



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 5, 2021 – 10:35 AM JST

PDB ID : 7EV7
Title : Bovine heart cytochrome c oxidase in the carbon monoxide-bound fully reduced state at a 50 K
Authors : Shimada, A.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2021-05-20
Resolution : 1.70 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 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 : 2.22
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) : 2.22

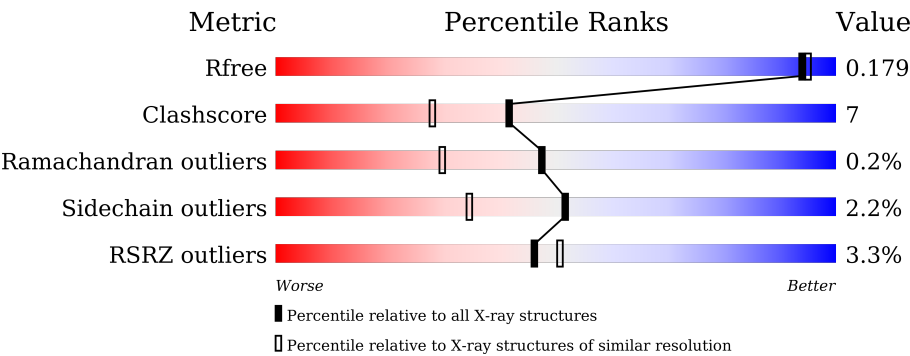
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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></div><div>87%12%.</div></div>
1	N	514	<div><div></div><div>87%13%</div></div>
2	B	227	<div><div>3%</div><div>80%18%.</div></div>
2	O	227	<div><div>2%</div><div>81%18%.</div></div>
3	C	261	<div><div></div><div>91%8%.</div></div>
3	P	261	<div><div>%</div><div>89%11%.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	A	602[A]	X	-	-	-
15	HEA	A	602[B]	X	-	-	-
15	HEA	A	602[C]	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	A	603	X	-	-	-
15	HEA	N	602[A]	X	-	-	-
15	HEA	N	602[B]	X	-	-	-
15	HEA	N	602[C]	X	-	-	-
15	HEA	N	603	X	-	-	-
18	NA	C	302	-	-	-	X
20	EDO	A	623	-	-	-	X
20	EDO	B	309	-	-	-	X
20	EDO	B	314	-	-	-	X
20	EDO	D	202	-	-	-	X
20	EDO	D	206	-	-	-	X
20	EDO	G	104	-	-	-	X
20	EDO	H	103	-	-	X	-
20	EDO	N	612	-	-	X	-
20	EDO	N	629	-	-	-	X
20	EDO	N	630	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34489 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	30	0
			4124	2750	635	698	41			
1	N	514	Total	C	N	O	S	0	28	0
			4116	2741	635	699	41			

- 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	11	0
			1869	1218	284	348	19			
2	O	227	Total	C	N	O	S	0	10	0
			1865	1216	284	346	19			

- 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	9	0
			2131	1422	337	357	15			
3	P	259	Total	C	N	O	S	0	11	0
			2141	1428	341	357	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	5	0
			1214	787	202	221	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1206	785	199	218	4			

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

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	94	Total	C	N	O	S	0	3	0
			723	447	129	142	5			
6	S	94	Total	C	N	O	S	0	3	0
			723	448	128	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			678	432	129	115	1	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	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	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

Continued on next page...

Continued from previous page...

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.

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			

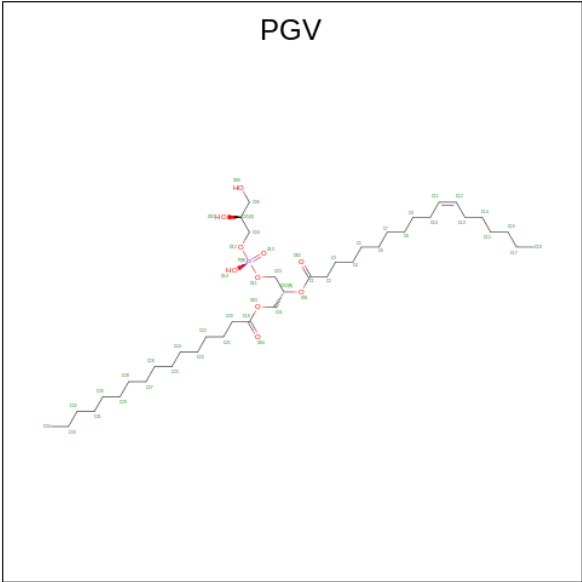
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			388	259	66	60	3			
12	Y	46	Total	C	N	O	S	0	4	0
			394	261	66	64	3			

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

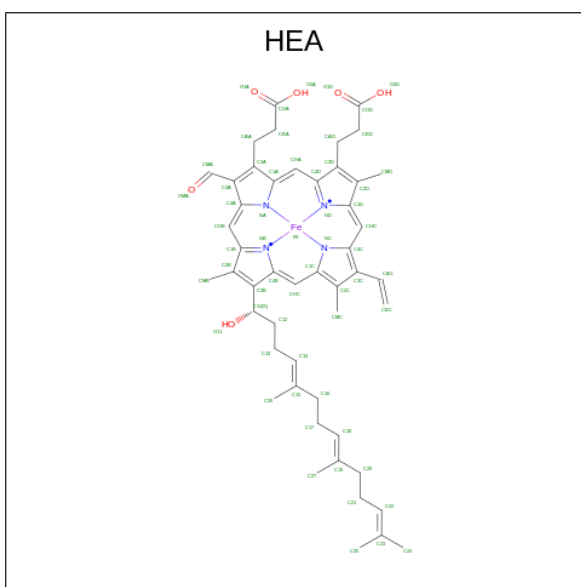
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is (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
14	A	1	Total	C	O	P	0	0
			51	40	10	1		
14	A	1	Total	C	O	P	0	0
			51	40	10	1		
14	C	1	Total	C	O	P	0	0
			51	40	10	1		
14	C	1	Total	C	O	P	0	0
			51	40	10	1		
14	N	1	Total	C	O	P	0	0
			51	40	10	1		
14	N	1	Total	C	O	P	0	0
			51	40	10	1		
14	P	1	Total	C	O	P	0	0
			51	40	10	1		
14	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 15 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	A	1	Total 79	C 67	Fe 1	N 4	O 7	0	1
15	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
15	N	1	Total 79	C 67	Fe 1	N 4	O 7	0	1
15	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 16 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

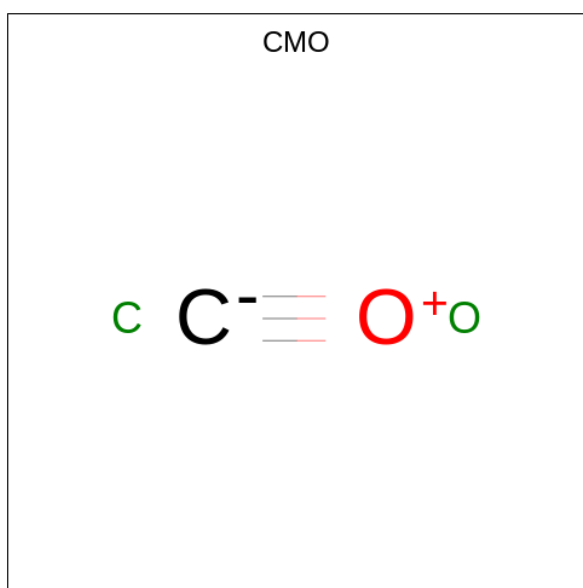
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	C	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		
18	P	1	Total	Na	0	0
			1	1		

- Molecule 19 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 20 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	H	1	Total	C	O	0	0
			4	2	2		
20	H	1	Total	C	O	0	0
			4	2	2		
20	H	1	Total	C	O	0	0
			4	2	2		
20	J	1	Total	C	O	0	0
			4	2	2		
20	J	1	Total	C	O	0	0
			4	2	2		
20	K	1	Total	C	O	0	0
			4	2	2		
20	K	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	L	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	M	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		
20	N	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

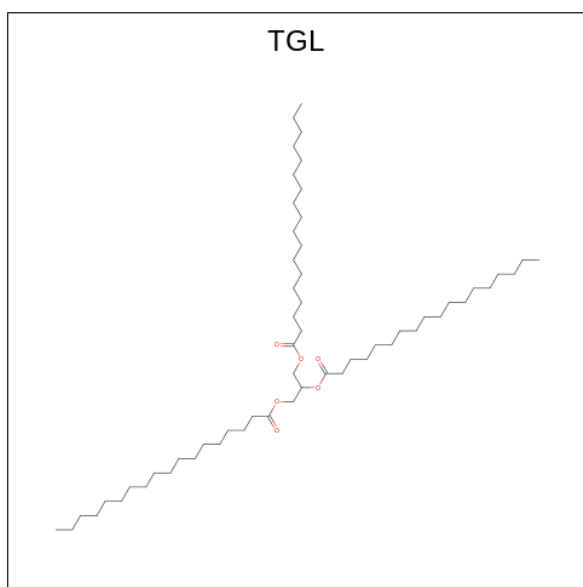
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4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

Continued on next page...

Continued from previous page...

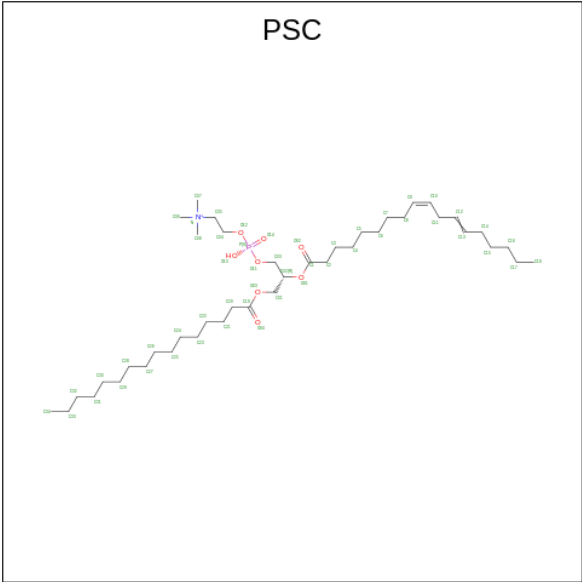
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	U	1	Total	C	O	0	0
			4	2	2		
20	V	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	W	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



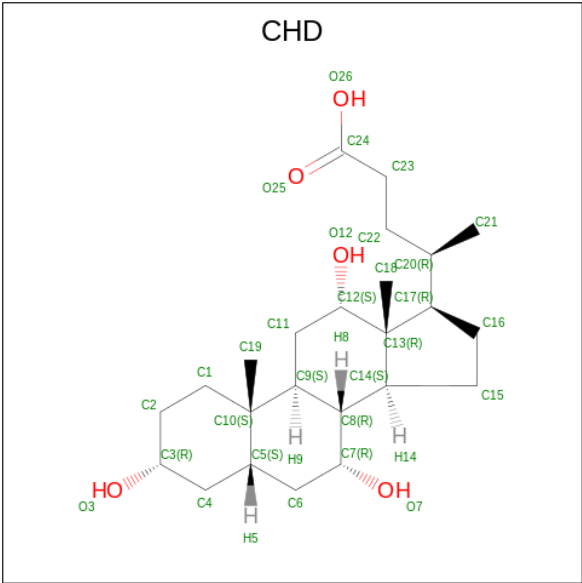
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



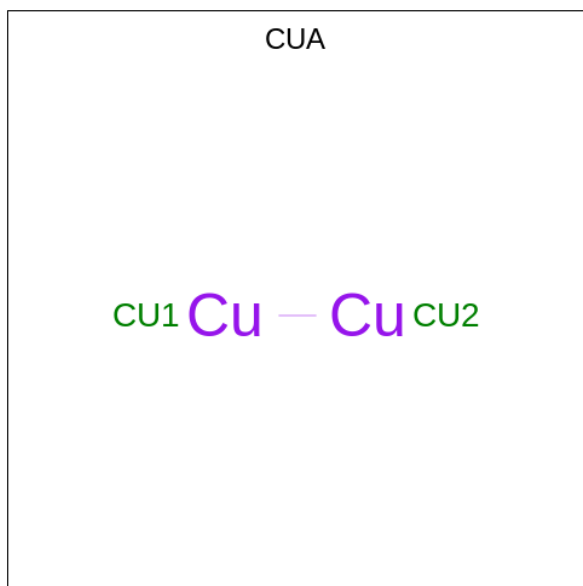
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

Continued on next page...

Continued from previous page...

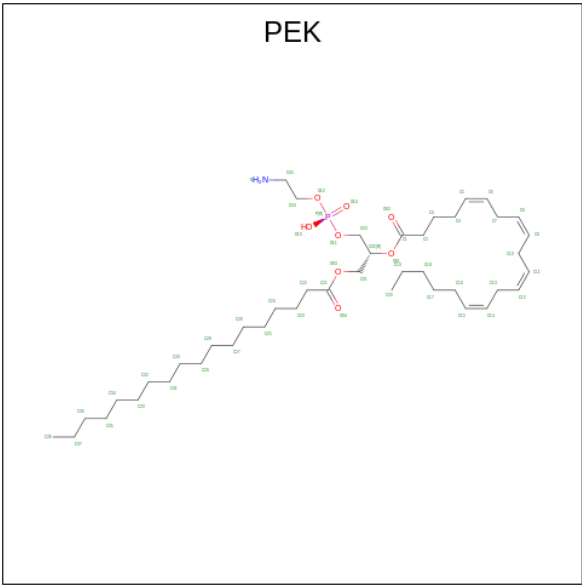
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	G	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0
23	Y	1	Total C O 29 24 5	0	0

- Molecule 24 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



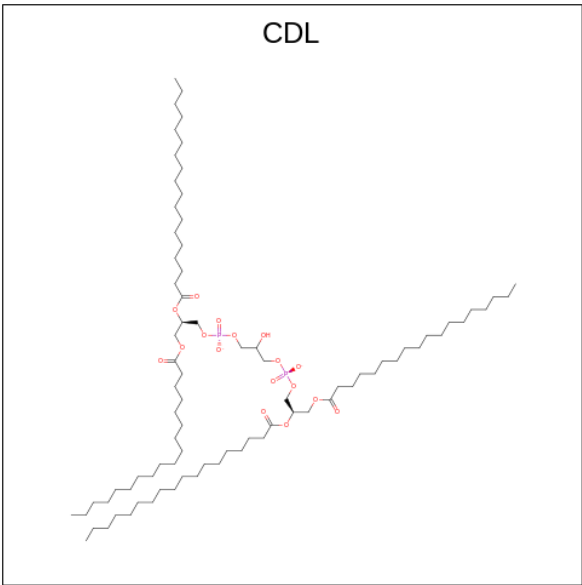
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

- Molecule 25 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).



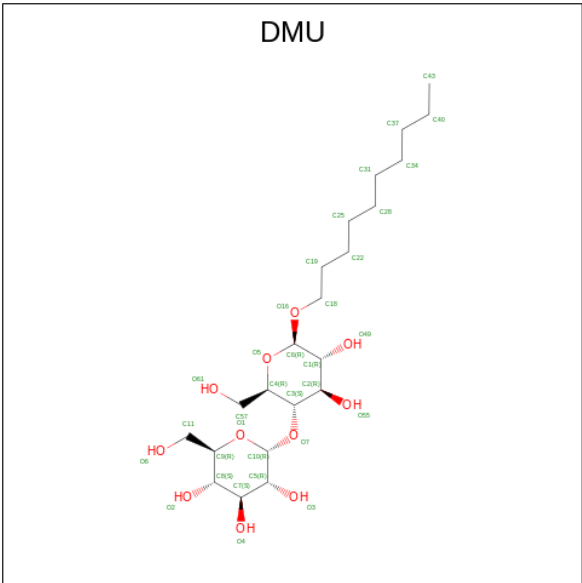
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 33 22 11	0	0
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	V	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

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

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

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	H	1	Total	O	P	0	0
			5	4	1		
29	U	1	Total	O	P	0	0
			5	4	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	255	Total	O	0	0
			255	255		
30	B	194	Total	O	0	2
			195	195		
30	C	142	Total	O	0	0
			142	142		
30	D	167	Total	O	0	0
			167	167		
30	E	120	Total	O	0	0
			120	120		
30	F	130	Total	O	0	0
			130	130		
30	G	67	Total	O	0	0
			67	67		
30	H	78	Total	O	0	0
			78	78		
30	I	53	Total	O	0	0
			53	53		
30	J	39	Total	O	0	0
			39	39		

Continued on next page...

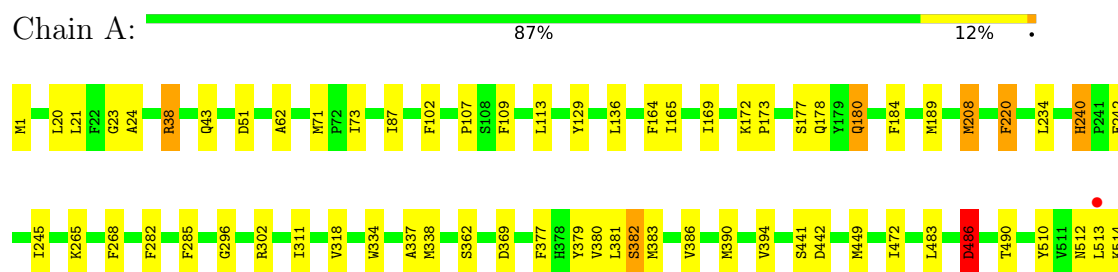
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	43	Total 43	O 43	0	0
30	L	38	Total 38	O 38	0	0
30	M	32	Total 32	O 32	0	0
30	N	240	Total 240	O 240	0	0
30	O	163	Total 164	O 164	0	1
30	P	138	Total 138	O 138	0	0
30	Q	85	Total 85	O 85	0	0
30	R	96	Total 96	O 96	0	0
30	S	129	Total 129	O 129	0	0
30	T	65	Total 65	O 65	0	0
30	U	72	Total 72	O 72	0	0
30	V	40	Total 40	O 40	0	0
30	W	45	Total 45	O 45	0	0
30	X	33	Total 33	O 33	0	0
30	Y	27	Total 27	O 27	0	0
30	Z	21	Total 21	O 21	0	0

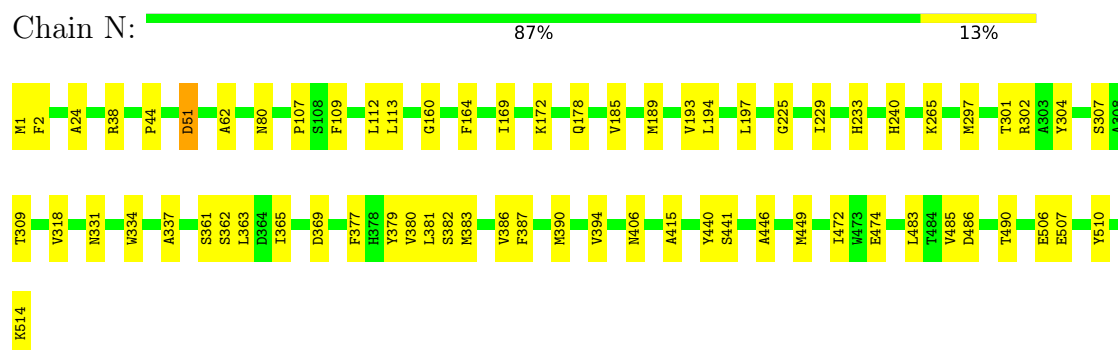
3 Residue-property plots

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.

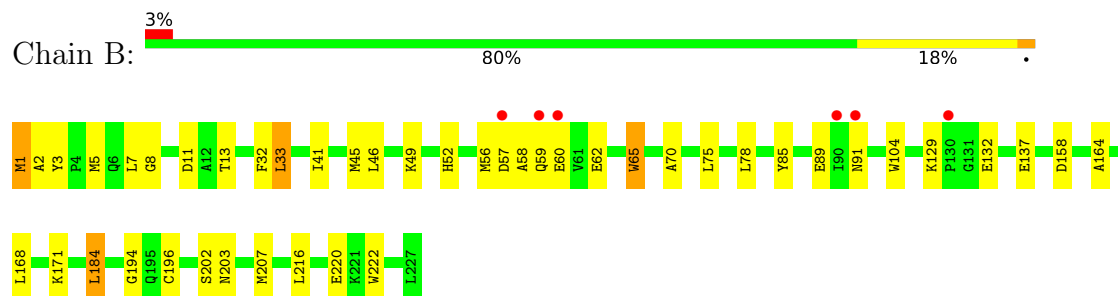
• Molecule 1: Cytochrome c oxidase subunit 1



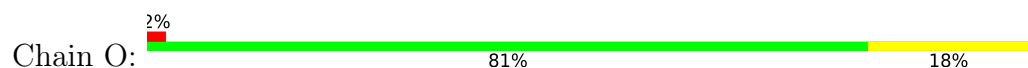
• Molecule 1: Cytochrome c oxidase subunit 1

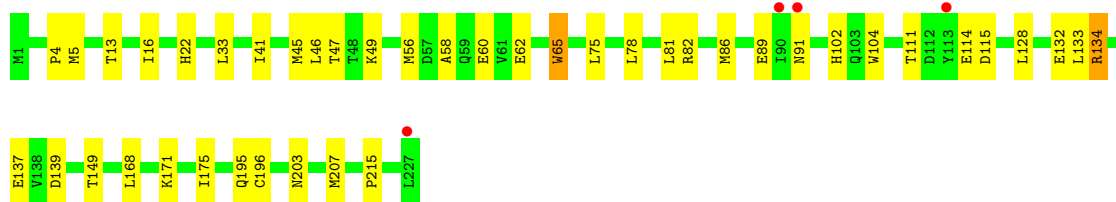


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 91% 8%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 11%



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 91% 6%



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 91% 6%



• Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 93% 2%

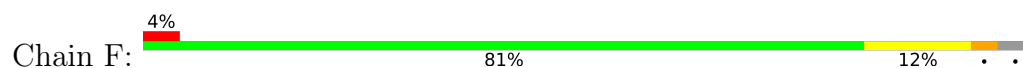


• Molecule 5: Cytochrome c oxidase subunit 5A

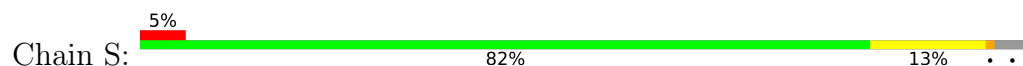
Chain R: 94% 2%



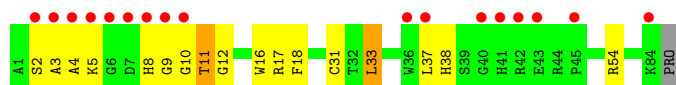
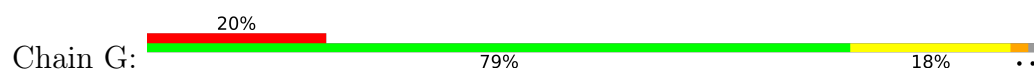
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



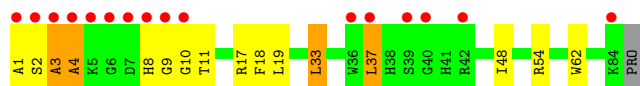
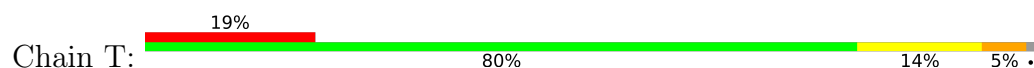
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



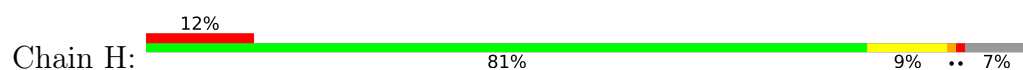
- Molecule 7: Cytochrome c oxidase subunit 6A2



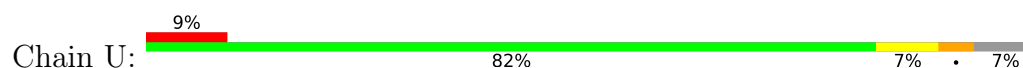
- Molecule 7: Cytochrome c oxidase subunit 6A2



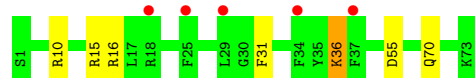
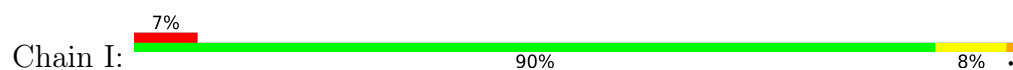
- Molecule 8: Cytochrome c oxidase subunit 6B1



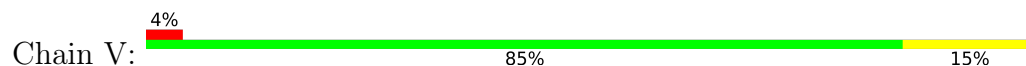
- Molecule 8: Cytochrome c oxidase subunit 6B1



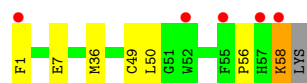
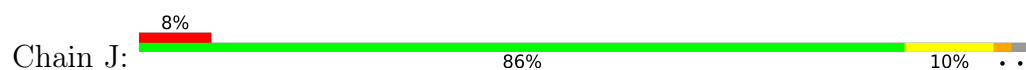
- Molecule 9: Cytochrome c oxidase subunit 6C



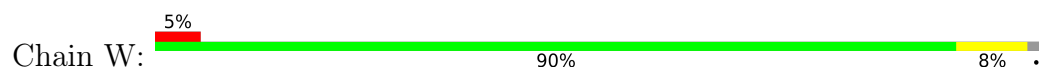
- Molecule 9: Cytochrome c oxidase subunit 6C



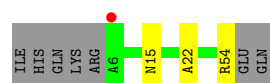
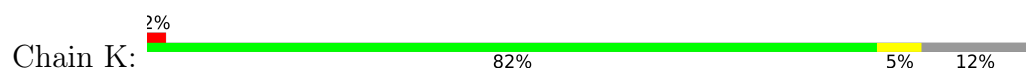
- Molecule 10: Cytochrome c oxidase subunit 7A1



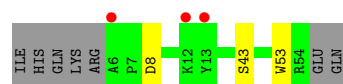
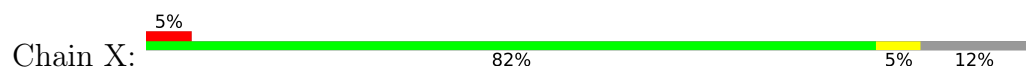
- Molecule 10: Cytochrome c oxidase subunit 7A1



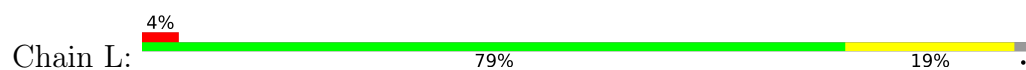
- Molecule 11: Cytochrome c oxidase subunit 7B



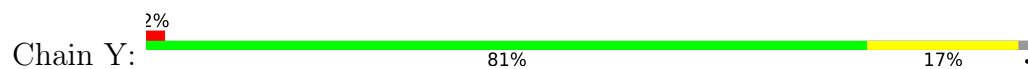
- Molecule 11: Cytochrome c oxidase subunit 7B



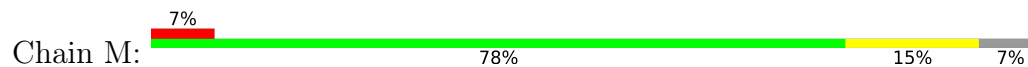
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



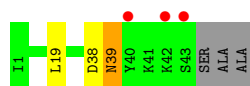
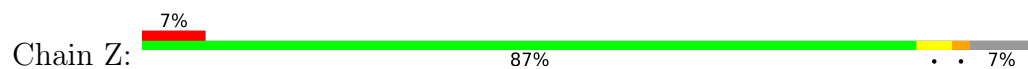
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.54Å 203.66Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 1.70 135.51 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.74-1.70) 99.6 (135.51-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.13-2998-000)	Depositor
R, R_{free}	0.159 , 0.178 0.159 , 0.179	Depositor DCC
R_{free} test set	35759 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34489	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: CMO, EDO, PGV, CUA, NA, PEK, ZN, PSC, CDL, FME, MG, CHD, DMU, SAC, CU, TPO, TGL, HEA, PO4

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	1.04	6/4390 (0.1%)	0.98	11/5989 (0.2%)
1	N	0.98	3/4371 (0.1%)	0.89	4/5964 (0.1%)
2	B	0.90	0/1961	0.94	6/2672 (0.2%)
2	O	0.81	2/1952 (0.1%)	0.87	4/2660 (0.2%)
3	C	0.94	1/2268 (0.0%)	0.82	0/3099
3	P	0.95	1/2289 (0.0%)	0.83	0/3126
4	D	0.83	0/1273	0.82	2/1716 (0.1%)
4	Q	0.60	0/1258	0.74	4/1696 (0.2%)
5	E	0.80	2/871 (0.2%)	0.76	1/1182 (0.1%)
5	R	0.63	0/871	0.66	0/1182
6	F	0.83	0/755	0.83	0/1026
6	S	0.77	1/755 (0.1%)	0.78	0/1025
7	G	0.81	0/690	0.70	0/937
7	T	0.72	0/698	0.74	0/948
8	H	0.87	0/682	0.80	0/921
8	U	0.74	0/682	0.72	0/921
9	I	0.68	0/605	0.72	1/802 (0.1%)
9	V	0.58	0/605	0.61	0/802
10	J	0.64	0/471	0.69	0/636
10	W	0.57	0/471	0.67	0/636
11	K	0.75	0/398	0.68	0/546
11	X	0.64	0/398	0.59	0/546
12	L	0.87	0/412	0.74	0/551
12	Y	0.80	0/430	0.65	0/575
13	M	0.80	0/345	0.72	0/470
13	Z	0.68	0/345	0.61	0/470
All	All	0.87	16/30246 (0.1%)	0.83	33/41098 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362[A]	SER	CB-OG	-7.75	1.32	1.42
1	A	362[B]	SER	CB-OG	-7.75	1.32	1.42
1	N	362[A]	SER	CB-OG	-6.02	1.34	1.42
1	N	362[B]	SER	CB-OG	-6.02	1.34	1.42
3	P	94	PHE	CE2-CZ	5.98	1.48	1.37
5	E	70	VAL	CB-CG2	5.65	1.64	1.52
1	A	102	PHE	CE2-CZ	5.60	1.48	1.37
1	A	184	PHE	CG-CD1	5.58	1.47	1.38
1	N	185	VAL	CB-CG2	5.40	1.64	1.52
1	A	184	PHE	CE2-CZ	5.32	1.47	1.37
1	A	220	PHE	CE1-CZ	5.31	1.47	1.37
3	C	102	TYR	CG-CD2	-5.29	1.32	1.39
6	S	73	TRP	CZ3-CH2	5.26	1.48	1.40
5	E	70	VAL	CB-CG1	-5.20	1.42	1.52
2	O	65[A]	TRP	CB-CG	-5.03	1.41	1.50
2	O	65[B]	TRP	CB-CG	-5.03	1.41	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-17.52	72.16	100.20
4	Q	20[A]	ARG	NE-CZ-NH2	-8.93	115.83	120.30
4	Q	20[B]	ARG	NE-CZ-NH2	-8.93	115.83	120.30
4	Q	20[A]	ARG	NE-CZ-NH1	8.19	124.40	120.30
4	Q	20[B]	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	A	38	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	208[A]	MET	CG-SD-CE	6.40	110.44	100.20
1	A	208[B]	MET	CG-SD-CE	6.40	110.44	100.20
2	O	65[A]	TRP	CA-CB-CG	6.26	125.59	113.70
2	O	65[B]	TRP	CA-CB-CG	6.26	125.59	113.70
9	I	55	ASP	CB-CG-OD1	6.04	123.73	118.30
2	O	139	ASP	CB-CG-OD1	5.97	123.67	118.30
1	N	486[A]	ASP	CB-CG-OD1	5.96	123.67	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	486[B]	ASP	CB-CG-OD1	5.96	123.67	118.30
2	B	45	MET	CG-SD-CE	5.76	109.42	100.20
1	A	302[A]	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-5.72	117.44	120.30
2	B	158	ASP	CB-CG-OD1	5.70	123.43	118.30
2	O	134	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	B	11	ASP	CB-CG-OD1	5.51	123.25	118.30
1	A	129	TYR	CB-CG-CD2	-5.43	117.75	121.00
1	N	51[A]	ASP	CB-CG-OD2	5.41	123.17	118.30
1	N	51[C]	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	38	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	486[A]	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	486[B]	ASP	CB-CG-OD2	5.32	123.09	118.30
2	B	65[A]	TRP	CA-CB-CG	5.28	123.72	113.70
2	B	65[B]	TRP	CA-CB-CG	5.28	123.72	113.70
1	A	442	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	B	184	LEU	CA-CB-CG	5.09	127.01	115.30
5	E	90	ARG	NE-CZ-NH2	-5.04	117.78	120.30
4	D	20[A]	ARG	NE-CZ-NH1	5.01	122.81	120.30
4	D	20[B]	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain

5.2 Too-close contacts

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	4124	0	4092	56	0
1	N	4116	0	4070	60	0
2	B	1869	0	1872	37	0
2	O	1865	0	1874	36	0
3	C	2131	0	2039	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2141	0	2056	38	0
4	D	1214	0	1205	15	0
4	Q	1206	0	1196	13	0
5	E	852	0	845	2	0
5	R	852	0	845	1	0
6	F	723	0	702	9	0
6	S	723	0	705	12	0
7	G	675	0	644	18	0
7	T	678	0	644	14	0
8	H	662	0	623	6	0
8	U	662	0	623	7	0
9	I	601	0	613	7	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	3	0
11	K	384	0	366	3	0
11	X	384	0	366	3	0
12	L	388	0	389	12	0
12	Y	394	0	385	8	0
13	M	335	0	352	9	0
13	Z	335	0	352	2	0
14	A	102	0	152	3	0
14	C	102	0	152	4	0
14	N	102	0	152	4	0
14	P	102	0	152	7	0
15	A	139	0	112	6	0
15	N	139	0	112	6	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	C	1	0	0	0	0
18	N	1	0	0	0	0
18	P	1	0	0	1	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	76	0	114	9	0
20	B	40	0	60	10	2
20	C	28	0	42	3	0
20	D	24	0	33	3	2
20	E	12	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	F	24	0	36	1	0
20	G	20	0	30	4	0
20	H	12	0	18	5	0
20	J	8	0	12	2	0
20	K	8	0	12	2	0
20	L	16	0	24	0	0
20	M	16	0	24	3	0
20	N	84	0	126	13	0
20	O	20	0	30	2	0
20	P	44	0	66	5	0
20	Q	8	0	12	0	0
20	R	20	0	30	1	0
20	S	44	0	66	2	0
20	T	8	0	12	0	0
20	U	4	0	6	1	0
20	V	4	0	6	0	0
20	W	12	0	18	2	0
20	Y	8	0	12	0	0
21	B	63	0	110	4	0
21	D	63	0	110	9	0
21	L	63	0	110	11	0
21	N	63	0	110	2	0
21	Q	63	0	110	7	0
21	Y	63	0	110	11	0
22	B	52	0	80	10	0
22	O	52	0	80	5	0
23	B	29	0	39	0	0
23	C	87	0	117	3	0
23	G	29	0	39	1	0
23	J	29	0	39	3	0
23	P	87	0	117	9	0
23	W	29	0	39	3	0
23	Y	29	0	39	4	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	159	0	231	8	0
25	P	159	0	231	15	0
26	C	100	0	156	13	0
26	G	100	0	156	18	0
26	P	100	0	156	20	0
26	T	100	0	156	11	0
27	C	66	0	84	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	G	33	0	42	1	0
27	M	66	0	84	0	0
27	P	99	0	124	6	0
27	V	33	0	42	4	0
27	Z	66	0	84	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	255	0	0	6	0
30	B	195	0	0	3	2
30	C	142	0	0	1	0
30	D	167	0	0	1	2
30	E	120	0	0	1	0
30	F	130	0	0	2	0
30	G	67	0	0	0	0
30	H	78	0	0	1	0
30	I	53	0	0	1	0
30	J	39	0	0	1	0
30	K	43	0	0	0	0
30	L	38	0	0	1	0
30	M	32	0	0	0	0
30	N	240	0	0	3	0
30	O	164	0	0	3	0
30	P	138	0	0	4	0
30	Q	85	0	0	4	0
30	R	96	0	0	1	0
30	S	129	0	0	6	0
30	T	65	0	0	0	0
30	U	72	0	0	2	0
30	V	40	0	0	1	0
30	W	45	0	0	3	0
30	X	33	0	0	1	0
30	Y	27	0	0	1	0
30	Z	21	0	0	0	0
All	All	34489	0	32823	452	4

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 7.

All (452) 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)
8:H:24:ASN:HD21	20:H:103:EDO:H21	1.24	0.98
6:F:75:HIS:H	6:F:80[A]:GLN:HE22	1.12	0.97
1:N:178[B]:GLN:NE2	30:N:701:HOH:O	1.99	0.95
6:S:75:HIS:H	6:S:80[A]:GLN:HE22	1.14	0.93
25:P:305:PEK:H041	7:T:17:ARG:HH22	1.32	0.93
11:K:15:ASN:H	20:K:102:EDO:H12	1.34	0.91
7:T:3:ALA:HA	7:T:4:ALA:HB2	1.55	0.89
22:B:302:PSC:H071	9:I:10:ARG:HH21	1.39	0.87
12:L:24[B]:MET:SD	30:L:223:HOH:O	2.33	0.86
21:D:201:TGL:H342	9:I:16:ARG:HE	1.42	0.85
20:A:609:EDO:H22	30:A:790:HOH:O	1.77	0.84
12:Y:42:HIS:HB2	23:Y:104:CHD:H12	1.59	0.83
12:L:13:PHE:HA	21:L:101:TGL:HC21	1.61	0.83
12:L:20:ARG:HH22	21:L:101:TGL:HC61	1.42	0.81
20:A:627:EDO:H12	30:A:756:HOH:O	1.81	0.80
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.63	0.80
2:B:8:GLY:H	20:B:310:EDO:H21	1.46	0.78
26:P:308:CDL:H862	26:P:308:CDL:H822	1.65	0.77
20:A:619:EDO:H12	20:F:103:EDO:H11	1.67	0.76
3:P:161[A]:GLN:HE22	25:P:305:PEK:H22	1.52	0.75
3:P:63:ARG:HE	26:P:308:CDL:HA21	1.52	0.75
3:P:67:PHE:HE2	26:P:308:CDL:H1	1.52	0.74
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.28	0.74
25:C:305:PEK:H042	7:G:17:ARG:HH12	1.53	0.73
1:N:390:MET:O	1:N:394[B]:VAL:HG12	1.89	0.72
1:A:318:VAL:HG22	2:B:65[A]:TRP:CD1	2.25	0.72
4:D:19[B]:ARG:NH1	30:D:301:HOH:O	2.22	0.71
2:B:7:LEU:HD11	21:B:301:TGL:H152	1.72	0.71
7:G:5:LYS:NZ	20:G:103:EDO:O2	2.21	0.71
1:N:164:PHE:CE2	20:N:612:EDO:H22	2.26	0.70
3:C:213:THR:HG23	26:C:308:CDL:H771	1.72	0.70
6:F:3:GLY:O	30:F:201:HOH:O	2.09	0.69
12:L:20:ARG:NH2	21:L:101:TGL:HC61	2.08	0.68
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.34	0.68
2:O:89:GLU:O	2:O:91:ASN:ND2	2.26	0.68
9:V:8:GLN:NE2	30:V:202:HOH:O	2.26	0.68
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.76	0.68
21:N:608:TGL:HA81	21:N:608:TGL:H141	1.75	0.68
3:P:70:HIS:HE1	20:P:319:EDO:H11	1.59	0.68
1:N:318:VAL:HG22	2:O:65[A]:TRP:CD1	2.29	0.67
1:A:510:TYR:OH	1:A:512[B]:ASN:OD1	2.03	0.67
13:M:1:ILE:HG23	20:M:103:EDO:H22	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:233:HIS:HE2	20:N:623:EDO:H22	1.61	0.65
7:G:8:HIS:CD2	7:G:9:GLY:H	2.14	0.65
14:P:306:PGV:H161	26:P:308:CDL:H651	1.78	0.65
3:C:67:PHE:HE2	26:C:308:CDL:H1	1.60	0.65
5:R:90:ARG:NH2	30:R:302:HOH:O	2.29	0.65
4:D:40:LEU:HB2	20:D:205:EDO:H21	1.79	0.65
3:P:180[B]:GLU:OE2	30:P:401:HOH:O	2.15	0.65
1:A:381[B]:LEU:HB2	15:A:603:HEA:CAC	2.27	0.64
18:P:302:NA:NA	30:P:505:HOH:O	1.70	0.64
1:N:80:ASN:HD21	20:N:612:EDO:H12	1.62	0.64
20:P:314:EDO:O2	30:P:402:HOH:O	2.15	0.64
13:M:7:LYS:NZ	20:M:104:EDO:H11	2.12	0.64
3:P:165:ILE:HG12	25:P:305:PEK:H9	1.77	0.64
13:M:7:LYS:HZ1	20:M:104:EDO:H11	1.63	0.64
6:S:80[B]:GLN:NE2	30:S:204:HOH:O	2.32	0.63
1:A:285:PHE:HB2	7:T:3:ALA:HB2	1.79	0.63
26:G:101:CDL:H322	26:G:101:CDL:HA62	1.80	0.63
10:J:36:MET:HG2	23:J:101:CHD:H222	1.79	0.62
14:P:306:PGV:H131	26:P:308:CDL:H591	1.81	0.62
7:T:8:HIS:CD2	7:T:9:GLY:H	2.17	0.62
2:B:85:TYR:CE2	26:T:101:CDL:H111	2.34	0.62
25:C:305:PEK:H042	7:G:17:ARG:NH1	2.15	0.62
1:N:415:ALA:HB1	21:Q:201:TGL:H121	1.80	0.62
2:O:13:THR:HB	2:O:168:LEU:HD23	1.81	0.62
26:G:101:CDL:H561	26:G:101:CDL:H771	1.82	0.62
3:P:51[B]:MET:SD	26:P:308:CDL:H621	2.40	0.61
1:A:113[B]:LEU:HD12	21:L:101:TGL:H131	1.81	0.61
27:C:310:DMU:H11	10:J:49:CYS:HB3	1.80	0.61
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.82	0.61
3:C:39:SER:OG	27:C:319:DMU:H30	2.00	0.61
3:P:213:THR:HG23	26:P:308:CDL:H761	1.82	0.61
12:Y:42:HIS:HB2	23:Y:104:CHD:H212	1.82	0.61
7:T:48:ILE:HG12	20:U:101:EDO:H12	1.81	0.61
26:C:308:CDL:H192	26:C:308:CDL:H622	1.83	0.61
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.82	0.60
1:N:474:GLU:OE2	20:N:619:EDO:H22	2.00	0.60
4:Q:20[A]:ARG:HG2	30:Q:362:HOH:O	2.01	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.46	0.60
1:N:507:GLU:H	20:N:618:EDO:H12	1.66	0.60
20:A:624:EDO:H22	21:L:101:TGL:HC51	1.84	0.60
3:C:91:VAL:O	3:C:95[B]:THR:HG23	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:27:VAL:HG21	27:V:102:DMU:H7	1.83	0.60
6:S:94:HIS:O	30:S:201:HOH:O	2.16	0.60
4:D:78:TRP:CA	21:D:201:TGL:HB22	2.31	0.59
1:N:51[C]:ASP:OD2	1:N:441:SER:OG	2.19	0.59
1:N:446:ALA:H	20:N:630:EDO:H21	1.67	0.59
2:O:56:MET:HB3	22:O:301:PSC:H231	1.85	0.59
23:J:101:CHD:H221	20:J:102:EDO:H22	1.84	0.59
2:B:222:TRP:HE1	20:B:312:EDO:C2	2.16	0.58
1:A:311[A]:ILE:HD13	26:T:101:CDL:H441	1.85	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.84	0.58
30:Q:312:HOH:O	20:R:203:EDO:H21	2.04	0.58
26:G:101:CDL:H141	26:G:101:CDL:H381	1.86	0.58
14:P:307:PGV:H032	30:P:499:HOH:O	2.03	0.58
7:G:12:GLY:HA3	20:G:107:EDO:H11	1.86	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.85	0.57
3:P:37:PHE:CE2	27:P:309:DMU:H12	2.38	0.57
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.86	0.57
3:C:210:ILE:HD13	14:C:306:PGV:H302	1.85	0.57
8:H:8:ILE:HG22	8:H:9:LYS:HD2	1.86	0.57
10:J:58:LYS:H	10:J:58:LYS:HD2	1.70	0.57
25:C:305:PEK:N	30:C:402:HOH:O	2.15	0.57
1:N:472:ILE:HG21	21:Y:101:TGL:H201	1.87	0.57
20:N:612:EDO:H11	30:N:922:HOH:O	2.05	0.57
11:K:15:ASN:N	20:K:102:EDO:H12	2.13	0.56
1:A:169:ILE:HD12	7:T:8:HIS:HB3	1.86	0.56
20:N:630:EDO:H11	2:O:133:LEU:HD22	1.87	0.56
3:P:210:ILE:HD13	14:P:306:PGV:H302	1.88	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.56
3:P:161[A]:GLN:NE2	25:P:305:PEK:H5	2.20	0.56
1:N:381[B]:LEU:HB2	15:N:603:HEA:CAC	2.36	0.56
2:B:203:ASN:ND2	30:B:405[A]:HOH:O	2.37	0.56
14:N:601:PGV:H301	13:Z:19:LEU:HD23	1.88	0.56
20:O:306:EDO:H21	8:U:24:ASN:HD21	1.70	0.56
12:Y:23:ALA:HB2	27:Z:102:DMU:H15	1.88	0.56
2:B:13:THR:HB	2:B:168:LEU:HD23	1.88	0.56
1:N:318:VAL:HG22	2:O:65[A]:TRP:HD1	1.68	0.56
3:C:224:LYS:CD	26:C:308:CDL:HB31	2.37	0.55
3:C:258:TRP:CD1	23:C:311:CHD:H161	2.41	0.55
20:A:614:EDO:H22	13:M:2:THR:HG23	1.89	0.55
12:Y:20:ARG:HH22	21:Y:101:TGL:HC62	1.72	0.55
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24[B]:MET:HG2	21:L:101:TGL:HA22	1.89	0.55
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.87	0.55
1:A:510:TYR:HE1	1:A:512[B]:ASN:ND2	2.06	0.54
25:C:303:PEK:H381	7:T:19:LEU:HD21	1.88	0.54
1:N:382[B]:SER:O	1:N:386:VAL:HB	2.08	0.54
15:N:603:HEA:HMC1	15:N:603:HEA:HBC1	1.89	0.54
26:T:101:CDL:H531	26:T:101:CDL:H262	1.89	0.54
1:A:24:ALA:HB2	15:A:602[A]:HEA:H253	1.89	0.54
4:Q:19[B]:ARG:HD3	4:Q:21:ASP:OD1	2.07	0.54
3:P:67:PHE:CE2	26:P:308:CDL:H1	2.39	0.54
25:P:305:PEK:H041	7:T:17:ARG:NH2	2.13	0.54
3:C:40[A]:MET:SD	27:G:108:DMU:O49	2.66	0.53
12:Y:24[A]:MET:SD	21:Y:101:TGL:H172	2.47	0.53
1:N:112:LEU:HG	30:N:916:HOH:O	2.06	0.53
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.07	0.53
1:A:486[A]:ASP:OD1	4:D:19[A]:ARG:HD2	2.09	0.53
30:F:214:HOH:O	20:J:103:EDO:H11	2.08	0.53
3:P:261:SER:OXT	23:P:310:CHD:H21	2.08	0.53
20:P:315:EDO:H11	20:W:104:EDO:H22	1.90	0.53
7:T:33:LEU:HD13	7:T:37:LEU:HD22	1.91	0.53
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.91	0.53
7:G:33:LEU:HB3	20:G:104:EDO:H22	1.91	0.53
2:O:62:GLU:HG2	2:O:65[A]:TRP:CE2	2.43	0.53
3:P:156:ARG:HE	23:P:311:CHD:C24	2.21	0.53
27:P:324:DMU:H1	7:T:62:TRP:HB2	1.91	0.53
3:P:259:TRP:O	23:P:310:CHD:O12	2.27	0.53
1:A:379:TYR:O	1:A:383[B]:MET:HB2	2.09	0.52
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.91	0.52
1:A:165:ILE:HG23	1:A:189[B]:MET:HE1	1.92	0.52
1:A:318:VAL:HG22	2:B:65[A]:TRP:HD1	1.71	0.52
4:D:78:TRP:CB	21:D:201:TGL:HB22	2.40	0.52
12:L:2[A]:HIS:CG	12:L:3:TYR:H	2.28	0.52
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.92	0.52
20:P:320:EDO:H12	6:S:52:ILE:HD11	1.92	0.51
30:A:763:HOH:O	20:H:103:EDO:H11	2.09	0.51
26:G:101:CDL:HB32	1:N:304:TYR:HD1	1.75	0.51
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.08	0.51
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.46	0.51
8:H:24:ASN:ND2	20:H:103:EDO:H21	2.09	0.51
12:Y:20:ARG:HH12	21:Y:101:TGL:HC42	1.76	0.51
20:C:316:EDO:O2	20:H:102:EDO:H22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:101:CDL:H381	2:O:81:LEU:HD12	1.93	0.51
4:Q:81:VAL:HG11	21:Q:201:TGL:HB62	1.91	0.51
3:P:258:TRP:CD1	23:P:310:CHD:H161	2.45	0.51
1:N:406:ASN:HD21	14:N:601:PGV:H22	1.76	0.51
14:N:609:PGV:H343	25:P:304:PEK:H381	1.93	0.51
3:P:51[A]:MET:SD	26:P:308:CDL:H612	2.50	0.51
8:U:8:ILE:HG22	8:U:9:LYS:HD2	1.93	0.51
25:C:305:PEK:H383	26:G:101:CDL:C27	2.42	0.51
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.92	0.50
3:C:51[A]:MET:SD	26:C:308:CDL:H611	2.51	0.50
10:W:36:MET:HG2	23:W:101:CHD:H222	1.93	0.50
1:N:113:LEU:HB2	21:Y:101:TGL:H301	1.92	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.93	0.50
4:Q:10:ASP:HB2	30:Q:302:HOH:O	2.10	0.50
10:W:54:SER:O	12:Y:46:LYS:HD3	2.10	0.50
1:A:382[B]:SER:O	1:A:386:VAL:HB	2.11	0.50
30:A:734:HOH:O	12:L:7:PRO:HG3	2.11	0.50
3:C:73:PRO:O	20:C:317:EDO:H12	2.12	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.93	0.50
25:C:303:PEK:H282	25:C:303:PEK:H322	1.93	0.50
2:O:82:ARG:NH2	30:O:404:HOH:O	2.44	0.50
3:C:106:LEU:HD13	14:C:307:PGV:H21	1.94	0.50
5:E:46:LYS:NZ	30:E:303:HOH:O	2.44	0.50
7:G:31:CYS:SG	26:G:101:CDL:H532	2.52	0.49
6:S:19:GLU:HG2	30:S:297:HOH:O	2.12	0.49
21:L:101:TGL:H231	21:L:101:TGL:HA92	1.94	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.49
2:B:49:LYS:HD2	4:D:20[B]:ARG:HH12	1.77	0.49
1:N:507:GLU:H	20:N:618:EDO:C1	2.24	0.49
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.94	0.49
7:G:4:ALA:HB1	1:N:194:LEU:HD12	1.95	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.49
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.47	0.49
15:A:603:HEA:HBC1	15:A:603:HEA:HMC1	1.94	0.49
8:U:37:HIS:HD2	30:U:201:HOH:O	1.96	0.49
12:L:26:THR:HG23	13:M:25:SER:CB	2.43	0.49
1:N:112:LEU:HD23	1:N:112:LEU:C	2.33	0.49
2:B:58:ALA:H	20:B:311:EDO:H21	1.78	0.49
20:B:309:EDO:H12	30:B:566:HOH:O	2.11	0.49
7:G:4:ALA:CB	1:N:194:LEU:HD12	2.43	0.49
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:224:LYS:HE3	26:P:308:CDL:H131	1.95	0.48
3:P:224:LYS:CD	26:P:308:CDL:HB31	2.42	0.48
25:P:304:PEK:H101	25:P:304:PEK:H42	1.95	0.48
2:O:82:ARG:HD2	30:O:401:HOH:O	2.13	0.48
4:D:20[B]:ARG:NE	5:E:73:ASP:OD2	2.42	0.48
26:G:101:CDL:H172	1:N:307:SER:CB	2.44	0.48
4:D:19[B]:ARG:HH21	4:D:21:ASP:CG	2.17	0.48
6:S:10:GLU:OE1	6:S:25:ARG:NH2	2.43	0.48
21:B:301:TGL:HC31	20:B:310:EDO:H12	1.96	0.48
3:C:131:LEU:HD21	26:G:101:CDL:HB61	1.96	0.48
7:G:4:ALA:HB2	1:N:197:LEU:HD12	1.96	0.48
3:C:224:LYS:HD3	26:C:308:CDL:HB31	1.94	0.48
7:G:38:HIS:CE1	26:G:101:CDL:H122	2.49	0.48
7:G:11:TPO:O2P	7:G:16:TRP:NE1	2.34	0.47
20:S:107:EDO:H11	30:S:278:HOH:O	2.14	0.47
2:B:52:HIS:HE1	22:B:302:PSC:H012	1.79	0.47
26:G:101:CDL:H181	20:G:104:EDO:O1	2.13	0.47
7:G:8:HIS:HD2	7:G:9:GLY:H	1.58	0.47
23:J:101:CHD:H193	23:J:101:CHD:H111	1.58	0.47
2:B:3:TYR:OH	20:B:310:EDO:H22	2.13	0.47
2:O:41:ILE:HD13	22:O:301:PSC:C34	2.44	0.47
2:O:22[A]:HIS:CE1	9:V:44:LYS:HG3	2.49	0.47
25:P:305:PEK:H203	25:P:305:PEK:H162	1.96	0.47
14:A:601:PGV:H311	13:M:19:LEU:HD23	1.97	0.47
1:A:43:GLN:HG3	20:A:623:EDO:H11	1.96	0.47
1:A:472:ILE:HG21	21:L:101:TGL:HA91	1.96	0.47
2:B:33[A]:LEU:HD13	9:I:31:PHE:CD2	2.50	0.47
3:C:37:PHE:CD2	27:C:310:DMU:H13	2.50	0.47
2:O:49:LYS:HD3	21:Q:201:TGL:HC71	1.96	0.47
2:O:82:ARG:NH1	30:O:401:HOH:O	2.25	0.47
3:P:161[A]:GLN:HE21	25:P:305:PEK:H5	1.77	0.47
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.55	0.47
1:A:51[C]:ASP:HB2	2:B:202:SER:O	2.15	0.47
30:B:552:HOH:O	21:D:201:TGL:HC61	2.15	0.47
3:P:259:TRP:HD1	23:P:310:CHD:H213	1.80	0.47
4:Q:78:TRP:N	21:Q:201:TGL:HB22	2.30	0.47
21:Y:101:TGL:HC71	21:Y:101:TGL:HC22	1.97	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
2:B:129:LYS:HG3	20:B:309:EDO:H21	1.97	0.46
1:N:297[B]:MET:HE3	1:N:301:THR:HG21	1.97	0.46
9:V:2:THR:OG1	9:V:3:ALA:N	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:24:ALA:HA	27:V:102:DMU:H8	1.97	0.46
27:P:324:DMU:H32	27:P:324:DMU:H3	1.67	0.46
6:S:94:HIS:HD2	30:S:314:HOH:O	1.99	0.46
8:H:37:HIS:HD2	8:H:40:GLU:OE2	1.99	0.46
23:P:310:CHD:H182	23:P:310:CHD:H8	1.60	0.46
1:A:510:TYR:CE1	1:A:512[B]:ASN:ND2	2.83	0.46
1:N:24:ALA:HB2	15:N:602[A]:HEA:H253	1.96	0.46
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.97	0.46
1:A:390:MET:O	1:A:394[A]:VAL:HG22	2.15	0.46
4:D:121:LYS:NZ	20:D:207:EDO:O2	2.49	0.46
2:O:58:ALA:O	2:O:62:GLU:HG3	2.16	0.46
10:J:56:PRO:HD3	12:L:46:LYS:HD2	1.97	0.46
1:N:510:TYR:HD2	20:S:107:EDO:H21	1.80	0.46
2:O:16:ILE:HD11	2:O:86:MET:HG2	1.97	0.46
3:P:67:PHE:HE2	26:P:308:CDL:C1	2.23	0.46
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.16	0.46
20:A:620:EDO:H11	12:L:10:ASN:HD22	1.80	0.46
26:T:101:CDL:H511	26:T:101:CDL:H231	1.98	0.46
2:B:56:MET:HA	22:B:302:PSC:H212	1.97	0.46
7:G:38:HIS:NE2	26:G:101:CDL:O1	2.35	0.46
3:P:160:LEU:HD13	23:P:311:CHD:H181	1.98	0.46
1:A:510:TYR:CZ	1:A:512[B]:ASN:OD1	2.69	0.46
14:A:601:PGV:H312	13:M:16:ALA:HA	1.97	0.46
1:A:164:PHE:CE2	20:A:609:EDO:H21	2.51	0.45
20:W:104:EDO:H21	30:W:216:HOH:O	2.16	0.45
22:O:301:PSC:H21	22:O:301:PSC:H02	1.86	0.45
4:Q:19[B]:ARG:HG2	4:Q:22:TYR:HB3	1.98	0.45
1:A:20:LEU:HB3	21:L:101:TGL:H221	1.98	0.45
21:B:301:TGL:H242	21:B:301:TGL:HA91	1.98	0.45
23:C:311:CHD:H111	23:C:311:CHD:H193	1.79	0.45
12:L:26:THR:HG23	13:M:25:SER:HB3	1.99	0.45
26:G:101:CDL:H651	26:G:101:CDL:H622	1.77	0.45
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.17	0.45
10:W:7:GLU:HG3	30:W:231:HOH:O	2.16	0.45
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.69	0.45
2:B:52:HIS:CE1	22:B:302:PSC:H012	2.51	0.45
1:A:381[B]:LEU:HB2	15:A:603:HEA:HAC	1.98	0.45
23:C:309:CHD:O25	10:J:1:PHE:N	2.43	0.45
1:N:160:GLY:CA	20:N:612:EDO:H21	2.47	0.45
6:F:51:SER:O	6:F:94:HIS:N	2.48	0.45
26:G:101:CDL:H422	26:G:101:CDL:H451	1.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:80:ASN:ND2	20:N:612:EDO:H12	2.30	0.45
20:N:630:EDO:H11	2:O:133:LEU:CD2	2.47	0.45
3:P:226:HIS:CE1	26:P:308:CDL:HB32	2.52	0.45
1:A:311[A]:ILE:CD1	26:T:101:CDL:H441	2.47	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.98	0.45
25:P:304:PEK:H42	25:P:304:PEK:H72	1.58	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.44
21:D:201:TGL:H241	21:D:201:TGL:HA92	2.00	0.44
7:G:4:ALA:HB1	1:N:193:VAL:HG12	2.00	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.44
1:A:51[A]:ASP:OD2	1:A:441:SER:OG	2.27	0.44
2:B:89:GLU:O	2:B:91:ASN:ND2	2.50	0.44
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.48	0.44
3:P:131:LEU:HD21	26:T:101:CDL:HB61	1.99	0.44
1:A:136[B]:LEU:HD11	30:A:945:HOH:O	2.16	0.44
7:T:1:ALA:HA	7:T:2:SER:HA	1.75	0.44
26:T:101:CDL:H771	26:T:101:CDL:H561	2.00	0.44
1:A:164:PHE:HE2	20:A:609:EDO:H21	1.82	0.44
4:D:78:TRP:HA	21:D:201:TGL:HB22	1.98	0.44
8:U:9:LYS:HB3	8:U:10:ASN:H	1.62	0.44
14:C:307:PGV:H272	14:C:307:PGV:H241	1.71	0.44
3:P:37:PHE:CD2	27:P:309:DMU:H12	2.53	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.52	0.44
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	1.99	0.44
3:C:244:PHE:HA	25:C:303:PEK:H101	1.98	0.44
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.99	0.44
1:A:334:TRP:CZ3	21:D:201:TGL:HA62	2.52	0.44
2:B:56:MET:HB3	22:B:302:PSC:H252	1.99	0.44
26:G:101:CDL:HB32	1:N:304:TYR:CD1	2.52	0.44
1:N:2:PHE:HZ	21:Y:101:TGL:HG32	1.82	0.44
6:F:53:THR:HG23	6:F:55:LYS:H	1.83	0.44
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.17	0.44
8:U:40:GLU:OE2	30:U:201:HOH:O	2.21	0.44
3:C:63:ARG:HH21	26:C:308:CDL:HA21	1.82	0.44
14:C:306:PGV:H172	26:C:308:CDL:H652	2.00	0.44
14:N:601:PGV:H042	14:N:601:PGV:H031	2.00	0.44
2:O:65[B]:TRP:HE1	22:O:301:PSC:H12	1.83	0.44
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.53	0.43
12:L:24[A]:MET:SD	21:L:101:TGL:H162	2.57	0.43
3:P:70:HIS:CE1	20:P:319:EDO:H11	2.46	0.43
1:A:208[B]:MET:HE1	1:A:234:LEU:CD1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.00	0.43
25:P:305:PEK:H042	6:S:1:ALA:HA	2.00	0.43
26:T:101:CDL:H651	26:T:101:CDL:H622	1.77	0.43
26:G:101:CDL:H511	26:G:101:CDL:H202	2.00	0.43
9:I:36:LYS:NZ	9:I:36:LYS:HB3	2.33	0.43
2:O:62:GLU:HG2	2:O:65[A]:TRP:CZ2	2.54	0.43
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.53	0.43
2:B:1:FME:HE2	2:B:2:ALA:O	2.18	0.43
3:C:73:PRO:HB3	20:C:317:EDO:H11	1.98	0.43
26:G:101:CDL:H522	26:G:101:CDL:H231	2.00	0.43
14:P:307:PGV:H242	14:P:307:PGV:H101	2.00	0.43
26:P:308:CDL:H711	26:P:308:CDL:H172	1.99	0.43
23:P:310:CHD:H232	23:P:310:CHD:H211	1.72	0.43
2:B:203:ASN:OD1	20:B:308:EDO:H21	2.18	0.43
8:H:9:LYS:HB3	8:H:10:ASN:H	1.53	0.43
3:P:244:PHE:HA	25:P:303:PEK:H101	2.01	0.43
21:Y:101:TGL:H182	21:Y:101:TGL:H342	1.89	0.43
23:Y:104:CHD:H193	23:Y:104:CHD:H111	1.86	0.43
2:O:4:PRO:HB2	11:X:43:SER:HA	2.01	0.43
9:V:20:HIS:HD2	27:V:102:DMU:H1	1.83	0.43
25:C:304:PEK:H71	25:C:304:PEK:H42	1.69	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.53	0.43
23:W:101:CHD:H221	30:W:218:HOH:O	2.19	0.43
1:A:334:TRP:HZ3	21:D:201:TGL:HA62	1.84	0.43
26:C:308:CDL:H822	26:C:308:CDL:H851	1.62	0.43
7:G:2:SER:HB3	25:P:303:PEK:H331	2.01	0.43
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.99	0.42
2:B:49:LYS:O	4:D:20[B]:ARG:NH2	2.50	0.42
15:N:603:HEA:HMC1	15:N:603:HEA:CBC	2.48	0.42
3:P:37:PHE:CD2	27:P:309:DMU:H9	2.53	0.42
2:B:62:GLU:HA	2:B:65[A]:TRP:CD1	2.54	0.42
3:C:67:PHE:HE2	26:C:308:CDL:C1	2.31	0.42
3:C:67:PHE:CE2	26:C:308:CDL:H1	2.48	0.42
26:C:308:CDL:H451	26:C:308:CDL:H421	1.73	0.42
10:J:7:GLU:HG3	30:J:227:HOH:O	2.18	0.42
20:O:306:EDO:C2	8:U:24:ASN:HD21	2.31	0.42
23:W:101:CHD:H211	23:W:101:CHD:H231	1.69	0.42
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.54	0.42
1:A:208[B]:MET:HE3	1:A:220:PHE:CZ	2.53	0.42
9:I:15:ARG:HG3	30:I:128:HOH:O	2.20	0.42
14:P:306:PGV:H172	26:P:308:CDL:H632	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:103:EDO:H22	30:H:248:HOH:O	2.18	0.42
23:P:310:CHD:H193	23:P:310:CHD:H111	1.79	0.42
1:A:21:LEU:HD23	21:L:101:TGL:H211	2.02	0.42
23:G:102:CHD:H12	23:G:102:CHD:H212	2.01	0.42
1:N:309:THR:HG22	15:N:603:HEA:HMB2	2.01	0.42
1:N:506:GLU:N	20:N:618:EDO:H11	2.35	0.42
25:P:305:PEK:C04	7:T:17:ARG:HH22	2.17	0.42
2:B:216:LEU:O	2:B:220:GLU:HG3	2.20	0.42
2:B:222:TRP:HE1	20:B:312:EDO:H22	1.84	0.42
20:B:312:EDO:H11	9:I:70:GLN:OE1	2.20	0.42
26:T:101:CDL:H312	26:T:101:CDL:HA62	1.67	0.42
2:B:41:ILE:HG21	22:B:302:PSC:H332	2.02	0.42
1:N:449:MET:SD	2:O:5:MET:HG2	2.60	0.42
6:S:94:HIS:NE2	30:S:205:HOH:O	2.36	0.42
1:A:240:HIS:CD2	1:A:240:HIS:C	2.93	0.41
3:C:51[B]:MET:SD	26:C:308:CDL:H232	2.60	0.41
6:F:64:GLU:O	6:F:65:ASP:HB2	2.20	0.41
1:N:331[B]:ASN:HD21	4:Q:21:ASP:HB3	1.84	0.41
2:O:111:THR:HA	2:O:114:GLU:O	2.19	0.41
4:Q:20[B]:ARG:HG3	30:Q:362:HOH:O	2.19	0.41
1:A:87:ILE:O	1:A:173:PRO:HD3	2.19	0.41
1:N:169:ILE:HD11	1:N:189[A]:MET:HE3	2.01	0.41
6:S:64:GLU:O	6:S:65:ASP:HB2	2.19	0.41
8:U:60:TYR:CD1	8:U:60:TYR:C	2.93	0.41
21:B:301:TGL:H241	21:B:301:TGL:H272	1.80	0.41
7:G:8:HIS:HA	7:G:11:TPO:HG23	2.02	0.41
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.81	0.41
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.41
21:Y:101:TGL:H232	21:Y:101:TGL:H202	1.57	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.02	0.41
2:B:70:ALA:HB1	26:T:101:CDL:H471	2.03	0.41
2:O:47:THR:HA	21:Q:201:TGL:HC81	2.01	0.41
1:A:268:PHE:HE2	22:B:302:PSC:H251	1.85	0.41
3:P:38:ASN:O	27:P:323:DMU:O3	2.36	0.41
9:V:27:VAL:HG11	27:V:102:DMU:H11	2.01	0.41
13:Z:39:ASN:OD1	13:Z:39:ASN:N	2.52	0.41
1:N:302[A]:ARG:NH2	1:N:365:ILE:HD11	2.35	0.41
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.35	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.95	0.41
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.09	0.41
22:B:302:PSC:H042	22:B:302:PSC:H063	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:MET:CE	11:K:22:ALA:HB2	2.51	0.41
1:N:2:PHE:CZ	21:Y:101:TGL:HG32	2.56	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.56	0.41
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	2.02	0.41
1:N:334:TRP:CE3	21:Q:201:TGL:HA31	2.55	0.41
1:N:383[A]:MET:HA	1:N:387:PHE:CD1	2.56	0.41
3:P:224:LYS:HD2	26:P:308:CDL:HB31	2.02	0.41
3:P:224:LYS:CE	26:P:308:CDL:H131	2.51	0.41
26:P:308:CDL:H161	26:P:308:CDL:H132	1.86	0.41
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	2.21	0.41
26:T:101:CDL:H832	26:T:101:CDL:H801	1.83	0.41
11:X:8:ASP:HB2	30:X:116:HOH:O	2.20	0.41
2:B:57:ASP:H	22:B:302:PSC:C21	2.34	0.41
21:Q:201:TGL:H363	9:V:16:ARG:HH21	1.86	0.41
12:Y:41:ARG:HH12	23:Y:104:CHD:H9	1.85	0.41
26:P:308:CDL:H452	26:P:308:CDL:H421	1.84	0.40
15:A:602[A]:HEA:H211	15:A:602[B]:HEA:H271	1.96	0.40
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.03	0.40
7:G:2:SER:OG	7:G:3:ALA:O	2.32	0.40
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.21	0.40
22:O:301:PSC:H261	22:O:301:PSC:H232	1.49	0.40
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.02	0.40
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.21	0.40
1:A:510:TYR:HE1	1:A:512[B]:ASN:HD21	1.70	0.40
30:A:899:HOH:O	13:M:41:LYS:HG2	2.21	0.40
22:B:302:PSC:H252	22:B:302:PSC:H221	1.74	0.40
14:P:307:PGV:H62	14:P:307:PGV:H31	1.85	0.40
14:A:601:PGV:H131	4:D:87:PHE:CD2	2.56	0.40
26:G:101:CDL:H381	2:O:81:LEU:CD1	2.50	0.40
21:N:608:TGL:HA91	21:N:608:TGL:H252	2.02	0.40
3:P:77:LYS:NZ	25:P:303:PEK:HN1	2.20	0.40
1:N:472:ILE:HD13	21:Y:101:TGL:H201	2.03	0.40
3:P:226:HIS:HE1	26:P:308:CDL:HB32	1.86	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:314:EDO:C2	20:D:206:EDO:C1[2_584]	1.49	0.71
30:B:479:HOH:O	30:D:306:HOH:O[2_584]	1.96	0.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:314:EDO:O2	20:D:206:EDO:C1[2_584]	1.97	0.23
30:B:551:HOH:O	30:D:426:HOH:O[2_584]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/514 (106%)	532 (98%)	11 (2%)	0	100	100
1	N	541/514 (105%)	532 (98%)	9 (2%)	0	100	100
2	B	236/227 (104%)	231 (98%)	5 (2%)	0	100	100
2	O	235/227 (104%)	228 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	260 (98%)	6 (2%)	0	100	100
3	P	268/261 (103%)	263 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	13	3
7	T	82/85 (96%)	73 (89%)	6 (7%)	3 (4%)	3	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	12	2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
12	Y	47/47 (100%)	46 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3616/3614 (100%)	3521 (97%)	87 (2%)	8 (0%)	47	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	T	4	ALA
7	G	10	GLY
8	H	8	ILE
8	H	9	LYS
7	T	3	ALA
8	H	45	ALA
7	T	10	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	455/426 (107%)	445 (98%)	10 (2%)	52	34
1	N	453/426 (106%)	447 (99%)	6 (1%)	69	56
2	B	221/210 (105%)	213 (96%)	8 (4%)	35	16
2	O	220/210 (105%)	212 (96%)	8 (4%)	35	16
3	C	233/226 (103%)	230 (99%)	3 (1%)	69	56
3	P	235/226 (104%)	232 (99%)	3 (1%)	69	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	133/129 (103%)	131 (98%)	2 (2%)	65	51
4	Q	131/129 (102%)	129 (98%)	2 (2%)	65	51
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	63
5	R	92/95 (97%)	91 (99%)	1 (1%)	73	63
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	3
6	S	81/81 (100%)	79 (98%)	2 (2%)	47	29
7	G	67/68 (98%)	63 (94%)	4 (6%)	19	6
7	T	68/68 (100%)	64 (94%)	4 (6%)	19	6
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	12
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	7
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	43
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	17
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	12
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	12
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	28
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	41/40 (102%)	41 (100%)	0	100	100
12	Y	43/40 (108%)	40 (93%)	3 (7%)	15	3
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	7
All	All	3152/3082 (102%)	3072 (98%)	80 (2%)	52	29

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	180	GLN
1	A	338	MET
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER
1	A	382[C]	SER
1	A	486[A]	ASP
1	A	486[B]	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	33[A]	LEU
2	B	33[B]	LEU
2	B	59	GLN
2	B	60[A]	GLU
2	B	60[B]	GLU
2	B	75	LEU
2	B	78	LEU
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	147	LYS
5	E	90	ARG
6	F	2	SER
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80[A]	GLN
6	F	80[B]	GLN
6	F	94	HIS
7	G	18	PHE
7	G	33	LEU
7	G	37	LEU
7	G	54	ARG
8	H	7	LYS
8	H	9	LYS
8	H	60	TYR
9	I	36	LYS
10	J	50	LEU
10	J	58	LYS
11	K	54	ARG
1	N	38	ARG
1	N	109	PHE
1	N	361	SER
1	N	363	LEU
1	N	369	ASP
1	N	485	VAL
2	O	33[A]	LEU
2	O	33[B]	LEU
2	O	60	GLU
2	O	75	LEU
2	O	78	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	115[A]	ASP
2	O	115[B]	ASP
2	O	171	LYS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	20[A]	ARG
4	Q	20[B]	ARG
5	R	80	GLU
6	S	80[A]	GLN
6	S	80[B]	GLN
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	54	ARG
8	U	7	LYS
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
9	V	15	ARG
9	V	29	LEU
10	W	50	LEU
10	W	58	LYS
12	Y	2[A]	HIS
12	Y	2[B]	HIS
12	Y	47	LYS
13	Z	38	ASP
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	91	ASN
3	C	38	ASN
3	C	68	GLN
4	D	109	HIS
7	G	8	HIS
8	H	37	HIS
10	J	57	HIS
13	M	39	ASN
2	O	91	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	101	HIS
4	Q	109	HIS
6	S	94	HIS
7	T	8	HIS
8	U	10	ASN
8	U	37	HIS
9	V	20	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	1.32	1 (12%)	10,14,16	0.79	0
9	SAC	I	1	9	7,8,9	0.63	0	8,9,11	0.94	0
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	0.83	0
7	TPO	G	11	7	8,10,11	1.32	1 (12%)	10,14,16	0.85	0
2	FME	O	1	2	8,9,10	0.87	0	7,9,11	0.94	0
2	FME	B	1	2	8,9,10	0.94	0	7,9,11	1.48	1 (14%)
1	FME	A	1	1	8,9,10	0.50	0	7,9,11	1.88	2 (28%)
1	FME	N	1	1	8,9,10	0.42	0	7,9,11	1.29	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	T	11	7	-	5/9/11/13	-
9	SAC	I	1	9	-	0/7/8/10	-
9	SAC	V	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.81	1.59	1.50
7	G	11	TPO	P-O1P	2.80	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.42	115.91	109.73
1	A	1	FME	CE-SD-CG	2.42	108.71	100.40
2	B	1	FME	O-C-CA	-2.19	119.03	124.78
1	N	1	FME	O-C-CA	-2.02	119.50	124.78

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	O-C-CA-CB
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
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CB-CG-SD-CE
9	V	1	SAC	N-CA-CB-OG
9	V	1	SAC	C-CA-CB-OG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	CA-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	2	0
2	B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 10 are monoatomic - leaving 199 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	$\# Z > 2$
20	EDO	F	107	-	3,3,3	0.36	0	2,2,2	0.57	0
20	EDO	A	610	-	3,3,3	0.90	0	2,2,2	1.03	0
20	EDO	W	103	-	3,3,3	0.87	0	2,2,2	0.44	0
20	EDO	R	202	-	3,3,3	0.61	0	2,2,2	0.22	0
20	EDO	A	613	-	3,3,3	0.72	0	2,2,2	0.37	0
20	EDO	C	317	-	3,3,3	0.39	0	2,2,2	0.03	0
20	EDO	B	312	-	3,3,3	0.58	0	2,2,2	0.20	0
20	EDO	M	103	-	3,3,3	0.46	0	2,2,2	0.13	0
21	TGL	L	101	-	62,62,62	1.06	3 (4%)	65,65,65	1.20	8 (12%)
25	PEK	C	305	-	52,52,52	0.94	2 (3%)	55,57,57	1.19	5 (9%)
21	TGL	N	608	-	62,62,62	1.02	3 (4%)	65,65,65	1.20	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	S	106	-	3,3,3	0.43	0	2,2,2	0.56	0
29	PO4	H	104	-	4,4,4	0.93	0	6,6,6	0.36	0
27	DMU	P	323	-	34,34,34	0.44	0	45,45,45	0.89	2 (4%)
20	EDO	N	628	-	3,3,3	0.42	0	2,2,2	1.09	0
20	EDO	O	305	-	3,3,3	0.47	0	2,2,2	0.22	0
20	EDO	Y	102	-	3,3,3	0.53	0	2,2,2	0.37	0
20	EDO	G	103	-	3,3,3	0.56	0	2,2,2	0.32	0
20	EDO	R	204	-	3,3,3	0.51	0	2,2,2	0.25	0
24	CUA	O	302	2	0,1,1	0.00	-	-		
20	EDO	A	625	-	3,3,3	0.54	0	2,2,2	0.83	0
20	EDO	H	101	-	3,3,3	0.43	0	2,2,2	0.53	0
20	EDO	T	103	-	3,3,3	0.57	0	2,2,2	0.53	0
20	EDO	D	202	-	3,3,3	0.60	0	2,2,2	0.20	0
27	DMU	G	108	-	34,34,34	0.48	0	45,45,45	1.17	3 (6%)
20	EDO	S	109	-	3,3,3	0.47	0	2,2,2	0.44	0
20	EDO	B	305	-	3,3,3	0.48	0	2,2,2	0.68	0
20	EDO	J	102	-	3,3,3	0.40	0	2,2,2	0.35	0
20	EDO	D	203	-	3,3,3	0.50	0	2,2,2	0.14	0
20	EDO	P	315	-	3,3,3	1.06	0	2,2,2	0.56	0
20	EDO	D	207	-	3,3,3	0.48	0	2,2,2	0.77	0
25	PEK	C	304	-	52,52,52	0.86	2 (3%)	55,57,57	1.07	3 (5%)
22	PSC	B	302	-	51,51,51	1.09	3 (5%)	57,59,59	1.34	7 (12%)
20	EDO	A	612	-	3,3,3	0.60	0	2,2,2	0.67	0
20	EDO	S	105	-	3,3,3	0.53	0	2,2,2	0.13	0
20	EDO	C	314	-	3,3,3	0.54	0	2,2,2	0.39	0
15	HEA	N	603	1	44,67,67	1.22	3 (6%)	37,103,103	1.63	9 (24%)
20	EDO	W	102	-	3,3,3	0.30	0	2,2,2	0.67	0
20	EDO	P	317	-	3,3,3	0.66	0	2,2,2	0.17	0
23	CHD	P	301	-	29,32,32	0.86	1 (3%)	48,51,51	1.50	10 (20%)
20	EDO	N	610	-	3,3,3	1.10	0	2,2,2	0.52	0
21	TGL	B	301	-	62,62,62	1.13	4 (6%)	65,65,65	1.29	5 (7%)
20	EDO	G	106	-	3,3,3	0.62	0	2,2,2	0.69	0
23	CHD	C	309	-	29,32,32	0.65	0	48,51,51	1.16	6 (12%)
20	EDO	N	618	-	3,3,3	0.77	0	2,2,2	1.14	0
20	EDO	P	318	-	3,3,3	0.74	0	2,2,2	0.11	0
20	EDO	O	307	-	3,3,3	0.49	0	2,2,2	0.27	0
20	EDO	P	319	-	3,3,3	0.95	0	2,2,2	0.45	0
20	EDO	L	102	-	3,3,3	0.54	0	2,2,2	0.09	0
23	CHD	Y	104	-	29,32,32	0.81	1 (3%)	48,51,51	1.85	14 (29%)
20	EDO	B	310	-	3,3,3	0.45	0	2,2,2	0.24	0
20	EDO	B	313	-	3,3,3	0.56	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	M	101	-	34,34,34	0.50	0	45,45,45	1.09	3 (6%)
20	EDO	B	311	-	3,3,3	0.54	0	2,2,2	0.11	0
20	EDO	M	102	-	3,3,3	0.47	0	2,2,2	0.34	0
20	EDO	N	623	-	3,3,3	0.52	0	2,2,2	0.39	0
20	EDO	P	322	-	3,3,3	0.54	0	2,2,2	0.33	0
20	EDO	A	616	-	3,3,3	0.43	0	2,2,2	0.64	0
23	CHD	W	101	-	29,32,32	0.64	1 (3%)	48,51,51	1.60	7 (14%)
27	DMU	V	102	-	34,34,34	0.55	1 (2%)	45,45,45	1.03	3 (6%)
20	EDO	V	101	-	3,3,3	0.48	0	2,2,2	0.42	0
20	EDO	N	617	-	3,3,3	0.32	0	2,2,2	0.81	0
14	PGV	C	307	-	50,50,50	0.96	2 (4%)	53,56,56	1.58	7 (13%)
20	EDO	B	307	-	3,3,3	0.59	0	2,2,2	0.22	0
20	EDO	B	308	-	3,3,3	0.59	0	2,2,2	0.41	0
20	EDO	Q	203	-	3,3,3	0.42	0	2,2,2	0.40	0
21	TGL	Y	101	-	62,62,62	1.02	3 (4%)	65,65,65	1.14	4 (6%)
20	EDO	G	105	-	3,3,3	0.54	0	2,2,2	0.15	0
20	EDO	A	611	-	3,3,3	0.67	0	2,2,2	0.59	0
20	EDO	A	609	-	3,3,3	0.46	0	2,2,2	0.50	0
29	PO4	U	102	-	4,4,4	0.98	0	6,6,6	0.40	0
20	EDO	J	103	-	3,3,3	0.40	0	2,2,2	0.49	0
27	DMU	Z	102	-	34,34,34	0.48	0	45,45,45	1.13	3 (6%)
20	EDO	N	626	-	3,3,3	0.35	0	2,2,2	0.33	0
20	EDO	P	314	-	3,3,3	0.42	0	2,2,2	0.78	0
20	EDO	N	613	-	3,3,3	0.45	0	2,2,2	0.46	0
20	EDO	N	625	-	3,3,3	0.71	0	2,2,2	0.30	0
20	EDO	N	612	-	3,3,3	0.52	0	2,2,2	0.67	0
21	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.00	6 (9%)
27	DMU	C	319	-	34,34,34	0.48	0	45,45,45	1.05	3 (6%)
15	HEA	N	602[A]	-	44,67,67	1.31	4 (9%)	37,103,103	2.33	11 (29%)
14	PGV	N	609	-	50,50,50	1.01	5 (10%)	53,56,56	1.12	3 (5%)
27	DMU	P	324	-	34,34,34	0.55	0	45,45,45	0.73	1 (2%)
26	CDL	T	101	-	99,99,99	1.30	12 (12%)	105,111,111	1.11	6 (5%)
22	PSC	O	301	-	51,51,51	1.10	3 (5%)	57,59,59	1.26	5 (8%)
20	EDO	C	316	-	3,3,3	0.89	0	2,2,2	0.61	0
20	EDO	F	103	-	3,3,3	0.44	0	2,2,2	0.16	0
20	EDO	F	106	-	3,3,3	0.90	0	2,2,2	0.42	0
23	CHD	J	101	-	29,32,32	0.70	1 (3%)	48,51,51	1.76	12 (25%)
19	CMO	N	607[A]	-	0,1,1	0.00	-	-		
20	EDO	P	313	-	3,3,3	0.43	0	2,2,2	0.30	0
20	EDO	N	630	-	3,3,3	0.39	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	P	310	-	29,32,32	0.78	1 (3%)	48,51,51	1.90	12 (25%)
20	EDO	S	108	-	3,3,3	0.72	0	2,2,2	0.42	0
14	PGV	A	608	-	50,50,50	0.88	2 (4%)	53,56,56	0.88	1 (1%)
20	EDO	L	103	-	3,3,3	0.57	0	2,2,2	0.11	0
20	EDO	K	102	-	3,3,3	0.50	0	2,2,2	0.21	0
20	EDO	G	104	-	3,3,3	0.44	0	2,2,2	0.52	0
20	EDO	P	316	-	3,3,3	0.67	0	2,2,2	0.36	0
25	PEK	C	303	-	52,52,52	0.93	2 (3%)	55,57,57	1.30	5 (9%)
20	EDO	U	101	-	3,3,3	0.61	0	2,2,2	0.27	0
20	EDO	O	306	-	3,3,3	0.52	0	2,2,2	0.17	0
23	CHD	G	102	-	29,32,32	0.93	0	48,51,51	1.42	7 (14%)
20	EDO	L	104	-	3,3,3	0.82	0	2,2,2	0.15	0
23	CHD	C	311	-	29,32,32	0.80	1 (3%)	48,51,51	1.80	10 (20%)
21	TGL	D	201	-	62,62,62	1.20	4 (6%)	65,65,65	0.94	5 (7%)
15	HEA	N	602[B]	-	44,67,67	1.23	4 (9%)	37,103,103	1.98	9 (24%)
20	EDO	S	110	-	3,3,3	0.66	0	2,2,2	0.66	0
20	EDO	A	622	-	3,3,3	0.33	0	2,2,2	0.57	0
15	HEA	A	603	1	44,67,67	1.17	4 (9%)	37,103,103	1.87	12 (32%)
20	EDO	N	629	-	3,3,3	0.41	0	2,2,2	0.35	0
20	EDO	E	203	-	3,3,3	0.55	0	2,2,2	0.51	0
27	DMU	C	310	-	34,34,34	0.42	0	45,45,45	0.88	0
20	EDO	A	618	-	3,3,3	0.42	0	2,2,2	0.51	0
14	PGV	P	306	-	50,50,50	0.77	1 (2%)	53,56,56	1.23	4 (7%)
19	CMO	N	607[B]	16	0,1,1	0.00	-	-		
19	CMO	A	607[A]	-	0,1,1	0.00	-	-		
20	EDO	K	101	-	3,3,3	0.68	0	2,2,2	0.12	0
20	EDO	N	615	-	3,3,3	0.51	0	2,2,2	0.38	0
20	EDO	R	205	-	3,3,3	0.53	0	2,2,2	0.21	0
20	EDO	D	206	20	3,3,3	0.43	0	2,2,2	0.40	0
20	EDO	A	620	-	3,3,3	0.63	0	2,2,2	1.08	0
23	CHD	C	301	-	29,32,32	1.02	3 (10%)	48,51,51	1.59	8 (16%)
20	EDO	R	203	-	3,3,3	0.55	0	2,2,2	0.25	0
14	PGV	P	307	-	50,50,50	0.97	2 (4%)	53,56,56	1.36	8 (15%)
20	EDO	P	312	-	3,3,3	0.47	0	2,2,2	1.02	0
20	EDO	S	103	-	3,3,3	0.83	0	2,2,2	0.11	0
23	CHD	B	303	-	29,32,32	1.14	2 (6%)	48,51,51	1.79	12 (25%)
14	PGV	N	601	-	50,50,50	0.92	2 (4%)	53,56,56	1.20	5 (9%)
20	EDO	A	627	-	3,3,3	0.83	0	2,2,2	0.56	0
25	PEK	P	305	-	52,52,52	0.96	2 (3%)	55,57,57	1.22	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PEK	P	304	-	52,52,52	0.70	2 (3%)	55,57,57	1.12	5 (9%)
20	EDO	M	105	-	3,3,3	1.17	0	2,2,2	0.72	0
20	EDO	O	303	-	3,3,3	0.87	0	2,2,2	0.46	0
20	EDO	Q	202	-	3,3,3	0.42	0	2,2,2	0.33	0
20	EDO	N	621	-	3,3,3	0.59	0	2,2,2	0.26	0
20	EDO	R	201	-	3,3,3	0.60	0	2,2,2	0.52	0
20	EDO	A	619	-	3,3,3	0.39	0	2,2,2	0.86	0
20	EDO	C	315	-	3,3,3	0.61	0	2,2,2	0.47	0
20	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.57	0
20	EDO	S	111	-	3,3,3	0.77	0	2,2,2	0.29	0
20	EDO	O	304	-	3,3,3	0.49	0	2,2,2	0.13	0
20	EDO	F	105	-	3,3,3	0.53	0	2,2,2	0.13	0
27	DMU	P	309	-	34,34,34	0.46	0	45,45,45	0.69	0
20	EDO	A	623	-	3,3,3	0.60	0	2,2,2	0.39	0
26	CDL	C	308	-	99,99,99	1.31	12 (12%)	105,111,111	1.23	9 (8%)
20	EDO	H	102	-	3,3,3	0.54	0	2,2,2	0.16	0
20	EDO	E	201	-	3,3,3	0.41	0	2,2,2	0.46	0
20	EDO	W	104	-	3,3,3	0.52	0	2,2,2	0.30	0
14	PGV	A	601	-	50,50,50	0.96	2 (4%)	53,56,56	1.08	4 (7%)
19	CMO	A	607[B]	16	0,1,1	0.00	-	-		
20	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.19	0
15	HEA	A	602[A]	-	44,67,67	1.37	6 (13%)	37,103,103	2.20	8 (21%)
20	EDO	T	102	-	3,3,3	0.69	0	2,2,2	0.94	0
20	EDO	P	321	-	3,3,3	0.59	0	2,2,2	0.49	0
20	EDO	Y	103	-	3,3,3	0.44	0	2,2,2	0.24	0
26	CDL	G	101	-	99,99,99	1.32	12 (12%)	105,111,111	1.46	11 (10%)
27	DMU	M	106	-	34,34,34	0.59	1 (2%)	45,45,45	1.19	4 (8%)
20	EDO	S	107	-	3,3,3	0.49	0	2,2,2	0.36	0
20	EDO	A	621	-	3,3,3	0.61	0	2,2,2	0.42	0
20	EDO	N	622	-	3,3,3	0.57	0	2,2,2	0.52	0
20	EDO	S	112	-	3,3,3	0.50	0	2,2,2	1.65	1 (50%)
26	CDL	P	308	-	99,99,99	1.34	12 (12%)	105,111,111	1.32	9 (8%)
20	EDO	A	624	-	3,3,3	0.40	0	2,2,2	0.64	0
20	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.31	0
20	EDO	N	624	-	3,3,3	0.61	0	2,2,2	0.28	0
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.86	2 (4%)
20	EDO	M	104	-	3,3,3	0.63	0	2,2,2	0.50	0
20	EDO	A	617	-	3,3,3	0.66	0	2,2,2	0.17	0
20	EDO	N	619	-	3,3,3	0.55	0	2,2,2	0.28	0
20	EDO	C	318	-	3,3,3	0.70	0	2,2,2	0.09	0
20	EDO	P	320	-	3,3,3	0.47	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	A	626	-	3,3,3	0.68	0	2,2,2	1.03	0
20	EDO	F	104	-	3,3,3	0.88	0	2,2,2	0.07	0
20	EDO	N	620	-	3,3,3	0.59	0	2,2,2	0.43	0
20	EDO	S	104	-	3,3,3	0.82	0	2,2,2	0.74	0
24	CUA	B	304	2	0,1,1	0.00	-	-		
14	PGV	C	306	-	50,50,50	0.80	2 (4%)	53,56,56	0.95	3 (5%)
20	EDO	A	615	-	3,3,3	0.63	0	2,2,2	0.17	0
20	EDO	B	306	-	3,3,3	0.82	0	2,2,2	0.34	0
20	EDO	C	312	-	3,3,3	0.75	0	2,2,2	0.11	0
20	EDO	C	313	-	3,3,3	0.77	0	2,2,2	0.30	0
20	EDO	L	105	-	3,3,3	0.56	0	2,2,2	0.29	0
23	CHD	P	311	-	29,32,32	0.72	0	48,51,51	1.21	7 (14%)
25	PEK	P	303	-	52,52,52	0.94	2 (3%)	55,57,57	1.15	5 (9%)
20	EDO	S	102	-	3,3,3	0.95	0	2,2,2	0.78	0
15	HEA	A	602[B]	-	44,67,67	1.38	6 (13%)	37,103,103	1.91	7 (18%)
20	EDO	H	103	-	3,3,3	0.50	0	2,2,2	0.18	0
20	EDO	D	205	-	3,3,3	0.69	0	2,2,2	0.42	0
20	EDO	N	616	-	3,3,3	0.53	0	2,2,2	0.39	0
20	EDO	E	202	-	3,3,3	0.65	0	2,2,2	0.07	0
20	EDO	B	314	20	3,3,3	0.48	0	2,2,2	0.39	0
20	EDO	B	309	-	3,3,3	0.42	0	2,2,2	0.10	0
20	EDO	G	107	-	3,3,3	0.72	0	2,2,2	0.13	0
20	EDO	N	627	-	3,3,3	0.44	0	2,2,2	0.48	0
20	EDO	N	611	-	3,3,3	0.68	0	2,2,2	0.56	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
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	W	103	-	-	1/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	C	317	-	-	0/1/1/1	-
20	EDO	B	312	-	-	0/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
21	TGL	L	101	-	-	29/65/65/65	-
25	PEK	C	305	-	-	19/56/56/56	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	N	608	-	-	19/65/65/65	-
20	EDO	S	106	-	-	0/1/1/1	-
27	DMU	P	323	-	-	3/19/59/59	0/2/2/2
20	EDO	N	628	-	-	1/1/1/1	-
20	EDO	O	305	-	-	1/1/1/1	-
20	EDO	Y	102	-	-	0/1/1/1	-
20	EDO	G	103	-	-	1/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-
15	HEA	A	602[C]	-	3/3/3/16	-	-
20	EDO	A	625	-	-	0/1/1/1	-
20	EDO	H	101	-	-	0/1/1/1	-
20	EDO	T	103	-	-	1/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
27	DMU	G	108	-	-	6/19/59/59	0/2/2/2
20	EDO	S	109	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
20	EDO	P	315	-	-	0/1/1/1	-
20	EDO	D	207	-	-	0/1/1/1	-
25	PEK	C	304	-	-	12/56/56/56	-
22	PSC	B	302	-	-	20/55/55/55	-
20	EDO	A	612	-	-	0/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
15	HEA	N	603	1	3/3/7/16	0/24/76/76	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	P	317	-	-	0/1/1/1	-
23	CHD	P	301	-	-	1/7/74/74	0/4/4/4
20	EDO	N	610	-	-	0/1/1/1	-
21	TGL	B	301	-	-	19/65/65/65	-
20	EDO	G	106	-	-	0/1/1/1	-
23	CHD	C	309	-	-	3/7/74/74	0/4/4/4
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	P	318	-	-	0/1/1/1	-
20	EDO	O	307	-	-	0/1/1/1	-
20	EDO	P	319	-	-	0/1/1/1	-
20	EDO	L	102	-	-	1/1/1/1	-
23	CHD	Y	104	-	-	7/7/74/74	0/4/4/4
20	EDO	B	310	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	B	313	-	-	1/1/1/1	-
27	DMU	M	101	-	-	7/19/59/59	0/2/2/2
20	EDO	B	311	-	-	0/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
20	EDO	N	623	-	-	1/1/1/1	-
20	EDO	P	322	-	-	0/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
23	CHD	W	101	-	-	6/7/74/74	0/4/4/4
27	DMU	V	102	-	-	11/19/59/59	0/2/2/2
20	EDO	V	101	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
14	PGV	C	307	-	-	12/55/55/55	-
20	EDO	B	307	-	-	1/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-
21	TGL	Y	101	-	-	30/65/65/65	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	J	103	-	-	1/1/1/1	-
27	DMU	Z	102	-	-	9/19/59/59	0/2/2/2
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	N	625	-	-	1/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	21/65/65/65	-
27	DMU	C	319	-	-	9/19/59/59	0/2/2/2
15	HEA	N	602[A]	-	3/3/7/16	0/24/76/76	-
14	PGV	N	609	-	-	5/55/55/55	-
27	DMU	P	324	-	-	13/19/59/59	0/2/2/2
26	CDL	T	101	-	-	36/110/110/110	-
22	PSC	O	301	-	-	20/55/55/55	-
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	F	106	-	-	0/1/1/1	-
23	CHD	J	101	-	-	7/7/74/74	0/4/4/4
20	EDO	P	313	-	-	1/1/1/1	-
20	EDO	N	630	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	P	310	-	-	1/7/74/74	0/4/4/4
20	EDO	S	108	-	-	1/1/1/1	-
14	PGV	A	608	-	-	8/55/55/55	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	K	102	-	-	0/1/1/1	-
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	P	316	-	-	1/1/1/1	-
25	PEK	C	303	-	-	21/56/56/56	-
20	EDO	U	101	-	-	0/1/1/1	-
20	EDO	O	306	-	-	1/1/1/1	-
23	CHD	G	102	-	-	0/7/74/74	0/4/4/4
20	EDO	L	104	-	-	1/1/1/1	-
23	CHD	C	311	-	-	1/7/74/74	0/4/4/4
21	TGL	D	201	-	-	19/65/65/65	-
15	HEA	N	602[B]	-	3/3/7/16	1/24/76/76	-
20	EDO	S	110	-	-	0/1/1/1	-
20	EDO	A	622	-	-	0/1/1/1	-
15	HEA	A	603	1	3/3/7/16	0/24/76/76	-
20	EDO	N	629	-	-	1/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
27	DMU	C	310	-	-	4/19/59/59	0/2/2/2
20	EDO	A	618	-	-	0/1/1/1	-
14	PGV	P	306	-	-	8/55/55/55	-
20	EDO	K	101	-	-	0/1/1/1	-
20	EDO	R	205	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	D	206	20	-	0/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-
23	CHD	C	301	-	-	0/7/74/74	0/4/4/4
20	EDO	R	203	-	-	0/1/1/1	-
14	PGV	P	307	-	-	10/55/55/55	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
23	CHD	B	303	-	-	0/7/74/74	0/4/4/4
14	PGV	N	601	-	-	20/55/55/55	-
20	EDO	A	627	-	-	0/1/1/1	-
25	PEK	P	305	-	-	21/56/56/56	-
25	PEK	P	304	-	-	9/56/56/56	-
20	EDO	M	105	-	-	1/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	Q	202	-	-	1/1/1/1	-
20	EDO	N	621	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	A	619	-	-	0/1/1/1	-
20	EDO	C	315	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	S	111	-	-	1/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
15	HEA	N	602[C]	-	3/3/3/16	-	-
27	DMU	P	309	-	-	6/19/59/59	0/2/2/2
20	EDO	A	623	-	-	0/1/1/1	-
26	CDL	C	308	-	-	38/110/110/110	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	W	104	-	-	1/1/1/1	-
14	PGV	A	601	-	-	11/55/55/55	-
20	EDO	A	614	-	-	0/1/1/1	-
15	HEA	A	602[A]	-	3/3/7/16	1/24/76/76	-
20	EDO	T	102	-	-	0/1/1/1	-
20	EDO	P	321	-	-	1/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
26	CDL	G	101	-	-	32/110/110/110	-
27	DMU	M	106	-	-	7/19/59/59	0/2/2/2
20	EDO	S	107	-	-	1/1/1/1	-
20	EDO	A	621	-	-	0/1/1/1	-
20	EDO	N	622	-	-	1/1/1/1	-
20	EDO	S	112	-	-	1/1/1/1	-
26	CDL	P	308	-	-	36/110/110/110	-
20	EDO	A	624	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	N	624	-	-	1/1/1/1	-
27	DMU	Z	101	-	-	2/19/59/59	0/2/2/2
20	EDO	M	104	-	-	1/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	C	318	-	-	0/1/1/1	-
20	EDO	P	320	-	-	0/1/1/1	-
20	EDO	A	626	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	620	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
14	PGV	C	306	-	-	10/55/55/55	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	L	105	-	-	0/1/1/1	-
23	CHD	P	311	-	-	3/7/74/74	0/4/4/4
25	PEK	P	303	-	-	19/56/56/56	-
20	EDO	S	102	-	-	0/1/1/1	-
15	HEA	A	602[B]	-	3/3/7/16	0/24/76/76	-
20	EDO	H	103	-	-	0/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	N	616	-	-	1/1/1/1	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	B	314	20	-	0/1/1/1	-
20	EDO	B	309	-	-	0/1/1/1	-
20	EDO	G	107	-	-	0/1/1/1	-
20	EDO	N	627	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OG2-CB1	5.06	1.48	1.34
21	B	301	TGL	OG3-CC1	4.91	1.47	1.33
21	B	301	TGL	OG1-CA1	4.83	1.47	1.33
26	G	101	CDL	OA8-CA7	4.62	1.46	1.33
14	A	601	PGV	O03-C19	4.60	1.46	1.33
26	P	308	CDL	OA8-CA7	4.58	1.46	1.33
25	P	303	PEK	O03-C21	4.55	1.46	1.33
21	Q	201	TGL	OG1-CA1	4.53	1.46	1.33
14	N	601	PGV	O03-C19	4.52	1.46	1.33
25	C	303	PEK	O03-C21	4.51	1.46	1.33
14	P	307	PGV	O03-C19	4.51	1.46	1.33
21	L	101	TGL	OG2-CB1	4.50	1.47	1.34
26	P	308	CDL	OB6-CB5	4.49	1.47	1.34
21	Y	101	TGL	OG1-CA1	4.48	1.46	1.33
26	P	308	CDL	OA6-CA5	4.48	1.46	1.34
21	N	608	TGL	OG2-CB1	4.47	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	301	TGL	OG2-CB1	4.46	1.46	1.34
21	Y	101	TGL	OG2-CB1	4.45	1.46	1.34
21	D	201	TGL	OG1-CA1	4.45	1.46	1.33
21	L	101	TGL	OG3-CC1	4.43	1.46	1.33
15	N	602[A]	HEA	C3B-C11	-4.42	1.49	1.52
25	P	305	PEK	O03-C21	4.35	1.46	1.33
22	O	301	PSC	O01-C1	4.33	1.46	1.34
25	C	305	PEK	O03-C21	4.32	1.46	1.33
21	L	101	TGL	OG1-CA1	4.31	1.45	1.33
14	C	307	PGV	O01-C1	4.29	1.46	1.34
21	N	608	TGL	OG3-CC1	4.29	1.45	1.33
25	P	305	PEK	O01-C1	4.27	1.46	1.34
26	T	101	CDL	OB8-CB7	4.27	1.45	1.33
26	C	308	CDL	OB8-CB7	4.27	1.45	1.33
14	C	307	PGV	O03-C19	4.26	1.45	1.33
21	Q	201	TGL	OG2-CB1	4.25	1.46	1.34
26	T	101	CDL	OB6-CB5	4.24	1.46	1.34
21	N	608	TGL	OG1-CA1	4.24	1.45	1.33
26	G	101	CDL	OB8-CB7	4.23	1.45	1.33
26	G	101	CDL	OB6-CB5	4.22	1.46	1.34
26	T	101	CDL	OA8-CA7	4.22	1.45	1.33
25	C	305	PEK	O01-C1	4.20	1.46	1.34
26	C	308	CDL	OA8-CA7	4.19	1.45	1.33
26	P	308	CDL	OB8-CB7	4.19	1.45	1.33
22	B	302	PSC	O01-C1	4.19	1.46	1.34
26	C	308	CDL	OB6-CB5	4.19	1.46	1.34
14	P	307	PGV	O01-C1	4.18	1.46	1.34
21	Y	101	TGL	OG3-CC1	4.13	1.45	1.33
25	P	303	PEK	O01-C1	4.11	1.45	1.34
26	C	308	CDL	OA6-CA5	4.10	1.45	1.34
26	G	101	CDL	OA6-CA5	4.09	1.45	1.34
22	B	302	PSC	O03-C19	4.06	1.45	1.33
21	D	201	TGL	OG3-CC1	4.02	1.45	1.33
22	O	301	PSC	O03-C19	4.01	1.45	1.33
15	N	602[A]	HEA	C3C-C2C	-4.01	1.34	1.40
15	N	602[B]	HEA	C3C-C2C	-4.01	1.34	1.40
21	Q	201	TGL	OG3-CC1	4.00	1.45	1.33
21	D	201	TGL	OB1-CB1	3.94	1.34	1.22
26	T	101	CDL	OA6-CA5	3.92	1.45	1.34
25	C	303	PEK	O01-C1	3.92	1.45	1.34
14	A	601	PGV	O01-C1	3.88	1.45	1.34
22	B	302	PSC	C13-C12	3.77	1.53	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601	PGV	O01-C1	3.76	1.44	1.34
22	O	301	PSC	C13-C12	3.73	1.53	1.31
15	A	602[A]	HEA	C3B-C11	-3.54	1.50	1.52
15	A	602[A]	HEA	CAA-C2A	3.52	1.58	1.52
15	A	602[B]	HEA	CAA-C2A	3.52	1.58	1.52
14	N	609	PGV	O01-C1	3.52	1.44	1.34
26	G	101	CDL	C42-C41	-3.47	1.32	1.51
15	N	603	HEA	CAD-C3D	3.42	1.57	1.52
26	C	308	CDL	C59-C58	-3.41	1.32	1.51
26	C	308	CDL	C82-C81	-3.41	1.32	1.51
26	P	308	CDL	C79-C78	-3.39	1.32	1.51
23	B	303	CHD	C11-C12	3.38	1.59	1.53
26	P	308	CDL	C82-C81	-3.35	1.32	1.51
26	G	101	CDL	C82-C81	-3.33	1.32	1.51
26	C	308	CDL	C62-C61	-3.33	1.32	1.51
26	T	101	CDL	C82-C81	-3.32	1.32	1.51
26	T	101	CDL	C62-C61	-3.30	1.33	1.51
26	T	101	CDL	C59-C58	-3.30	1.33	1.51
26	C	308	CDL	C79-C78	-3.29	1.33	1.51
26	P	308	CDL	C59-C58	-3.27	1.33	1.51
26	T	101	CDL	C22-C21	-3.26	1.33	1.51
26	C	308	CDL	C39-C38	-3.23	1.33	1.51
15	A	602[A]	HEA	CAD-C3D	3.23	1.56	1.52
15	A	602[B]	HEA	CAD-C3D	3.23	1.56	1.52
25	C	304	PEK	O03-C21	3.22	1.42	1.33
26	G	101	CDL	C62-C61	-3.22	1.33	1.51
25	C	304	PEK	O01-C1	3.21	1.43	1.34
26	G	101	CDL	C39-C38	-3.21	1.33	1.51
26	G	101	CDL	C79-C78	-3.20	1.33	1.51
26	G	101	CDL	C59-C58	-3.20	1.33	1.51
26	P	308	CDL	C19-C18	-3.19	1.33	1.51
26	T	101	CDL	C79-C78	-3.19	1.33	1.51
26	P	308	CDL	C39-C38	-3.19	1.33	1.51
26	C	308	CDL	C42-C41	-3.18	1.33	1.51
15	A	602[B]	HEA	O11-C11	3.18	1.50	1.42
26	T	101	CDL	C19-C18	-3.17	1.33	1.51
26	C	308	CDL	C22-C21	-3.17	1.33	1.51
26	P	308	CDL	C62-C61	-3.15	1.33	1.51
26	C	308	CDL	C19-C18	-3.15	1.33	1.51
26	P	308	CDL	C22-C21	-3.14	1.34	1.51
26	P	308	CDL	C42-C41	-3.14	1.34	1.51
26	G	101	CDL	C22-C21	-3.13	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	101	CDL	C19-C18	-3.09	1.34	1.51
26	T	101	CDL	C42-C41	-3.07	1.34	1.51
26	T	101	CDL	C39-C38	-3.06	1.34	1.51
15	A	603	HEA	CMC-C2C	2.91	1.57	1.51
23	B	303	CHD	C11-C9	2.90	1.58	1.53
14	A	608	PGV	O01-C1	2.77	1.42	1.34
15	N	603	HEA	C3A-C2A	-2.76	1.36	1.40
15	A	602[A]	HEA	C3C-C2C	-2.76	1.36	1.40
15	A	602[B]	HEA	C3C-C2C	-2.76	1.36	1.40
14	N	609	PGV	O03-C19	2.76	1.41	1.33
15	A	602[A]	HEA	C3A-C2A	-2.67	1.36	1.40
15	A	602[B]	HEA	C3A-C2A	-2.67	1.36	1.40
15	N	602[B]	HEA	O11-C11	2.65	1.48	1.42
25	P	304	PEK	O03-C21	2.64	1.41	1.33
15	N	603	HEA	O11-C11	2.63	1.48	1.42
14	C	306	PGV	O01-C1	2.46	1.41	1.34
15	A	603	HEA	C3B-C11	2.43	1.54	1.52
15	A	603	HEA	C3C-C2C	-2.41	1.37	1.40
14	A	608	PGV	O01-C02	-2.39	1.40	1.46
27	M	106	DMU	O16-C6	2.34	1.44	1.40
23	C	311	CHD	C13-C14	-2.31	1.51	1.55
14	N	609	PGV	O01-C02	-2.30	1.40	1.46
14	P	306	PGV	P-O14	-2.26	1.44	1.55
23	C	301	CHD	C11-C9	2.26	1.57	1.53
25	P	304	PEK	C05-C04	2.25	1.59	1.50
23	J	101	CHD	C13-C14	-2.24	1.51	1.55
23	P	310	CHD	C13-C14	-2.24	1.51	1.55
15	N	602[A]	HEA	C3C-CAC	2.21	1.52	1.47
15	N	602[B]	HEA	C3C-CAC	2.21	1.52	1.47
14	N	609	PGV	O03-C01	2.18	1.50	1.45
15	N	602[A]	HEA	CAD-C3D	2.17	1.55	1.52
15	N	602[B]	HEA	CAD-C3D	2.17	1.55	1.52
14	C	306	PGV	O01-C02	-2.13	1.41	1.46
23	Y	104	CHD	C13-C14	-2.12	1.51	1.55
14	N	609	PGV	C03-C02	2.10	1.57	1.50
23	C	301	CHD	O12-C12	2.09	1.47	1.43
23	P	301	CHD	C11-C9	2.08	1.57	1.53
23	W	101	CHD	C13-C14	-2.07	1.52	1.55
23	C	301	CHD	C13-C12	-2.04	1.51	1.54
27	V	102	DMU	O16-C6	2.04	1.43	1.40
15	A	602[A]	HEA	C1D-C2D	-2.04	1.38	1.42
15	A	602[B]	HEA	C1D-C2D	-2.04	1.38	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	603	HEA	O11-C11	2.02	1.47	1.42
21	B	301	TGL	OC1-CC1	-2.02	1.16	1.22

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[A]	HEA	C13-C12-C11	-8.27	101.93	114.35
15	A	602[A]	HEA	C13-C12-C11	-6.51	104.56	114.35
23	P	310	CHD	C13-C14-C8	-6.48	106.46	114.74
15	N	602[A]	HEA	C1B-C2B-C3B	-6.40	102.54	107.00
15	N	602[B]	HEA	C1B-C2B-C3B	-6.40	102.54	107.00
26	G	101	CDL	OA6-CA5-C11	5.94	124.31	111.50
14	C	307	PGV	O01-C1-C2	5.92	124.25	111.50
21	B	301	TGL	OG2-CB1-CB2	5.50	123.36	111.50
23	C	311	CHD	C13-C14-C8	-5.26	108.02	114.74
14	P	307	PGV	O03-C19-C20	5.18	128.15	111.91
14	N	601	PGV	O01-C1-C2	5.17	122.64	111.50
22	B	302	PSC	O01-C1-C2	5.14	122.58	111.50
23	B	303	CHD	C11-C9-C10	-5.09	108.47	113.73
22	O	301	PSC	O01-C1-C2	5.08	122.45	111.50
25	C	305	PEK	O01-C1-C2	5.06	122.42	111.50
21	N	608	TGL	OG2-CB1-CB2	5.04	122.37	111.50
15	A	602[A]	HEA	CAA-CBA-CGA	-5.00	104.28	112.67
15	A	602[B]	HEA	CAA-CBA-CGA	-5.00	104.28	112.67
14	C	307	PGV	O03-C19-C20	4.97	127.50	111.91
23	W	101	CHD	C1-C10-C5	4.95	115.08	107.77
25	C	303	PEK	O01-C1-C2	4.86	121.97	111.50
26	G	101	CDL	OB6-CB5-C51	4.76	121.77	111.50
26	C	308	CDL	OB6-CB5-C51	4.76	121.77	111.50
26	P	308	CDL	OB6-CB5-C51	4.74	121.72	111.50
15	A	603	HEA	CAD-CBD-CGD	-4.73	104.73	112.67
26	G	101	CDL	OA8-CA7-C31	4.69	126.62	111.91
23	P	310	CHD	C11-C12-C13	4.67	116.03	111.24
26	T	101	CDL	OB6-CB5-C51	4.65	121.53	111.50
15	A	602[A]	HEA	CMB-C2B-C3B	4.58	133.65	124.69
15	A	602[B]	HEA	CMB-C2B-C3B	4.58	133.65	124.69
23	C	311	CHD	C11-C12-C13	4.57	115.94	111.24
15	A	603	HEA	C1B-C2B-C3B	-4.57	103.82	107.00
26	P	308	CDL	OA6-CA5-C11	4.45	121.08	111.50
25	C	303	PEK	C02-O01-C1	-4.43	106.88	117.79
23	J	101	CHD	C11-C9-C10	-4.40	109.19	113.73
15	N	602[A]	HEA	CMB-C2B-C3B	4.35	133.21	124.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[B]	HEA	CMB-C2B-C3B	4.35	133.21	124.69
23	C	301	CHD	C18-C13-C12	4.31	113.45	109.07
15	A	602[B]	HEA	C13-C12-C11	-4.27	107.93	114.35
25	P	305	PEK	O01-C1-C2	4.27	120.70	111.50
14	P	307	PGV	O01-C1-C2	4.27	120.70	111.50
21	L	101	TGL	OG2-CB1-CB2	4.18	120.50	111.50
26	P	308	CDL	OB8-CB7-C71	4.17	124.99	111.91
23	C	301	CHD	C22-C20-C17	-4.13	101.75	110.28
15	A	602[A]	HEA	C1B-C2B-C3B	-4.12	104.13	107.00
15	A	602[B]	HEA	C1B-C2B-C3B	-4.12	104.13	107.00
21	Y	101	TGL	OG2-CB1-CB2	4.09	120.31	111.50
15	A	602[A]	HEA	CMB-C2B-C1B	-4.07	122.21	128.46
15	A	602[B]	HEA	CMB-C2B-C1B	-4.07	122.21	128.46
25	P	303	PEK	O01-C1-C2	4.04	120.20	111.50
23	Y	104	CHD	C13-C17-C20	-4.03	114.69	119.50
25	P	305	PEK	O03-C21-C22	3.94	124.28	111.91
23	Y	104	CHD	C5-C4-C3	-3.93	106.98	112.76
27	V	102	DMU	O1-C10-C5	3.93	118.66	110.35
14	P	306	PGV	O01-C1-O02	-3.91	114.26	123.70
15	N	603	HEA	CAD-CBD-CGD	-3.91	106.12	112.67
23	J	101	CHD	C6-C5-C4	-3.87	106.73	111.19
15	N	602[B]	HEA	C13-C12-C11	-3.85	108.56	114.35
23	J	101	CHD	C13-C17-C20	-3.83	114.92	119.50
23	P	310	CHD	C11-C9-C10	-3.75	109.86	113.73
23	J	101	CHD	C19-C10-C9	-3.74	106.03	111.18
23	W	101	CHD	C1-C10-C9	-3.72	105.50	111.35
23	J	101	CHD	C10-C9-C8	-3.71	107.84	111.82
22	O	301	PSC	C03-C02-C01	-3.70	103.03	111.79
23	C	301	CHD	C1-C2-C3	-3.69	105.73	110.47
23	W	101	CHD	C11-C9-C10	-3.67	109.94	113.73
21	B	301	TGL	OG3-CC1-CC2	3.63	123.29	111.91
23	P	310	CHD	C9-C11-C12	3.62	119.08	114.30
23	C	311	CHD	C11-C9-C10	-3.60	110.02	113.73
26	G	101	CDL	CA6-OA8-CA7	3.59	130.42	117.12
14	A	601	PGV	O01-C1-C2	3.58	119.22	111.50
23	C	311	CHD	C9-C11-C12	3.58	119.02	114.30
26	P	308	CDL	OA8-CA7-C31	3.53	122.99	111.91
23	Y	104	CHD	C17-C13-C14	3.53	103.65	100.09
14	N	609	PGV	O01-C1-O02	-3.53	115.18	123.70
26	C	308	CDL	OB8-CB7-C71	3.52	122.96	111.91
27	Z	102	DMU	C10-C5-C7	3.52	117.32	110.00
21	Q	201	TGL	OG1-CA1-CA2	3.50	122.88	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	602[A]	HEA	C26-C15-C16	3.47	121.11	115.27
27	Z	102	DMU	O1-C10-C5	3.46	117.67	110.35
15	N	603	HEA	C13-C12-C11	-3.44	109.17	114.35
23	B	303	CHD	C22-C23-C24	-3.43	106.21	113.59
23	Y	104	CHD	C1-C2-C3	3.42	114.86	110.47
23	G	102	CHD	C11-C9-C10	-3.41	110.21	113.73
26	G	101	CDL	OA6-CA5-OA7	-3.41	115.46	123.70
25	P	303	PEK	O03-C21-C22	3.41	122.61	111.91
23	Y	104	CHD	C9-C8-C7	-3.41	107.80	111.88
23	P	301	CHD	C22-C23-C24	-3.40	106.28	113.59
22	B	302	PSC	O01-C02-C03	3.40	120.71	108.40
26	P	308	CDL	CB4-OB6-CB5	-3.37	109.51	117.79
23	W	101	CHD	C6-C5-C4	-3.36	107.32	111.19
26	G	101	CDL	CA4-OA6-CA5	-3.35	109.54	117.79
15	N	602[A]	HEA	CAA-CBA-CGA	-3.26	107.19	112.67
15	N	602[B]	HEA	CAA-CBA-CGA	-3.26	107.19	112.67
21	L	101	TGL	OG3-CC1-OC1	-3.26	115.36	123.59
14	P	306	PGV	C03-C02-C01	-3.26	104.08	111.79
14	C	306	PGV	C21-C20-C19	-3.25	101.79	113.62
23	Y	104	CHD	C10-C9-C8	-3.25	108.33	111.82
14	N	601	PGV	O01-C1-O02	-3.25	115.85	123.70
26	G	101	CDL	OA8-CA7-OA9	-3.24	115.41	123.59
23	B	303	CHD	C9-C11-C12	-3.24	110.03	114.30
23	B	303	CHD	C19-C10-C5	-3.21	104.91	110.36
23	Y	104	CHD	C6-C5-C10	3.19	116.05	112.66
21	B	301	TGL	OG1-CA1-CA2	3.18	121.88	111.91
25	C	303	PEK	O03-C21-C22	3.18	121.88	111.91
14	C	307	PGV	C01-O03-C19	3.17	128.85	117.12
23	G	102	CHD	C13-C17-C20	-3.14	115.74	119.50
27	M	106	DMU	C10-O7-C3	-3.13	110.21	117.96
15	N	603	HEA	C1B-C2B-C3B	-3.10	104.84	107.00
27	G	108	DMU	C7-C8-C9	3.10	115.76	110.24
25	C	304	PEK	O03-C21-C22	3.08	121.56	111.91
15	A	603	HEA	C27-C19-C20	3.08	120.44	115.27
22	O	301	PSC	C21-C20-C19	-3.06	102.48	113.62
14	C	307	PGV	C02-O01-C1	-3.06	110.27	117.79
26	C	308	CDL	CB4-OB6-CB5	-3.04	110.31	117.79
23	J	101	CHD	C1-C2-C3	3.04	114.37	110.47
23	Y	104	CHD	C13-C14-C8	-3.04	110.86	114.74
26	T	101	CDL	OA6-CA5-C11	3.02	118.00	111.50
27	V	102	DMU	C10-C5-C7	3.00	116.25	110.00
23	B	303	CHD	C6-C5-C4	-3.00	107.74	111.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	201	TGL	OG1-CA1-CA2	2.99	121.28	111.91
21	N	608	TGL	OG3-CC1-CC2	2.98	121.27	111.91
25	P	304	PEK	O11-P-O14	-2.98	97.44	109.07
15	N	603	HEA	C27-C19-C20	2.97	120.28	115.27
25	C	305	PEK	O03-C21-C22	2.97	121.21	111.91
23	B	303	CHD	O12-C12-C13	-2.96	106.02	111.03
25	C	305	PEK	C02-O01-C1	-2.96	110.50	117.79
15	A	602[A]	HEA	C25-C23-C24	2.93	121.08	114.60
25	C	303	PEK	O01-C1-O02	-2.93	116.62	123.70
15	N	602[B]	HEA	C27-C19-C20	2.93	120.19	115.27
21	Q	201	TGL	OG2-CB1-CB2	2.91	117.77	111.50
14	N	609	PGV	O03-C19-O04	-2.89	116.30	123.59
23	P	301	CHD	C21-C20-C22	-2.89	105.84	110.36
25	P	305	PEK	O03-C21-O04	-2.89	116.31	123.59
14	C	307	PGV	O03-C19-O04	-2.87	116.35	123.59
26	G	101	CDL	CB6-CB4-CB3	-2.86	105.01	111.79
27	M	101	DMU	C18-O16-C6	-2.86	109.10	113.84
23	C	311	CHD	C14-C8-C9	-2.86	105.78	109.71
15	A	603	HEA	CBD-CAD-C3D	2.85	117.74	112.49
26	C	308	CDL	OA8-CA7-C31	2.85	120.85	111.91
23	C	311	CHD	C14-C13-C12	2.84	110.05	107.40
21	L	101	TGL	CC3-CC2-CC1	2.82	123.88	113.62
23	B	303	CHD	O12-C12-C11	2.81	114.85	109.12
27	G	108	DMU	C8-C7-C5	2.79	115.70	110.82
23	C	311	CHD	C22-C23-C24	-2.79	107.59	113.59
15	N	603	HEA	CBA-CAA-C2A	-2.79	107.33	112.48
23	W	101	CHD	C4-C5-C10	2.79	115.62	112.66
21	N	608	TGL	OG1-CA1-CA2	2.78	120.63	111.91
14	N	601	PGV	O03-C19-C20	2.78	120.63	111.91
15	A	603	HEA	C20-C19-C18	-2.78	115.50	121.12
14	P	307	PGV	C21-C20-C19	-2.77	103.56	113.62
26	P	308	CDL	OB8-CB7-OB9	-2.75	116.65	123.59
15	N	602[A]	HEA	CMB-C2B-C1B	-2.74	124.25	128.46
15	N	602[B]	HEA	CMB-C2B-C1B	-2.74	124.25	128.46
14	A	601	PGV	O03-C19-C20	2.74	120.51	111.91
23	W	101	CHD	C4-C3-C2	-2.73	107.30	110.55
15	N	602[A]	HEA	C26-C15-C16	2.72	119.84	115.27
27	G	108	DMU	C10-O7-C3	-2.71	111.25	117.96
23	P	310	CHD	C14-C13-C12	2.71	109.93	107.40
14	C	307	PGV	O01-C1-O02	-2.71	117.16	123.70
25	P	304	PEK	O03-C21-C22	2.69	120.36	111.91
15	A	603	HEA	CMC-C2C-C1C	-2.68	124.34	128.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	101	TGL	OG3-CC1-CC2	2.68	120.31	111.91
15	A	602[B]	HEA	C13-C14-C15	-2.67	121.22	127.66
23	G	102	CHD	C6-C5-C4	-2.67	108.11	111.19
23	B	303	CHD	C16-C17-C13	2.66	106.16	103.55
22	B	302	PSC	C04-C05-N	-2.66	106.91	115.78
21	Y	101	TGL	OG1-CA1-CA2	2.65	120.21	111.91
25	P	305	PEK	C02-O01-C1	-2.63	111.31	117.79
27	C	319	DMU	C10-O1-C9	2.62	118.83	113.69
25	C	304	PEK	O11-P-O14	-2.61	98.85	109.07
23	P	301	CHD	C6-C7-C8	-2.61	108.70	111.48
27	P	324	DMU	O7-C10-C5	2.57	114.75	108.10
23	P	301	CHD	O12-C12-C11	2.56	114.34	109.12
21	L	101	TGL	OG1-CA1-CA2	2.55	119.91	111.91
23	P	311	CHD	C22-C23-C24	-2.55	108.11	113.59
23	P	310	CHD	C17-C13-C14	2.54	102.65	100.09
26	G	101	CDL	CB4-OB6-CB5	-2.53	111.56	117.79
15	N	602[A]	HEA	C3C-C4C-NC	2.53	112.48	109.21
15	N	602[B]	HEA	C3C-C4C-NC	2.53	112.48	109.21
23	C	309	CHD	C16-C17-C13	2.52	106.03	103.55
21	L	101	TGL	OG3-CC1-CC2	2.52	119.82	111.91
23	C	301	CHD	C22-C23-C24	-2.52	108.17	113.59
21	N	608	TGL	CG3-CG2-CG1	-2.52	105.83	111.79
26	C	308	CDL	OA6-CA5-C11	2.51	116.92	111.50
27	Z	102	DMU	C10-O7-C3	-2.51	111.75	117.96
27	M	106	DMU	C10-C5-C7	2.51	115.22	110.00
26	T	101	CDL	OA8-CA7-C31	2.50	119.77	111.91
23	Y	104	CHD	C9-C10-C5	2.50	112.09	108.58
23	B	303	CHD	C1-C10-C5	2.50	111.47	107.77
26	T	101	CDL	CB6-CB4-CB3	-2.49	105.89	111.79
26	P	308	CDL	OA8-CA7-OA9	-2.49	117.30	123.59
14	P	307	PGV	O03-C19-O04	-2.47	117.35	123.59
21	Q	201	TGL	OG1-CA1-OA1	-2.47	117.35	123.59
15	A	602[A]	HEA	O11-C11-C3B	-2.47	104.88	112.00
21	D	201	TGL	CB3-CB2-CB1	2.47	122.59	113.62
21	Q	201	TGL	CG2-OG2-CB1	-2.46	111.75	117.79
23	J	101	CHD	C4-C3-C2	-2.45	107.63	110.55
21	D	201	TGL	OG1-CA1-OA1	-2.45	117.41	123.59
23	P	301	CHD	C22-C20-C17	-2.44	105.24	110.28
15	N	602[B]	HEA	C13-C14-C15	-2.43	121.80	127.66
25	C	304	PEK	O01-C1-C2	2.43	116.75	111.50
25	C	305	PEK	O03-C21-O04	-2.43	117.45	123.59
23	P	301	CHD	C6-C5-C4	-2.43	108.39	111.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	302	PSC	C3-C2-C1	-2.43	104.79	113.62
23	G	102	CHD	C11-C12-C13	2.42	113.73	111.24
23	G	102	CHD	C19-C10-C1	-2.42	104.36	108.26
21	L	101	TGL	CG3-CG2-CG1	-2.41	106.08	111.79
14	P	306	PGV	O01-C1-C2	2.41	116.69	111.50
23	P	311	CHD	C13-C14-C8	-2.40	111.67	114.74
21	B	301	TGL	CG3-CG2-CG1	-2.40	106.11	111.79
25	P	303	PEK	O03-C21-O04	-2.40	117.54	123.59
22	O	301	PSC	C14-C13-C12	-2.40	106.33	124.73
14	A	601	PGV	C02-O01-C1	-2.39	111.91	117.79
26	T	101	CDL	CB4-OB6-CB5	-2.38	111.92	117.79
15	A	603	HEA	CMC-C2C-C3C	2.38	129.13	124.68
22	O	301	PSC	O01-C1-O02	-2.37	117.96	123.70
14	P	307	PGV	O04-C19-C20	-2.37	114.48	123.73
15	N	602[A]	HEA	C16-C15-C14	-2.36	116.33	121.12
15	A	603	HEA	C16-C15-C14	-2.36	116.34	121.12
23	P	310	CHD	C14-C8-C9	-2.36	106.47	109.71
23	P	311	CHD	C15-C14-C13	2.36	105.86	103.55
23	P	311	CHD	C16-C17-C13	2.35	105.86	103.55
23	C	311	CHD	C16-C17-C20	-2.35	108.50	112.15
23	J	101	CHD	C13-C14-C8	-2.35	111.74	114.74
23	J	101	CHD	C14-C8-C9	2.34	112.92	109.71
23	J	101	CHD	C9-C8-C7	-2.34	109.08	111.88
20	S	112	EDO	O2-C2-C1	-2.34	95.08	111.91
21	Q	201	TGL	OG3-CC1-CC2	2.34	119.24	111.91
15	A	603	HEA	C21-C20-C19	2.33	120.66	112.98
23	Y	104	CHD	C23-C22-C20	-2.33	111.58	114.72
21	D	201	TGL	CG3-OG3-CC1	2.33	125.74	117.12
15	A	603	HEA	CAA-CBA-CGA	-2.33	108.77	112.67
25	P	304	PEK	C03-C02-C01	-2.33	106.29	111.79
23	W	101	CHD	C13-C17-C20	-2.32	116.72	119.50
15	N	603	HEA	C21-C22-C23	-2.32	119.81	127.75
23	B	303	CHD	C13-C17-C20	-2.31	116.73	119.50
27	M	101	DMU	C31-C28-C25	-2.31	102.69	114.42
15	A	602[B]	HEA	C21-C20-C19	-2.31	105.39	112.98
23	G	102	CHD	C22-C23-C24	-2.30	108.64	113.59
26	T	101	CDL	OB6-CB5-OB7	-2.30	118.15	123.70
22	B	302	PSC	O01-C1-O02	-2.29	118.16	123.70
26	C	308	CDL	OB8-CB7-OB9	-2.29	117.80	123.59
21	Q	201	TGL	OG3-CC1-OC1	-2.29	117.82	123.59
26	C	308	CDL	C80-C79-C78	2.28	126.03	114.42
14	P	306	PGV	C21-C20-C19	-2.28	105.33	113.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	307	PGV	C3-C2-C1	-2.28	105.34	113.62
26	P	308	CDL	C72-C71-CB7	-2.28	105.34	113.62
23	C	301	CHD	O3-C3-C2	-2.27	104.39	110.16
21	B	301	TGL	CB3-CB2-CB1	-2.27	105.38	113.62
27	P	323	DMU	C10-O1-C9	2.26	118.13	113.69
21	L	101	TGL	OG2-CB1-OB1	-2.26	118.23	123.70
26	C	308	CDL	OB6-CB5-OB7	-2.26	118.23	123.70
23	C	309	CHD	C13-C14-C8	-2.25	111.86	114.74
15	N	603	HEA	CBD-CAD-C3D	2.25	116.64	112.49
26	G	101	CDL	OB6-CB5-OB7	-2.25	118.27	123.70
25	C	305	PEK	O01-C1-O02	-2.25	118.27	123.70
15	N	603	HEA	C21-C20-C19	2.25	120.37	112.98
23	J	101	CHD	C1-C10-C5	2.24	111.09	107.77
23	C	309	CHD	C22-C23-C24	-2.24	108.78	113.59
14	P	307	PGV	C02-O01-C1	-2.24	112.28	117.79
22	B	302	PSC	O03-C01-C02	-2.24	101.93	108.43
14	C	307	PGV	C21-C20-C19	-2.23	105.50	113.62
23	Y	104	CHD	C19-C10-C9	-2.23	108.11	111.18
14	A	601	PGV	C4-C3-C2	-2.22	105.20	113.19
27	V	102	DMU	C10-O1-C9	2.22	118.05	113.69
23	P	310	CHD	C9-C8-C7	2.21	114.52	111.88
23	C	311	CHD	C1-C10-C5	2.21	111.03	107.77
14	C	306	PGV	O01-C02-C03	-2.20	100.45	108.40
25	P	304	PEK	O13-P-O14	2.19	123.08	112.24
23	P	310	CHD	C1-C10-C5	2.19	111.00	107.77
27	Z	101	DMU	C10-O7-C3	-2.18	112.56	117.96
23	C	301	CHD	C6-C7-C8	-2.18	109.15	111.48
23	C	311	CHD	C22-C20-C17	-2.18	105.79	110.28
22	B	302	PSC	C01-O03-C19	2.18	125.18	117.12
23	P	301	CHD	C9-C11-C12	-2.17	111.43	114.30
23	C	309	CHD	C23-C22-C20	-2.17	111.80	114.72
23	P	310	CHD	C16-C17-C20	-2.17	108.79	112.15
23	P	301	CHD	C10-C9-C8	-2.17	109.49	111.82
23	G	102	CHD	C13-C14-C8	-2.16	111.97	114.74
23	P	310	CHD	C22-C23-C24	-2.16	108.95	113.59
25	P	304	PEK	O03-C21-O04	-2.16	118.15	123.59
15	A	603	HEA	C13-C12-C11	-2.15	111.11	114.35
23	C	309	CHD	C14-C8-C9	-2.15	106.76	109.71
23	P	311	CHD	C19-C10-C9	-2.15	108.23	111.18
21	L	101	TGL	C21-C20-CA9	-2.15	103.53	114.42
23	C	309	CHD	C15-C14-C13	2.15	105.66	103.55
15	N	602[A]	HEA	C25-C23-C24	2.14	119.34	114.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	323	DMU	O1-C9-C8	2.14	113.58	109.69
23	P	301	CHD	O12-C12-C13	-2.14	107.42	111.03
25	C	303	PEK	O03-C21-O04	-2.13	118.22	123.59
27	M	101	DMU	C22-C19-C18	-2.12	104.08	113.49
23	Y	104	CHD	O12-C12-C11	2.12	113.45	109.12
21	D	201	TGL	OG3-CG3-CG2	-2.12	102.25	108.43
23	P	311	CHD	C11-C9-C10	-2.12	111.54	113.73
23	B	303	CHD	C16-C17-C20	-2.12	108.86	112.15
27	C	319	DMU	C6-C1-C2	2.12	114.41	110.00
25	P	303	PEK	C03-C02-C01	-2.11	106.80	111.79
27	C	319	DMU	O1-C9-C8	2.11	113.52	109.69
23	J	101	CHD	C17-C13-C14	2.10	102.21	100.09
14	N	609	PGV	O03-C19-C20	2.10	118.50	111.91
23	Y	104	CHD	C11-C9-C10	-2.09	111.57	113.73
14	C	306	PGV	O01-C1-C2	2.08	115.99	111.50
27	M	106	DMU	O7-C3-C4	2.08	115.15	109.45
23	C	301	CHD	O12-C12-C13	-2.08	107.51	111.03
27	M	106	DMU	C2-C3-C4	-2.08	106.16	110.93
23	B	303	CHD	C10-C9-C8	2.06	114.03	111.82
14	P	307	PGV	C01-O03-C19	2.06	124.76	117.12
15	N	602[A]	HEA	CAD-C3D-C2D	2.06	133.17	127.25
15	N	602[B]	HEA	CAD-C3D-C2D	2.06	133.17	127.25
14	N	601	PGV	C02-O01-C1	-2.06	112.72	117.79
23	C	301	CHD	C19-C10-C1	-2.05	104.96	108.26
25	P	305	PEK	C01-O03-C21	2.05	124.71	117.12
27	Z	101	DMU	C34-C31-C28	-2.05	104.04	114.42
21	Y	101	TGL	OG3-CC1-OC1	-2.05	118.43	123.59
23	P	301	CHD	C19-C10-C1	-2.04	104.97	108.26
26	C	308	CDL	OA6-CA4-CA3	2.04	115.79	108.40
15	A	603	HEA	CBA-CAA-C2A	-2.04	108.72	112.48
15	N	603	HEA	CAA-CBA-CGA	-2.03	109.26	112.67
14	A	608	PGV	O03-C19-C20	2.03	118.29	111.91
15	N	602[A]	HEA	O11-C11-C3B	-2.03	106.15	112.00
23	Y	104	CHD	C22-C23-C24	-2.03	109.23	113.59
26	P	308	CDL	CA6-CA4-CA3	-2.03	106.99	111.79
23	P	310	CHD	C14-C8-C7	2.03	114.49	111.81
26	G	101	CDL	OA8-CA6-CA4	-2.02	102.56	108.43
23	P	311	CHD	C5-C4-C3	-2.01	109.80	112.76
25	P	303	PEK	C01-O03-C21	2.00	124.54	117.12
14	N	601	PGV	O01-C02-C03	2.00	115.64	108.40

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	602[A]	HEA	NB
15	A	602[A]	HEA	ND
15	A	602[A]	HEA	NA
15	A	602[B]	HEA	NB
15	A	602[B]	HEA	ND
15	A	602[B]	HEA	NA
15	A	602[C]	HEA	NB
15	A	602[C]	HEA	ND
15	A	602[C]	HEA	NA
15	A	603	HEA	NB
15	A	603	HEA	ND
15	A	603	HEA	NA
15	N	602[A]	HEA	NB
15	N	602[A]	HEA	ND
15	N	602[A]	HEA	NA
15	N	602[B]	HEA	NB
15	N	602[B]	HEA	ND
15	N	602[B]	HEA	NA
15	N	602[C]	HEA	NB
15	N	602[C]	HEA	ND
15	N	602[C]	HEA	NA
15	N	603	HEA	NB
15	N	603	HEA	ND
15	N	603	HEA	NA

All (652) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	PGV	O04-C19-O03-C01
14	A	601	PGV	C20-C19-O03-C01
14	C	307	PGV	C04-O12-P-O13
14	C	307	PGV	O04-C19-O03-C01
14	C	307	PGV	C20-C19-O03-C01
14	N	601	PGV	C2-C1-O01-C02
14	N	601	PGV	O04-C19-O03-C01
14	N	601	PGV	C20-C19-O03-C01
14	P	306	PGV	C10-C11-C12-C13
14	P	307	PGV	O04-C19-O03-C01
14	P	307	PGV	C20-C19-O03-C01
20	M	105	EDO	O1-C1-C2-O2
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	Y	101	TGL	CB2-CB1-OG2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	B	302	PSC	C04-O12-P-O11
22	B	302	PSC	C04-O12-P-O13
22	B	302	PSC	C04-O12-P-O14
22	B	302	PSC	C2-C1-O01-C02
22	O	301	PSC	C03-O11-P-O13
22	O	301	PSC	C03-O11-P-O14
22	O	301	PSC	O02-C1-O01-C02
22	O	301	PSC	C2-C1-O01-C02
25	C	303	PEK	C03-O11-P-O13
25	C	303	PEK	C03-O11-P-O14
25	C	303	PEK	O04-C21-O03-C01
25	C	303	PEK	C22-C21-O03-C01
25	C	305	PEK	O04-C21-O03-C01
25	C	305	PEK	C22-C21-O03-C01
25	C	305	PEK	C5-C6-C7-C8
25	P	303	PEK	O04-C21-O03-C01
25	P	303	PEK	C22-C21-O03-C01
25	P	303	PEK	C4-C5-C6-C7
25	P	305	PEK	O04-C21-O03-C01
25	P	305	PEK	C22-C21-O03-C01
26	C	308	CDL	CA2-OA2-PA1-OA3
26	C	308	CDL	C11-CA5-OA6-CA4
26	C	308	CDL	OA9-CA7-OA8-CA6
26	C	308	CDL	C31-CA7-OA8-CA6
26	C	308	CDL	CB3-OB5-PB2-OB4
26	G	101	CDL	CA3-OA5-PA1-OA3
26	G	101	CDL	CB3-OB5-PB2-OB2
26	P	308	CDL	CA2-OA2-PA1-OA3
26	P	308	CDL	CA3-OA5-PA1-OA3
26	P	308	CDL	OA9-CA7-OA8-CA6
26	P	308	CDL	C31-CA7-OA8-CA6
26	P	308	CDL	CB2-OB2-PB2-OB3
26	P	308	CDL	CB3-OB5-PB2-OB4
26	T	101	CDL	CA2-OA2-PA1-OA5
26	T	101	CDL	CA3-OA5-PA1-OA2
26	T	101	CDL	OA9-CA7-OA8-CA6
26	T	101	CDL	C31-CA7-OA8-CA6
27	P	324	DMU	O5-C6-O16-C18
27	P	324	DMU	C5-C10-O7-C3
27	Z	102	DMU	C1-C6-O16-C18
27	Z	102	DMU	O5-C6-O16-C18
27	Z	102	DMU	C19-C18-O16-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	G	101	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	C31-CA7-OA8-CA6
23	J	101	CHD	C21-C20-C22-C23
27	P	324	DMU	O1-C10-O7-C3
14	A	601	PGV	O02-C1-O01-C02
14	N	601	PGV	O02-C1-O01-C02
21	Y	101	TGL	OB1-CB1-OG2-CG2
22	B	302	PSC	O02-C1-O01-C02
26	C	308	CDL	OA7-CA5-OA6-CA4
27	V	102	DMU	C5-C10-O7-C3
27	P	324	DMU	O6-C11-C9-O1
23	W	101	CHD	C21-C20-C22-C23
23	Y	104	CHD	C21-C20-C22-C23
27	V	102	DMU	O6-C11-C9-O1
14	N	601	PGV	C10-C11-C12-C13
25	C	303	PEK	C4-C5-C6-C7
25	C	305	PEK	C4-C5-C6-C7
25	C	305	PEK	C13-C14-C15-C16
27	V	102	DMU	O1-C10-O7-C3
23	C	309	CHD	C17-C20-C22-C23
27	P	324	DMU	O6-C11-C9-C8
27	G	108	DMU	O5-C4-C57-O61
27	V	102	DMU	O5-C4-C57-O61
14	A	601	PGV	C2-C1-O01-C02
21	L	101	TGL	CC3-CC4-CC5-CC6
26	P	308	CDL	C80-C81-C82-C83
23	P	311	CHD	C17-C20-C22-C23
27	M	106	DMU	O5-C4-C57-O61
27	P	324	DMU	C3-C4-C57-O61
27	V	102	DMU	O6-C11-C9-C8
23	C	309	CHD	C21-C20-C22-C23
23	P	311	CHD	C21-C20-C22-C23
26	C	308	CDL	C57-C58-C59-C60
27	P	324	DMU	O5-C4-C57-O61
27	M	106	DMU	C3-C4-C57-O61
21	Y	101	TGL	CA2-CA1-OG1-CG1
23	Y	104	CHD	C20-C22-C23-C24
27	Z	102	DMU	O5-C4-C57-O61
27	V	102	DMU	C3-C4-C57-O61
26	G	101	CDL	CA7-C31-C32-C33
21	Y	101	TGL	OA1-CA1-OG1-CG1
14	P	307	PGV	C1-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	C	303	PEK	C7-C8-C9-C10
25	C	305	PEK	C10-C11-C12-C13
25	P	305	PEK	C13-C14-C15-C16
21	Y	101	TGL	CC1-CC2-CC3-CC4
23	Y	104	CHD	C17-C20-C22-C23
21	L	101	TGL	CC6-CC7-CC8-CC9
20	N	618	EDO	O1-C1-C2-O2
21	Q	201	TGL	CA9-C20-C21-C22
23	W	101	CHD	C20-C22-C23-C24
22	O	301	PSC	C23-C24-C25-C26
27	P	309	DMU	C5-C10-O7-C3
26	C	308	CDL	C42-C43-C44-C45
27	C	310	DMU	O16-C18-C19-C22
27	P	309	DMU	O16-C18-C19-C22
27	C	319	DMU	O6-C11-C9-C8
27	V	102	DMU	O5-C6-O16-C18
27	M	106	DMU	O16-C18-C19-C22
27	Z	102	DMU	O16-C18-C19-C22
14	C	307	PGV	O12-C04-C05-O05
27	P	324	DMU	O16-C18-C19-C22
27	G	108	DMU	C3-C4-C57-O61
21	Q	201	TGL	CB2-CB1-OG2-CG2
14	C	307	PGV	C04-O12-P-O11
22	O	301	PSC	C03-O11-P-O12
25	C	303	PEK	C03-O11-P-O12
26	C	308	CDL	CB3-OB5-PB2-OB2
26	P	308	CDL	CB3-OB5-PB2-OB2
27	C	319	DMU	O5-C4-C57-O61
27	P	309	DMU	O1-C10-O7-C3
26	G	101	CDL	C80-C81-C82-C83
27	C	319	DMU	O6-C11-C9-O1
14	C	307	PGV	O12-C04-C05-C06
21	Q	201	TGL	OB1-CB1-OG2-CG2
25	C	303	PEK	O02-C1-O01-C02
23	C	309	CHD	C20-C22-C23-C24
23	P	311	CHD	C20-C22-C23-C24
25	C	303	PEK	C2-C1-O01-C02
27	Z	102	DMU	C28-C31-C34-C37
21	L	101	TGL	CC2-CC1-OG3-CG3
21	D	201	TGL	CA9-C20-C21-C22
21	Y	101	TGL	C12-C13-C14-C29
21	N	608	TGL	OB1-CB1-OG2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	D	201	TGL	CB1-CB2-CB3-CB4
21	L	101	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	CB2-CB3-CB4-CB5
21	Y	101	TGL	CC4-CC5-CC6-CC7
22	B	302	PSC	C11-C10-C9-C8
25	P	304	PEK	C7-C8-C9-C10
26	P	308	CDL	C57-C58-C59-C60
21	N	608	TGL	CB1-CB2-CB3-CB4
21	L	101	TGL	CA2-CA1-OG1-CG1
14	P	306	PGV	C24-C25-C26-C27
21	L	101	TGL	CC2-CC3-CC4-CC5
21	L	101	TGL	CA9-C20-C21-C22
26	T	101	CDL	C77-C78-C79-C80
21	D	201	TGL	CA6-CA7-CA8-CA9
26	T	101	CDL	CA5-C11-C12-C13
21	Q	201	TGL	C20-C21-C22-C23
21	Y	101	TGL	CC3-CC4-CC5-CC6
26	C	308	CDL	C20-C21-C22-C23
26	P	308	CDL	C77-C78-C79-C80
27	C	310	DMU	C31-C34-C37-C40
27	C	319	DMU	C3-C4-C57-O61
21	D	201	TGL	CC7-CC8-CC9-C15
21	N	608	TGL	CB4-CB5-CB6-CB7
26	C	308	CDL	C40-C41-C42-C43
27	G	108	DMU	C28-C31-C34-C37
26	T	101	CDL	OB7-CB5-OB6-CB4
21	N	608	TGL	CB2-CB1-OG2-CG2
26	P	308	CDL	C51-CB5-OB6-CB4
26	T	101	CDL	C51-CB5-OB6-CB4
21	B	301	TGL	C11-C12-C13-C14
21	B	301	TGL	C21-C22-C23-C24
21	N	608	TGL	CB3-CB4-CB5-CB6
21	Y	101	TGL	CC5-CC6-CC7-CC8
21	N	608	TGL	C10-C11-C12-C13
26	G	101	CDL	C20-C21-C22-C23
27	C	319	DMU	C22-C25-C28-C31
21	L	101	TGL	CB3-CB4-CB5-CB6
21	L	101	TGL	CB7-CB8-CB9-C10
21	Q	201	TGL	CC5-CC6-CC7-CC8
21	Y	101	TGL	CB7-CB8-CB9-C10
21	B	301	TGL	CA5-CA6-CA7-CA8
21	Q	201	TGL	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
22	O	301	PSC	C30-C31-C32-C33
26	C	308	CDL	C17-C18-C19-C20
23	J	101	CHD	C20-C22-C23-C24
21	L	101	TGL	CC9-C15-C16-C17
14	N	601	PGV	C2-C3-C4-C5
14	P	306	PGV	C7-C8-C9-C10
21	D	201	TGL	C11-C10-CB9-CB8
21	L	101	TGL	CB9-C10-C11-C12
27	M	106	DMU	C28-C31-C34-C37
21	B	301	TGL	OB1-CB1-OG2-CG2
14	C	306	PGV	C7-C8-C9-C10
21	L	101	TGL	C12-C13-C14-C29
14	N	601	PGV	C1-C2-C3-C4
21	Q	201	TGL	CC1-CC2-CC3-CC4
21	B	301	TGL	CB2-CB1-OG2-CG2
26	G	101	CDL	C51-CB5-OB6-CB4
27	V	102	DMU	C25-C28-C31-C34
23	P	310	CHD	C21-C20-C22-C23
25	P	304	PEK	C22-C23-C24-C25
26	G	101	CDL	C13-C14-C15-C16
21	L	101	TGL	CA3-CA4-CA5-CA6
21	L	101	TGL	OA1-CA1-OG1-CG1
21	D	201	TGL	CA3-CA4-CA5-CA6
26	C	308	CDL	OB7-CB5-OB6-CB4
26	G	101	CDL	OB7-CB5-OB6-CB4
26	P	308	CDL	OB7-CB5-OB6-CB4
21	Y	101	TGL	C21-C22-C23-C24
25	C	304	PEK	C26-C27-C28-C29
21	Q	201	TGL	C18-C19-C33-C34
20	A	620	EDO	O1-C1-C2-O2
20	D	202	EDO	O1-C1-C2-O2
20	N	629	EDO	O1-C1-C2-O2
20	O	305	EDO	O1-C1-C2-O2
20	P	313	EDO	O1-C1-C2-O2
20	R	204	EDO	O1-C1-C2-O2
20	S	111	EDO	O1-C1-C2-O2
20	S	112	EDO	O1-C1-C2-O2
20	W	102	EDO	O1-C1-C2-O2
21	B	301	TGL	C20-C21-C22-C23
14	C	307	PGV	C2-C1-O01-C02
21	B	301	TGL	CB1-CB2-CB3-CB4
27	Z	102	DMU	C3-C4-C57-O61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	Y	101	TGL	C22-C23-C24-C25
21	L	101	TGL	OC1-CC1-OG3-CG3
25	C	304	PEK	C16-C17-C18-C19
26	G	101	CDL	C37-C38-C39-C40
21	D	201	TGL	OB1-CB1-OG2-CG2
26	G	101	CDL	OA7-CA5-OA6-CA4
21	B	301	TGL	CC2-CC1-OG3-CG3
26	T	101	CDL	C20-C21-C22-C23
27	M	106	DMU	C18-C19-C22-C25
21	Y	101	TGL	C19-C33-C34-C35
21	D	201	TGL	CB2-CB1-OG2-CG2
25	C	305	PEK	C2-C1-O01-C02
26	C	308	CDL	C51-CB5-OB6-CB4
26	G	101	CDL	C11-CA5-OA6-CA4
26	C	308	CDL	C77-C78-C79-C80
26	T	101	CDL	C54-C55-C56-C57
14	C	306	PGV	C20-C21-C22-C23
26	C	308	CDL	C36-C37-C38-C39
14	C	307	PGV	O02-C1-O01-C02
25	C	305	PEK	O02-C1-O01-C02
21	Q	201	TGL	C16-C17-C18-C19
27	C	319	DMU	C19-C22-C25-C28
21	L	101	TGL	C21-C22-C23-C24
27	M	106	DMU	C25-C28-C31-C34
25	P	303	PEK	C30-C31-C32-C33
27	G	108	DMU	C31-C34-C37-C40
14	C	306	PGV	C10-C11-C12-C13
27	G	108	DMU	O6-C11-C9-O1
21	D	201	TGL	CC6-CC7-CC8-CC9
21	D	201	TGL	C20-C21-C22-C23
25	P	303	PEK	C2-C1-O01-C02
27	C	319	DMU	C25-C28-C31-C34
26	P	308	CDL	CA2-OA2-PA1-OA5
21	Y	101	TGL	C11-C12-C13-C14
26	G	101	CDL	C60-C61-C62-C63
21	Q	201	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	CC6-CC7-CC8-CC9
21	Y	101	TGL	C24-C25-C26-C27
22	O	301	PSC	C22-C23-C24-C25
26	G	101	CDL	C55-C56-C57-C58
27	P	323	DMU	O6-C11-C9-C8
25	P	303	PEK	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	M	106	DMU	C31-C34-C37-C40
26	T	101	CDL	CA7-C31-C32-C33
21	B	301	TGL	C12-C13-C14-C29
26	C	308	CDL	C41-C42-C43-C44
26	T	101	CDL	C60-C61-C62-C63
14	N	601	PGV	O03-C01-C02-C03
25	P	305	PEK	O03-C01-C02-C03
26	C	308	CDL	CB3-CB4-CB6-OB8
14	N	609	PGV	C10-C11-C12-C13
21	Y	101	TGL	CA3-CA4-CA5-CA6
21	D	201	TGL	CC4-CC5-CC6-CC7
21	L	101	TGL	C17-C18-C19-C33
26	P	308	CDL	CA5-C11-C12-C13
25	P	305	PEK	C34-C35-C36-C37
27	P	309	DMU	O6-C11-C9-O1
14	N	609	PGV	C27-C28-C29-C30
22	O	301	PSC	C20-C19-O03-C01
27	C	319	DMU	C34-C37-C40-C43
27	P	323	DMU	C34-C37-C40-C43
25	C	303	PEK	C29-C30-C31-C32
25	P	304	PEK	C13-C14-C15-C16
23	Y	104	CHD	C13-C17-C20-C21
14	P	307	PGV	C2-C1-O01-C02
22	B	302	PSC	O03-C01-C02-O01
21	B	301	TGL	CC4-CC5-CC6-CC7
25	P	303	PEK	O02-C1-O01-C02
23	W	101	CHD	C17-C20-C22-C23
14	A	601	PGV	C20-C21-C22-C23
21	B	301	TGL	CA9-C20-C21-C22
26	G	101	CDL	C32-C31-CA7-OA8
21	B	301	TGL	C25-C26-C27-C28
21	N	608	TGL	C29-C30-C31-C32
21	Q	201	TGL	CB2-CB3-CB4-CB5
14	A	608	PGV	C10-C11-C12-C13
25	C	304	PEK	C7-C8-C9-C10
25	P	305	PEK	C10-C11-C12-C13
21	D	201	TGL	OG3-CC1-CC2-CC3
14	A	601	PGV	C01-C02-C03-O11
25	P	305	PEK	C01-C02-C03-O11
26	P	308	CDL	OA5-CA3-CA4-CA6
21	N	608	TGL	C20-C21-C22-C23
23	Y	104	CHD	C16-C17-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	Y	101	TGL	C23-C24-C25-C26
26	G	101	CDL	C57-C58-C59-C60
26	G	101	CDL	CB5-C51-C52-C53
26	G	101	CDL	C61-C62-C63-C64
26	P	308	CDL	C41-C42-C43-C44
27	Z	101	DMU	O16-C18-C19-C22
14	A	601	PGV	C19-C20-C21-C22
26	C	308	CDL	C60-C61-C62-C63
14	P	306	PGV	C02-C03-O11-P
26	T	101	CDL	C61-C62-C63-C64
25	C	303	PEK	C33-C34-C35-C36
21	Q	201	TGL	CG1-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-C03
26	T	101	CDL	CA3-CA4-CA6-OA8
26	P	308	CDL	C36-C37-C38-C39
25	C	304	PEK	C4-C5-C6-C7
25	C	304	PEK	C13-C14-C15-C16
26	P	308	CDL	C12-C13-C14-C15
22	B	302	PSC	C9-C10-C11-C12
22	B	302	PSC	C10-C11-C12-C13
22	O	301	PSC	C9-C10-C11-C12
22	O	301	PSC	C10-C11-C12-C13
25	C	303	PEK	C5-C6-C7-C8
25	C	303	PEK	C11-C10-C9-C8
25	C	303	PEK	C9-C10-C11-C12
25	C	303	PEK	C11-C12-C13-C14
25	C	303	PEK	C12-C13-C14-C15
25	C	304	PEK	C9-C10-C11-C12
25	C	304	PEK	C11-C12-C13-C14
25	C	304	PEK	C12-C13-C14-C15
25	C	305	PEK	C6-C7-C8-C9
25	C	305	PEK	C11-C10-C9-C8
25	C	305	PEK	C9-C10-C11-C12
25	C	305	PEK	C11-C12-C13-C14
25	C	305	PEK	C12-C13-C14-C15
25	P	303	PEK	C5-C6-C7-C8
25	P	303	PEK	C6-C7-C8-C9
25	P	303	PEK	C11-C10-C9-C8
25	P	303	PEK	C9-C10-C11-C12
25	P	303	PEK	C11-C12-C13-C14
25	P	303	PEK	C12-C13-C14-C15
25	P	304	PEK	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	P	304	PEK	C9-C10-C11-C12
25	P	304	PEK	C11-C12-C13-C14
25	P	304	PEK	C12-C13-C14-C15
25	P	305	PEK	C5-C6-C7-C8
25	P	305	PEK	C6-C7-C8-C9
25	P	305	PEK	C11-C10-C9-C8
25	P	305	PEK	C9-C10-C11-C12
25	P	305	PEK	C11-C12-C13-C14
25	P	305	PEK	C12-C13-C14-C15
26	P	308	CDL	CB2-OB2-PB2-OB5
21	B	301	TGL	OC1-CC1-OG3-CG3
21	L	101	TGL	CA5-CA6-CA7-CA8
26	P	308	CDL	OA5-CA3-CA4-OA6
22	O	301	PSC	O04-C19-O03-C01
26	C	308	CDL	CB7-C71-C72-C73
21	Q	201	TGL	CC3-CC4-CC5-CC6
14	N	601	PGV	O03-C01-C02-O01
21	Q	201	TGL	OG2-CG2-CG3-OG3
26	C	308	CDL	OB6-CB4-CB6-OB8
23	J	101	CHD	C13-C17-C20-C22
23	Y	104	CHD	C13-C17-C20-C22
14	P	307	PGV	O02-C1-O01-C02
23	C	311	CHD	C21-C20-C22-C23
20	F	107	EDO	O1-C1-C2-O2
20	G	103	EDO	O1-C1-C2-O2
20	N	624	EDO	O1-C1-C2-O2
25	P	305	PEK	O02-C1-O01-C02
26	G	101	CDL	C42-C43-C44-C45
23	J	101	CHD	C16-C17-C20-C22
23	Y	104	CHD	C16-C17-C20-C22
26	G	101	CDL	O1-C1-CB2-OB2
25	P	303	PEK	C32-C33-C34-C35
21	D	201	TGL	CC2-CC3-CC4-CC5
22	B	302	PSC	C24-C25-C26-C27
27	Z	101	DMU	C22-C25-C28-C31
14	N	601	PGV	C03-C02-O01-C1
22	B	302	PSC	C03-C02-O01-C1
27	P	323	DMU	O16-C18-C19-C22
26	P	308	CDL	C52-C53-C54-C55
21	L	101	TGL	OG1-CG1-CG2-CG3
26	G	101	CDL	OB5-CB3-CB4-OB6
14	A	608	PGV	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	J	101	CHD	C13-C17-C20-C21
25	C	303	PEK	C34-C35-C36-C37
21	L	101	TGL	OG1-CG1-CG2-OG2
21	L	101	TGL	OG2-CG2-CG3-OG3
21	Y	101	TGL	OG1-CG1-CG2-OG2
21	Y	101	TGL	OG2-CG2-CG3-OG3
25	P	305	PEK	O03-C01-C02-O01
26	P	308	CDL	OB6-CB4-CB6-OB8
26	T	101	CDL	OA6-CA4-CA6-OA8
27	M	101	DMU	O6-C11-C9-C8
21	N	608	TGL	CA5-CA6-CA7-CA8
27	C	310	DMU	C18-C19-C22-C25
14	C	307	PGV	C03-O11-P-O12
26	C	308	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CA3-OA5-PA1-OA2
26	P	308	CDL	CA3-OA5-PA1-OA2
14	P	307	PGV	C3-C4-C5-C6
21	Y	101	TGL	CA6-CA7-CA8-CA9
14	C	306	PGV	C02-C03-O11-P
21	L	101	TGL	C15-C16-C17-C18
14	C	307	PGV	C04-O12-P-O14
26	G	101	CDL	CB3-OB5-PB2-OB4
26	P	308	CDL	CB2-OB2-PB2-OB4
26	T	101	CDL	CA2-OA2-PA1-OA4
26	T	101	CDL	CA3-OA5-PA1-OA4
14	N	601	PGV	C01-C02-C03-O11
25	C	305	PEK	C01-C02-C03-O11
26	C	308	CDL	OA5-CA3-CA4-CA6
21	Q	201	TGL	C16-C15-CC9-CC8
20	M	104	EDO	O1-C1-C2-O2
20	N	623	EDO	O1-C1-C2-O2
20	Q	203	EDO	O1-C1-C2-O2
21	Y	101	TGL	CB9-C10-C11-C12
25	P	305	PEK	C33-C34-C35-C36
22	O	301	PSC	C11-C10-C9-C8
22	O	301	PSC	C19-C20-C21-C22
21	D	201	TGL	C18-C19-C33-C34
21	Q	201	TGL	C33-C34-C35-C36
21	Y	101	TGL	CC7-CC8-CC9-C15
27	P	324	DMU	C28-C31-C34-C37
14	A	601	PGV	O01-C02-C03-O11
26	T	101	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	P	309	DMU	C22-C25-C28-C31
21	D	201	TGL	C16-C15-CC9-CC8
21	L	101	TGL	CG1-CG2-CG3-OG3
21	Y	101	TGL	CG1-CG2-CG3-OG3
22	B	302	PSC	O12-C04-C05-N
26	P	308	CDL	CB3-CB4-CB6-OB8
25	P	303	PEK	C7-C8-C9-C10
25	P	304	PEK	C4-C5-C6-C7
27	P	324	DMU	C19-C22-C25-C28
21	N	608	TGL	CC7-CC8-CC9-C15
25	P	305	PEK	C17-C18-C19-C20
23	J	101	CHD	C17-C20-C22-C23
26	T	101	CDL	C12-C11-CA5-OA6
14	N	601	PGV	C19-C20-C21-C22
27	P	324	DMU	C18-C19-C22-C25
27	M	101	DMU	C19-C22-C25-C28
21	N	608	TGL	CA4-CA5-CA6-CA7
23	J	101	CHD	C16-C17-C20-C21
25	C	304	PEK	C10-C11-C12-C13
21	N	608	TGL	C12-C13-C14-C29
14	N	601	PGV	O12-C04-C05-O05
21	Y	101	TGL	C29-C30-C31-C32
27	M	101	DMU	C34-C37-C40-C43
27	C	319	DMU	C28-C31-C34-C37
14	C	306	PGV	C25-C26-C27-C28
26	P	308	CDL	C60-C61-C62-C63
25	P	305	PEK	O01-C02-C03-O11
27	V	102	DMU	C2-C3-O7-C10
27	V	102	DMU	C4-C3-O7-C10
21	B	301	TGL	C11-C10-CB9-CB8
20	A	617	EDO	O1-C1-C2-O2
20	B	307	EDO	O1-C1-C2-O2
20	D	205	EDO	O1-C1-C2-O2
20	L	102	EDO	O1-C1-C2-O2
20	N	612	EDO	O1-C1-C2-O2
20	N	625	EDO	O1-C1-C2-O2
20	O	306	EDO	O1-C1-C2-O2
20	P	316	EDO	O1-C1-C2-O2
20	P	321	EDO	O1-C1-C2-O2
20	S	108	EDO	O1-C1-C2-O2
25	P	305	PEK	C2-C1-O01-C02
22	O	301	PSC	O03-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	T	101	CDL	OB6-CB4-CB6-OB8
26	T	101	CDL	C37-C38-C39-C40
22	O	301	PSC	C04-O12-P-O11
26	C	308	CDL	CA3-OA5-PA1-OA2
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CB2-OB2-PB2-OB5
26	T	101	CDL	CB2-OB2-PB2-OB5
26	T	101	CDL	CB3-OB5-PB2-OB2
14	C	306	PGV	C1-C2-C3-C4
14	C	307	PGV	O03-C01-C02-C03
22	O	301	PSC	O03-C01-C02-C03
26	T	101	CDL	C43-C44-C45-C46
14	N	609	PGV	C11-C12-C13-C14
27	M	101	DMU	C25-C28-C31-C34
26	C	308	CDL	C76-C77-C78-C79
21	Y	101	TGL	C15-C16-C17-C18
26	P	308	CDL	C31-C32-C33-C34
22	B	302	PSC	C7-C8-C9-C10
26	T	101	CDL	C17-C18-C19-C20
14	A	601	PGV	C23-C24-C25-C26
26	T	101	CDL	C11-C12-C13-C14
26	G	101	CDL	OB5-CB3-CB4-CB6
26	T	101	CDL	OB5-CB3-CB4-CB6
21	N	608	TGL	CB9-C10-C11-C12
26	T	101	CDL	OA5-CA3-CA4-OA6
15	N	602[B]	HEA	C26-C15-C16-C17
21	B	301	TGL	C15-C16-C17-C18
14	N	609	PGV	C26-C27-C28-C29
22	O	301	PSC	O03-C01-C02-O01
21	L	101	TGL	CC4-CC5-CC6-CC7
21	Y	101	TGL	C20-C21-C22-C23
26	C	308	CDL	C37-C38-C39-C40
22	B	302	PSC	C3-C4-C5-C6
27	P	324	DMU	C34-C37-C40-C43
26	P	308	CDL	C75-C76-C77-C78
20	A	609	EDO	O1-C1-C2-O2
14	P	306	PGV	C1-C2-C3-C4
21	L	101	TGL	CA1-CA2-CA3-CA4
21	B	301	TGL	CC2-CC3-CC4-CC5
21	L	101	TGL	C22-C23-C24-C25
25	P	303	PEK	O03-C01-C02-C03
25	C	305	PEK	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	C	306	PGV	C24-C25-C26-C27
26	T	101	CDL	C81-C82-C83-C84
26	P	308	CDL	C17-C18-C19-C20
14	N	601	PGV	C21-C22-C23-C24
14	N	601	PGV	C11-C12-C13-C14
22	B	302	PSC	C12-C13-C14-C15
25	C	303	PEK	C6-C7-C8-C9
25	C	304	PEK	C5-C6-C7-C8
21	N	608	TGL	CC5-CC6-CC7-CC8
22	B	302	PSC	C29-C30-C31-C32
26	P	308	CDL	C37-C38-C39-C40
23	W	101	CHD	C13-C17-C20-C21
22	B	302	PSC	C20-C21-C22-C23
27	M	101	DMU	C22-C25-C28-C31
21	D	201	TGL	CC3-CC4-CC5-CC6
22	B	302	PSC	C1-C2-C3-C4
21	Q	201	TGL	CC9-C15-C16-C17
21	B	301	TGL	OG1-CG1-CG2-OG2
25	P	303	PEK	O03-C01-C02-O01
26	G	101	CDL	OB6-CB4-CB6-OB8
14	A	608	PGV	C23-C24-C25-C26
27	V	102	DMU	C22-C25-C28-C31
26	C	308	CDL	C39-C40-C41-C42
26	G	101	CDL	C40-C41-C42-C43
26	T	101	CDL	C80-C81-C82-C83
27	Z	102	DMU	O6-C11-C9-O1
26	P	308	CDL	C83-C84-C85-C86
26	P	308	CDL	C58-C59-C60-C61
14	A	608	PGV	C25-C26-C27-C28
20	S	107	EDO	O1-C1-C2-O2
20	W	103	EDO	O1-C1-C2-O2
26	C	308	CDL	C82-C83-C84-C85
21	B	301	TGL	CC9-C15-C16-C17
21	D	201	TGL	OC1-CC1-CC2-CC3
21	N	608	TGL	C13-C14-C29-C30
21	Q	201	TGL	C12-C13-C14-C29
14	P	306	PGV	C9-C10-C11-C12
14	P	307	PGV	C9-C10-C11-C12
25	C	305	PEK	O01-C02-C03-O11
26	C	308	CDL	OA5-CA3-CA4-OA6
21	N	608	TGL	C16-C15-CC9-CC8
14	A	608	PGV	O03-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	N	608	TGL	C14-C29-C30-C31
14	A	608	PGV	C31-C32-C33-C34
21	B	301	TGL	C24-C25-C26-C27
21	L	101	TGL	C16-C15-CC9-CC8
14	N	609	PGV	O03-C19-C20-C21
26	G	101	CDL	C15-C16-C17-C18
14	A	601	PGV	C15-C16-C17-C18
26	T	101	CDL	C40-C41-C42-C43
15	A	602[A]	HEA	C27-C19-C20-C21
14	C	307	PGV	C1-C2-C3-C4
14	N	601	PGV	C9-C10-C11-C12
25	C	304	PEK	C14-C15-C16-C17
26	G	101	CDL	C52-C53-C54-C55
27	M	101	DMU	C28-C31-C34-C37
23	W	101	CHD	C13-C17-C20-C22
21	N	608	TGL	C21-C22-C23-C24
27	C	310	DMU	C22-C25-C28-C31
27	P	324	DMU	C31-C34-C37-C40
21	Y	101	TGL	C10-C11-C12-C13
26	P	308	CDL	C13-C14-C15-C16
14	A	608	PGV	C11-C12-C13-C14
25	C	305	PEK	C3-C4-C5-C6
25	P	303	PEK	C3-C4-C5-C6
25	P	305	PEK	C14-C15-C16-C17
21	Y	101	TGL	OG1-CG1-CG2-CG3
21	Q	201	TGL	CB3-CB4-CB5-CB6
21	D	201	TGL	CB5-CB6-CB7-CB8
26	P	308	CDL	C52-C51-CB5-OB6
20	L	104	EDO	O1-C1-C2-O2
20	N	616	EDO	O1-C1-C2-O2
20	N	622	EDO	O1-C1-C2-O2
20	N	628	EDO	O1-C1-C2-O2
20	Q	202	EDO	O1-C1-C2-O2
26	T	101	CDL	C57-C58-C59-C60
14	C	306	PGV	C11-C12-C13-C14
22	O	301	PSC	C7-C8-C9-C10
25	C	303	PEK	O03-C21-C22-C23
26	C	308	CDL	C32-C31-CA7-OA8
14	N	601	PGV	O03-C19-C20-C21
21	N	608	TGL	OG2-CG2-CG3-OG3
23	W	101	CHD	C16-C17-C20-C22
27	M	101	DMU	O16-C18-C19-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	T	101	CDL	C32-C31-CA7-OA8
14	P	307	PGV	C11-C12-C13-C14
25	P	304	PEK	C14-C15-C16-C17
26	C	308	CDL	C52-C51-CB5-OB6
26	C	308	CDL	C35-C36-C37-C38
22	O	301	PSC	C12-C13-C14-C15
25	C	305	PEK	C14-C15-C16-C17
25	P	305	PEK	C3-C4-C5-C6
14	C	306	PGV	C9-C10-C11-C12
26	P	308	CDL	C52-C51-CB5-OB7
14	P	307	PGV	C28-C29-C30-C31
14	P	306	PGV	C05-C04-O12-P
22	B	302	PSC	C22-C23-C24-C25
26	C	308	CDL	CA3-OA5-PA1-OA3
26	C	308	CDL	CB2-OB2-PB2-OB3
26	G	101	CDL	CA2-OA2-PA1-OA3
20	A	626	EDO	O1-C1-C2-O2
20	B	313	EDO	O1-C1-C2-O2
20	J	103	EDO	O1-C1-C2-O2
20	T	103	EDO	O1-C1-C2-O2
20	W	104	EDO	O1-C1-C2-O2
14	A	608	PGV	C26-C27-C28-C29
14	P	306	PGV	C27-C28-C29-C30
25	C	303	PEK	O04-C21-C22-C23
25	C	305	PEK	C23-C24-C25-C26
26	T	101	CDL	C32-C31-CA7-OA9
14	A	601	PGV	O03-C19-C20-C21
26	C	308	CDL	C55-C56-C57-C58
27	Z	102	DMU	C22-C25-C28-C31
26	C	308	CDL	C52-C51-CB5-OB7
23	P	301	CHD	C16-C17-C20-C22
26	P	308	CDL	C61-C62-C63-C64
25	P	303	PEK	C14-C15-C16-C17
26	T	101	CDL	C52-C51-CB5-OB6
21	Q	201	TGL	CA4-CA5-CA6-CA7
21	D	201	TGL	OC1-CC1-OG3-CG3
14	C	306	PGV	C05-C04-O12-P
25	C	303	PEK	C02-C03-O11-P
14	N	601	PGV	O04-C19-C20-C21
21	Q	201	TGL	OG3-CC1-CC2-CC3
25	C	304	PEK	C22-C23-C24-C25
26	C	308	CDL	C32-C31-CA7-OA9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	P	309	DMU	C19-C18-O16-C6
14	N	601	PGV	C11-C10-C9-C8
27	G	108	DMU	C4-C3-O7-C10
26	T	101	CDL	C31-C32-C33-C34
14	P	307	PGV	O01-C1-C2-C3
26	C	308	CDL	C38-C39-C40-C41
14	N	601	PGV	O01-C1-C2-C3

There are no ring outliers.

89 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	C	317	EDO	2	0
20	B	312	EDO	3	0
20	M	103	EDO	1	0
21	L	101	TGL	11	0
25	C	305	PEK	4	0
21	N	608	TGL	2	0
27	P	323	DMU	1	0
20	G	103	EDO	1	0
20	D	202	EDO	1	0
27	G	108	DMU	1	0
20	J	102	EDO	1	0
20	P	315	EDO	1	0
20	D	207	EDO	1	0
25	C	304	PEK	1	0
22	B	302	PSC	10	0
15	N	603	HEA	4	0
21	B	301	TGL	4	0
23	C	309	CHD	1	0
20	N	618	EDO	3	0
20	P	319	EDO	2	0
23	Y	104	CHD	4	0
20	B	310	EDO	3	0
20	B	311	EDO	1	0
20	N	623	EDO	1	0
23	W	101	CHD	3	0
27	V	102	DMU	4	0
14	C	307	PGV	2	0
20	B	308	EDO	1	0
21	Y	101	TGL	11	0
20	A	609	EDO	3	0

Continued on next page...

Continued from previous page...

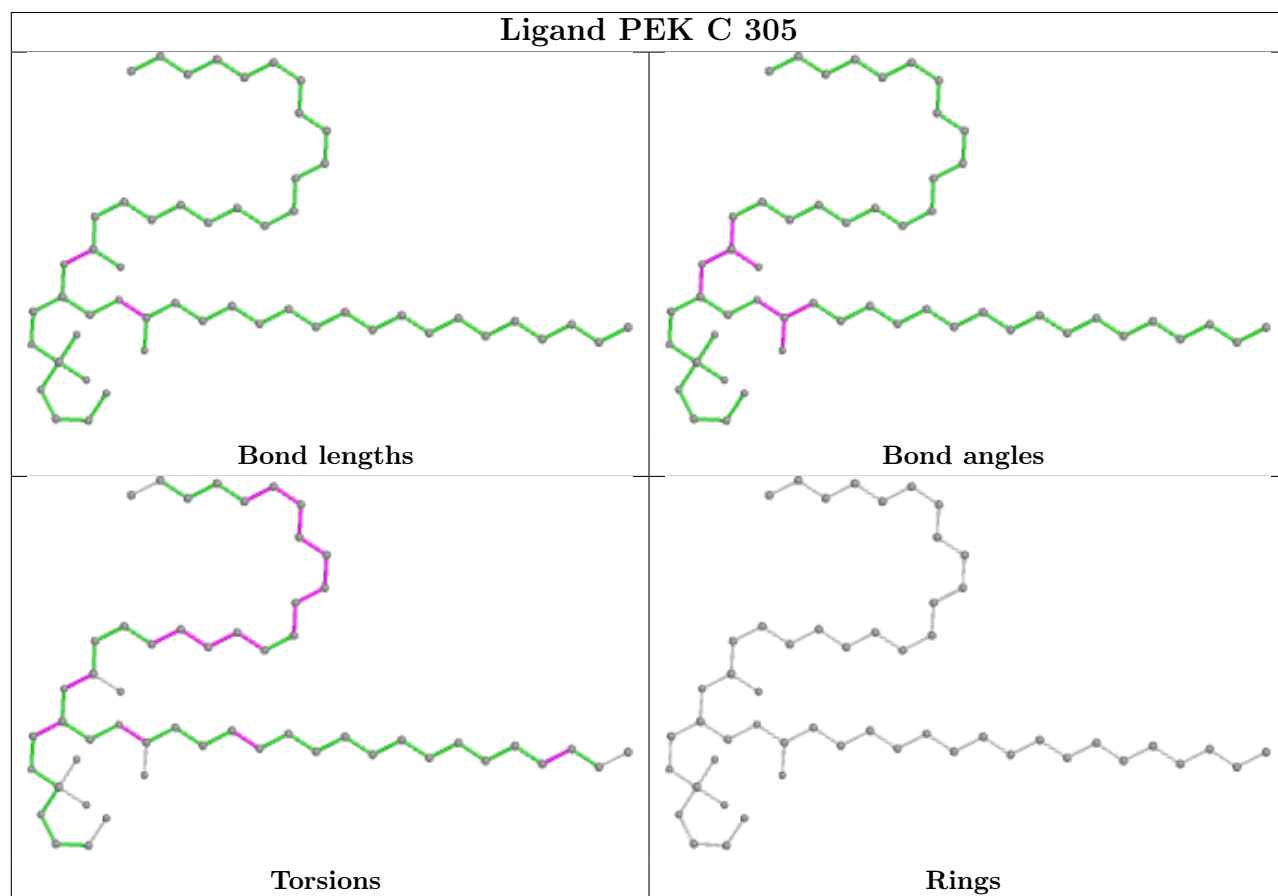
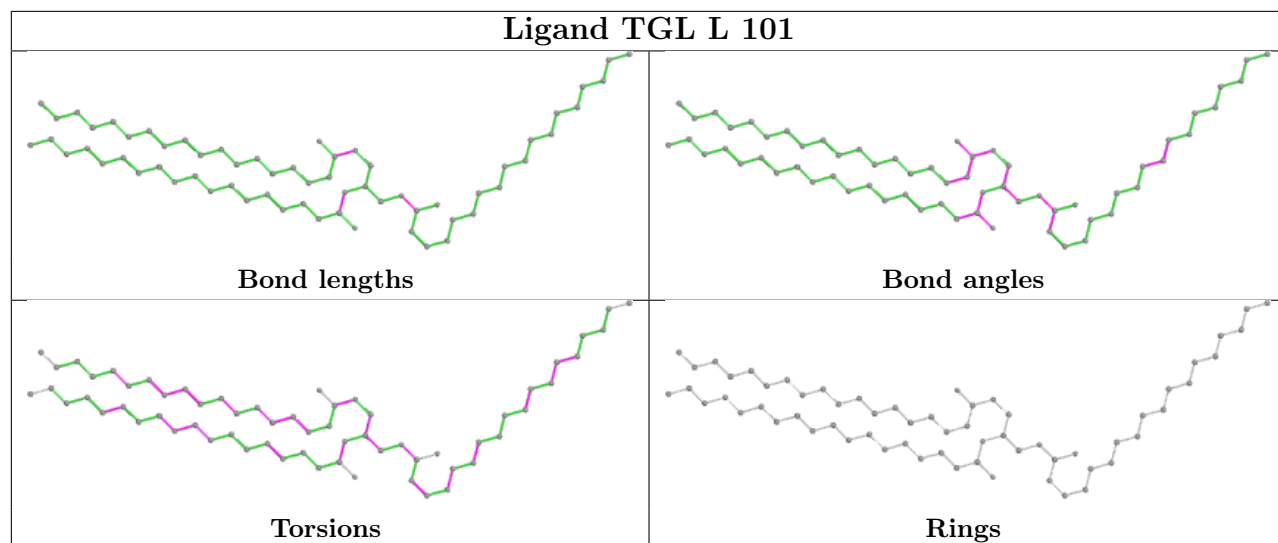
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	103	EDO	1	0
27	Z	102	DMU	1	0
20	P	314	EDO	1	0
20	N	612	EDO	5	0
21	Q	201	TGL	7	0
27	C	319	DMU	1	0
15	N	602[A]	HEA	2	0
14	N	609	PGV	1	0
27	P	324	DMU	2	0
26	T	101	CDL	11	0
22	O	301	PSC	5	0
20	C	316	EDO	1	0
20	F	103	EDO	1	0
23	J	101	CHD	3	0
20	N	630	EDO	3	0
23	P	310	CHD	7	0
20	K	102	EDO	2	0
20	G	104	EDO	2	0
25	C	303	PEK	3	0
20	U	101	EDO	1	0
20	O	306	EDO	2	0
23	G	102	CHD	1	0
23	C	311	CHD	2	0
21	D	201	TGL	9	0
15	A	603	HEA	3	0
27	C	310	DMU	2	0
14	P	306	PGV	4	0
20	D	206	EDO	0	2
20	A	620	EDO	1	0
20	R	203	EDO	1	0
14	P	307	PGV	3	0
14	N	601	PGV	3	0
20	A	627	EDO	1	0
25	P	305	PEK	9	0
25	P	304	PEK	3	0
20	A	619	EDO	1	0
27	P	309	DMU	3	0
20	A	623	EDO	1	0
26	C	308	CDL	13	0
20	H	102	EDO	1	0
20	W	104	EDO	2	0
14	A	601	PGV	3	0

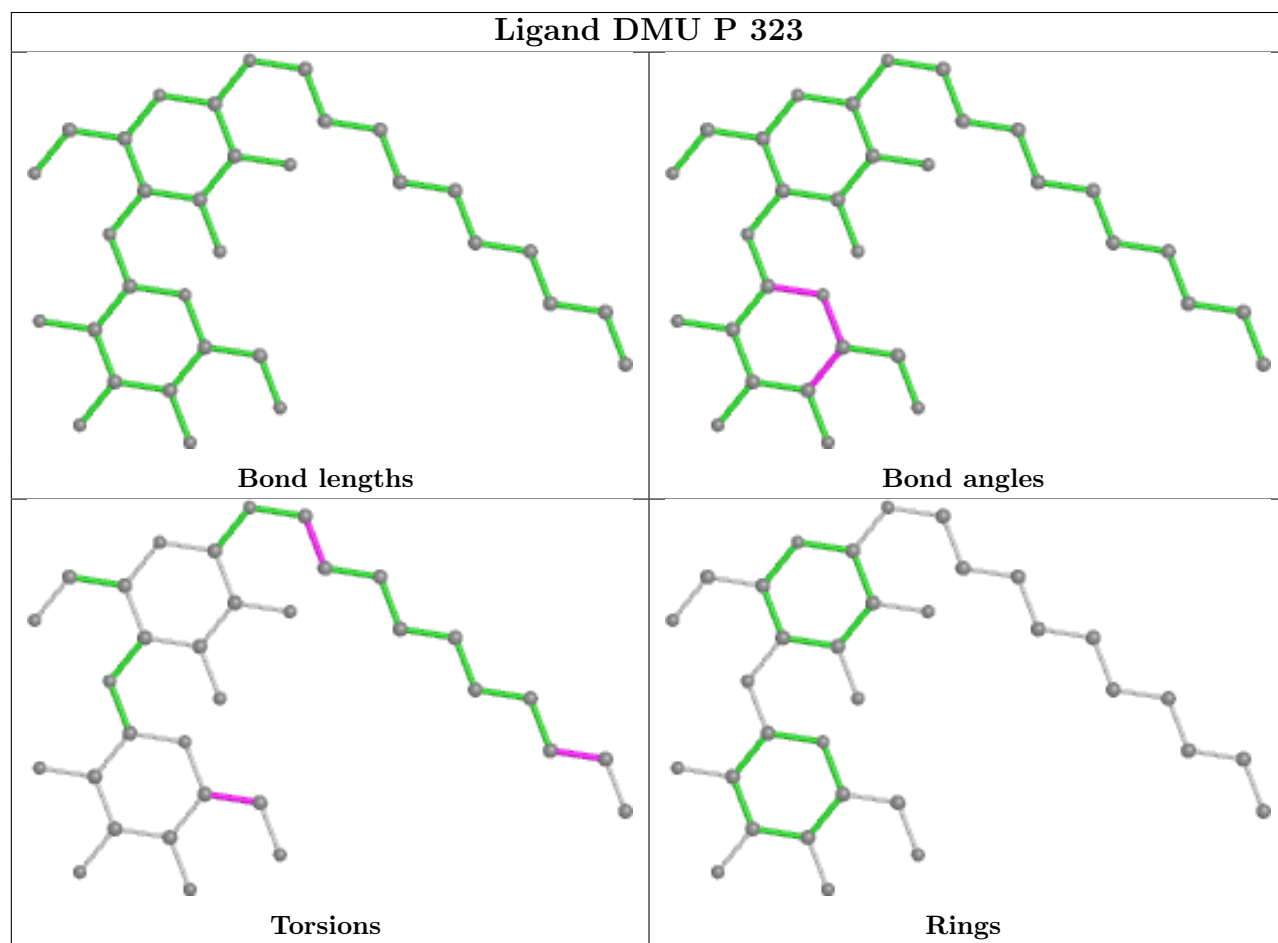
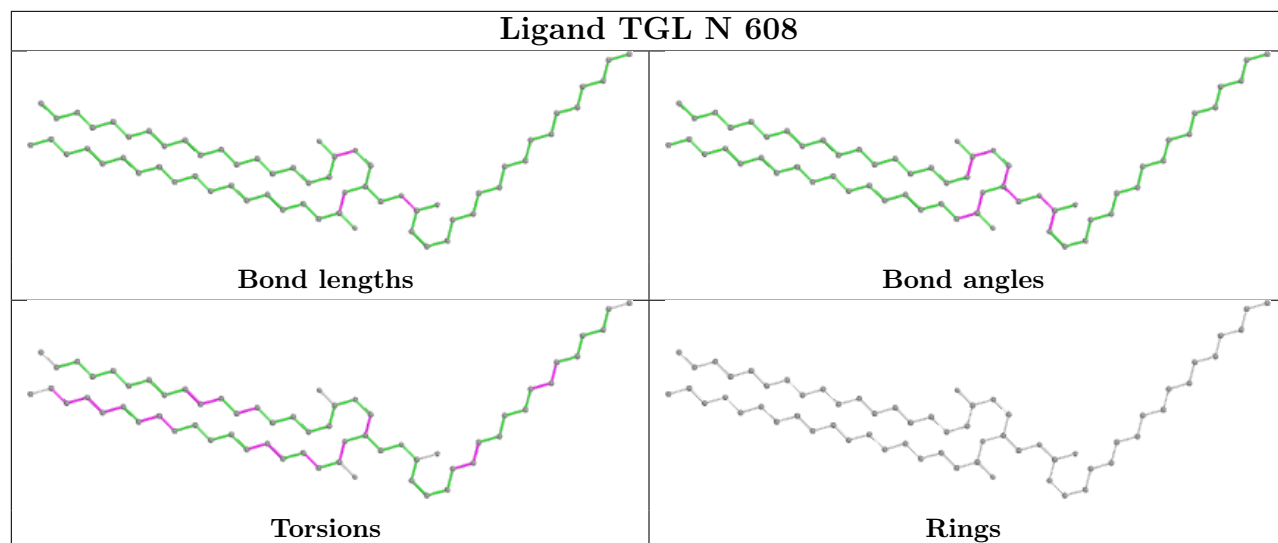
Continued on next page...

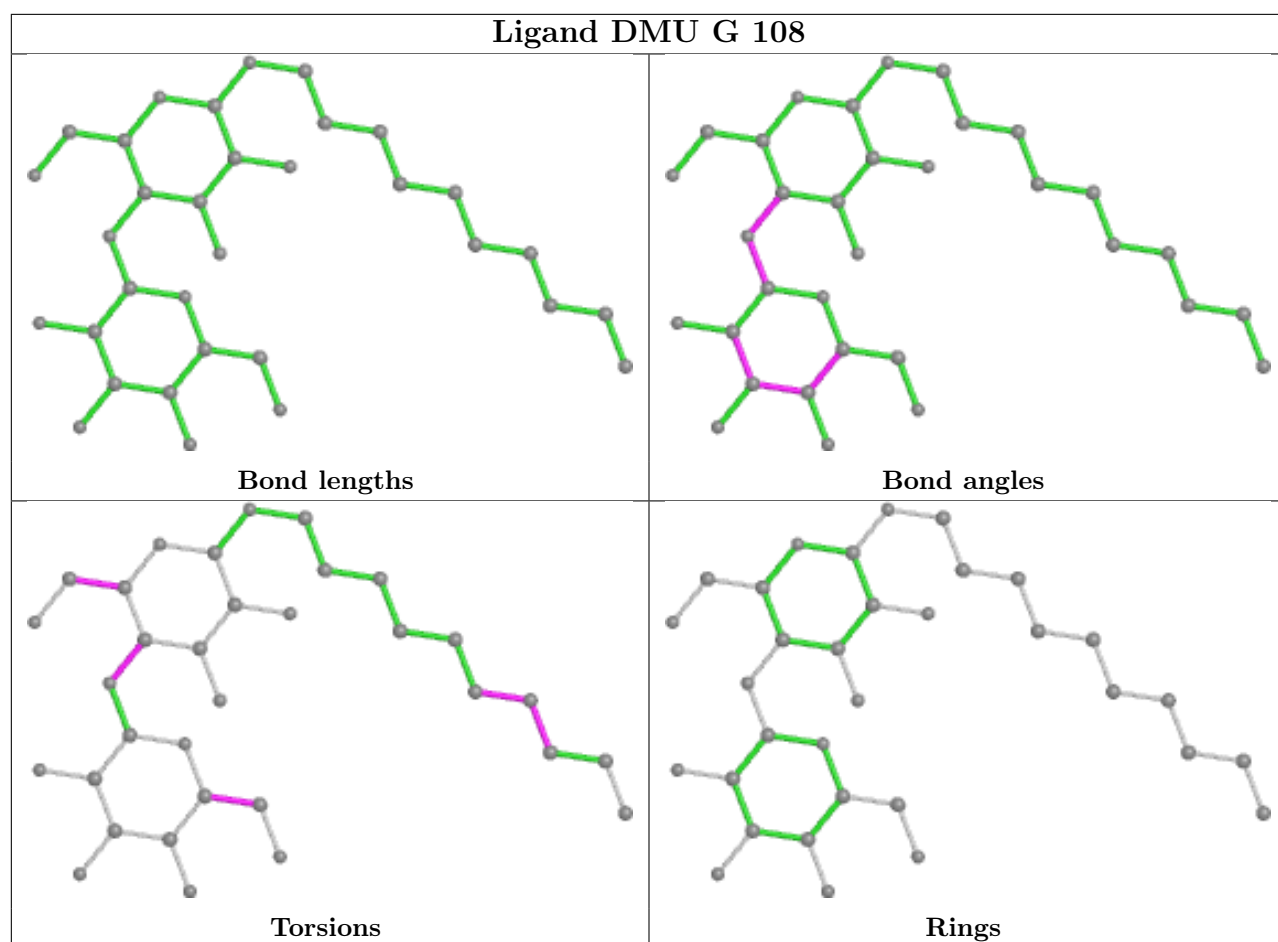
Continued from previous page...

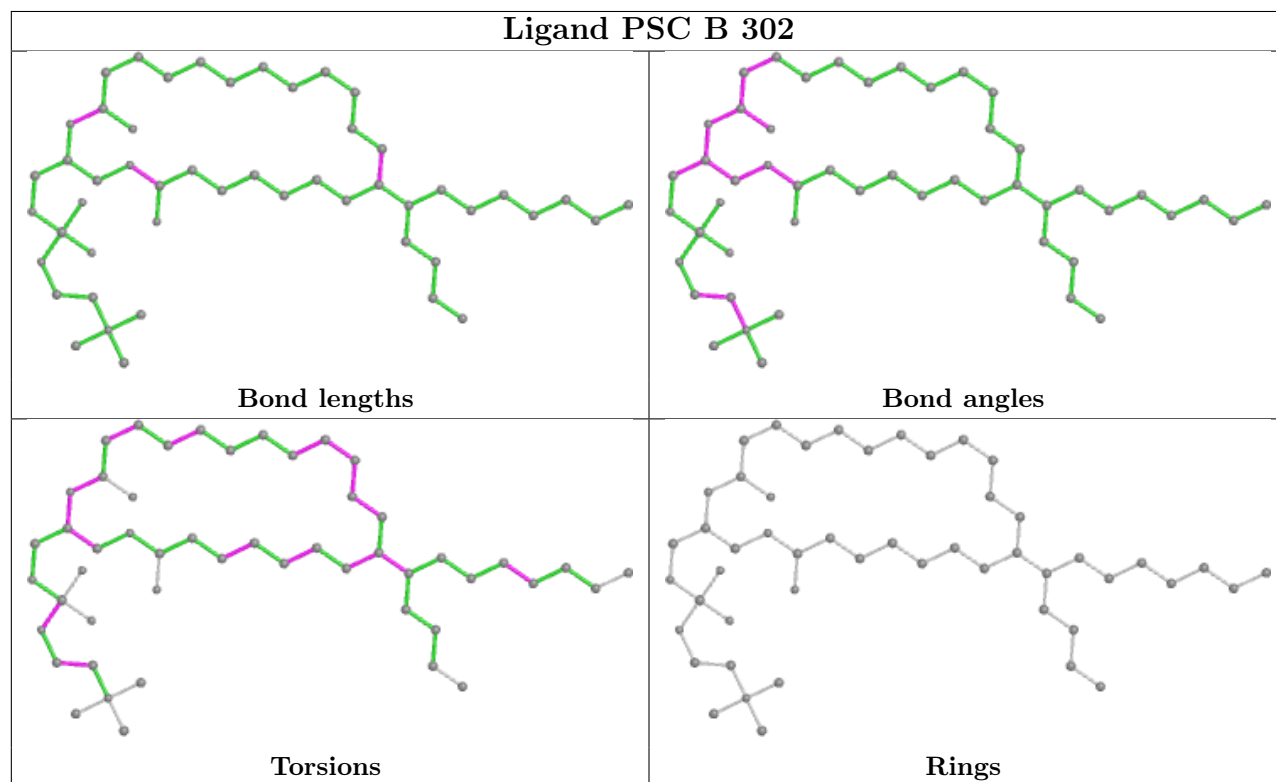
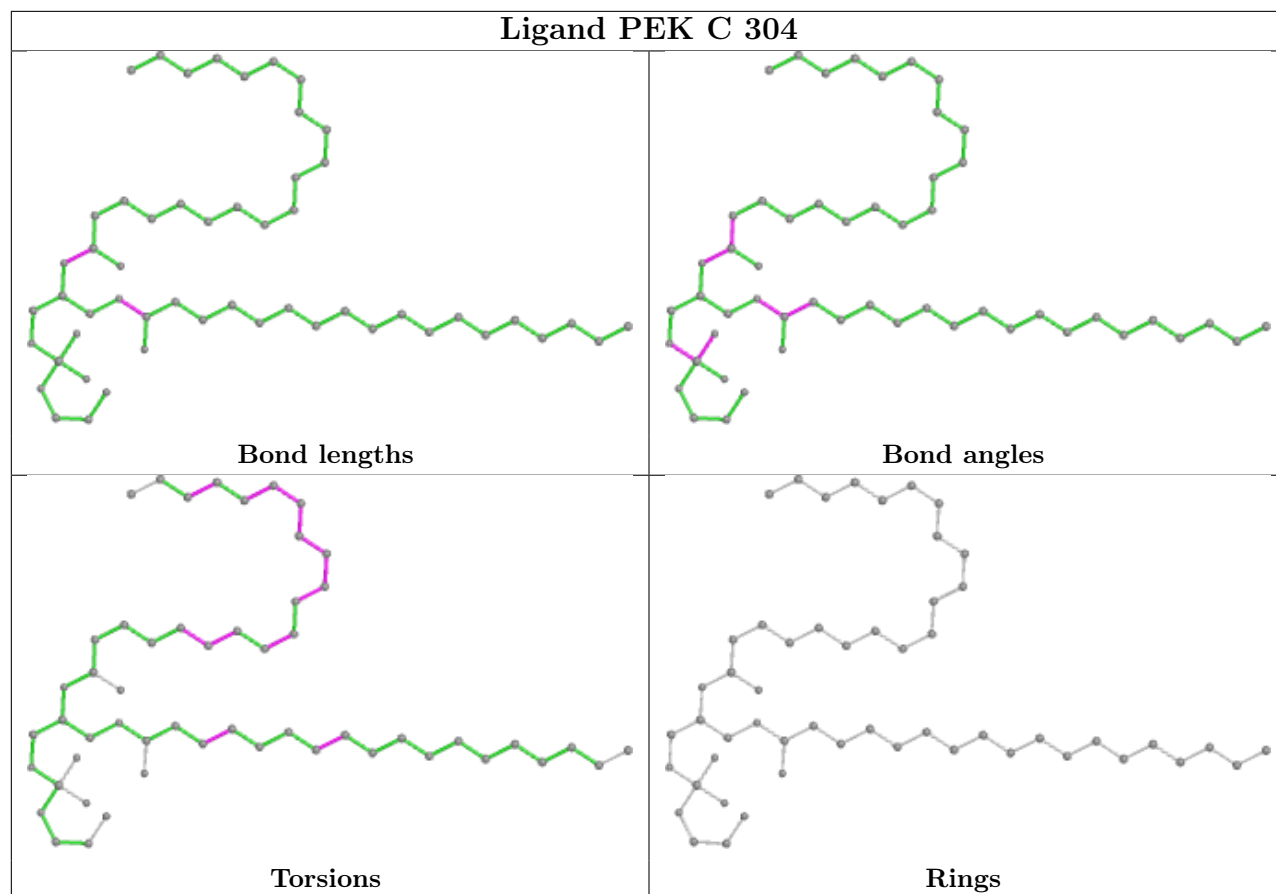
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	614	EDO	1	0
15	A	602[A]	HEA	3	0
26	G	101	CDL	18	0
20	S	107	EDO	2	0
26	P	308	CDL	20	0
20	A	624	EDO	1	0
20	M	104	EDO	2	0
20	N	619	EDO	1	0
20	P	320	EDO	1	0
14	C	306	PGV	2	0
23	P	311	CHD	2	0
25	P	303	PEK	3	0
20	H	103	EDO	4	0
20	D	205	EDO	1	0
20	B	314	EDO	0	2
20	B	309	EDO	2	0
20	G	107	EDO	1	0

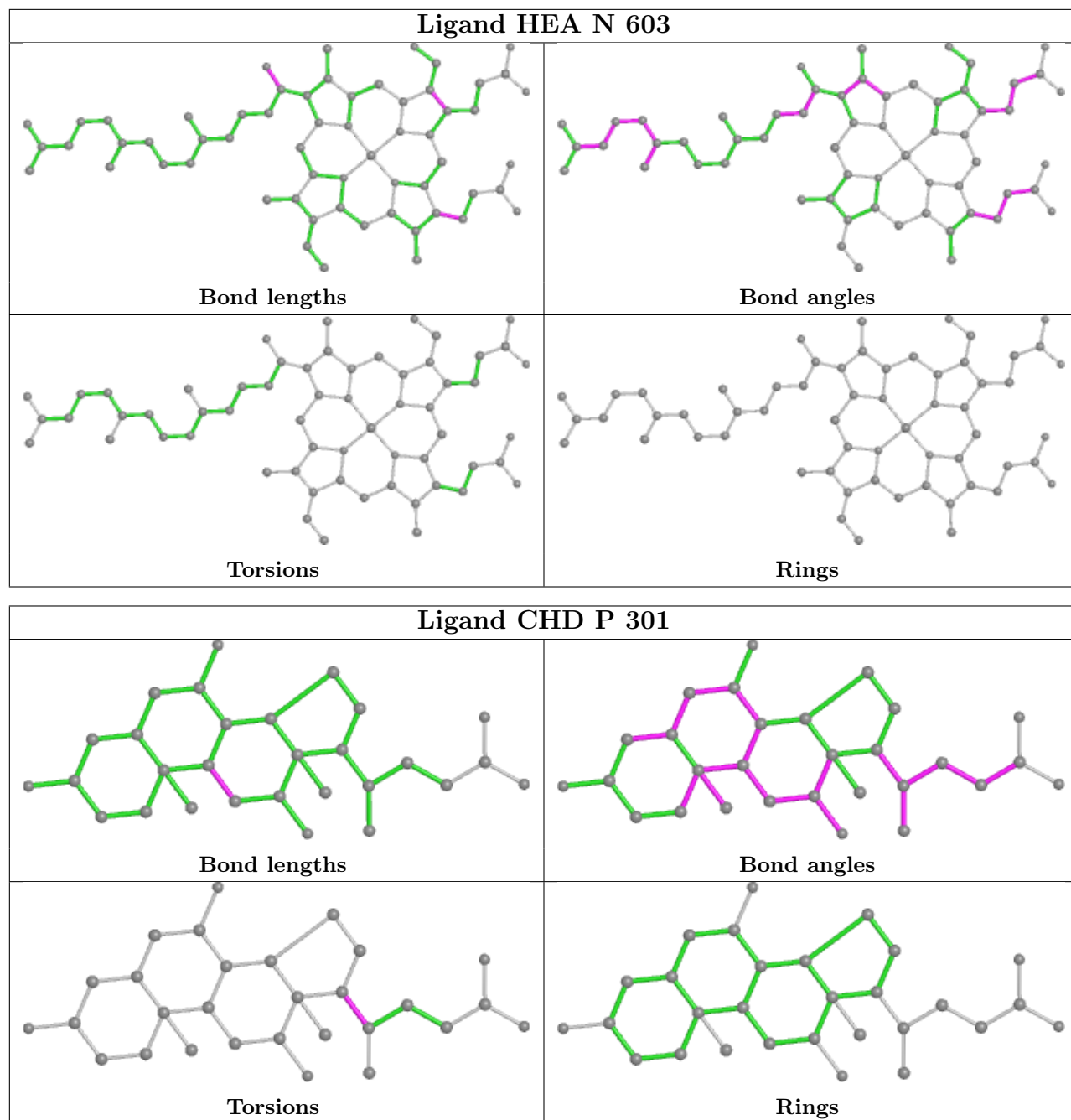
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



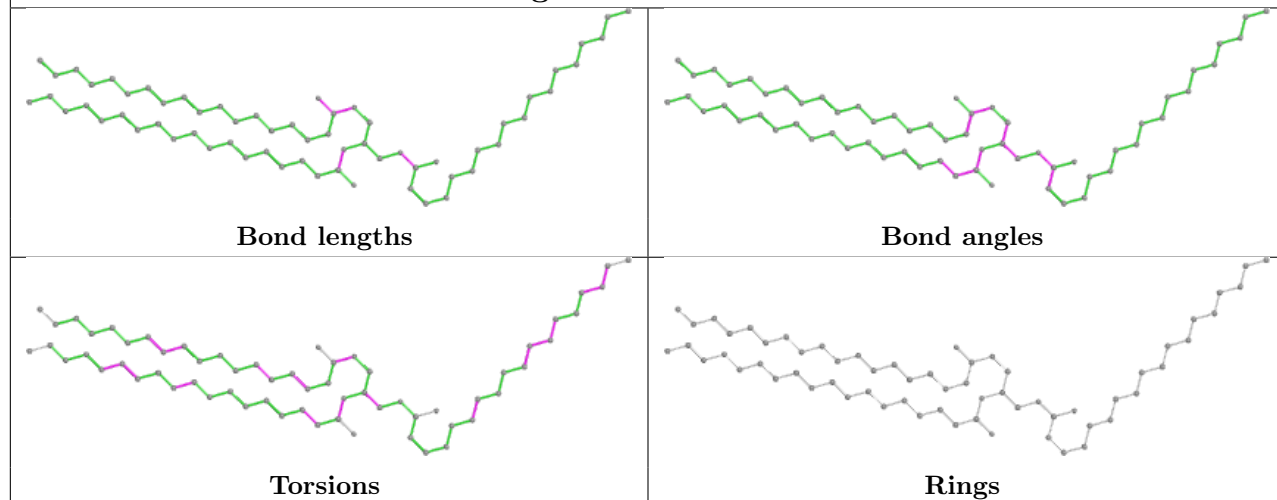




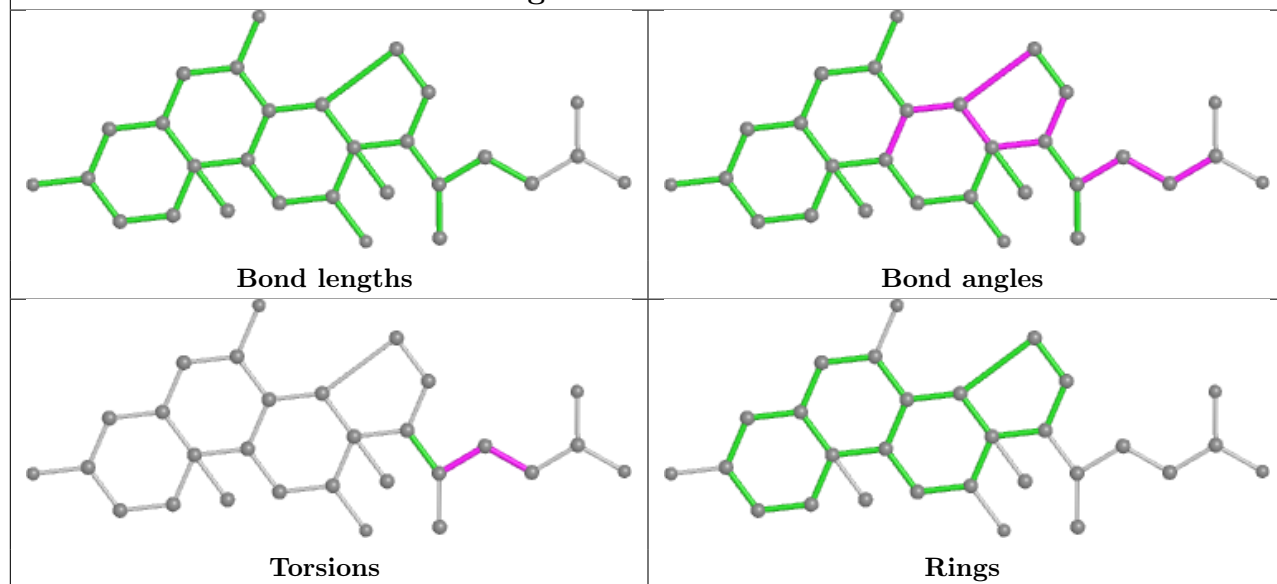


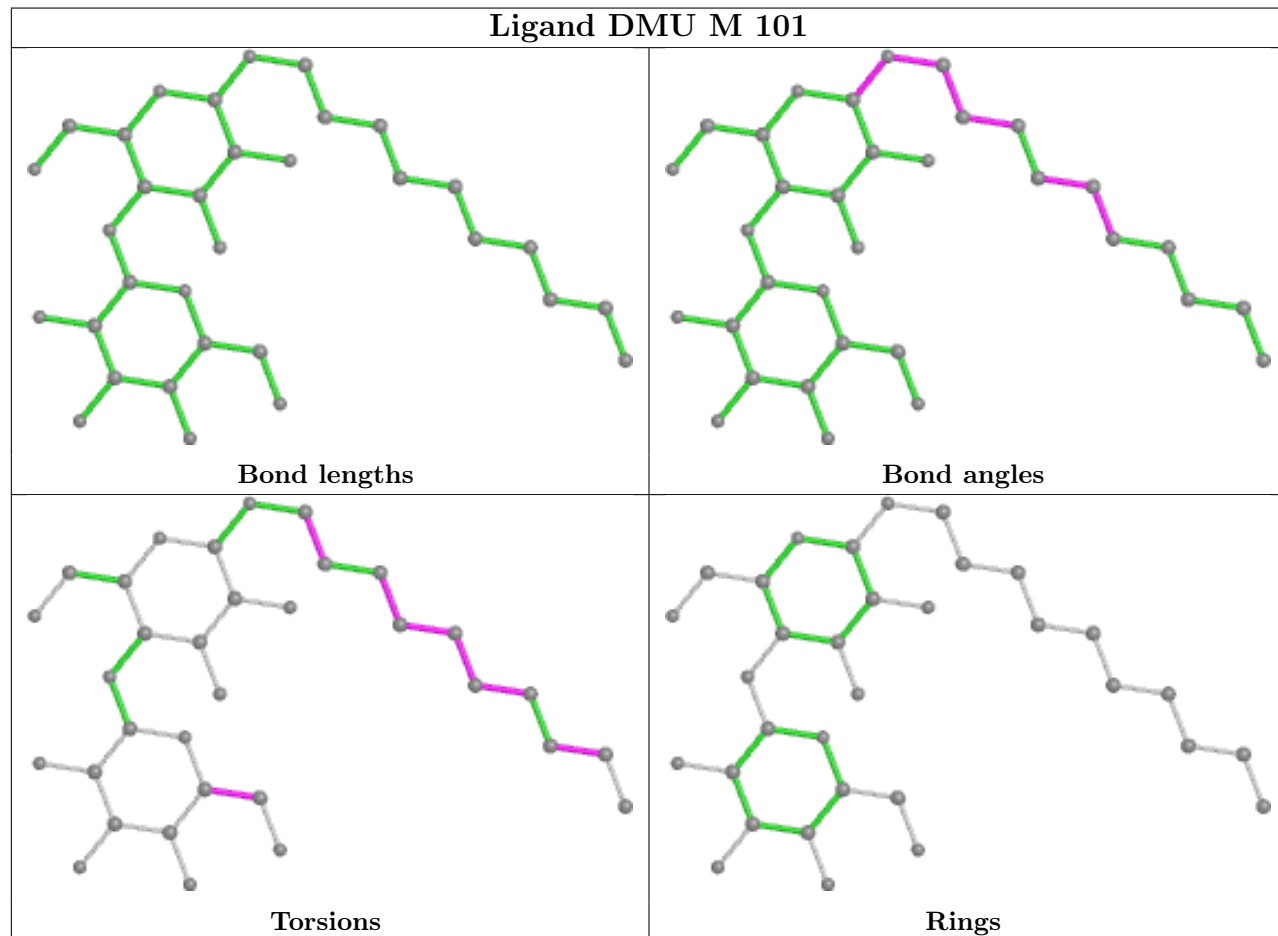
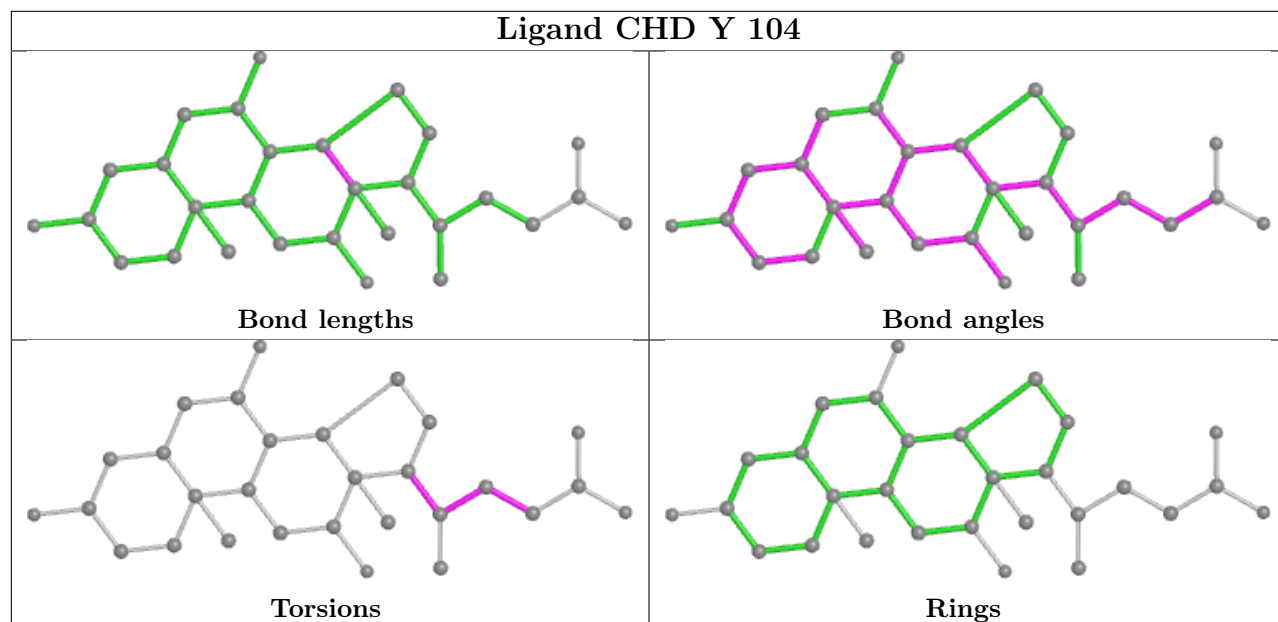


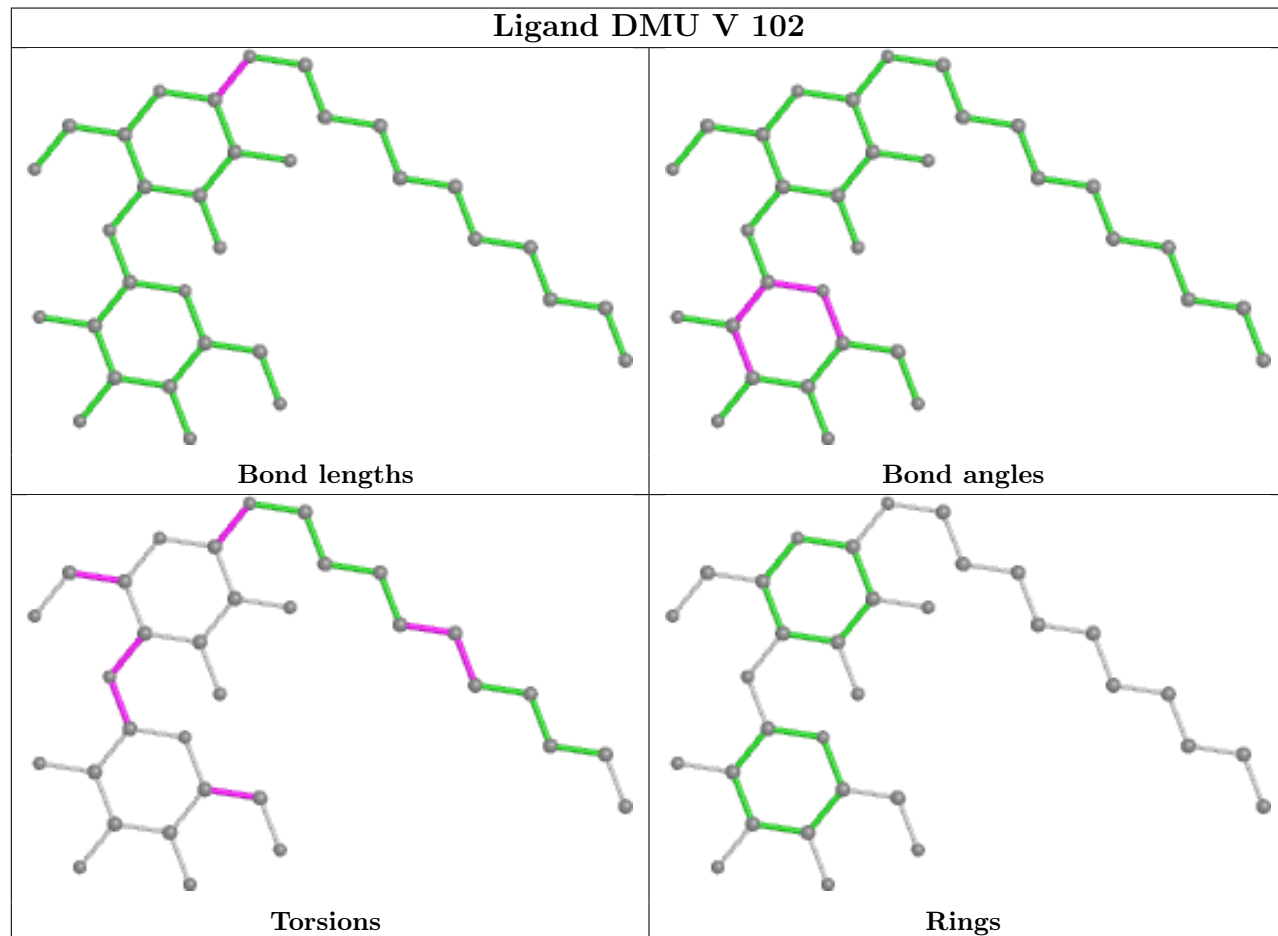
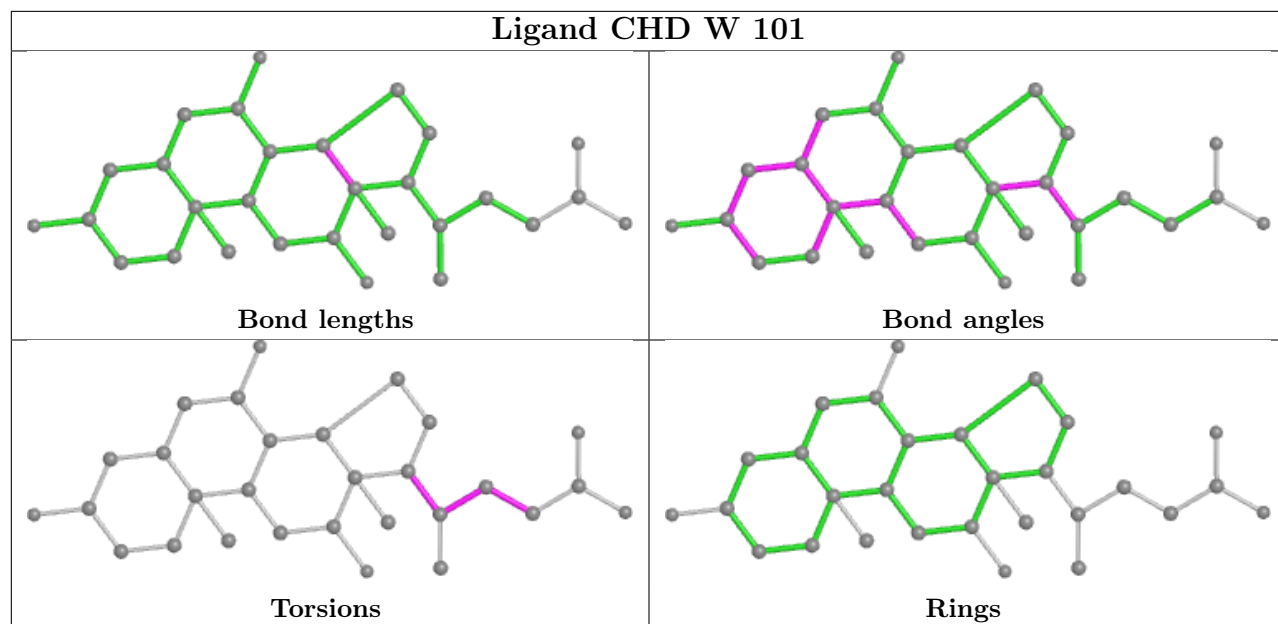
Ligand TGL B 301

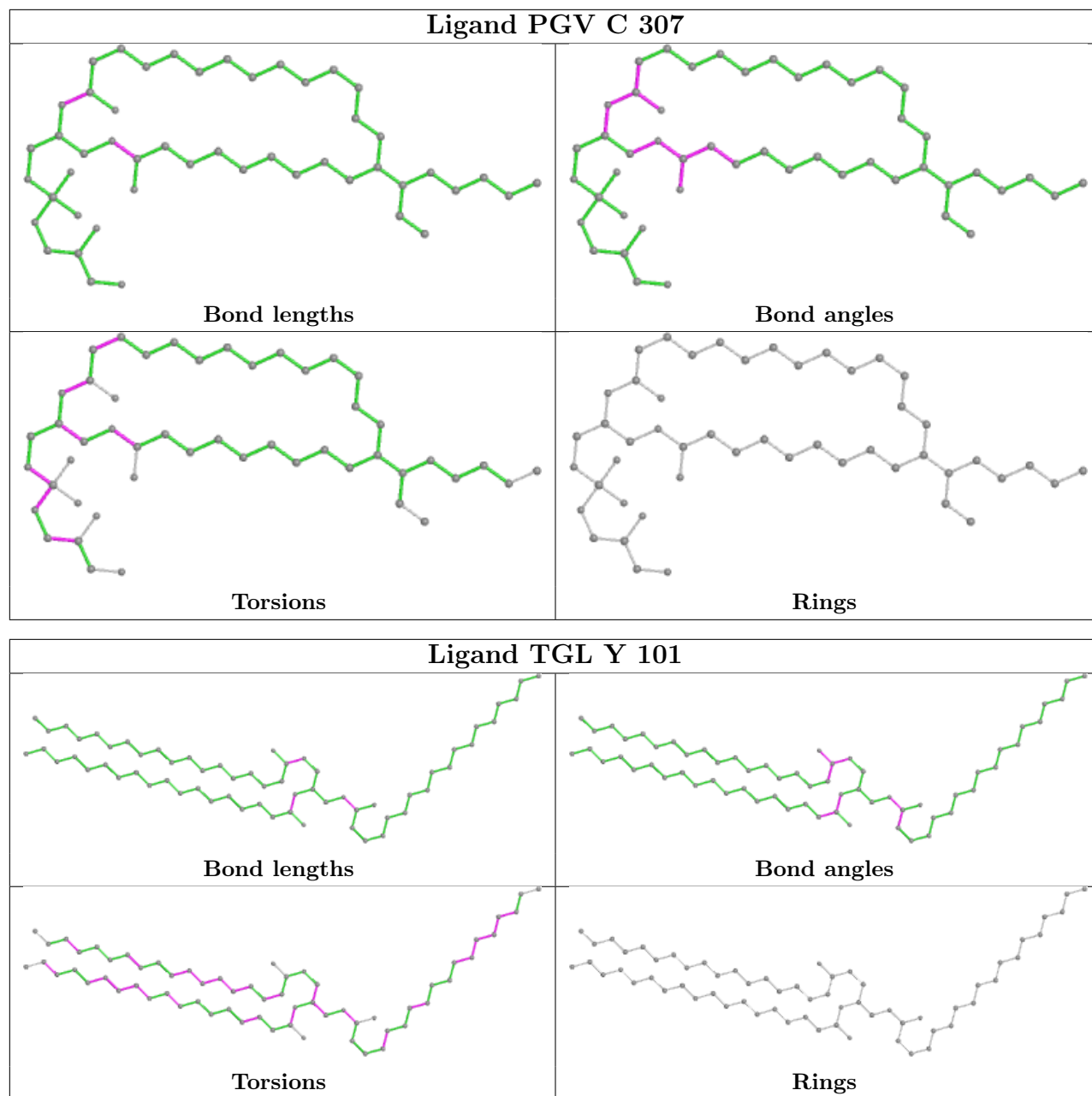


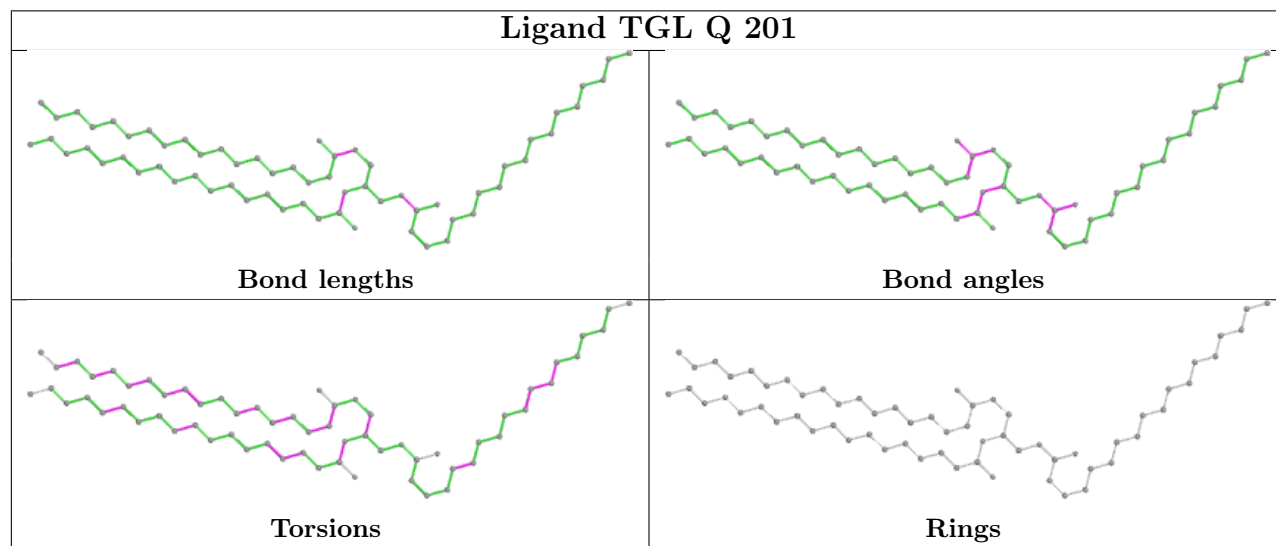
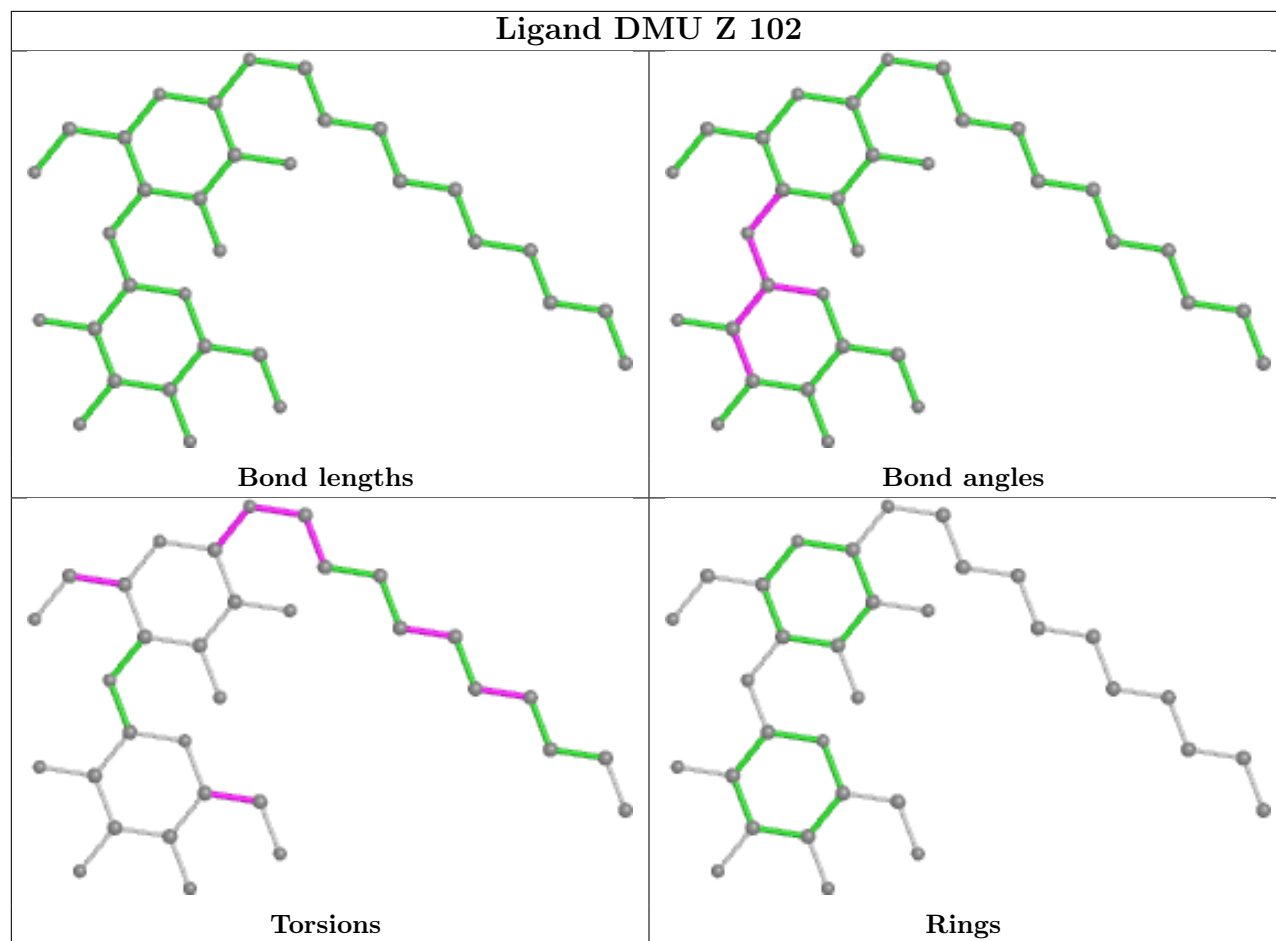
Ligand CHD C 309

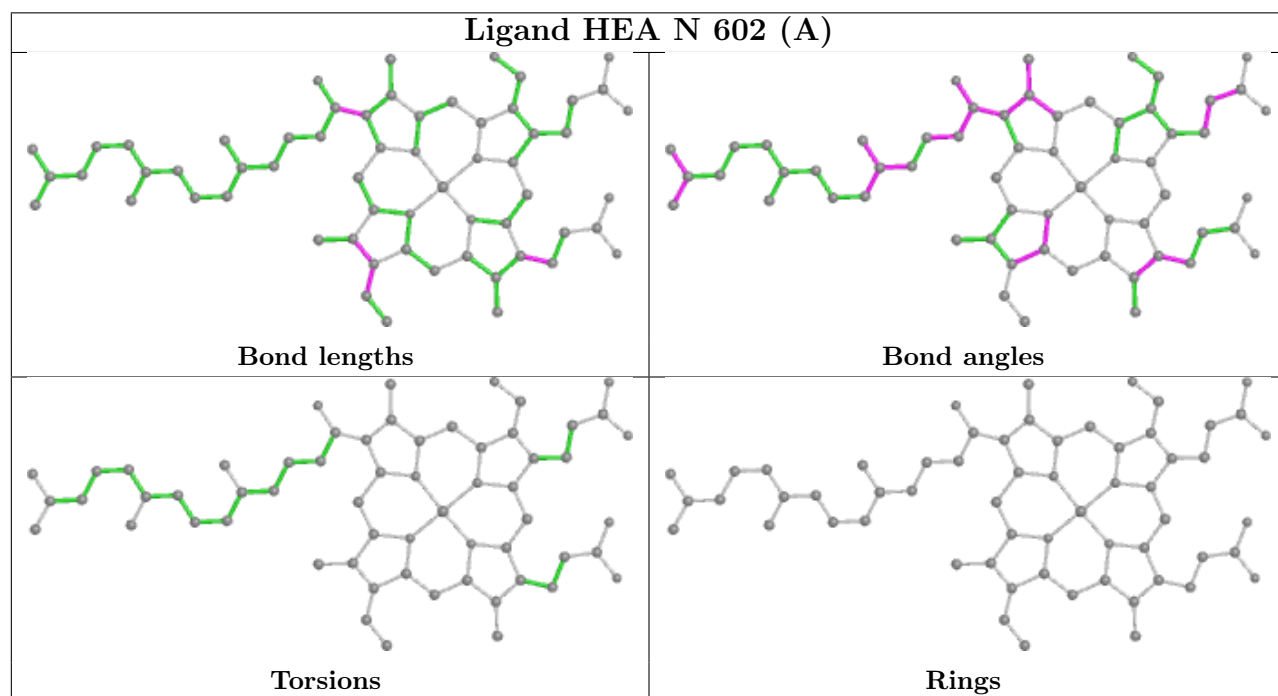
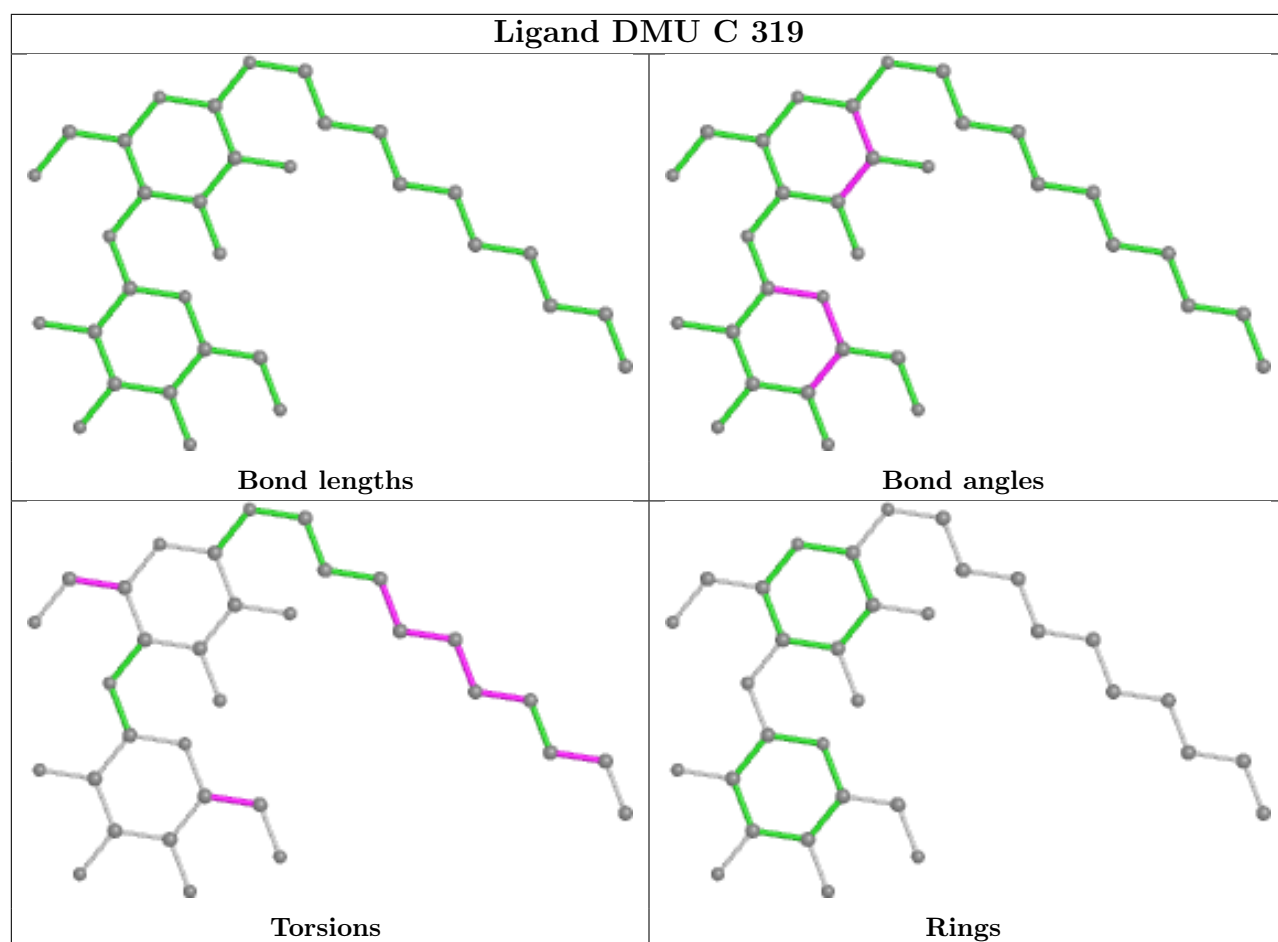


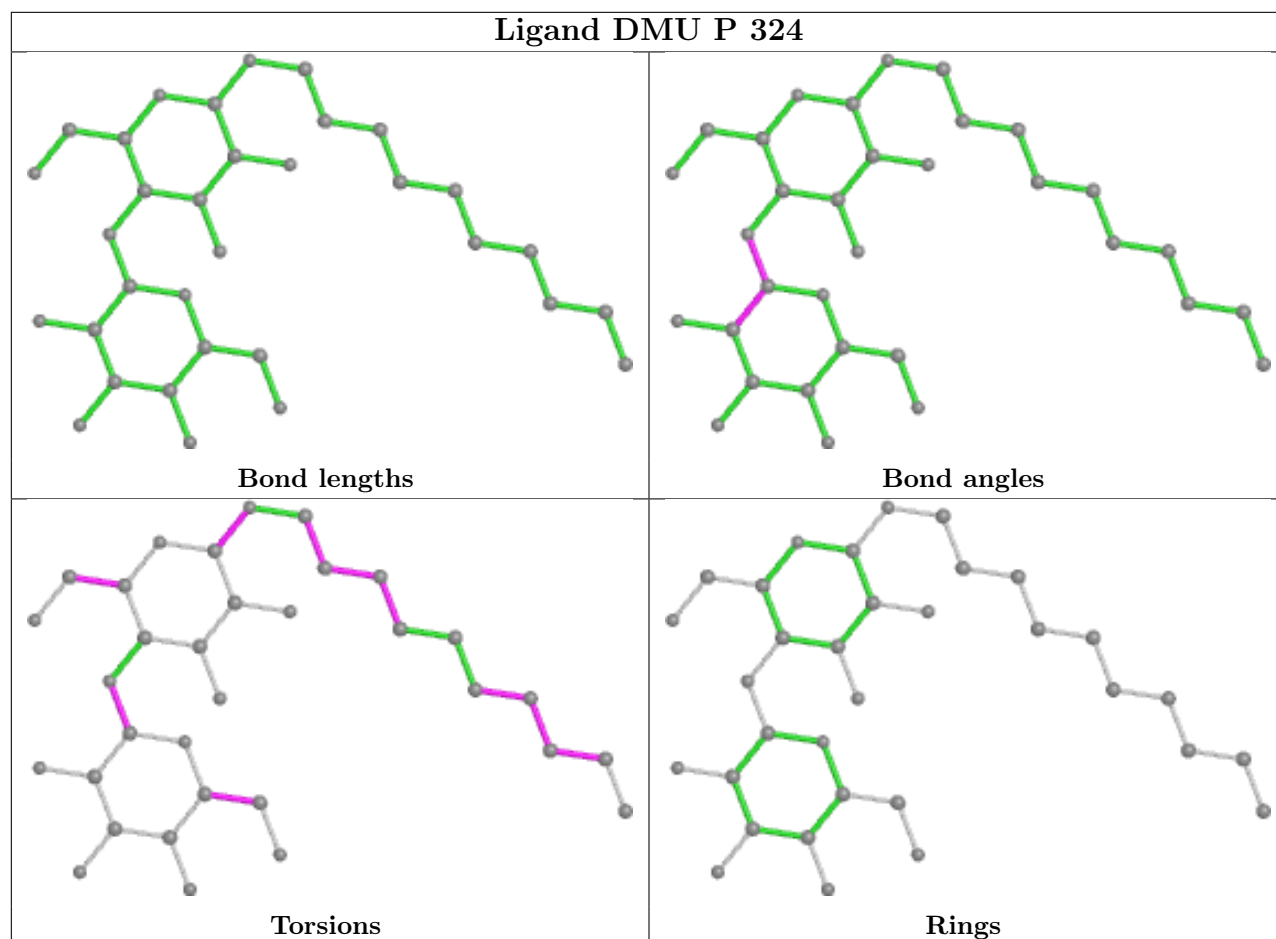
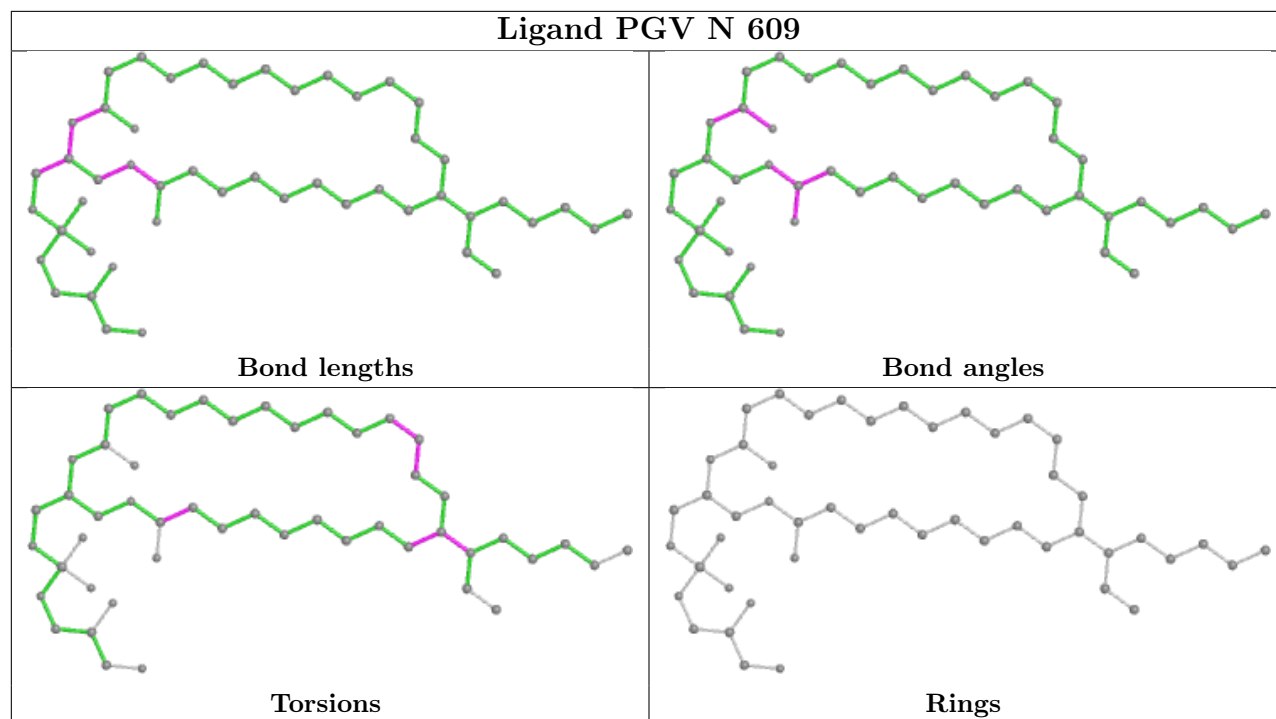


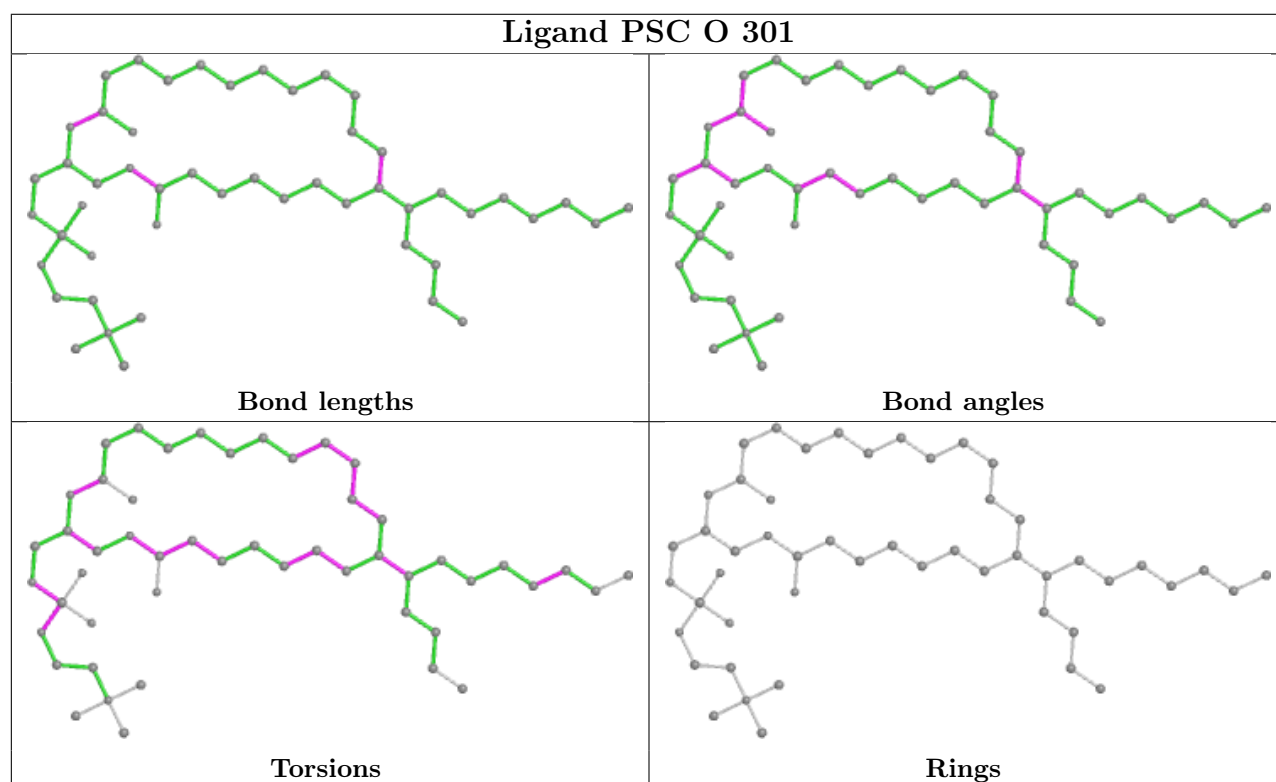
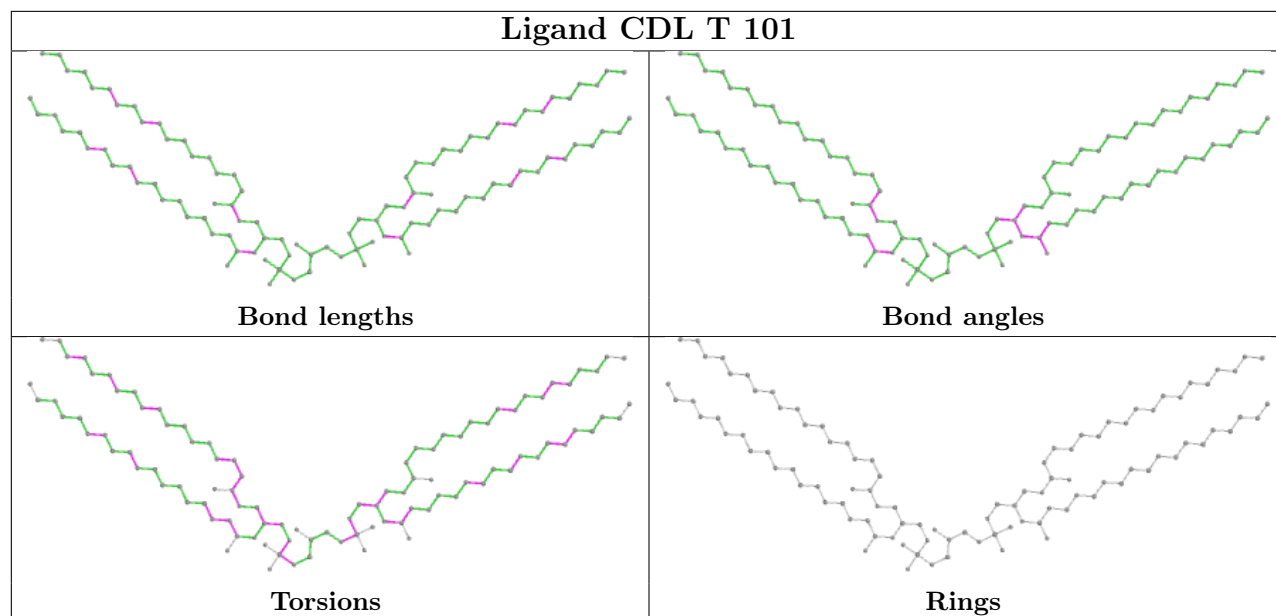




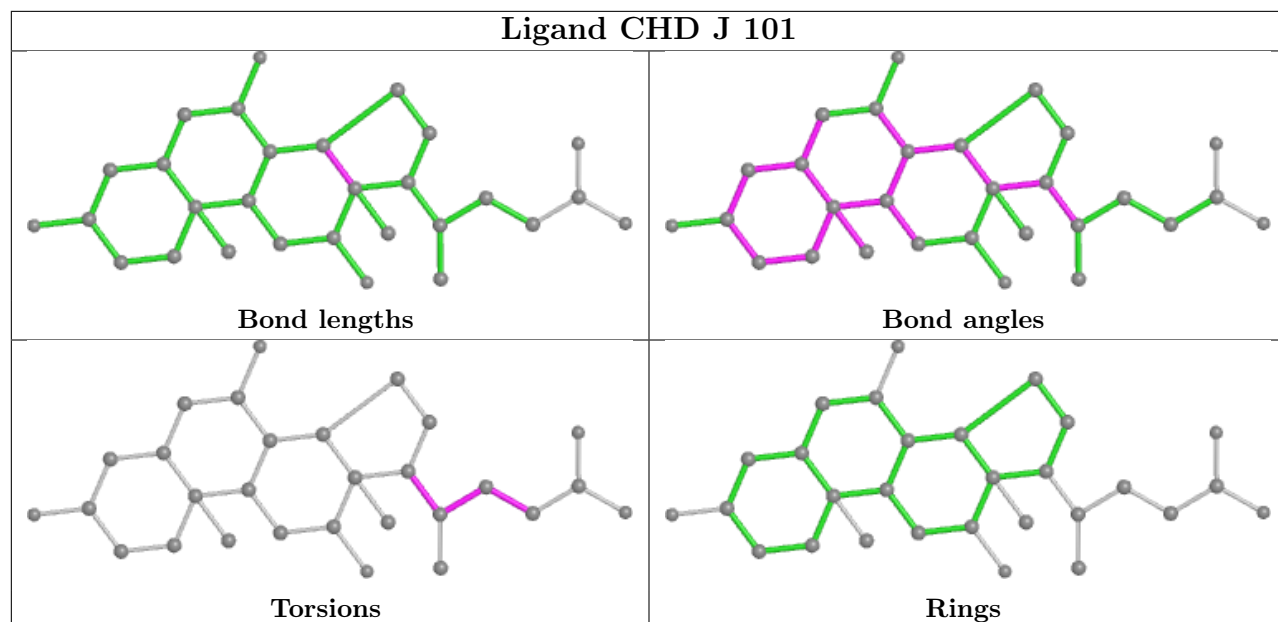




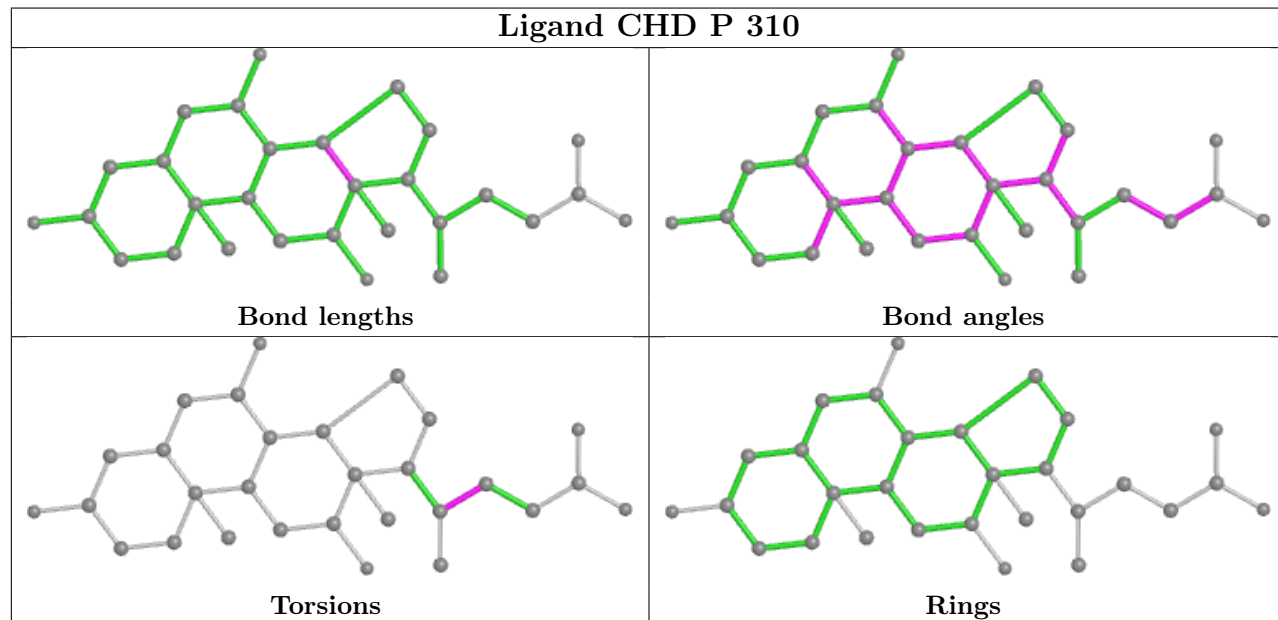


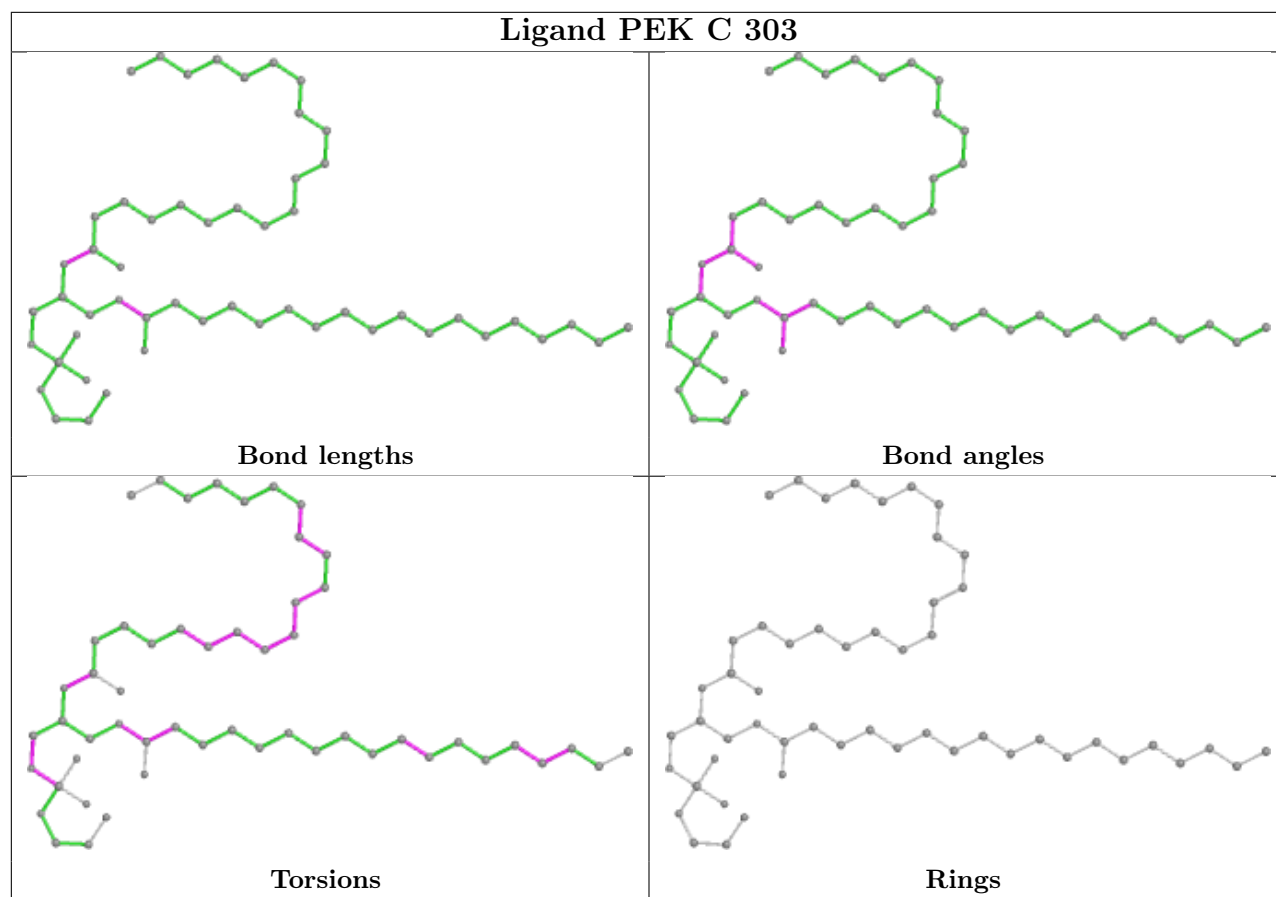
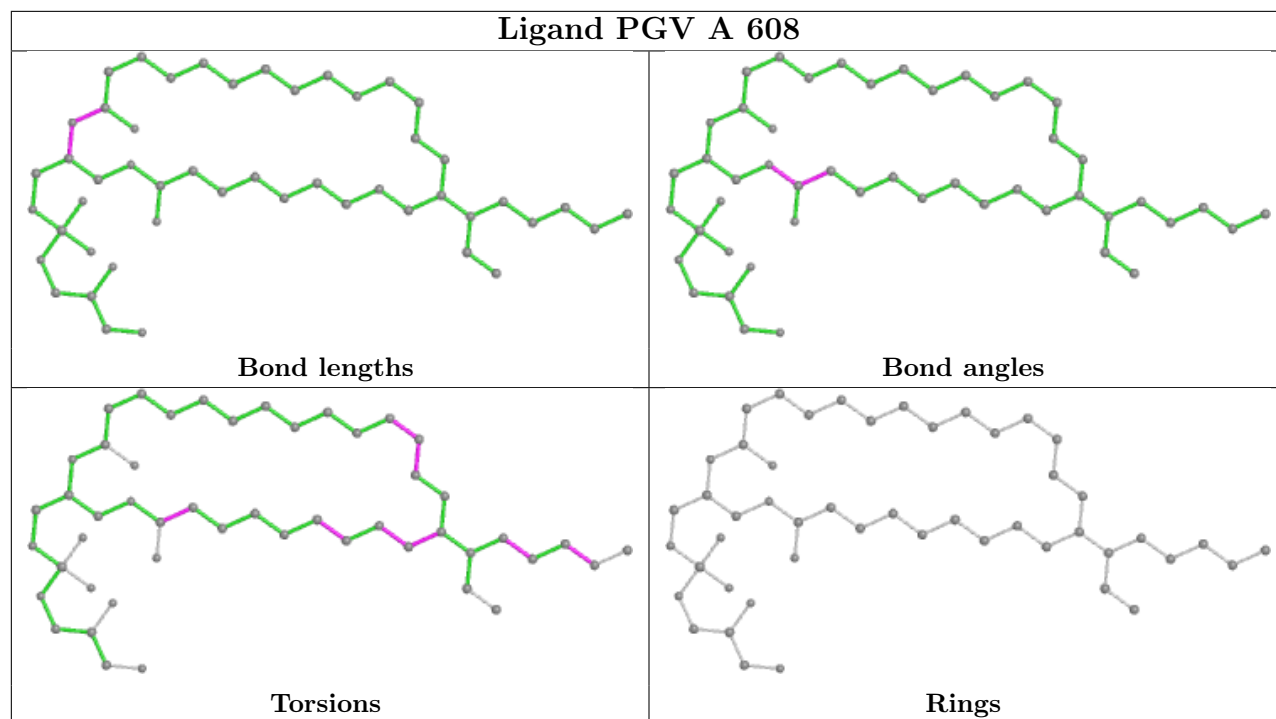


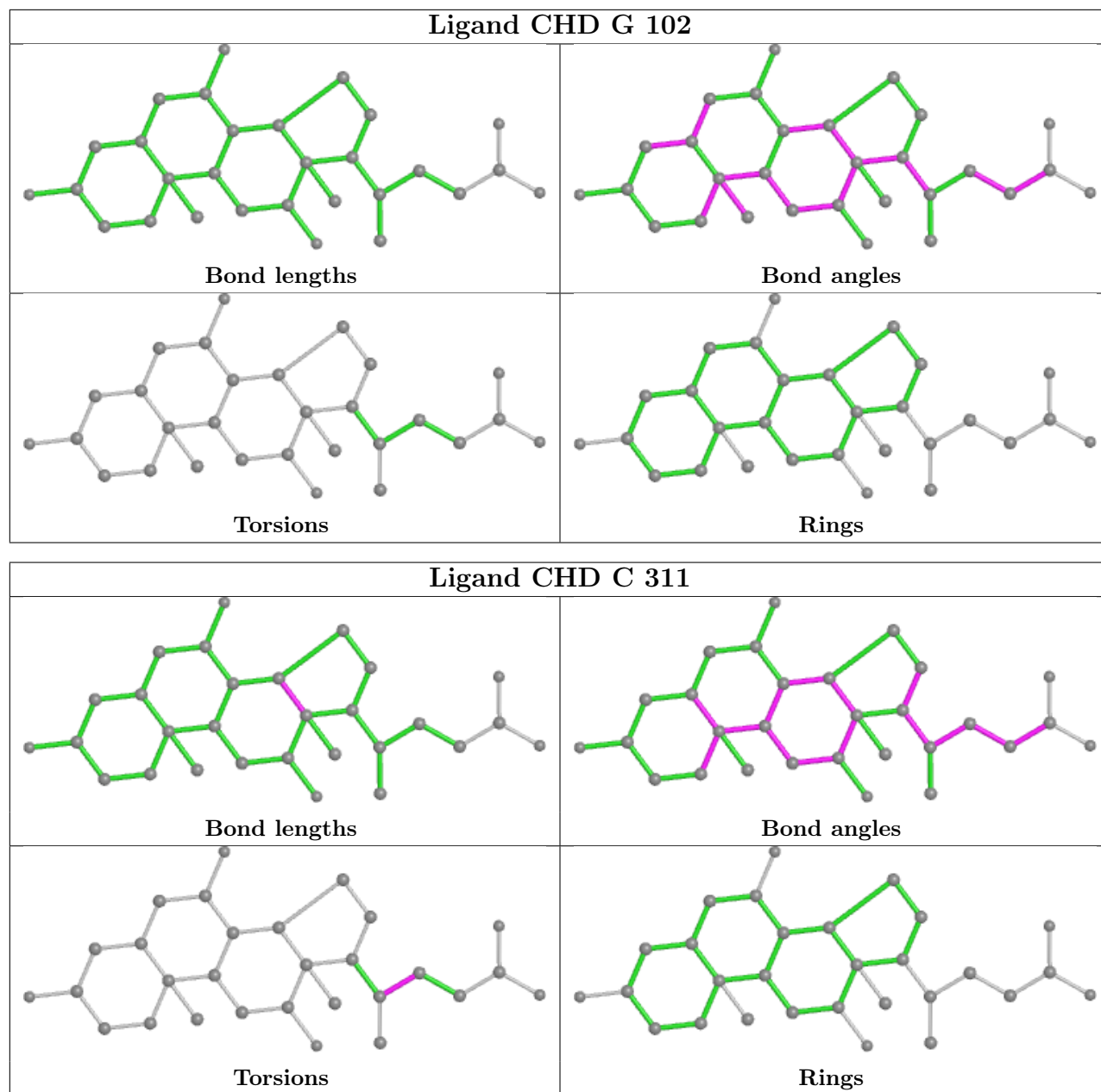
Ligand CHD J 101

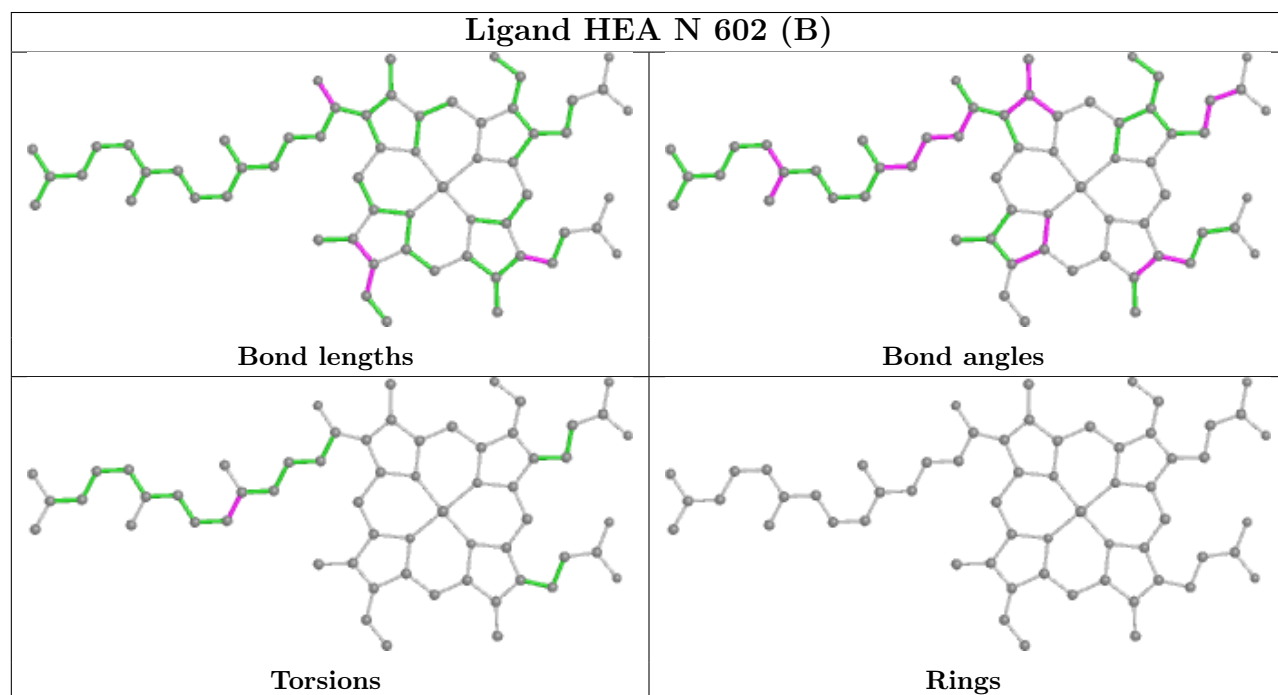
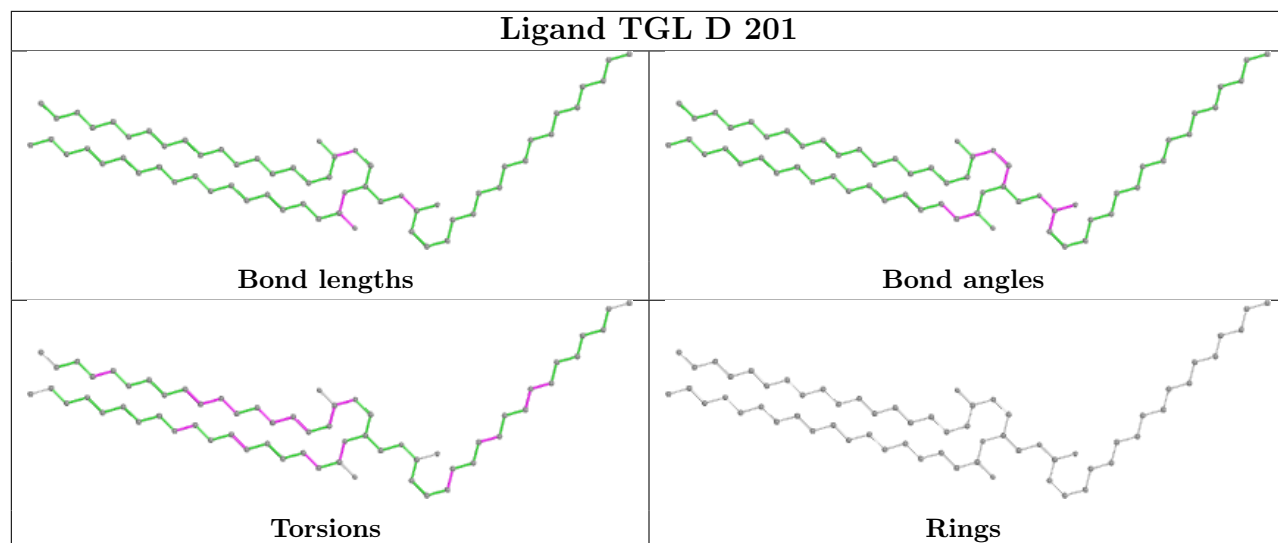


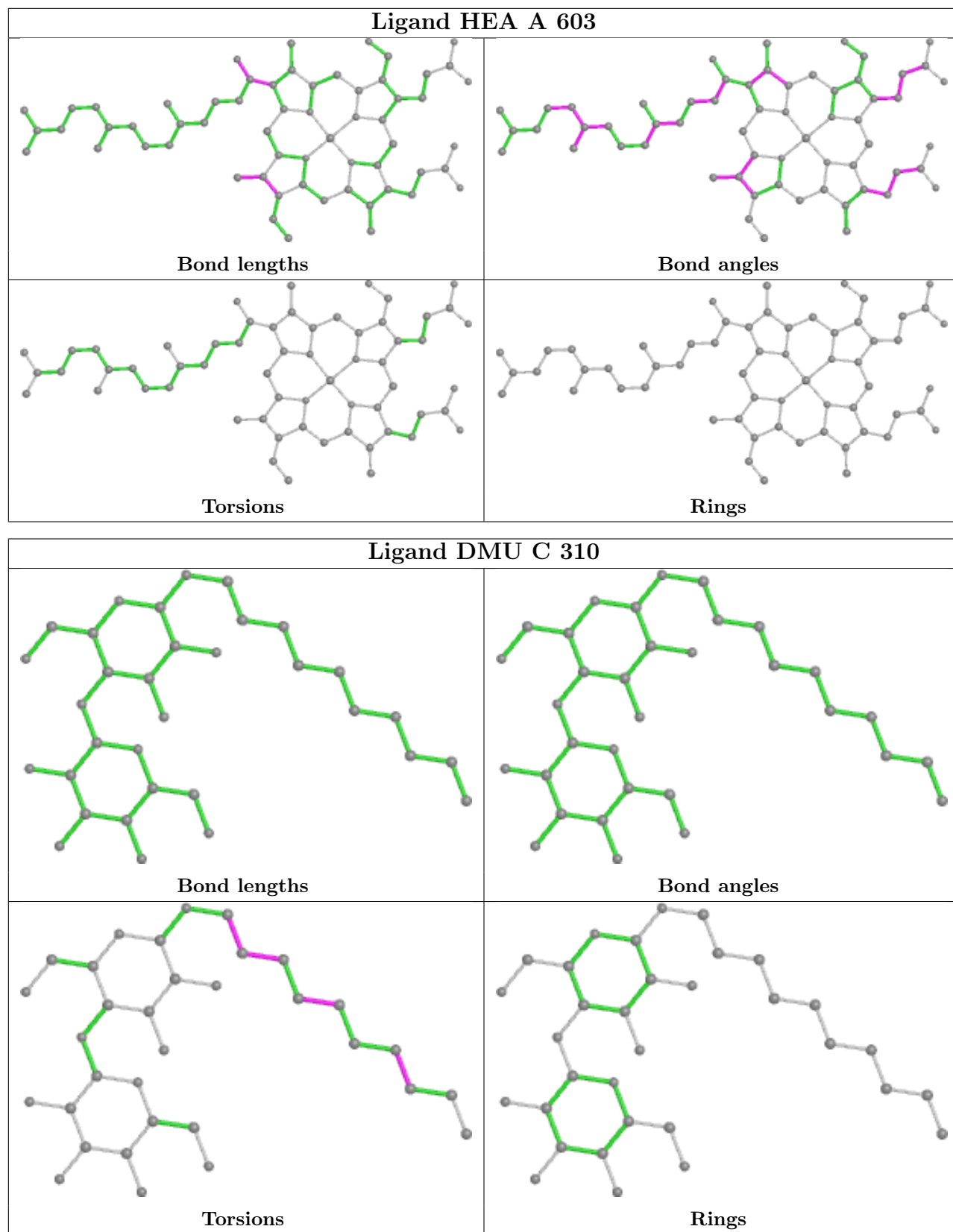
Ligand CHD P 310



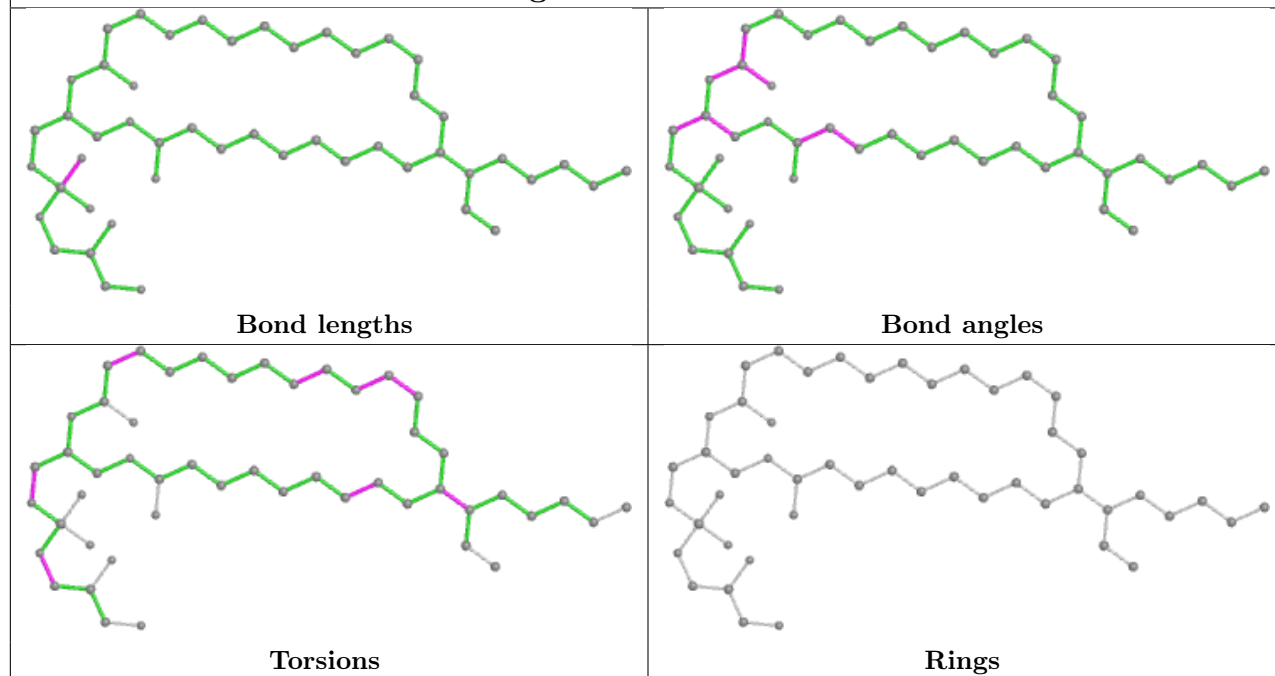




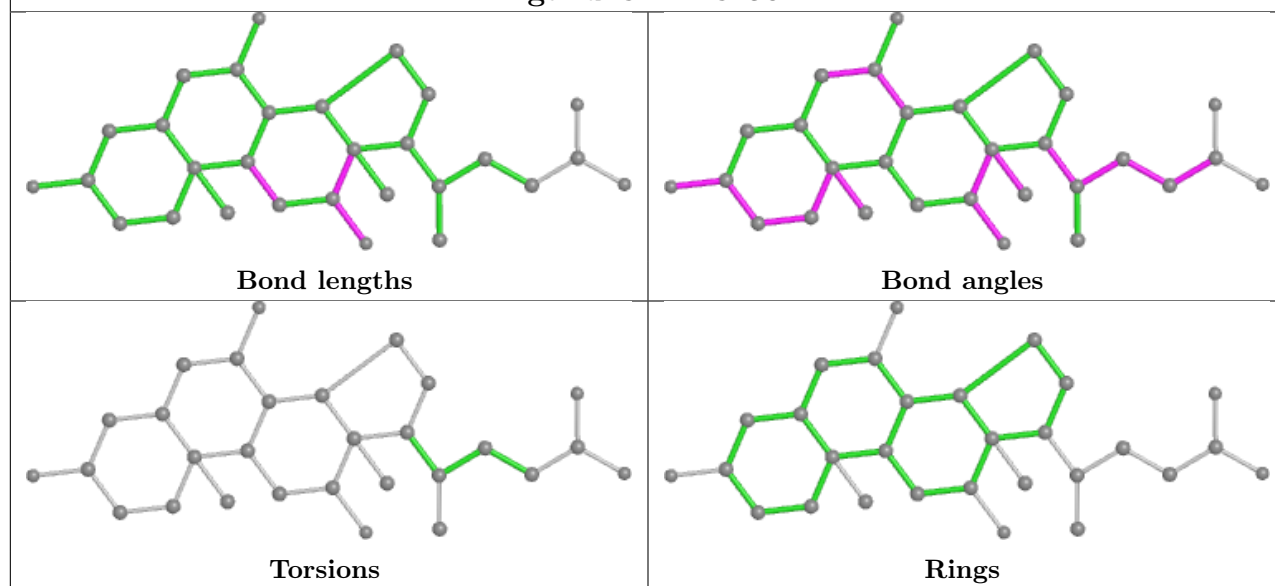




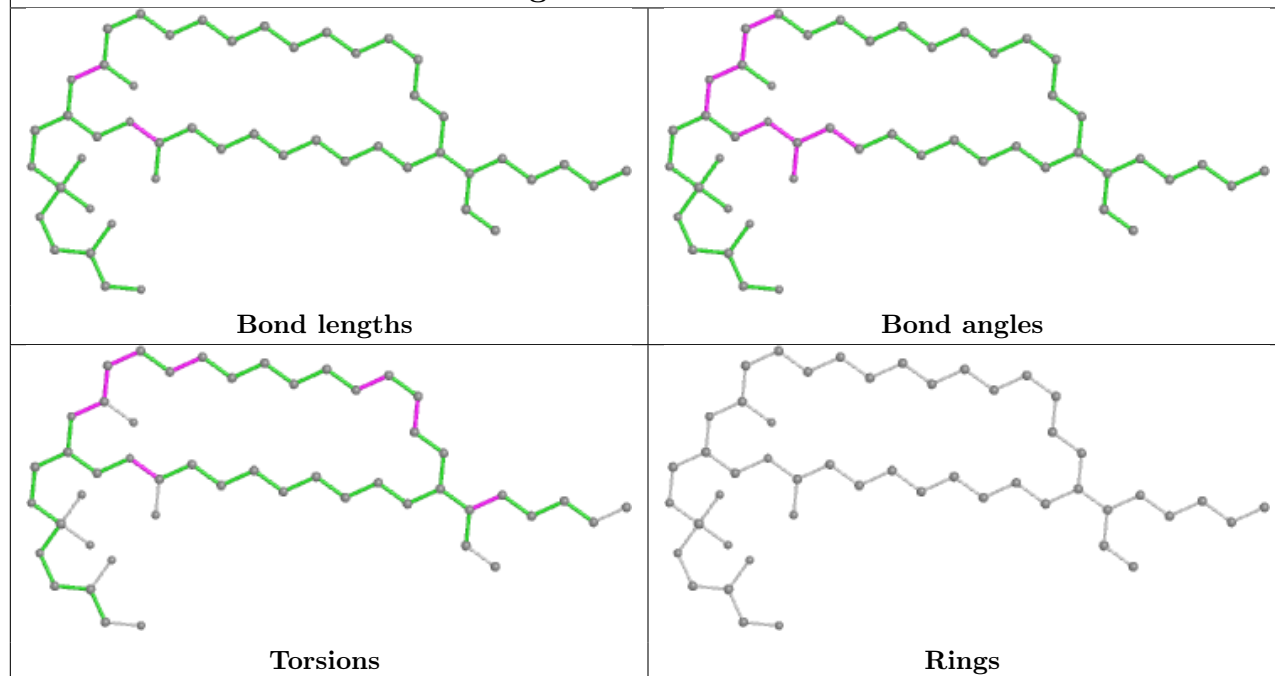
Ligand PGV P 306



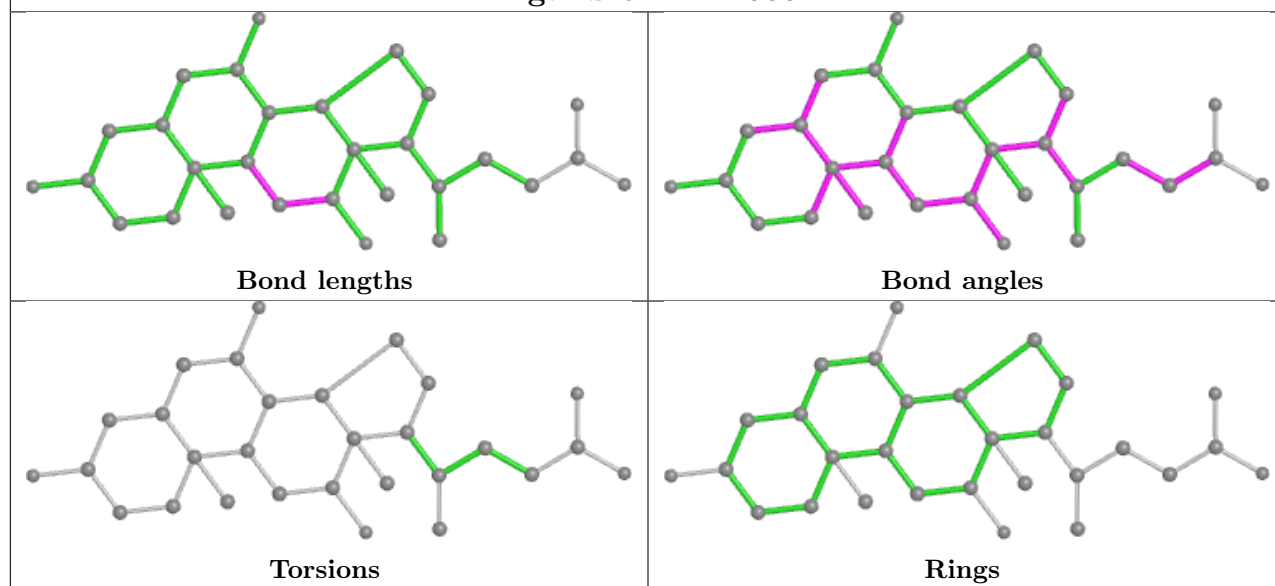
Ligand CHD C 301

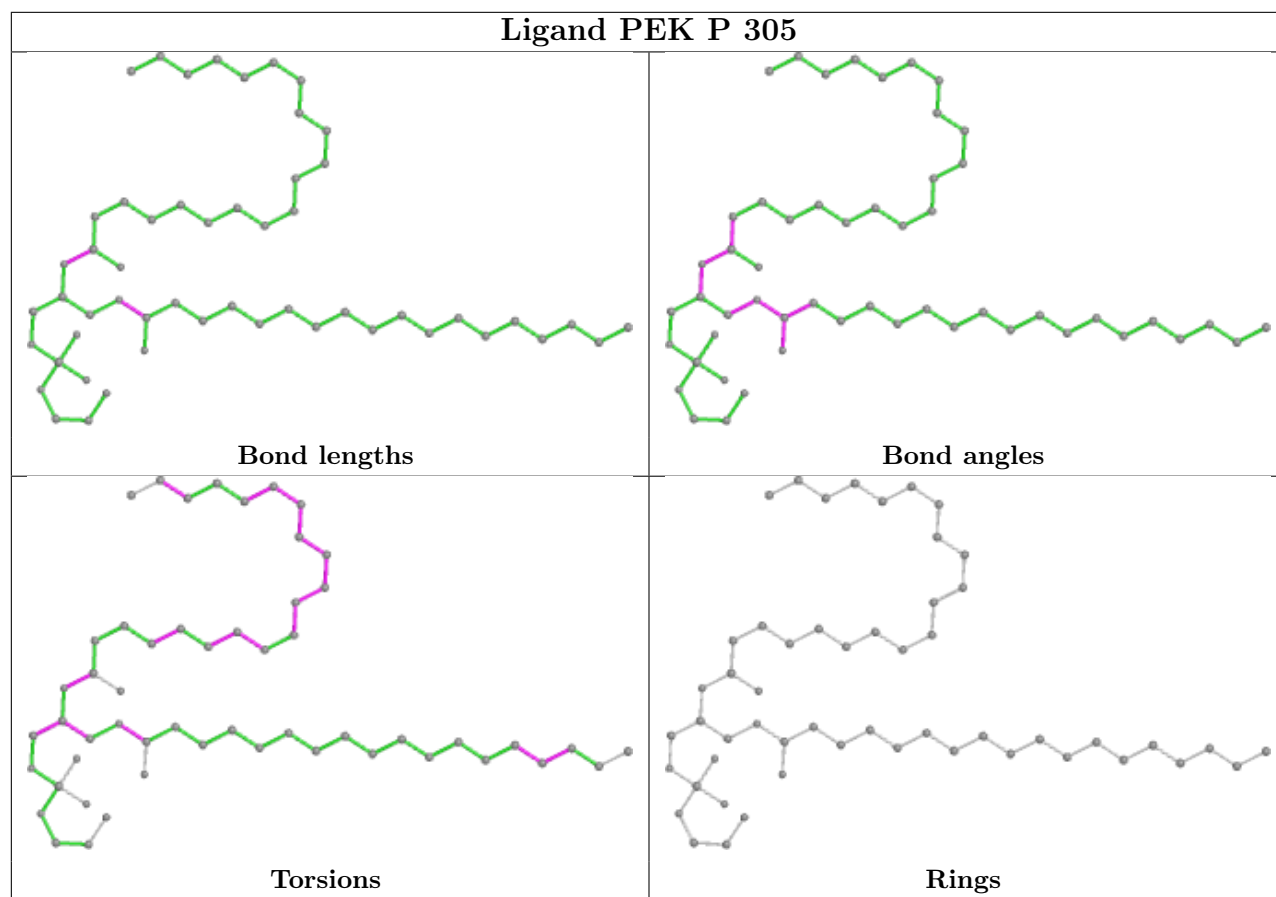
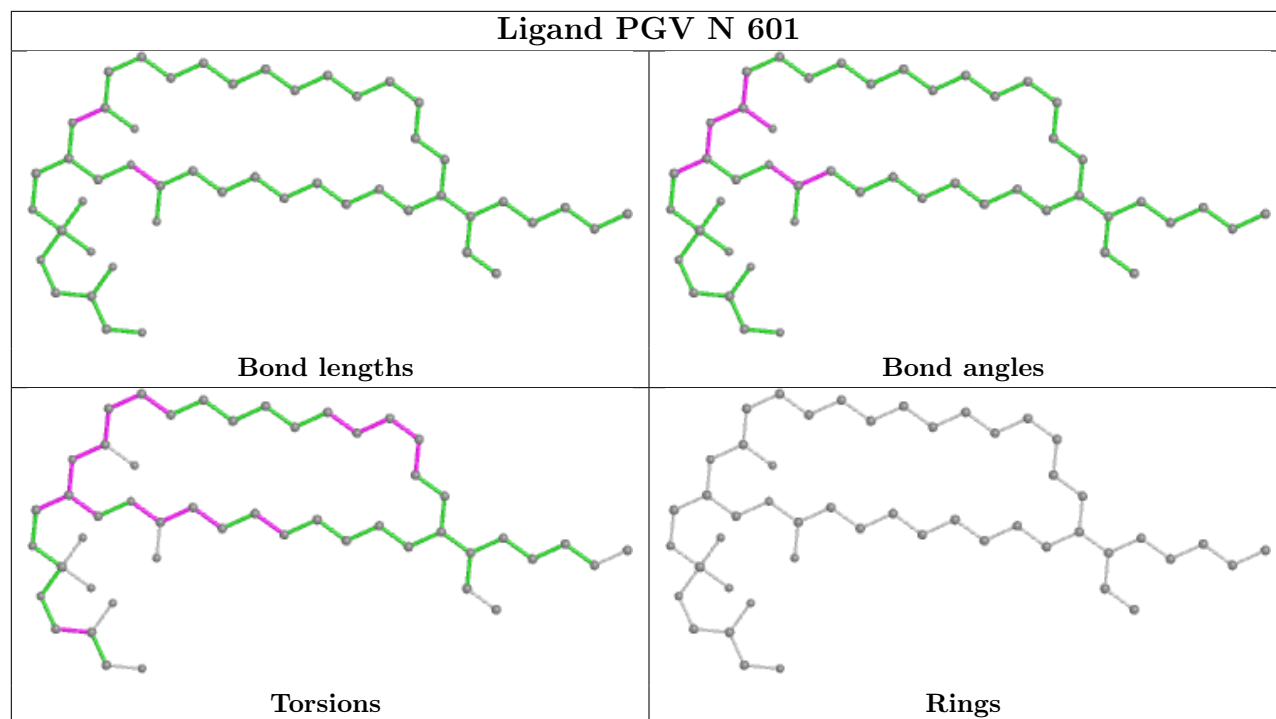


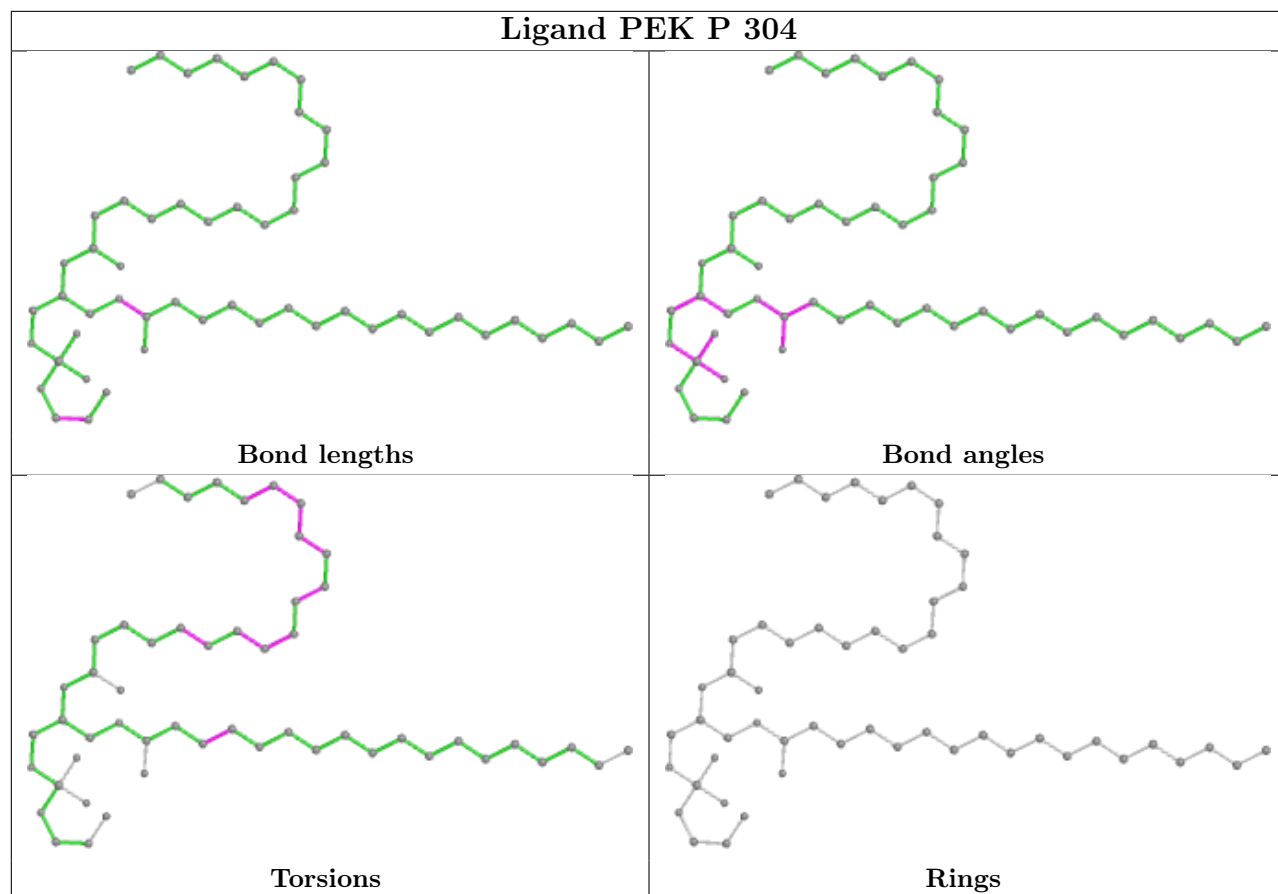
Ligand PGV P 307

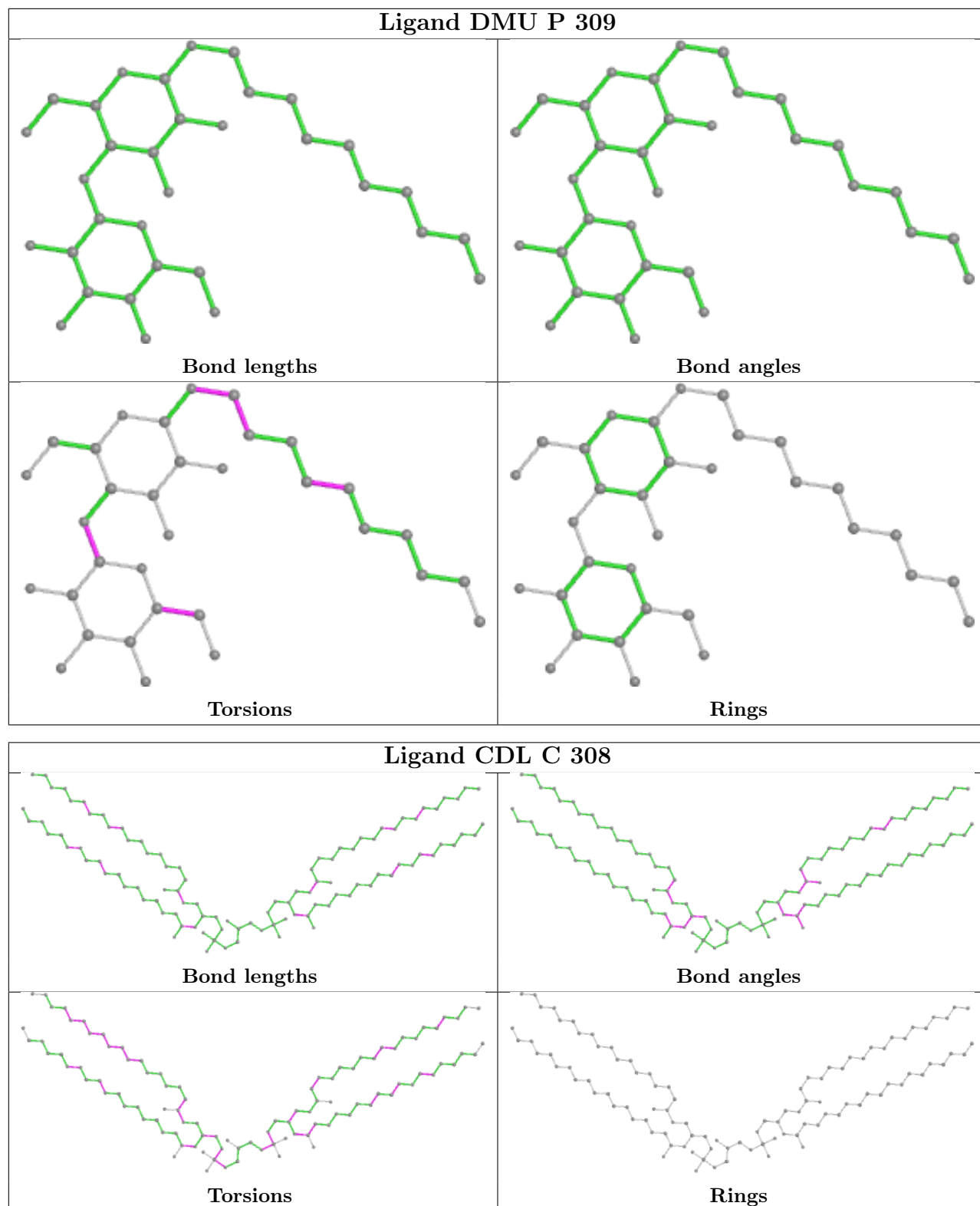


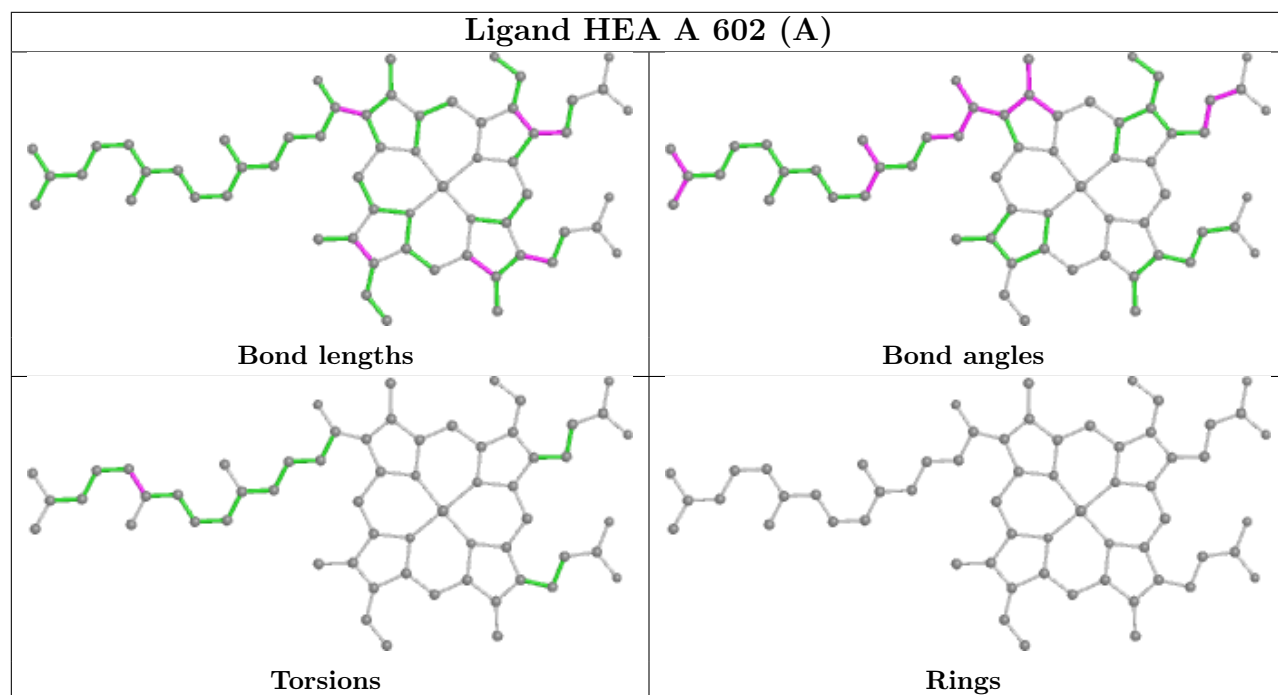
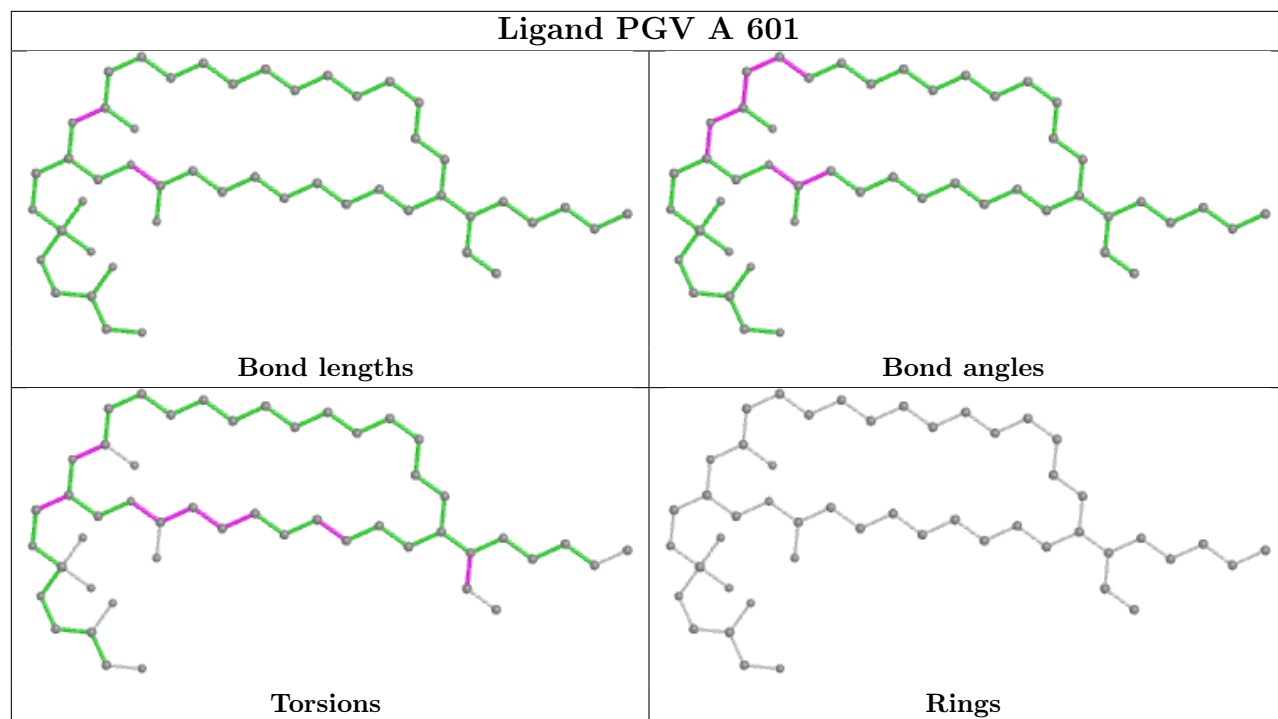
Ligand CHD B 303

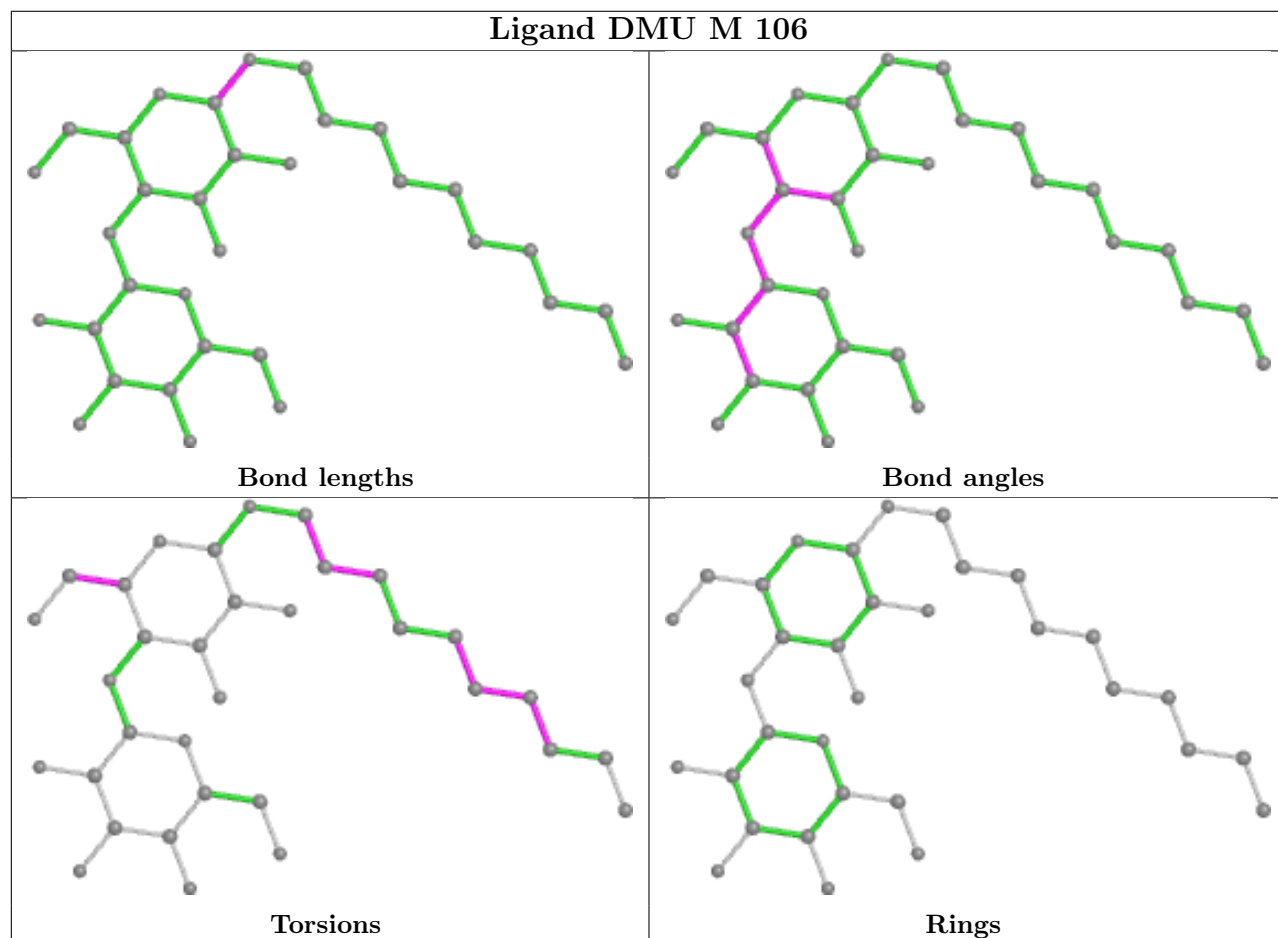
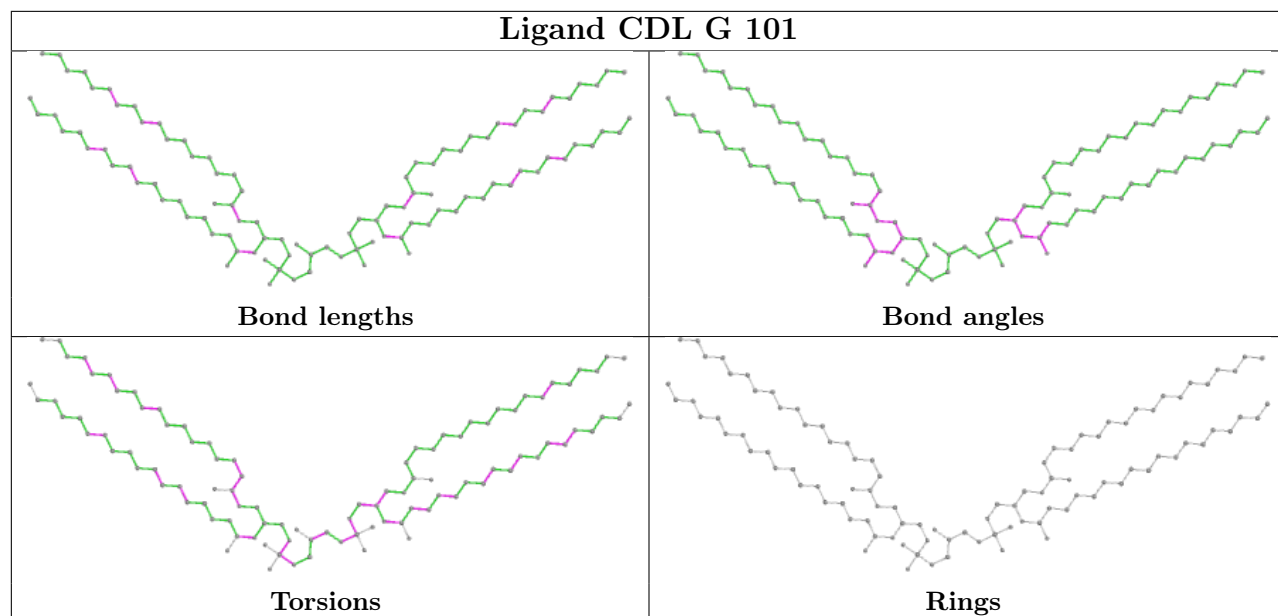


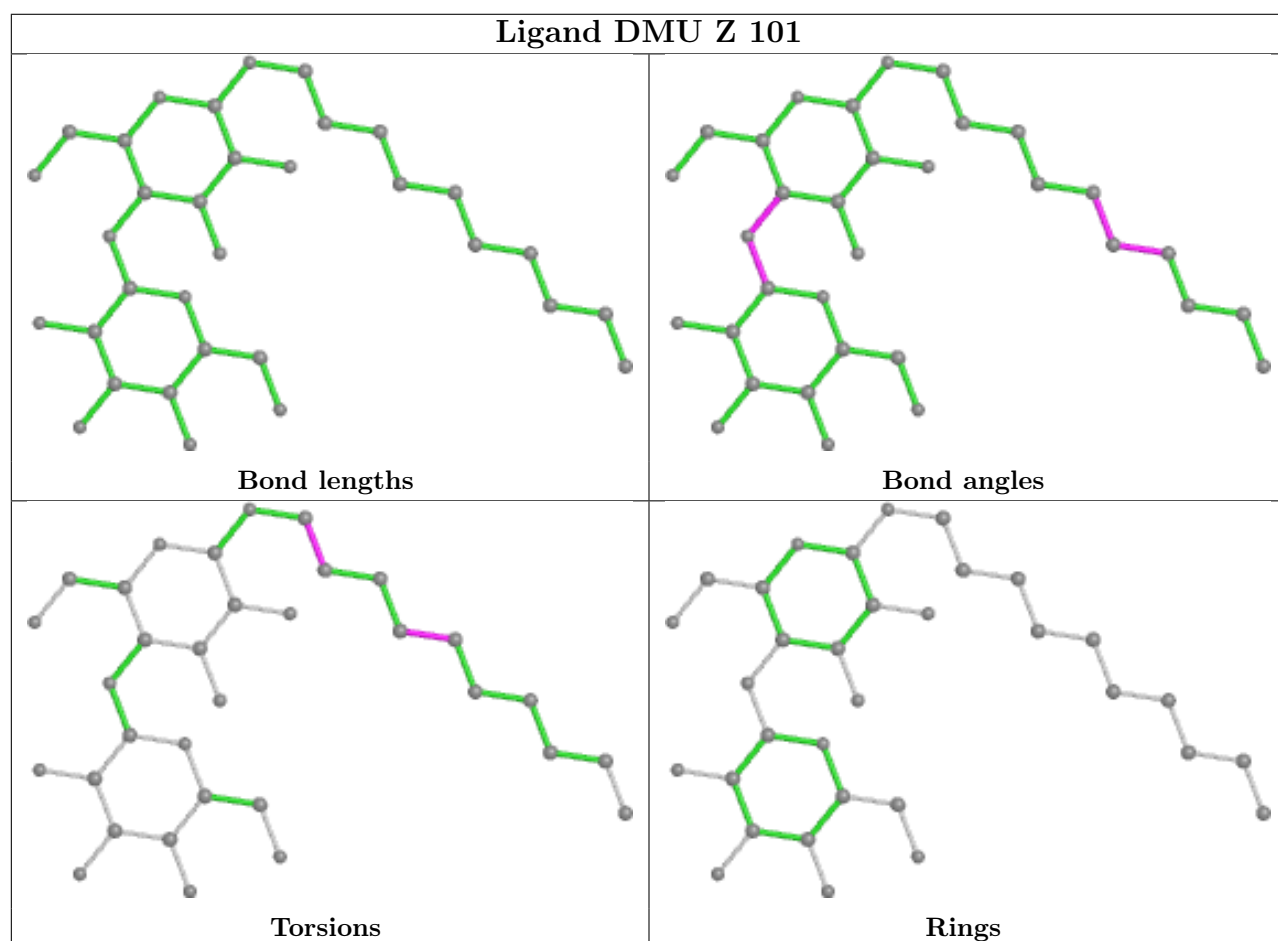
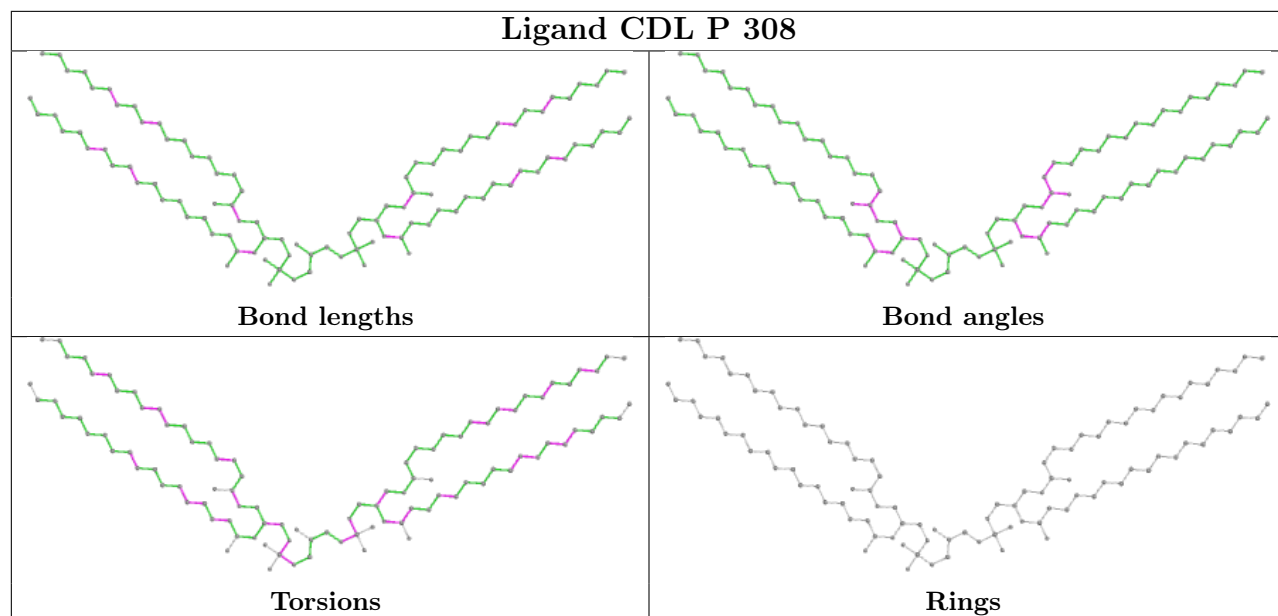


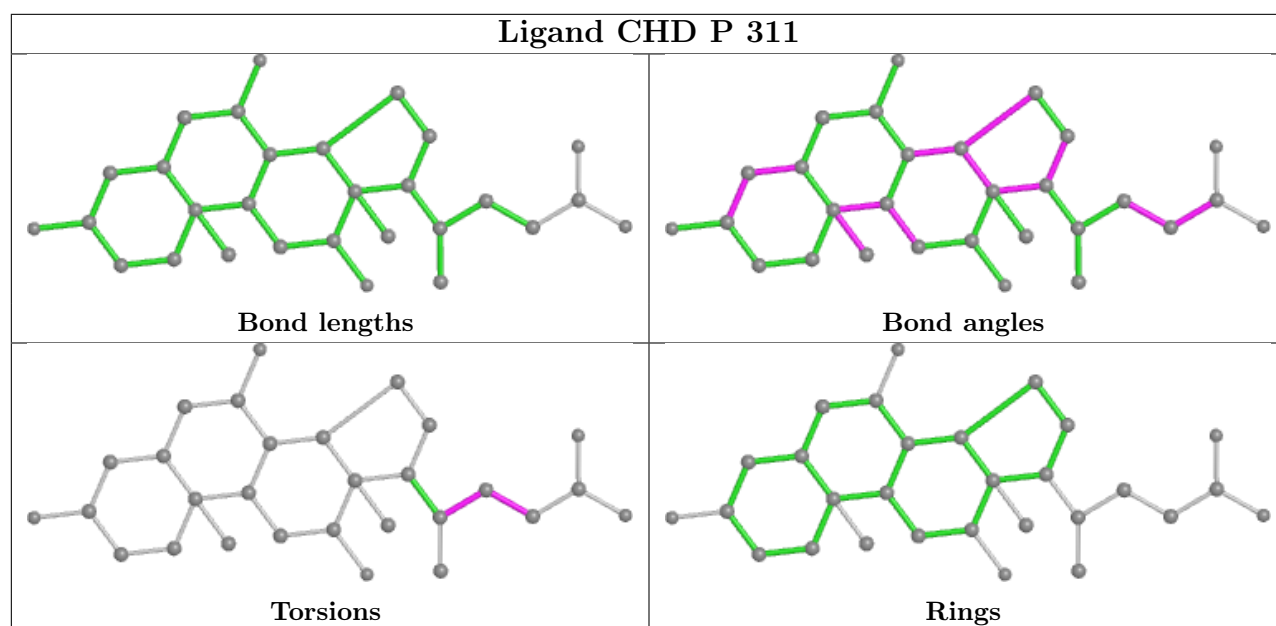
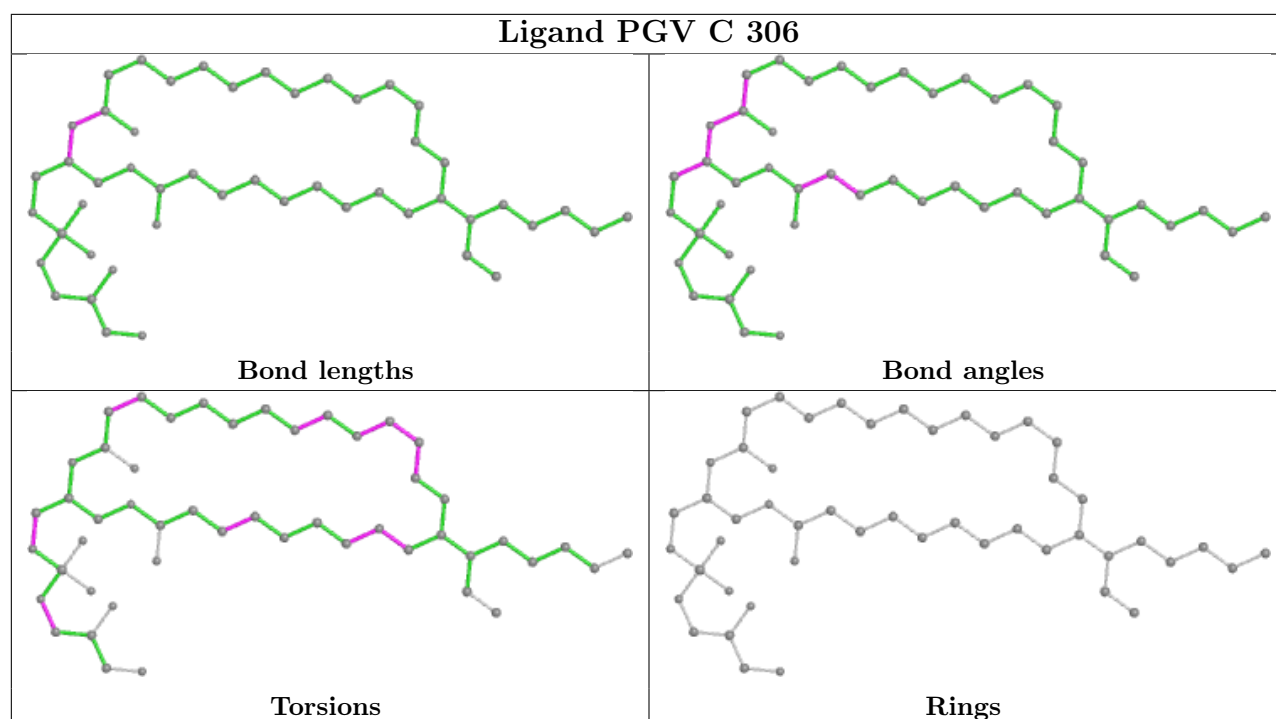


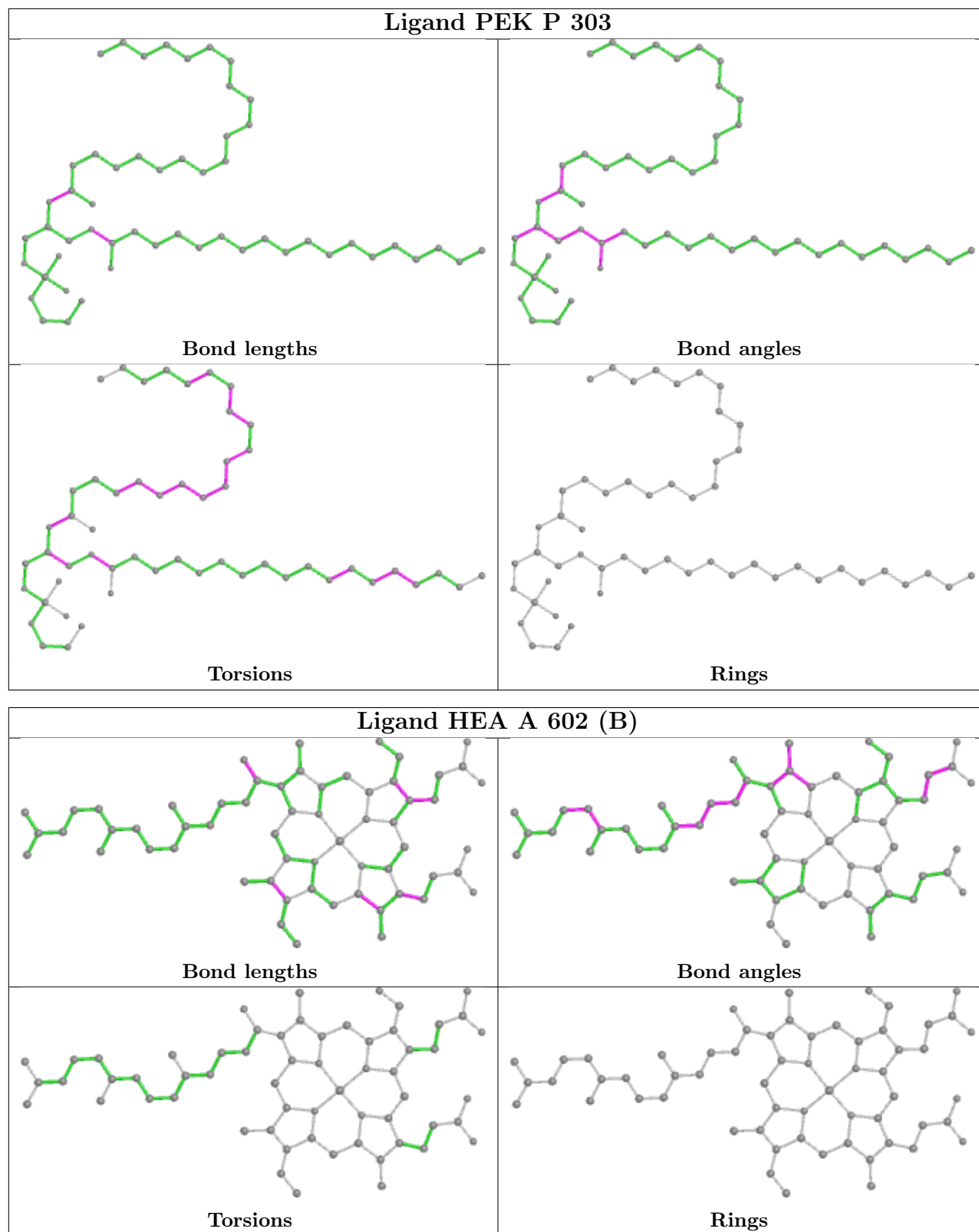












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.12	1 (0%) 95 95	18, 23, 30, 74	0
1	N	513/514 (99%)	-0.16	0 100 100	19, 25, 33, 69	0
2	B	226/227 (99%)	-0.08	6 (2%) 54 58	21, 29, 53, 108	0
2	O	226/227 (99%)	-0.13	4 (1%) 68 72	25, 34, 62, 118	0
3	C	259/261 (99%)	-0.14	0 100 100	20, 26, 39, 84	0
3	P	259/261 (99%)	-0.04	2 (0%) 86 88	20, 27, 40, 108	0
4	D	144/147 (97%)	-0.28	1 (0%) 87 90	25, 32, 50, 86	0
4	Q	144/147 (97%)	0.90	10 (6%) 16 19	30, 44, 89, 254	0
5	E	105/109 (96%)	-0.24	2 (1%) 66 70	26, 31, 57, 134	0
5	R	105/109 (96%)	-0.20	2 (1%) 66 70	26, 38, 64, 127	0
6	F	94/98 (95%)	0.04	4 (4%) 35 39	22, 32, 61, 160	0
6	S	94/98 (95%)	0.08	5 (5%) 26 29	22, 31, 58, 169	0
7	G	83/85 (97%)	1.01	17 (20%) 1 0	25, 33, 142, 185	0
7	T	83/85 (97%)	1.02	16 (19%) 1 1	24, 36, 141, 185	0
8	H	79/85 (92%)	0.44	10 (12%) 3 4	26, 35, 117, 150	0
8	U	79/85 (92%)	0.40	8 (10%) 7 8	30, 40, 135, 187	0
9	I	72/73 (98%)	0.18	5 (6%) 16 19	28, 42, 71, 85	0
9	V	72/73 (98%)	0.35	3 (4%) 36 40	28, 49, 81, 147	0
10	J	58/59 (98%)	0.30	5 (8%) 10 12	26, 36, 78, 150	0
10	W	58/59 (98%)	0.10	3 (5%) 27 30	27, 37, 80, 213	0
11	K	49/56 (87%)	-0.09	1 (2%) 65 69	28, 36, 50, 82	0
11	X	49/56 (87%)	0.17	3 (6%) 21 23	35, 44, 76, 96	0
12	L	46/47 (97%)	-0.02	2 (4%) 35 39	24, 29, 44, 108	0
12	Y	46/47 (97%)	-0.00	1 (2%) 62 66	28, 34, 63, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.16	3 (6%)	16	18	24, 29, 69, 120	0
13	Z	43/46 (93%)	0.39	3 (6%)	16	18	31, 37, 96, 250	0
All	All	3542/3614 (98%)	0.04	117 (3%)	46	51	18, 30, 66, 254	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	42.6
4	Q	6	VAL	26.1
4	Q	4	SER	22.7
6	F	1	ALA	15.3
7	T	3	ALA	12.1
7	G	8	HIS	12.1
13	Z	42	LYS	11.5
7	G	4	ALA	10.7
7	G	3	ALA	10.1
6	S	1	ALA	9.9
7	T	1	ALA	9.3
10	J	58	LYS	9.1
4	Q	7	LYS	8.6
7	T	36	TRP	8.6
4	Q	8	SER	8.5
6	S	94	HIS	8.3
7	T	8	HIS	8.2
10	W	58	LYS	7.8
8	H	8	ILE	7.8
7	T	7[A]	ASP	7.2
8	U	8	ILE	7.1
12	Y	47	LYS	6.9
5	R	5	HIS	6.6
7	T	5	LYS	6.5
13	Z	43	SER	6.3
2	O	90	ILE	6.3
8	U	47	GLY	6.3
7	G	2	SER	6.2
7	G	5	LYS	6.2
8	H	46	LYS	6.0
7	G	36	TRP	5.9
7	G	10	GLY	5.7
9	V	37	PHE	5.6
7	T	10	GLY	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	6	GLY	5.5
13	M	43	SER	5.5
7	G	7	ASP	5.4
6	S	2	SER	5.4
8	H	9	LYS	5.2
12	L	2[A]	HIS	5.2
7	T	4	ALA	5.1
8	H	44	THR	5.1
7	G	9	GLY	5.1
7	T	42	ARG	5.0
4	Q	9	GLU	4.9
10	J	1	PHE	4.9
7	T	2	SER	4.7
8	U	9	LYS	4.6
7	G	42	ARG	4.6
8	U	46	LYS	4.5
2	B	90	ILE	4.4
12	L	47	LYS	4.4
8	H	45	ALA	4.2
5	R	109	VAL	4.2
5	E	5	HIS	4.1
2	O	227	LEU	4.0
9	I	37	PHE	4.0
9	I	29	LEU	4.0
8	H	47	GLY	4.0
8	H	48	GLY	3.9
10	W	1	PHE	3.9
8	U	45	ALA	3.9
7	T	9	GLY	3.8
4	Q	10	ASP	3.8
10	J	57	HIS	3.7
10	W	57	HIS	3.7
4	Q	51	LEU	3.5
6	F	2	SER	3.5
13	M	42	LYS	3.5
10	J	55	PHE	3.4
13	Z	40	TYR	3.4
2	O	91	ASN	3.2
11	K	6	ALA	3.2
11	X	6	ALA	3.2
8	H	7	LYS	3.1
9	I	25	PHE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	V	34	PHE	3.0
7	T	39	SER	3.0
7	T	6	GLY	3.0
8	U	10	ASN	3.0
7	T	84	LYS	3.0
6	F	3	GLY	2.9
7	T	40	GLY	2.9
7	T	37	LEU	2.9
8	U	44	THR	2.9
3	P	3	HIS	2.9
2	B	91	ASN	2.8
6	S	3	GLY	2.8
7	G	41	HIS	2.8
7	G	37	LEU	2.7
6	F	94	HIS	2.6
2	O	113	TYR	2.6
13	M	40	TYR	2.6
6	S	93	PRO	2.6
10	J	52	TRP	2.5
2	B	59	GLN	2.5
4	D	4	SER	2.5
4	Q	17[A]	VAL	2.4
11	X	13	TYR	2.3
7	G	40	GLY	2.3
3	P	37	PHE	2.3
2	B	57	ASP	2.3
9	V	2	THR	2.3
8	U	7	LYS	2.2
8	H	10	ASN	2.2
7	G	45	PRO	2.2
9	I	34	PHE	2.2
9	I	18	ARG	2.2
8	H	42	ALA	2.2
1	A	513	LEU	2.1
2	B	60[A]	GLU	2.1
7	G	43	GLU	2.1
11	X	12	LYS	2.1
4	Q	19[A]	ARG	2.1
7	G	84	LYS	2.0
2	B	130	PRO	2.0
5	E	109	VAL	2.0

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

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	0.13	0.55	140,173,213,214	0
7	TPO	G	11	11/12	0.47	0.46	130,158,180,180	0
9	SAC	V	1	9/10	0.58	0.39	179,194,204,205	0
9	SAC	I	1	9/10	0.66	0.41	124,152,158,159	0
1	FME	A	1	10/11	0.94	0.11	35,41,68,72	0
2	FME	B	1	10/11	0.97	0.11	27,29,34,51	0
1	FME	N	1	10/11	0.97	0.09	35,41,68,69	0
2	FME	O	1	10/11	0.98	0.10	34,36,41,51	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
18	NA	C	302	1/1	-0.24	1.00	809,809,809,809	0
20	EDO	N	619	4/4	0.20	0.38	85,86,89,89	0
20	EDO	A	614	4/4	0.25	0.36	108,110,111,113	0
20	EDO	D	206	4/4	0.28	0.52	167,169,170,172	0
20	EDO	D	202	4/4	0.29	0.48	83,91,98,99	0
27	DMU	P	324	33/33	0.29	0.27	56,122,149,154	0
20	EDO	N	629	4/4	0.33	0.42	110,114,115,115	0
20	EDO	N	623	4/4	0.33	0.36	90,91,93,94	0
20	EDO	K	102	4/4	0.35	0.34	97,97,98,99	0
20	EDO	B	309	4/4	0.36	0.42	98,99,99,100	0
20	EDO	S	105	4/4	0.38	0.30	84,88,90,91	0
20	EDO	L	104	4/4	0.43	0.17	58,59,60,60	0
20	EDO	P	319	4/4	0.43	0.30	47,54,56,58	0
27	DMU	V	102	33/33	0.43	0.38	71,155,170,171	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	D	203	4/4	0.48	0.24	85,87,90,91	0
20	EDO	B	314	4/4	0.50	0.52	167,168,169,169	0
23	CHD	C	311	29/29	0.51	0.36	104,140,160,162	0
20	EDO	C	313	4/4	0.53	0.32	56,66,73,73	0
20	EDO	O	305	4/4	0.54	0.35	89,94,97,99	0
20	EDO	P	316	4/4	0.55	0.26	53,58,65,66	0
20	EDO	M	103	4/4	0.55	0.36	91,92,94,96	0
20	EDO	B	310	4/4	0.56	0.33	89,94,97,99	0
25	PEK	P	305	53/53	0.56	0.33	39,89,206,231	0
20	EDO	W	104	4/4	0.57	0.25	80,83,86,86	0
20	EDO	O	307	4/4	0.57	0.27	85,87,88,89	0
20	EDO	D	205	4/4	0.57	0.29	60,62,71,74	0
20	EDO	B	311	4/4	0.57	0.28	79,80,81,82	0
20	EDO	B	312	4/4	0.57	0.39	59,63,64,66	0
20	EDO	W	103	4/4	0.58	0.16	47,49,56,57	0
20	EDO	U	101	4/4	0.59	0.34	67,70,71,72	0
26	CDL	G	101	100/100	0.59	0.34	55,112,187,207	0
21	TGL	Q	201	63/63	0.60	0.20	53,80,101,104	0
27	DMU	C	310	33/33	0.61	0.33	48,101,111,113	0
27	DMU	P	309	33/33	0.61	0.29	46,101,136,137	0
20	EDO	M	105	4/4	0.61	0.22	35,47,53,56	0
26	CDL	T	101	100/100	0.61	0.32	58,102,162,185	0
14	PGV	P	307	51/51	0.62	0.30	65,96,161,165	0
23	CHD	P	310	29/29	0.62	0.30	92,136,146,150	0
20	EDO	G	105	4/4	0.62	0.17	74,75,75,77	0
20	EDO	N	618	4/4	0.63	0.19	41,41,44,47	0
20	EDO	N	630	4/4	0.63	0.53	94,94,94,97	0
14	PGV	C	307	51/51	0.63	0.28	51,91,167,179	0
20	EDO	N	612	4/4	0.63	0.37	42,50,50,54	0
23	CHD	Y	104	29/29	0.64	0.32	94,123,130,131	0
25	PEK	P	303	53/53	0.64	0.29	47,94,170,176	0
23	CHD	W	101	29/29	0.64	0.28	97,102,131,133	0
20	EDO	P	320	4/4	0.65	0.22	85,85,87,88	0
27	DMU	C	319	33/33	0.65	0.24	50,98,119,120	0
23	CHD	J	101	29/29	0.65	0.25	101,111,135,139	0
26	CDL	P	308	100/100	0.65	0.33	43,112,160,168	0
20	EDO	P	315	4/4	0.65	0.28	32,50,59,60	0
20	EDO	S	111	4/4	0.66	0.36	49,52,60,60	0
27	DMU	M	106	33/33	0.67	0.28	59,101,127,131	0
20	EDO	M	104	4/4	0.67	0.15	57,58,58,66	0
25	PEK	C	305	53/53	0.68	0.27	47,79,141,144	0
27	DMU	G	108	33/33	0.68	0.27	61,124,156,158	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	DMU	Z	102	33/33	0.68	0.28	75,102,117,127	0
20	EDO	R	205	4/4	0.69	0.20	68,73,75,76	0
21	TGL	L	101	63/63	0.69	0.28	30,76,115,139	0
29	PO4	U	102	5/5	0.69	0.24	157,157,158,159	0
25	PEK	C	303	53/53	0.71	0.35	46,134,181,186	0
23	CHD	P	311	29/29	0.71	0.18	80,96,107,109	0
20	EDO	R	202	4/4	0.71	0.16	60,61,61,67	0
20	EDO	O	306	4/4	0.71	0.35	73,80,80,82	0
14	PGV	N	601	51/51	0.74	0.28	45,87,144,151	0
20	EDO	B	305	4/4	0.74	0.18	50,52,54,54	0
20	EDO	B	307	4/4	0.74	0.19	60,61,66,67	0
20	EDO	R	203	4/4	0.74	0.15	60,64,66,68	0
21	TGL	Y	101	63/63	0.74	0.25	42,68,122,141	0
26	CDL	C	308	100/100	0.74	0.29	41,94,151,153	0
22	PSC	B	302	52/52	0.76	0.32	44,121,206,217	0
20	EDO	A	623	4/4	0.76	0.49	51,66,75,81	0
20	EDO	C	317	4/4	0.76	0.25	75,78,78,79	0
20	EDO	G	104	4/4	0.76	0.56	107,109,111,112	0
23	CHD	C	309	29/29	0.77	0.17	68,78,95,97	0
21	TGL	D	201	63/63	0.77	0.20	36,71,99,104	0
20	EDO	R	204	4/4	0.78	0.18	68,68,69,70	0
20	EDO	P	321	4/4	0.78	0.26	53,61,65,68	0
20	EDO	A	617	4/4	0.78	0.22	52,56,61,62	0
20	EDO	H	101	4/4	0.78	0.14	56,57,62,63	0
20	EDO	N	625	4/4	0.80	0.24	54,56,58,59	0
20	EDO	P	313	4/4	0.80	0.11	60,62,63,63	0
20	EDO	S	108	4/4	0.80	0.16	43,53,63,69	0
14	PGV	A	601	51/51	0.81	0.28	32,79,182,190	0
20	EDO	F	105	4/4	0.81	0.21	65,68,73,75	0
21	TGL	N	608	63/63	0.81	0.20	52,73,109,113	0
20	EDO	P	322	4/4	0.81	0.12	57,58,58,60	0
20	EDO	S	110	4/4	0.81	0.14	51,53,58,58	0
20	EDO	N	616	4/4	0.83	0.10	61,62,63,65	0
20	EDO	J	102	4/4	0.83	0.34	111,111,113,114	0
21	TGL	B	301	63/63	0.83	0.17	45,67,109,115	0
20	EDO	L	102	4/4	0.84	0.12	68,70,71,73	0
27	DMU	P	323	33/33	0.85	0.14	51,88,98,100	0
20	EDO	C	314	4/4	0.85	0.22	54,57,62,63	0
20	EDO	P	314	4/4	0.85	0.14	49,50,55,55	0
20	EDO	V	101	4/4	0.85	0.20	60,65,68,71	0
20	EDO	L	105	4/4	0.85	0.09	53,55,57,59	0
20	EDO	A	624	4/4	0.86	0.15	58,59,60,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	PSC	O	301	52/52	0.86	0.30	35,100,221,227	0
20	EDO	Q	202	4/4	0.86	0.15	65,67,71,77	0
20	EDO	E	202	4/4	0.87	0.12	53,54,56,60	0
20	EDO	N	617	4/4	0.88	0.18	61,65,70,71	0
20	EDO	Y	102	4/4	0.88	0.08	59,59,61,65	0
20	EDO	G	103	4/4	0.88	0.14	45,49,51,54	0
20	EDO	D	207	4/4	0.88	0.15	44,44,49,54	0
20	EDO	M	102	4/4	0.88	0.14	61,67,68,69	0
20	EDO	N	615	4/4	0.88	0.11	55,57,57,61	0
20	EDO	H	103	4/4	0.88	0.20	34,38,43,45	0
20	EDO	A	621	4/4	0.89	0.14	40,47,52,55	0
20	EDO	H	102	4/4	0.89	0.24	50,50,54,55	0
20	EDO	N	621	4/4	0.89	0.16	47,49,49,50	0
27	DMU	Z	101	33/33	0.89	0.13	37,45,63,69	0
20	EDO	A	622	4/4	0.89	0.15	63,65,67,67	0
20	EDO	G	107	4/4	0.89	0.11	35,50,57,58	0
20	EDO	N	627	4/4	0.90	0.19	64,65,67,70	0
20	EDO	N	628	4/4	0.90	0.15	33,42,47,50	0
20	EDO	S	107	4/4	0.90	0.36	56,62,64,66	0
20	EDO	A	609	4/4	0.90	0.41	32,46,54,57	0
20	EDO	C	318	4/4	0.90	0.20	39,53,59,60	0
20	EDO	Q	203	4/4	0.90	0.19	47,58,58,61	0
20	EDO	J	103	4/4	0.90	0.18	57,61,65,72	0
20	EDO	P	318	4/4	0.90	0.17	38,42,46,46	0
20	EDO	C	316	4/4	0.90	0.18	31,39,40,41	0
20	EDO	S	106	4/4	0.91	0.15	40,51,51,56	0
20	EDO	S	112	4/4	0.91	0.25	39,43,45,46	0
20	EDO	L	103	4/4	0.91	0.11	56,58,59,64	0
27	DMU	M	101	33/33	0.91	0.10	34,40,57,62	0
20	EDO	A	612	4/4	0.91	0.16	39,41,42,42	0
20	EDO	B	308	4/4	0.91	0.28	46,50,51,52	0
20	EDO	A	620	4/4	0.92	0.17	37,40,42,47	0
20	EDO	D	204[A]	4/4	0.92	0.23	46,55,59,64	1
20	EDO	A	625	4/4	0.92	0.10	50,54,60,61	0
20	EDO	B	313	4/4	0.92	0.16	39,44,47,48	0
20	EDO	W	102	4/4	0.92	0.19	58,59,62,67	0
20	EDO	A	626	4/4	0.92	0.23	30,36,48,52	0
20	EDO	A	613	4/4	0.92	0.15	37,40,48,50	0
20	EDO	N	624	4/4	0.92	0.19	29,40,56,67	0
20	EDO	Y	103	4/4	0.92	0.22	57,57,61,63	0
20	EDO	F	103	4/4	0.92	0.26	38,52,57,58	0
20	EDO	N	626	4/4	0.92	0.19	59,60,63,65	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	A	615	4/4	0.93	0.19	36,41,50,51	0
20	EDO	A	627	4/4	0.93	0.17	27,31,37,41	0
20	EDO	F	104	4/4	0.93	0.09	32,37,37,42	0
29	PO4	H	104	5/5	0.93	0.15	90,91,95,96	0
20	EDO	E	201	4/4	0.93	0.10	59,62,66,68	0
20	EDO	T	103	4/4	0.94	0.19	40,46,48,51	0
20	EDO	S	103	4/4	0.94	0.08	33,34,38,38	0
20	EDO	A	618	4/4	0.94	0.15	30,42,54,61	0
20	EDO	N	614	4/4	0.94	0.11	36,37,41,44	0
23	CHD	P	301	29/29	0.94	0.08	24,27,32,34	0
20	EDO	O	304	4/4	0.94	0.16	40,40,44,46	0
20	EDO	S	104	4/4	0.95	0.11	28,29,31,32	0
20	EDO	A	610	4/4	0.95	0.11	27,27,31,32	0
20	EDO	F	107	4/4	0.95	0.16	43,45,57,66	0
20	EDO	C	315	4/4	0.95	0.16	29,34,42,48	0
23	CHD	C	301	29/29	0.95	0.08	23,27,31,33	0
25	PEK	P	304	53/53	0.95	0.12	25,44,95,99	0
20	EDO	R	201	4/4	0.95	0.09	40,40,41,41	0
20	EDO	O	303	4/4	0.95	0.09	29,29,30,30	0
20	EDO	A	616	4/4	0.95	0.21	28,36,38,38	0
20	EDO	C	312	4/4	0.95	0.07	31,34,34,35	0
20	EDO	K	101	4/4	0.95	0.07	49,49,50,53	0
20	EDO	A	619	4/4	0.95	0.28	33,35,47,48	0
20	EDO	N	610	4/4	0.96	0.11	26,26,26,31	0
23	CHD	G	102	29/29	0.96	0.08	22,24,28,36	0
25	PEK	C	304	53/53	0.96	0.13	26,43,87,91	0
20	EDO	T	102	4/4	0.96	0.12	31,31,36,38	0
14	PGV	C	306	51/51	0.96	0.12	21,28,77,81	0
23	CHD	B	303	29/29	0.96	0.08	22,25,33,38	0
20	EDO	N	620	4/4	0.96	0.10	37,38,41,42	0
20	EDO	P	317	4/4	0.96	0.17	36,39,40,42	0
18	NA	P	302	1/1	0.97	0.31	17,17,17,17	1
19	CMO	N	607[A]	2/2	0.97	0.22	19,19,19,19	2
19	CMO	N	607[B]	2/2	0.97	0.22	18,18,18,19	2
14	PGV	P	306	51/51	0.97	0.12	21,30,78,81	0
20	EDO	G	106	4/4	0.97	0.09	28,30,34,36	0
14	PGV	A	608	51/51	0.97	0.11	21,26,56,58	0
20	EDO	N	611	4/4	0.97	0.12	36,39,40,41	0
20	EDO	N	622	4/4	0.97	0.17	30,36,38,39	0
14	PGV	N	609	51/51	0.97	0.11	22,27,56,61	0
20	EDO	N	613	4/4	0.97	0.11	22,26,27,30	0
20	EDO	S	109	4/4	0.97	0.18	28,39,46,47	0

Continued on next page...

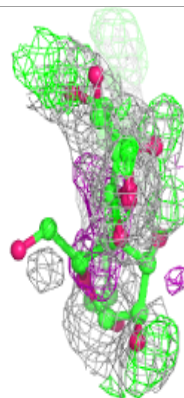
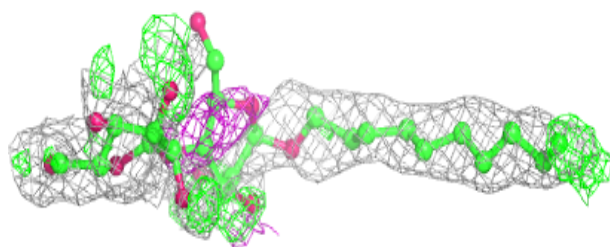
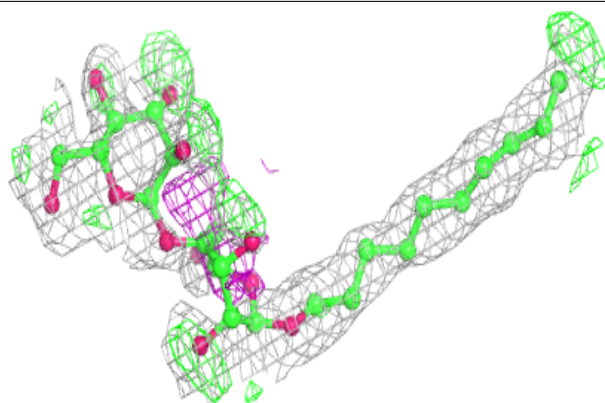
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	P	312	4/4	0.97	0.12	28,34,39,47	0
20	EDO	F	106	4/4	0.97	0.12	29,31,32,35	0
15	HEA	A	602[B]	60/60	0.98	0.10	18,21,28,30	18
19	CMO	A	607[A]	2/2	0.98	0.23	16,16,16,16	2
19	CMO	A	607[B]	2/2	0.98	0.23	16,16,16,16	2
15	HEA	A	602[C]	43/60	0.98	0.10	18,20,22,25	1
24	CUA	O	302	2/2	0.98	0.11	25,25,25,25	0
20	EDO	S	102	4/4	0.98	0.08	22,23,23,23	0
20	EDO	B	306	4/4	0.98	0.10	23,23,26,30	0
15	HEA	A	603	60/60	0.98	0.09	18,20,27,30	0
20	EDO	E	203	4/4	0.98	0.08	36,39,40,41	0
15	HEA	N	602[A]	60/60	0.98	0.10	21,25,30,32	18
15	HEA	N	602[B]	60/60	0.98	0.10	21,25,30,32	18
15	HEA	N	602[C]	43/60	0.98	0.10	21,24,26,27	1
15	HEA	N	603	60/60	0.98	0.09	19,23,28,30	0
15	HEA	A	602[A]	60/60	0.98	0.10	18,21,28,29	18
18	NA	N	606	1/1	0.99	0.07	31,31,31,31	0
17	MG	A	605	1/1	0.99	0.09	22,22,22,22	0
20	EDO	F	102	4/4	0.99	0.09	22,23,23,25	0
24	CUA	B	304	2/2	0.99	0.12	21,21,21,21	0
17	MG	N	605	1/1	0.99	0.12	26,26,26,26	0
28	ZN	F	101	1/1	0.99	0.12	27,27,27,27	0
16	CU	N	604	1/1	0.99	0.15	23,23,23,23	0
20	EDO	A	611	4/4	0.99	0.12	21,23,24,27	0
28	ZN	S	101	1/1	1.00	0.13	27,27,27,27	0
18	NA	A	606	1/1	1.00	0.08	26,26,26,26	0
16	CU	A	604	1/1	1.00	0.14	20,20,20,20	0

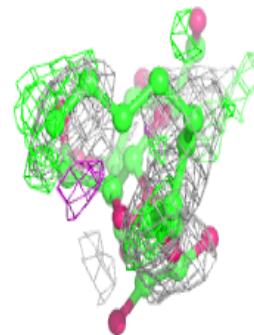
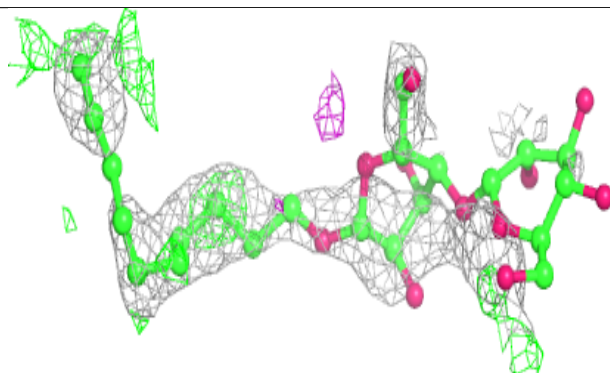
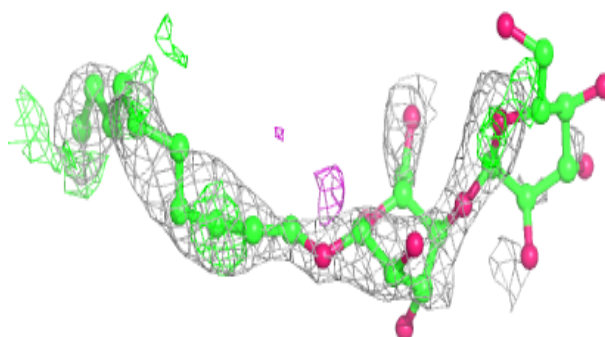
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DMU P 324:

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

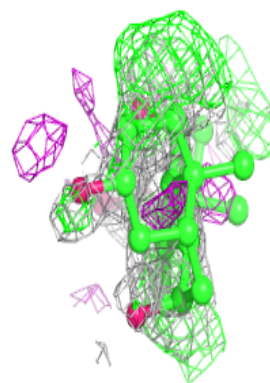
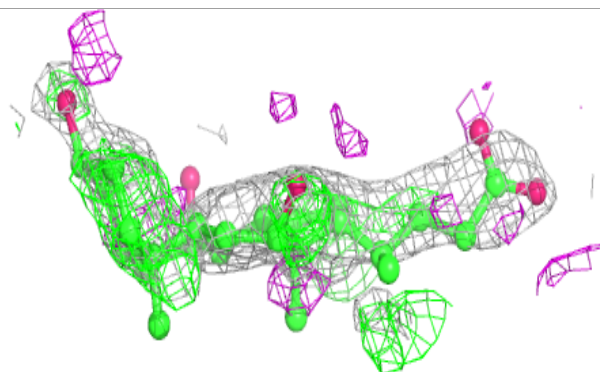
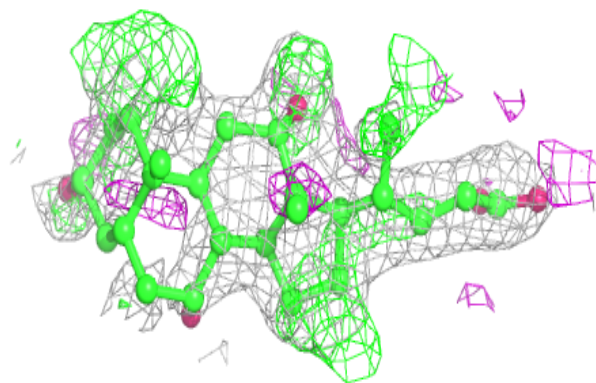
**Electron density around DMU V 102:**

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



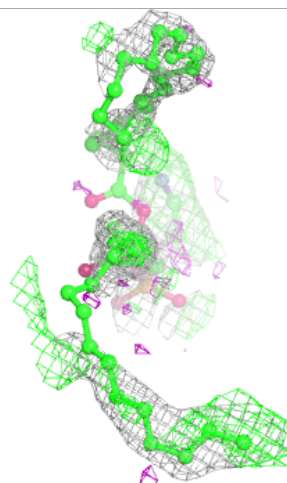
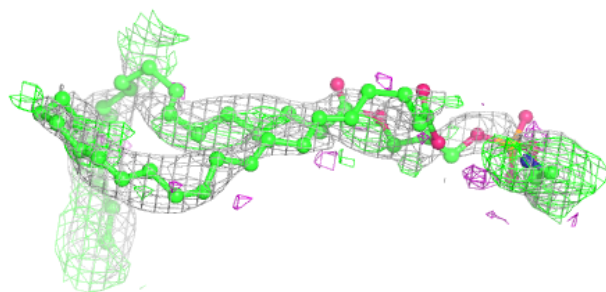
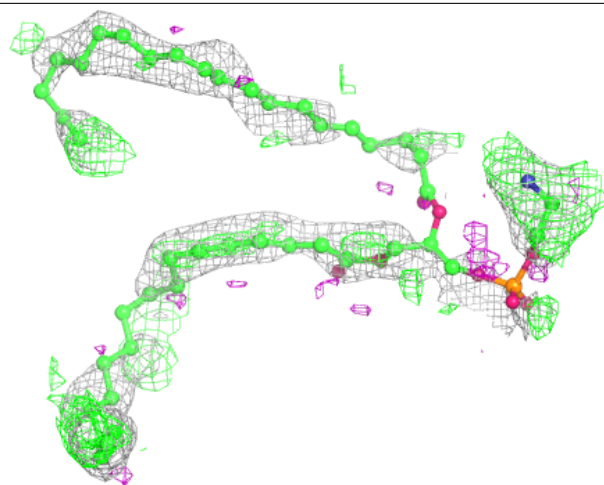
Electron density around CHD C 311:

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



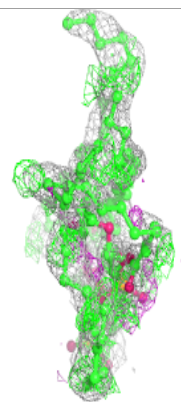
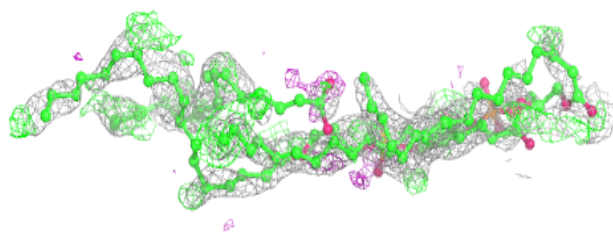
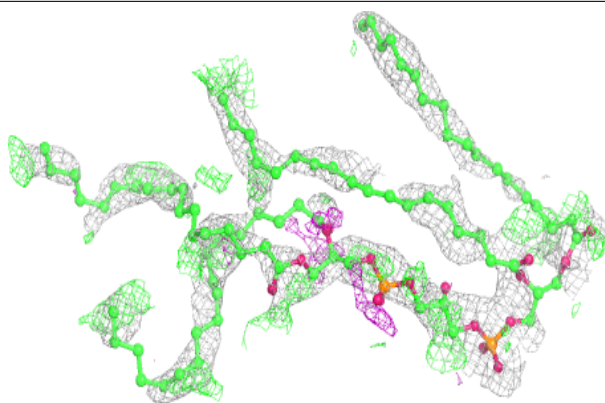
Electron density around PEK P 305:

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

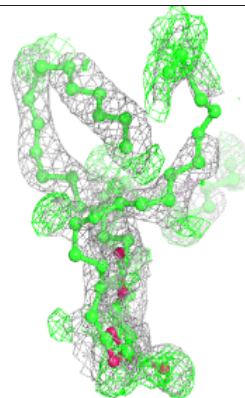
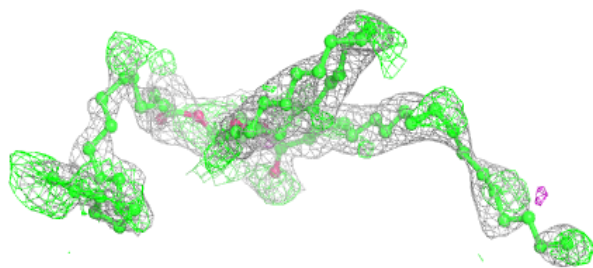
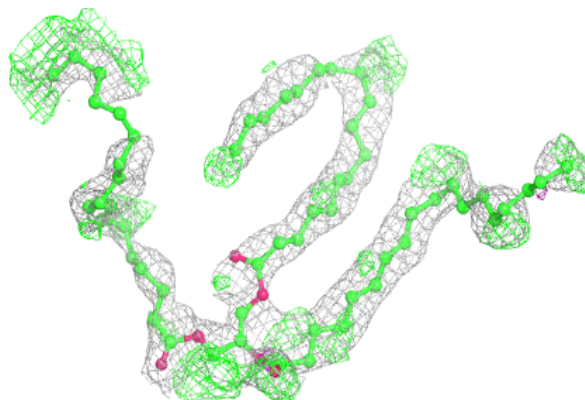


Electron density around CDL G 101:

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

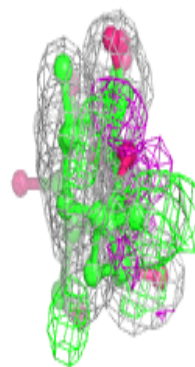
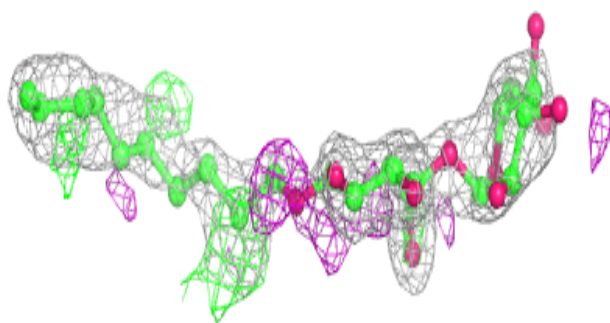
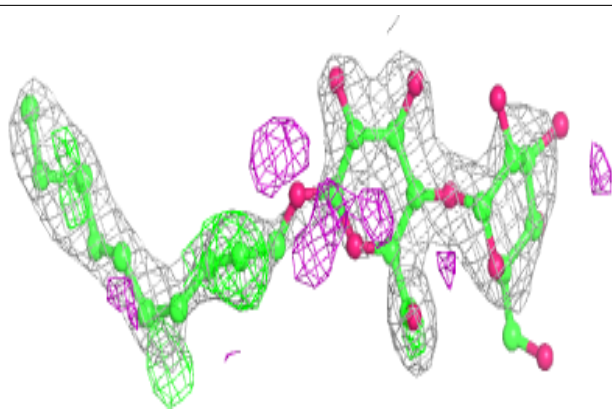
**Electron density around TGL Q 201:**

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

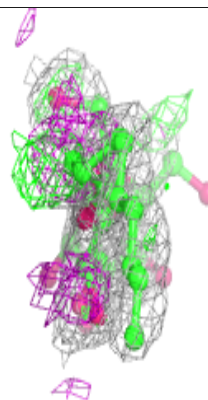
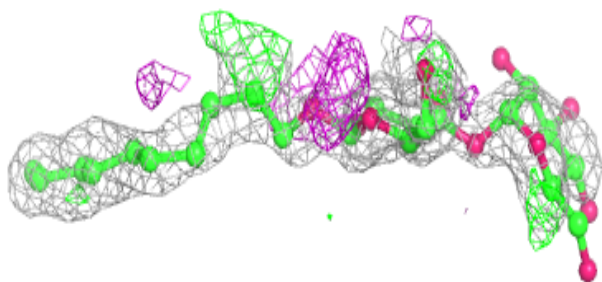
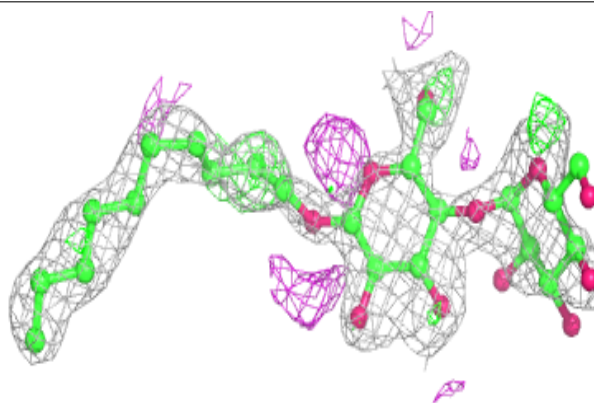


Electron density around DMU C 310:

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

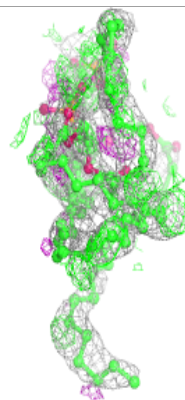
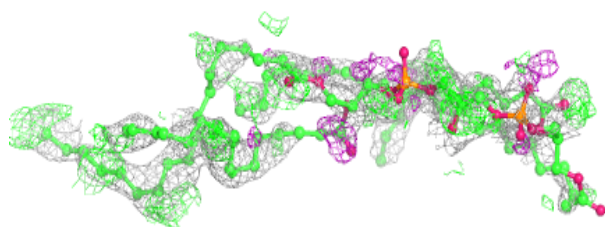
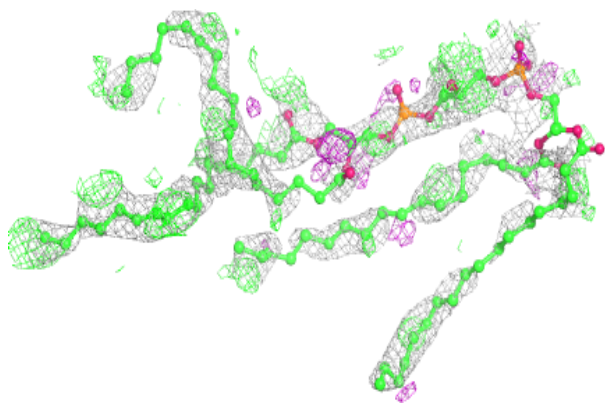
**Electron density around DMU P 309:**

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

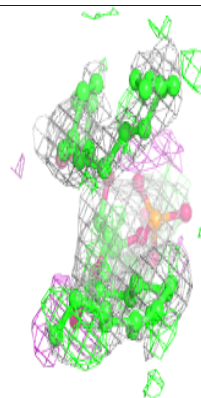
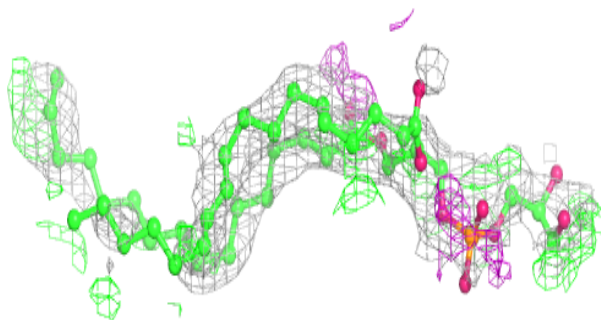
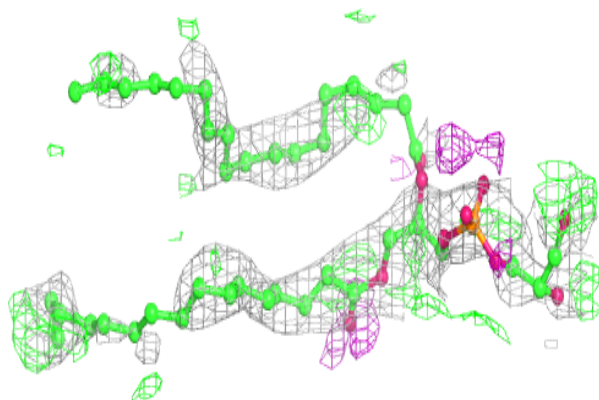


Electron density around CDL T 101:

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

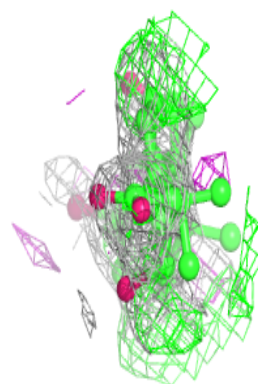
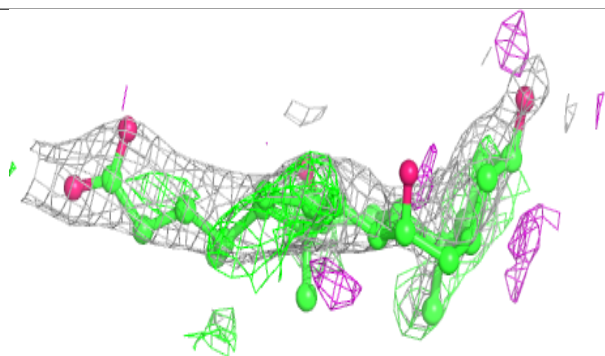
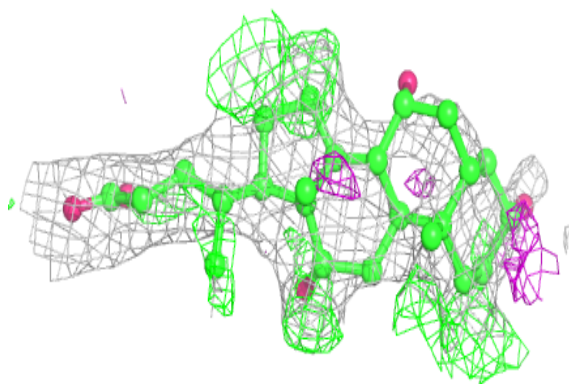
**Electron density around PGV P 307:**

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

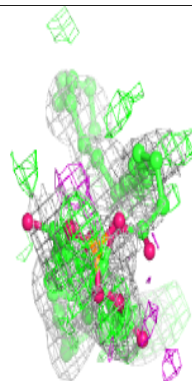
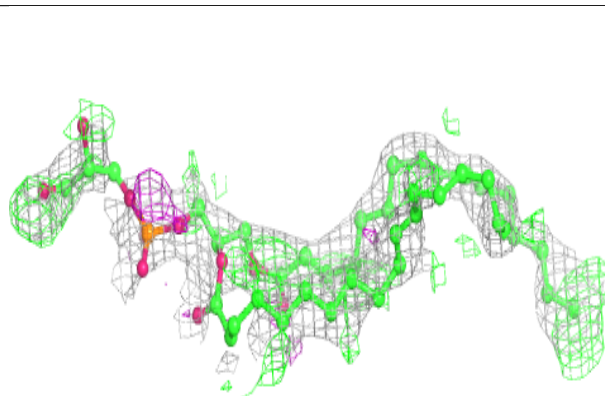
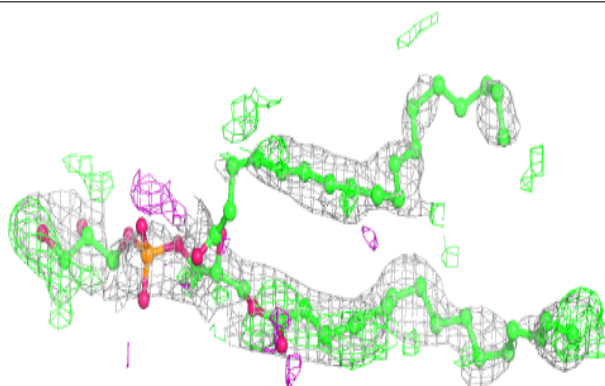


Electron density around CHD P 310:

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

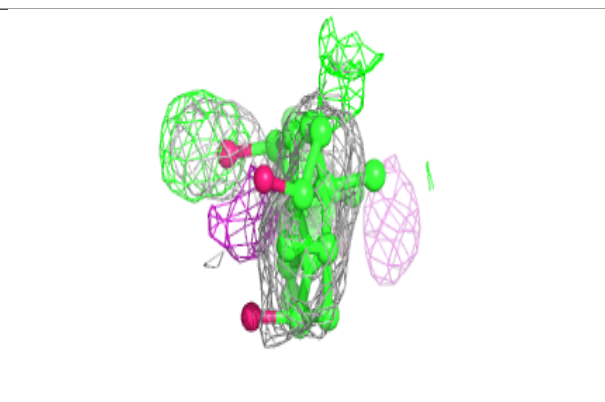
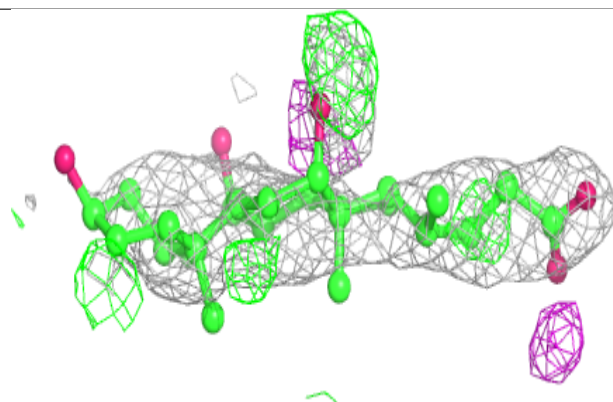
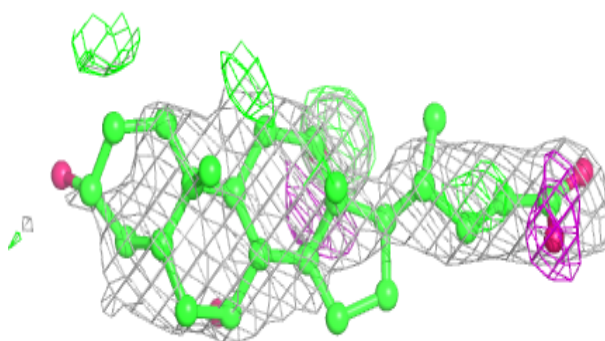
**Electron density around PGV C 307:**

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

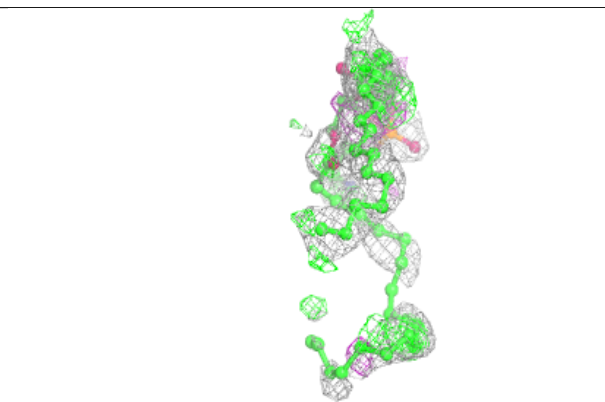
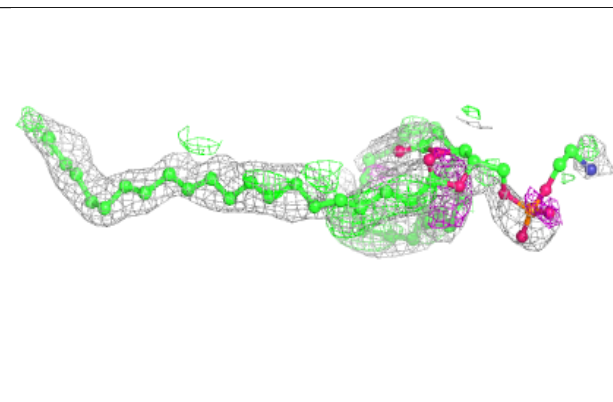
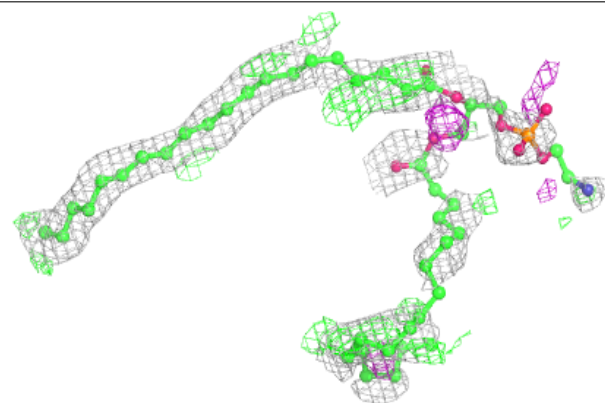


Electron density around CHD Y 104:

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

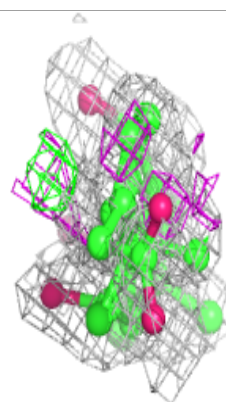
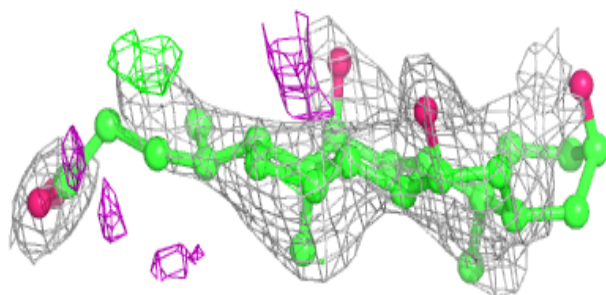
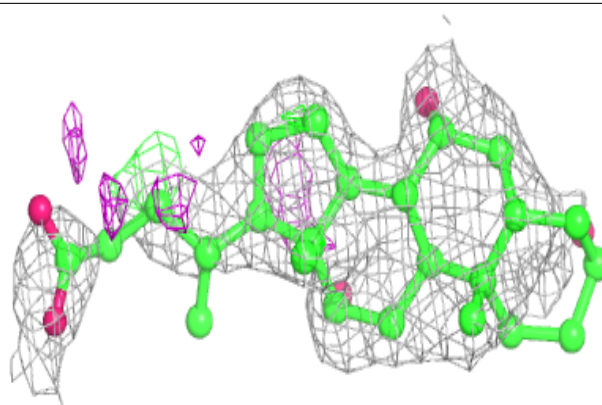
**Electron density around PEK P 303:**

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

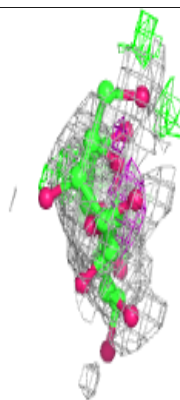
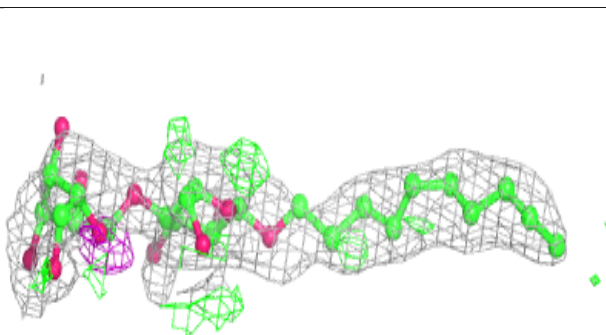
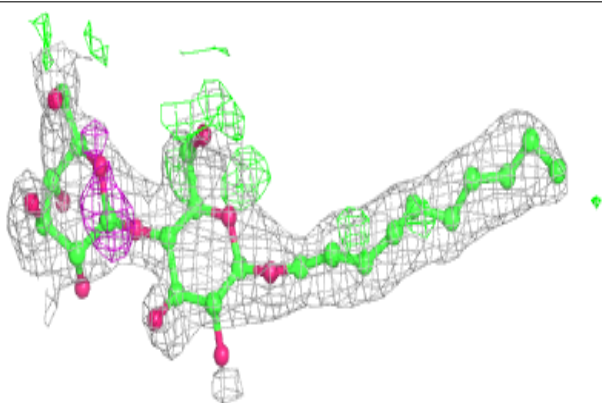


Electron density around CHD W 101:

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

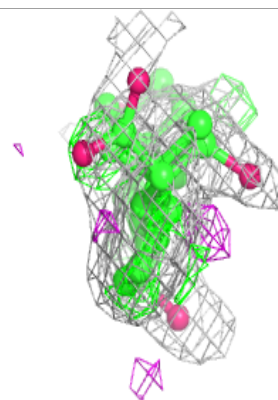
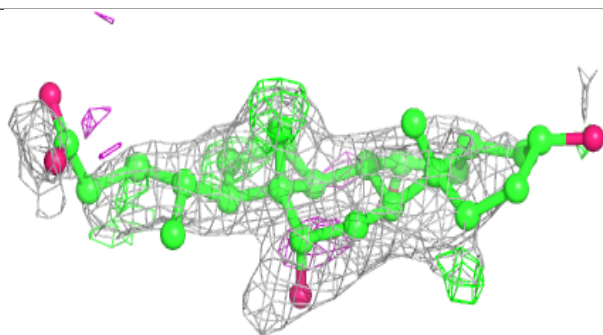
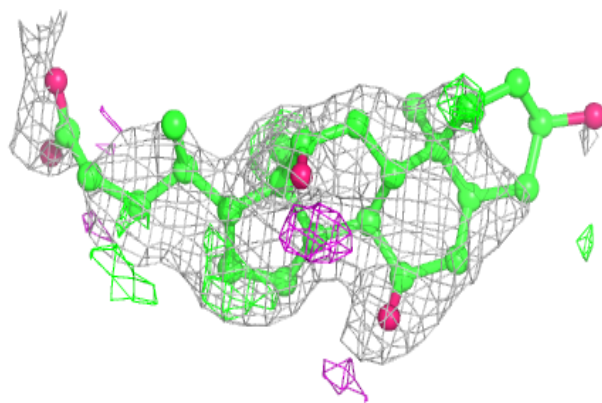
**Electron density around DMU C 319:**

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



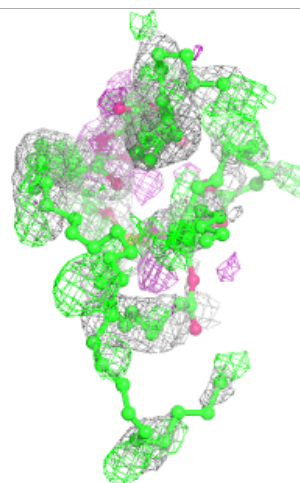
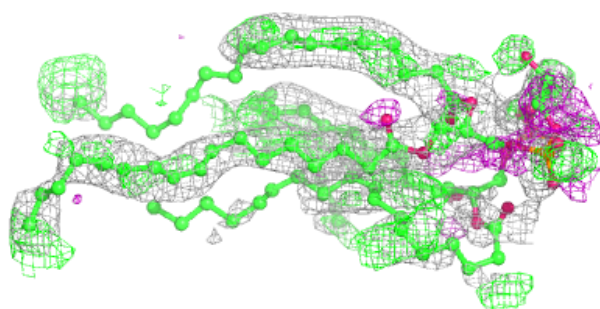
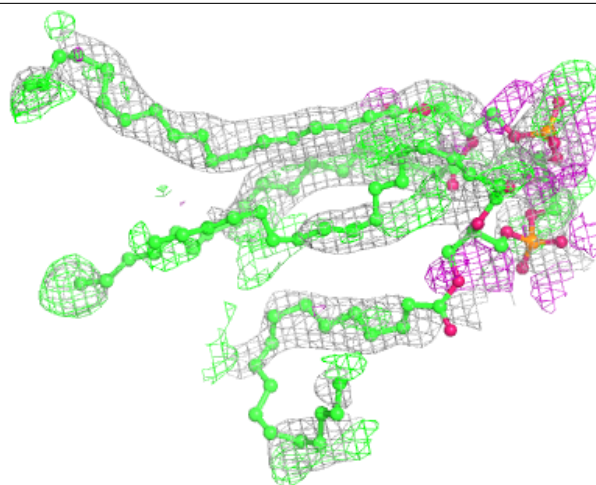
Electron density around CHD J 101:

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



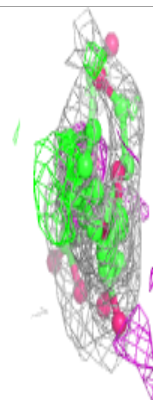
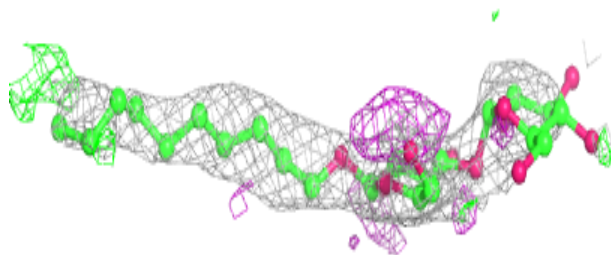
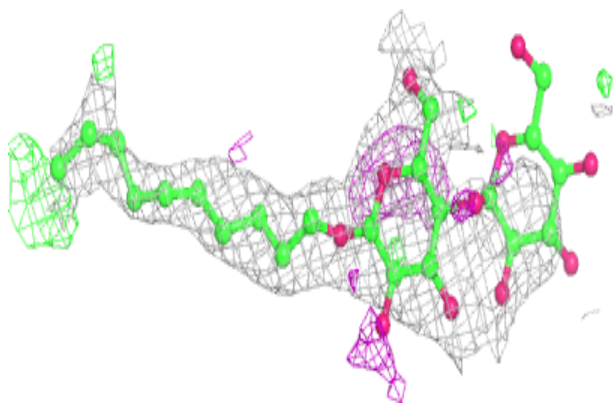
Electron density around CDL P 308:

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



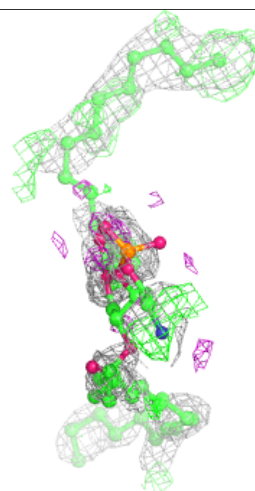
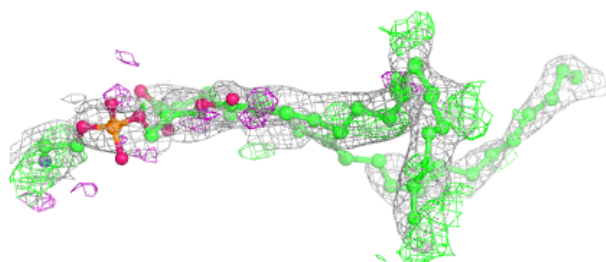
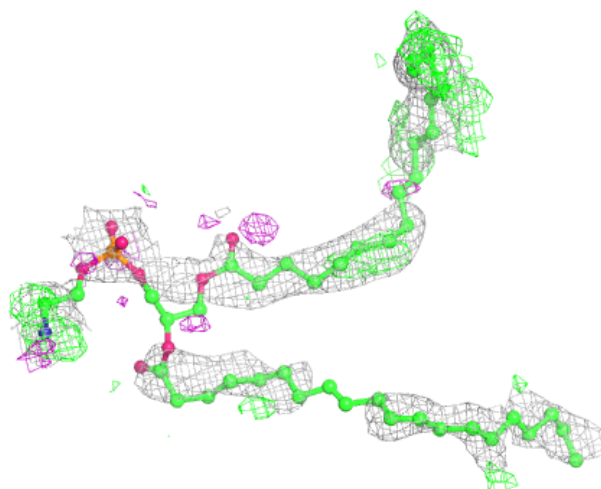
Electron density around DMU M 106:

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



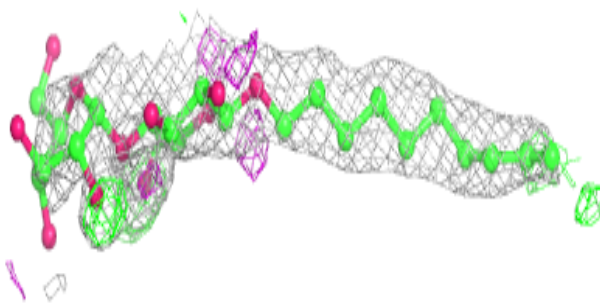
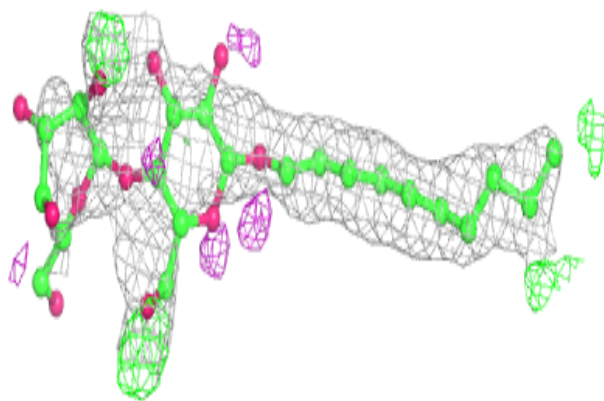
Electron density around PEK C 305:

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

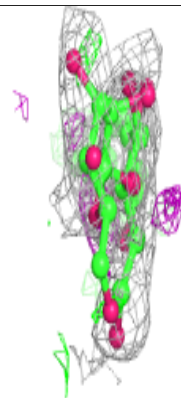
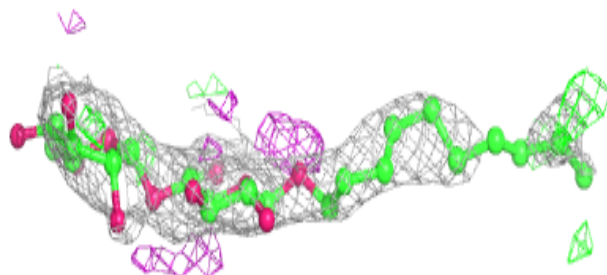
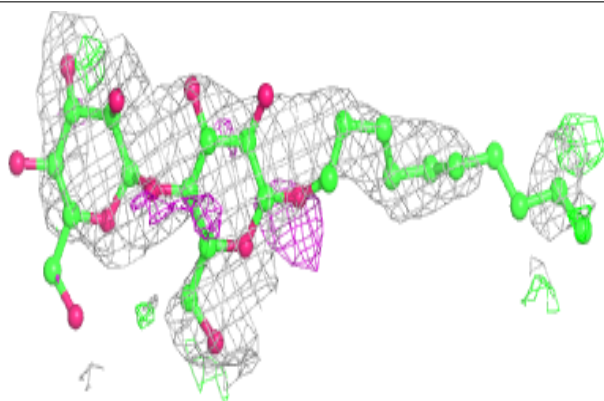


Electron density around DMU G 108:

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

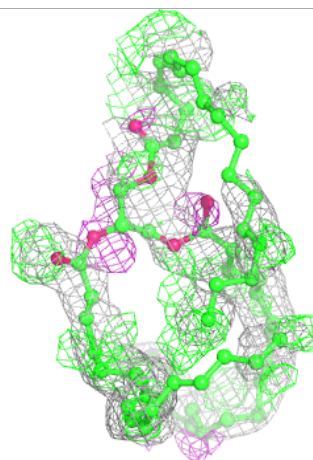
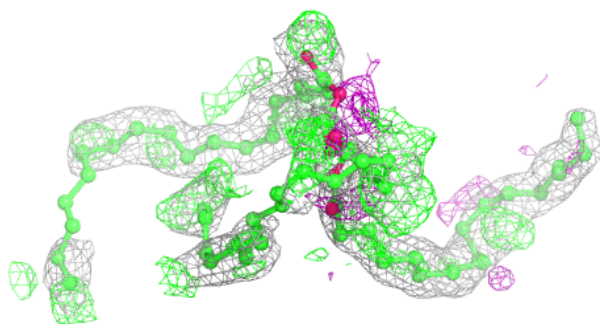
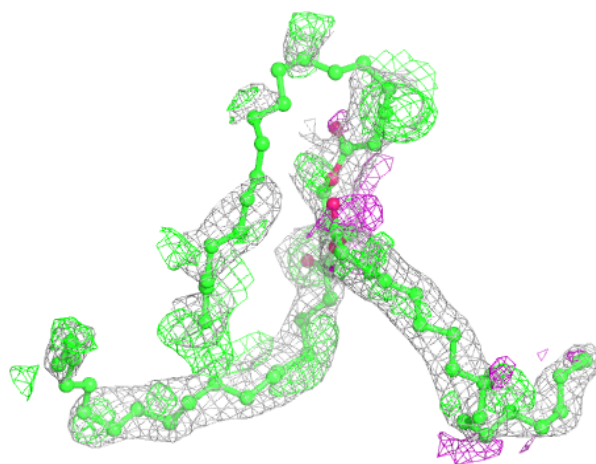
**Electron density around DMU Z 102:**

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



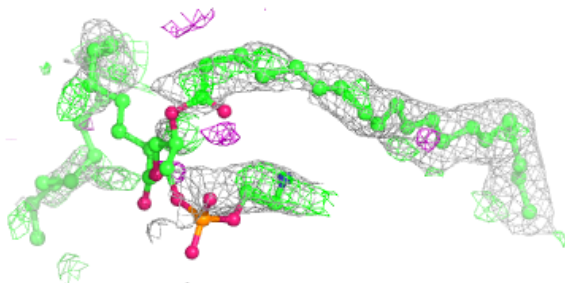
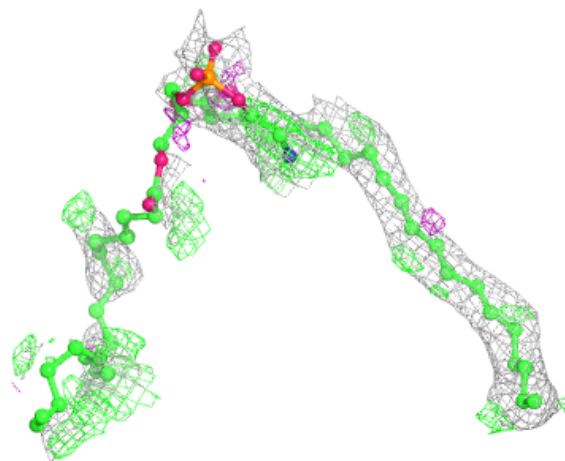
Electron density around TGL L 101:

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



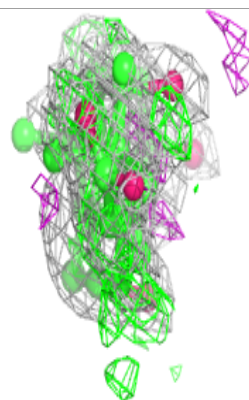
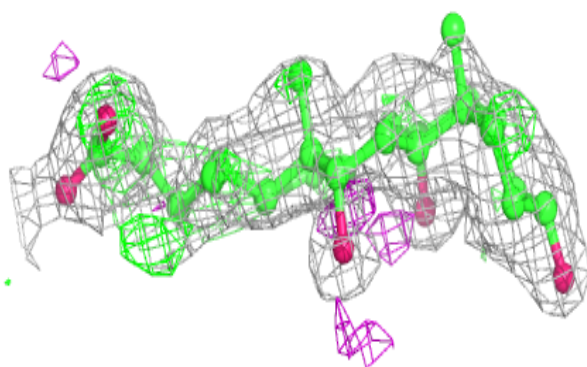
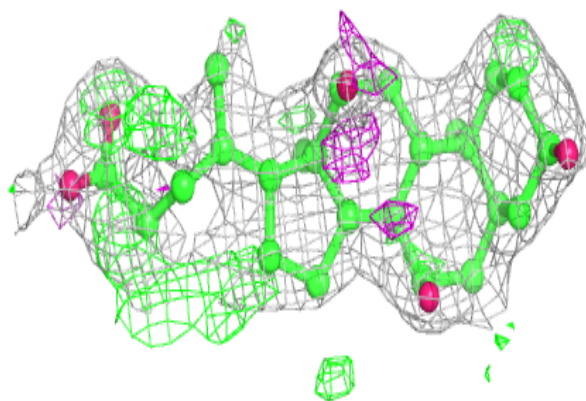
Electron density around PEK C 303:

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

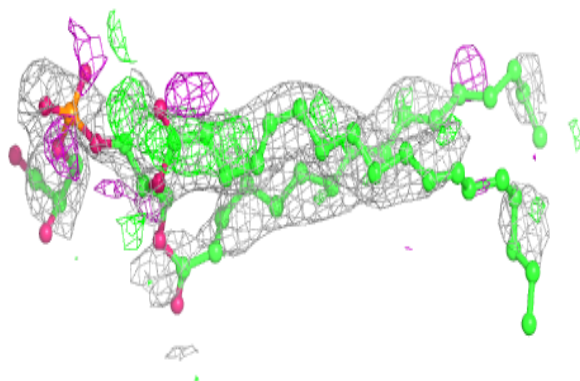
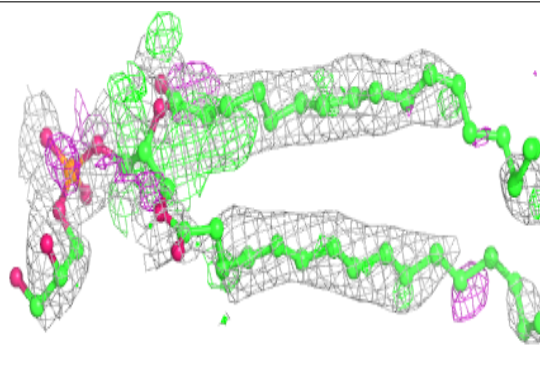


Electron density around CHD P 311:

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

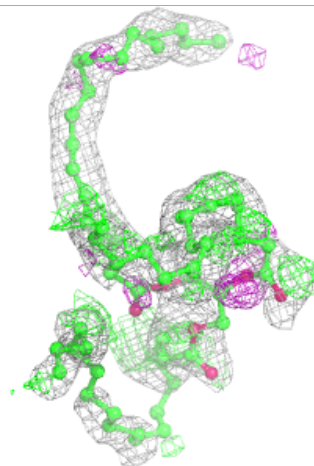
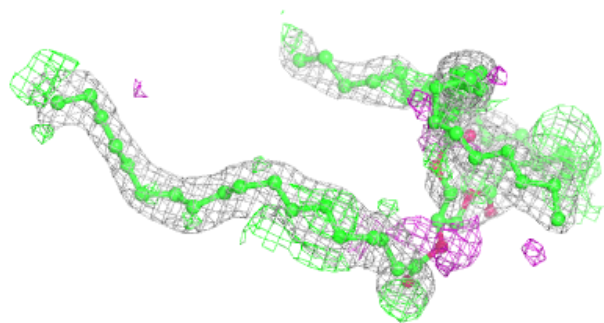
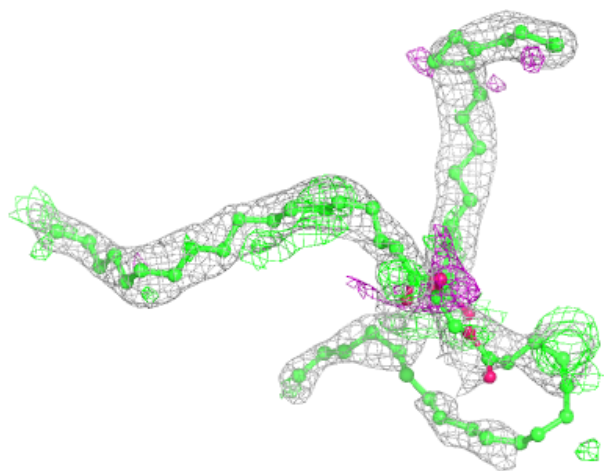
**Electron density around PGV N 601:**

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



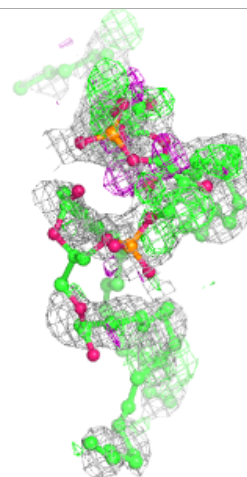
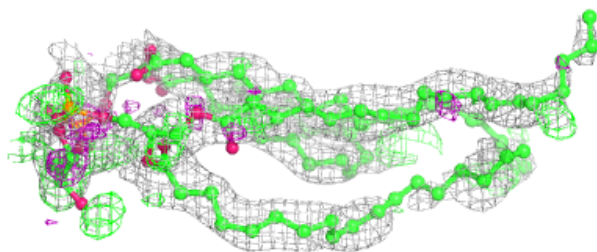
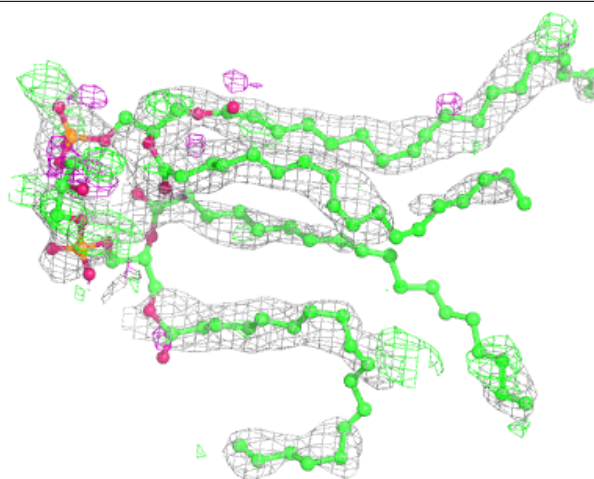
Electron density around TGL Y 101:

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



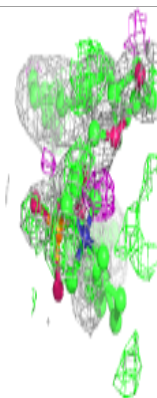
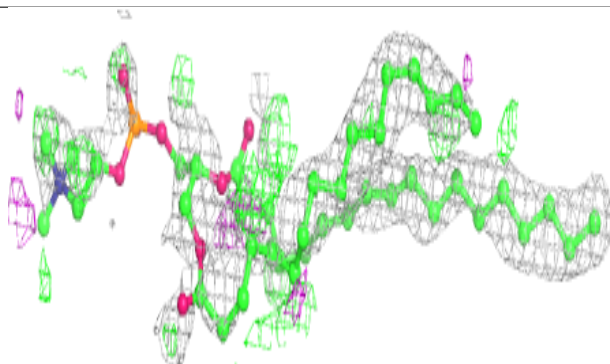
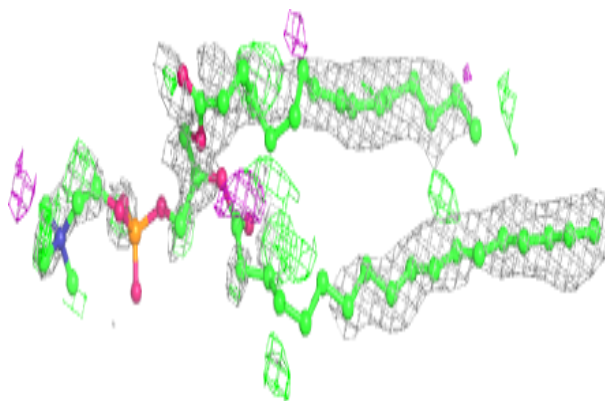
Electron density around CDL C 308:

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

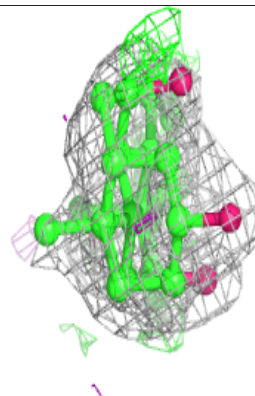
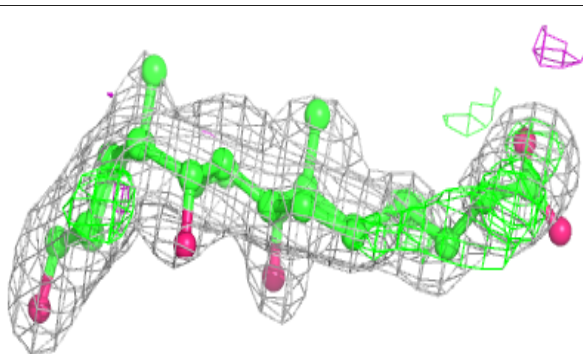
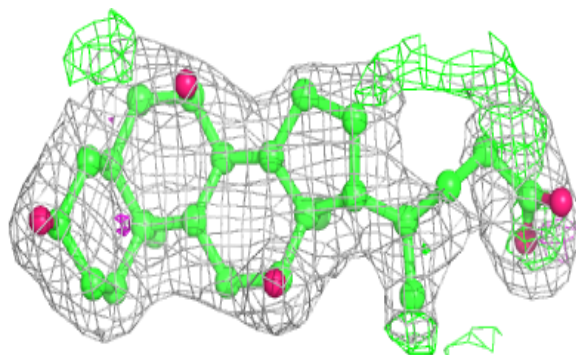


Electron density around PSC B 302:

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

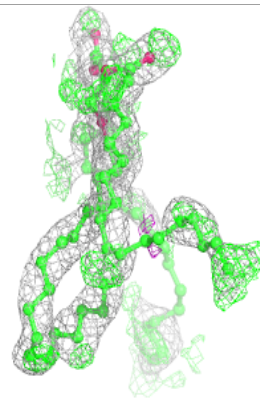
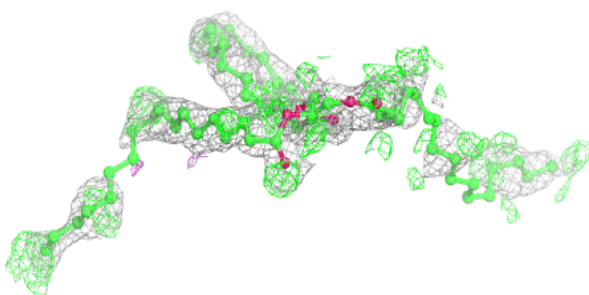
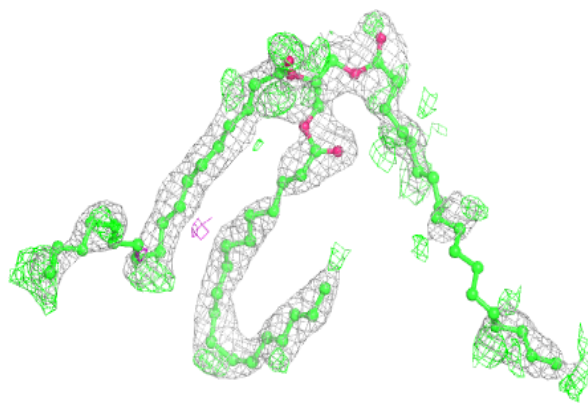
**Electron density around CHD C 309:**

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

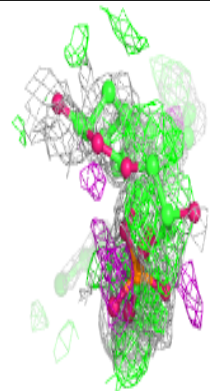
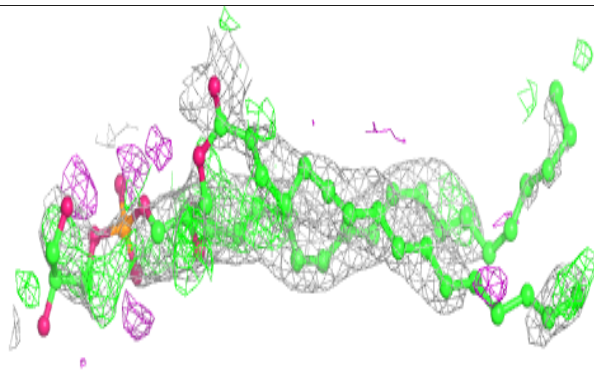
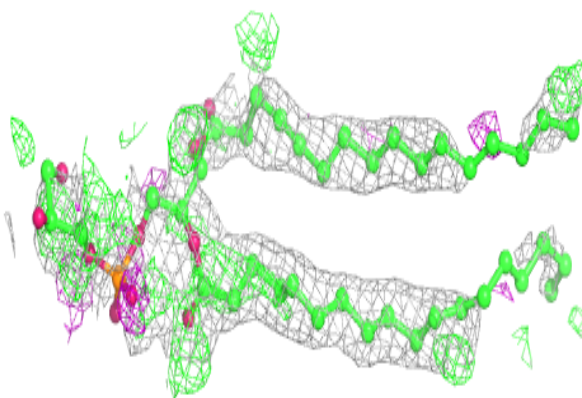


Electron density around TGL D 201:

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

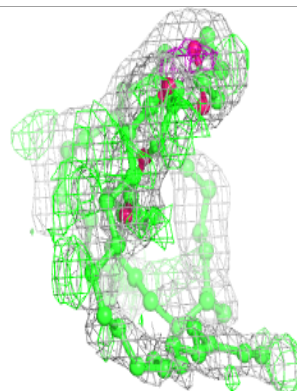
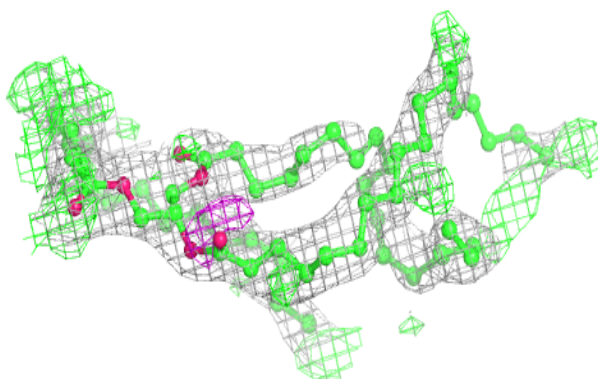
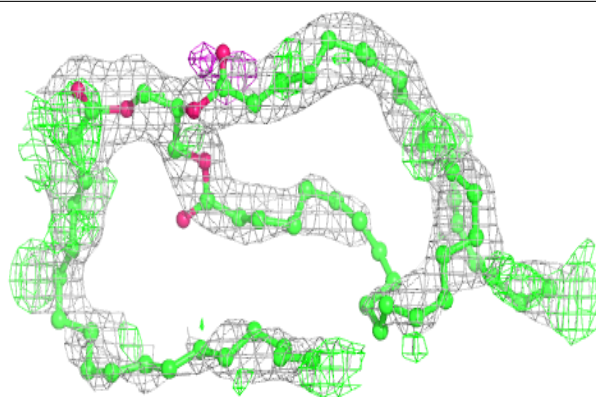
**Electron density around PGV A 601:**

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

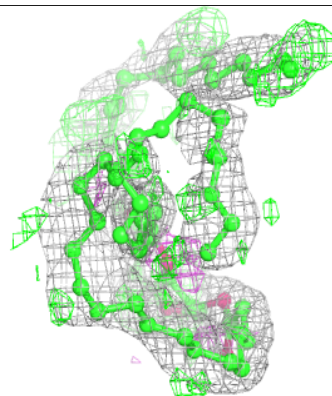
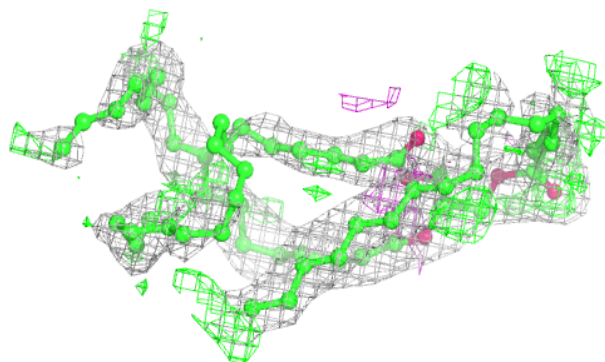
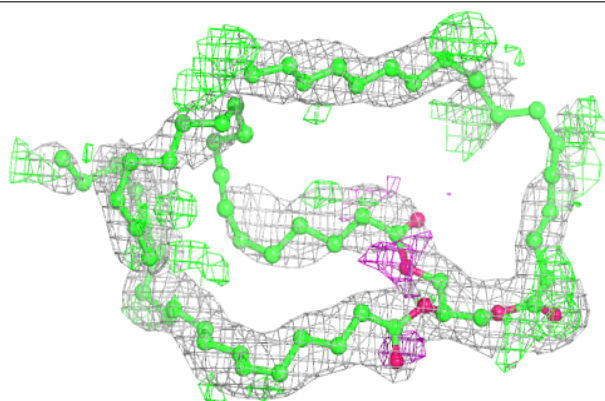


Electron density around TGL N 608:

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

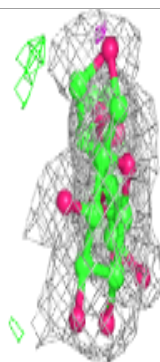
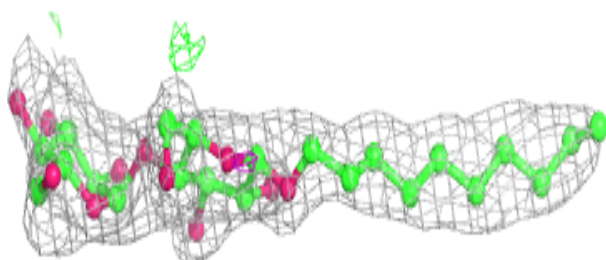
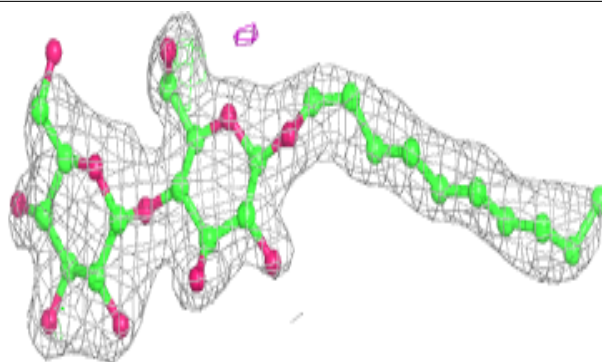
**Electron density around TGL B 301:**

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

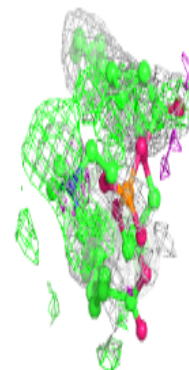
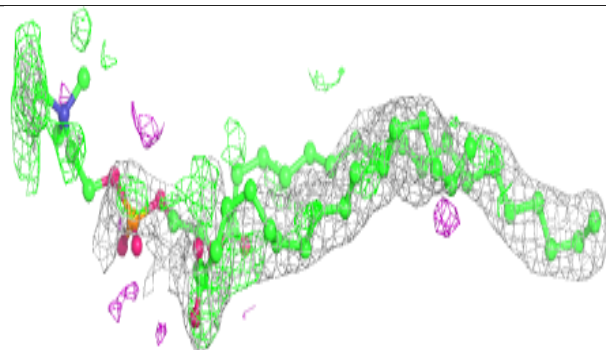
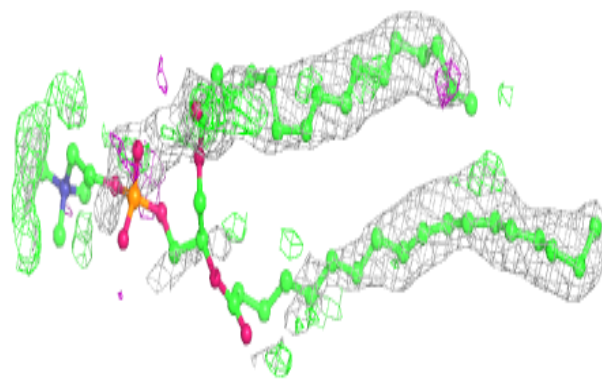


Electron density around DMU P 323:

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

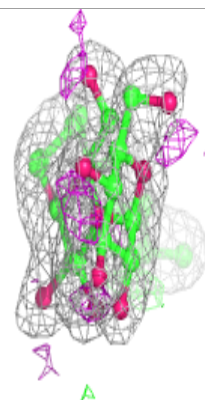
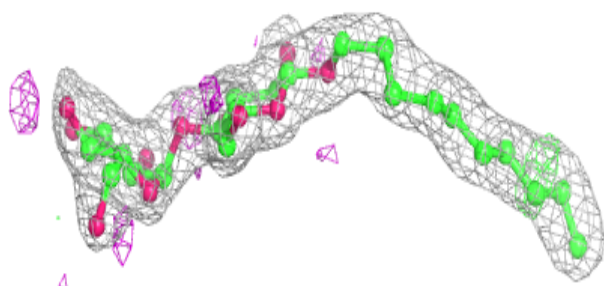
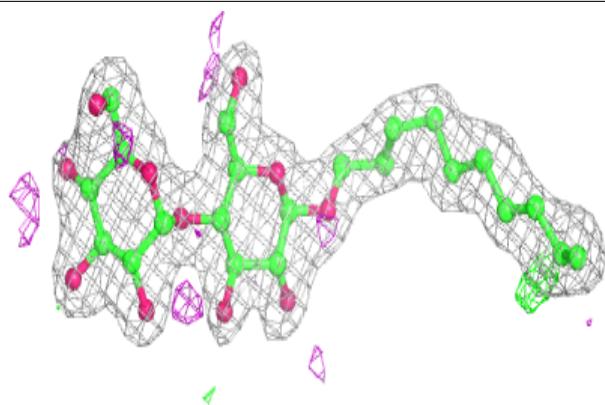
**Electron density around PSC O 301:**

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

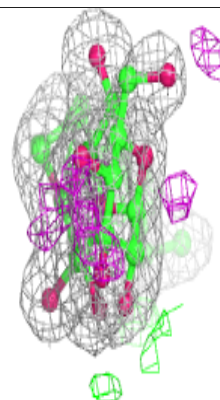
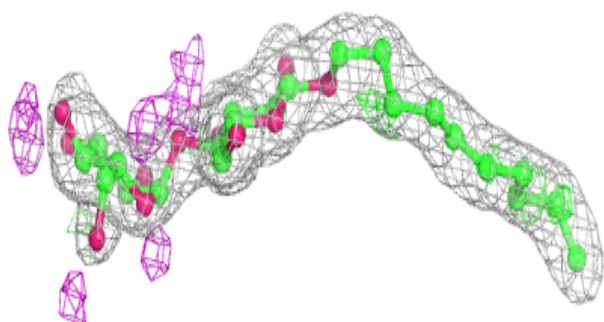
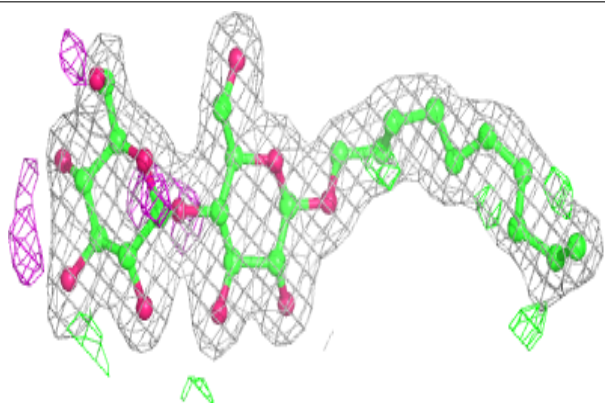


Electron density around DMU Z 101:

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

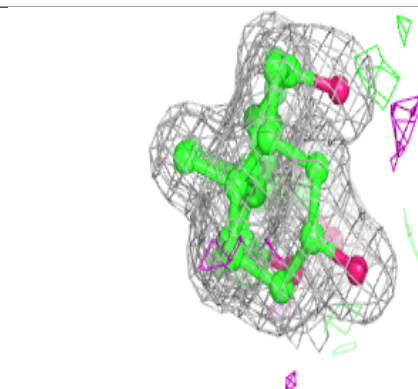
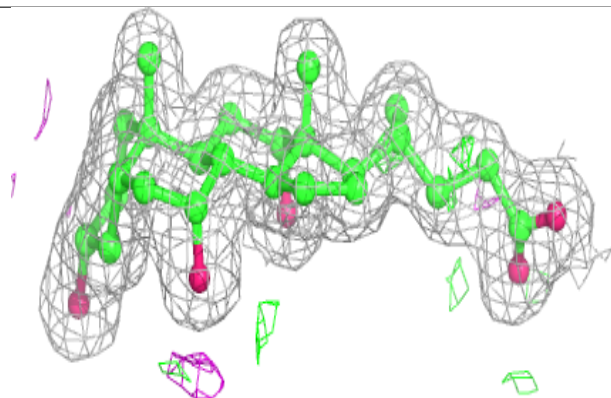
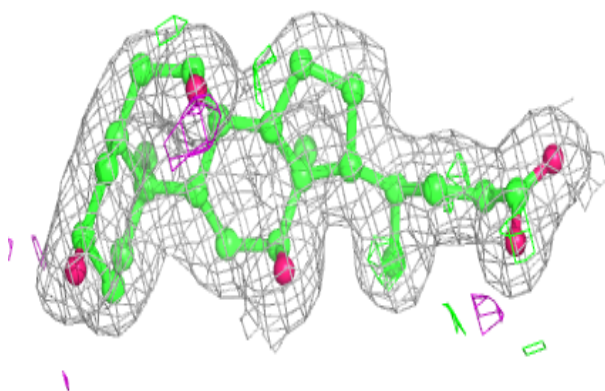
**Electron density around DMU M 101:**

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

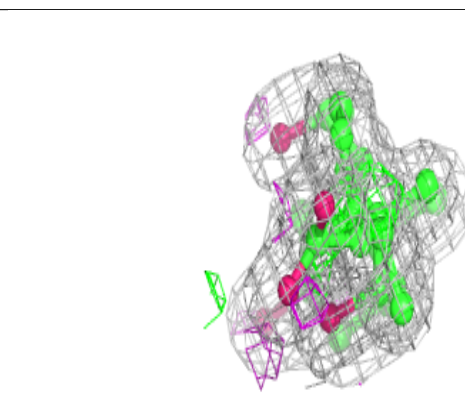
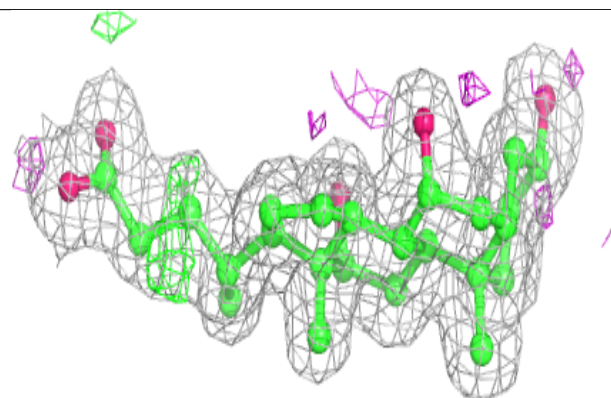
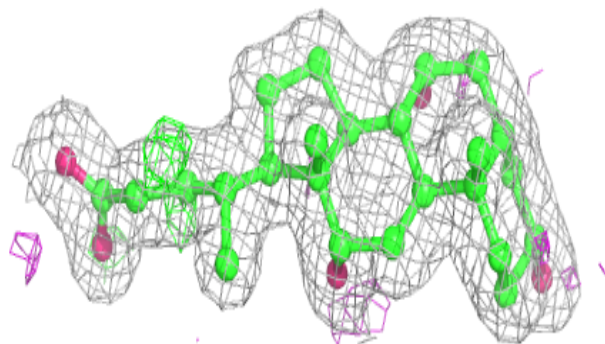


Electron density around CHD P 301:

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

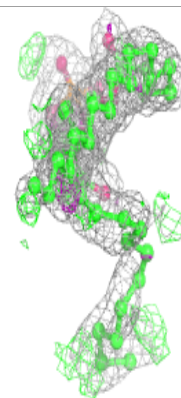
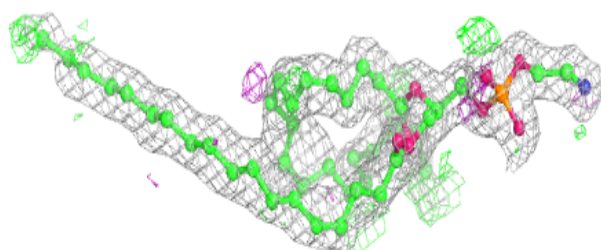
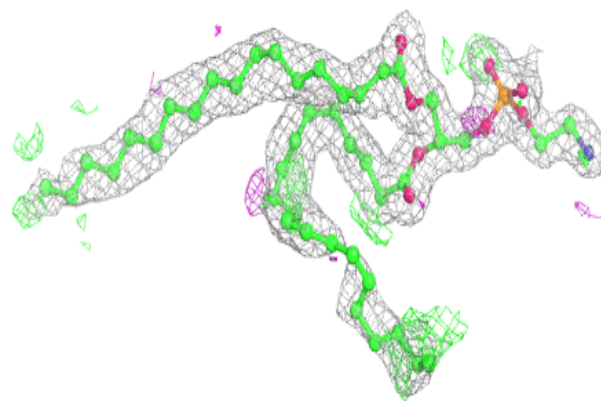
**Electron density around CHD C 301:**

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

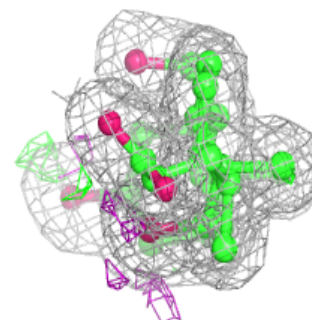
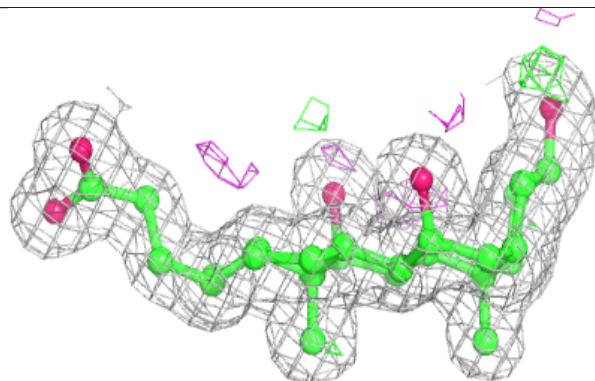
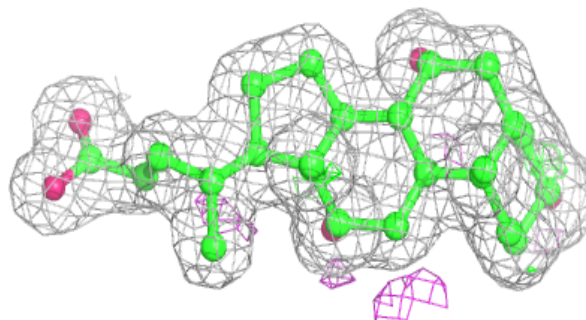


Electron density around PEK P 304:

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

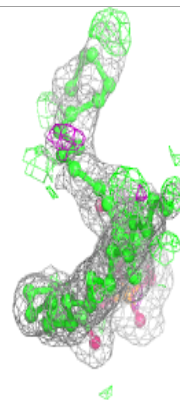
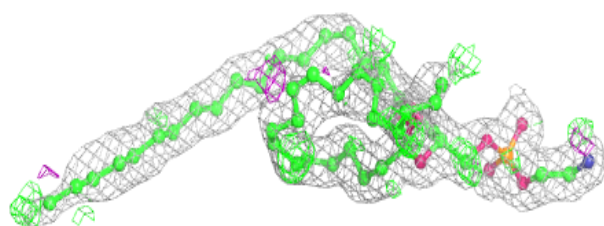
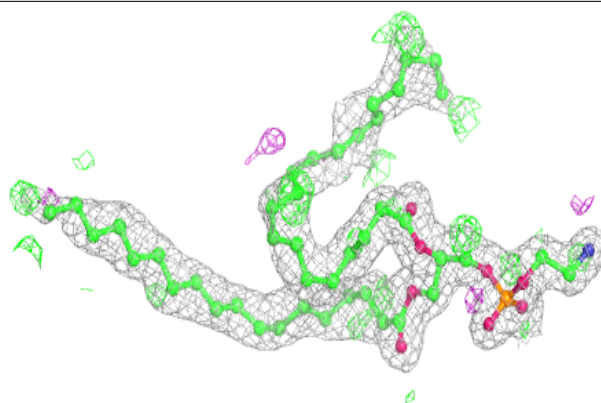
**Electron density around CHD G 102:**

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

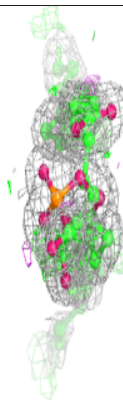
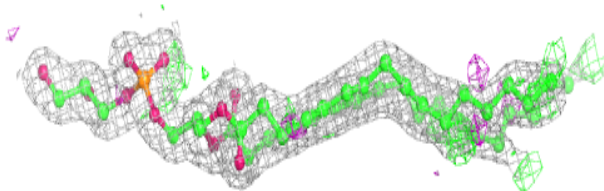
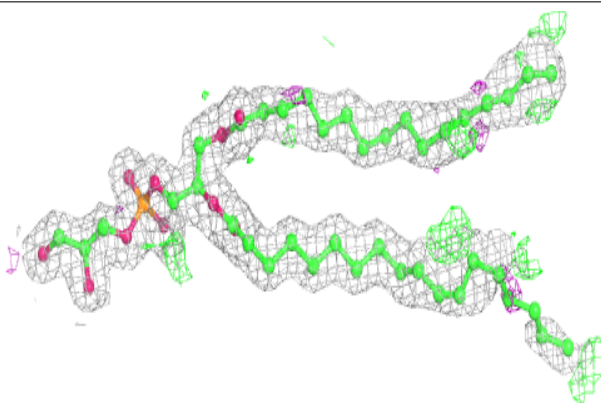


Electron density around PEK C 304:

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

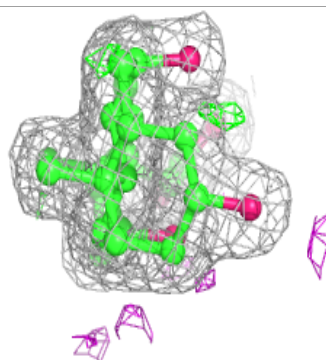
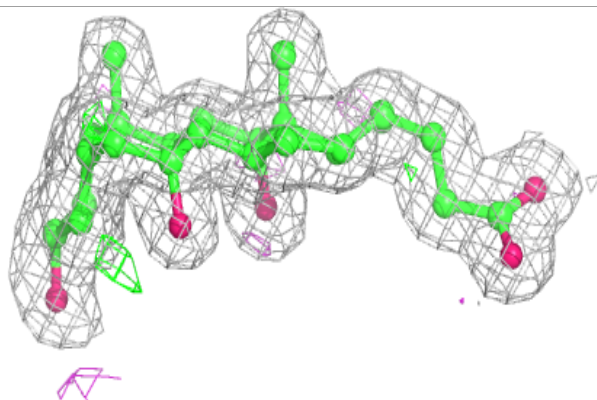
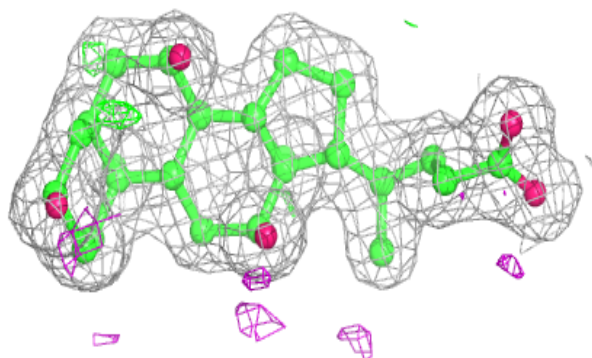
**Electron density around PGV C 306:**

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

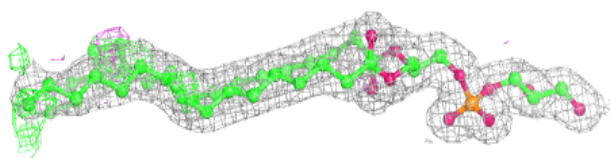
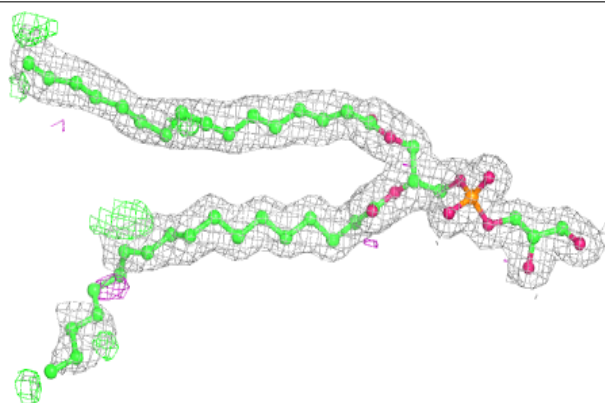


Electron density around CHD B 303:

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

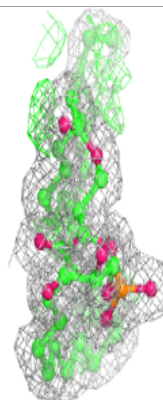
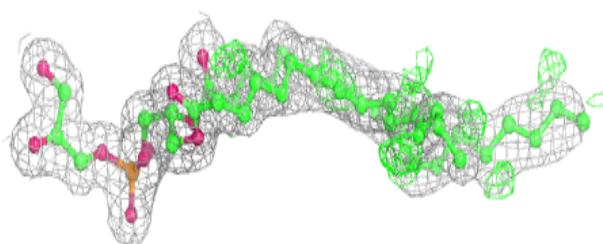
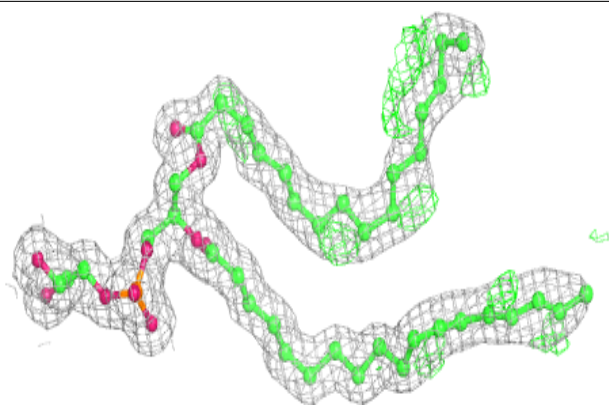
**Electron density around PGV P 306:**

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

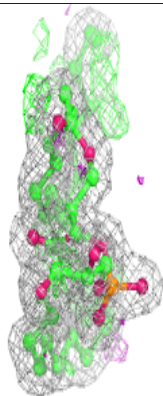
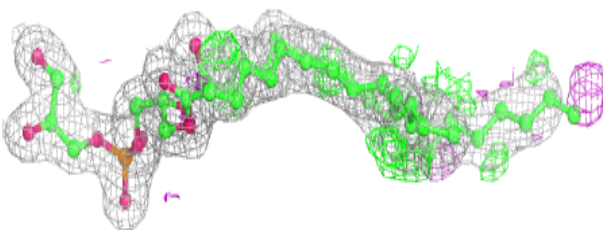
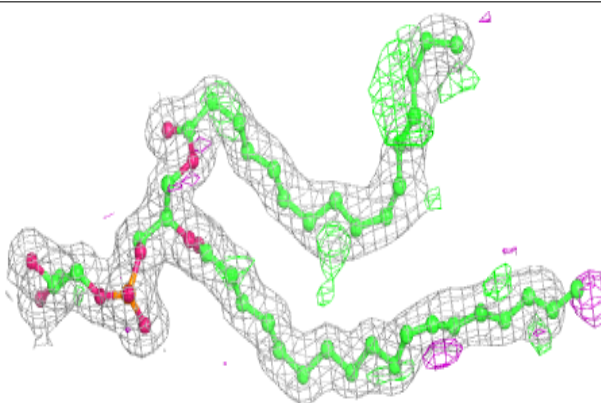


Electron density around PGV A 608:

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

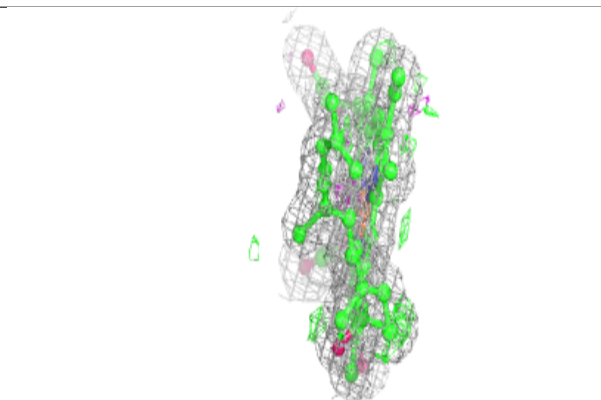
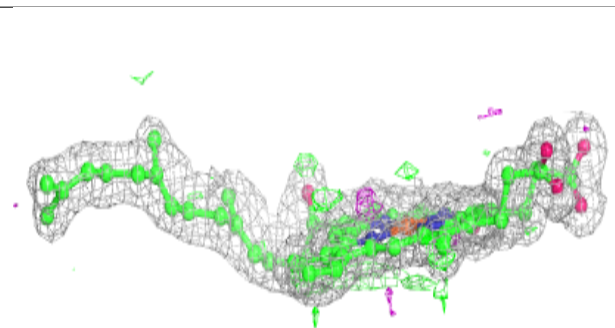
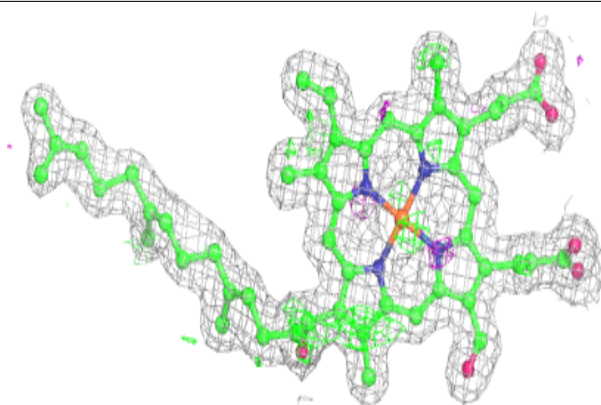
**Electron density around PGV N 609:**

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

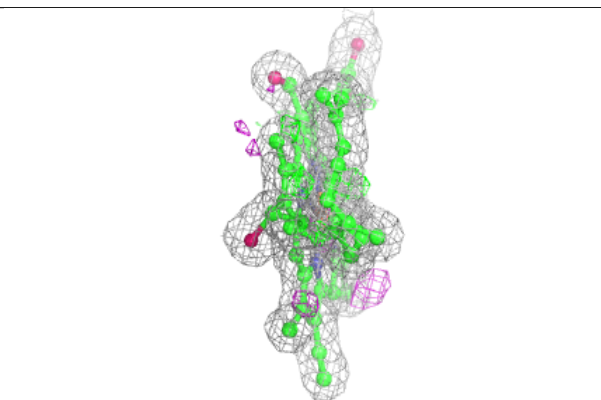
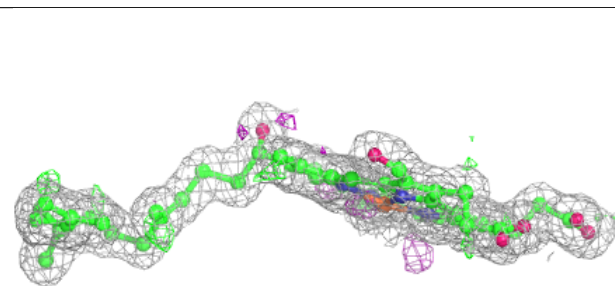
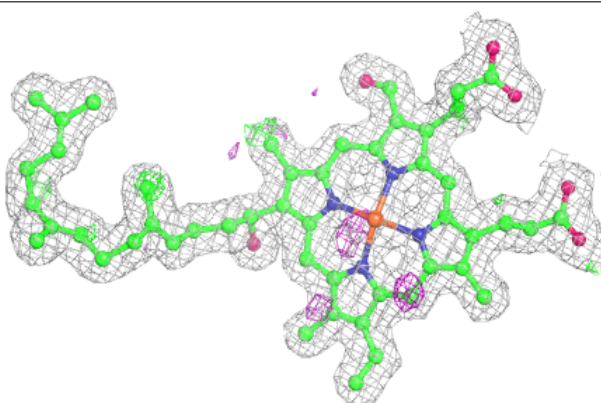


Electron density around HEA A 602 (B):

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

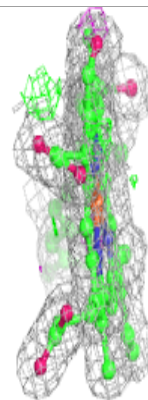
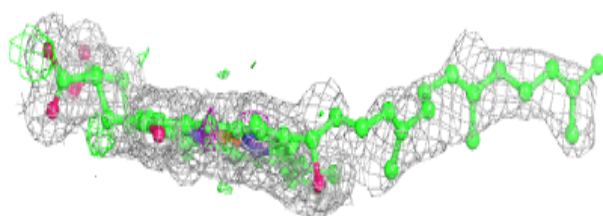
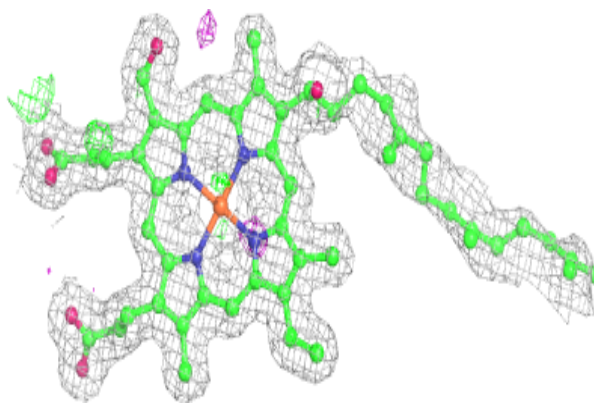
**Electron density around HEA A 603:**

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

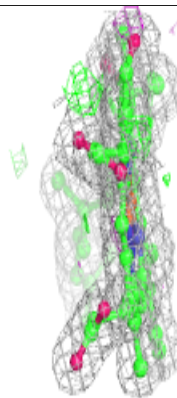
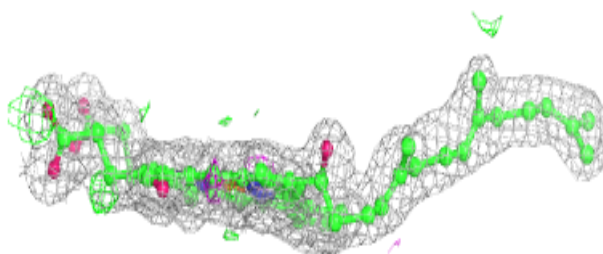
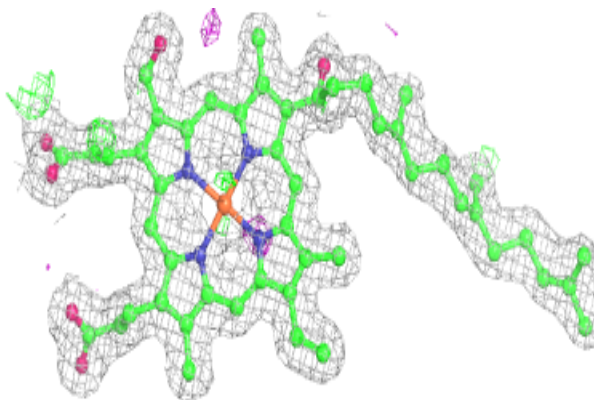


Electron density around HEA N 602 (A):

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

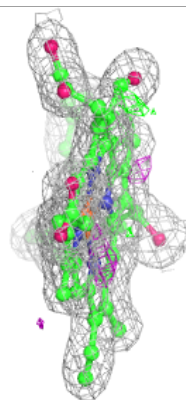
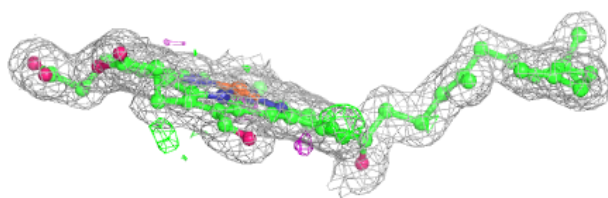
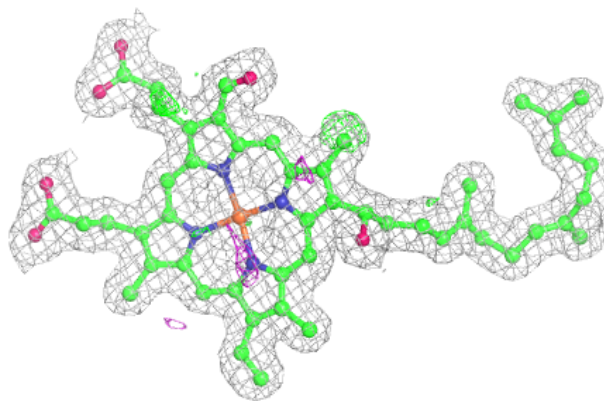
**Electron density around HEA N 602 (B):**

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

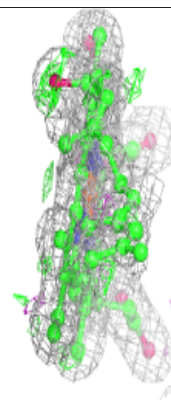
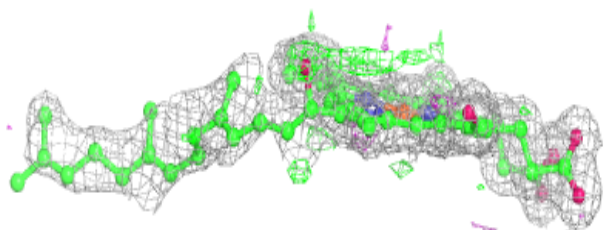
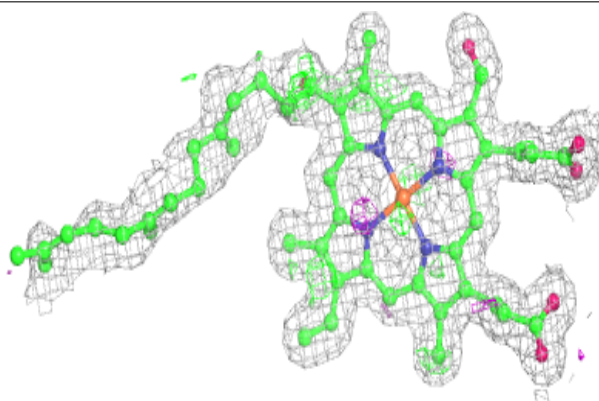


Electron density around HEA N 603:

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

**Electron density around HEA A 602 (A):**

$2mF_o-DF_c$ (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.