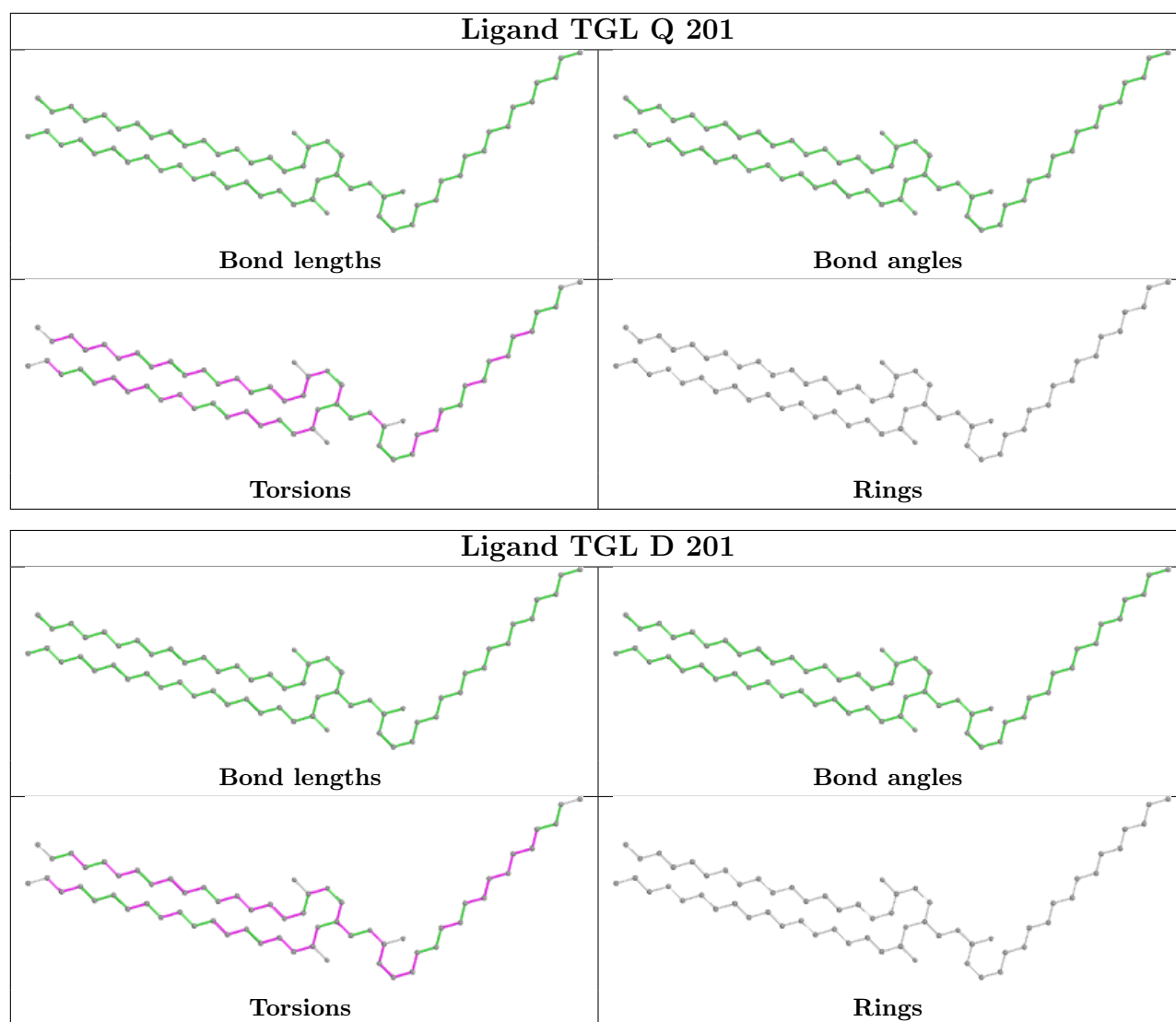
Ligand PEK T 102



Ligand CHD W 302







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.08	4 (0%) 86 91	26, 32, 41, 78	0
1	N	513/514 (99%)	-0.11	2 (0%) 92 96	28, 36, 47, 75	0
2	B	226/227 (99%)	-0.38	2 (0%) 84 90	27, 39, 73, 116	0
2	O	226/227 (99%)	-0.25	5 (2%) 62 72	32, 45, 76, 100	0
3	C	259/261 (99%)	-0.57	0 100 100	27, 36, 49, 93	0
3	P	259/261 (99%)	-0.59	1 (0%) 92 96	30, 37, 54, 93	0
4	D	144/147 (97%)	-0.45	2 (1%) 75 83	31, 41, 63, 89	0
4	Q	144/147 (97%)	0.47	15 (10%) 6 10	39, 56, 89, 170	0
5	E	105/109 (96%)	-0.38	3 (2%) 51 62	33, 42, 68, 114	0
5	R	105/109 (96%)	-0.19	4 (3%) 40 53	38, 50, 73, 112	0
6	F	98/98 (100%)	0.34	6 (6%) 21 31	31, 41, 94, 178	0
6	S	98/98 (100%)	-0.05	6 (6%) 21 31	32, 43, 99, 135	0
7	G	83/85 (97%)	0.63	15 (18%) 1 2	32, 44, 113, 120	0
7	T	83/85 (97%)	0.81	21 (25%) 0 1	33, 48, 112, 144	0
8	H	79/85 (92%)	0.39	10 (12%) 3 6	32, 45, 104, 110	0
8	U	79/85 (92%)	0.36	9 (11%) 5 7	37, 51, 110, 154	0
9	I	72/73 (98%)	0.60	12 (16%) 1 2	34, 51, 82, 107	0
9	V	72/73 (98%)	0.54	10 (13%) 2 4	40, 58, 82, 98	0
10	J	58/59 (98%)	-0.03	5 (8%) 10 16	35, 46, 73, 110	0
10	W	58/59 (98%)	0.19	5 (8%) 10 16	38, 51, 86, 128	0
11	K	49/56 (87%)	0.05	2 (4%) 37 49	33, 45, 64, 70	0
11	X	49/56 (87%)	0.74	6 (12%) 4 7	45, 55, 81, 110	0
12	L	46/47 (97%)	-0.42	0 100 100	30, 37, 56, 112	0
12	Y	46/47 (97%)	-0.29	2 (4%) 35 47	36, 47, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.15	2 (4%) 31 44	31, 38, 74, 96	0
13	Z	43/46 (93%)	0.18	6 (13%) 2 4	40, 48, 83, 126	0
All	All	3550/3614 (98%)	-0.08	155 (4%) 34 46	26, 40, 77, 178	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	18.6
6	F	97	ALA	11.9
4	Q	5	VAL	11.3
4	Q	4	SER	9.8
6	F	96	LEU	9.4
10	W	58	LYS	9.1
7	G	2	SER	9.0
9	I	37	PHE	8.7
6	F	98	HIS	8.4
11	X	6	ALA	8.2
5	R	109	VAL	8.1
7	G	3	ALA	7.8
8	U	8	ILE	7.8
7	T	1	ALA	7.1
4	Q	7	LYS	6.7
8	U	7	LYS	6.7
8	H	45	ALA	6.4
5	R	5	HIS	6.2
13	Z	42	LYS	6.2
8	H	46	LYS	5.8
2	O	90	ILE	5.7
10	J	1	PHE	5.6
9	V	37	PHE	5.6
5	E	5	HIS	5.6
11	X	7	PRO	5.5
8	H	44	THR	5.3
7	T	42	ARG	5.1
10	J	58	LYS	5.0
13	Z	43	SER	4.9
6	F	95	GLN	4.8
7	T	40	GLY	4.7
6	S	98	HIS	4.6
7	T	36	TRP	4.6
7	G	84	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
7	G	41	HIS	4.4
2	O	227	LEU	4.4
4	Q	147	LYS	4.3
5	E	109	VAL	4.2
9	I	25	PHE	4.2
9	V	34	PHE	4.1
10	W	57	HIS	4.0
9	I	26	MET	4.0
7	T	43	GLU	4.0
9	I	34	PHE	3.9
11	X	34	THR	3.7
7	G	42	ARG	3.6
9	I	33	THR	3.6
7	T	45	PRO	3.6
10	W	48	TYR	3.6
7	T	2	SER	3.6
8	H	48	GLY	3.6
9	I	29	LEU	3.5
6	S	96	LEU	3.5
9	V	2	THR	3.4
7	T	41	HIS	3.4
9	I	19	PHE	3.4
7	T	3	ALA	3.4
7	T	47	PHE	3.3
4	Q	8	SER	3.3
9	V	53	ASN	3.3
6	S	97	ALA	3.3
8	U	48	GLY	3.3
2	B	90	ILE	3.3
7	G	36	TRP	3.3
2	O	113	TYR	3.2
8	U	10	ASN	3.2
7	T	46	ALA	3.2
4	D	147	LYS	3.1
6	F	3	GLY	3.1
9	V	26	MET	3.1
11	X	13	TYR	3.1
2	O	91	ASN	3.1
7	G	4	ALA	3.1
8	U	49	ASP	3.1
13	Z	39	ASN	3.1
8	H	47	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
4	Q	73	ARG	3.0
7	T	39	SER	2.9
8	H	42	ALA	2.9
10	J	57	HIS	2.9
9	V	33	THR	2.9
11	K	6	ALA	2.9
7	G	10	GLY	2.9
12	Y	47	LYS	2.8
9	I	18	ARG	2.8
7	G	5	LYS	2.8
7	G	9	GLY	2.8
9	I	30	GLY	2.8
9	V	30	GLY	2.8
7	T	33	LEU	2.8
7	G	40	GLY	2.8
11	K	7	PRO	2.8
7	T	5	LYS	2.8
8	U	45	ALA	2.7
9	V	25	PHE	2.7
4	Q	43	LYS	2.7
7	G	33	LEU	2.7
4	Q	39	ALA	2.7
11	X	12	LYS	2.7
7	T	48	ILE	2.7
7	T	9	GLY	2.6
7	T	10	GLY	2.6
7	G	43	GLU	2.6
9	I	22	VAL	2.6
9	I	21	ILE	2.6
5	R	108	LYS	2.6
8	H	36	PHE	2.5
4	Q	78	TRP	2.5
7	T	82	TYR	2.5
4	Q	35	ALA	2.5
8	U	80	THR	2.5
5	E	7	THR	2.4
13	M	40	TYR	2.4
9	V	29	LEU	2.4
9	I	23	GLY	2.4
13	M	35	TYR	2.4
8	U	47	GLY	2.4
4	Q	50	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	366	VAL	2.4
4	Q	48	TRP	2.3
2	O	92	ASN	2.3
8	H	10	ASN	2.3
6	S	1	ALA	2.3
2	B	40	TYR	2.2
13	Z	35	TYR	2.2
9	V	32	ALA	2.2
10	J	2	GLU	2.2
6	S	94	HIS	2.2
6	F	27	GLY	2.2
13	Z	40	TYR	2.2
7	T	6	GLY	2.2
6	S	25	ARG	2.1
12	Y	20	ARG	2.1
4	D	102	TYR	2.1
7	T	84	LYS	2.1
5	R	79	LYS	2.1
8	U	44	THR	2.1
1	A	257	ILE	2.1
4	Q	141	ASP	2.1
7	G	35	SER	2.1
3	P	182	TYR	2.1
10	W	1	PHE	2.1
7	G	7	ASP	2.0
1	A	367	LEU	2.0
10	J	30	ILE	2.0
11	X	47	ARG	2.0
10	W	52	TRP	2.0
1	N	383	MET	2.0
8	H	79	GLY	2.0
4	Q	46	ALA	2.0
1	A	389	ILE	2.0
1	N	381	LEU	2.0
7	T	37	LEU	2.0
8	H	43	MET	2.0
13	Z	13	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	T	11	11/12	0.69	0.26	86,110,136,136	0
7	TPO	G	11	11/12	0.71	0.24	65,112,161,163	0
1	FME	A	1	10/11	0.92	0.16	44,54,81,85	0
2	FME	O	1	10/11	0.95	0.15	43,47,55,60	0
1	FME	N	1	10/11	0.96	0.18	49,54,81,82	0
2	FME	B	1	10/11	0.98	0.13	38,39,50,58	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
19	EDO	A	617	4/4	0.17	0.64	94,103,106,110	0
29	SAC	V	101	9/10	0.25	0.90	113,120,131,132	0
29	SAC	I	101	9/10	0.27	0.41	98,111,125,128	0
26	DMU	G	101	33/33	0.41	0.47	78,110,150,153	0
19	EDO	G	109	4/4	0.46	0.34	91,103,104,105	0
19	EDO	G	105	4/4	0.57	0.31	76,80,85,86	0
19	EDO	Z	1601	4/4	0.61	0.17	77,84,85,86	0
26	DMU	C	311	33/33	0.62	0.27	82,113,128,132	0
27	PEK	C	313	53/53	0.62	0.32	60,84,139,156	0
23	PSC	B	303	52/52	0.64	0.35	59,111,180,194	0
25	CDL	C	310	100/100	0.65	0.28	61,107,147,165	0
17	PGV	C	303	51/51	0.66	0.26	66,98,125,151	0
24	CHD	T	105	29/29	0.66	0.26	88,161,180,184	0
19	EDO	D	205	4/4	0.67	0.46	91,98,101,105	0
19	EDO	B	309	4/4	0.69	0.23	65,72,78,81	0
22	TGL	Q	201	63/63	0.69	0.26	66,92,121,137	0
27	PEK	P	305	53/53	0.70	0.26	63,98,164,174	0
19	EDO	N	614	4/4	0.70	0.41	63,63,67,73	0
19	EDO	V	103	4/4	0.70	0.23	82,90,92,93	0
22	TGL	Y	101	63/63	0.71	0.27	52,69,126,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	EDO	N	608	4/4	0.71	0.49	47,51,52,56	0
26	DMU	C	312	33/33	0.72	0.35	70,103,119,133	0
25	CDL	T	103	100/100	0.72	0.29	59,107,145,164	0
27	PEK	G	103	53/53	0.73	0.27	65,97,166,172	0
27	PEK	P	301	53/53	0.73	0.24	59,87,135,155	0
19	EDO	B	311	4/4	0.73	0.28	91,92,93,96	0
23	PSC	R	201	52/52	0.73	0.36	56,99,184,199	0
19	EDO	E	204	4/4	0.73	0.20	64,64,64,70	0
19	EDO	N	612	4/4	0.74	0.38	78,79,85,87	0
19	EDO	Q	204	4/4	0.74	0.35	68,76,83,84	0
19	EDO	A	608	4/4	0.75	0.28	47,56,59,61	0
17	PGV	P	307	51/51	0.76	0.29	69,104,132,144	0
22	TGL	D	201	63/63	0.77	0.24	48,82,100,115	0
25	CDL	P	308	100/100	0.77	0.25	51,90,120,128	0
19	EDO	P	314	4/4	0.77	0.26	67,74,77,79	0
17	PGV	N	617	51/51	0.78	0.32	51,90,145,155	0
19	EDO	L	102	4/4	0.79	0.26	63,64,64,65	0
22	TGL	L	101	63/63	0.79	0.22	43,70,121,131	0
22	TGL	N	604	63/63	0.79	0.27	58,91,131,137	0
19	EDO	J	103	4/4	0.79	0.21	52,57,63,64	0
26	DMU	P	303	33/33	0.81	0.31	54,103,121,129	0
26	DMU	Q	206	33/33	0.81	0.28	53,68,83,92	0
19	EDO	O	302	4/4	0.81	0.20	68,74,75,80	0
19	EDO	S	105	4/4	0.81	0.21	67,68,70,71	0
19	EDO	P	310	4/4	0.81	0.24	61,67,71,78	0
19	EDO	D	202	4/4	0.81	0.22	53,67,72,74	0
24	CHD	Y	102	29/29	0.81	0.29	82,140,163,186	0
25	CDL	C	304	100/100	0.81	0.26	52,92,118,123	0
19	EDO	D	206	4/4	0.82	0.26	55,56,57,61	0
19	EDO	J	102	4/4	0.82	0.20	74,77,77,79	0
19	EDO	N	610	4/4	0.83	0.28	66,69,69,72	0
19	EDO	K	101	4/4	0.83	0.20	58,60,61,61	0
19	EDO	O	303	4/4	0.83	0.25	69,73,77,81	0
22	TGL	B	302	63/63	0.83	0.25	49,85,110,116	0
19	EDO	C	306	4/4	0.84	0.17	44,45,48,49	0
19	EDO	S	104	4/4	0.84	0.20	71,79,81,82	0
19	EDO	N	616	4/4	0.84	0.25	70,70,73,74	0
17	PGV	A	604	51/51	0.85	0.24	48,83,126,130	0
19	EDO	C	309	4/4	0.85	0.22	78,78,78,81	0
19	EDO	J	104	4/4	0.85	0.21	67,74,78,79	0
19	EDO	V	102	4/4	0.85	0.25	72,80,81,88	0
26	DMU	D	208	33/33	0.85	0.23	42,53,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	I	102	4/4	0.85	0.10	60,65,66,68	0
19	EDO	K	102	4/4	0.85	0.20	62,64,64,66	0
19	EDO	B	308	4/4	0.86	0.28	63,65,72,74	0
19	EDO	B	310	4/4	0.86	0.14	57,60,62,64	0
19	EDO	W	303	4/4	0.86	0.11	82,85,85,86	0
19	EDO	G	106	4/4	0.86	0.18	54,60,62,69	0
19	EDO	G	107	4/4	0.86	0.21	60,62,62,62	0
24	CHD	W	302	29/29	0.87	0.30	66,74,96,98	0
19	EDO	B	305	4/4	0.87	0.16	55,62,66,67	0
24	CHD	J	101	29/29	0.88	0.30	53,72,92,93	0
19	EDO	R	203	4/4	0.88	0.18	64,65,66,68	0
19	EDO	A	612	4/4	0.88	0.14	54,63,65,65	0
15	MG	N	602	1/1	0.88	0.11	35,35,35,35	0
19	EDO	F	703	4/4	0.89	0.22	53,69,73,77	0
19	EDO	S	103	4/4	0.89	0.23	73,74,74,77	0
19	EDO	P	311	4/4	0.89	0.21	68,72,74,76	0
19	EDO	C	308	4/4	0.90	0.12	74,78,79,80	0
19	EDO	I	103	4/4	0.91	0.21	61,62,67,68	0
19	EDO	D	207	4/4	0.91	0.25	64,65,68,73	0
19	EDO	A	610	4/4	0.91	0.26	41,42,45,49	0
19	EDO	Q	205	4/4	0.91	0.21	61,69,79,83	0
19	EDO	N	613	4/4	0.92	0.15	51,64,70,75	0
19	EDO	D	203	4/4	0.92	0.17	53,57,61,62	0
19	EDO	M	701	4/4	0.92	0.20	67,69,70,75	0
19	EDO	J	105	4/4	0.92	0.14	58,62,62,66	0
19	EDO	W	301	4/4	0.92	0.27	69,75,80,80	0
27	PEK	T	102	53/53	0.92	0.22	35,54,100,105	0
19	EDO	D	204	4/4	0.92	0.17	65,67,69,70	0
19	EDO	A	613	4/4	0.92	0.18	56,65,70,76	0
19	EDO	B	306	4/4	0.93	0.18	55,59,62,65	0
19	EDO	Q	202	4/4	0.93	0.16	61,64,68,76	0
24	CHD	C	305	29/29	0.93	0.22	53,55,59,63	0
19	EDO	A	611	4/4	0.93	0.14	64,65,67,68	0
19	EDO	N	615	4/4	0.93	0.20	56,57,60,60	0
19	EDO	R	202	4/4	0.93	0.19	57,58,60,60	0
19	EDO	A	616	4/4	0.93	0.24	68,69,72,72	0
19	EDO	S	102	4/4	0.93	0.15	37,38,39,39	0
19	EDO	E	205	4/4	0.94	0.24	60,69,70,70	0
19	EDO	C	307	4/4	0.94	0.14	66,66,70,76	0
19	EDO	P	312	4/4	0.94	0.28	53,56,57,58	0
19	EDO	P	313	4/4	0.94	0.13	51,52,54,59	0
19	EDO	N	611	4/4	0.94	0.20	65,68,70,73	0

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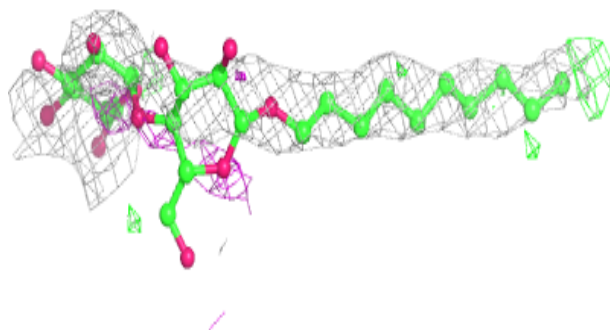
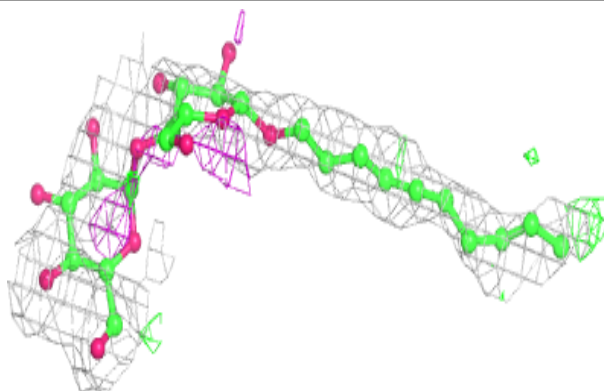
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	E	203	4/4	0.94	0.16	54,55,58,59	0
15	MG	A	602	1/1	0.94	0.11	31,31,31,31	0
17	PGV	C	302	51/51	0.95	0.23	30,44,100,102	0
19	EDO	B	307	4/4	0.95	0.08	64,68,70,70	0
19	EDO	T	104	4/4	0.95	0.32	58,60,63,64	0
24	CHD	P	309	29/29	0.95	0.21	55,63,68,74	0
19	EDO	A	614	4/4	0.95	0.22	55,56,57,57	0
19	EDO	A	615	4/4	0.95	0.19	61,66,67,68	0
24	CHD	T	101	29/29	0.96	0.10	32,38,43,47	0
27	PEK	G	102	53/53	0.96	0.21	32,53,88,100	0
19	EDO	A	609	4/4	0.96	0.18	30,33,33,35	0
19	EDO	B	304	4/4	0.96	0.17	32,35,36,39	0
19	EDO	F	704	4/4	0.96	0.17	37,39,41,42	0
19	EDO	G	104	4/4	0.96	0.26	37,39,40,42	0
19	EDO	Q	203	4/4	0.96	0.07	58,62,64,66	0
17	PGV	A	605	51/51	0.96	0.23	28,44,72,73	0
18	HEA	N	606	60/60	0.97	0.17	25,37,47,59	0
17	PGV	P	306	51/51	0.97	0.17	30,45,87,88	0
19	EDO	N	607	4/4	0.97	0.15	35,35,36,36	0
24	CHD	C	301	29/29	0.97	0.10	35,37,40,44	0
19	EDO	F	701	4/4	0.97	0.17	43,44,45,46	0
19	EDO	N	609	4/4	0.97	0.12	51,52,53,53	0
24	CHD	P	304	29/29	0.97	0.10	31,35,38,40	0
19	EDO	E	201	4/4	0.97	0.14	47,48,49,49	0
19	EDO	E	202	4/4	0.97	0.16	49,53,54,54	0
17	PGV	P	302	51/51	0.97	0.22	28,51,74,75	0
18	HEA	A	607	60/60	0.98	0.16	25,31,54,63	0
18	HEA	N	605	60/60	0.98	0.13	28,31,38,40	0
16	NA	A	603	1/1	0.98	0.08	30,30,30,30	0
21	CUA	O	301	2/2	0.98	0.08	35,35,35,37	0
24	CHD	G	108	29/29	0.98	0.08	32,35,39,41	0
18	HEA	A	606	60/60	0.98	0.13	25,28,37,40	0
21	CUA	B	301	2/2	0.99	0.07	30,30,30,31	0
16	NA	N	603	1/1	0.99	0.06	32,32,32,32	0
20	OH	A	618	1/1	1.00	0.13	21,21,21,21	1
20	OH	N	618	1/1	1.00	0.13	18,18,18,18	1
28	ZN	F	702	1/1	1.00	0.06	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.05	39,39,39,39	0
14	CU	A	601	1/1	1.00	0.12	31,31,31,31	0
14	CU	N	601	1/1	1.00	0.12	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

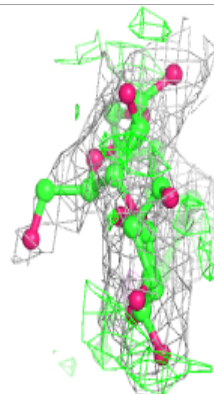
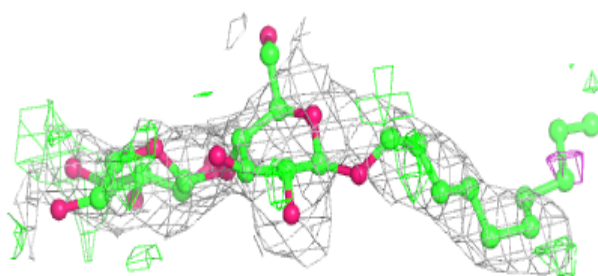
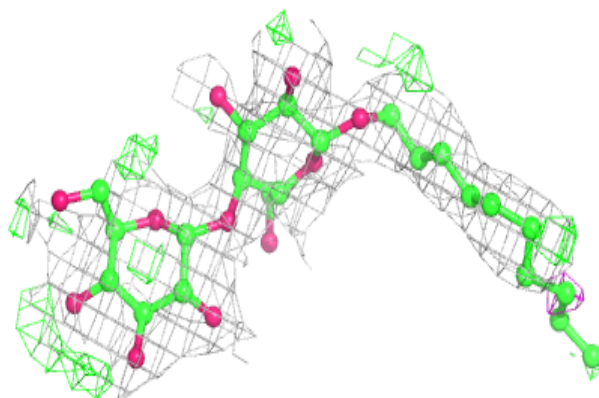
Electron density around DMU G 101:

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



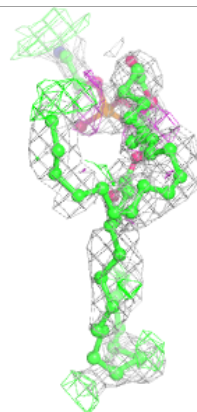
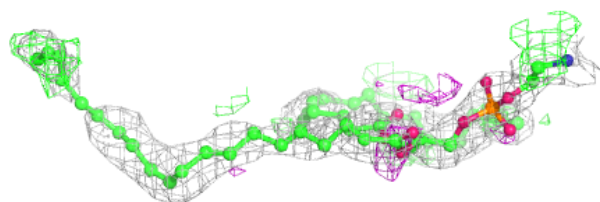
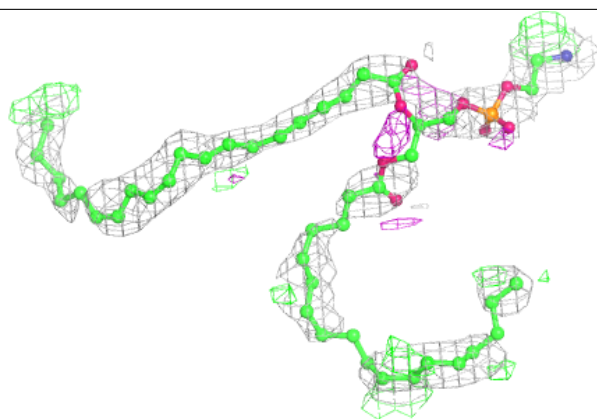
Electron density around DMU C 311:

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

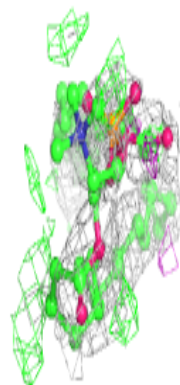
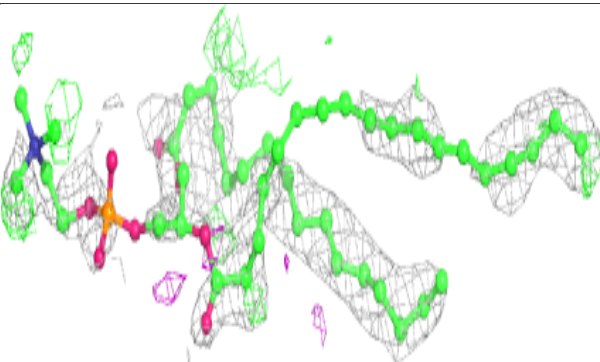
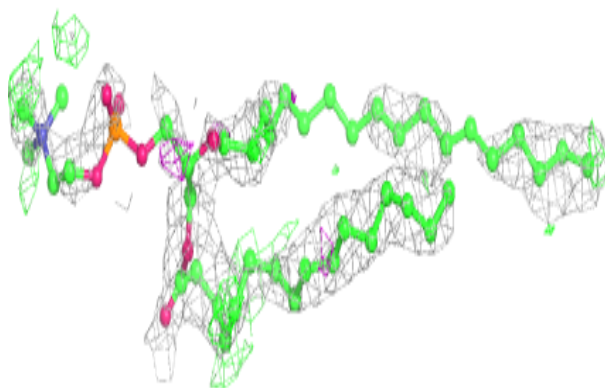


Electron density around PEK C 313:

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

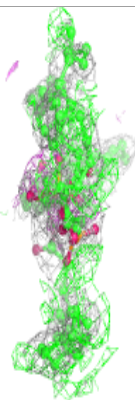
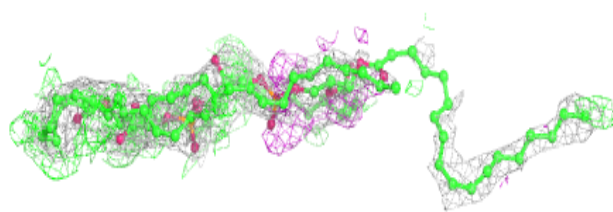
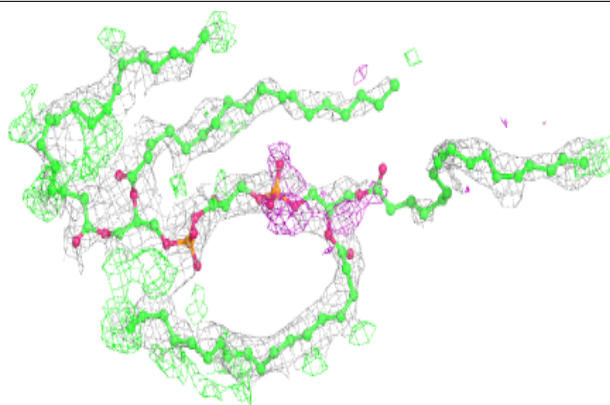
**Electron density around PSC B 303:**

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

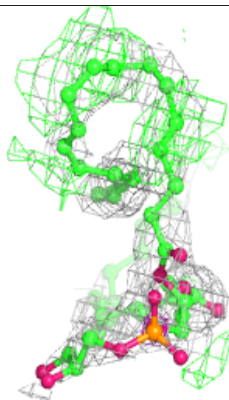
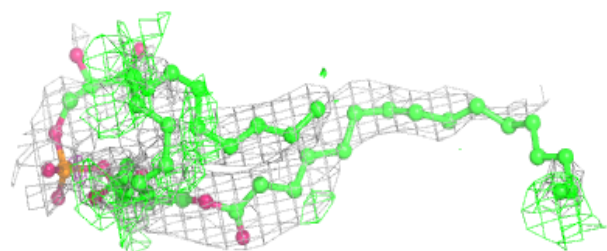
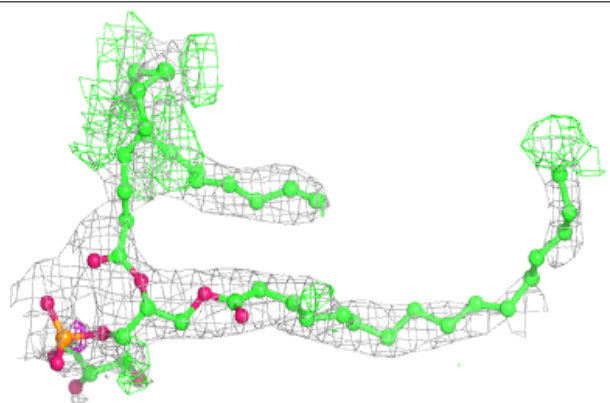


Electron density around CDL C 310:

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

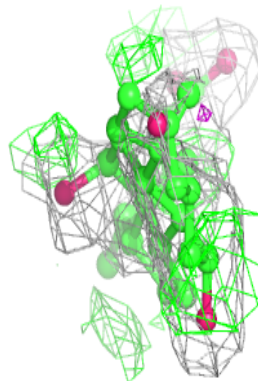
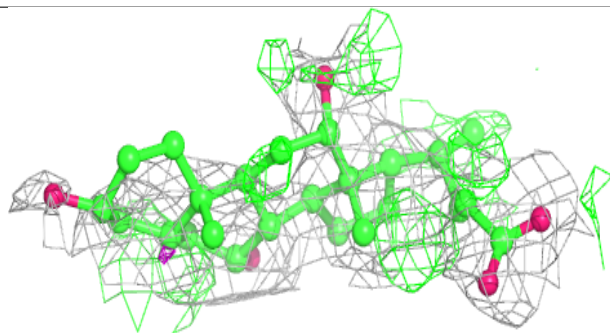
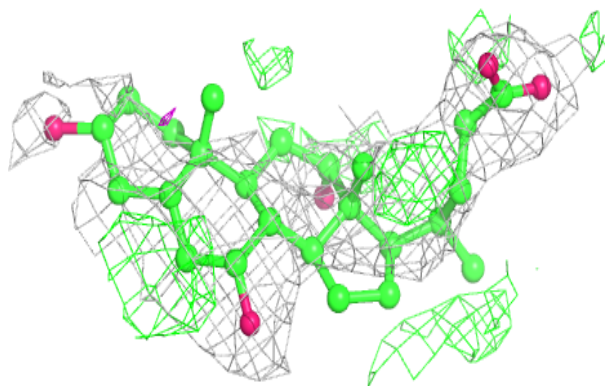
**Electron density around PGV C 303:**

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

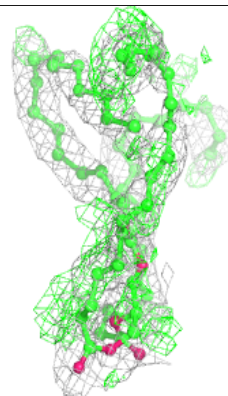
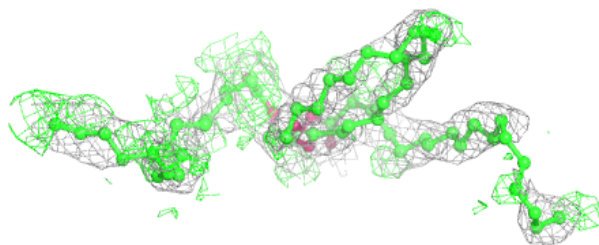
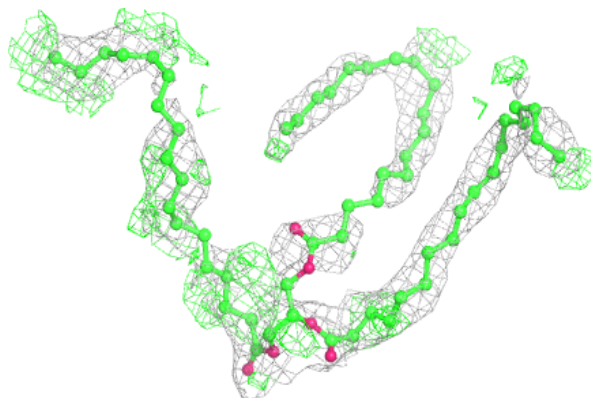


Electron density around CHD T 105:

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

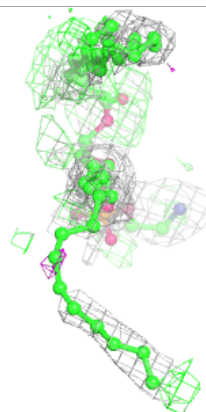
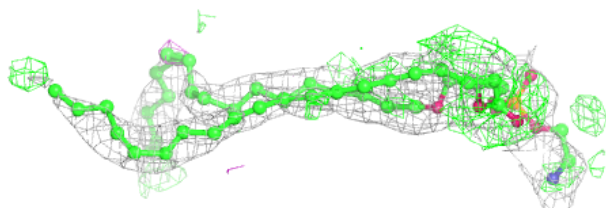
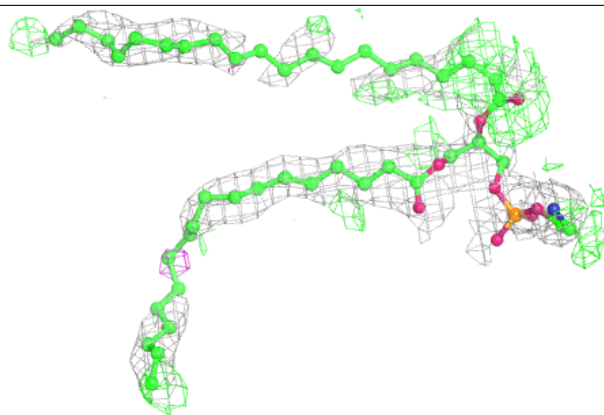
**Electron density around TGL Q 201:**

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

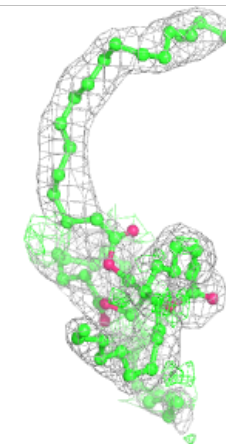
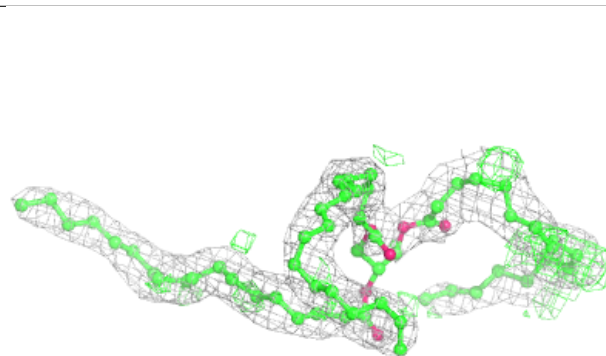
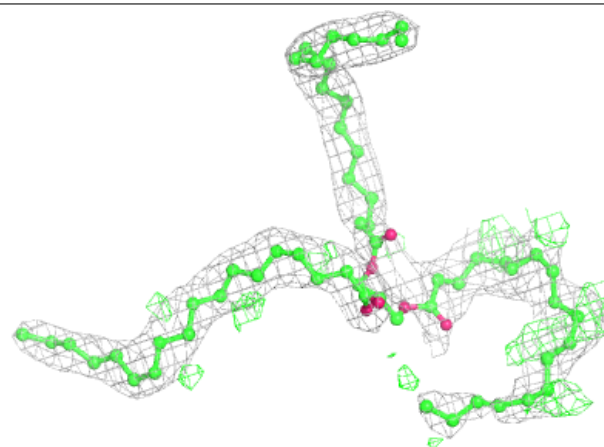


Electron density around PEK P 305:

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

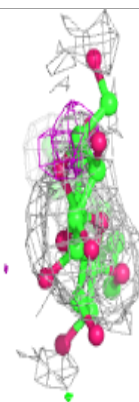
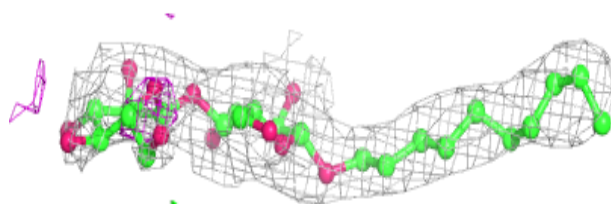
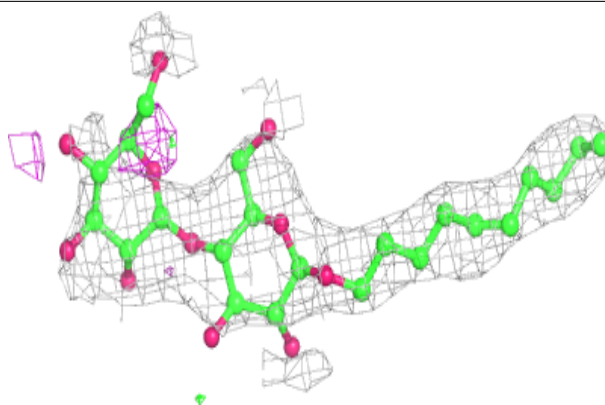
**Electron density around TGL Y 101:**

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

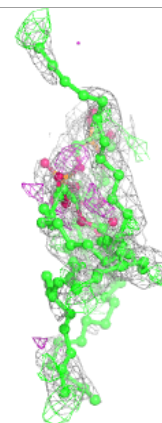
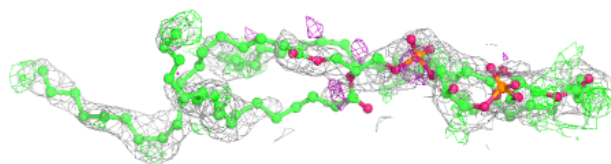
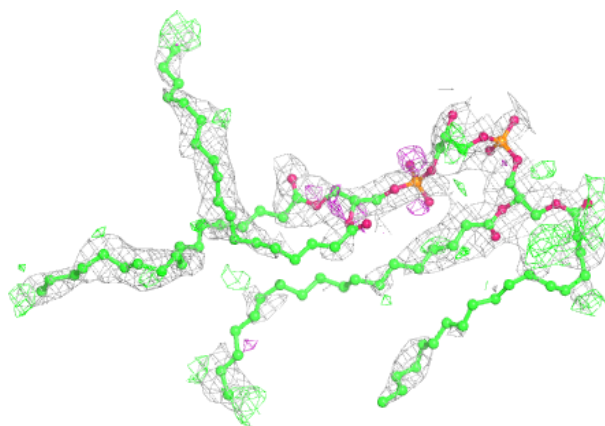


Electron density around DMU C 312:

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

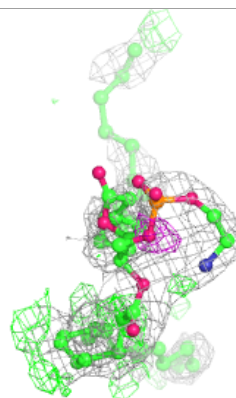
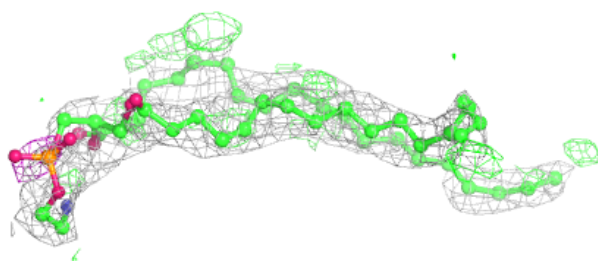
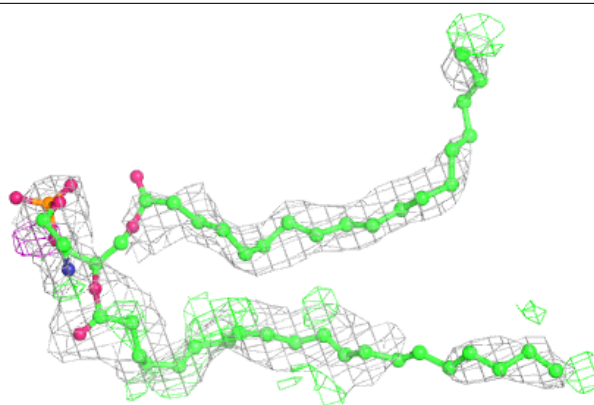
**Electron density around CDL T 103:**

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

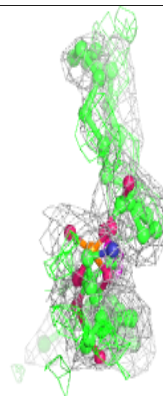
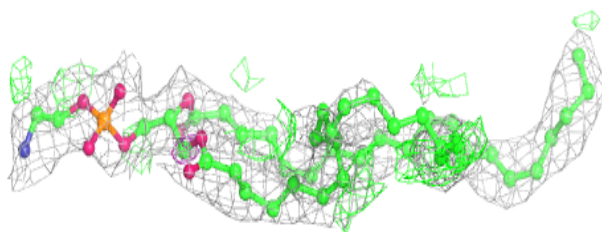
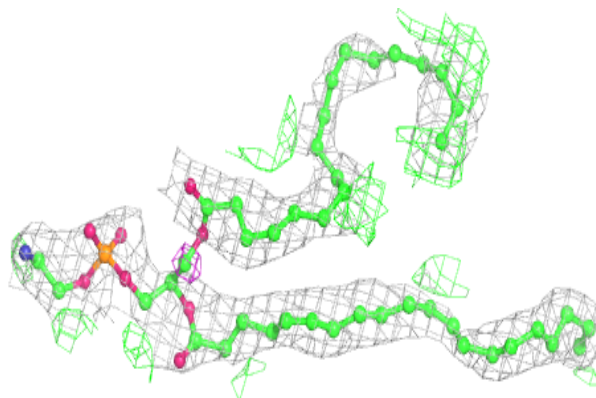


Electron density around PEK G 103:

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

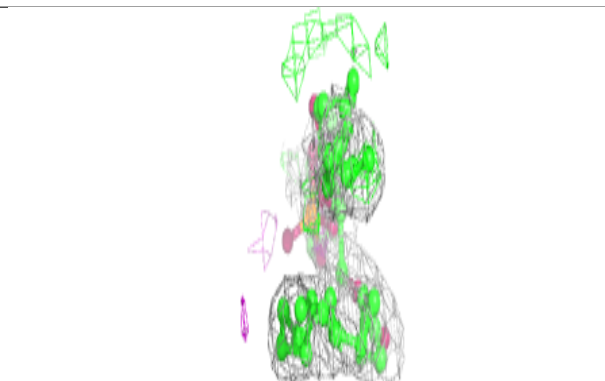
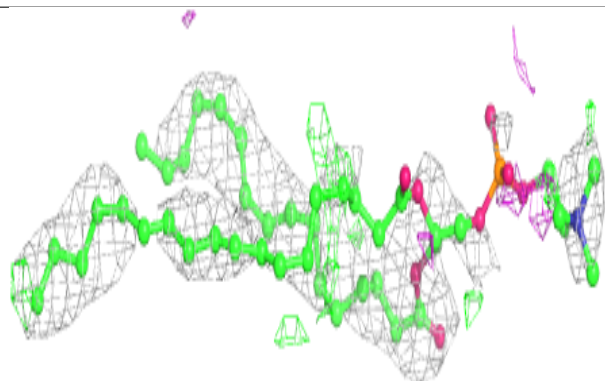
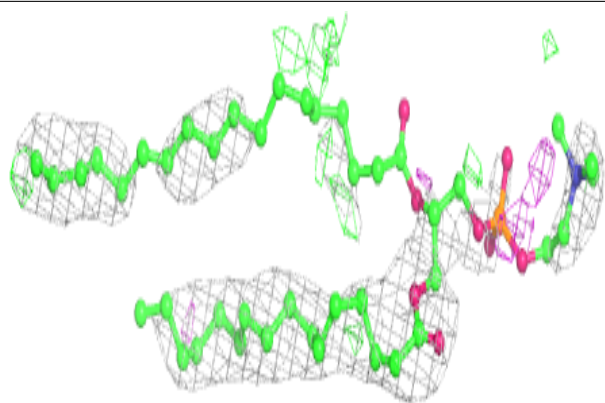
**Electron density around PEK P 301:**

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

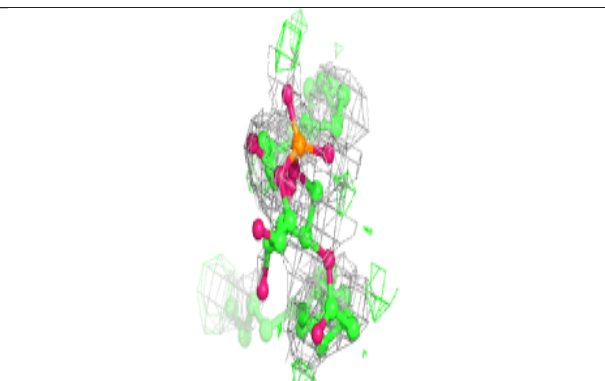
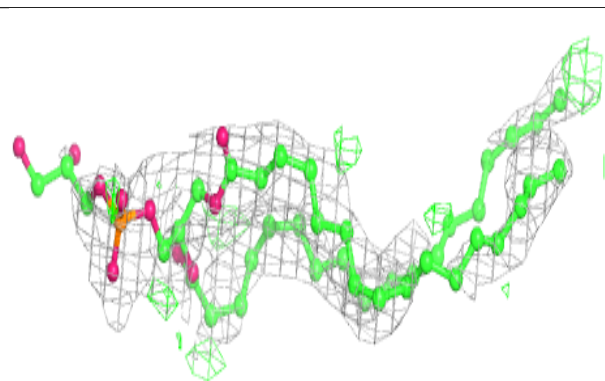
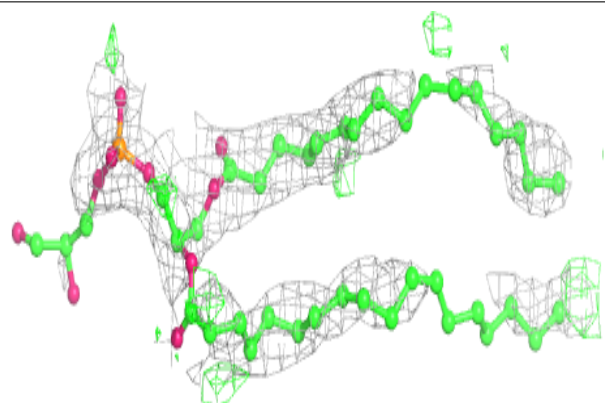


Electron density around PSC R 201:

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

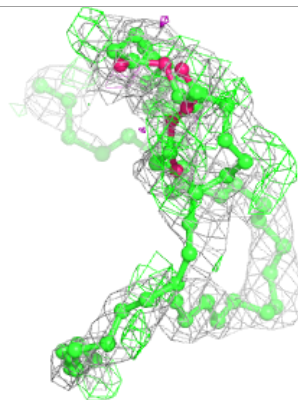
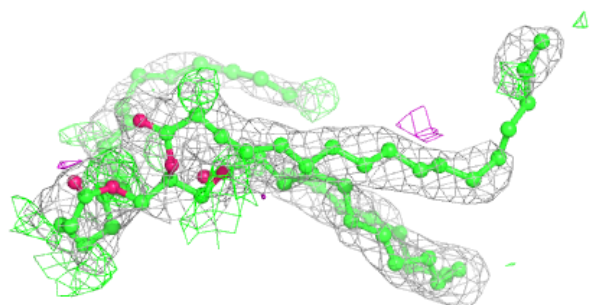
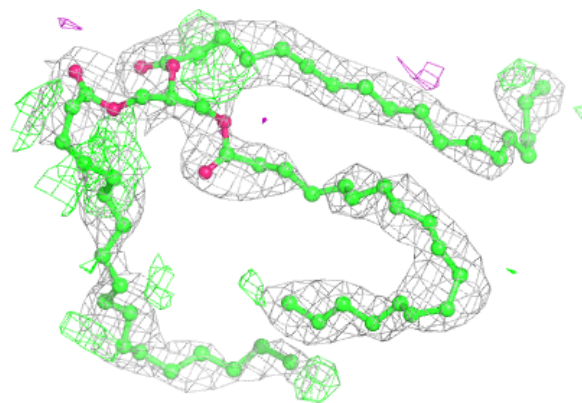
**Electron density around PGV P 307:**

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

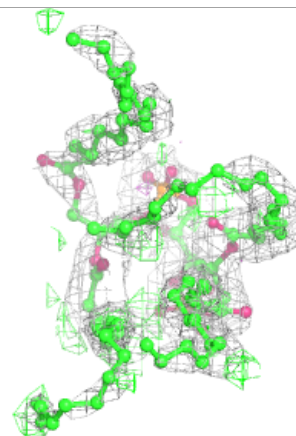
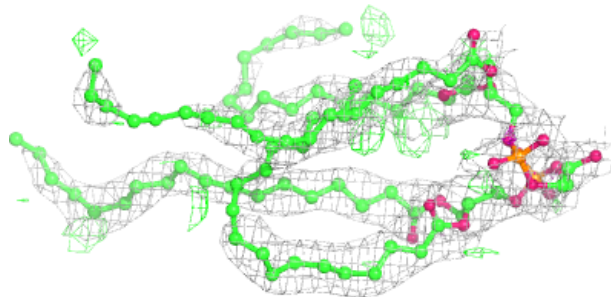
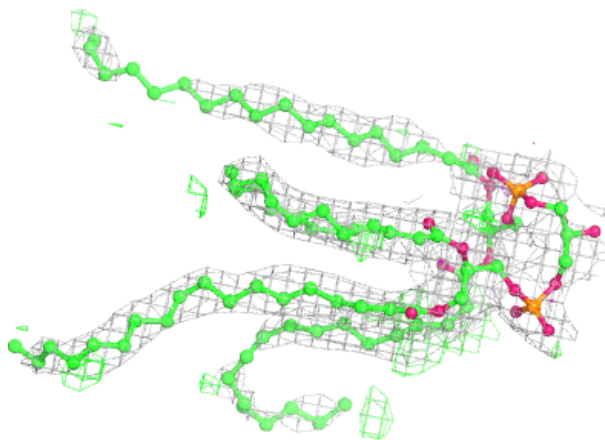


Electron density around TGL D 201:

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

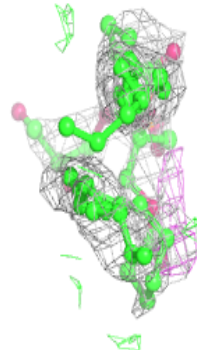
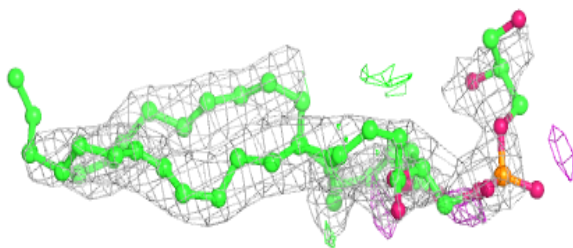
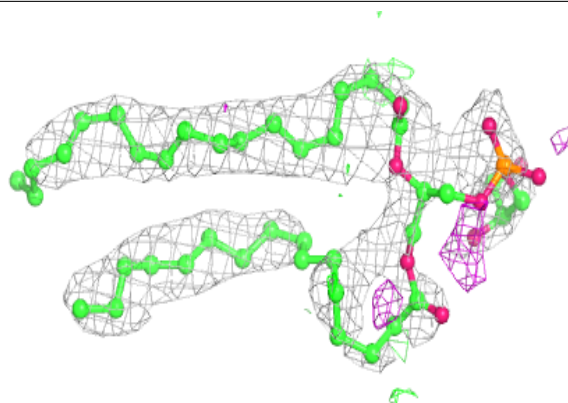
**Electron density around CDL P 308:**

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



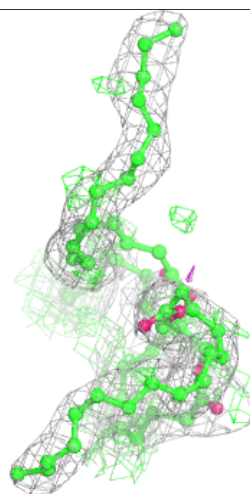
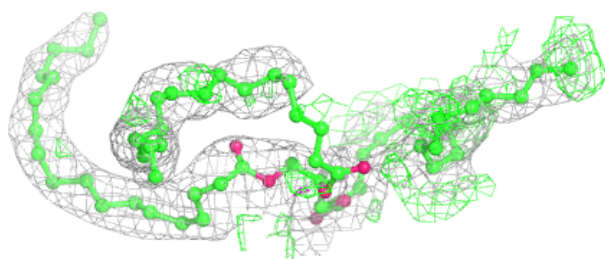
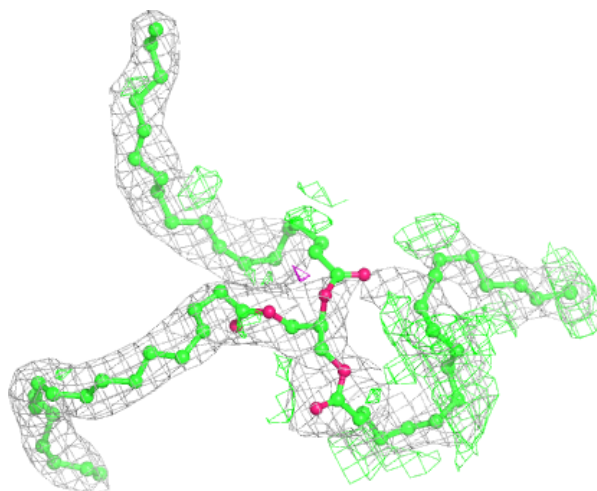
Electron density around PGV N 617:

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



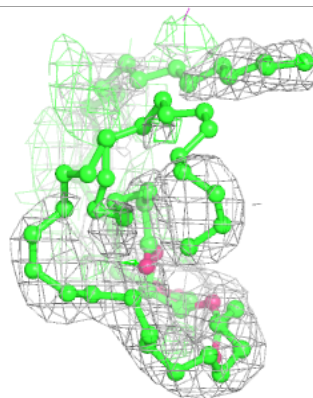
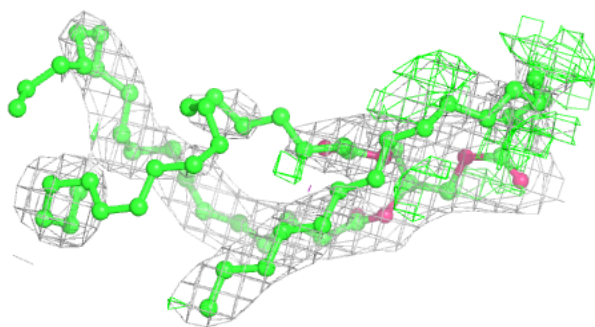
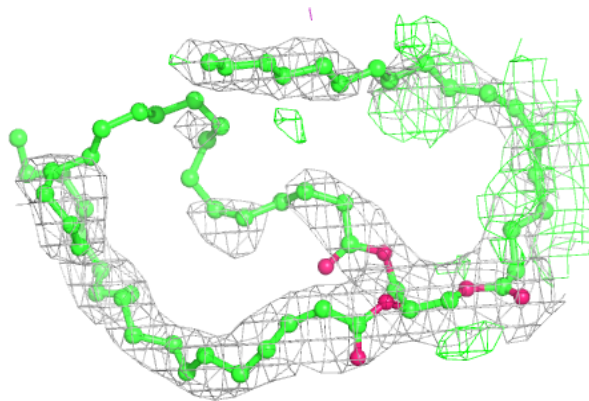
Electron density around TGL L 101:

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

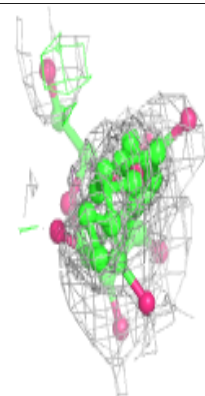
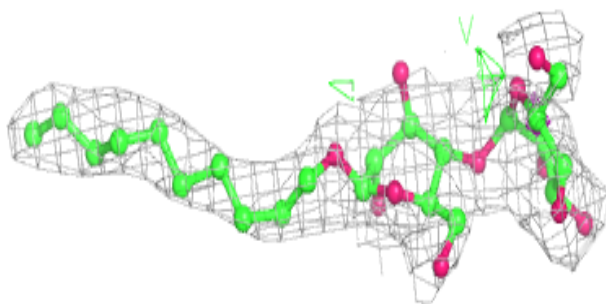
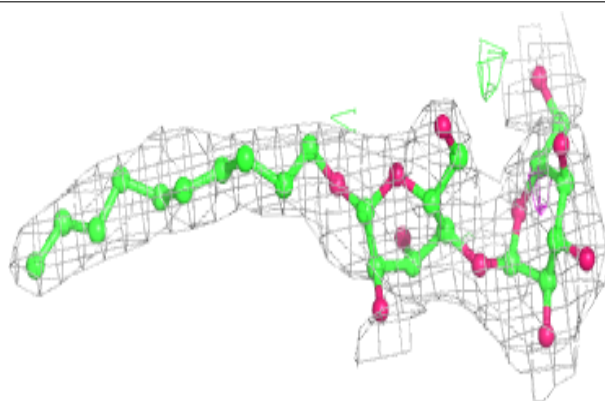


Electron density around TGL N 604:

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

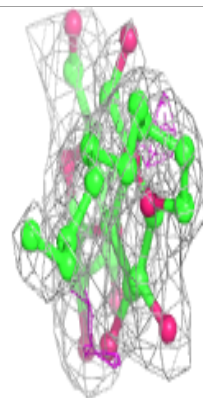
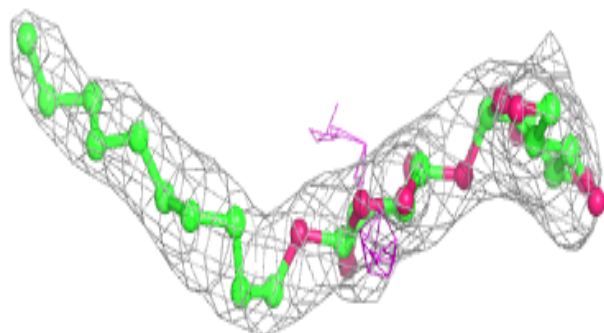
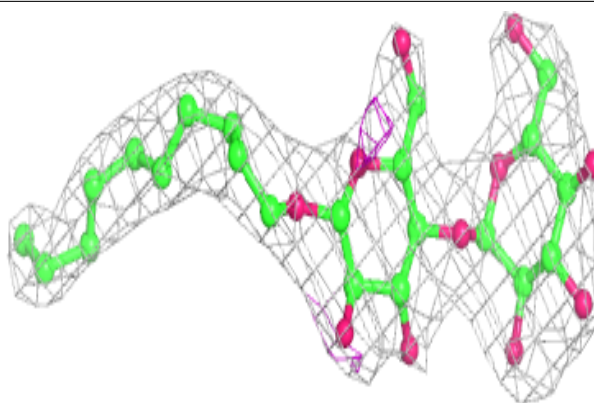
**Electron density around DMU P 303:**

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

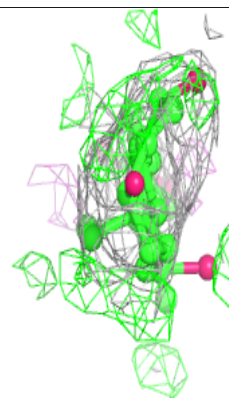
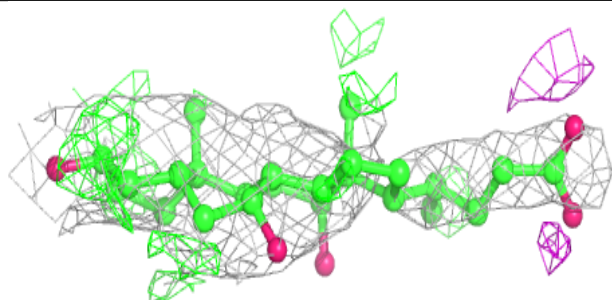
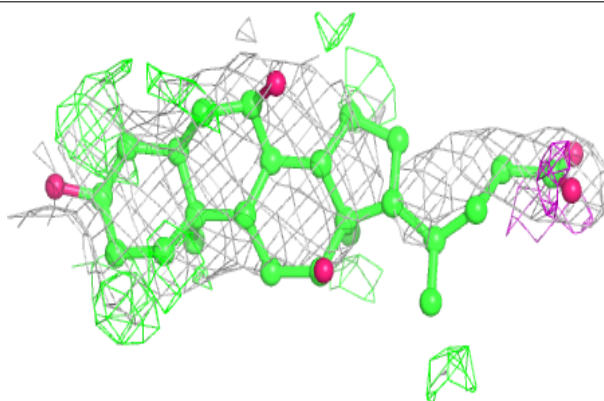


Electron density around DMU Q 206:

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

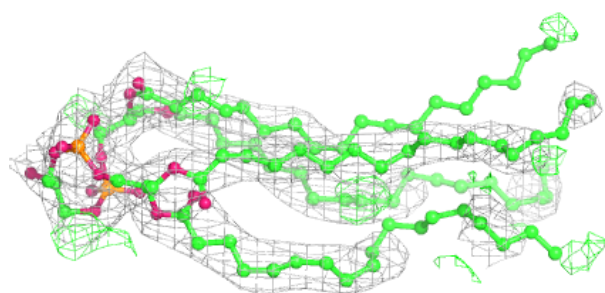
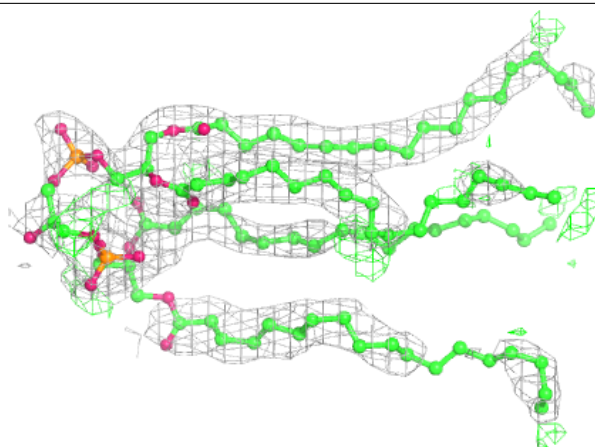
**Electron density around CHD Y 102:**

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

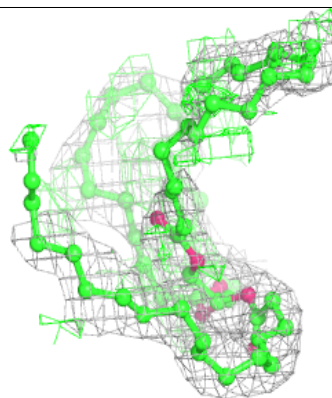
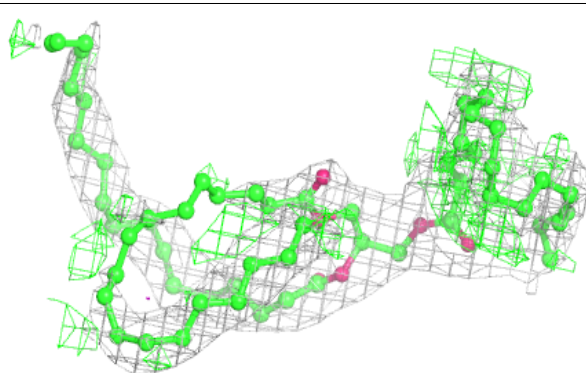
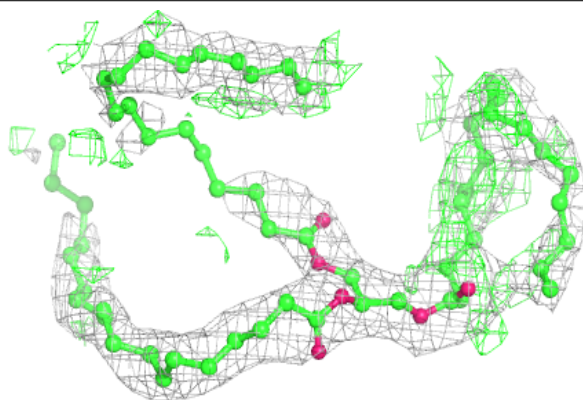


Electron density around CDL C 304:

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

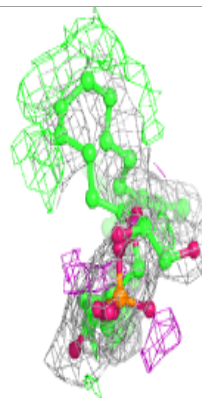
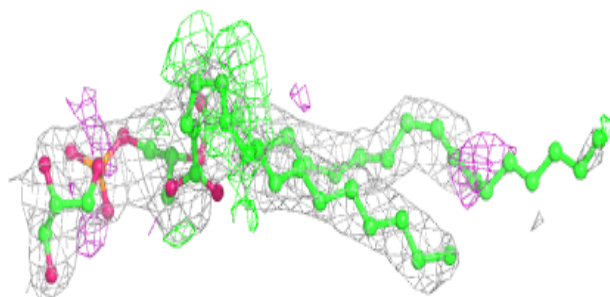
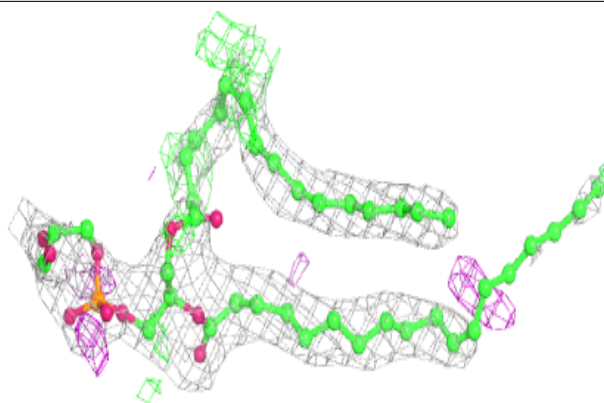
**Electron density around TGL B 302:**

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

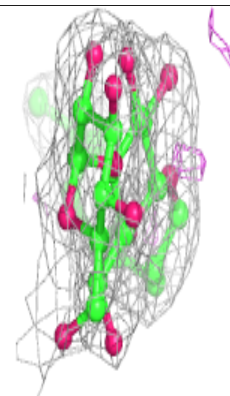
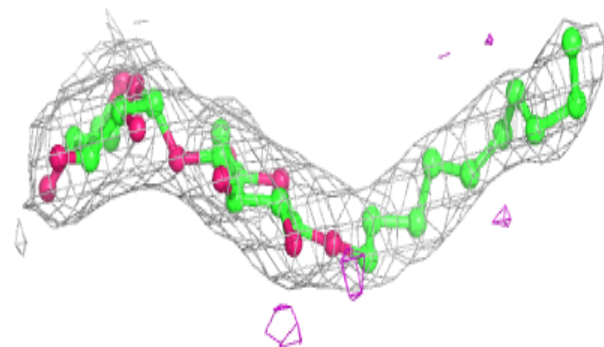
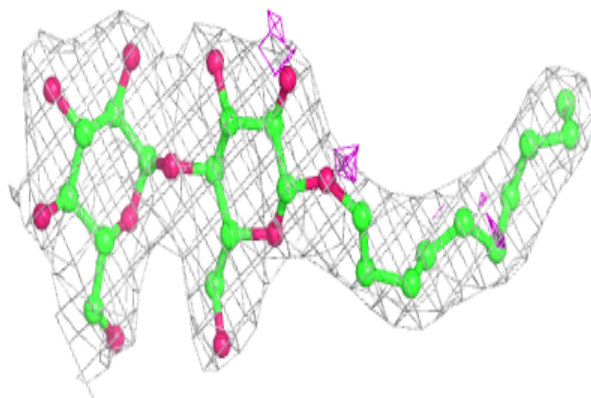


Electron density around PGV A 604:

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

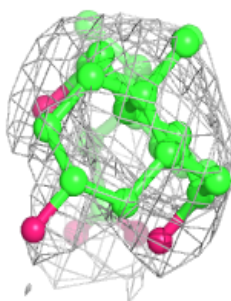
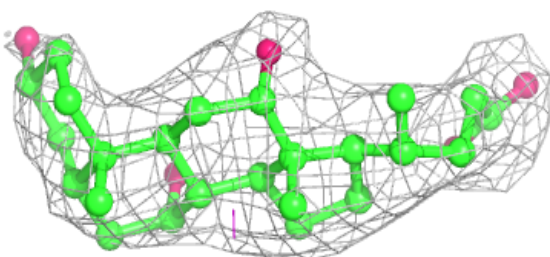
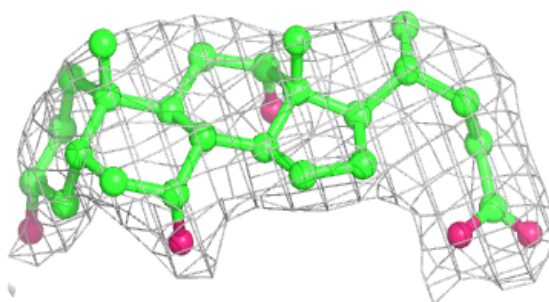
**Electron density around DMU D 208:**

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

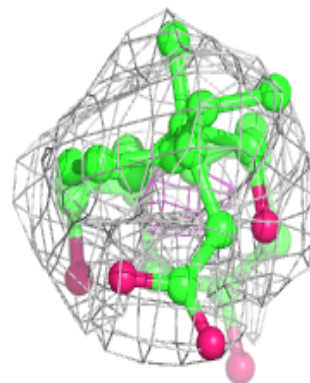
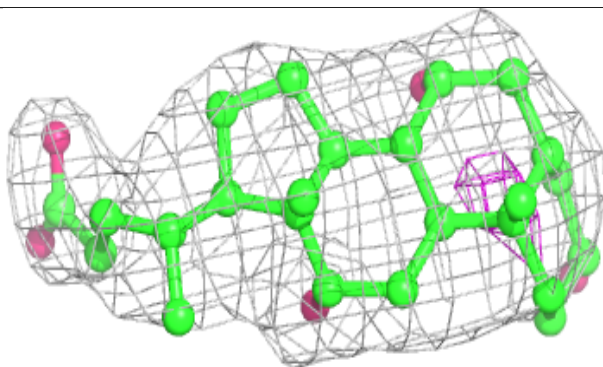
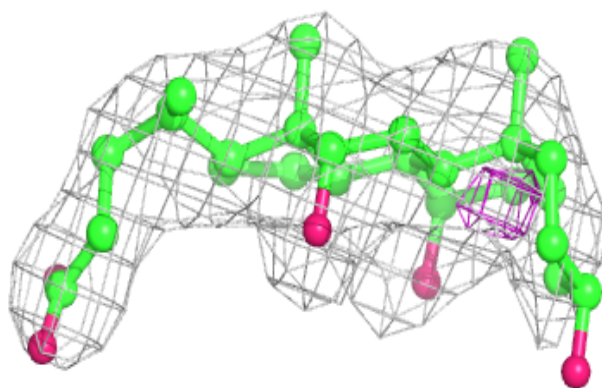


Electron density around CHD W 302:

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

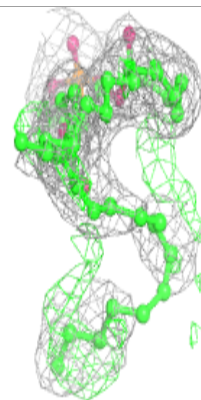
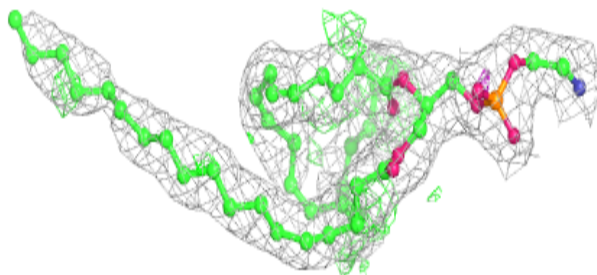
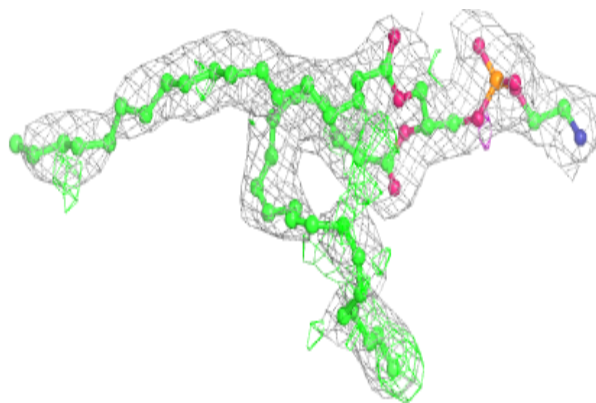
**Electron density around CHD J 101:**

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

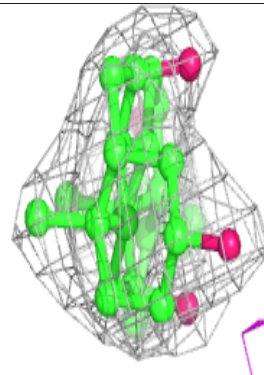
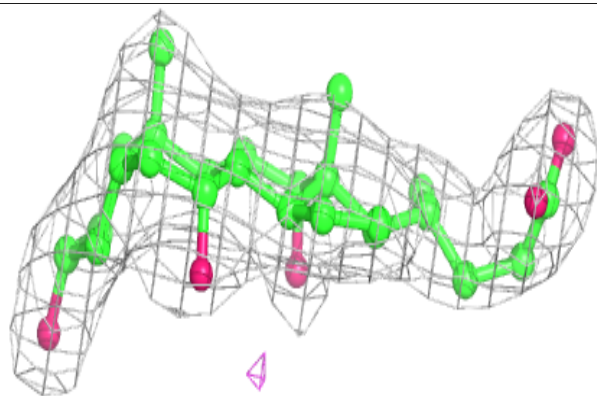
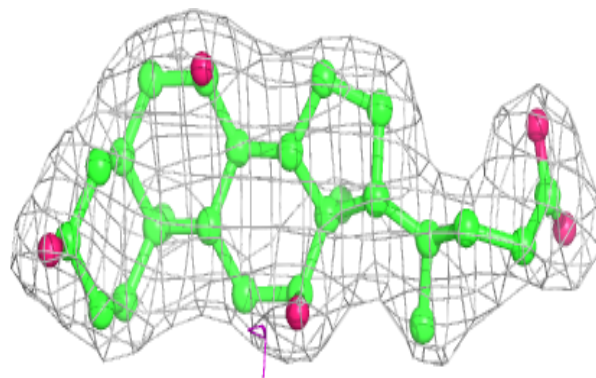


Electron density around PEK T 102:

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

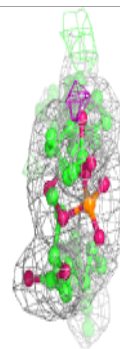
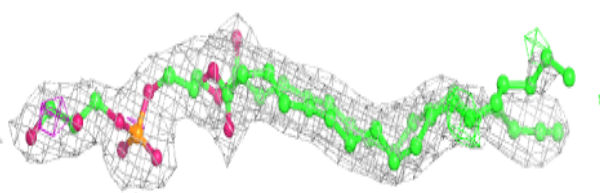
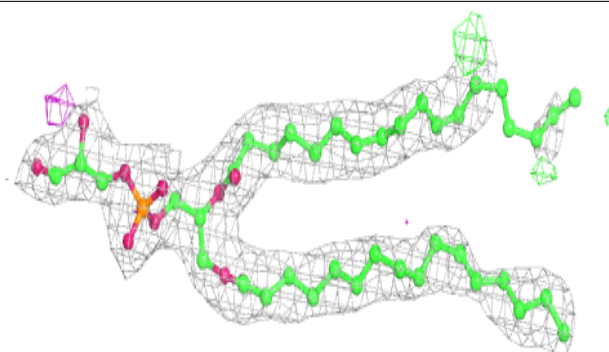
**Electron density around CHD C 305:**

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

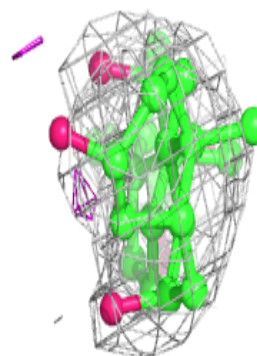
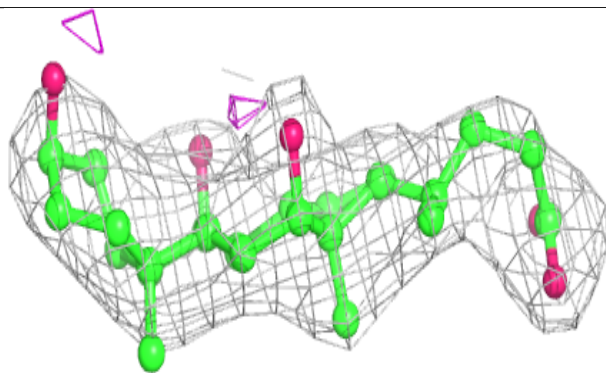
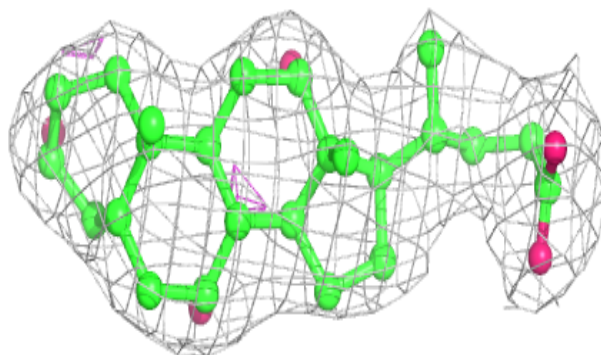


Electron density around PGV C 302:

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

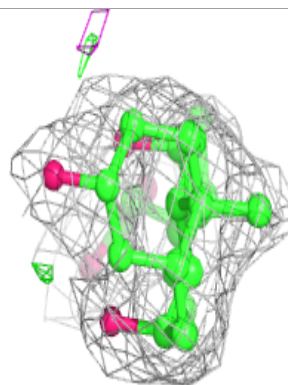
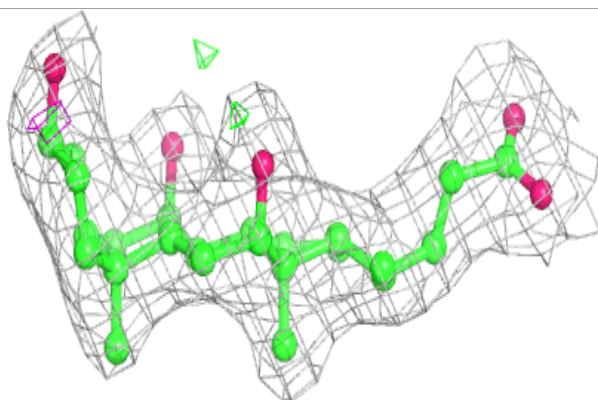
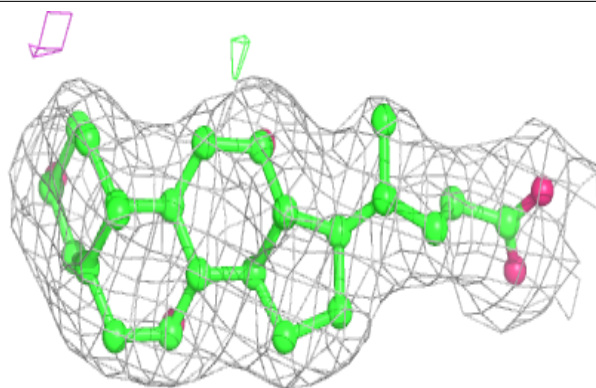
**Electron density around CHD P 309:**

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

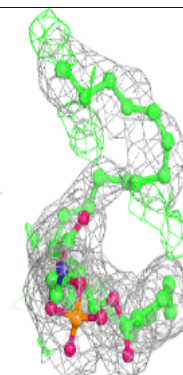
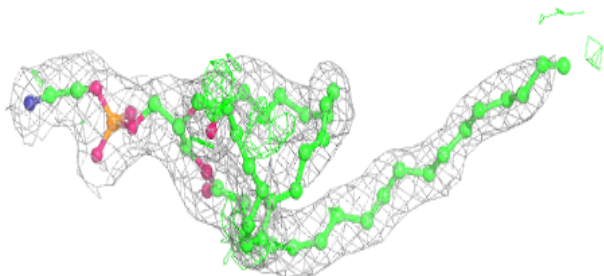
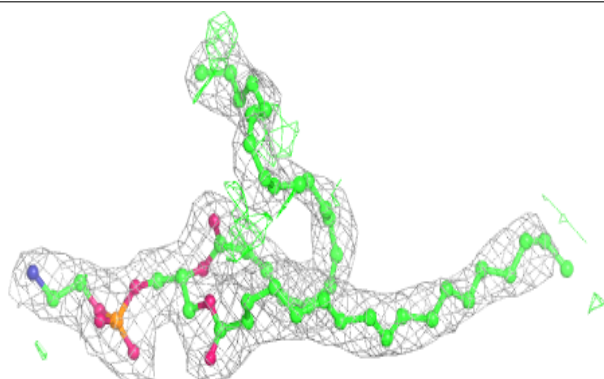


Electron density around CHD T 101:

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

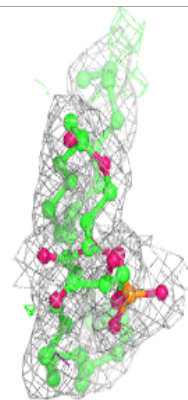
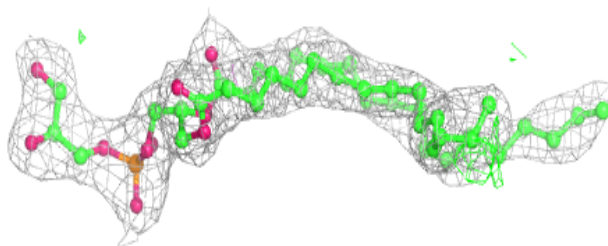
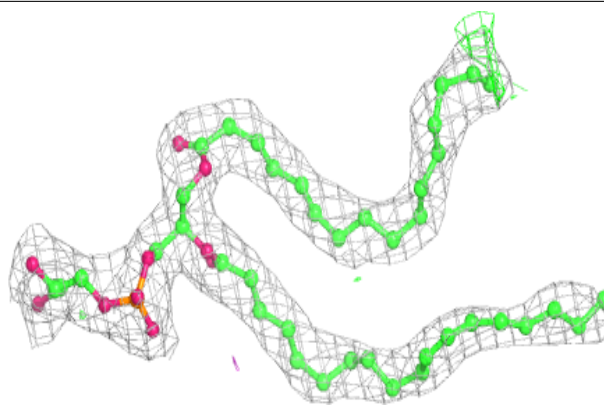
**Electron density around PEK G 102:**

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

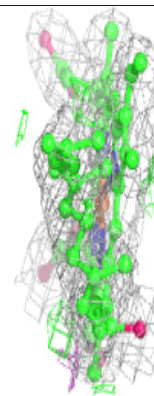
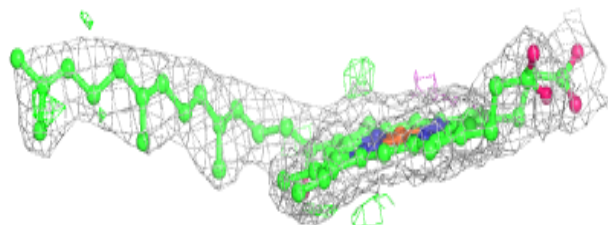
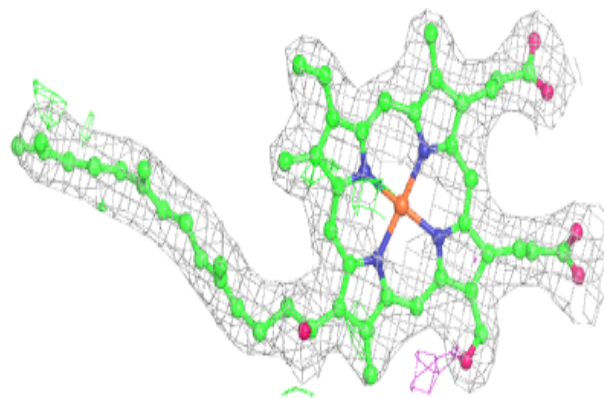


Electron density around PGV A 605:

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

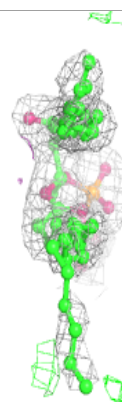
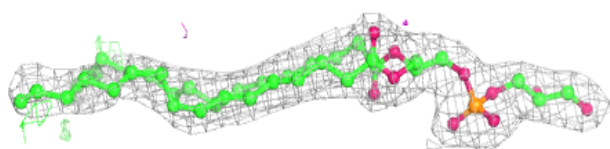
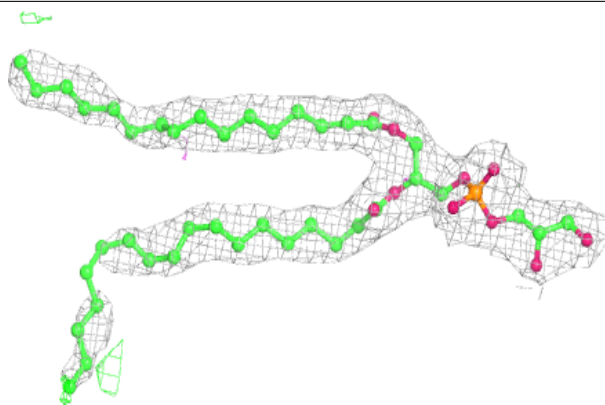
**Electron density around HEA N 606:**

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

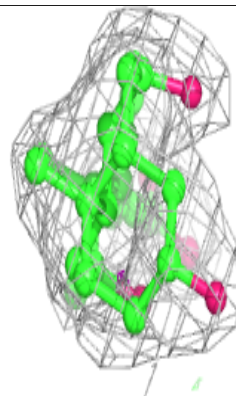
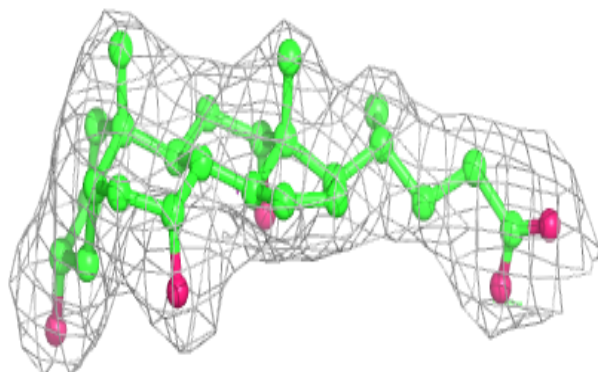
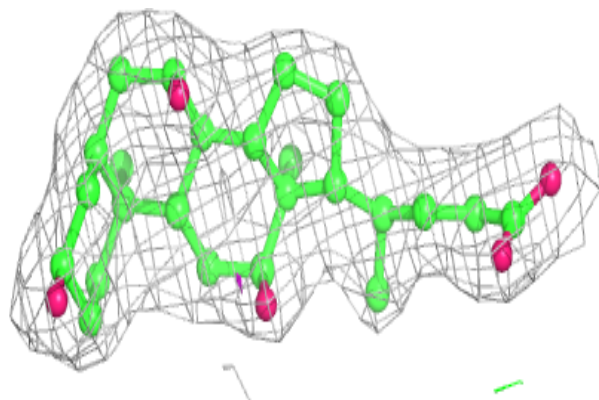


Electron density around PGV P 306:

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

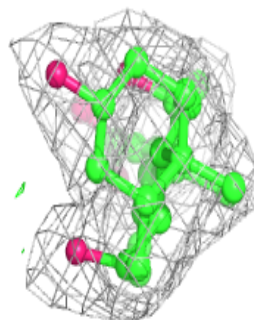
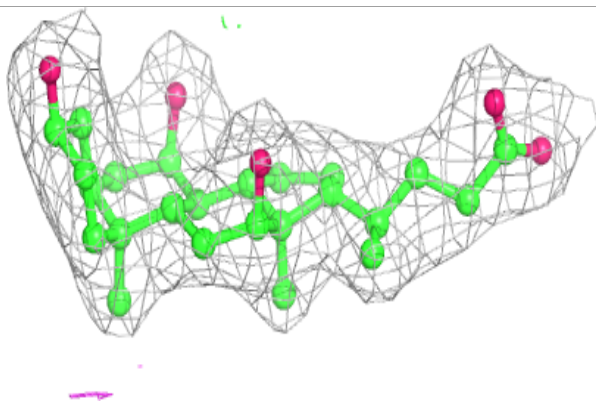
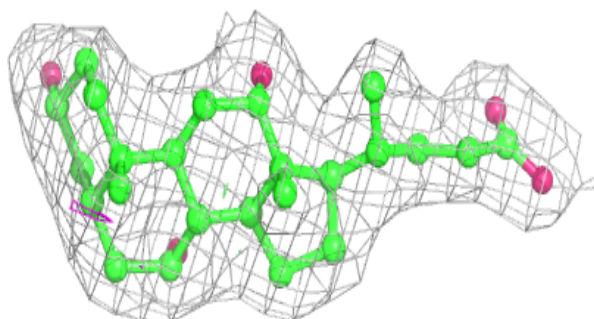
**Electron density around CHD C 301:**

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

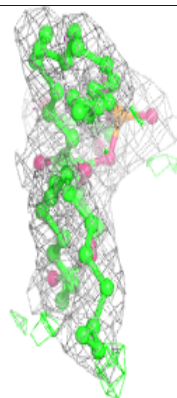
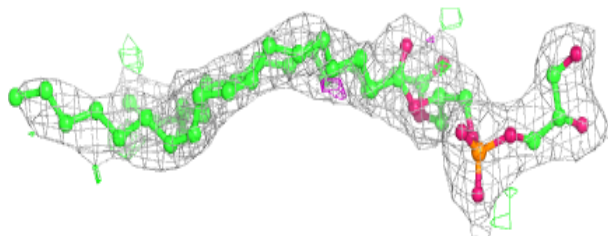
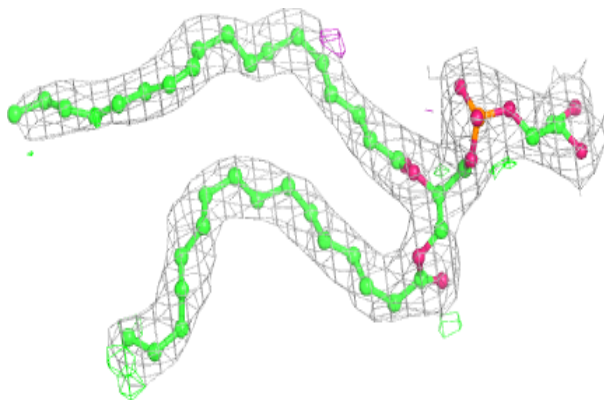


Electron density around CHD P 304:

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

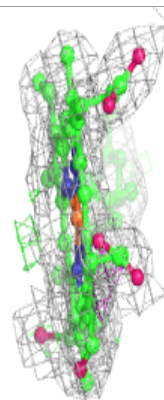
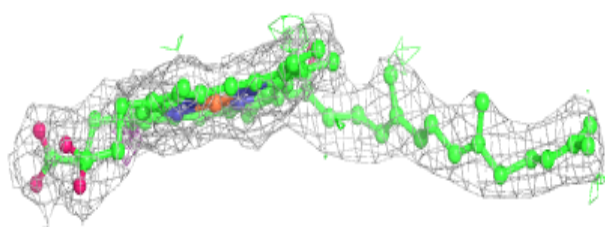
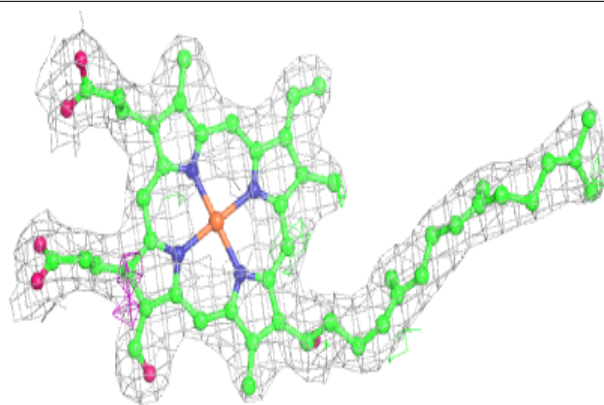
**Electron density around PGV P 302:**

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

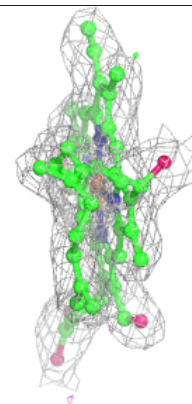
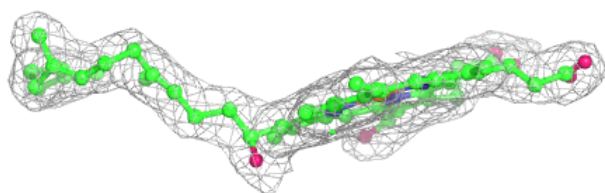
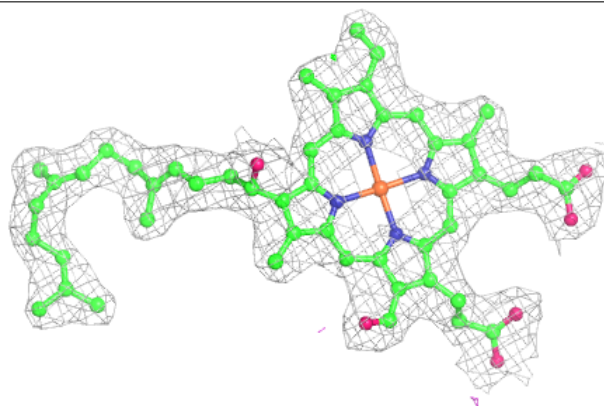


Electron density around HEA A 607:

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

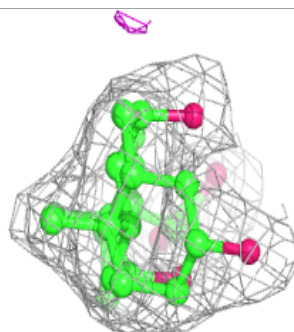
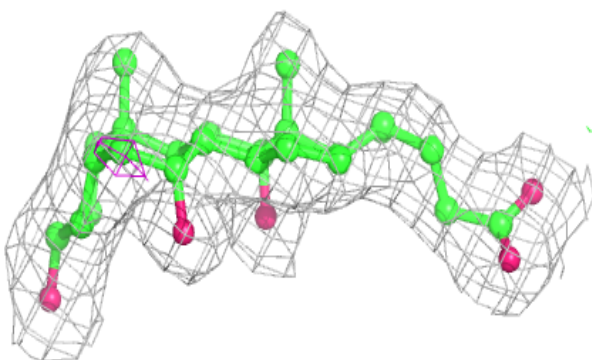
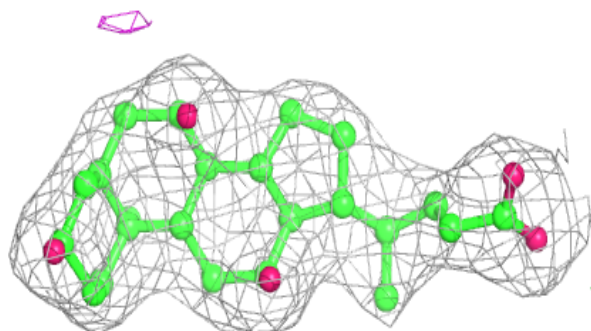
**Electron density around HEA N 605:**

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

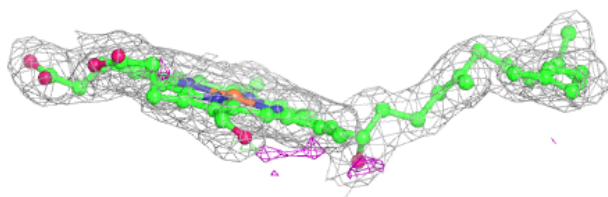
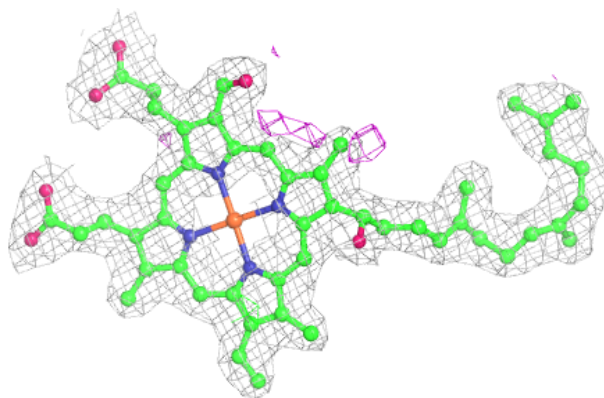


Electron density around CHD G 108:

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

**Electron density around HEA A 606:**

$2mF_o-DF_c$ (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.