



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 12, 2022 – 08:43 PM JST

PDB ID : 7YPY
Title : Bovine heart cytochrome c oxidase in fully oxidized state at 1.5 angstrom resolution
Authors : Shimada, A.; Tsukihara, T.
Deposited on : 2022-08-05
Resolution : 1.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

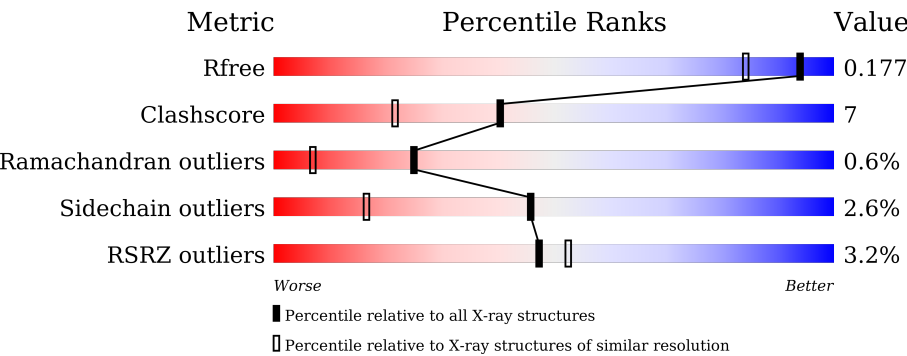
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 1.50 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.



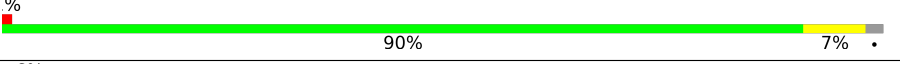
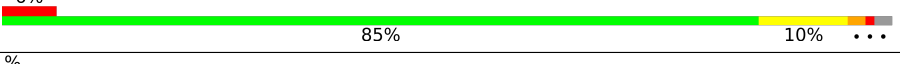
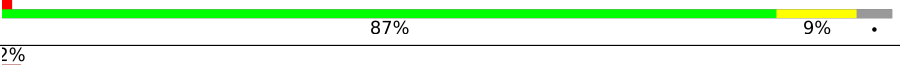
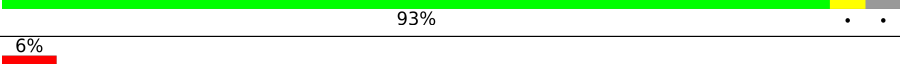

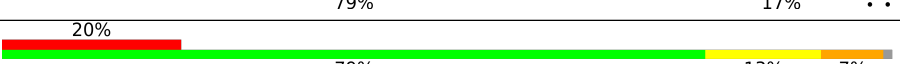
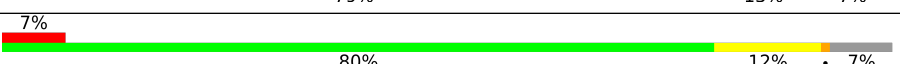
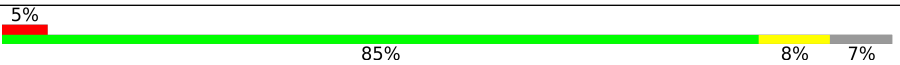

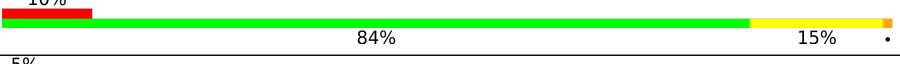
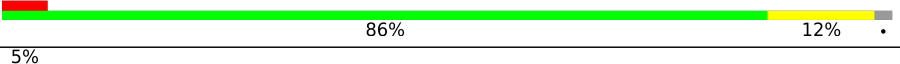
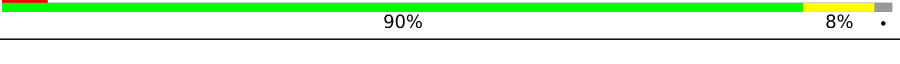

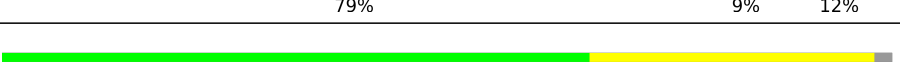





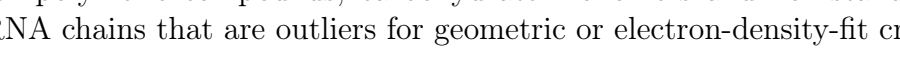
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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></div><div></div><div></div><div></div></div> <div>86%13%.</div>
1	N	514	<div><div></div><div></div><div></div><div></div><div></div></div> <div>90%8%.</div>
2	B	227	<div><div></div><div></div><div></div><div></div><div></div></div> <div>%78%22%.</div>
2	O	227	<div><div></div><div></div><div></div><div></div><div></div></div> <div>2%83%16%</div>
3	C	261	<div><div></div><div></div><div></div><div></div><div></div></div> <div>87%12%.</div>
3	P	261	<div><div></div><div></div><div></div><div></div><div></div></div> <div>85%13%..</div>

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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	
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	
14	T	85	

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	601[A]	X	-	-	-
15	HEA	A	601[B]	X	-	-	-
15	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	HEA	N	601[A]	X	-	-	-
15	HEA	N	601[B]	X	-	-	-
15	HEA	N	602	X	-	-	-
22	EDO	A	610	-	-	X	-
22	EDO	A	621	-	-	X	-
22	EDO	A	622	-	-	-	X
22	EDO	A	625	-	-	X	-
22	EDO	J	103	-	-	-	X
22	EDO	N	622	-	-	X	-
23	DMU	A	628	-	-	-	X
23	DMU	I	101	-	-	-	X
23	DMU	K	101	-	-	-	X
23	DMU	K	102	-	-	-	X
23	DMU	K	104	-	-	-	X
23	DMU	K	105	-	-	-	X
23	DMU	K	106	-	-	-	X
23	DMU	X	102	-	-	-	X
23	DMU	X	103	-	-	-	X
23	DMU	X	105	-	-	-	X
23	DMU	X	106	-	-	-	X
23	DMU	X	107	-	-	-	X
25	CHD	X	101	-	-	-	X
27	CDL	T	102	-	-	X	-
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 35132 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	40	0
			4164	2775	638	707	44			
1	N	514	Total	C	N	O	S	0	38	0
			4156	2772	634	706	44			

- 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
			1854	1207	283	345	19			
2	O	227	Total	C	N	O	S	0	8	0
			1848	1200	284	345	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	10	0
			2138	1428	340	355	15			
3	P	259	Total	C	N	O	S	0	10	0
			2137	1427	340	356	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	4	0
			1208	788	198	218	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1209	788	199	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			858	547	147	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			758	469	135	148	6			
6	S	98	Total	C	N	O	S	0	2	0
			753	467	134	146	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	C	N	O	P	S	0	2	0
			682	437	129	114	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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			
10	W	58	Total	C	N	O	S	0	1	0
			464	299	78	84	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	2	0
			388	253	65	67	3			
11	X	49	Total	C	N	O	S	0	2	0
			388	253	65	67	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	4	0
			390	260	65	62	3			

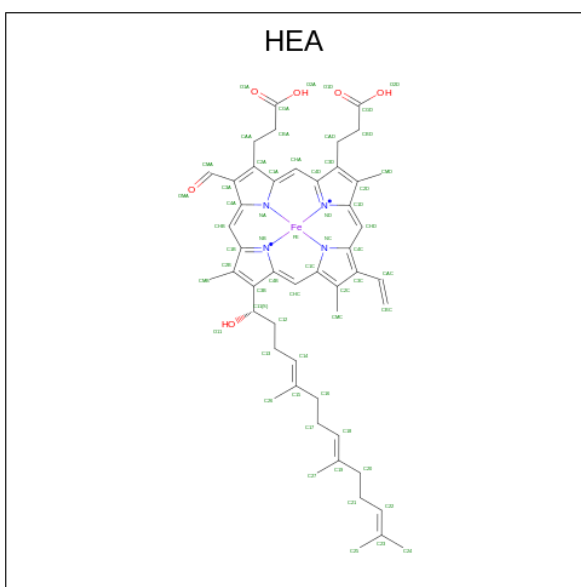
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B, mitochondrial.

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

- Molecule 14 is a protein called Cytochrome c oxidase subunit 6A2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	84	Total	C	N	O	S	0	2	0
			678	437	129	111	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	C	Fe	N	O	
			69	58	1	4	6	0
15	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
15	N	1	Total	C	Fe	N	O	
			69	58	1	4	6	0
15	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

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

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

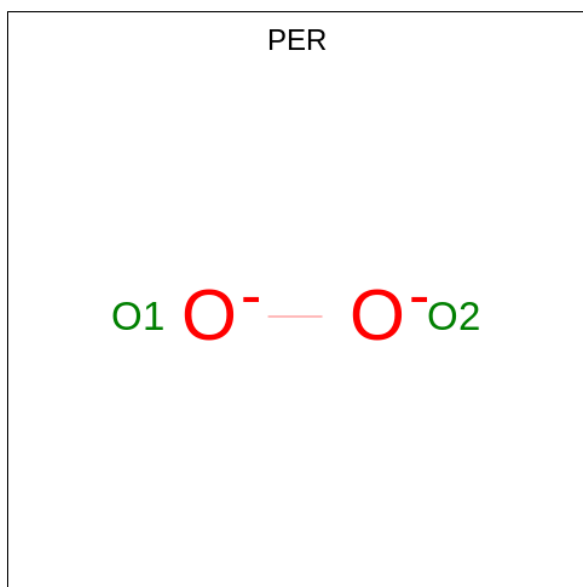
- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

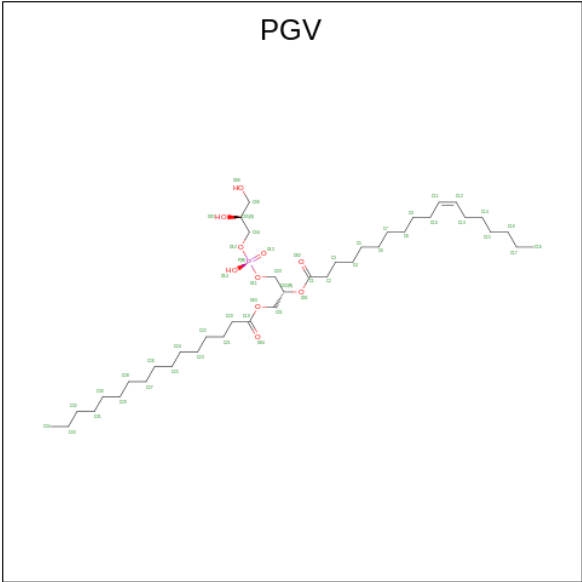
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



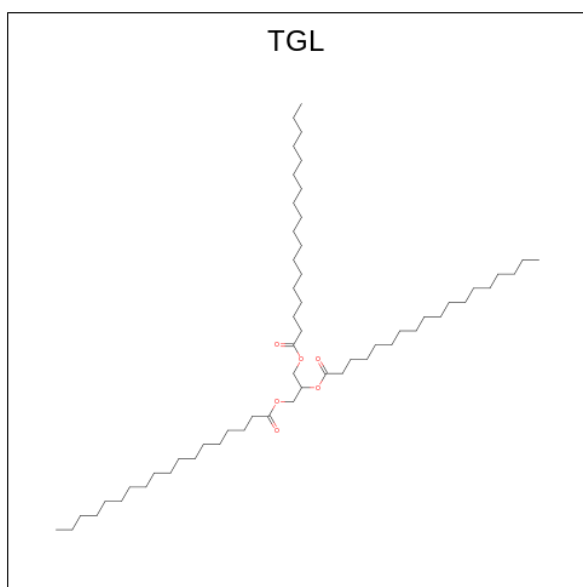
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P) (labeled as "Ligand of Interest" by depositor).



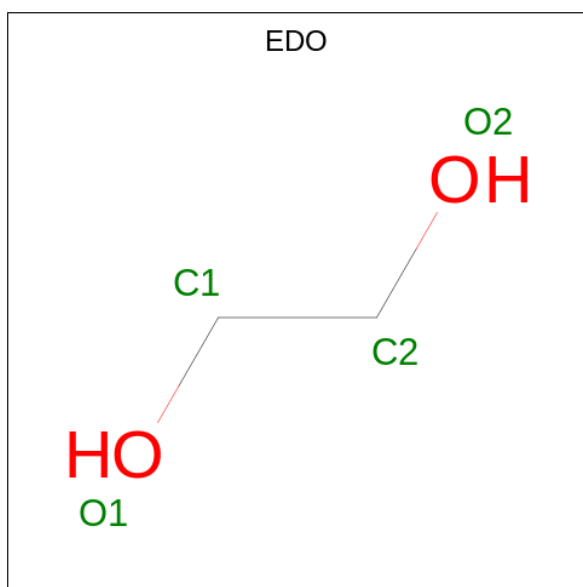
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			48	37	10	1		
20	G	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	Q	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			63	57	6		
21	B	1	Total	C	O	0	0
			62	56	6		
21	D	1	Total	C	O	0	0
			62	56	6		
21	O	1	Total	C	O	0	0
			60	54	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	E	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	F	1	Total	C	O	0	0
			4	2	2		
22	G	1	Total	C	O	0	0
			4	2	2		
22	G	1	Total	C	O	0	0
			4	2	2		
22	G	1	Total	C	O	0	0
			4	2	2		
22	H	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	J	1	Total	C	O	0	0
			4	2	2		
22	L	1	Total	C	O	0	0
			4	2	2		
22	L	1	Total	C	O	0	0
			4	2	2		
22	L	1	Total	C	O	0	0
			4	2	2		
22	M	1	Total	C	O	0	0
			4	2	2		
22	M	1	Total	C	O	0	0
			4	2	2		

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

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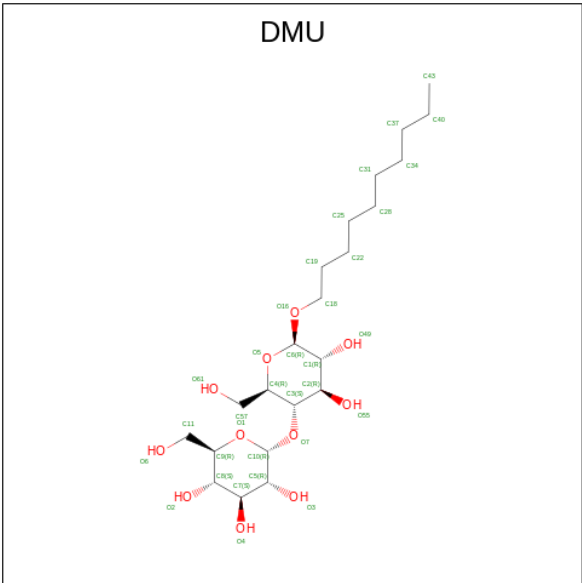
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	P	1	Total	C	O	0	0
			4	2	2		
22	Q	1	Total	C	O	0	0
			4	2	2		
22	Q	1	Total	C	O	0	0
			4	2	2		
22	R	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	S	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	T	1	Total	C	O	0	0
			4	2	2		
22	V	1	Total	C	O	0	0
			4	2	2		
22	W	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	Y	1	Total	C	O	0	0
			4	2	2		
22	Y	1	Total	C	O	0	0
			4	2	2		
22	Z	1	Total	C	O	0	0
			4	2	2		

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁) (labeled as "Ligand of Interest" by depositor).



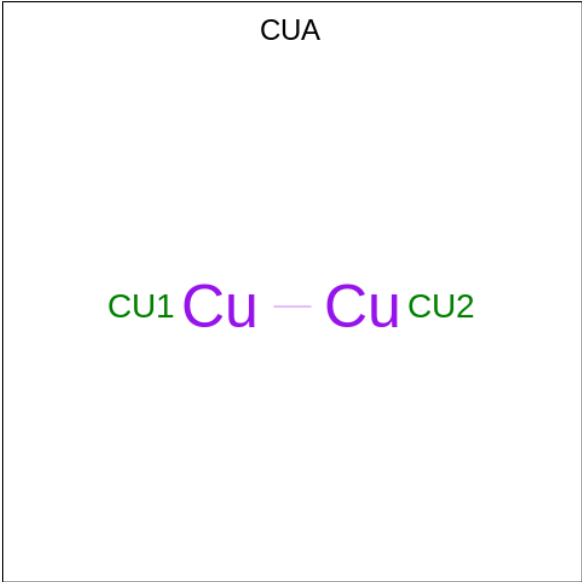
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			33	22	11		
23	C	1	Total	C	O	0	0
			33	22	11		
23	C	1	Total	C	O	0	0
			33	22	11		
23	C	1	Total	C	O	0	0
			33	22	11		
23	C	1	Total	C	O	0	0
			33	22	11		
23	D	1	Total	C	O	0	0
			33	22	11		
23	I	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			33	22	11		

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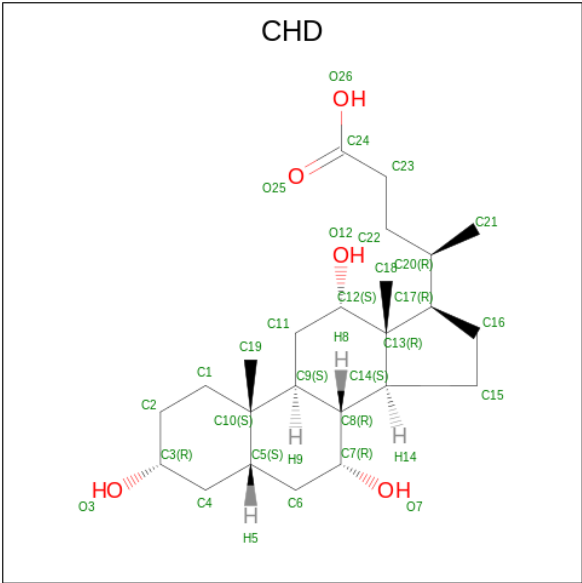
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	K	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			32	22	10		
23	K	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			33	22	11		
23	K	1	Total	C	O	0	0
			33	22	11		
23	L	1	Total	C	O	0	0
			33	22	11		
23	M	1	Total	C	O	0	0
			33	22	11		
23	O	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	X	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

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



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

- Molecule 25 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



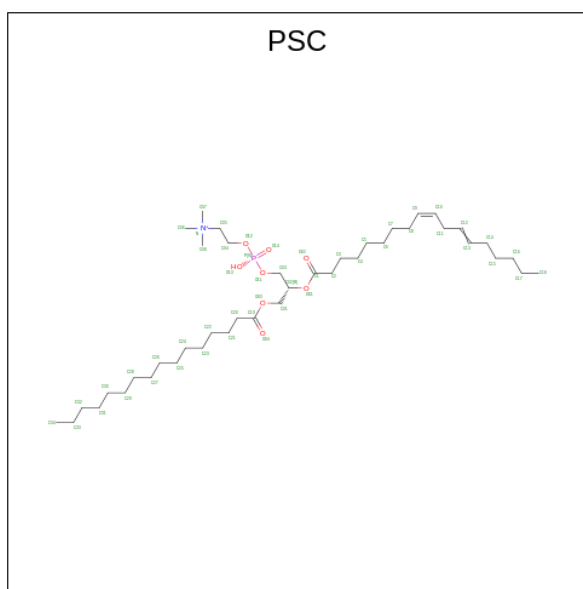
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			29	24	5		
25	C	1	Total	C	O	0	0
			29	24	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			29	24	5		
25	L	1	Total	C	O	0	0
			29	24	5		
25	O	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		
25	P	1	Total	C	O	0	0
			29	24	5		
25	X	1	Total	C	O	0	0
			29	24	5		
25	Y	1	Total	C	O	0	0
			29	24	5		

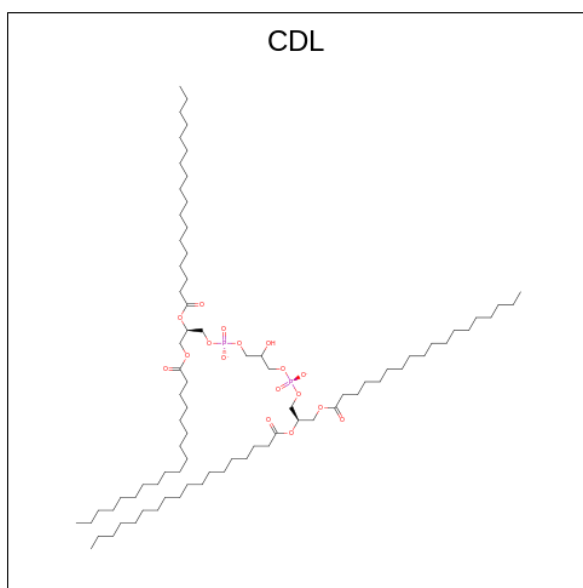
- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

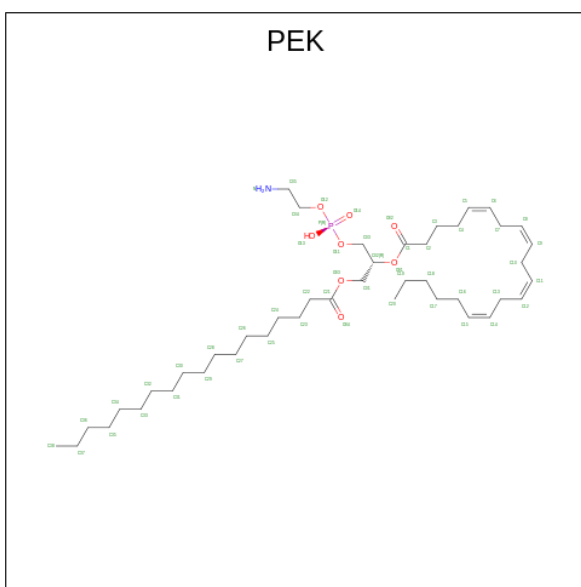
- Molecule 27 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	C	1	Total	C	O	P	0	0
			89	71	16	2		
27	G	1	Total	C	O	P	0	0
			100	81	17	2		
27	P	1	Total	C	O	P	0	0
			90	72	16	2		
27	T	1	Total	C	O	P	0	0
			98	79	17	2		

- Molecule 28 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) (labeled as "Ligand of Interest" by depositor).

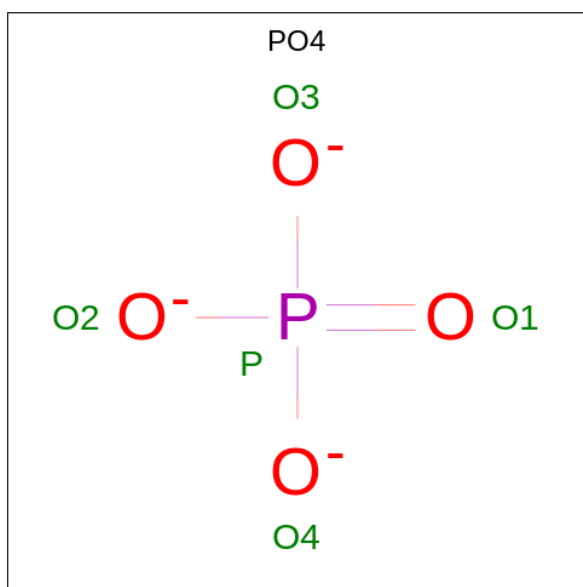


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	C	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	O	P		0	0
			50	41	8	1			

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 30 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 31 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	A	264	Total	O	0	9
			264	264		
31	B	218	Total	O	0	6
			219	219		
31	C	142	Total	O	0	0
			142	142		
31	D	212	Total	O	0	0
			212	212		
31	E	159	Total	O	0	0
			159	159		
31	F	156	Total	O	0	0
			156	156		
31	G	78	Total	O	0	0
			78	78		
31	H	102	Total	O	0	0
			102	102		
31	I	65	Total	O	0	0
			65	65		
31	J	48	Total	O	0	0
			48	48		

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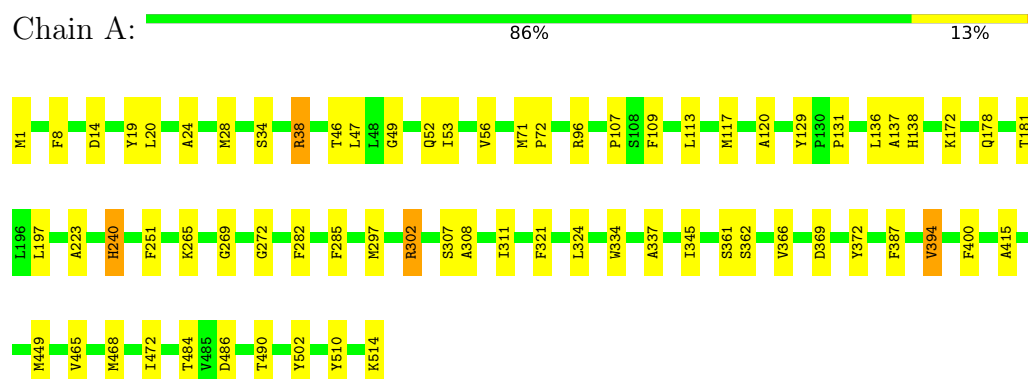
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	K	40	Total 40	O 40	0	0
31	L	36	Total 36	O 36	0	2
31	M	34	Total 34	O 34	0	0
31	N	260	Total 260	O 260	0	13
31	O	184	Total 185	O 185	0	6
31	P	139	Total 139	O 139	0	0
31	Q	97	Total 97	O 97	0	0
31	R	110	Total 110	O 110	0	0
31	S	135	Total 135	O 135	0	0
31	T	60	Total 60	O 60	0	0
31	U	79	Total 79	O 79	0	0
31	V	50	Total 50	O 50	0	0
31	W	40	Total 40	O 40	0	0
31	X	31	Total 31	O 31	0	0
31	Y	30	Total 30	O 30	0	0
31	Z	22	Total 22	O 22	0	0

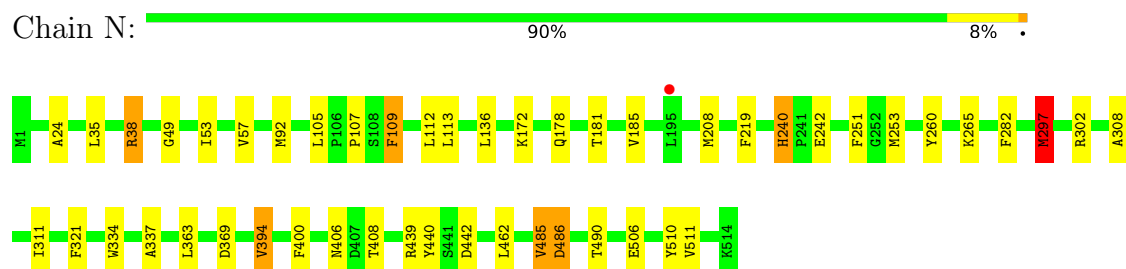
3 Residue-property plots

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.

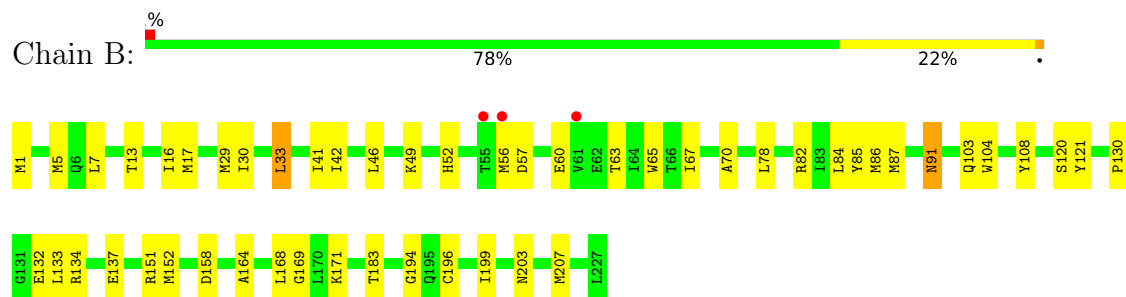
• Molecule 1: Cytochrome c oxidase subunit 1



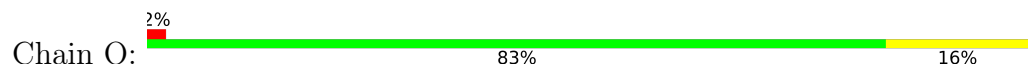
• Molecule 1: Cytochrome c oxidase subunit 1

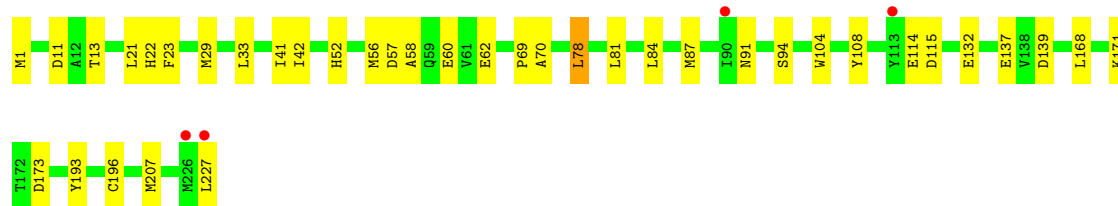


• Molecule 2: Cytochrome c oxidase subunit 2



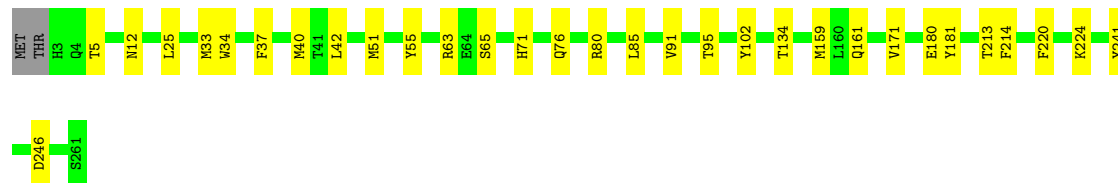
• Molecule 2: Cytochrome c oxidase subunit 2





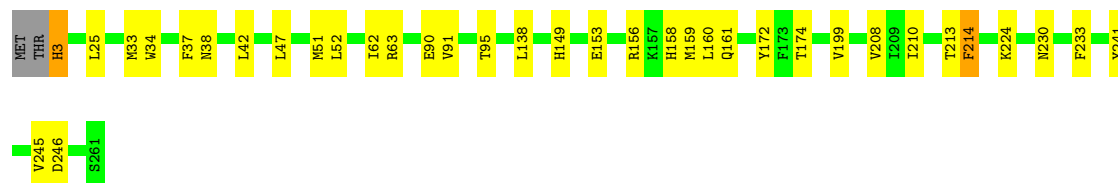
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 12%



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 85% 13%



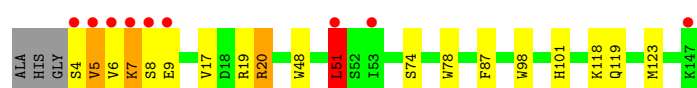
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 90% 7%



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

Chain Q: 85% 10% 5%

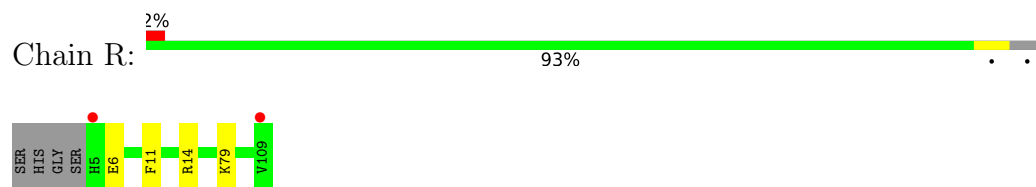


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

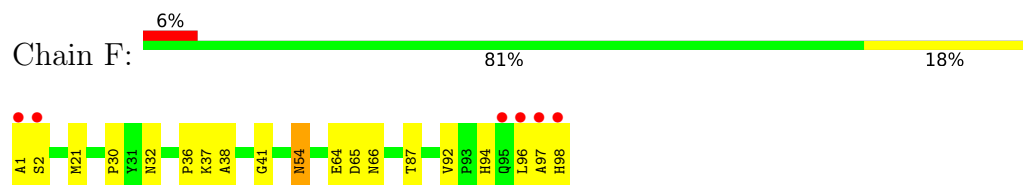
Chain E: 87% 9%



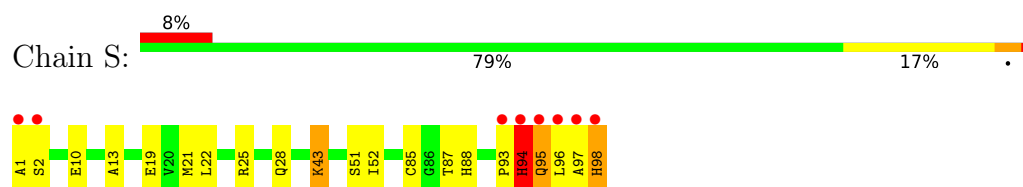
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



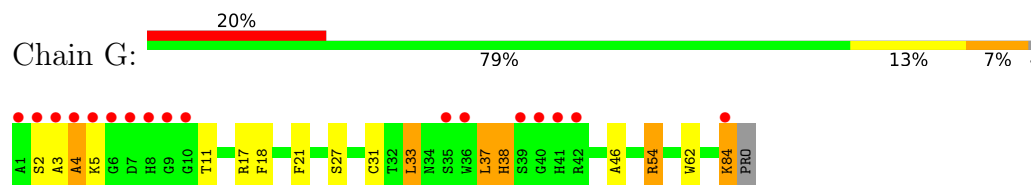
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



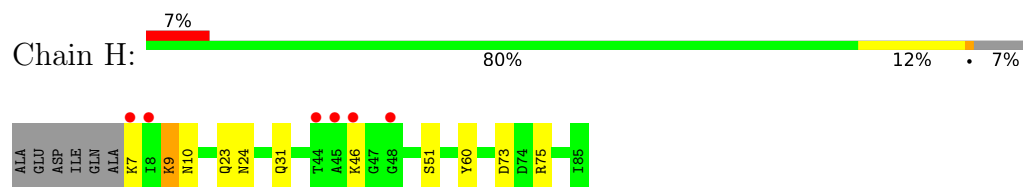
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



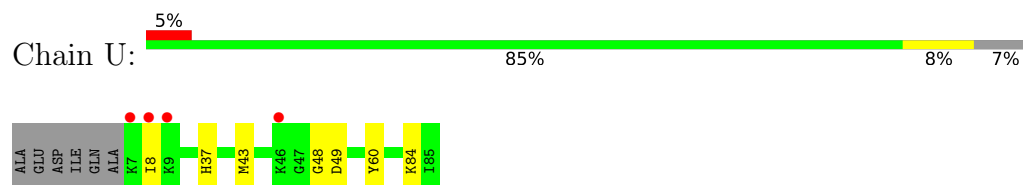
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



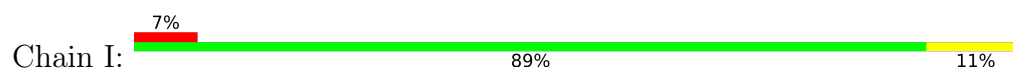
- Molecule 8: Cytochrome c oxidase subunit 6B1

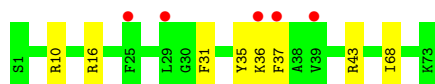


- Molecule 8: Cytochrome c oxidase subunit 6B1

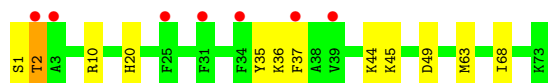
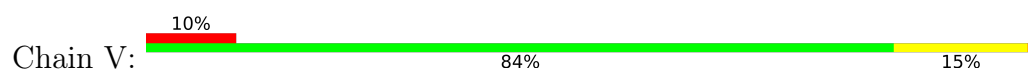


- Molecule 9: Cytochrome c oxidase subunit 6C

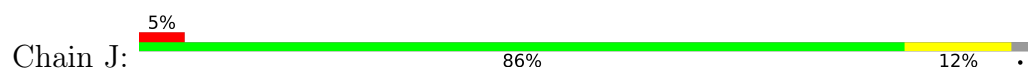




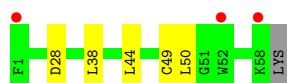
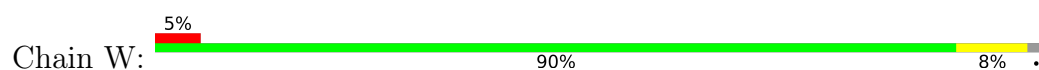
- Molecule 9: Cytochrome c oxidase subunit 6C



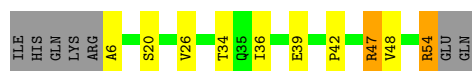
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



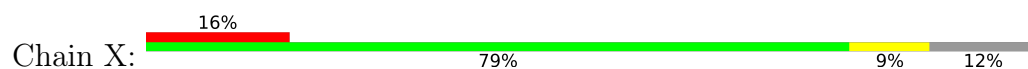
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



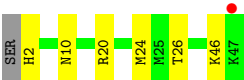
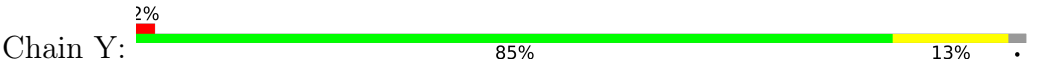
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



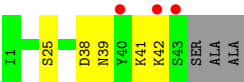
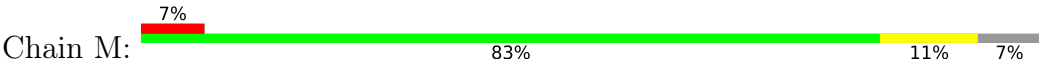
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



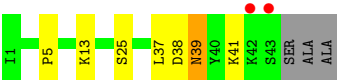
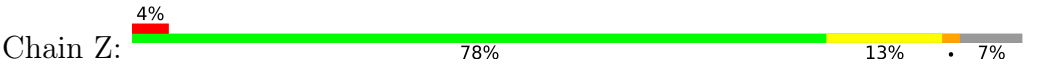
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



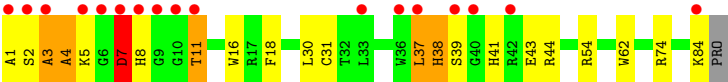
• Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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



• Molecule 14: Cytochrome c oxidase subunit 6A2, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.94Å 204.40Å 177.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.95 – 1.50 89.10 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.95-1.50) 98.2 (89.10-1.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.40Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.159 , 0.177 0.160 , 0.177	Depositor DCC
R_{free} test set	63174 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35132	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: CHD, PSC, CUA, EDO, FME, DMU, PGV, CU, MG, SAC, ZN, CDL, HEA, TGL, PER, TPO, PEK, NA, 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	1.09	10/4467 (0.2%)	1.14	18/6094 (0.3%)
1	N	0.98	4/4445 (0.1%)	0.99	11/6066 (0.2%)
2	B	0.98	3/1952 (0.2%)	1.08	6/2658 (0.2%)
2	O	0.82	1/1929 (0.1%)	0.94	6/2626 (0.2%)
3	C	0.98	3/2278 (0.1%)	0.95	6/3112 (0.2%)
3	P	0.96	1/2277 (0.0%)	0.90	4/3110 (0.1%)
4	D	0.96	0/1266	0.90	2/1706 (0.1%)
4	Q	0.60	0/1259	0.72	3/1698 (0.2%)
5	E	0.83	1/871 (0.1%)	0.92	4/1182 (0.3%)
5	R	0.69	0/882	0.73	0/1196
6	F	0.88	0/795	0.87	0/1079
6	S	0.77	0/780	0.87	0/1058
7	G	0.79	0/708	0.89	1/961 (0.1%)
8	H	0.89	0/682	0.92	2/921 (0.2%)
8	U	0.71	0/682	0.78	0/921
9	I	0.79	0/605	0.83	2/802 (0.2%)
9	V	0.72	0/605	0.73	1/802 (0.1%)
10	J	0.57	0/471	0.71	1/636 (0.2%)
10	W	0.54	0/480	0.66	1/648 (0.2%)
11	K	0.87	0/413	0.83	1/566 (0.2%)
11	X	0.57	0/413	0.63	0/566
12	L	1.06	1/393 (0.3%)	0.90	0/526
12	Y	0.73	0/427	0.71	0/570
13	M	0.94	0/345	0.89	0/470
13	Z	0.69	0/345	0.69	0/470
14	T	0.75	0/716	0.80	0/974
All	All	0.91	24/30486 (0.1%)	0.94	69/41418 (0.2%)

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
6	S	0	2
All	All	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	241	TYR	CE1-CZ	-6.16	1.30	1.38
5	E	70	VAL	CB-CG1	-5.91	1.40	1.52
1	A	362[A]	SER	CB-OG	-5.90	1.34	1.42
1	A	362[B]	SER	CB-OG	-5.90	1.34	1.42
3	C	76	GLN	CD-OE1	5.81	1.36	1.24
1	N	242	GLU	CD-OE2	5.70	1.31	1.25
2	B	152	MET	CB-CG	-5.59	1.33	1.51
1	A	394[A]	VAL	CB-CG2	-5.53	1.41	1.52
1	A	394[B]	VAL	CB-CG2	-5.53	1.41	1.52
1	N	394[A]	VAL	CB-CG2	-5.51	1.41	1.52
1	N	394[B]	VAL	CB-CG2	-5.51	1.41	1.52
2	B	121	TYR	CE2-CZ	5.48	1.45	1.38
2	B	120	SER	CB-OG	-5.39	1.35	1.42
12	L	37	PHE	CE2-CZ	5.37	1.47	1.37
1	A	502	TYR	CD1-CE1	5.32	1.47	1.39
3	C	102	TYR	CG-CD1	-5.14	1.32	1.39
2	O	193	TYR	CD1-CE1	5.08	1.47	1.39
1	N	92	MET	CB-CG	5.06	1.67	1.51
1	A	189[A]	MET	CG-SD	-5.06	1.68	1.81
1	A	189[B]	MET	CG-SD	-5.06	1.68	1.81
1	A	34[A]	SER	CB-OG	-5.04	1.35	1.42
1	A	34[B]	SER	CB-OG	-5.04	1.35	1.42
1	A	307	SER	CB-OG	5.04	1.48	1.42
3	P	90	GLU	CG-CD	-5.01	1.44	1.51

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	38	ARG	NE-CZ-NH1	11.34	125.97	120.30
4	Q	20	ARG	NE-CZ-NH2	-8.88	115.86	120.30
9	I	16	ARG	NE-CZ-NH2	-8.77	115.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	153	GLU	OE1-CD-OE2	8.19	133.13	123.30
8	H	75	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	A	400	PHE	CB-CG-CD2	-7.99	115.21	120.80
1	N	251	PHE	CB-CG-CD1	-7.80	115.34	120.80
1	N	38	ARG	NE-CZ-NH1	7.61	124.11	120.30
4	Q	20	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	19	TYR	CB-CG-CD1	-7.47	116.52	121.00
1	A	251	PHE	CB-CG-CD1	-7.35	115.66	120.80
1	A	14	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	8	PHE	CB-CG-CD1	7.25	125.88	120.80
5	E	40	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	442	ASP	CB-CG-OD2	-7.11	111.90	118.30
2	O	173	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	8	PHE	CB-CG-CD2	-6.96	115.92	120.80
4	D	20	ARG	NE-CZ-NH1	6.85	123.72	120.30
2	B	134	ARG	NE-CZ-NH2	-6.85	116.88	120.30
4	Q	51	LEU	CA-CB-CG	6.72	130.77	115.30
10	W	28	ASP	CB-CG-OD2	-6.64	112.33	118.30
5	E	73	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	442	ASP	CB-CG-OD1	6.55	124.19	118.30
10	J	28	ASP	CB-CG-OD2	-6.50	112.45	118.30
2	O	11	ASP	CB-CG-OD1	6.49	124.14	118.30
1	N	38	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	387	PHE	CB-CG-CD1	-6.27	116.41	120.80
5	E	30	ARG	NE-CZ-NH2	-6.09	117.26	120.30
2	O	108	TYR	CB-CG-CD1	-6.07	117.36	121.00
4	D	20	ARG	NE-CZ-NH2	-6.03	117.28	120.30
11	K	47	ARG	NE-CZ-NH1	5.99	123.29	120.30
9	I	43	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	302[A]	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	A	129	TYR	CB-CG-CD1	-5.87	117.48	121.00
1	N	400	PHE	CB-CG-CD2	-5.82	116.72	120.80
2	B	158	ASP	CB-CG-OD1	5.72	123.45	118.30
1	N	440	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	N	439	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	N	442	ASP	CB-CG-OD1	5.58	123.32	118.30
3	C	181	TYR	CB-CG-CD2	-5.55	117.67	121.00
2	B	56[A]	MET	CG-SD-CE	5.52	109.04	100.20
2	B	56[B]	MET	CG-SD-CE	5.52	109.04	100.20
2	O	173	ASP	CB-CG-OD2	-5.50	113.35	118.30
3	P	233	PHE	CB-CG-CD2	-5.47	116.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	253	MET	CG-SD-CE	-5.46	91.46	100.20
2	O	139	ASP	CB-CG-OD1	5.46	123.21	118.30
7	G	54	ARG	NE-CZ-NH2	-5.41	117.60	120.30
3	P	241	TYR	CB-CG-CD1	-5.37	117.78	121.00
3	C	80[A]	ARG	NE-CZ-NH2	-5.34	117.63	120.30
3	C	80[B]	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	N	297[A]	MET	CB-CG-SD	5.34	128.41	112.40
1	N	297[B]	MET	CB-CG-SD	5.34	128.41	112.40
3	P	214	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	A	251	PHE	CB-CG-CD2	5.26	124.48	120.80
1	A	372	TYR	CB-CG-CD1	-5.23	117.86	121.00
9	V	10	ARG	NE-CZ-NH2	-5.14	117.73	120.30
5	E	66	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	C	241	TYR	CB-CG-CD1	-5.11	117.94	121.00
2	O	21	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	A	439	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	N	442	ASP	CB-CG-OD2	-5.08	113.73	118.30
2	B	151	ARG	NE-CZ-NH1	5.06	122.83	120.30
8	H	73	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	96	ARG	NE-CZ-NH2	-5.03	117.79	120.30
3	C	80[A]	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	C	80[B]	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	B	108	TYR	CZ-CE2-CD2	-5.00	115.30	119.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
6	S	94	HIS	Peptide

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	4164	0	4140	66	0
1	N	4156	0	4141	46	0
2	B	1854	0	1861	35	0
2	O	1848	0	1847	21	0
3	C	2138	0	2061	27	0
3	P	2137	0	2057	37	0
4	D	1208	0	1199	11	0
4	Q	1209	0	1202	17	0
5	E	852	0	845	2	0
5	R	858	0	854	4	0
6	F	758	0	739	17	0
6	S	753	0	736	16	0
7	G	682	0	650	14	0
8	H	662	0	623	5	0
8	U	662	0	623	2	0
9	I	601	0	613	4	0
9	V	601	0	613	6	0
10	J	460	0	459	5	0
10	W	464	0	461	3	0
11	K	388	0	372	9	0
11	X	388	0	372	5	0
12	L	380	0	380	16	0
12	Y	390	0	390	5	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	T	678	0	651	20	0
15	A	129	0	88	4	0
15	N	129	0	88	4	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	N	1	0	0	0	0
19	A	2	0	0	1	0
19	N	2	0	0	1	0
20	A	102	0	152	2	0
20	C	99	0	143	1	0
20	G	51	0	76	2	0
20	N	51	0	76	1	0
20	P	51	0	76	1	0
20	Q	51	0	76	5	0
21	A	63	0	110	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	62	0	105	6	0
21	D	62	0	105	12	0
21	O	60	0	101	4	0
21	Q	63	0	110	8	0
21	Y	63	0	110	8	0
22	A	72	0	107	26	0
22	B	20	0	30	1	0
22	C	24	0	36	1	0
22	D	16	0	24	2	0
22	E	12	0	18	0	0
22	F	24	0	35	0	0
22	G	12	0	18	1	0
22	H	4	0	6	1	0
22	J	20	0	30	1	0
22	L	12	0	18	0	0
22	M	8	0	12	1	0
22	N	68	0	102	12	0
22	O	8	0	12	0	0
22	P	24	0	36	1	0
22	Q	8	0	12	1	0
22	R	4	0	6	0	0
22	S	32	0	48	6	0
22	T	16	0	24	0	0
22	V	4	0	6	2	0
22	W	4	0	6	1	0
22	Y	8	0	12	0	0
22	Z	4	0	6	0	0
23	A	33	0	42	1	0
23	C	132	0	168	6	0
23	D	33	0	42	1	0
23	I	33	0	42	4	0
23	K	197	0	250	8	0
23	L	33	0	42	4	0
23	M	33	0	42	1	0
23	O	33	0	42	0	0
23	P	99	0	126	10	0
23	X	198	0	252	10	0
23	Z	33	0	42	0	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	B	29	0	39	0	0
25	C	58	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	L	29	0	39	1	0
25	O	29	0	39	1	0
25	P	58	0	78	3	0
25	X	29	0	36	7	0
25	Y	29	0	39	0	0
26	B	52	0	80	11	0
26	O	51	0	75	9	0
27	C	89	0	126	8	0
27	G	100	0	156	18	0
27	P	90	0	133	11	0
27	T	98	0	149	21	0
28	C	158	0	226	20	0
28	P	106	0	154	7	0
28	T	50	0	71	5	0
29	F	1	0	0	0	0
29	S	1	0	0	0	0
30	H	5	0	0	0	0
30	U	5	0	0	0	0
31	A	264	0	0	12	0
31	B	219	0	0	3	0
31	C	142	0	0	3	0
31	D	212	0	0	1	0
31	E	159	0	0	0	0
31	F	156	0	0	1	0
31	G	78	0	0	0	0
31	H	102	0	0	3	0
31	I	65	0	0	1	0
31	J	48	0	0	1	0
31	K	40	0	0	2	0
31	L	36	0	0	2	0
31	M	34	0	0	0	0
31	N	260	0	0	5	0
31	O	185	0	0	0	0
31	P	139	0	0	2	0
31	Q	97	0	0	0	0
31	R	110	0	0	1	0
31	S	135	0	0	2	0
31	T	60	0	0	2	0
31	U	79	0	0	1	0
31	V	50	0	0	0	0
31	W	40	0	0	0	0
31	X	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Y	30	0	0	0	0
31	Z	22	0	0	0	0
All	All	35132	0	33221	471	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (471) 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)
19:A:606:PER:O2	19:A:606:PER:O1	1.55	1.24
19:N:606:PER:O2	19:N:606:PER:O1	1.55	1.21
4:D:78:TRP:HB3	21:D:201:TGL:HB21	1.38	1.02
12:Y:20:ARG:HH22	21:Y:101:TGL:HC51	1.26	0.96
27:G:101:CDL:H241	27:G:101:CDL:H541	1.52	0.91
28:C:305:PEK:H041	7:G:17:ARG:HH12	1.33	0.90
8:H:24:ASN:HD21	22:H:101:EDO:H22	1.34	0.90
1:N:113:LEU:HB2	21:Y:101:TGL:H301	1.53	0.88
1:A:510:TYR:HA	22:A:625:EDO:H21	1.58	0.84
22:A:626:EDO:H22	31:A:913:HOH:O	1.77	0.84
22:N:622:EDO:H22	31:N:787:HOH:O	1.78	0.83
22:A:610:EDO:H11	22:A:620:EDO:H22	1.62	0.81
4:D:78:TRP:CB	21:D:201:TGL:HB21	2.11	0.81
3:C:161[A]:GLN:HE22	28:C:305:PEK:H22	1.46	0.80
12:L:2:HIS:CG	12:L:3:TYR:H	2.02	0.78
2:B:130:PRO:HB3	22:D:202:EDO:H21	1.68	0.76
28:P:301:PEK:H331	28:P:301:PEK:H131	1.68	0.76
12:L:42:HIS:HB2	23:L:105:DMU:H6	1.68	0.75
15:A:602:HEA:HBC1	15:A:602:HEA:HMC1	1.70	0.74
3:C:51[A]:MET:SD	27:C:302:CDL:H621	2.27	0.74
1:A:136[B]:LEU:HD11	31:A:954:HOH:O	1.89	0.73
1:A:223:ALA:HB2	22:A:610:EDO:H21	1.70	0.73
15:N:602:HEA:HBC1	15:N:602:HEA:HMC1	1.71	0.72
3:P:33:MET:SD	23:P:305:DMU:H8	2.30	0.71
6:F:94:HIS:NE2	6:F:98:HIS:HA	2.05	0.71
1:A:137:ALA:HA	22:A:619:EDO:H21	1.71	0.71
22:A:610:EDO:H12	22:B:308:EDO:H12	1.73	0.70
11:K:20:SER:HA	23:K:105:DMU:H5	1.72	0.70
1:A:272:GLY:H	22:A:621:EDO:H11	1.56	0.69
14:T:38:HIS:HD2	27:T:102:CDL:H1	1.56	0.69
3:P:224:LYS:HD2	27:P:303:CDL:HB31	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:308:DMU:H9	10:J:49:CYS:HB3	1.73	0.69
14:T:11:THR:HG23	14:T:16:TRP:HE1	1.57	0.68
3:C:33:MET:HE1	3:C:42:LEU:H	1.59	0.68
1:N:485[A]:VAL:HG21	22:N:613:EDO:H12	1.75	0.68
6:S:95:GLN:NE2	6:S:98:HIS:OXT	2.27	0.68
3:C:91:VAL:O	3:C:95[B]:THR:HG23	1.95	0.67
6:F:30:PRO:O	6:F:98:HIS:HB2	1.94	0.67
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.34	0.67
3:P:213:THR:HG23	27:P:303:CDL:H771	1.77	0.66
9:V:20:HIS:HE1	22:V:101:EDO:H12	1.59	0.66
23:X:103:DMU:H2	31:X:203:HOH:O	1.95	0.66
3:P:63:ARG:HE	27:P:303:CDL:CA2	2.09	0.65
31:N:867:HOH:O	6:S:95:GLN:HB2	1.95	0.65
26:B:304:PSC:H071	9:I:10:ARG:HH21	1.62	0.65
3:P:51[A]:MET:SD	27:P:303:CDL:H621	2.37	0.65
3:P:91:VAL:O	3:P:95[B]:THR:HG23	1.96	0.65
1:N:406:ASN:HD21	20:Q:201:PGV:H21	1.62	0.64
3:P:149:HIS:NE2	22:P:313:EDO:H12	2.11	0.64
3:P:34:TRP:HE1	23:P:314:DMU:C57	2.10	0.64
14:T:38:HIS:CD2	27:T:102:CDL:H1	2.31	0.64
1:A:486[B]:ASP:OD1	31:A:701:HOH:O	2.15	0.64
3:C:63:ARG:HE	27:C:302:CDL:CA2	2.11	0.64
2:O:41:ILE:HD13	26:O:304:PSC:H321	1.80	0.64
1:A:465:VAL:HA	22:A:622:EDO:H21	1.79	0.64
6:S:51:SER:O	6:S:94:HIS:HA	1.98	0.64
1:N:485[A]:VAL:CG2	22:N:613:EDO:H12	2.28	0.63
11:X:40:TRP:CD1	23:X:103:DMU:H7	2.33	0.63
1:A:302[B]:ARG:NH1	31:A:706:HOH:O	2.31	0.62
1:A:484[A]:THR:HG22	31:A:915:HOH:O	1.99	0.62
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.79	0.62
23:K:105:DMU:H20	23:K:106:DMU:H16	1.82	0.62
21:D:201:TGL:H242	21:D:201:TGL:HA91	1.81	0.62
7:G:27:SER:HB3	27:G:101:CDL:H562	1.80	0.62
26:O:304:PSC:H12	26:O:304:PSC:H322	1.81	0.61
14:T:31:CYS:SG	27:T:102:CDL:H562	2.41	0.61
23:C:316:DMU:H23	10:J:41:GLY:HA3	1.81	0.61
23:L:105:DMU:H5	31:L:212:HOH:O	1.99	0.61
3:P:33:MET:HE1	3:P:42:LEU:H	1.66	0.61
1:A:20:LEU:HB3	21:A:609:TGL:H221	1.83	0.61
3:C:12:ASN:HD21	22:C:313:EDO:H12	1.64	0.61
7:G:46:ALA:HA	22:G:105:EDO:H11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:26:VAL:HG13	23:K:101:DMU:H11	1.83	0.61
3:C:5:THR:HB	6:F:98:HIS:HD2	1.66	0.61
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.83	0.60
2:B:13:THR:HB	2:B:168:LEU:HD23	1.84	0.60
12:L:41:ARG:HH12	23:L:105:DMU:H2	1.65	0.60
3:P:161[A]:GLN:HE22	28:T:101:PEK:H5	1.67	0.60
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.66	0.60
4:Q:78:TRP:CA	21:Q:202:TGL:HB22	2.32	0.60
1:N:511:VAL:H	22:N:622:EDO:H21	1.67	0.59
2:B:7:LEU:HD12	21:B:301:TGL:HC52	1.83	0.59
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.03	0.59
22:A:625:EDO:H22	6:F:36:PRO:CD	2.33	0.59
12:L:2:HIS:CD2	12:L:3:TYR:H	2.20	0.59
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.84	0.59
9:V:45:LYS:NZ	9:V:49:ASP:OD2	2.34	0.59
27:G:101:CDL:H201	27:G:101:CDL:H511	1.85	0.59
1:A:178[B]:GLN:HG3	14:T:7:ASP:OD2	2.03	0.58
3:C:5:THR:CB	6:F:98:HIS:HD2	2.16	0.58
11:K:6:ALA:N	31:K:201:HOH:O	2.35	0.58
3:C:161[A]:GLN:NE2	28:C:305:PEK:H22	2.15	0.58
20:A:608:PGV:H152	20:A:608:PGV:H321	1.85	0.57
4:D:4:SER:N	31:D:302:HOH:O	2.37	0.57
1:N:297[A]:MET:SD	1:N:302:ARG:HG2	2.44	0.57
20:C:306:PGV:H161	27:T:102:CDL:H621	1.85	0.57
1:A:334:TRP:CZ3	21:D:201:TGL:HA52	2.39	0.57
1:N:308:ALA:O	1:N:311[B]:ILE:HG12	2.05	0.57
2:B:52:HIS:HE1	26:B:304:PSC:H212	1.70	0.56
1:A:302[B]:ARG:NE	1:A:361[B]:SER:OG	2.35	0.56
6:S:19:GLU:HG2	31:S:298:HOH:O	2.04	0.56
27:T:102:CDL:H751	27:T:102:CDL:H572	1.85	0.56
22:A:610:EDO:H22	31:A:754:HOH:O	2.05	0.56
20:G:102:PGV:H11	25:P:306:CHD:H152	1.87	0.56
1:N:408:THR:HB	20:Q:201:PGV:H51	1.87	0.56
21:B:301:TGL:HA72	21:B:301:TGL:H142	1.88	0.56
11:K:36:ILE:HA	23:K:103:DMU:H36	1.87	0.56
1:A:282:PHE:HA	14:T:4:ALA:HB3	1.87	0.56
1:A:285:PHE:CD2	14:T:4:ALA:HB2	2.40	0.56
11:X:16:ALA:HA	25:X:101:CHD:H192	1.88	0.56
3:C:85:LEU:HD21	28:C:309:PEK:H281	1.88	0.55
28:C:307:PEK:H101	28:C:307:PEK:H42	1.89	0.55
1:N:297[A]:MET:CG	1:N:302:ARG:HG3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:304:PSC:H061	5:E:8:ASP:OD1	2.07	0.55
23:X:105:DMU:H32	23:X:106:DMU:H30	1.87	0.55
7:G:38:HIS:CE1	27:G:101:CDL:H111	2.42	0.55
23:C:317:DMU:H2	7:G:62:TRP:HB2	1.89	0.55
22:A:613:EDO:H12	31:A:737:HOH:O	2.07	0.54
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.08	0.54
1:N:181[B]:THR:HG23	1:N:185:VAL:HB	1.89	0.54
3:P:37:PHE:CE2	23:P:305:DMU:H13	2.42	0.54
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.89	0.54
2:B:52:HIS:CE1	26:B:304:PSC:H212	2.42	0.54
14:T:31:CYS:SG	27:T:102:CDL:H532	2.47	0.54
2:O:22[A]:HIS:CE1	9:V:44:LYS:HG3	2.43	0.54
12:L:2:HIS:CG	12:L:3:TYR:N	2.71	0.54
1:A:120:ALA:HB2	22:A:623:EDO:H12	1.89	0.54
1:A:272:GLY:N	22:A:621:EDO:H11	2.23	0.54
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.54
20:Q:201:PGV:H042	20:Q:201:PGV:H031	1.90	0.54
1:A:272:GLY:H	22:A:621:EDO:C1	2.21	0.54
2:B:42:ILE:HG21	21:D:201:TGL:H231	1.90	0.53
2:O:42:ILE:HG21	21:Q:202:TGL:H232	1.89	0.53
27:G:101:CDL:H222	27:G:101:CDL:H531	1.91	0.53
2:O:84:LEU:HD12	2:O:87[A]:MET:CE	2.39	0.53
27:T:102:CDL:H252	27:T:102:CDL:H541	1.89	0.53
7:G:31:CYS:SG	27:G:101:CDL:H551	2.48	0.53
27:G:101:CDL:H761	1:N:282:PHE:HZ	1.72	0.53
6:S:94:HIS:ND1	6:S:95:GLN:O	2.41	0.53
23:K:102:DMU:H36	23:K:102:DMU:H29	1.91	0.53
3:P:52:LEU:HD23	27:P:303:CDL:H382	1.91	0.53
4:D:78:TRP:HB3	21:D:201:TGL:CB2	2.27	0.53
1:A:468:MET:HG3	31:A:938:HOH:O	2.08	0.52
27:G:101:CDL:H352	2:O:78:LEU:HD12	1.91	0.52
1:N:297[A]:MET:SD	1:N:302:ARG:CG	2.97	0.52
21:A:609:TGL:HC32	12:L:20:ARG:HH12	1.74	0.52
28:C:305:PEK:H383	27:G:101:CDL:H271	1.90	0.52
3:P:199:VAL:HA	28:P:307:PEK:H42	1.92	0.52
1:A:197:LEU:HD11	28:C:309:PEK:H332	1.90	0.52
20:A:607:PGV:H183	28:C:307:PEK:H322	1.91	0.52
4:D:78:TRP:CA	21:D:201:TGL:HB21	2.39	0.52
1:N:35[B]:LEU:HD21	1:N:462:LEU:HB2	1.92	0.52
27:G:101:CDL:H371	2:O:81:LEU:HD12	1.91	0.52
23:X:107:DMU:O1	23:X:107:DMU:H2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486[B]:ASP:OD2	4:D:19:ARG:HD2	2.10	0.51
1:N:334:TRP:CE3	21:Q:202:TGL:HA31	2.45	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.92	0.51
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.08	0.51
1:A:324[B]:LEU:HD11	1:A:345:ILE:HG21	1.91	0.51
11:K:39:GLU:HB3	31:K:209:HOH:O	2.09	0.51
3:P:95[B]:THR:HG22	28:P:301:PEK:H172	1.93	0.51
5:R:6:GLU:OE2	5:R:14[A]:ARG:NH2	2.37	0.51
2:B:57:ASP:H	26:B:304:PSC:H201	1.76	0.50
1:A:321:PHE:CD1	2:B:65:TRP:HB2	2.45	0.50
1:A:486[B]:ASP:OD2	4:D:17[B]:VAL:HG21	2.10	0.50
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.50
1:N:334:TRP:CD1	21:Q:202:TGL:HC41	2.47	0.50
23:P:314:DMU:H3	14:T:62:TRP:HA	1.93	0.50
11:K:42:PRO:O	11:K:47:ARG:NH2	2.45	0.50
22:N:609:EDO:H21	31:N:795:HOH:O	2.12	0.50
21:A:609:TGL:CC5	12:L:20:ARG:HH22	2.24	0.49
31:B:435:HOH:O	23:I:101:DMU:H29	2.12	0.49
1:N:506:GLU:OE2	3:P:3:HIS:HD2	1.94	0.49
2:B:30:ILE:HG12	23:I:101:DMU:H12	1.93	0.49
1:N:486[B]:ASP:OD2	4:Q:19[B]:ARG:HD2	2.12	0.49
23:P:315:DMU:H22	10:W:38:LEU:HA	1.94	0.49
1:A:194:LEU:CD1	14:T:4:ALA:HB1	2.42	0.49
3:P:33:MET:CE	3:P:42:LEU:H	2.25	0.49
27:G:101:CDL:H471	2:O:70:ALA:HB1	1.94	0.49
1:A:46:THR:HG22	1:A:49[B]:GLY:H	1.78	0.49
28:C:305:PEK:H282	25:O:303:CHD:H11	1.93	0.49
1:N:109:PHE:CE2	21:Y:101:TGL:H312	2.48	0.49
3:P:161[A]:GLN:HE22	28:T:101:PEK:H22	1.78	0.49
28:P:301:PEK:H312	28:P:301:PEK:H11	1.95	0.49
10:J:52:TRP:O	10:J:57:HIS:HE1	1.96	0.48
12:Y:24[B]:MET:HG2	21:Y:101:TGL:HA22	1.95	0.48
3:C:161[A]:GLN:NE2	28:C:305:PEK:H5	2.28	0.48
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.43	0.48
11:X:19:ALA:HB3	25:X:101:CHD:H5	1.95	0.48
23:X:106:DMU:H36	23:X:106:DMU:O55	2.12	0.48
1:A:472:ILE:HG21	21:A:609:TGL:HA91	1.94	0.48
1:N:49[B]:GLY:HA3	13:Z:41:LYS:HE3	1.96	0.48
1:N:510:TYR:HA	22:N:622:EDO:H21	1.94	0.48
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:32:TYR:CZ	22:J:104:EDO:H22	2.48	0.48
3:P:160:LEU:HD13	25:P:304:CHD:H181	1.96	0.48
25:X:101:CHD:H193	25:X:101:CHD:H111	1.51	0.48
27:T:102:CDL:H511	27:T:102:CDL:H181	1.95	0.48
4:Q:5:VAL:H	13:Z:5:PRO:HD2	1.79	0.48
1:A:47:LEU:HD12	22:M:102:EDO:H22	1.96	0.48
23:C:317:DMU:H2	7:G:62:TRP:CB	2.44	0.48
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.43	0.48
1:A:285:PHE:CE2	14:T:4:ALA:HB2	2.48	0.48
1:A:321:PHE:HA	1:A:324[B]:LEU:HD22	1.94	0.48
27:P:303:CDL:OB9	27:P:303:CDL:H541	2.14	0.48
21:Q:202:TGL:H242	21:Q:202:TGL:HA92	1.96	0.48
3:C:246:ASP:HB2	31:C:510:HOH:O	2.13	0.47
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.96	0.47
22:A:625:EDO:H22	6:F:36:PRO:HD3	1.96	0.47
3:C:220:PHE:CE2	27:C:302:CDL:H192	2.50	0.47
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.97	0.47
1:N:113:LEU:CB	21:Y:101:TGL:H301	2.34	0.47
2:B:91:ASN:OD1	2:B:183[A]:THR:HG21	2.14	0.47
1:N:113:LEU:HB2	21:Y:101:TGL:C32	2.44	0.47
27:G:101:CDL:H441	1:N:311[B]:ILE:HG22	1.96	0.47
3:P:246:ASP:HB2	31:P:508:HOH:O	2.14	0.47
3:C:171:VAL:HG22	27:C:302:CDL:H852	1.97	0.47
6:S:22:LEU:HD12	31:S:307:HOH:O	2.14	0.47
23:X:105:DMU:O3	23:X:105:DMU:H29	2.15	0.47
1:A:49[B]:GLY:HA3	13:M:41:LYS:HE3	1.97	0.47
28:P:301:PEK:H312	28:P:301:PEK:C11	2.45	0.47
3:P:172:TYR:CZ	28:T:101:PEK:H191	2.50	0.46
4:Q:87[B]:PHE:HE1	25:X:101:CHD:H231	1.80	0.46
3:C:37:PHE:CG	23:C:308:DMU:H6	2.50	0.46
4:D:115:TRP:CE3	22:D:202:EDO:H11	2.50	0.46
4:Q:101:HIS:HB2	23:X:104:DMU:O49	2.15	0.46
2:B:41[A]:ILE:HD13	26:B:304:PSC:H342	1.96	0.46
2:B:85:TYR:CE1	27:T:102:CDL:OA7	2.69	0.46
3:C:134:THR:HG21	27:G:101:CDL:H611	1.97	0.46
21:O:301:TGL:H111	21:O:301:TGL:HA72	1.98	0.46
2:B:70:ALA:HB1	27:T:102:CDL:H461	1.97	0.46
31:B:515:HOH:O	23:I:101:DMU:H1	2.15	0.46
12:L:26:THR:HG23	13:M:25:SER:CB	2.46	0.46
12:L:43:GLN:HG3	31:L:234:HOH:O	2.15	0.46
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.96	0.46
6:S:1:ALA:HB2	28:T:101:PEK:O13	2.15	0.46
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
3:C:224:LYS:CD	27:C:302:CDL:HB31	2.45	0.46
1:N:486[A]:ASP:OD2	4:Q:17[A]:VAL:HG11	2.16	0.46
26:O:304:PSC:H081	5:R:11:PHE:HB2	1.97	0.46
23:P:305:DMU:H10	10:W:49:CYS:HB3	1.98	0.46
6:S:13:ALA:O	22:S:108:EDO:H11	2.16	0.46
23:K:101:DMU:O6	23:K:101:DMU:O2	2.31	0.46
22:N:624:EDO:H22	22:S:103:EDO:H21	1.97	0.46
21:O:301:TGL:HC71	21:O:301:TGL:H152	1.55	0.46
4:Q:7:LYS:H	4:Q:7:LYS:HG3	1.60	0.46
11:X:19:ALA:CB	25:X:101:CHD:H5	2.46	0.46
1:N:112:LEU:HD23	1:N:112:LEU:C	2.36	0.46
4:Q:78:TRP:N	21:Q:202:TGL:HB22	2.31	0.46
14:T:1:ALA:O	14:T:2:SER:OG	2.32	0.46
1:A:113[B]:LEU:HD13	12:L:39:ILE:HD11	1.98	0.46
1:A:415:ALA:HB1	21:D:201:TGL:H131	1.98	0.46
1:N:24:ALA:HB2	15:N:601[B]:HEA:H253	1.97	0.46
3:P:158:HIS:CE1	6:S:1:ALA:HA	2.50	0.46
1:A:223:ALA:CB	22:A:610:EDO:H21	2.43	0.45
2:B:70:ALA:HB1	27:T:102:CDL:C46	2.47	0.45
28:C:305:PEK:H042	6:F:1:ALA:CB	2.45	0.45
21:A:609:TGL:HC51	12:L:20:ARG:HH22	1.80	0.45
22:A:612:EDO:H12	31:A:804:HOH:O	2.17	0.45
3:C:180[B]:GLU:HG2	31:C:450:HOH:O	2.15	0.45
20:G:102:PGV:H332	20:G:102:PGV:H301	1.74	0.45
27:P:303:CDL:H561	27:P:303:CDL:H532	1.73	0.45
27:T:102:CDL:H521	27:T:102:CDL:H551	1.79	0.45
1:A:366[B]:VAL:CG1	2:B:169:GLY:HA2	2.47	0.45
21:A:609:TGL:HC31	12:L:14:SER:H	1.81	0.45
2:B:82:ARG:HH11	2:B:86:MET:HE3	1.82	0.45
7:G:33:LEU:O	7:G:37:LEU:HB2	2.17	0.45
8:H:23:GLN:HG3	31:H:248:HOH:O	2.16	0.45
28:P:301:PEK:H242	28:P:301:PEK:H272	1.56	0.45
3:C:33:MET:CE	3:C:42:LEU:H	2.27	0.45
3:P:34:TRP:HE1	23:P:314:DMU:H30	1.82	0.45
14:T:37:LEU:HD23	27:T:102:CDL:H361	1.99	0.45
22:A:625:EDO:H11	6:F:32:ASN:OD1	2.16	0.45
22:N:622:EDO:H11	22:S:107:EDO:H22	1.97	0.45
14:T:11:THR:HG23	14:T:16:TRP:NE1	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:K:104:DMU:O61	23:K:104:DMU:H35	2.16	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.45
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.45
6:F:21[B]:MET:HB2	6:F:21[B]:MET:HE2	1.60	0.45
11:K:47:ARG:HG2	11:K:48:VAL:HG23	1.99	0.45
1:N:297[A]:MET:HG2	1:N:302:ARG:HG3	1.98	0.45
1:N:485[A]:VAL:HG22	31:N:881:HOH:O	2.16	0.45
14:T:41:HIS:HB3	14:T:74:ARG:NH1	2.32	0.45
2:B:49:LYS:HE3	21:D:201:TGL:HC71	1.98	0.45
8:H:46:LYS:HG2	31:H:271:HOH:O	2.17	0.45
2:O:57:ASP:N	26:O:304:PSC:H202	2.32	0.45
3:P:37:PHE:CD2	23:P:305:DMU:H13	2.52	0.45
4:Q:119:GLN:O	4:Q:123:MET:HG3	2.17	0.45
14:T:2:SER:HA	14:T:3:ALA:O	2.17	0.45
1:A:71[A]:MET:HB2	1:A:72:PRO:HD3	1.98	0.44
1:N:511:VAL:N	22:N:622:EDO:H21	2.32	0.44
3:P:138:LEU:HD12	27:T:102:CDL:H592	1.98	0.44
8:U:43:MET:O	8:U:48:GLY:HA3	2.16	0.44
1:A:52[A]:GLN:OE1	22:A:613:EDO:H22	2.17	0.44
3:C:213:THR:HG23	27:C:302:CDL:H771	1.99	0.44
10:J:7:GLU:HG3	31:J:227:HOH:O	2.17	0.44
21:Y:101:TGL:HA91	21:Y:101:TGL:H222	1.61	0.44
1:A:194:LEU:HD11	14:T:4:ALA:HB1	1.99	0.44
6:F:87[B]:THR:HG21	31:F:294:HOH:O	2.17	0.44
3:P:161[A]:GLN:NE2	28:T:101:PEK:H5	2.32	0.44
22:S:108:EDO:O2	22:W:101:EDO:H11	2.18	0.44
15:A:601[A]:HEA:H271	15:A:601[A]:HEA:H212	1.55	0.44
23:D:206:DMU:O1	23:D:206:DMU:H2	2.18	0.44
1:N:510:TYR:HD2	22:S:107:EDO:H21	1.82	0.44
21:O:301:TGL:H271	21:O:301:TGL:H222	1.99	0.44
3:P:62:ILE:HD12	27:P:303:CDL:H511	1.98	0.44
3:P:174:THR:HG21	27:P:303:CDL:H851	1.98	0.44
27:T:102:CDL:H782	27:T:102:CDL:H581	1.99	0.44
21:Y:101:TGL:HC22	21:Y:101:TGL:HC52	1.57	0.44
23:C:318:DMU:H35	23:C:318:DMU:H30	1.99	0.44
8:U:37:HIS:HE1	31:U:202:HOH:O	2.00	0.44
4:D:98:TRP:CE2	23:M:101:DMU:H11	2.53	0.44
23:P:314:DMU:H4	23:P:314:DMU:H36	1.72	0.44
23:A:628:DMU:H36	23:A:628:DMU:H2	1.64	0.44
2:O:52:HIS:HE1	26:O:304:PSC:H012	1.82	0.44
3:P:210:ILE:HD13	20:P:302:PGV:H301	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:14[B]:ARG:HG2	31:R:335:HOH:O	2.18	0.44
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.99	0.43
11:K:54:ARG:HE	11:K:54:ARG:HB3	1.55	0.43
1:N:511:VAL:H	22:N:622:EDO:C2	2.30	0.43
14:T:44:ARG:NH1	31:T:201:HOH:O	2.18	0.43
1:A:117[A]:MET:HE1	23:L:105:DMU:H8	2.00	0.43
21:A:609:TGL:HA62	12:L:25:MET:HG2	2.00	0.43
3:C:55:TYR:OH	27:C:302:CDL:HA62	2.18	0.43
28:C:307:PEK:H221	28:C:307:PEK:H251	1.79	0.43
1:N:136[B]:LEU:HD11	31:T:252:HOH:O	2.18	0.43
3:P:156:ARG:HE	25:P:304:CHD:C24	2.31	0.43
31:A:739:HOH:O	12:L:7:PRO:HG3	2.17	0.43
11:K:34:THR:HG22	23:K:102:DMU:H6	2.01	0.43
22:A:619:EDO:H12	2:B:103:GLN:OE1	2.18	0.43
2:B:7:LEU:HD11	21:B:301:TGL:HC81	2.00	0.43
4:D:127:LYS:HD2	31:I:245:HOH:O	2.17	0.43
20:N:607:PGV:H343	20:N:607:PGV:H311	1.85	0.43
26:O:304:PSC:H311	26:O:304:PSC:H282	1.37	0.43
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.43
6:S:28:GLN:HE22	6:S:98:HIS:HA	1.83	0.43
28:C:305:PEK:H331	28:C:305:PEK:H362	1.57	0.43
21:B:301:TGL:H142	21:B:301:TGL:H112	1.86	0.43
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.49	0.43
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.54	0.43
28:C:305:PEK:H222	7:G:21:PHE:CD2	2.53	0.43
6:S:52:ILE:HA	6:S:94:HIS:CD2	2.54	0.43
21:A:609:TGL:HC41	21:A:609:TGL:OC1	2.18	0.43
26:B:304:PSC:H183	23:I:101:DMU:H25	1.99	0.43
28:C:307:PEK:H42	28:C:307:PEK:H72	1.77	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.46	0.43
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.58	0.43
4:Q:78:TRP:HA	21:Q:202:TGL:HB22	1.99	0.43
27:T:102:CDL:H541	27:T:102:CDL:H231	2.01	0.43
21:D:201:TGL:HC32	21:D:201:TGL:HG12	2.00	0.43
28:P:301:PEK:H371	28:P:301:PEK:H192	2.01	0.43
6:S:95:GLN:HB2	6:S:96:LEU:HA	2.00	0.43
2:B:29[B]:MET:HB2	9:I:35:TYR:CE2	2.54	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.42
21:B:301:TGL:H221	21:B:301:TGL:H252	1.80	0.42
4:Q:6:VAL:HG12	4:Q:7:LYS:HG3	2.01	0.42
1:A:439:ARG:O	31:A:702[B]:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:A:609:TGL:HC22	21:A:609:TGL:HC52	1.81	0.42
3:C:180[B]:GLU:HG3	31:C:447:HOH:O	2.17	0.42
1:N:297[A]:MET:SD	1:N:302:ARG:HG3	2.59	0.42
4:Q:98:TRP:HB2	23:X:104:DMU:H18	2.01	0.42
27:T:102:CDL:H511	27:T:102:CDL:H202	2.01	0.42
23:X:103:DMU:H11	23:X:103:DMU:H16	1.86	0.42
1:A:429:HIS:HB3	21:B:301:TGL:HB31	2.01	0.42
2:B:16[B]:ILE:HG23	31:B:519:HOH:O	2.19	0.42
2:B:63:THR:O	2:B:67:ILE:HG12	2.19	0.42
27:T:102:CDL:H581	27:T:102:CDL:C79	2.49	0.42
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	2.01	0.42
31:A:940:HOH:O	21:D:201:TGL:HC31	2.18	0.42
13:M:42:LYS:HD2	13:M:42:LYS:HA	1.87	0.42
1:N:321:PHE:CZ	26:O:304:PSC:H162	2.54	0.42
1:N:363[A]:LEU:HG	2:O:23:PHE:HD1	1.85	0.42
3:P:224:LYS:CD	27:P:303:CDL:HB31	2.45	0.42
22:A:611:EDO:H11	12:L:10:ASN:HD22	1.84	0.42
6:S:10:GLU:OE1	6:S:25:ARG:NH1	2.51	0.42
9:V:20:HIS:CE1	22:V:101:EDO:H12	2.49	0.42
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.01	0.42
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.34	0.42
1:N:208[A]:MET:HG2	1:N:219:PHE:CE1	2.54	0.42
31:N:893:HOH:O	4:Q:20:ARG:HG3	2.19	0.42
14:T:30:LEU:HD21	27:T:102:CDL:H471	2.01	0.42
27:T:102:CDL:H782	27:T:102:CDL:H561	2.02	0.42
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.55	0.42
26:O:304:PSC:H221	26:O:304:PSC:H252	1.54	0.42
4:Q:101:HIS:ND1	23:X:104:DMU:H5	2.35	0.42
2:B:16[A]:ILE:HG21	2:B:87:MET:HG2	2.01	0.42
7:G:84:LYS:N	7:G:84:LYS:HD2	2.35	0.42
2:O:29[B]:MET:HB2	9:V:35:TYR:CE2	2.55	0.42
21:D:201:TGL:H241	21:D:201:TGL:H212	1.76	0.42
25:L:104:CHD:H193	25:L:104:CHD:H111	1.74	0.42
2:O:114:GLU:HG3	2:O:227:LEU:HD21	2.02	0.42
21:A:609:TGL:H231	21:A:609:TGL:HA92	2.02	0.41
6:F:64:GLU:O	6:F:65:ASP:HB2	2.20	0.41
7:G:37:LEU:HD21	27:G:101:CDL:H361	2.01	0.41
27:G:101:CDL:H321	27:G:101:CDL:CA6	2.50	0.41
27:G:101:CDL:H321	27:G:101:CDL:HA62	2.01	0.41
1:A:24:ALA:HB2	15:A:601[B]:HEA:H253	2.02	0.41
21:A:609:TGL:HC62	22:A:627:EDO:H21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:C:305:PEK:H383	27:G:101:CDL:C27	2.50	0.41
1:A:439:ARG:HD3	2:B:199:ILE:HB	2.03	0.41
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.61	0.41
26:B:304:PSC:H042	26:B:304:PSC:H063	1.77	0.41
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.19	0.41
20:Q:201:PGV:H151	20:Q:201:PGV:H12	1.74	0.41
3:C:224:LYS:HD3	27:C:302:CDL:HB31	2.03	0.41
25:C:303:CHD:H162	25:C:303:CHD:H222	1.64	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.02	0.41
3:P:38:ASN:HA	31:P:433:HOH:O	2.20	0.41
6:S:43:LYS:HD3	6:S:88:HIS:CE1	2.55	0.41
1:A:28[A]:MET:CE	15:A:601[A]:HEA:H273	2.50	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.94	0.41
1:A:269:GLY:CA	22:A:621:EDO:H12	2.51	0.41
9:I:68:ILE:HD13	9:I:68:ILE:HG21	1.86	0.41
1:N:105:LEU:HD11	22:N:609:EDO:H12	2.03	0.41
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB2	1.76	0.41
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.50	0.41
28:C:309:PEK:H15	28:C:309:PEK:H181	1.82	0.41
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	2.01	0.41
1:A:131:PRO:HB3	22:A:620:EDO:H12	2.03	0.41
1:A:172:LYS:HD2	1:A:181[A]:THR:CG2	2.51	0.41
1:N:240:HIS:CD2	1:N:240:HIS:C	2.94	0.41
15:N:601[A]:HEA:H212	15:N:601[A]:HEA:H271	1.59	0.41
3:P:34:TRP:HE1	23:P:314:DMU:H29	1.83	0.41
21:A:609:TGL:HC52	21:A:609:TGL:HC82	1.85	0.41
2:B:133[B]:LEU:HD13	4:D:122:ARG:NH1	2.36	0.41
26:B:304:PSC:H292	26:B:304:PSC:H262	1.79	0.41
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.56	0.41
28:C:305:PEK:H041	7:G:17:ARG:NH1	2.16	0.41
27:G:101:CDL:H362	27:G:101:CDL:H122	2.03	0.41
8:H:31:GLN:NE2	31:H:201:HOH:O	2.41	0.41
10:W:44:LEU:HD23	10:W:44:LEU:HA	1.88	0.41
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.91	0.41
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.56	0.41
5:E:6:GLU:OE2	5:E:14:ARG:NH2	2.52	0.41
1:N:260:TYR:OH	1:N:485[A]:VAL:HG22	2.21	0.41
21:Q:202:TGL:HG2	21:Q:202:TGL:H151	2.02	0.41
22:Q:203:EDO:H22	22:S:104:EDO:H11	2.03	0.41
28:C:307:PEK:H161	28:C:307:PEK:H132	1.65	0.40
1:N:53[B]:ILE:O	1:N:57:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:610:EDO:H22	12:Y:10:ASN:HD22	1.86	0.40
25:X:101:CHD:H222	25:X:101:CHD:H162	1.49	0.40
12:Y:26:THR:HG23	13:Z:25:SER:HB2	2.03	0.40
6:F:92:VAL:HG23	6:F:92:VAL:O	2.22	0.40
15:N:602:HEA:H243	2:O:69:PRO:HB3	2.02	0.40
2:O:56:MET:CG	26:O:304:PSC:H211	2.51	0.40
14:T:30:LEU:HD21	27:T:102:CDL:C47	2.51	0.40
25:X:101:CHD:H191	25:X:101:CHD:H8	1.82	0.40
22:A:617:EDO:H22	6:F:66:ASN:ND2	2.36	0.40
25:C:303:CHD:H112	25:C:303:CHD:H12A	1.85	0.40
3:P:52:LEU:CD2	27:P:303:CDL:H382	2.52	0.40
13:Z:39:ASN:OD1	13:Z:39:ASN:N	2.55	0.40
1:A:361[A]:SER:OG	2:B:84:LEU:HD13	2.21	0.40
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.56	0.40
3:C:95[B]:THR:HG22	28:C:309:PEK:H172	2.03	0.40
21:O:301:TGL:HA42	21:O:301:TGL:HA71	1.90	0.40
20:Q:201:PGV:H162	20:Q:201:PGV:H312	2.02	0.40
5:R:79:LYS:HD2	5:R:79:LYS:HA	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/514 (107%)	537 (97%)	15 (3%)	0	100	100
1	N	550/514 (107%)	534 (97%)	16 (3%)	0	100	100
2	B	236/227 (104%)	231 (98%)	5 (2%)	0	100	100
2	O	233/227 (103%)	226 (97%)	7 (3%)	0	100	100
3	C	267/261 (102%)	262 (98%)	5 (2%)	0	100	100
3	P	267/261 (102%)	262 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	146/147 (99%)	143 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	139 (96%)	5 (3%)	1 (1%)	22	6
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	104/109 (95%)	104 (100%)	0	0	100	100
6	F	100/98 (102%)	96 (96%)	3 (3%)	1 (1%)	15	3
6	S	98/98 (100%)	92 (94%)	2 (2%)	4 (4%)	3	0
7	G	83/85 (98%)	70 (84%)	9 (11%)	4 (5%)	2	0
8	H	77/85 (91%)	71 (92%)	6 (8%)	0	100	100
8	U	77/85 (91%)	72 (94%)	3 (4%)	2 (3%)	5	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	1 (1%)	1 (1%)	11	1
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
11	X	49/56 (88%)	48 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	48/47 (102%)	46 (96%)	1 (2%)	1 (2%)	7	1
13	M	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
14	T	84/85 (99%)	71 (84%)	7 (8%)	6 (7%)	1	0
All	All	3649/3614 (101%)	3529 (97%)	100 (3%)	20 (0%)	25	9

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
6	S	94	HIS
14	T	5	LYS
14	T	8	HIS
8	U	8	ILE
8	U	49	ASP
6	F	97	ALA
14	T	4	ALA
14	T	39	SER
7	G	5	LYS

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Mol	Chain	Res	Type
7	G	37	LEU
6	S	2	SER
6	S	97	ALA
9	V	2	THR
12	Y	46	LYS
7	G	3	ALA
6	S	95	GLN
14	T	3	ALA
14	T	7	ASP
4	Q	5	VAL

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	465/426 (109%)	461 (99%)	4 (1%)	78	61
1	N	463/426 (109%)	454 (98%)	9 (2%)	57	27
2	B	221/210 (105%)	216 (98%)	5 (2%)	50	20
2	O	218/210 (104%)	211 (97%)	7 (3%)	39	10
3	C	234/226 (104%)	232 (99%)	2 (1%)	78	61
3	P	234/226 (104%)	230 (98%)	4 (2%)	60	33
4	D	132/129 (102%)	129 (98%)	3 (2%)	50	20
4	Q	131/129 (102%)	125 (95%)	6 (5%)	27	5
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	22
5	R	93/95 (98%)	93 (100%)	0	100	100
6	F	85/81 (105%)	80 (94%)	5 (6%)	19	2
6	S	83/81 (102%)	81 (98%)	2 (2%)	49	19
7	G	69/68 (102%)	63 (91%)	6 (9%)	10	0
8	H	71/75 (95%)	66 (93%)	5 (7%)	15	1
8	U	71/75 (95%)	69 (97%)	2 (3%)	43	14
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	54 (95%)	3 (5%)	22	3
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	50/50 (100%)	49 (98%)	1 (2%)	55	25
11	K	41/46 (89%)	40 (98%)	1 (2%)	49	19
11	X	41/46 (89%)	40 (98%)	1 (2%)	49	19
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	16
12	Y	43/40 (108%)	42 (98%)	1 (2%)	50	20
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	3
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	1
14	T	70/69 (101%)	62 (89%)	8 (11%)	5	0
All	All	3183/3083 (103%)	3098 (97%)	85 (3%)	46	15

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	369	ASP
2	B	33	LEU
2	B	60	GLU
2	B	78	LEU
2	B	91	ASN
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
4	D	31[A]	LYS
4	D	31[B]	LYS
4	D	58	GLU
5	E	5	HIS
5	E	90	ARG
6	F	2	SER
6	F	37	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	96	LEU
7	G	2	SER
7	G	18	PHE

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Mol	Chain	Res	Type
7	G	33	LEU
7	G	38	HIS
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	10	ASN
8	H	51	SER
8	H	60	TYR
9	I	36	LYS
9	I	37	PHE
11	K	54	ARG
12	L	47	LYS
13	M	38	ASP
13	M	39	ASN
1	N	38	ARG
1	N	109	PHE
1	N	297[A]	MET
1	N	297[B]	MET
1	N	369	ASP
1	N	485[A]	VAL
1	N	485[B]	VAL
1	N	486[A]	ASP
1	N	486[B]	ASP
2	O	33	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	171	LYS
3	P	3	HIS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	7	LYS
4	Q	8	SER
4	Q	9	GLU
4	Q	51	LEU
4	Q	74	SER
6	S	43	LYS

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Mol	Chain	Res	Type
6	S	98	HIS
14	T	7	ASP
14	T	11	THR
14	T	18	PHE
14	T	37	LEU
14	T	38	HIS
14	T	43	GLU
14	T	54	ARG
14	T	84	LYS
8	U	60	TYR
8	U	84	LYS
9	V	2	THR
9	V	36	LYS
9	V	37	PHE
10	W	50	LEU
11	X	47	ARG
12	Y	2	HIS
13	Z	13	LYS
13	Z	38	ASP
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	52	HIS
6	F	98	HIS
10	J	57	HIS
12	L	2	HIS
1	N	178	GLN
3	P	3	HIS
4	Q	109	HIS
14	T	8	HIS
14	T	34	ASN
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	1.36	2 (25%)	7,9,11	1.60	2 (28%)
9	SAC	I	1	9	7,8,9	0.60	0	8,9,11	0.86	0
9	SAC	V	1	9	7,8,9	0.60	0	8,9,11	0.90	1 (12%)
1	FME	N	1	1	8,9,10	0.52	0	7,9,11	1.11	0
2	FME	O	1	2	8,9,10	0.89	0	7,9,11	1.26	2 (28%)
1	FME	A	1	1	8,9,10	0.53	0	7,9,11	1.30	1 (14%)
7	TPO	G	11	7	8,10,11	1.34	1 (12%)	10,14,16	0.67	0

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.74	1.59	1.50
2	B	1	FME	CG-SD	-2.38	1.68	1.81
2	B	1	FME	CB-CG	2.33	1.60	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-2.62	105.66	112.95
2	B	1	FME	O-C-CA	-2.57	118.04	124.78
2	O	1	FME	CG-CB-CA	-2.37	106.37	112.95
1	A	1	FME	O1-CN-N	-2.24	119.36	125.27
9	V	1	SAC	O-C-CA	-2.13	119.19	124.78
2	O	1	FME	O-C-CA	-2.13	119.20	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 182 ligands modelled in this entry, 8 are monoatomic - leaving 174 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
22	EDO	P	308	-	3,3,3	0.42	0	2,2,2	0.30	0
23	DMU	L	105	-	34,34,34	0.48	1 (2%)	45,45,45	1.04	1 (2%)
23	DMU	K	104	-	34,34,34	0.53	0	45,45,45	1.19	4 (8%)
23	DMU	D	206	-	34,34,34	0.53	0	45,45,45	1.40	7 (15%)
22	EDO	N	610	-	3,3,3	0.40	0	2,2,2	0.48	0
22	EDO	A	617	-	3,3,3	0.67	0	2,2,2	0.10	0
22	EDO	A	627	-	3,3,3	0.44	0	2,2,2	0.70	0
21	TGL	O	301	-	59,59,62	1.04	3 (5%)	62,62,65	1.02	5 (8%)
28	PEK	C	305	-	52,52,52	1.01	2 (3%)	55,57,57	1.38	8 (14%)
22	EDO	N	621	-	3,3,3	0.70	0	2,2,2	0.25	0
21	TGL	D	201	-	61,61,62	1.20	6 (9%)	64,64,65	1.18	6 (9%)
22	EDO	S	109	-	3,3,3	0.92	0	2,2,2	0.57	0
23	DMU	I	101	-	34,34,34	0.49	0	45,45,45	1.05	3 (6%)
26	PSC	O	304	-	50,50,51	1.15	3 (6%)	56,58,59	1.51	9 (16%)
22	EDO	D	202	-	3,3,3	0.33	0	2,2,2	0.53	0
15	HEA	A	601[B]	-	57,67,67	1.69	12 (21%)	61,103,103	2.16	21 (34%)
22	EDO	C	312	-	3,3,3	0.59	0	2,2,2	0.38	0
22	EDO	P	312	-	3,3,3	0.40	0	2,2,2	0.53	0
22	EDO	O	305	-	3,3,3	0.48	0	2,2,2	0.24	0
22	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.93	0
22	EDO	Y	103	-	3,3,3	0.45	0	2,2,2	0.37	0
23	DMU	K	101	-	34,34,34	0.59	1 (2%)	45,45,45	1.54	10 (22%)
22	EDO	V	101	-	3,3,3	0.50	0	2,2,2	0.22	0
25	CHD	L	104	-	32,32,32	0.67	0	51,51,51	2.25	15 (29%)
15	HEA	A	601[A]	-	57,67,67	1.66	12 (21%)	61,103,103	1.99	20 (32%)
19	PER	A	606	15,16	0,1,1	-	-	-	-	-
22	EDO	O	306	-	3,3,3	0.76	0	2,2,2	0.89	0
22	EDO	A	618	-	3,3,3	1.14	0	2,2,2	0.74	0
25	CHD	P	304	-	32,32,32	0.83	1 (3%)	51,51,51	1.34	8 (15%)
30	PO4	U	101	-	4,4,4	1.08	0	6,6,6	0.37	0
22	EDO	J	101	-	3,3,3	0.56	0	2,2,2	0.09	0
23	DMU	P	314	-	34,34,34	0.57	0	45,45,45	1.39	8 (17%)
22	EDO	N	619	-	3,3,3	0.74	0	2,2,2	0.36	0
15	HEA	A	602	1,19	57,67,67	1.65	11 (19%)	61,103,103	1.92	18 (29%)
20	PGV	C	301	-	50,50,50	0.90	4 (8%)	53,56,56	0.99	4 (7%)
22	EDO	F	105	-	3,3,3	0.79	0	2,2,2	0.44	0
22	EDO	A	622	-	3,3,3	0.56	0	2,2,2	0.40	0
22	EDO	T	106	-	3,3,3	0.49	0	2,2,2	0.36	0
24	CUA	O	302	2	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	DMU	M	101	-	34,34,34	0.58	0	45,45,45	1.18	3 (6%)
22	EDO	M	102	-	3,3,3	0.46	0	2,2,2	0.13	0
22	EDO	S	103	-	3,3,3	0.34	0	2,2,2	0.56	0
22	EDO	S	107	-	3,3,3	0.47	0	2,2,2	0.31	0
22	EDO	F	103	-	3,3,3	0.60	0	2,2,2	0.65	0
22	EDO	C	310	-	3,3,3	0.94	0	2,2,2	0.09	0
22	EDO	P	310	-	3,3,3	0.78	0	2,2,2	0.31	0
22	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.49	0
23	DMU	X	103	-	34,34,34	0.56	0	45,45,45	1.35	5 (11%)
23	DMU	X	107	-	34,34,34	0.64	1 (2%)	45,45,45	1.29	7 (15%)
28	PEK	C	309	-	52,52,52	1.00	2 (3%)	55,57,57	1.11	4 (7%)
22	EDO	A	619	-	3,3,3	0.57	0	2,2,2	0.50	0
22	EDO	N	614	-	3,3,3	1.23	0	2,2,2	0.24	0
23	DMU	A	628	-	34,34,34	0.59	0	45,45,45	1.12	5 (11%)
28	PEK	P	307	-	52,52,52	0.67	1 (1%)	55,57,57	1.25	4 (7%)
23	DMU	K	105	-	34,34,34	0.53	0	45,45,45	1.19	5 (11%)
22	EDO	N	615	-	3,3,3	0.69	0	2,2,2	0.13	0
22	EDO	A	623	-	3,3,3	0.90	0	2,2,2	0.38	0
22	EDO	C	311	-	3,3,3	0.51	0	2,2,2	0.35	0
22	EDO	P	311	-	3,3,3	0.54	0	2,2,2	0.49	0
20	PGV	Q	201	-	50,50,50	0.96	2 (4%)	53,56,56	1.26	4 (7%)
23	DMU	K	103	-	33,33,34	0.54	0	41,43,45	1.10	3 (7%)
28	PEK	C	307	-	51,51,52	0.76	1 (1%)	54,56,57	1.05	3 (5%)
22	EDO	G	103	-	3,3,3	0.53	0	2,2,2	0.11	0
21	TGL	Y	101	-	62,62,62	1.09	3 (4%)	65,65,65	1.25	6 (9%)
22	EDO	D	204	-	3,3,3	0.68	0	2,2,2	0.32	0
22	EDO	N	623	-	3,3,3	0.49	0	2,2,2	0.19	0
22	EDO	J	104	-	3,3,3	0.49	0	2,2,2	0.49	0
22	EDO	S	108	-	3,3,3	0.59	0	2,2,2	0.03	0
23	DMU	P	315	-	34,34,34	0.49	0	45,45,45	1.11	2 (4%)
27	CDL	G	101	-	99,99,99	1.32	12 (12%)	105,111,111	1.34	11 (10%)
22	EDO	N	609	-	3,3,3	1.14	0	2,2,2	0.96	0
15	HEA	N	601[B]	-	57,67,67	1.69	14 (24%)	61,103,103	2.00	18 (29%)
21	TGL	A	609	-	62,62,62	1.10	3 (4%)	65,65,65	1.43	10 (15%)
22	EDO	J	103	-	3,3,3	0.48	0	2,2,2	0.29	0
15	HEA	N	602	1,19	57,67,67	1.53	12 (21%)	61,103,103	2.01	18 (29%)
28	PEK	P	301	-	52,52,52	0.96	2 (3%)	55,57,57	1.21	4 (7%)
23	DMU	K	102	-	34,34,34	0.60	1 (2%)	45,45,45	0.97	3 (6%)
22	EDO	R	201	-	3,3,3	0.52	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	P	309	-	3,3,3	0.39	0	2,2,2	0.75	0
22	EDO	T	104	-	3,3,3	0.86	0	2,2,2	0.56	0
22	EDO	A	615	-	3,3,3	0.62	0	2,2,2	0.02	0
22	EDO	A	626	-	3,3,3	0.37	0	2,2,2	0.79	0
15	HEA	N	601[A]	-	57,67,67	1.70	14 (24%)	61,103,103	2.01	19 (31%)
22	EDO	Z	102	-	3,3,3	0.50	0	2,2,2	0.37	0
22	EDO	A	620	-	3,3,3	0.42	0	2,2,2	0.34	0
22	EDO	N	620	-	3,3,3	0.44	0	2,2,2	0.27	0
25	CHD	O	303	-	32,32,32	0.93	1 (3%)	51,51,51	1.37	8 (15%)
22	EDO	B	308	-	3,3,3	0.64	0	2,2,2	0.46	0
22	EDO	N	624	-	3,3,3	0.45	0	2,2,2	0.29	0
22	EDO	E	201	-	3,3,3	0.51	0	2,2,2	0.51	0
22	EDO	E	203	-	3,3,3	0.71	0	2,2,2	0.37	0
24	CUA	B	302	2	0,1,1	-	-	-	-	-
25	CHD	C	304	-	32,32,32	1.20	2 (6%)	51,51,51	1.60	11 (21%)
23	DMU	C	308	-	34,34,34	0.57	0	45,45,45	0.90	2 (4%)
22	EDO	A	610	-	3,3,3	0.22	0	2,2,2	0.27	0
22	EDO	Q	204	-	3,3,3	0.78	0	2,2,2	0.56	0
22	EDO	A	625	-	3,3,3	0.44	0	2,2,2	0.21	0
22	EDO	B	306	-	3,3,3	0.96	0	2,2,2	0.24	0
22	EDO	F	106	-	3,3,3	0.52	0	2,2,2	0.21	0
22	EDO	N	612	-	3,3,3	0.59	0	2,2,2	0.46	0
22	EDO	P	313	-	3,3,3	0.59	0	2,2,2	0.33	0
22	EDO	G	104	-	3,3,3	0.68	0	2,2,2	0.63	0
22	EDO	N	608	-	3,3,3	0.47	0	2,2,2	0.34	0
25	CHD	B	303	-	32,32,32	1.09	2 (6%)	51,51,51	1.48	10 (19%)
22	EDO	B	305	-	3,3,3	0.33	0	2,2,2	0.51	0
22	EDO	S	105	-	3,3,3	0.68	0	2,2,2	0.77	0
19	PER	N	606	15,16	0,1,1	-	-	-	-	-
22	EDO	C	313	-	3,3,3	0.64	0	2,2,2	0.17	0
22	EDO	A	612	-	3,3,3	0.91	0	2,2,2	0.66	0
20	PGV	A	607	-	50,50,50	0.94	2 (4%)	53,56,56	0.96	3 (5%)
22	EDO	W	101	-	3,3,3	0.48	0	2,2,2	0.13	0
22	EDO	A	624	-	3,3,3	1.01	0	2,2,2	0.90	0
22	EDO	F	107	-	3,3,3	0.70	0	2,2,2	1.39	0
28	PEK	T	101	-	49,49,52	1.01	2 (4%)	53,54,57	1.31	6 (11%)
23	DMU	C	318	-	34,34,34	0.64	1 (2%)	45,45,45	1.28	5 (11%)
20	PGV	N	607	-	50,50,50	1.15	5 (10%)	53,56,56	1.22	3 (5%)
22	EDO	C	314	-	3,3,3	0.52	0	2,2,2	0.47	0
22	EDO	N	617	-	3,3,3	0.38	0	2,2,2	0.36	0
22	EDO	S	102	-	3,3,3	0.59	0	2,2,2	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	A	613	-	3,3,3	0.52	0	2,2,2	0.13	0
23	DMU	X	102	-	34,34,34	0.60	1 (2%)	45,45,45	1.24	5 (11%)
22	EDO	G	105	-	3,3,3	0.48	0	2,2,2	0.34	0
21	TGL	Q	202	-	62,62,62	1.09	4 (6%)	65,65,65	0.89	3 (4%)
23	DMU	O	307	-	34,34,34	0.53	0	45,45,45	1.18	6 (13%)
20	PGV	A	608	-	50,50,50	1.05	4 (8%)	53,56,56	1.19	4 (7%)
22	EDO	D	203	-	3,3,3	0.78	0	2,2,2	0.28	0
22	EDO	H	101	-	3,3,3	0.38	0	2,2,2	0.23	0
22	EDO	T	105	-	3,3,3	0.52	0	2,2,2	0.25	0
22	EDO	Q	203	-	3,3,3	0.64	0	2,2,2	0.70	0
22	EDO	N	622	-	3,3,3	0.78	0	2,2,2	0.29	0
23	DMU	X	104	-	34,34,34	0.53	0	45,45,45	1.16	5 (11%)
22	EDO	J	105	-	3,3,3	0.56	0	2,2,2	0.28	0
23	DMU	P	305	-	34,34,34	0.60	1 (2%)	45,45,45	0.83	0
22	EDO	Y	102	-	3,3,3	0.48	0	2,2,2	0.51	0
25	CHD	Y	104	-	32,32,32	0.71	0	51,51,51	2.24	16 (31%)
22	EDO	T	103	-	3,3,3	0.46	0	2,2,2	0.28	0
22	EDO	A	611	-	3,3,3	0.81	0	2,2,2	0.67	0
22	EDO	A	621	-	3,3,3	0.35	0	2,2,2	0.42	0
22	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.55	0
23	DMU	Z	101	-	34,34,34	0.53	1 (2%)	45,45,45	0.84	1 (2%)
22	EDO	F	102	-	3,3,3	0.90	0	2,2,2	0.33	0
27	CDL	T	102	-	97,97,99	1.33	12 (12%)	103,109,111	1.32	8 (7%)
25	CHD	X	101	-	32,32,32	0.85	1 (3%)	51,51,51	2.16	19 (37%)
20	PGV	C	306	-	47,47,50	1.03	2 (4%)	50,53,56	1.57	7 (14%)
22	EDO	N	613	-	3,3,3	0.52	0	2,2,2	0.88	0
22	EDO	J	102	-	3,3,3	0.38	0	2,2,2	0.16	0
22	EDO	A	616	-	3,3,3	0.81	0	2,2,2	0.33	0
22	EDO	L	103	-	3,3,3	0.42	0	2,2,2	0.36	0
22	EDO	N	611	-	3,3,3	0.42	0	2,2,2	0.57	0
22	EDO	C	315	-	3,3,3	1.16	0	2,2,2	0.57	0
22	EDO	M	103	-	3,3,3	0.33	0	2,2,2	0.99	0
22	EDO	F	104	-	3,3,3	0.43	0	2,2,2	0.33	0
20	PGV	P	302	-	50,50,50	0.79	2 (4%)	53,56,56	0.99	2 (3%)
22	EDO	S	106	-	3,3,3	0.70	0	2,2,2	0.08	0
22	EDO	B	309	-	3,3,3	0.58	0	2,2,2	0.19	0
30	PO4	H	102	-	4,4,4	0.96	0	6,6,6	0.51	0
25	CHD	C	303	-	32,32,32	0.86	1 (3%)	51,51,51	1.64	11 (21%)
23	DMU	X	106	-	34,34,34	0.60	0	45,45,45	1.81	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	CDL	C	302	-	86,86,99	1.52	14 (16%)	90,94,111	1.56	13 (14%)
22	EDO	L	102	-	3,3,3	0.40	0	2,2,2	0.80	0
22	EDO	S	104	-	3,3,3	0.61	0	2,2,2	0.69	0
21	TGL	B	301	-	61,61,62	1.06	3 (4%)	64,64,65	1.10	3 (4%)
22	EDO	L	101	-	3,3,3	0.83	0	2,2,2	0.53	0
22	EDO	D	205	-	3,3,3	0.69	0	2,2,2	0.26	0
20	PGV	G	102	-	50,50,50	0.97	2 (4%)	53,56,56	1.15	5 (9%)
22	EDO	B	307	-	3,3,3	0.81	0	2,2,2	0.40	0
23	DMU	C	317	-	34,34,34	0.49	0	45,45,45	1.41	8 (17%)
27	CDL	P	303	-	88,88,99	1.38	11 (12%)	95,98,111	1.59	13 (13%)
23	DMU	K	106	-	34,34,34	0.59	0	45,45,45	1.10	3 (6%)
25	CHD	P	306	-	32,32,32	0.97	1 (3%)	51,51,51	1.40	8 (15%)
22	EDO	E	202	-	3,3,3	0.37	0	2,2,2	0.49	0
23	DMU	X	105	-	34,34,34	0.66	1 (2%)	45,45,45	1.32	7 (15%)
23	DMU	C	316	-	34,34,34	0.60	1 (2%)	45,45,45	1.20	4 (8%)
26	PSC	B	304	-	51,51,51	1.09	3 (5%)	57,59,59	1.36	6 (10%)

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
22	EDO	P	308	-	-	0/1/1/1	-
23	DMU	L	105	-	-	11/19/59/59	0/2/2/2
23	DMU	K	104	-	-	10/19/59/59	0/2/2/2
23	DMU	D	206	-	-	9/19/59/59	0/2/2/2
22	EDO	N	610	-	-	1/1/1/1	-
22	EDO	A	617	-	-	1/1/1/1	-
22	EDO	A	627	-	-	1/1/1/1	-
21	TGL	O	301	-	-	24/62/62/65	-
28	PEK	C	305	-	-	27/56/56/56	-
22	EDO	N	621	-	-	1/1/1/1	-
21	TGL	D	201	-	-	26/64/64/65	-
22	EDO	S	109	-	-	0/1/1/1	-
23	DMU	I	101	-	-	9/19/59/59	0/2/2/2
26	PSC	O	304	-	-	29/54/54/55	-
22	EDO	D	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEA	A	601[B]	-	3/3/7/16	6/32/76/76	-
22	EDO	C	312	-	-	0/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
22	EDO	O	305	-	-	0/1/1/1	-
22	EDO	N	618	-	-	1/1/1/1	-
22	EDO	Y	103	-	-	0/1/1/1	-
23	DMU	K	101	-	-	7/19/59/59	0/2/2/2
22	EDO	V	101	-	-	0/1/1/1	-
25	CHD	L	104	-	-	5/9/74/74	1/4/4/4
15	HEA	A	601[A]	-	3/3/7/16	8/32/76/76	-
22	EDO	O	306	-	-	0/1/1/1	-
22	EDO	A	618	-	-	0/1/1/1	-
25	CHD	P	304	-	-	7/9/74/74	0/4/4/4
22	EDO	J	101	-	-	1/1/1/1	-
23	DMU	P	314	-	-	5/19/59/59	0/2/2/2
22	EDO	N	619	-	-	0/1/1/1	-
15	HEA	A	602	1,19	3/3/7/16	4/32/76/76	-
20	PGV	C	301	-	-	9/55/55/55	-
22	EDO	F	105	-	-	0/1/1/1	-
22	EDO	A	622	-	-	0/1/1/1	-
22	EDO	T	106	-	-	0/1/1/1	-
23	DMU	M	101	-	-	4/19/59/59	0/2/2/2
22	EDO	M	102	-	-	0/1/1/1	-
22	EDO	S	103	-	-	1/1/1/1	-
22	EDO	S	107	-	-	1/1/1/1	-
22	EDO	F	103	-	-	0/1/1/1	-
22	EDO	C	310	-	-	0/1/1/1	-
22	EDO	P	310	-	-	0/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
23	DMU	X	103	-	-	9/19/59/59	0/2/2/2
23	DMU	X	107	-	-	9/19/59/59	0/2/2/2
28	PEK	C	309	-	-	17/56/56/56	-
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
23	DMU	A	628	-	-	4/19/59/59	0/2/2/2
28	PEK	P	307	-	-	11/56/56/56	-
23	DMU	K	105	-	-	9/19/59/59	0/2/2/2
22	EDO	N	615	-	-	1/1/1/1	-
22	EDO	A	623	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	C	311	-	-	0/1/1/1	-
22	EDO	P	311	-	-	0/1/1/1	-
20	PGV	Q	201	-	-	11/55/55/55	-
23	DMU	K	103	-	-	10/19/55/59	0/2/2/2
28	PEK	C	307	-	-	14/55/55/56	-
22	EDO	G	103	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	35/65/65/65	-
22	EDO	D	204	-	-	0/1/1/1	-
22	EDO	N	623	-	-	1/1/1/1	-
22	EDO	J	104	-	-	1/1/1/1	-
22	EDO	S	108	-	-	0/1/1/1	-
23	DMU	P	315	-	-	1/19/59/59	0/2/2/2
27	CDL	G	101	-	-	37/110/110/110	-
22	EDO	N	609	-	-	1/1/1/1	-
15	HEA	N	601[B]	-	3/3/7/16	2/32/76/76	-
21	TGL	A	609	-	-	30/65/65/65	-
22	EDO	J	103	-	-	0/1/1/1	-
15	HEA	N	602	1,19	3/3/7/16	4/32/76/76	-
28	PEK	P	301	-	-	22/56/56/56	-
23	DMU	K	102	-	-	6/19/59/59	0/2/2/2
22	EDO	R	201	-	-	0/1/1/1	-
22	EDO	P	309	-	-	1/1/1/1	-
22	EDO	T	104	-	-	0/1/1/1	-
22	EDO	A	615	-	-	0/1/1/1	-
22	EDO	A	626	-	-	1/1/1/1	-
15	HEA	N	601[A]	-	3/3/7/16	6/32/76/76	-
22	EDO	Z	102	-	-	1/1/1/1	-
22	EDO	A	620	-	-	0/1/1/1	-
22	EDO	N	620	-	-	1/1/1/1	-
25	CHD	O	303	-	-	2/9/74/74	0/4/4/4
22	EDO	B	308	-	-	0/1/1/1	-
22	EDO	N	624	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	E	203	-	-	0/1/1/1	-
25	CHD	C	304	-	-	2/9/74/74	0/4/4/4
23	DMU	C	308	-	-	7/19/59/59	0/2/2/2
22	EDO	A	610	-	-	1/1/1/1	-
22	EDO	Q	204	-	-	0/1/1/1	-
22	EDO	A	625	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	B	306	-	-	0/1/1/1	-
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	N	612	-	-	0/1/1/1	-
22	EDO	P	313	-	-	0/1/1/1	-
22	EDO	G	104	-	-	0/1/1/1	-
22	EDO	N	608	-	-	1/1/1/1	-
25	CHD	B	303	-	-	2/9/74/74	0/4/4/4
22	EDO	B	305	-	-	0/1/1/1	-
22	EDO	S	105	-	-	0/1/1/1	-
22	EDO	C	313	-	-	1/1/1/1	-
22	EDO	A	612	-	-	0/1/1/1	-
20	PGV	A	607	-	-	5/55/55/55	-
22	EDO	W	101	-	-	0/1/1/1	-
22	EDO	A	624	-	-	0/1/1/1	-
22	EDO	F	107	-	-	0/1/1/1	-
28	PEK	T	101	-	-	24/51/51/56	-
23	DMU	C	318	-	-	9/19/59/59	0/2/2/2
20	PGV	N	607	-	-	7/55/55/55	-
22	EDO	C	314	-	-	0/1/1/1	-
22	EDO	N	617	-	-	1/1/1/1	-
22	EDO	S	102	-	-	0/1/1/1	-
22	EDO	A	613	-	-	1/1/1/1	-
23	DMU	X	102	-	-	8/19/59/59	0/2/2/2
22	EDO	G	105	-	-	0/1/1/1	-
21	TGL	Q	202	-	-	21/65/65/65	-
23	DMU	O	307	-	-	5/19/59/59	0/2/2/2
20	PGV	A	608	-	-	14/55/55/55	-
22	EDO	D	203	-	-	0/1/1/1	-
22	EDO	H	101	-	-	0/1/1/1	-
22	EDO	T	105	-	-	0/1/1/1	-
22	EDO	Q	203	-	-	0/1/1/1	-
22	EDO	N	622	-	-	0/1/1/1	-
23	DMU	X	104	-	-	6/19/59/59	0/2/2/2
22	EDO	J	105	-	-	0/1/1/1	-
23	DMU	P	305	-	-	5/19/59/59	0/2/2/2
22	EDO	Y	102	-	-	1/1/1/1	-
25	CHD	Y	104	-	-	4/9/74/74	0/4/4/4
22	EDO	T	103	-	-	0/1/1/1	-
22	EDO	A	611	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	621	-	-	0/1/1/1	-
22	EDO	A	614	-	-	0/1/1/1	-
23	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
22	EDO	F	102	-	-	0/1/1/1	-
27	CDL	T	102	-	-	34/108/108/110	-
25	CHD	X	101	-	-	8/9/74/74	0/4/4/4
20	PGV	C	306	-	-	9/52/52/55	-
22	EDO	N	613	-	-	0/1/1/1	-
22	EDO	J	102	-	-	1/1/1/1	-
22	EDO	A	616	-	-	0/1/1/1	-
22	EDO	L	103	-	-	0/1/1/1	-
22	EDO	N	611	-	-	1/1/1/1	-
22	EDO	C	315	-	-	0/1/1/1	-
22	EDO	M	103	-	-	1/1/1/1	-
22	EDO	F	104	-	-	1/1/1/1	-
20	PGV	P	302	-	-	9/55/55/55	-
22	EDO	S	106	-	-	0/1/1/1	-
22	EDO	B	309	-	-	0/1/1/1	-
25	CHD	C	303	-	-	7/9/74/74	0/4/4/4
23	DMU	X	106	-	-	7/19/59/59	0/2/2/2
27	CDL	C	302	-	-	24/89/89/110	-
22	EDO	L	102	-	-	0/1/1/1	-
22	EDO	S	104	-	-	0/1/1/1	-
21	TGL	B	301	-	-	26/64/64/65	-
22	EDO	L	101	-	-	1/1/1/1	-
22	EDO	D	205	-	-	0/1/1/1	-
20	PGV	G	102	-	-	15/55/55/55	-
22	EDO	B	307	-	-	0/1/1/1	-
23	DMU	C	317	-	-	3/19/59/59	0/2/2/2
27	CDL	P	303	-	-	30/94/94/110	-
23	DMU	K	106	-	-	13/19/59/59	0/2/2/2
25	CHD	P	306	-	-	2/9/74/74	0/4/4/4
22	EDO	E	202	-	-	1/1/1/1	-
23	DMU	X	105	-	-	10/19/59/59	0/2/2/2
23	DMU	C	316	-	-	6/19/59/59	0/2/2/2
26	PSC	B	304	-	-	18/55/55/55	-

All (204) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	C	302	CDL	OA6-CA5	5.77	1.46	1.33
21	A	609	TGL	OG3-CC1	5.06	1.48	1.33
21	Y	101	TGL	OG3-CC1	4.86	1.47	1.33
26	O	304	PSC	O01-C1	4.80	1.47	1.34
28	C	305	PEK	O03-C21	4.76	1.47	1.33
21	Q	202	TGL	OG2-CB1	4.71	1.47	1.34
21	B	301	TGL	OG1-CA1	4.71	1.47	1.33
20	C	306	PGV	O03-C19	4.69	1.47	1.33
27	P	303	CDL	OB8-CB7	4.69	1.47	1.33
21	A	609	TGL	OG2-CB1	4.68	1.47	1.34
21	Y	101	TGL	OG2-CB1	4.67	1.47	1.34
15	A	602	HEA	CHD-C1D	4.66	1.46	1.35
27	P	303	CDL	OA8-CA7	4.62	1.46	1.33
21	O	301	TGL	OG3-CC1	4.62	1.46	1.33
28	C	309	PEK	O03-C21	4.60	1.46	1.33
28	T	101	PEK	O03-C21	4.59	1.46	1.33
27	P	303	CDL	OA6-CA5	4.59	1.47	1.34
27	T	102	CDL	OA8-CA7	4.55	1.46	1.33
21	B	301	TGL	OG3-CC1	4.54	1.46	1.33
20	A	608	PGV	O03-C19	4.52	1.46	1.33
28	P	301	PEK	O01-C1	4.51	1.47	1.34
27	G	101	CDL	OA8-CA7	4.51	1.46	1.33
28	C	309	PEK	O01-C1	4.51	1.47	1.34
21	D	201	TGL	OG1-CA1	4.50	1.46	1.33
27	G	101	CDL	OB8-CB7	4.50	1.46	1.33
27	T	102	CDL	OB8-CB7	4.49	1.46	1.33
27	C	302	CDL	OA8-CA7	4.48	1.46	1.33
21	Y	101	TGL	OG1-CA1	4.48	1.46	1.33
20	Q	201	PGV	O03-C19	4.45	1.46	1.33
26	B	304	PSC	O01-C1	4.44	1.46	1.34
20	G	102	PGV	O03-C19	4.44	1.46	1.33
15	A	602	HEA	C3C-C2C	-4.41	1.34	1.40
28	P	301	PEK	O03-C21	4.37	1.46	1.33
21	Q	202	TGL	OG1-CA1	4.34	1.46	1.33
27	G	101	CDL	OA6-CA5	4.33	1.46	1.34
21	A	609	TGL	OG1-CA1	4.31	1.45	1.33
21	Q	202	TGL	OG3-CC1	4.30	1.45	1.33
20	Q	201	PGV	O01-C1	4.29	1.46	1.34
21	O	301	TGL	OG1-CA1	4.26	1.45	1.33
27	G	101	CDL	OB6-CB5	4.26	1.46	1.34
27	C	302	CDL	OB8-CB7	4.25	1.45	1.33
21	O	301	TGL	OG2-CB1	4.23	1.46	1.34
20	G	102	PGV	O01-C1	4.22	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	102	CDL	OB6-CB5	4.21	1.46	1.34
15	N	601[A]	HEA	CHC-C4B	4.19	1.45	1.35
15	N	601[B]	HEA	CHC-C4B	4.19	1.45	1.35
15	N	601[A]	HEA	C4B-NB	-4.19	1.33	1.40
15	N	601[B]	HEA	C4B-NB	-4.19	1.33	1.40
20	C	306	PGV	O01-C1	4.17	1.46	1.34
27	T	102	CDL	OA6-CA5	4.12	1.45	1.34
28	T	101	PEK	O01-C1	4.07	1.45	1.34
28	C	305	PEK	O01-C1	4.01	1.45	1.34
21	D	201	TGL	OG3-CC1	3.94	1.44	1.33
15	A	602	HEA	CHC-C4B	3.93	1.45	1.35
26	O	304	PSC	C13-C12	3.93	1.54	1.31
20	N	607	PGV	O01-C02	-3.93	1.36	1.46
21	B	301	TGL	OG2-CB1	3.89	1.45	1.34
15	N	601[A]	HEA	C1D-C2D	-3.89	1.37	1.44
15	N	601[B]	HEA	C1D-C2D	-3.89	1.37	1.44
26	B	304	PSC	O03-C19	3.87	1.44	1.33
26	O	304	PSC	O03-C19	3.86	1.44	1.33
20	A	608	PGV	O01-C1	3.80	1.45	1.34
15	N	602	HEA	CHD-C1D	3.79	1.44	1.35
15	A	601[A]	HEA	C1D-ND	-3.78	1.33	1.40
15	A	601[B]	HEA	C1D-ND	-3.78	1.33	1.40
15	A	601[A]	HEA	C3C-C2C	-3.73	1.35	1.40
15	A	601[B]	HEA	C3C-C2C	-3.73	1.35	1.40
26	B	304	PSC	C13-C12	3.73	1.53	1.31
21	D	201	TGL	OG2-CB1	3.68	1.44	1.34
21	D	201	TGL	OB1-CB1	3.63	1.33	1.22
27	P	303	CDL	OB6-CB5	3.53	1.44	1.34
27	C	302	CDL	C79-C78	-3.53	1.31	1.51
15	A	601[A]	HEA	CHD-C1D	3.49	1.43	1.35
15	A	601[B]	HEA	CHD-C1D	3.49	1.43	1.35
27	C	302	CDL	C82-C81	-3.42	1.32	1.51
15	A	601[A]	HEA	C3A-C2A	-3.37	1.35	1.40
15	A	601[B]	HEA	C3A-C2A	-3.37	1.35	1.40
20	P	302	PGV	P-O14	-3.35	1.39	1.55
27	T	102	CDL	C59-C58	-3.35	1.32	1.51
27	C	302	CDL	C59-C58	-3.32	1.32	1.51
27	G	101	CDL	C59-C58	-3.32	1.33	1.51
27	P	303	CDL	C79-C78	-3.30	1.33	1.51
27	P	303	CDL	C59-C58	-3.28	1.33	1.51
27	C	302	CDL	OB6-CB5	3.28	1.43	1.34
27	P	303	CDL	C62-C61	-3.28	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	102	CDL	C42-C41	-3.27	1.33	1.51
27	C	302	CDL	C62-C61	-3.26	1.33	1.51
27	C	302	CDL	C19-C18	-3.26	1.33	1.51
15	N	601[A]	HEA	CMB-C2B	3.24	1.57	1.50
15	N	601[B]	HEA	CMB-C2B	3.24	1.57	1.50
27	T	102	CDL	C62-C61	-3.24	1.33	1.51
27	C	302	CDL	C22-C21	-3.23	1.33	1.51
27	P	303	CDL	C39-C38	-3.23	1.33	1.51
27	T	102	CDL	C82-C81	-3.22	1.33	1.51
20	N	607	PGV	O01-C1	3.21	1.43	1.34
27	P	303	CDL	C82-C81	-3.21	1.33	1.51
15	A	601[A]	HEA	C1D-C2D	-3.21	1.38	1.44
15	A	601[B]	HEA	C1D-C2D	-3.21	1.38	1.44
27	G	101	CDL	C82-C81	-3.20	1.33	1.51
27	P	303	CDL	C42-C41	-3.19	1.33	1.51
27	G	101	CDL	C62-C61	-3.18	1.33	1.51
27	C	302	CDL	C42-C41	-3.16	1.33	1.51
27	C	302	CDL	C39-C38	-3.15	1.33	1.51
27	G	101	CDL	C79-C78	-3.14	1.34	1.51
27	T	102	CDL	C22-C21	-3.13	1.34	1.51
21	D	201	TGL	CB2-CB1	3.12	1.59	1.50
27	T	102	CDL	C79-C78	-3.12	1.34	1.51
27	G	101	CDL	C39-C38	-3.11	1.34	1.51
27	T	102	CDL	C19-C18	-3.10	1.34	1.51
28	P	307	PEK	O03-C21	3.10	1.42	1.33
27	G	101	CDL	C19-C18	-3.08	1.34	1.51
15	N	602	HEA	C1D-ND	-3.06	1.35	1.40
27	T	102	CDL	C39-C38	-3.05	1.34	1.51
27	G	101	CDL	C42-C41	-3.04	1.34	1.51
25	C	304	CHD	O12-C12	3.00	1.48	1.43
27	G	101	CDL	C22-C21	-3.00	1.34	1.51
15	A	602	HEA	C2A-C1A	-2.95	1.35	1.42
25	C	304	CHD	O25-C24	2.92	1.31	1.22
15	A	601[A]	HEA	CHC-C4B	2.88	1.42	1.35
15	A	601[B]	HEA	CHC-C4B	2.88	1.42	1.35
15	N	601[A]	HEA	O11-C11	2.85	1.49	1.42
15	N	601[B]	HEA	O11-C11	2.85	1.49	1.42
20	A	608	PGV	O02-C1	2.84	1.31	1.22
15	A	602	HEA	C1D-ND	-2.83	1.35	1.40
28	C	307	PEK	O03-C21	2.83	1.41	1.33
15	A	602	HEA	C1D-C2D	-2.83	1.39	1.44
15	A	601[A]	HEA	C16-C17	-2.76	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	601[B]	HEA	C16-C17	-2.76	1.44	1.53
15	N	602	HEA	CBA-CGA	2.73	1.56	1.50
23	P	305	DMU	O16-C6	2.72	1.44	1.40
27	C	302	CDL	OA6-CA4	-2.72	1.43	1.46
15	N	602	HEA	C3C-C2C	-2.68	1.36	1.40
25	B	303	CHD	C11-C9	2.67	1.58	1.53
15	N	602	HEA	O11-C11	2.66	1.48	1.42
25	O	303	CHD	C10-C9	-2.64	1.51	1.56
15	A	601[A]	HEA	CMB-C2B	2.62	1.56	1.50
15	A	601[B]	HEA	CMB-C2B	2.62	1.56	1.50
15	N	601[A]	HEA	O2D-CGD	-2.62	1.21	1.30
15	N	601[B]	HEA	O2D-CGD	-2.62	1.21	1.30
15	N	601[A]	HEA	CMD-C2D	2.57	1.56	1.50
15	N	601[B]	HEA	CMD-C2D	2.57	1.56	1.50
15	N	601[A]	HEA	C1B-C2B	-2.57	1.39	1.44
15	N	601[B]	HEA	C1B-C2B	-2.57	1.39	1.44
15	N	601[A]	HEA	CHD-C1D	2.56	1.41	1.35
15	N	601[B]	HEA	CHD-C1D	2.56	1.41	1.35
27	P	303	CDL	C19-C18	-2.53	1.33	1.51
15	N	602	HEA	C3D-C2D	-2.51	1.31	1.36
15	N	602	HEA	FE-NB	2.48	2.09	1.96
15	A	602	HEA	O1D-CGD	2.45	1.30	1.22
23	C	318	DMU	O16-C6	2.44	1.44	1.40
15	N	601[A]	HEA	O1D-CGD	2.40	1.30	1.22
15	N	601[B]	HEA	O1D-CGD	2.40	1.30	1.22
20	A	607	PGV	O01-C1	2.39	1.41	1.34
20	N	607	PGV	C03-C02	2.38	1.58	1.50
15	A	602	HEA	C18-C19	2.38	1.38	1.33
23	X	102	DMU	O16-C6	2.37	1.44	1.40
15	N	601[A]	HEA	O1A-CGA	2.37	1.30	1.22
15	N	601[B]	HEA	O1A-CGA	2.37	1.30	1.22
15	N	602	HEA	C2A-C1A	-2.35	1.37	1.42
15	A	601[A]	HEA	O2A-CGA	-2.35	1.22	1.30
15	A	601[B]	HEA	O2A-CGA	-2.35	1.22	1.30
15	A	602	HEA	O1A-CGA	2.34	1.29	1.22
23	X	105	DMU	O16-C6	2.31	1.44	1.40
20	A	607	PGV	C03-C02	2.31	1.57	1.50
20	C	301	PGV	O01-C02	-2.29	1.40	1.46
15	N	602	HEA	C1D-C2D	-2.28	1.40	1.44
20	C	301	PGV	O03-C01	2.25	1.50	1.45
20	N	607	PGV	C01-C02	2.25	1.57	1.50
20	N	607	PGV	O04-C19	-2.25	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	316	DMU	O16-C6	2.23	1.44	1.40
21	D	201	TGL	OG2-CG2	-2.22	1.41	1.46
20	A	608	PGV	O01-C02	-2.22	1.41	1.46
15	N	601[A]	HEA	C4D-ND	-2.22	1.34	1.38
15	N	601[B]	HEA	C4D-ND	-2.22	1.34	1.38
20	P	302	PGV	O01-C02	-2.20	1.41	1.46
23	X	107	DMU	O16-C6	2.19	1.43	1.40
15	N	601[A]	HEA	C12-C11	-2.19	1.49	1.52
15	N	601[B]	HEA	C12-C11	-2.19	1.49	1.52
27	C	302	CDL	PB2-OB3	2.18	1.57	1.50
15	A	602	HEA	CBD-CGD	2.18	1.55	1.50
25	B	303	CHD	C10-C9	-2.18	1.52	1.56
25	P	306	CHD	O25-C24	2.17	1.29	1.22
21	Q	202	TGL	OB1-CB1	2.17	1.29	1.22
23	K	102	DMU	O16-C6	2.16	1.43	1.40
15	N	602	HEA	C4C-CHD	2.16	1.47	1.41
23	K	101	DMU	O16-C6	2.15	1.43	1.40
20	C	301	PGV	P-O14	-2.15	1.45	1.55
15	N	602	HEA	C4D-C3D	-2.14	1.41	1.45
15	A	601[A]	HEA	CAD-C3D	2.14	1.56	1.51
15	A	601[B]	HEA	CAD-C3D	2.14	1.56	1.51
15	N	601[A]	HEA	CBD-CGD	2.14	1.55	1.50
15	N	601[B]	HEA	CBD-CGD	2.14	1.55	1.50
25	C	303	CHD	C13-C14	-2.14	1.51	1.55
15	N	602	HEA	C14-C15	2.12	1.38	1.33
25	X	101	CHD	C13-C14	-2.10	1.51	1.55
15	A	601[A]	HEA	CBA-CGA	2.07	1.55	1.50
15	A	601[B]	HEA	CBA-CGA	2.07	1.55	1.50
23	Z	101	DMU	O16-C6	2.03	1.43	1.40
20	C	301	PGV	C20-C19	2.03	1.56	1.50
15	A	602	HEA	C1B-NB	-2.03	1.34	1.38
15	A	601[A]	HEA	CBD-CGD	2.03	1.55	1.50
15	A	601[B]	HEA	CBD-CGD	2.03	1.55	1.50
23	L	105	DMU	O16-C6	2.01	1.43	1.40
25	P	304	CHD	C13-C14	-2.00	1.52	1.55

All (501) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	302	CDL	CB4-OB6-CB5	-6.42	101.99	117.79
25	L	104	CHD	C6-C5-C4	-6.23	104.02	111.19
27	G	101	CDL	OB6-CB5-C51	6.16	124.77	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	104	CHD	C6-C5-C4	-5.99	104.30	111.19
15	N	602	HEA	C3C-C4C-NC	5.87	116.80	109.21
28	P	307	PEK	C2-C3-C4	5.83	123.61	113.23
20	C	306	PGV	O01-C1-C2	5.81	124.02	111.50
15	A	601[A]	HEA	C2D-C1D-ND	5.80	116.71	109.84
15	A	601[B]	HEA	C2D-C1D-ND	5.80	116.71	109.84
27	T	102	CDL	OB6-CB5-C51	5.77	123.94	111.50
15	N	602	HEA	C4D-CHA-C1A	5.74	130.13	122.56
25	Y	104	CHD	C21-C20-C17	5.72	121.69	112.92
27	P	303	CDL	CB4-OB6-CB5	-5.66	103.86	117.79
26	O	304	PSC	O01-C1-C2	5.58	123.52	111.50
25	X	101	CHD	C19-C10-C9	-5.55	103.53	111.18
21	A	609	TGL	OG2-CB1-CB2	5.55	123.46	111.50
27	P	303	CDL	C52-C51-CB5	-5.49	93.66	113.62
26	B	304	PSC	O01-C1-C2	5.48	123.31	111.50
21	Y	101	TGL	OG2-CB1-CB2	5.40	123.15	111.50
15	A	601[B]	HEA	C27-C19-C20	5.38	124.32	115.27
25	L	104	CHD	C11-C9-C10	-5.34	108.22	113.73
15	N	601[A]	HEA	C3C-C4C-NC	5.33	116.10	109.21
15	N	601[B]	HEA	C3C-C4C-NC	5.33	116.10	109.21
27	T	102	CDL	OA6-CA5-C11	5.17	122.65	111.50
20	C	306	PGV	O03-C19-C20	5.14	128.03	111.91
25	Y	104	CHD	C1-C10-C5	5.13	115.36	107.77
21	B	301	TGL	OG2-CB1-CB2	5.13	122.56	111.50
21	D	201	TGL	CG2-OG2-CB1	-4.98	105.52	117.79
25	L	104	CHD	C21-C20-C17	4.88	120.39	112.92
25	C	303	CHD	C14-C13-C12	4.84	111.91	107.40
27	C	302	CDL	OA6-CA5-OA7	-4.76	119.51	125.57
25	X	101	CHD	C11-C9-C10	-4.74	108.84	113.73
20	A	608	PGV	C3-C2-C1	4.69	130.68	113.62
20	N	607	PGV	O01-C1-O02	-4.65	112.47	123.70
28	C	305	PEK	O03-C21-C22	4.64	126.47	111.91
25	X	101	CHD	C17-C13-C12	-4.58	113.48	117.67
25	L	104	CHD	C13-C17-C20	4.56	124.94	119.50
28	P	301	PEK	O01-C1-C2	4.55	121.32	111.50
20	Q	201	PGV	C02-O01-C1	-4.54	106.60	117.79
15	A	602	HEA	C4D-CHA-C1A	4.54	128.55	122.56
28	T	101	PEK	O03-C21-C22	4.53	126.14	111.91
25	Y	104	CHD	C14-C8-C7	4.53	117.81	111.81
27	G	101	CDL	OA6-CA5-C11	4.46	121.10	111.50
27	P	303	CDL	OA6-CA5-C11	4.44	121.08	111.50
15	N	601[A]	HEA	CHA-C4D-ND	4.36	129.17	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	601[B]	HEA	CHA-C4D-ND	4.36	129.17	124.43
23	X	103	DMU	O5-C4-C3	4.33	118.87	109.75
27	C	302	CDL	C52-C51-CB5	-4.30	97.98	113.62
25	C	303	CHD	C13-C17-C20	-4.30	114.36	119.50
25	L	104	CHD	C14-C13-C12	4.30	111.40	107.40
27	P	303	CDL	OB8-CB7-C71	4.22	125.15	111.91
25	C	304	CHD	C18-C13-C12	4.21	113.35	109.07
25	X	101	CHD	C5-C4-C3	-4.19	106.60	112.76
27	P	303	CDL	OB6-CB5-C51	4.16	120.46	111.50
23	K	105	DMU	O7-C3-C2	4.12	118.25	107.28
20	G	102	PGV	O03-C19-C20	4.12	124.83	111.91
23	X	102	DMU	O5-C4-C3	4.07	118.33	109.75
25	X	101	CHD	C4-C3-C2	-4.07	105.69	110.55
28	C	309	PEK	O01-C1-C2	4.06	120.24	111.50
15	N	601[A]	HEA	O2A-CGA-CBA	4.04	127.00	114.03
15	N	601[B]	HEA	O2A-CGA-CBA	4.04	127.00	114.03
23	D	206	DMU	C10-O7-C3	4.02	127.91	117.96
23	D	206	DMU	O7-C3-C2	3.99	117.89	107.28
20	Q	201	PGV	O01-C1-C2	3.95	120.01	111.50
15	N	601[A]	HEA	CHC-C4B-NB	3.94	129.24	124.38
15	N	601[B]	HEA	CHC-C4B-NB	3.94	129.24	124.38
15	N	601[A]	HEA	OMA-CMA-C3A	-3.92	116.36	124.91
15	N	601[B]	HEA	OMA-CMA-C3A	-3.92	116.36	124.91
27	G	101	CDL	OA8-CA7-C31	3.90	124.16	111.91
15	A	601[A]	HEA	CHA-C4D-C3D	-3.88	119.14	124.84
15	A	601[B]	HEA	CHA-C4D-C3D	-3.88	119.14	124.84
15	A	602	HEA	C3C-C4C-NC	3.87	114.22	109.21
23	C	317	DMU	C10-O7-C3	-3.87	108.38	117.96
23	C	318	DMU	C10-O1-C9	3.87	121.28	113.69
23	K	106	DMU	C10-C5-C7	3.87	118.05	110.00
23	X	106	DMU	C10-O1-C9	3.86	121.26	113.69
25	Y	104	CHD	C11-C9-C10	-3.85	109.75	113.73
15	A	601[A]	HEA	C1D-ND-C4D	-3.83	101.12	105.07
15	A	601[B]	HEA	C1D-ND-C4D	-3.83	101.12	105.07
15	N	601[A]	HEA	CMB-C2B-C1B	-3.83	119.21	125.04
15	N	601[B]	HEA	CMB-C2B-C1B	-3.83	119.21	125.04
23	M	101	DMU	C18-O16-C6	-3.81	107.52	113.84
25	L	104	CHD	C11-C12-C13	3.81	115.16	111.24
26	B	304	PSC	O01-C02-C03	3.81	122.18	108.40
28	C	309	PEK	O03-C21-C22	3.79	123.80	111.91
23	K	101	DMU	C6-O5-C4	3.77	121.10	113.69
26	O	304	PSC	O03-C01-C02	-3.76	97.48	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	102	DMU	O7-C3-C4	3.76	119.76	109.45
27	C	302	CDL	OB6-CB5-C51	3.76	119.59	111.50
15	N	602	HEA	O1A-CGA-CBA	-3.75	111.04	123.08
23	A	628	DMU	C6-C1-C2	3.75	117.80	110.00
23	L	105	DMU	O7-C3-C2	3.74	117.23	107.28
23	C	318	DMU	O1-C9-C8	3.73	116.46	109.69
23	X	106	DMU	C10-O7-C3	-3.69	108.84	117.96
25	P	304	CHD	C13-C17-C20	-3.68	115.10	119.50
15	A	602	HEA	C2D-C1D-ND	3.68	114.19	109.84
28	P	301	PEK	C02-O01-C1	-3.66	108.79	117.79
25	X	101	CHD	C18-C13-C12	3.65	112.78	109.07
23	X	105	DMU	O16-C6-C1	3.61	113.94	108.30
25	X	101	CHD	C10-C9-C8	-3.61	107.94	111.82
28	C	305	PEK	O03-C21-O04	-3.56	114.60	123.59
15	A	602	HEA	CMB-C2B-C1B	3.55	130.45	125.04
23	X	103	DMU	C6-O5-C4	3.55	120.66	113.69
15	A	601[A]	HEA	C13-C12-C11	-3.54	109.03	114.35
15	A	601[B]	HEA	C13-C12-C11	-3.54	109.03	114.35
15	A	601[A]	HEA	C3D-C4D-ND	3.53	113.78	110.36
15	A	601[B]	HEA	C3D-C4D-ND	3.53	113.78	110.36
23	X	107	DMU	C6-C1-C2	3.53	117.35	110.00
15	N	602	HEA	CAD-CBD-CGD	-3.52	106.03	113.60
23	X	105	DMU	C8-C7-C5	-3.52	104.68	110.82
15	A	602	HEA	C20-C19-C18	-3.51	114.01	121.12
23	C	317	DMU	C8-C7-C5	3.51	116.95	110.82
23	C	316	DMU	O1-C10-C5	3.49	117.73	110.35
23	X	103	DMU	C10-O1-C9	3.48	120.52	113.69
15	A	601[B]	HEA	C17-C18-C19	3.48	136.03	127.66
28	C	305	PEK	O01-C1-C2	3.47	118.98	111.50
25	X	101	CHD	C9-C11-C12	3.46	118.88	114.30
28	T	101	PEK	O01-C1-C2	3.46	118.96	111.50
15	A	601[B]	HEA	C21-C22-C23	-3.45	115.95	127.75
15	N	602	HEA	C3B-C4B-NB	-3.45	105.75	109.84
21	O	301	TGL	OG2-CB1-CB2	3.44	118.91	111.50
20	P	302	PGV	O01-C1-O02	-3.43	115.41	123.70
25	Y	104	CHD	C14-C13-C12	3.43	110.59	107.40
15	A	602	HEA	CAD-CBD-CGD	-3.43	106.23	113.60
23	M	101	DMU	O5-C6-O16	-3.39	101.95	109.97
23	X	102	DMU	C6-O5-C4	3.38	120.33	113.69
23	X	106	DMU	O55-C2-C3	3.38	118.90	109.94
27	C	302	CDL	OA8-CA7-C31	3.37	122.50	111.91
28	C	307	PEK	O03-C21-C22	3.37	122.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	316	DMU	C10-C5-C7	3.37	117.01	110.00
21	A	609	TGL	OG3-CC1-CC2	3.36	122.47	111.91
23	K	101	DMU	O5-C4-C3	3.36	116.83	109.75
23	X	106	DMU	O1-C9-C8	3.35	115.78	109.69
15	A	601[B]	HEA	C20-C19-C18	-3.35	114.34	121.12
23	X	106	DMU	C7-C8-C9	3.35	116.21	110.24
27	T	102	CDL	CB4-OB6-CB5	-3.34	109.56	117.79
25	L	104	CHD	C10-C9-C8	3.34	115.41	111.82
25	P	306	CHD	C22-C20-C17	-3.34	103.39	110.28
15	N	601[A]	HEA	C16-C15-C14	-3.33	114.37	121.12
15	N	601[B]	HEA	C16-C15-C14	-3.33	114.37	121.12
15	N	601[B]	HEA	C27-C19-C20	3.31	120.84	115.27
25	X	101	CHD	C5-C6-C7	-3.30	110.83	114.46
27	P	303	CDL	OA8-CA7-C31	3.28	122.20	111.91
23	X	104	DMU	C10-O7-C3	-3.28	109.86	117.96
26	O	304	PSC	O01-C02-C03	3.27	120.26	108.40
25	P	306	CHD	C19-C10-C1	-3.27	102.99	108.26
25	L	104	CHD	C9-C10-C5	3.25	113.14	108.58
26	O	304	PSC	C01-O03-C19	3.23	129.09	117.12
15	A	601[A]	HEA	C4A-CHB-C1B	-3.23	118.29	122.56
15	A	601[B]	HEA	C4A-CHB-C1B	-3.23	118.29	122.56
27	G	101	CDL	CB4-OB6-CB5	-3.23	109.84	117.79
15	A	602	HEA	C13-C12-C11	-3.23	109.50	114.35
28	T	101	PEK	O13-P-O14	3.22	123.28	110.68
25	B	303	CHD	C11-C9-C10	-3.22	110.41	113.73
23	P	314	DMU	O7-C10-C5	3.19	116.37	108.10
15	N	601[A]	HEA	C26-C15-C16	3.19	120.64	115.27
15	N	601[B]	HEA	C26-C15-C16	3.19	120.64	115.27
25	C	303	CHD	C9-C11-C12	-3.17	110.11	114.30
23	O	307	DMU	O1-C10-C5	3.16	117.03	110.35
21	A	609	TGL	OG3-CC1-OC1	-3.16	115.62	123.59
20	G	102	PGV	O03-C19-O04	-3.16	115.63	123.59
28	C	305	PEK	C36-C35-C34	-3.15	98.45	114.42
25	C	304	CHD	C23-C22-C20	-3.14	108.78	114.52
27	T	102	CDL	OA8-CA7-C31	3.14	121.77	111.91
23	X	106	DMU	C1-C2-C3	-3.13	102.53	109.68
25	L	104	CHD	C14-C8-C7	3.13	115.96	111.81
23	O	307	DMU	C10-C5-C7	3.13	116.51	110.00
23	K	101	DMU	O1-C10-C5	3.13	116.97	110.35
23	X	106	DMU	O1-C10-C5	3.11	116.94	110.35
28	T	101	PEK	C01-O03-C21	3.10	128.59	117.12
15	A	602	HEA	CMD-C2D-C1D	3.08	129.74	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	601[A]	HEA	O1A-CGA-CBA	-3.08	113.19	123.08
15	A	601[B]	HEA	O1A-CGA-CBA	-3.08	113.19	123.08
25	C	304	CHD	C22-C23-C24	-3.07	104.37	112.51
15	A	602	HEA	C2B-C1B-NB	3.06	113.55	109.88
23	X	107	DMU	C1-C2-C3	3.03	116.61	109.68
27	T	102	CDL	OA6-CA5-OA7	-3.03	116.37	123.70
25	P	306	CHD	C21-C20-C22	-3.03	105.62	110.36
15	A	602	HEA	O1D-CGD-CBD	-3.03	113.36	123.08
15	A	602	HEA	O1A-CGA-CBA	-3.03	113.36	123.08
23	X	106	DMU	O7-C10-C5	3.02	115.94	108.10
25	L	104	CHD	C1-C10-C9	-3.02	106.60	111.35
23	C	318	DMU	C7-C8-C9	3.02	115.62	110.24
27	G	101	CDL	OB6-CB5-OB7	-3.01	116.42	123.70
23	K	104	DMU	O16-C6-C1	3.01	113.00	108.30
21	D	201	TGL	OG3-CC1-OC1	-3.01	116.00	123.59
28	C	305	PEK	C01-O03-C21	3.00	128.24	117.12
28	P	307	PEK	C3-C2-C1	-3.00	102.71	113.62
26	O	304	PSC	C21-C20-C19	-3.00	102.72	113.62
15	N	602	HEA	CHB-C1B-NB	3.00	127.69	124.43
23	X	106	DMU	O7-C3-C2	3.00	115.25	107.28
21	B	301	TGL	OG1-CA1-CA2	2.99	121.29	111.91
23	P	314	DMU	O16-C6-C1	2.99	112.96	108.30
15	N	602	HEA	CHA-C4D-C3D	2.97	129.21	124.84
25	P	304	CHD	C13-C14-C8	-2.96	110.96	114.74
21	O	301	TGL	OG1-CA1-CA2	2.95	121.18	111.91
27	C	302	CDL	OB8-CB7-C71	2.95	121.17	111.91
27	C	302	CDL	OB2-PB2-OB5	-2.95	98.88	106.73
23	X	107	DMU	O7-C3-C2	2.95	115.13	107.28
25	B	303	CHD	C18-C13-C17	-2.95	106.59	111.21
28	T	101	PEK	O03-C21-O04	-2.94	116.17	123.59
23	X	103	DMU	O1-C9-C8	2.94	115.03	109.69
25	C	304	CHD	C6-C7-C8	-2.92	108.36	111.48
21	Q	202	TGL	OG3-CC1-CC2	2.92	121.06	111.91
23	C	317	DMU	C10-C5-C7	2.91	116.05	110.00
25	C	304	CHD	C17-C13-C12	-2.90	115.02	117.67
23	A	628	DMU	C1-C2-C3	2.90	116.30	109.68
23	P	314	DMU	O7-C3-C2	2.89	114.98	107.28
15	N	601[A]	HEA	O1D-CGD-CBD	-2.89	113.79	123.08
15	N	601[B]	HEA	O1D-CGD-CBD	-2.89	113.79	123.08
23	P	314	DMU	O1-C9-C8	2.89	114.95	109.69
20	C	306	PGV	C02-O01-C1	-2.89	110.68	117.79
20	C	306	PGV	O03-C19-O04	-2.89	116.30	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	306	PGV	O01-C1-O02	-2.89	116.72	123.70
15	N	602	HEA	CHA-C4D-ND	-2.88	121.30	124.43
20	A	608	PGV	O03-C19-C20	2.88	120.94	111.91
28	P	301	PEK	O03-C21-C22	2.88	120.94	111.91
15	N	602	HEA	C4B-NB-C1B	2.87	108.04	105.07
26	B	304	PSC	O01-C1-O02	-2.87	116.76	123.70
27	T	102	CDL	CA4-OA6-CA5	-2.87	110.73	117.79
25	L	104	CHD	C1-C2-C3	2.86	114.14	110.47
27	P	303	CDL	OB2-PB2-OB5	-2.86	99.13	106.73
20	Q	201	PGV	O03-C19-C20	2.86	120.87	111.91
15	A	601[A]	HEA	CMB-C2B-C1B	-2.85	120.69	125.04
15	A	601[B]	HEA	CMB-C2B-C1B	-2.85	120.69	125.04
15	N	602	HEA	O2A-CGA-O1A	2.84	130.38	123.30
23	K	104	DMU	C18-O16-C6	-2.84	109.13	113.84
15	N	601[A]	HEA	CHA-C4D-C3D	-2.84	120.67	124.84
15	N	601[B]	HEA	CHA-C4D-C3D	-2.84	120.67	124.84
25	Y	104	CHD	C13-C17-C20	2.83	122.88	119.50
23	K	103	DMU	C10-O1-C9	2.83	119.23	113.69
20	N	607	PGV	O02-C1-C2	2.82	134.74	123.73
23	A	628	DMU	O7-C3-C2	2.82	114.78	107.28
25	X	101	CHD	C14-C8-C7	2.81	115.53	111.81
23	K	105	DMU	C1-C2-C3	-2.81	103.28	109.68
23	K	104	DMU	C10-O1-C9	2.80	119.19	113.69
25	P	304	CHD	C11-C9-C10	-2.80	110.84	113.73
15	A	601[A]	HEA	C25-C23-C24	2.80	120.78	114.60
25	Y	104	CHD	C17-C13-C12	-2.79	115.12	117.67
25	C	303	CHD	C16-C17-C20	2.78	116.46	112.15
23	K	101	DMU	O5-C6-C1	2.78	116.24	110.35
25	X	101	CHD	C23-C22-C20	-2.76	109.47	114.52
27	G	101	CDL	OA8-CA7-OA9	-2.76	116.62	123.59
23	M	101	DMU	C28-C25-C22	-2.75	100.46	114.42
25	Y	104	CHD	C21-C20-C22	-2.73	106.08	110.36
15	A	602	HEA	O2D-CGD-CBD	2.73	122.79	114.03
25	Y	104	CHD	C19-C10-C1	-2.73	103.87	108.26
21	D	201	TGL	OG1-CA1-CA2	2.73	120.46	111.91
25	B	303	CHD	C16-C17-C13	2.72	106.22	103.55
15	A	601[A]	HEA	C1D-C2D-C3D	-2.72	104.09	106.96
15	A	601[B]	HEA	C1D-C2D-C3D	-2.72	104.09	106.96
23	X	105	DMU	O1-C9-C11	2.72	113.19	106.44
23	K	104	DMU	O1-C9-C8	2.71	114.62	109.69
15	A	602	HEA	C21-C20-C19	2.70	121.86	112.98
23	I	101	DMU	C18-O16-C6	-2.69	109.38	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	303	CHD	C23-C22-C20	-2.69	109.61	114.52
27	P	303	CDL	OB4-PB2-OB3	2.68	121.19	110.68
20	N	607	PGV	O03-C19-O04	-2.68	116.82	123.59
23	C	317	DMU	O1-C10-C5	2.67	116.00	110.35
15	N	601[A]	HEA	CAA-CBA-CGA	-2.67	106.28	113.76
15	N	601[B]	HEA	CAA-CBA-CGA	-2.67	106.28	113.76
15	N	601[A]	HEA	O2A-CGA-O1A	-2.67	116.65	123.30
15	N	601[B]	HEA	O2A-CGA-O1A	-2.67	116.65	123.30
23	C	308	DMU	C18-O16-C6	-2.66	109.42	113.84
21	B	301	TGL	CB3-CB2-CB1	-2.64	104.01	113.62
23	P	314	DMU	C10-O1-C9	2.64	118.87	113.69
21	Q	202	TGL	OG1-CA1-CA2	2.64	120.18	111.91
20	A	608	PGV	C4-C3-C2	-2.64	103.71	113.19
25	B	303	CHD	C1-C10-C9	2.64	115.50	111.35
25	B	303	CHD	C13-C14-C8	-2.63	111.38	114.74
23	K	103	DMU	O1-C10-C5	2.63	115.92	110.35
23	I	101	DMU	C6-O5-C4	-2.63	108.53	113.69
27	T	102	CDL	CB6-CB4-CB3	-2.63	105.58	111.79
23	K	101	DMU	C10-O7-C3	-2.62	111.48	117.96
21	D	201	TGL	OG2-CB1-OB1	-2.62	117.38	123.70
26	O	304	PSC	C02-O01-C1	2.62	124.23	117.79
23	C	316	DMU	C6-C1-C2	2.61	115.43	110.00
25	O	303	CHD	C11-C9-C10	-2.60	111.04	113.73
15	N	601[A]	HEA	O2D-CGD-CBD	2.60	122.39	114.03
15	N	601[B]	HEA	O2D-CGD-CBD	2.60	122.39	114.03
23	C	318	DMU	C10-C5-C7	2.60	115.41	110.00
25	P	304	CHD	C14-C8-C9	-2.60	106.14	109.71
23	O	307	DMU	C10-O1-C9	2.60	118.79	113.69
15	N	601[A]	HEA	C27-C19-C18	-2.60	117.01	123.68
25	Y	104	CHD	C4-C3-C2	-2.59	107.46	110.55
27	G	101	CDL	CA4-OA6-CA5	-2.59	111.43	117.79
20	G	102	PGV	O01-C1-C2	2.58	117.06	111.50
27	C	302	CDL	OB4-PB2-OB3	2.58	120.76	110.68
23	X	106	DMU	C8-C7-C5	2.58	115.32	110.82
27	P	303	CDL	OA6-CA4-CA3	2.57	117.71	108.40
25	L	104	CHD	C18-C13-C14	-2.56	107.20	111.21
21	Y	101	TGL	OG1-CA1-CA2	2.56	119.95	111.91
23	C	317	DMU	C7-C8-C9	2.56	114.81	110.24
23	D	206	DMU	C1-C2-C3	2.56	115.53	109.68
23	P	314	DMU	C18-O16-C6	-2.56	109.59	113.84
20	A	608	PGV	O01-C1-O02	2.56	129.89	123.70
25	Y	104	CHD	C1-C2-C3	-2.56	107.19	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	T	102	CDL	OB6-CB5-OB7	-2.55	117.54	123.70
25	O	303	CHD	C6-C7-C8	-2.55	108.76	111.48
25	B	303	CHD	C19-C10-C5	-2.55	106.05	110.36
23	C	316	DMU	C10-O1-C9	2.54	118.68	113.69
15	A	602	HEA	O2A-CGA-CBA	2.54	122.20	114.03
23	P	314	DMU	O5-C6-O16	-2.54	103.96	109.97
25	O	303	CHD	C4-C3-C2	-2.54	107.52	110.55
23	K	101	DMU	C10-O1-C9	2.54	118.67	113.69
20	P	302	PGV	C03-C02-C01	-2.53	105.79	111.79
28	C	307	PEK	O11-P-O14	-2.53	99.17	109.07
25	P	304	CHD	C1-C2-C3	2.53	113.71	110.47
15	N	601[A]	HEA	C27-C19-C20	2.52	119.51	115.27
15	A	601[A]	HEA	CMC-C2C-C1C	-2.51	124.61	128.46
15	A	601[B]	HEA	CMC-C2C-C1C	-2.51	124.61	128.46
27	P	303	CDL	OB8-CB7-OB9	-2.50	117.27	123.59
15	A	602	HEA	C1B-C2B-C3B	-2.50	103.81	106.80
15	A	602	HEA	C17-C18-C19	-2.50	121.64	127.66
25	C	303	CHD	C22-C23-C24	-2.50	105.87	112.51
23	D	206	DMU	O7-C10-O1	2.49	117.64	110.67
25	X	101	CHD	C13-C14-C8	-2.48	111.57	114.74
21	Q	202	TGL	OG3-CC1-OC1	-2.46	117.37	123.59
25	P	304	CHD	C17-C13-C14	2.46	102.57	100.09
25	B	303	CHD	C5-C4-C3	-2.46	109.15	112.76
23	D	206	DMU	C10-O1-C9	2.46	118.51	113.69
15	N	601[A]	HEA	C17-C18-C19	-2.45	121.75	127.66
28	C	305	PEK	C02-O01-C1	-2.45	111.76	117.79
28	C	309	PEK	O03-C21-O04	-2.45	117.42	123.59
25	C	303	CHD	C17-C13-C14	-2.45	97.63	100.09
23	X	105	DMU	C10-O1-C9	2.44	118.48	113.69
23	K	106	DMU	O7-C3-C2	2.43	113.75	107.28
25	X	101	CHD	C1-C2-C3	2.43	113.58	110.47
23	K	101	DMU	C6-C1-C2	2.43	115.05	110.00
25	Y	104	CHD	C4-C5-C10	2.42	115.23	112.66
15	A	602	HEA	CMB-C2B-C3B	-2.42	125.73	130.34
20	G	102	PGV	C03-C02-C01	-2.41	106.09	111.79
26	B	304	PSC	C02-O01-C1	2.40	123.71	117.79
21	A	609	TGL	OG1-CA1-CA2	2.40	119.43	111.91
20	C	301	PGV	C22-C21-C20	2.39	121.78	113.19
23	K	102	DMU	C6-O5-C4	2.39	118.38	113.69
25	C	304	CHD	C14-C8-C7	-2.39	108.64	111.81
15	N	601[A]	HEA	CHC-C4B-C3B	-2.38	119.66	125.80
15	N	601[B]	HEA	CHC-C4B-C3B	-2.38	119.66	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	601[A]	HEA	C25-C23-C22	-2.38	115.76	122.65
20	C	301	PGV	O01-C1-O02	-2.38	117.95	123.70
20	A	607	PGV	O01-C1-O02	-2.38	117.95	123.70
23	X	107	DMU	C7-C8-C9	-2.38	106.00	110.24
21	Y	101	TGL	OG2-CB1-OB1	-2.37	117.97	123.70
23	X	105	DMU	O7-C3-C2	2.37	113.58	107.28
15	N	602	HEA	C21-C20-C19	2.37	120.77	112.98
23	X	104	DMU	O1-C10-C5	2.37	115.36	110.35
26	B	304	PSC	O03-C01-C02	-2.37	101.54	108.43
26	O	304	PSC	O01-C1-O02	-2.36	117.99	123.70
23	K	105	DMU	O55-C2-C3	2.36	116.20	109.94
28	P	307	PEK	O03-C21-C22	2.36	119.32	111.91
23	D	206	DMU	C6-O5-C4	-2.36	109.06	113.69
15	A	601[A]	HEA	C26-C15-C16	2.35	119.23	115.27
15	A	601[B]	HEA	C26-C15-C16	2.35	119.23	115.27
23	X	106	DMU	C6-C1-C2	-2.35	105.10	110.00
23	C	317	DMU	O5-C4-C57	2.35	112.28	106.44
15	N	601[A]	HEA	C1B-C2B-C3B	2.35	109.61	106.80
15	N	601[B]	HEA	C1B-C2B-C3B	2.35	109.61	106.80
23	P	315	DMU	C1-C2-C3	2.34	115.03	109.68
23	X	106	DMU	C2-C3-C4	-2.33	105.58	110.93
23	O	307	DMU	O5-C4-C3	2.33	114.67	109.75
15	N	602	HEA	CMC-C2C-C1C	-2.33	124.88	128.46
23	X	104	DMU	C10-O1-C9	2.33	118.26	113.69
23	X	106	DMU	C10-C5-C7	2.33	114.84	110.00
23	O	307	DMU	O16-C6-C1	2.32	111.93	108.30
21	A	609	TGL	C20-CA9-CA8	-2.32	102.63	114.42
23	K	101	DMU	C2-C3-C4	2.32	116.25	110.93
15	N	602	HEA	CMB-C2B-C1B	2.31	128.56	125.04
15	N	602	HEA	C25-C23-C22	-2.30	115.99	122.65
25	B	303	CHD	O3-C3-C4	-2.30	105.27	109.85
23	C	317	DMU	O5-C4-C3	-2.30	104.91	109.75
27	G	101	CDL	OA6-CA5-OA7	-2.30	118.16	123.70
23	X	107	DMU	C10-C5-C7	2.29	114.77	110.00
25	C	303	CHD	C14-C8-C7	-2.29	108.77	111.81
23	K	105	DMU	C7-C8-C9	-2.29	106.16	110.24
23	K	101	DMU	C7-C8-C9	-2.28	106.16	110.24
23	P	314	DMU	C10-C5-C7	2.28	114.75	110.00
20	C	306	PGV	C21-C20-C19	-2.28	105.32	113.62
21	Y	101	TGL	C26-C25-C24	-2.28	102.85	114.42
27	C	302	CDL	OA8-CA7-OA9	-2.27	117.86	123.59
21	O	301	TGL	OG3-CC1-CC2	2.26	119.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	X	101	CHD	O7-C7-C8	2.26	114.48	109.43
25	C	303	CHD	C11-C12-C13	-2.26	108.92	111.24
23	P	315	DMU	C6-C1-C2	2.25	114.69	110.00
23	C	318	DMU	C8-C7-C5	2.25	114.75	110.82
25	Y	104	CHD	C9-C11-C12	-2.25	111.33	114.30
27	P	303	CDL	PB2-OB5-CB3	2.24	124.47	118.30
21	A	609	TGL	OG2-CG2-CG3	2.24	116.50	108.40
23	X	103	DMU	C7-C8-C9	2.24	114.23	110.24
28	P	307	PEK	O11-P-O14	-2.24	100.33	109.07
27	P	303	CDL	OB5-PB2-OB3	2.23	112.73	106.47
25	Y	104	CHD	C5-C6-C7	2.23	116.92	114.46
23	K	101	DMU	C1-C2-C3	2.23	114.77	109.68
15	A	601[A]	HEA	CHA-C4D-ND	2.22	126.84	124.43
15	A	601[B]	HEA	CHA-C4D-ND	2.22	126.84	124.43
25	O	303	CHD	C5-C6-C7	2.21	116.91	114.46
23	K	102	DMU	O1-C9-C11	2.21	111.94	106.44
23	X	106	DMU	C18-O16-C6	-2.21	110.17	113.84
25	X	101	CHD	C16-C17-C13	2.21	105.72	103.55
20	Q	201	PGV	O03-C19-O04	-2.21	118.01	123.59
20	A	607	PGV	O03-C19-O04	-2.21	118.02	123.59
21	A	609	TGL	CG3-CG2-CG1	-2.21	106.56	111.79
23	O	307	DMU	C18-O16-C6	-2.20	110.19	113.84
25	C	303	CHD	C11-C9-C10	-2.20	111.46	113.73
23	X	102	DMU	C2-C3-C4	2.20	115.96	110.93
23	D	206	DMU	C6-C1-C2	2.20	114.57	110.00
27	C	302	CDL	C61-C60-C59	-2.19	103.29	114.42
25	O	303	CHD	C21-C20-C17	-2.19	109.56	112.92
25	X	101	CHD	C11-C12-C13	2.19	113.50	111.24
25	B	303	CHD	C10-C9-C8	2.19	114.17	111.82
27	C	302	CDL	C78-C77-C76	-2.19	103.30	114.42
20	G	102	PGV	C01-O03-C19	2.19	125.23	117.12
27	G	101	CDL	OB8-CB7-C71	2.18	118.76	111.91
21	A	609	TGL	OG2-CB1-OB1	-2.18	118.43	123.70
25	P	306	CHD	C22-C23-C24	-2.18	106.71	112.51
25	O	303	CHD	C4-C5-C10	-2.18	110.34	112.66
25	C	304	CHD	C21-C20-C17	2.18	116.25	112.92
15	A	601[A]	HEA	C2B-C1B-NB	2.18	112.49	109.88
15	A	601[B]	HEA	C2B-C1B-NB	2.18	112.49	109.88
25	X	101	CHD	C11-C9-C8	2.18	114.06	110.88
25	L	104	CHD	C1-C10-C5	2.17	110.98	107.77
25	L	104	CHD	C17-C13-C12	-2.17	115.69	117.67
21	Y	101	TGL	OG3-CC1-CC2	2.17	118.70	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	C	307	PEK	C2-C3-C4	2.16	117.08	113.23
25	P	306	CHD	C16-C17-C20	-2.16	108.81	112.15
25	C	303	CHD	C14-C8-C9	-2.14	106.77	109.71
20	C	301	PGV	C21-C20-C19	-2.14	105.84	113.62
23	K	103	DMU	O5-C4-C57	2.14	111.75	106.44
21	O	301	TGL	OG1-CA1-OA1	-2.14	118.20	123.59
27	P	303	CDL	OA8-CA7-OA9	-2.13	118.21	123.59
15	A	601[A]	HEA	O2A-CGA-CBA	2.13	120.87	114.03
15	A	601[B]	HEA	O2A-CGA-CBA	2.13	120.87	114.03
23	X	104	DMU	C6-C1-C2	-2.13	105.56	110.00
23	X	107	DMU	O5-C6-C1	2.13	114.85	110.35
15	A	601[A]	HEA	C4B-NB-C1B	-2.12	102.88	105.07
15	A	601[B]	HEA	C4B-NB-C1B	-2.12	102.88	105.07
20	C	301	PGV	C04-C05-C06	-2.12	104.13	111.67
25	X	101	CHD	C21-C20-C17	-2.12	109.68	112.92
21	D	201	TGL	OG1-CA1-OA1	-2.12	118.25	123.59
26	O	304	PSC	C03-C02-C01	-2.12	106.78	111.79
15	A	601[A]	HEA	C16-C17-C18	2.12	118.83	111.88
15	N	602	HEA	C20-C19-C18	-2.11	116.84	121.12
15	N	601[A]	HEA	O1A-CGA-CBA	-2.11	116.30	123.08
15	N	601[B]	HEA	O1A-CGA-CBA	-2.11	116.30	123.08
23	Z	101	DMU	O1-C9-C8	2.11	113.53	109.69
21	A	609	TGL	CA5-CA4-CA3	-2.11	103.72	114.42
25	O	303	CHD	O12-C12-C13	-2.11	107.47	111.03
15	N	602	HEA	O2D-CGD-O1D	2.11	128.55	123.30
25	L	104	CHD	C14-C8-C9	-2.10	106.82	109.71
23	X	102	DMU	O1-C9-C11	2.10	111.66	106.44
28	C	309	PEK	O01-C1-O02	-2.10	118.63	123.70
23	C	308	DMU	C25-C22-C19	-2.10	103.77	114.42
25	C	304	CHD	C1-C2-C3	-2.10	107.78	110.47
23	X	105	DMU	C2-C3-C4	-2.10	106.12	110.93
15	A	601[A]	HEA	C3C-C4C-NC	2.09	111.92	109.21
15	A	601[B]	HEA	C3C-C4C-NC	2.09	111.92	109.21
15	A	601[A]	HEA	CHD-C1D-C2D	-2.09	120.94	126.72
15	A	601[B]	HEA	CHD-C1D-C2D	-2.09	120.94	126.72
23	X	107	DMU	C10-O1-C9	2.09	117.79	113.69
23	A	628	DMU	C8-C7-C5	-2.09	107.17	110.82
25	X	101	CHD	C6-C5-C4	-2.09	108.78	111.19
26	O	304	PSC	C28-C27-C26	-2.09	103.82	114.42
25	C	304	CHD	C19-C10-C1	-2.08	104.91	108.26
25	P	306	CHD	C1-C10-C9	2.07	114.61	111.35
25	P	304	CHD	C16-C17-C13	2.07	105.59	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	104	CHD	C1-C10-C9	-2.07	108.09	111.35
20	A	607	PGV	C22-C21-C20	2.07	120.64	113.19
25	P	304	CHD	C23-C22-C20	-2.07	110.73	114.52
20	C	306	PGV	O04-C19-C20	-2.07	115.66	123.73
23	I	101	DMU	O16-C6-C1	2.06	111.53	108.30
21	O	301	TGL	CG3-OG3-CC1	2.06	124.75	117.12
23	K	106	DMU	C7-C8-C9	-2.06	106.56	110.24
21	A	609	TGL	OG2-CG2-CG1	2.06	115.85	108.40
21	Y	101	TGL	OG2-CG2-CG1	2.05	115.84	108.40
23	K	105	DMU	C10-C5-C7	2.05	114.27	110.00
27	G	101	CDL	OB8-CB7-OB9	-2.05	118.42	123.59
15	N	602	HEA	C13-C12-C11	-2.05	111.27	114.35
23	X	105	DMU	O1-C9-C8	2.05	113.42	109.69
27	C	302	CDL	C84-C83-C82	-2.05	104.03	114.42
23	C	317	DMU	C18-O16-C6	-2.05	110.45	113.84
28	T	101	PEK	O01-C1-O02	-2.05	118.76	123.70
25	O	303	CHD	C16-C17-C20	-2.04	108.98	112.15
23	X	104	DMU	C1-C2-C3	-2.04	105.02	109.68
28	C	305	PEK	O01-C1-O02	-2.04	118.77	123.70
25	P	306	CHD	C5-C4-C3	-2.04	109.76	112.76
25	B	303	CHD	C1-C10-C5	2.04	110.79	107.77
26	B	304	PSC	C04-C05-N	-2.04	108.98	115.78
21	D	201	TGL	CC3-CC2-CC1	-2.04	106.22	113.62
23	X	106	DMU	O7-C3-C4	2.04	115.03	109.45
23	X	102	DMU	C7-C8-C9	-2.03	106.62	110.24
15	A	602	HEA	CMC-C2C-C3C	2.03	128.47	124.68
23	A	628	DMU	O5-C6-C1	2.03	114.64	110.35
27	G	101	CDL	C40-C39-C38	2.03	124.71	114.42
25	P	306	CHD	C15-C14-C13	-2.02	101.57	103.55
15	N	601[B]	HEA	C17-C18-C19	2.02	132.52	127.66
25	C	304	CHD	C1-C10-C5	2.02	110.75	107.77
28	P	301	PEK	C3-C4-C5	-2.02	100.88	112.43
15	N	602	HEA	C4B-C3B-C2B	2.01	110.85	107.41
28	C	305	PEK	O13-P-O14	2.01	122.18	112.24
25	C	304	CHD	C22-C20-C17	-2.01	106.13	110.28
27	C	302	CDL	CA6-CA4-CA3	-2.01	107.04	111.79

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	A	601[A]	HEA	ND
15	A	601[A]	HEA	NA

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Mol	Chain	Res	Type	Atom
15	A	601[A]	HEA	NB
15	A	601[B]	HEA	ND
15	A	601[B]	HEA	NA
15	A	601[B]	HEA	NB
15	A	602	HEA	ND
15	A	602	HEA	NA
15	A	602	HEA	NB
15	N	601[A]	HEA	ND
15	N	601[A]	HEA	NA
15	N	601[A]	HEA	NB
15	N	601[B]	HEA	ND
15	N	601[B]	HEA	NA
15	N	601[B]	HEA	NB
15	N	602	HEA	ND
15	N	602	HEA	NA
15	N	602	HEA	NB

All (819) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	A	601[A]	HEA	C18-C19-C20-C21
15	A	601[A]	HEA	C27-C19-C20-C21
20	A	608	PGV	C2-C1-O01-C02
20	A	608	PGV	O04-C19-O03-C01
20	A	608	PGV	C20-C19-O03-C01
20	C	306	PGV	C2-C1-O01-C02
20	C	306	PGV	O04-C19-O03-C01
20	C	306	PGV	C20-C19-O03-C01
20	G	102	PGV	O04-C19-O03-C01
20	G	102	PGV	C20-C19-O03-C01
20	Q	201	PGV	O04-C19-O03-C01
20	Q	201	PGV	C20-C19-O03-C01
20	Q	201	PGV	C10-C11-C12-C13
21	D	201	TGL	CB2-CB1-OG2-CG2
23	D	206	DMU	O5-C6-O16-C18
23	K	101	DMU	C1-C6-O16-C18
23	K	101	DMU	O5-C6-O16-C18
23	K	101	DMU	C19-C18-O16-C6
23	K	102	DMU	C1-C6-O16-C18
23	K	102	DMU	O5-C6-O16-C18
23	K	104	DMU	C19-C18-O16-C6
23	K	106	DMU	O5-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
23	P	314	DMU	C19-C18-O16-C6
23	X	102	DMU	C1-C6-O16-C18
23	X	102	DMU	O5-C6-O16-C18
23	X	103	DMU	C19-C18-O16-C6
23	X	107	DMU	C1-C6-O16-C18
23	X	107	DMU	O5-C6-O16-C18
25	C	303	CHD	C13-C17-C20-C21
25	C	303	CHD	C13-C17-C20-C22
25	C	303	CHD	C16-C17-C20-C22
25	Y	104	CHD	C13-C17-C20-C21
26	B	304	PSC	C04-O12-P-O13
26	B	304	PSC	O02-C1-O01-C02
26	B	304	PSC	C2-C1-O01-C02
26	O	304	PSC	C03-O11-P-O13
26	O	304	PSC	O02-C1-O01-C02
26	O	304	PSC	C2-C1-O01-C02
26	O	304	PSC	C11-C12-C13-C14
27	C	302	CDL	OA7-CA5-OA6-CA4
27	C	302	CDL	OA9-CA7-OA8-CA6
27	C	302	CDL	C31-CA7-OA8-CA6
27	C	302	CDL	CB3-OB5-PB2-OB4
27	G	101	CDL	CA2-OA2-PA1-OA3
27	G	101	CDL	CA2-OA2-PA1-OA4
27	G	101	CDL	CA2-OA2-PA1-OA5
27	G	101	CDL	CA3-OA5-PA1-OA3
27	G	101	CDL	CB3-OB5-PB2-OB2
27	G	101	CDL	CB3-OB5-PB2-OB3
27	P	303	CDL	CA3-OA5-PA1-OA2
27	P	303	CDL	CA3-OA5-PA1-OA3
27	P	303	CDL	OA9-CA7-OA8-CA6
27	P	303	CDL	C31-CA7-OA8-CA6
27	T	102	CDL	CA2-OA2-PA1-OA3
27	T	102	CDL	CA3-OA5-PA1-OA2
27	T	102	CDL	CA3-OA5-PA1-OA3
27	T	102	CDL	OA9-CA7-OA8-CA6
27	T	102	CDL	C31-CA7-OA8-CA6
27	T	102	CDL	CB2-OB2-PB2-OB3
27	T	102	CDL	CB3-OB5-PB2-OB2
27	T	102	CDL	CB3-OB5-PB2-OB3
28	C	305	PEK	C03-O11-P-O13
28	C	305	PEK	C04-O12-P-O13
28	C	305	PEK	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
28	C	305	PEK	O04-C21-O03-C01
28	C	305	PEK	C22-C21-O03-C01
28	C	309	PEK	O04-C21-O03-C01
28	C	309	PEK	C22-C21-O03-C01
28	P	301	PEK	O04-C21-O03-C01
28	P	301	PEK	C22-C21-O03-C01
28	P	301	PEK	C12-C13-C14-C15
28	T	101	PEK	C03-O11-P-O12
28	T	101	PEK	C03-O11-P-O13
28	T	101	PEK	C03-O11-P-O14
28	T	101	PEK	O04-C21-O03-C01
28	T	101	PEK	C22-C21-O03-C01
28	T	101	PEK	C5-C6-C7-C8
23	K	102	DMU	C4-C3-O7-C10
23	K	105	DMU	C2-C3-O7-C10
23	D	206	DMU	C2-C3-O7-C10
23	L	105	DMU	C2-C3-O7-C10
27	G	101	CDL	OA9-CA7-OA8-CA6
23	C	318	DMU	O1-C10-O7-C3
23	A	628	DMU	C2-C3-O7-C10
23	D	206	DMU	O1-C10-O7-C3
23	K	106	DMU	O1-C10-O7-C3
23	O	307	DMU	O1-C10-O7-C3
23	X	105	DMU	O1-C10-O7-C3
27	G	101	CDL	C31-CA7-OA8-CA6
23	C	318	DMU	O6-C11-C9-C8
25	C	303	CHD	C16-C17-C20-C21
25	L	104	CHD	C13-C17-C20-C21
25	L	104	CHD	C16-C17-C20-C22
20	A	608	PGV	O02-C1-O01-C02
20	C	306	PGV	O02-C1-O01-C02
21	D	201	TGL	OB1-CB1-OG2-CG2
23	I	101	DMU	C2-C3-O7-C10
23	K	103	DMU	O6-C11-C9-O1
25	L	104	CHD	C16-C17-C20-C21
25	Y	104	CHD	C16-C17-C20-C22
25	L	104	CHD	C13-C17-C20-C22
28	C	305	PEK	C10-C11-C12-C13
28	C	309	PEK	C10-C11-C12-C13
28	T	101	PEK	C13-C14-C15-C16
21	D	201	TGL	C21-C22-C23-C24
23	X	107	DMU	C2-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
27	G	101	CDL	C80-C81-C82-C83
23	X	105	DMU	O6-C11-C9-C8
23	K	104	DMU	O5-C4-C57-O61
23	P	314	DMU	O5-C4-C57-O61
23	X	105	DMU	O5-C4-C57-O61
23	C	316	DMU	O5-C4-C57-O61
23	X	103	DMU	O5-C4-C57-O61
23	X	105	DMU	O6-C11-C9-O1
23	I	101	DMU	C3-C4-C57-O61
23	L	105	DMU	C3-C4-C57-O61
27	C	302	CDL	C51-CB5-OB6-CB4
23	I	101	DMU	O6-C11-C9-O1
23	L	105	DMU	O6-C11-C9-C8
27	T	102	CDL	C60-C61-C62-C63
21	Y	101	TGL	CC5-CC6-CC7-CC8
23	K	103	DMU	O6-C11-C9-C8
25	X	101	CHD	C17-C20-C22-C23
23	K	104	DMU	O6-C11-C9-O1
23	X	107	DMU	O5-C4-C57-O61
23	C	316	DMU	C3-C4-C57-O61
27	C	302	CDL	C80-C81-C82-C83
27	G	101	CDL	C40-C41-C42-C43
23	C	318	DMU	O6-C11-C9-O1
23	L	105	DMU	O5-C4-C57-O61
15	N	601[A]	HEA	C27-C19-C20-C21
23	X	103	DMU	C3-C4-C57-O61
15	N	601[A]	HEA	C18-C19-C20-C21
25	X	101	CHD	C21-C20-C22-C23
23	C	317	DMU	O5-C4-C57-O61
23	K	105	DMU	O5-C4-C57-O61
23	L	105	DMU	O6-C11-C9-O1
15	N	601[A]	HEA	C15-C16-C17-C18
23	K	106	DMU	C3-C4-C57-O61
28	T	101	PEK	C10-C11-C12-C13
23	M	101	DMU	C28-C31-C34-C37
21	A	609	TGL	CB2-CB1-OG2-CG2
23	K	105	DMU	O6-C11-C9-C8
21	A	609	TGL	OB1-CB1-OG2-CG2
27	C	302	CDL	OB7-CB5-OB6-CB4
23	K	104	DMU	O6-C11-C9-C8
21	D	201	TGL	CC2-CC1-OG3-CG3
23	P	314	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
25	X	101	CHD	C13-C17-C20-C22
25	Y	104	CHD	C13-C17-C20-C22
25	P	304	CHD	C17-C20-C22-C23
23	C	317	DMU	C3-C4-C57-O61
23	K	105	DMU	C3-C4-C57-O61
23	X	105	DMU	C3-C4-C57-O61
23	X	107	DMU	C3-C4-C57-O61
23	C	308	DMU	C19-C22-C25-C28
23	O	307	DMU	O6-C11-C9-C8
20	G	102	PGV	C1-C2-C3-C4
21	B	301	TGL	CB1-CB2-CB3-CB4
23	X	103	DMU	C1-C6-O16-C18
27	T	102	CDL	OB6-CB4-CB6-OB8
23	I	101	DMU	O5-C4-C57-O61
23	P	314	DMU	C4-C3-O7-C10
25	X	101	CHD	C16-C17-C20-C21
20	Q	201	PGV	C2-C1-O01-C02
23	X	106	DMU	O1-C10-O7-C3
21	D	201	TGL	OC1-CC1-OG3-CG3
25	C	303	CHD	C17-C20-C22-C23
23	X	104	DMU	O6-C11-C9-O1
25	P	304	CHD	C21-C20-C22-C23
28	C	305	PEK	C4-C5-C6-C7
23	K	106	DMU	O5-C4-C57-O61
26	O	304	PSC	C19-C20-C21-C22
23	X	106	DMU	O6-C11-C9-O1
27	P	303	CDL	C80-C81-C82-C83
27	T	102	CDL	C40-C41-C42-C43
23	D	206	DMU	O16-C18-C19-C22
22	A	627	EDO	O1-C1-C2-O2
25	X	101	CHD	C13-C17-C20-C21
23	P	305	DMU	O16-C18-C19-C22
25	C	303	CHD	C21-C20-C22-C23
23	X	103	DMU	O5-C6-O16-C18
15	A	601[A]	HEA	C15-C16-C17-C18
21	Y	101	TGL	CB7-CB8-CB9-C10
20	Q	201	PGV	O02-C1-O01-C02
28	C	309	PEK	C13-C14-C15-C16
27	P	303	CDL	C51-CB5-OB6-CB4
20	G	102	PGV	C03-O11-P-O12
26	B	304	PSC	C04-O12-P-O11
26	O	304	PSC	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
26	O	304	PSC	C04-O12-P-O11
28	C	305	PEK	C04-O12-P-O11
23	I	101	DMU	O1-C10-O7-C3
23	Z	101	DMU	O16-C18-C19-C22
21	B	301	TGL	OB1-CB1-OG2-CG2
27	P	303	CDL	OB7-CB5-OB6-CB4
26	O	304	PSC	C04-C05-N-C07
20	G	102	PGV	C6-C7-C8-C9
23	K	104	DMU	C3-C4-C57-O61
21	B	301	TGL	C21-C20-CA9-CA8
27	T	102	CDL	C57-C58-C59-C60
21	B	301	TGL	CB2-CB1-OG2-CG2
28	C	309	PEK	C2-C1-O01-C02
21	A	609	TGL	C19-C33-C34-C35
21	B	301	TGL	CA5-CA6-CA7-CA8
21	Y	101	TGL	CB6-CB7-CB8-CB9
28	P	301	PEK	C24-C25-C26-C27
21	B	301	TGL	CC7-CC8-CC9-C15
21	D	201	TGL	CB9-C10-C11-C12
21	Q	202	TGL	C11-C10-CB9-CB8
21	Q	202	TGL	CA9-C20-C21-C22
21	Y	101	TGL	CB5-CB6-CB7-CB8
26	O	304	PSC	C03-C02-O01-C1
21	Y	101	TGL	OB1-CB1-OG2-CG2
28	C	309	PEK	O02-C1-O01-C02
27	C	302	CDL	CB7-C71-C72-C73
21	A	609	TGL	CC6-CC7-CC8-CC9
21	O	301	TGL	CB6-CB7-CB8-CB9
23	X	103	DMU	C31-C34-C37-C40
28	P	307	PEK	C26-C27-C28-C29
28	C	307	PEK	C7-C8-C9-C10
20	P	302	PGV	C7-C8-C9-C10
21	A	609	TGL	CA5-CA6-CA7-CA8
21	D	201	TGL	CC4-CC5-CC6-CC7
23	K	105	DMU	C22-C25-C28-C31
27	G	101	CDL	C57-C58-C59-C60
28	C	309	PEK	C28-C29-C30-C31
21	B	301	TGL	C17-C18-C19-C33
21	O	301	TGL	CB7-CB8-CB9-C10
21	O	301	TGL	C24-C25-C26-C27
23	K	104	DMU	O16-C18-C19-C22
23	X	102	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
23	O	307	DMU	O6-C11-C9-O1
20	A	608	PGV	C19-C20-C21-C22
21	D	201	TGL	CA1-CA2-CA3-CA4
23	K	103	DMU	O5-C6-O16-C18
23	K	105	DMU	C1-C6-O16-C18
27	G	101	CDL	OB6-CB4-CB6-OB8
23	K	101	DMU	O16-C18-C19-C22
23	K	105	DMU	O6-C11-C9-O1
21	O	301	TGL	CB4-CB5-CB6-CB7
27	G	101	CDL	C20-C21-C22-C23
21	Q	202	TGL	C18-C19-C33-C34
23	C	308	DMU	C22-C25-C28-C31
27	G	101	CDL	C60-C61-C62-C63
25	L	104	CHD	C20-C22-C23-C24
20	C	301	PGV	C7-C8-C9-C10
27	T	102	CDL	C53-C54-C55-C56
20	C	306	PGV	C04-C05-C06-O06
25	Y	104	CHD	C16-C17-C20-C21
21	Y	101	TGL	CB2-CB1-OG2-CG2
21	A	609	TGL	CA9-C20-C21-C22
21	D	201	TGL	C20-C21-C22-C23
23	C	318	DMU	C28-C31-C34-C37
23	K	103	DMU	C25-C28-C31-C34
27	G	101	CDL	C17-C18-C19-C20
21	A	609	TGL	CB5-CB6-CB7-CB8
21	A	609	TGL	CC3-CC4-CC5-CC6
21	D	201	TGL	C16-C15-CC9-CC8
21	Q	202	TGL	C19-C33-C34-C35
23	C	308	DMU	C28-C31-C34-C37
23	L	105	DMU	C28-C31-C34-C37
27	C	302	CDL	C59-C60-C61-C62
23	K	101	DMU	O5-C4-C57-O61
23	C	318	DMU	C19-C22-C25-C28
23	K	106	DMU	C2-C3-O7-C10
28	P	301	PEK	C25-C26-C27-C28
20	A	608	PGV	C7-C8-C9-C10
21	A	609	TGL	C18-C19-C33-C34
21	Q	202	TGL	CA4-CA5-CA6-CA7
21	Q	202	TGL	CC5-CC6-CC7-CC8
23	M	101	DMU	C19-C22-C25-C28
27	G	101	CDL	C14-C15-C16-C17
23	X	107	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
23	Z	101	DMU	C25-C28-C31-C34
27	C	302	CDL	C60-C61-C62-C63
23	K	101	DMU	C18-C19-C22-C25
23	C	317	DMU	C19-C18-O16-C6
23	X	102	DMU	C19-C18-O16-C6
23	X	104	DMU	C19-C18-O16-C6
21	A	609	TGL	CB2-CB3-CB4-CB5
20	C	301	PGV	C19-C20-C21-C22
27	P	303	CDL	C77-C78-C79-C80
27	T	102	CDL	C17-C18-C19-C20
28	P	301	PEK	C4-C5-C6-C7
27	P	303	CDL	C72-C73-C74-C75
21	O	301	TGL	CB5-CB6-CB7-CB8
21	O	301	TGL	CC7-CC8-CC9-C15
21	Q	202	TGL	CB2-CB1-OG2-CG2
23	P	305	DMU	C18-C19-C22-C25
21	O	301	TGL	C23-C24-C25-C26
21	Y	101	TGL	CA3-CA4-CA5-CA6
25	X	101	CHD	C16-C17-C20-C22
27	G	101	CDL	O1-C1-CA2-OA2
21	D	201	TGL	CB4-CB5-CB6-CB7
23	K	103	DMU	C22-C25-C28-C31
23	K	106	DMU	C4-C3-O7-C10
21	Q	202	TGL	CB5-CB6-CB7-CB8
23	K	106	DMU	C22-C25-C28-C31
23	L	105	DMU	C31-C34-C37-C40
23	Z	101	DMU	C22-C25-C28-C31
21	Q	202	TGL	OB1-CB1-OG2-CG2
28	P	301	PEK	O02-C1-O01-C02
23	K	102	DMU	C18-C19-C22-C25
23	C	316	DMU	C18-C19-C22-C25
26	O	304	PSC	C04-C05-N-C06
22	A	613	EDO	O1-C1-C2-O2
22	A	619	EDO	O1-C1-C2-O2
22	C	313	EDO	O1-C1-C2-O2
22	N	610	EDO	O1-C1-C2-O2
22	N	620	EDO	O1-C1-C2-O2
28	P	301	PEK	C2-C1-O01-C02
23	I	101	DMU	O16-C18-C19-C22
23	C	318	DMU	C18-C19-C22-C25
23	X	105	DMU	C18-C19-C22-C25
15	A	601[B]	HEA	C27-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
20	A	608	PGV	C11-C10-C9-C8
21	B	301	TGL	CA2-CA1-OG1-CG1
23	K	104	DMU	C28-C31-C34-C37
23	I	101	DMU	O6-C11-C9-C8
21	A	609	TGL	C16-C15-CC9-CC8
21	D	201	TGL	CC3-CC4-CC5-CC6
21	D	201	TGL	C21-C20-CA9-CA8
21	O	301	TGL	CC6-CC7-CC8-CC9
21	B	301	TGL	CA2-CA3-CA4-CA5
27	P	303	CDL	C36-C37-C38-C39
21	A	609	TGL	C17-C18-C19-C33
21	D	201	TGL	CA3-CA4-CA5-CA6
21	O	301	TGL	CB2-CB1-OG2-CG2
21	Q	202	TGL	CA7-CA8-CA9-C20
21	Y	101	TGL	CA6-CA7-CA8-CA9
21	B	301	TGL	C12-C13-C14-C29
21	O	301	TGL	OB1-CB1-OG2-CG2
21	A	609	TGL	CA1-CA2-CA3-CA4
21	Y	101	TGL	C20-C21-C22-C23
27	G	101	CDL	C43-C44-C45-C46
23	K	106	DMU	C1-C6-O16-C18
26	O	304	PSC	O03-C01-C02-O01
20	P	302	PGV	C30-C31-C32-C33
26	O	304	PSC	C04-C05-N-C08
23	K	103	DMU	C28-C31-C34-C37
23	X	103	DMU	C28-C31-C34-C37
23	A	628	DMU	O5-C4-C57-O61
21	D	201	TGL	C10-C11-C12-C13
21	A	609	TGL	C21-C22-C23-C24
21	Q	202	TGL	CA5-CA6-CA7-CA8
27	C	302	CDL	C36-C37-C38-C39
28	T	101	PEK	C7-C8-C9-C10
23	K	104	DMU	C25-C28-C31-C34
27	C	302	CDL	C77-C78-C79-C80
27	P	303	CDL	C11-C12-C13-C14
21	B	301	TGL	OA1-CA1-OG1-CG1
21	Y	101	TGL	CC9-C15-C16-C17
23	K	105	DMU	C25-C28-C31-C34
23	X	102	DMU	C18-C19-C22-C25
26	O	304	PSC	C01-C02-C03-O11
27	C	302	CDL	OA5-CA3-CA4-CA6
21	O	301	TGL	C21-C20-CA9-CA8

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Mol	Chain	Res	Type	Atoms
23	K	106	DMU	C25-C28-C31-C34
20	G	102	PGV	C3-C4-C5-C6
27	T	102	CDL	C20-C21-C22-C23
23	L	105	DMU	C18-C19-C22-C25
23	X	103	DMU	O6-C11-C9-O1
27	C	302	CDL	C57-C58-C59-C60
27	P	303	CDL	C60-C61-C62-C63
23	C	316	DMU	O16-C18-C19-C22
21	Q	202	TGL	CB4-CB5-CB6-CB7
21	Y	101	TGL	CC3-CC4-CC5-CC6
27	P	303	CDL	C11-CA5-OA6-CA4
21	D	201	TGL	CA9-C20-C21-C22
23	K	102	DMU	C25-C28-C31-C34
21	O	301	TGL	C19-C33-C34-C35
23	P	305	DMU	C22-C25-C28-C31
26	O	304	PSC	O03-C01-C02-C03
27	T	102	CDL	CB3-CB4-CB6-OB8
28	P	307	PEK	C7-C8-C9-C10
21	O	301	TGL	CA5-CA6-CA7-CA8
27	T	102	CDL	C84-C85-C86-C87
23	C	316	DMU	O6-C11-C9-C8
23	L	105	DMU	C34-C37-C40-C43
26	B	304	PSC	C26-C27-C28-C29
27	T	102	CDL	C14-C15-C16-C17
23	L	105	DMU	C19-C22-C25-C28
27	P	303	CDL	C42-C43-C44-C45
23	K	103	DMU	C1-C6-O16-C18
20	A	608	PGV	C20-C21-C22-C23
21	B	301	TGL	C13-C14-C29-C30
23	X	102	DMU	O5-C4-C57-O61
20	Q	201	PGV	C19-C20-C21-C22
23	K	101	DMU	O6-C11-C9-O1
23	O	307	DMU	O5-C4-C57-O61
21	Y	101	TGL	CG1-CG2-OG2-CB1
26	B	304	PSC	C03-C02-O01-C1
28	C	305	PEK	C16-C17-C18-C19
23	P	305	DMU	O6-C11-C9-O1
28	C	305	PEK	C13-C14-C15-C16
28	P	307	PEK	C13-C14-C15-C16
22	F	104	EDO	O1-C1-C2-O2
21	B	301	TGL	C18-C19-C33-C34
23	I	101	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
23	D	206	DMU	C1-C6-O16-C18
27	C	302	CDL	OB6-CB4-CB6-OB8
27	G	101	CDL	OA6-CA4-CA6-OA8
23	A	628	DMU	C34-C37-C40-C43
27	P	303	CDL	C31-C32-C33-C34
27	P	303	CDL	OA7-CA5-OA6-CA4
21	Y	101	TGL	C17-C18-C19-C33
23	X	103	DMU	O16-C18-C19-C22
21	D	201	TGL	C19-C33-C34-C35
21	B	301	TGL	C16-C17-C18-C19
21	Y	101	TGL	C29-C30-C31-C32
23	P	314	DMU	C2-C3-O7-C10
23	X	104	DMU	C25-C28-C31-C34
23	X	106	DMU	C22-C25-C28-C31
20	P	302	PGV	C31-C32-C33-C34
21	Y	101	TGL	CA9-C20-C21-C22
23	I	101	DMU	C4-C3-O7-C10
28	P	307	PEK	C22-C23-C24-C25
23	X	106	DMU	C2-C3-O7-C10
21	A	609	TGL	C29-C30-C31-C32
23	K	103	DMU	C34-C37-C40-C43
20	P	302	PGV	C10-C11-C12-C13
28	P	301	PEK	C7-C8-C9-C10
26	B	304	PSC	C01-C02-C03-O11
27	G	101	CDL	OB5-CB3-CB4-CB6
27	P	303	CDL	OA5-CA3-CA4-CA6
27	T	102	CDL	OB5-CB3-CB4-CB6
28	T	101	PEK	C01-C02-C03-O11
21	B	301	TGL	CC2-CC1-OG3-CG3
27	P	303	CDL	C59-C60-C61-C62
27	T	102	CDL	C81-C82-C83-C84
28	C	307	PEK	C23-C24-C25-C26
27	T	102	CDL	C52-C53-C54-C55
21	D	201	TGL	CC9-C15-C16-C17
21	Y	101	TGL	C24-C25-C26-C27
27	G	101	CDL	CB3-CB4-CB6-OB8
28	P	301	PEK	O03-C01-C02-C03
28	T	101	PEK	O03-C01-C02-C03
20	A	607	PGV	C10-C11-C12-C13
20	N	607	PGV	C10-C11-C12-C13
28	C	307	PEK	C13-C14-C15-C16
23	X	106	DMU	C4-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
26	O	304	PSC	C29-C30-C31-C32
20	G	102	PGV	C23-C24-C25-C26
26	O	304	PSC	C4-C5-C6-C7
23	Z	101	DMU	C34-C37-C40-C43
26	B	304	PSC	C9-C10-C11-C12
26	B	304	PSC	C10-C11-C12-C13
26	O	304	PSC	C9-C10-C11-C12
26	O	304	PSC	C10-C11-C12-C13
28	C	305	PEK	C5-C6-C7-C8
28	C	305	PEK	C6-C7-C8-C9
28	C	305	PEK	C11-C10-C9-C8
28	C	305	PEK	C9-C10-C11-C12
28	C	305	PEK	C11-C12-C13-C14
28	C	305	PEK	C12-C13-C14-C15
28	C	307	PEK	C6-C7-C8-C9
28	C	307	PEK	C9-C10-C11-C12
28	C	307	PEK	C11-C12-C13-C14
28	C	309	PEK	C5-C6-C7-C8
28	C	309	PEK	C11-C12-C13-C14
28	C	309	PEK	C12-C13-C14-C15
28	P	301	PEK	C5-C6-C7-C8
28	P	301	PEK	C11-C10-C9-C8
28	P	301	PEK	C9-C10-C11-C12
28	P	301	PEK	C11-C12-C13-C14
28	P	307	PEK	C9-C10-C11-C12
28	P	307	PEK	C11-C12-C13-C14
28	T	101	PEK	C6-C7-C8-C9
28	T	101	PEK	C11-C10-C9-C8
28	T	101	PEK	C9-C10-C11-C12
28	T	101	PEK	C11-C12-C13-C14
28	T	101	PEK	C12-C13-C14-C15
27	P	303	CDL	OA5-CA3-CA4-OA6
27	C	302	CDL	C40-C41-C42-C43
23	K	104	DMU	C31-C34-C37-C40
28	C	309	PEK	C4-C5-C6-C7
27	G	101	CDL	CA2-C1-CB2-OB2
23	C	318	DMU	O16-C18-C19-C22
20	P	302	PGV	C02-C03-O11-P
23	D	206	DMU	C3-C4-C57-O61
21	D	201	TGL	C23-C24-C25-C26
27	T	102	CDL	C83-C84-C85-C86
23	K	106	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
23	X	104	DMU	O16-C18-C19-C22
27	T	102	CDL	C75-C76-C77-C78
22	A	610	EDO	O1-C1-C2-O2
22	A	611	EDO	O1-C1-C2-O2
22	A	617	EDO	O1-C1-C2-O2
22	J	101	EDO	O1-C1-C2-O2
22	N	608	EDO	O1-C1-C2-O2
22	N	623	EDO	O1-C1-C2-O2
23	K	104	DMU	C34-C37-C40-C43
21	Q	202	TGL	CC9-C15-C16-C17
23	K	102	DMU	O16-C18-C19-C22
28	C	309	PEK	C1-C2-C3-C4
21	O	301	TGL	CC4-CC5-CC6-CC7
20	N	607	PGV	C29-C30-C31-C32
28	C	305	PEK	C7-C8-C9-C10
23	X	102	DMU	C22-C25-C28-C31
27	G	101	CDL	C37-C38-C39-C40
28	T	101	PEK	C28-C29-C30-C31
21	B	301	TGL	CB9-C10-C11-C12
27	C	302	CDL	C61-C62-C63-C64
21	Y	101	TGL	CA2-CA1-OG1-CG1
21	Q	202	TGL	C17-C18-C19-C33
21	B	301	TGL	CC4-CC5-CC6-CC7
21	Y	101	TGL	CC7-CC8-CC9-C15
26	B	304	PSC	C27-C28-C29-C30
21	A	609	TGL	CG1-CG2-OG2-CB1
23	Z	101	DMU	O6-C11-C9-C8
23	C	316	DMU	O6-C11-C9-O1
28	C	307	PEK	C22-C23-C24-C25
23	K	105	DMU	O5-C6-O16-C18
21	Y	101	TGL	C22-C23-C24-C25
21	A	609	TGL	OG1-CG1-CG2-CG3
27	T	102	CDL	CA3-CA4-CA6-OA8
23	C	318	DMU	C3-C4-C57-O61
21	Y	101	TGL	OA1-CA1-OG1-CG1
26	B	304	PSC	O01-C02-C03-O11
27	C	302	CDL	OA5-CA3-CA4-OA6
27	G	101	CDL	OB5-CB3-CB4-OB6
27	T	102	CDL	OB5-CB3-CB4-OB6
28	T	101	PEK	O01-C02-C03-O11
20	G	102	PGV	O12-C04-C05-O05
21	Y	101	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	OC1-CC1-OG3-CG3
21	O	301	TGL	CC5-CC6-CC7-CC8
21	Y	101	TGL	OG1-CG1-CG2-OG2
27	T	102	CDL	OA6-CA4-CA6-OA8
28	C	305	PEK	O03-C01-C02-O01
28	P	301	PEK	O03-C01-C02-O01
28	T	101	PEK	O03-C01-C02-O01
27	P	303	CDL	CA2-OA2-PA1-OA3
21	A	609	TGL	CA4-CA5-CA6-CA7
20	C	306	PGV	O05-C05-C06-O06
20	A	608	PGV	C23-C24-C25-C26
21	Y	101	TGL	CB4-CB5-CB6-CB7
28	P	307	PEK	C4-C5-C6-C7
23	X	105	DMU	C28-C31-C34-C37
21	A	609	TGL	C11-C10-CB9-CB8
20	N	607	PGV	C26-C27-C28-C29
23	K	106	DMU	C19-C22-C25-C28
27	T	102	CDL	C37-C38-C39-C40
27	G	101	CDL	CA3-OA5-PA1-OA2
27	T	102	CDL	CA2-OA2-PA1-OA5
27	T	102	CDL	CB2-OB2-PB2-OB5
28	C	305	PEK	C03-O11-P-O12
20	C	301	PGV	C02-C03-O11-P
20	G	102	PGV	C02-C03-O11-P
20	P	302	PGV	C24-C25-C26-C27
20	A	608	PGV	C03-O11-P-O13
20	G	102	PGV	C03-O11-P-O13
26	O	304	PSC	C03-O11-P-O14
26	O	304	PSC	C04-O12-P-O13
20	A	608	PGV	C01-C02-C03-O11
28	C	305	PEK	C01-C02-C03-O11
21	A	609	TGL	C21-C20-CA9-CA8
22	A	623	EDO	O1-C1-C2-O2
22	E	202	EDO	O1-C1-C2-O2
22	N	615	EDO	O1-C1-C2-O2
26	B	304	PSC	C31-C32-C33-C34
26	O	304	PSC	C11-C10-C9-C8
27	G	101	CDL	C36-C37-C38-C39
21	Y	101	TGL	CB3-CB4-CB5-CB6
23	Z	101	DMU	C28-C31-C34-C37
27	C	302	CDL	C34-C35-C36-C37
21	Q	202	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
23	X	104	DMU	C22-C25-C28-C31
23	X	106	DMU	C19-C18-O16-C6
23	O	307	DMU	C25-C28-C31-C34
28	P	301	PEK	C30-C31-C32-C33
21	O	301	TGL	CB1-CB2-CB3-CB4
23	P	305	DMU	C3-C4-C57-O61
21	D	201	TGL	CG1-CG2-CG3-OG3
21	Y	101	TGL	OG1-CG1-CG2-CG3
26	B	304	PSC	C23-C24-C25-C26
26	O	304	PSC	O12-C04-C05-N
27	C	302	CDL	CB3-CB4-CB6-OB8
28	C	305	PEK	O03-C01-C02-C03
20	Q	201	PGV	O03-C01-C02-O01
21	A	609	TGL	OG1-CG1-CG2-OG2
27	P	303	CDL	OB6-CB4-CB6-OB8
28	C	309	PEK	C32-C33-C34-C35
21	Y	101	TGL	CC2-CC3-CC4-CC5
21	Q	202	TGL	C23-C24-C25-C26
23	X	107	DMU	O1-C10-O7-C3
20	G	102	PGV	C29-C30-C31-C32
21	D	201	TGL	CC5-CC6-CC7-CC8
26	O	304	PSC	C6-C7-C8-C9
27	P	303	CDL	C40-C41-C42-C43
28	C	307	PEK	C25-C26-C27-C28
28	C	307	PEK	O03-C21-C22-C23
21	A	609	TGL	C20-C21-C22-C23
23	K	106	DMU	O16-C18-C19-C22
28	P	307	PEK	C14-C15-C16-C17
25	P	304	CHD	C13-C17-C20-C21
28	C	307	PEK	C17-C18-C19-C20
27	G	101	CDL	OB7-CB5-OB6-CB4
23	P	315	DMU	C18-C19-C22-C25
21	Q	202	TGL	CB3-CB4-CB5-CB6
26	O	304	PSC	O01-C02-C03-O11
23	K	103	DMU	O5-C4-C57-O61
27	G	101	CDL	C77-C78-C79-C80
15	A	601[B]	HEA	C18-C19-C20-C21
22	D	202	EDO	O1-C1-C2-O2
22	J	102	EDO	O1-C1-C2-O2
22	L	101	EDO	O1-C1-C2-O2
22	N	621	EDO	O1-C1-C2-O2
20	A	607	PGV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	O	304	PSC	C21-C22-C23-C24
21	D	201	TGL	OG2-CG2-CG3-OG3
27	C	302	CDL	CA3-OA5-PA1-OA2
27	G	101	CDL	CB2-OB2-PB2-OB5
26	B	304	PSC	O03-C01-C02-C03
27	G	101	CDL	CA3-CA4-CA6-OA8
27	P	303	CDL	CB3-CB4-CB6-OB8
23	D	206	DMU	O5-C4-C57-O61
28	C	309	PEK	C21-C22-C23-C24
21	Y	101	TGL	C10-C11-C12-C13
23	C	308	DMU	O6-C11-C9-O1
20	P	302	PGV	C11-C12-C13-C14
20	G	102	PGV	O12-C04-C05-C06
25	P	304	CHD	C13-C17-C20-C22
28	P	307	PEK	C2-C3-C4-C5
20	A	608	PGV	C10-C11-C12-C13
15	A	601[A]	HEA	CAD-CBD-CGD-O1D
15	A	601[B]	HEA	CAD-CBD-CGD-O1D
21	O	301	TGL	CA9-C20-C21-C22
27	P	303	CDL	C53-C54-C55-C56
21	D	201	TGL	OG3-CC1-CC2-CC3
20	Q	201	PGV	C5-C6-C7-C8
21	A	609	TGL	CB3-CB4-CB5-CB6
23	M	101	DMU	C22-C25-C28-C31
23	X	102	DMU	C19-C22-C25-C28
20	C	301	PGV	C10-C11-C12-C13
28	C	307	PEK	C4-C5-C6-C7
25	O	303	CHD	C22-C23-C24-O25
25	P	304	CHD	C22-C23-C24-O26
21	Y	101	TGL	CC6-CC7-CC8-CC9
28	C	305	PEK	C27-C28-C29-C30
26	B	304	PSC	C12-C13-C14-C15
25	O	303	CHD	C22-C23-C24-O26
22	S	107	EDO	O1-C1-C2-O2
26	O	304	PSC	C28-C29-C30-C31
23	X	104	DMU	O6-C11-C9-C8
20	N	607	PGV	C23-C24-C25-C26
27	G	101	CDL	CB2-C1-CA2-OA2
25	B	303	CHD	C22-C23-C24-O25
27	P	303	CDL	C35-C36-C37-C38
20	C	301	PGV	C27-C28-C29-C30
23	D	206	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
27	G	101	CDL	C41-C42-C43-C44
28	C	307	PEK	C28-C29-C30-C31
15	A	602	HEA	CAA-CBA-CGA-O1A
28	P	301	PEK	C01-C02-O01-C1
21	A	609	TGL	C22-C23-C24-C25
20	C	301	PGV	C26-C27-C28-C29
20	A	607	PGV	C11-C12-C13-C14
26	O	304	PSC	C7-C8-C9-C10
26	O	304	PSC	C12-C13-C14-C15
28	C	305	PEK	C14-C15-C16-C17
15	N	601[A]	HEA	CAD-CBD-CGD-O1D
15	N	601[B]	HEA	CAD-CBD-CGD-O1D
25	X	101	CHD	C22-C23-C24-O25
28	C	305	PEK	C35-C36-C37-C38
28	C	309	PEK	C11-C10-C9-C8
28	P	301	PEK	C6-C7-C8-C9
28	P	307	PEK	C5-C6-C7-C8
21	O	301	TGL	C17-C18-C19-C33
21	O	301	TGL	OC1-CC1-OG3-CG3
23	X	107	DMU	O16-C18-C19-C22
25	B	303	CHD	C22-C23-C24-O26
26	B	304	PSC	C20-C21-C22-C23
27	C	302	CDL	C63-C64-C65-C66
20	G	102	PGV	C30-C31-C32-C33
27	T	102	CDL	C23-C24-C25-C26
23	C	318	DMU	C31-C34-C37-C40
15	N	602	HEA	CAA-CBA-CGA-O2A
15	A	602	HEA	CAA-CBA-CGA-O2A
20	C	306	PGV	C14-C15-C16-C17
21	A	609	TGL	C13-C14-C29-C30
21	D	201	TGL	CB5-CB6-CB7-CB8
23	C	308	DMU	C18-C19-C22-C25
15	A	601[A]	HEA	C16-C17-C18-C19
20	A	607	PGV	C23-C24-C25-C26
21	A	609	TGL	OG2-CB1-CB2-CB3
27	G	101	CDL	C32-C31-CA7-OA8
27	G	101	CDL	C22-C23-C24-C25
22	J	104	EDO	O1-C1-C2-O2
22	M	103	EDO	O1-C1-C2-O2
22	N	618	EDO	O1-C1-C2-O2
22	P	309	EDO	O1-C1-C2-O2
22	P	312	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	S	103	EDO	O1-C1-C2-O2
21	O	301	TGL	CC2-CC1-OG3-CG3
23	L	105	DMU	C25-C28-C31-C34
15	N	602	HEA	CAD-CBD-CGD-O2D
28	C	309	PEK	C30-C31-C32-C33
21	B	301	TGL	C19-C33-C34-C35
25	P	304	CHD	C16-C17-C20-C22
26	O	304	PSC	C20-C21-C22-C23
20	G	102	PGV	C25-C26-C27-C28
20	A	608	PGV	C11-C12-C13-C14
20	C	301	PGV	C11-C12-C13-C14
20	Q	201	PGV	C9-C10-C11-C12
28	C	309	PEK	C14-C15-C16-C17
20	G	102	PGV	C26-C27-C28-C29
21	Q	202	TGL	C20-C21-C22-C23
15	A	602	HEA	CAD-CBD-CGD-O1D
25	P	304	CHD	C22-C23-C24-O25
23	D	206	DMU	C28-C31-C34-C37
21	Y	101	TGL	C25-C26-C27-C28
21	Q	202	TGL	OG2-CG2-CG3-OG3
15	N	602	HEA	CAD-CBD-CGD-O1D
20	N	607	PGV	C30-C31-C32-C33
27	C	302	CDL	CB3-OB5-PB2-OB2
15	N	602	HEA	CAA-CBA-CGA-O1A
21	B	301	TGL	CA1-CA2-CA3-CA4
21	Y	101	TGL	C16-C15-CC9-CC8
21	B	301	TGL	OG3-CC1-CC2-CC3
28	C	305	PEK	C2-C3-C4-C5
27	P	303	CDL	C78-C79-C80-C81
15	A	602	HEA	CAD-CBD-CGD-O2D
20	P	302	PGV	C9-C10-C11-C12
26	B	304	PSC	C7-C8-C9-C10
28	C	307	PEK	C14-C15-C16-C17
28	P	301	PEK	C14-C15-C16-C17
28	T	101	PEK	C14-C15-C16-C17
28	P	301	PEK	C03-C02-O01-C1
28	P	301	PEK	C27-C28-C29-C30
27	C	302	CDL	C58-C59-C60-C61
25	P	306	CHD	C22-C23-C24-O26
21	A	609	TGL	OA1-CA1-OG1-CG1
23	K	103	DMU	C3-C4-C57-O61
20	N	607	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
28	C	305	PEK	C3-C4-C5-C6
28	P	301	PEK	C3-C4-C5-C6
21	A	609	TGL	CB6-CB7-CB8-CB9
25	X	101	CHD	C22-C23-C24-O26
21	Y	101	TGL	CB9-C10-C11-C12
21	O	301	TGL	OA1-CA1-OG1-CG1
21	D	201	TGL	OG1-CA1-CA2-CA3
25	C	303	CHD	C22-C23-C24-O25
25	P	306	CHD	C22-C23-C24-O25
20	Q	201	PGV	C2-C3-C4-C5
27	G	101	CDL	C31-C32-C33-C34
27	T	102	CDL	C16-C17-C18-C19
21	O	301	TGL	C12-C13-C14-C29
22	N	617	EDO	O1-C1-C2-O2
20	C	301	PGV	C9-C10-C11-C12
23	X	107	DMU	C4-C3-O7-C10
27	P	303	CDL	C82-C83-C84-C85
28	T	101	PEK	C29-C30-C31-C32
21	Y	101	TGL	CA7-CA8-CA9-C20
21	O	301	TGL	OG2-CG2-CG3-OG3
20	C	306	PGV	C9-C10-C11-C12
23	K	106	DMU	C28-C31-C34-C37
21	Y	101	TGL	CC2-CC1-OG3-CG3
15	N	601[A]	HEA	C19-C20-C21-C22
20	A	608	PGV	C14-C15-C16-C17
21	B	301	TGL	C16-C15-CC9-CC8
15	A	601[A]	HEA	CAD-CBD-CGD-O2D
15	A	601[B]	HEA	CAD-CBD-CGD-O2D
27	T	102	CDL	C32-C31-CA7-OA8
15	N	601[A]	HEA	CAD-CBD-CGD-O2D
15	N	601[B]	HEA	CAD-CBD-CGD-O2D
25	C	304	CHD	C22-C23-C24-O25
21	D	201	TGL	OA1-CA1-CA2-CA3
23	C	308	DMU	C31-C34-C37-C40
20	C	306	PGV	C11-C12-C13-C14
21	Q	202	TGL	CA6-CA7-CA8-CA9
21	Y	101	TGL	CA2-CA3-CA4-CA5
23	C	308	DMU	C3-C4-C57-O61
23	M	101	DMU	C34-C37-C40-C43
28	C	307	PEK	C26-C27-C28-C29
21	A	609	TGL	CA2-CA1-OG1-CG1
21	O	301	TGL	CA2-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
21	Q	202	TGL	CC2-CC3-CC4-CC5
23	X	106	DMU	C5-C10-O7-C3
20	P	302	PGV	C15-C16-C17-C18
23	X	105	DMU	C25-C28-C31-C34
21	Y	101	TGL	OC1-CC1-OG3-CG3
20	A	607	PGV	O03-C19-C20-C21
27	G	101	CDL	OA7-CA5-OA6-CA4
20	C	301	PGV	C05-C04-O12-P
21	A	609	TGL	C14-C29-C30-C31
21	B	301	TGL	OC1-CC1-CC2-CC3
23	A	628	DMU	C1-C6-O16-C18
28	C	305	PEK	C03-O11-P-O14
23	X	105	DMU	C5-C10-O7-C3
25	C	304	CHD	C22-C23-C24-O26
28	T	101	PEK	C25-C26-C27-C28
22	A	625	EDO	O1-C1-C2-O2
22	A	626	EDO	O1-C1-C2-O2
22	N	609	EDO	O1-C1-C2-O2
22	N	611	EDO	O1-C1-C2-O2
22	Y	102	EDO	O1-C1-C2-O2
22	Z	102	EDO	O1-C1-C2-O2
27	T	102	CDL	C79-C80-C81-C82
27	P	303	CDL	C33-C34-C35-C36
20	Q	201	PGV	C01-C02-O01-C1
27	T	102	CDL	OB9-CB7-OB8-CB6
15	A	601[A]	HEA	CAA-CBA-CGA-O2A
15	A	601[B]	HEA	CAA-CBA-CGA-O2A
21	B	301	TGL	CC9-C15-C16-C17
27	P	303	CDL	C32-C31-CA7-OA8
21	B	301	TGL	OG1-CA1-CA2-CA3
28	T	101	PEK	O02-C1-O01-C02
27	P	303	CDL	C32-C31-CA7-OA9
26	B	304	PSC	C22-C23-C24-C25
23	X	105	DMU	C19-C18-O16-C6
20	N	607	PGV	O03-C19-C20-C21
28	P	307	PEK	C17-C18-C19-C20
15	A	601[A]	HEA	CAA-CBA-CGA-O1A
15	A	601[B]	HEA	CAA-CBA-CGA-O1A
27	G	101	CDL	O1-C1-CB2-OB2
28	T	101	PEK	C3-C4-C5-C6
21	B	301	TGL	OA1-CA1-CA2-CA3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	L	104	CHD	C1-C10-C2-C3-C4-C5

95 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	105	DMU	4	0
23	K	104	DMU	1	0
23	D	206	DMU	1	0
22	N	610	EDO	1	0
22	A	617	EDO	1	0
22	A	627	EDO	1	0
21	O	301	TGL	4	0
28	C	305	PEK	11	0
21	D	201	TGL	12	0
23	I	101	DMU	4	0
26	O	304	PSC	9	0
22	D	202	EDO	2	0
15	A	601[B]	HEA	1	0
23	K	101	DMU	2	0
22	V	101	EDO	2	0
25	L	104	CHD	1	0
15	A	601[A]	HEA	2	0
19	A	606	PER	1	0
25	P	304	CHD	2	0
23	P	314	DMU	5	0
15	A	602	HEA	1	0
22	A	622	EDO	2	0
23	M	101	DMU	1	0
22	M	102	EDO	1	0
22	S	103	EDO	1	0
22	S	107	EDO	2	0
23	X	103	DMU	3	0
23	X	107	DMU	1	0
28	C	309	PEK	4	0
22	A	619	EDO	2	0
23	A	628	DMU	1	0
28	P	307	PEK	1	0
23	K	105	DMU	2	0
22	A	623	EDO	1	0
20	Q	201	PGV	5	0
23	K	103	DMU	1	0
28	C	307	PEK	5	0
21	Y	101	TGL	8	0
22	J	104	EDO	1	0

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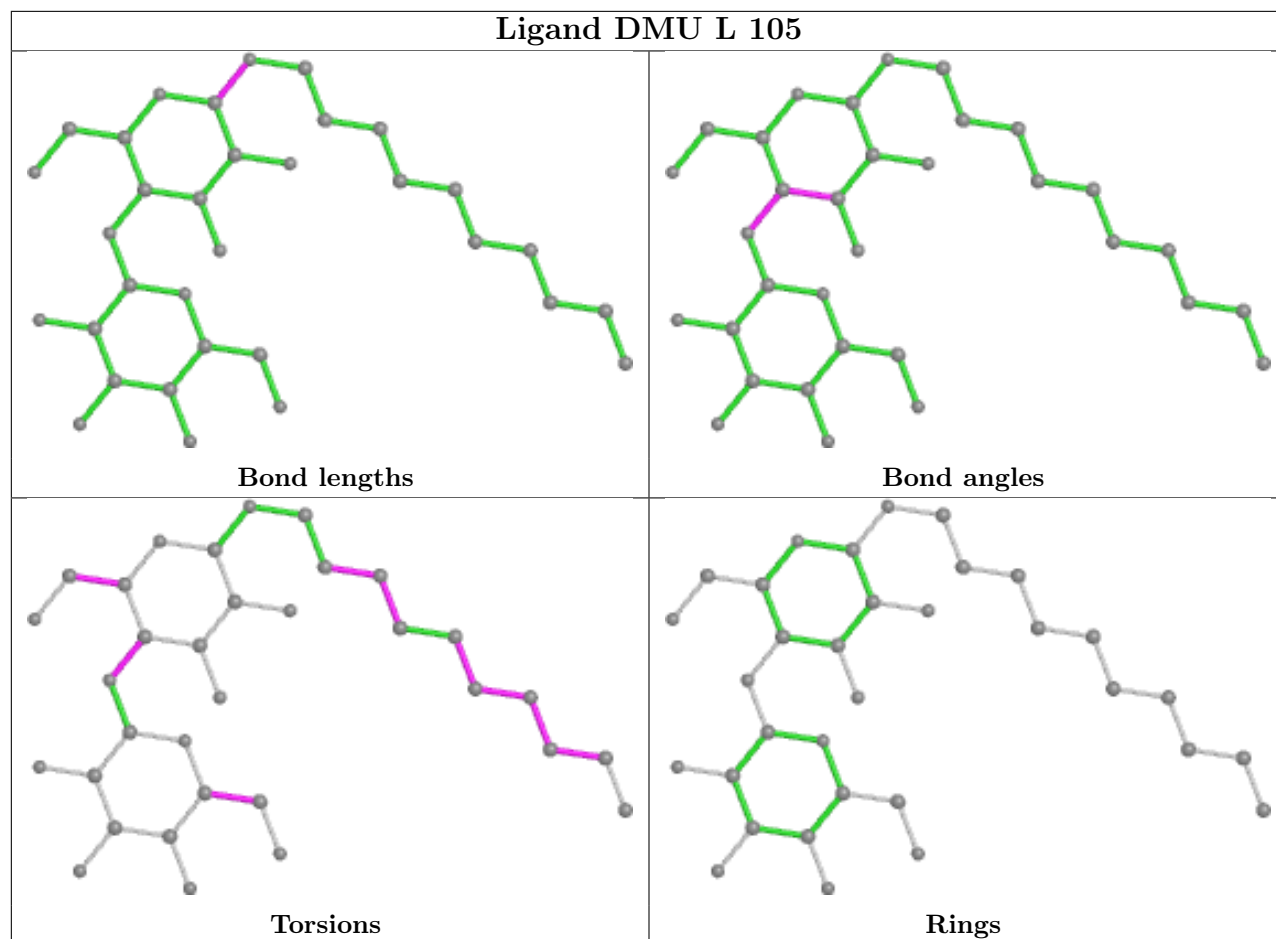
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	S	108	EDO	2	0
23	P	315	DMU	1	0
27	G	101	CDL	18	0
22	N	609	EDO	2	0
15	N	601[B]	HEA	1	0
21	A	609	TGL	12	0
15	N	602	HEA	2	0
28	P	301	PEK	6	0
23	K	102	DMU	2	0
22	A	626	EDO	1	0
15	N	601[A]	HEA	1	0
22	A	620	EDO	2	0
25	O	303	CHD	1	0
22	B	308	EDO	1	0
22	N	624	EDO	1	0
23	C	308	DMU	2	0
22	A	610	EDO	5	0
22	A	625	EDO	4	0
22	P	313	EDO	1	0
19	N	606	PER	1	0
22	C	313	EDO	1	0
22	A	612	EDO	1	0
20	A	607	PGV	1	0
22	W	101	EDO	1	0
28	T	101	PEK	5	0
23	C	318	DMU	1	0
20	N	607	PGV	1	0
22	A	613	EDO	2	0
22	G	105	EDO	1	0
21	Q	202	TGL	8	0
20	A	608	PGV	1	0
22	H	101	EDO	1	0
22	Q	203	EDO	1	0
22	N	622	EDO	6	0
23	X	104	DMU	3	0
23	P	305	DMU	4	0
22	A	611	EDO	1	0
22	A	621	EDO	4	0
27	T	102	CDL	21	0
25	X	101	CHD	7	0
20	C	306	PGV	1	0
22	N	613	EDO	2	0

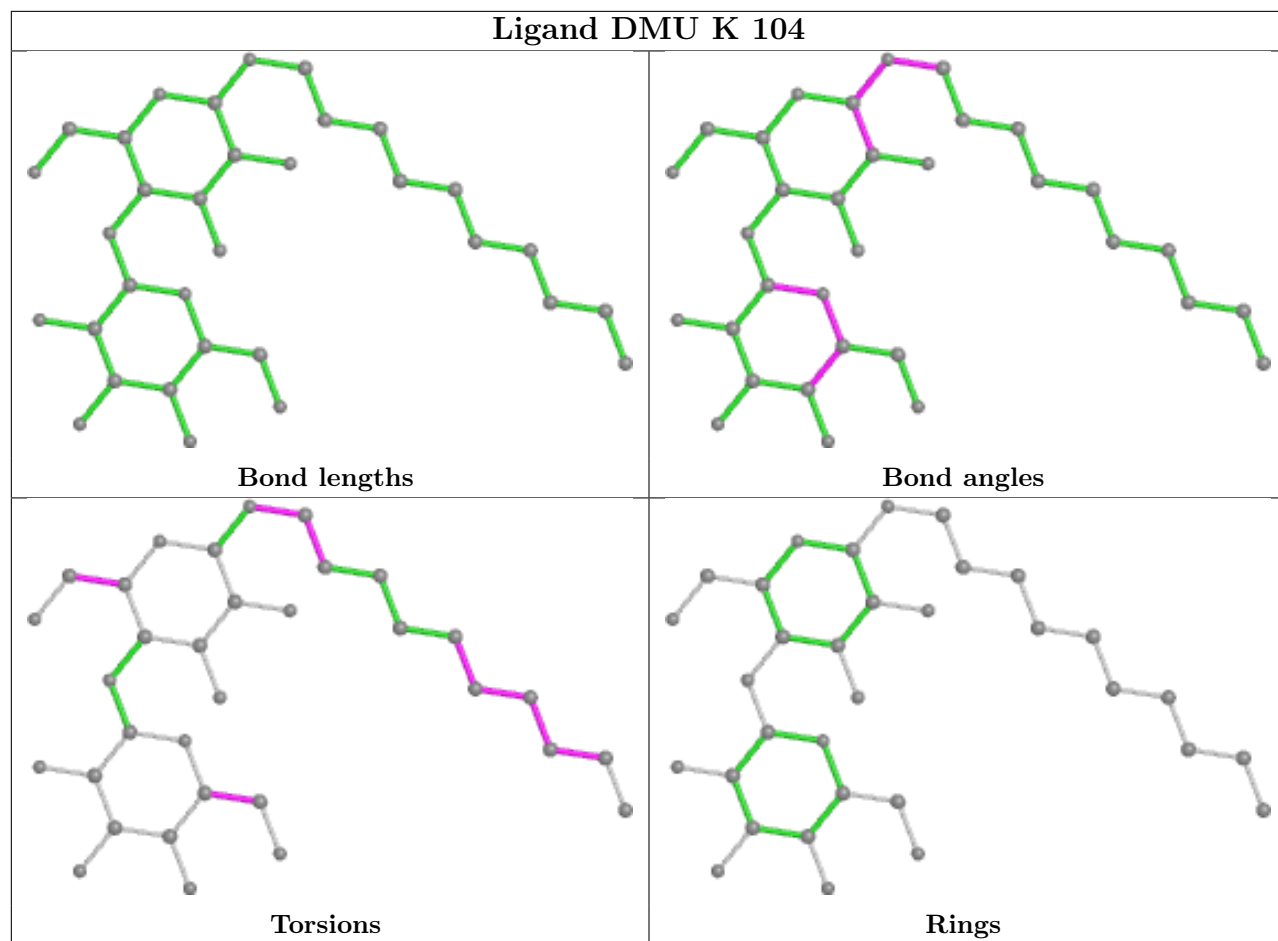
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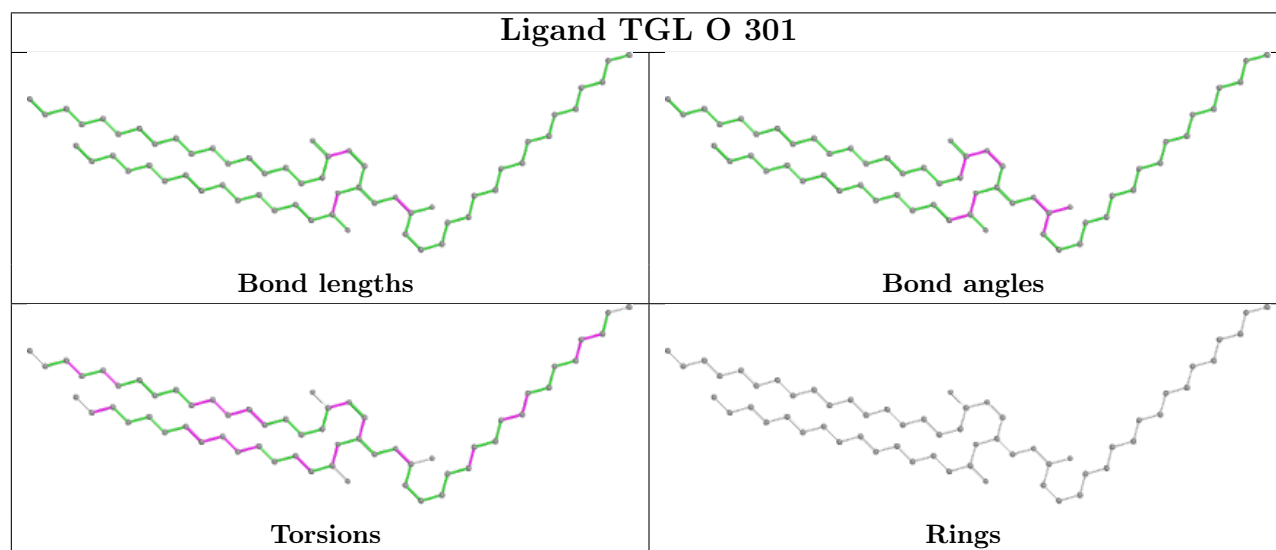
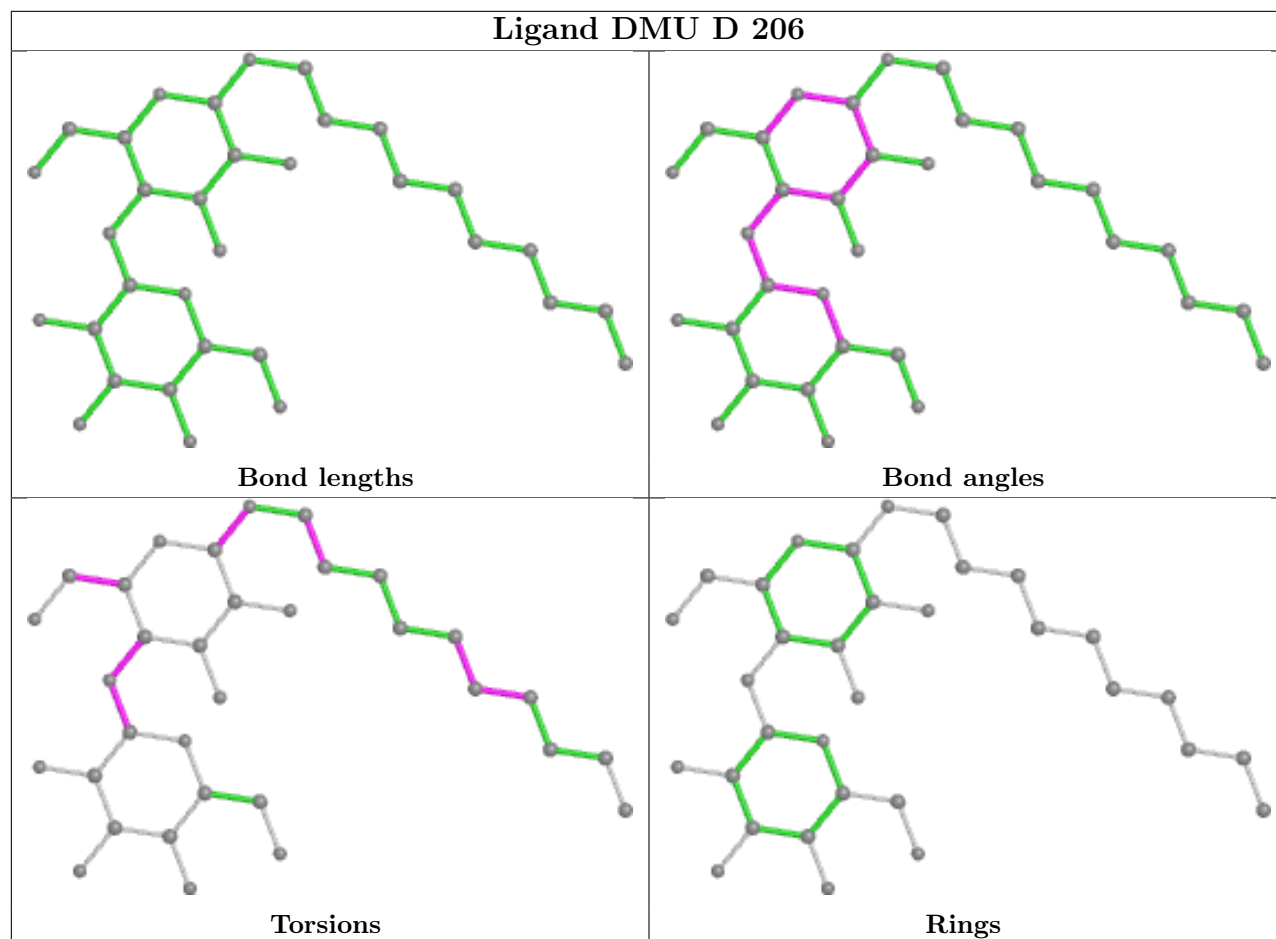
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	P	302	PGV	1	0
25	C	303	CHD	2	0
23	X	106	DMU	2	0
27	C	302	CDL	8	0
22	S	104	EDO	1	0
21	B	301	TGL	6	0
20	G	102	PGV	2	0
23	C	317	DMU	2	0
27	P	303	CDL	11	0
23	K	106	DMU	1	0
25	P	306	CHD	1	0
23	X	105	DMU	2	0
23	C	316	DMU	1	0
26	B	304	PSC	11	0

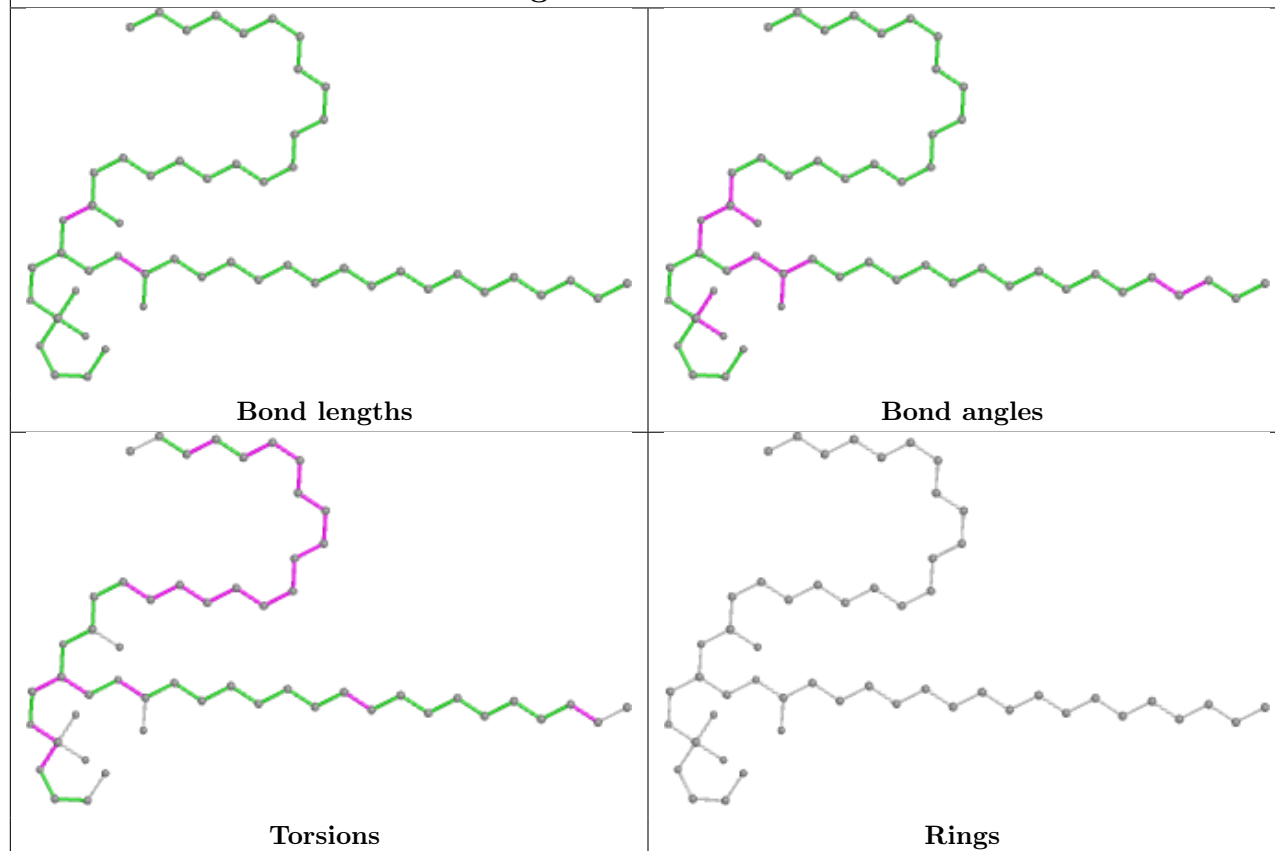
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



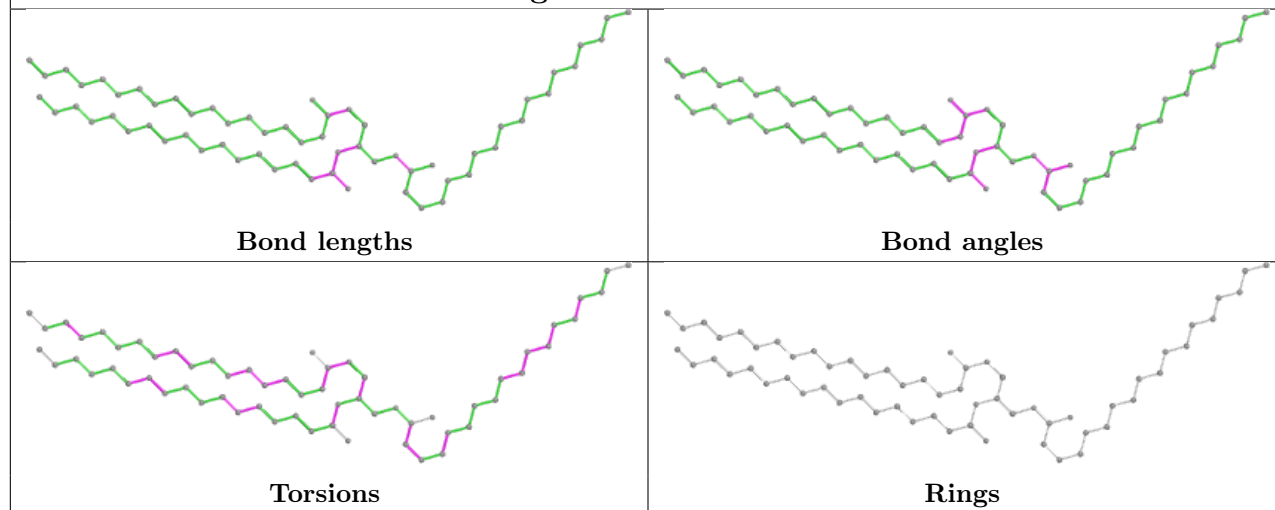




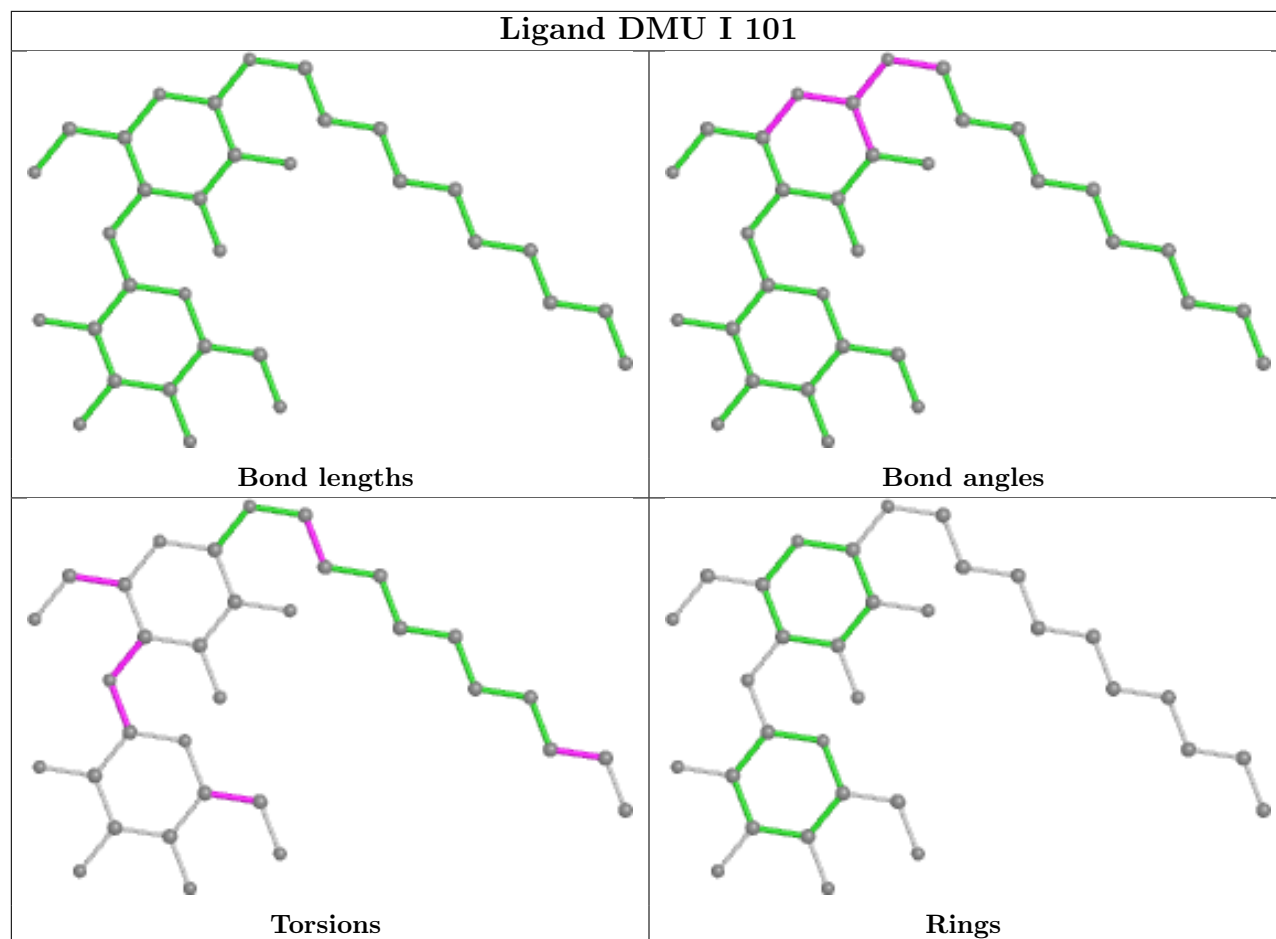
Ligand PEK C 305



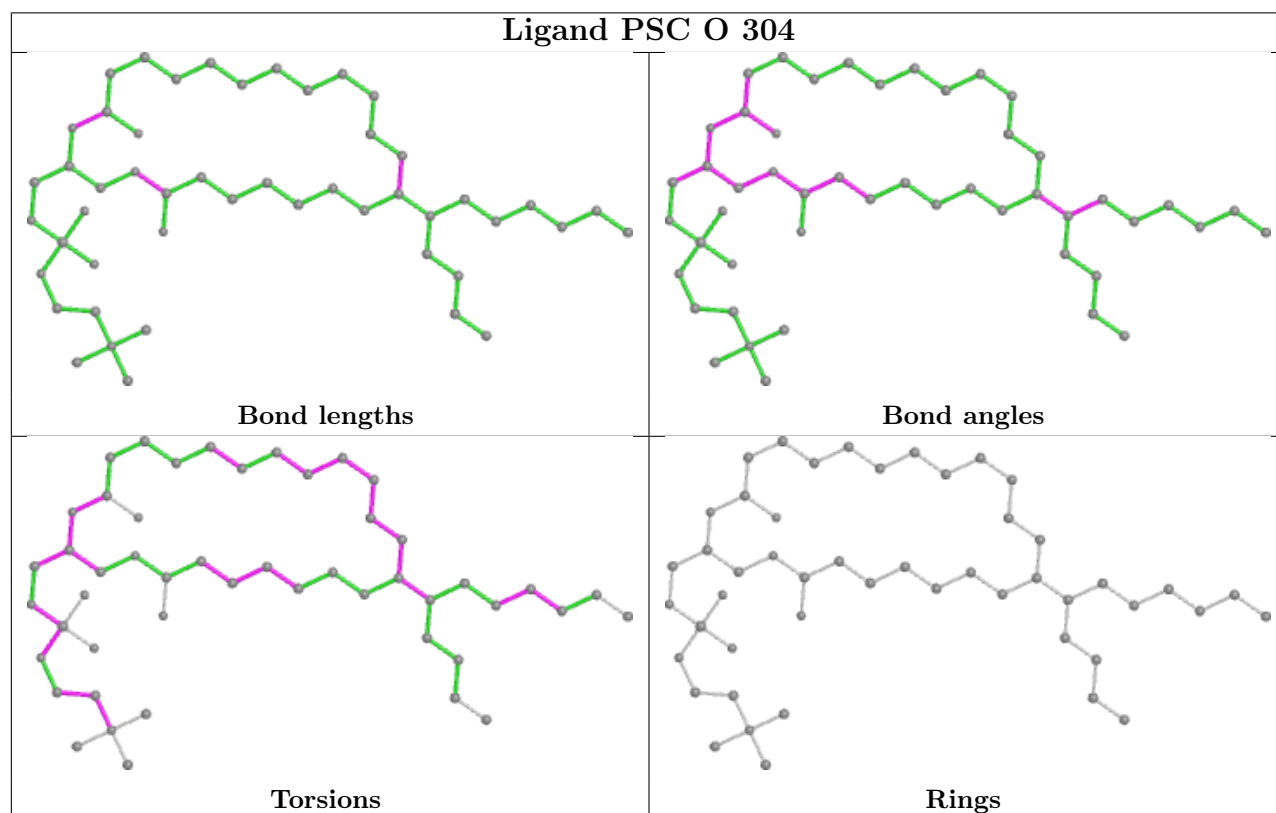
Ligand TGL D 201



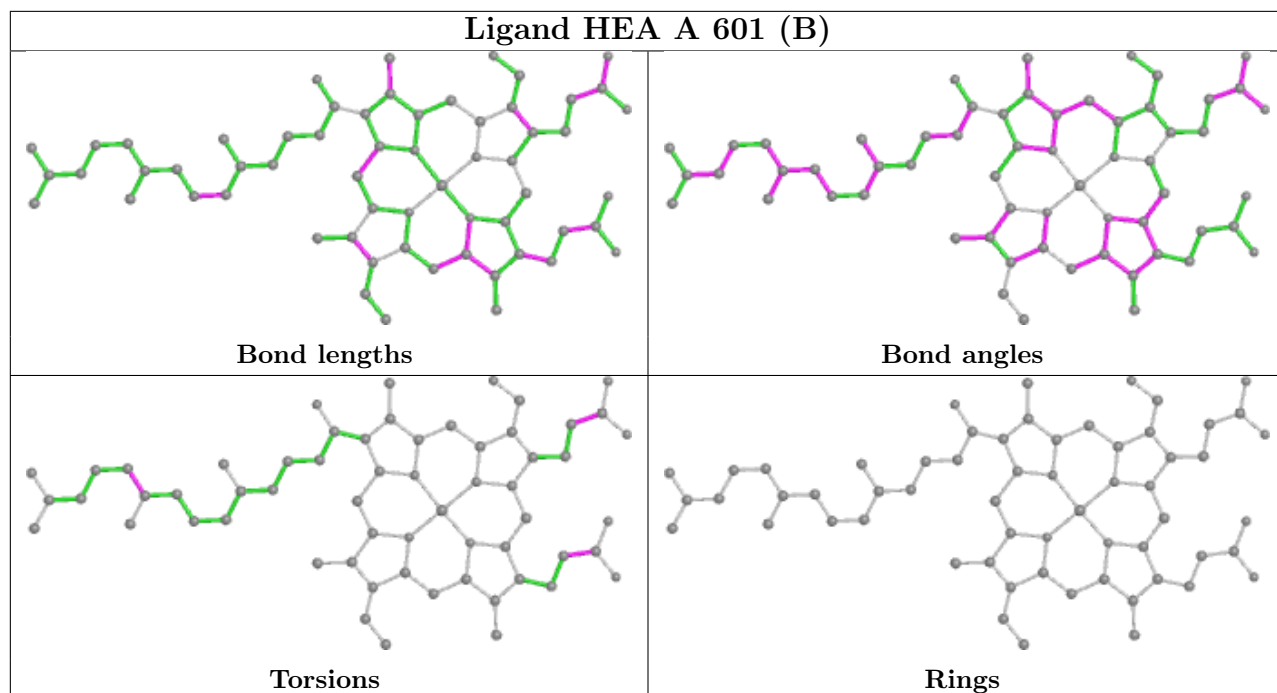
Ligand DMU I 101



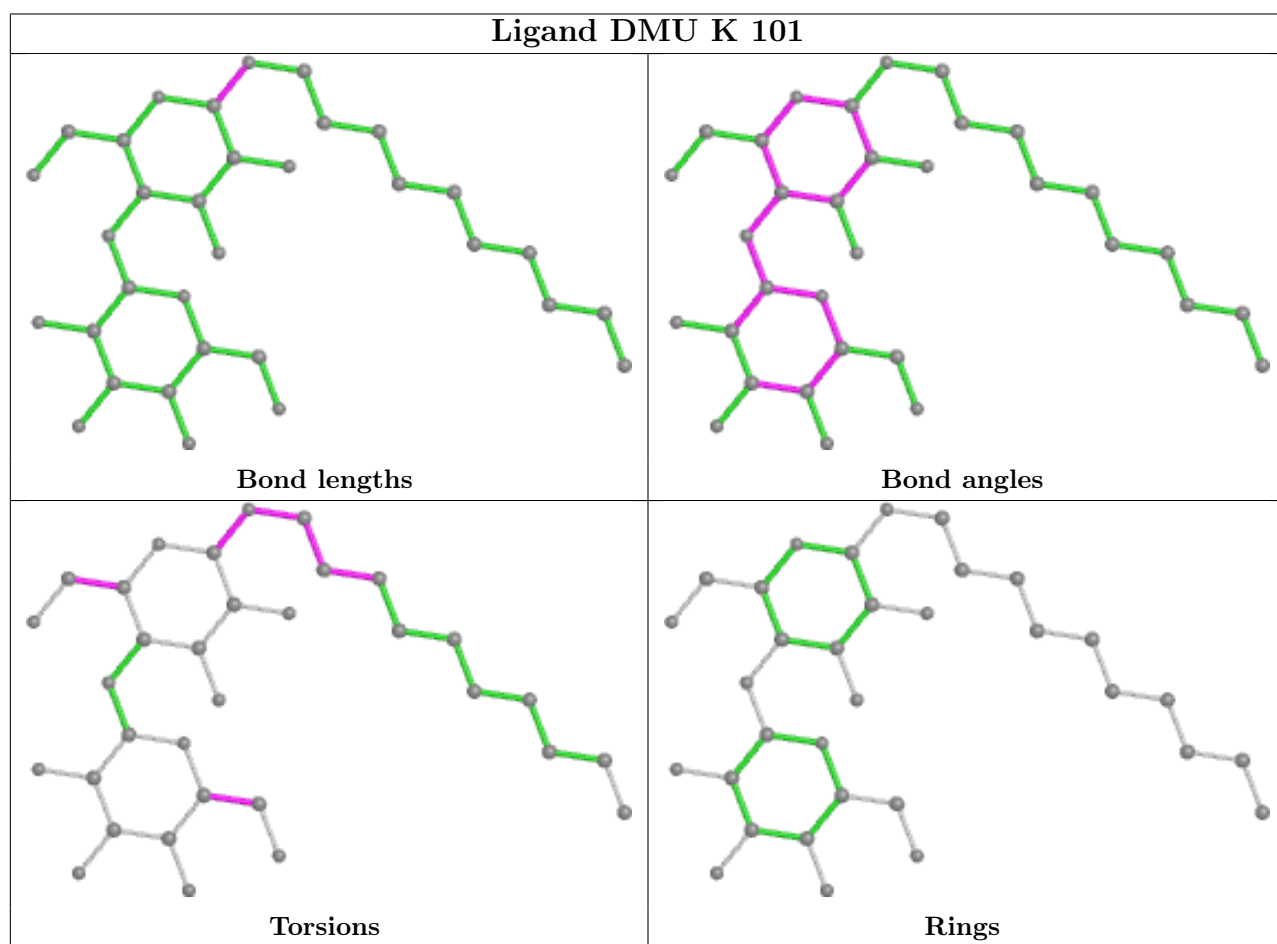
Ligand PSC O 304

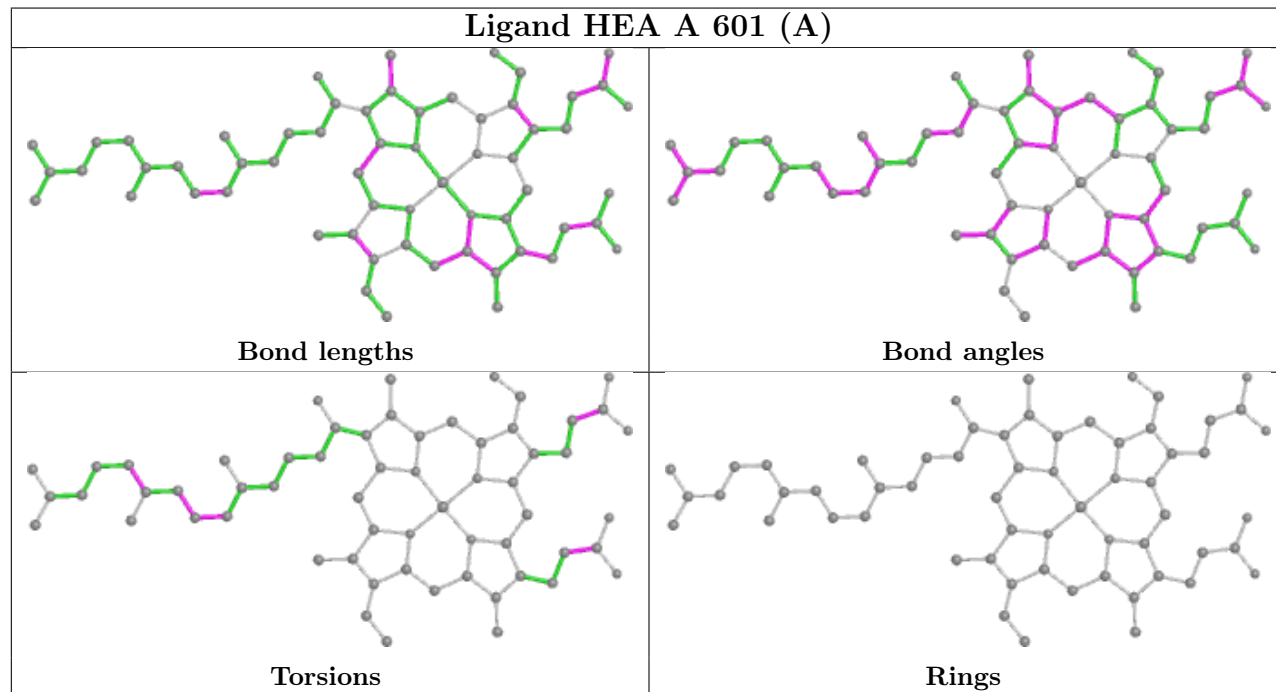
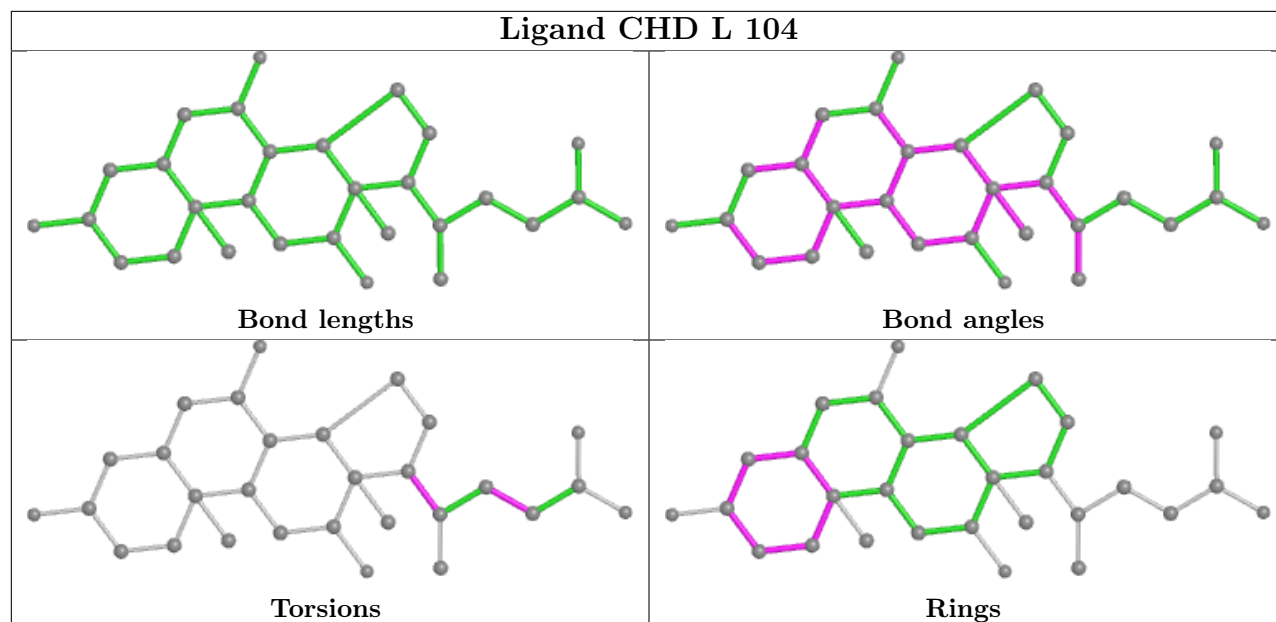


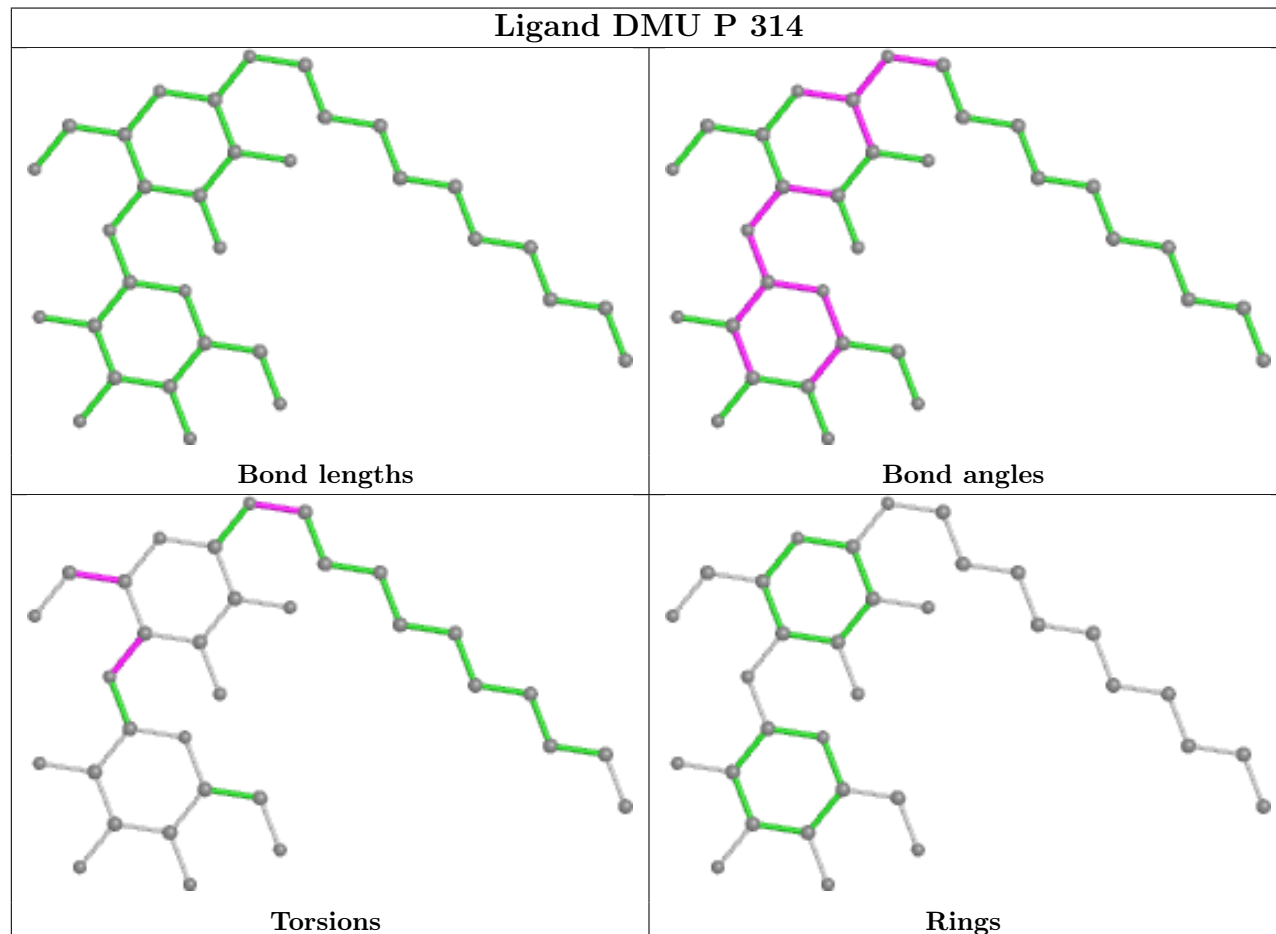
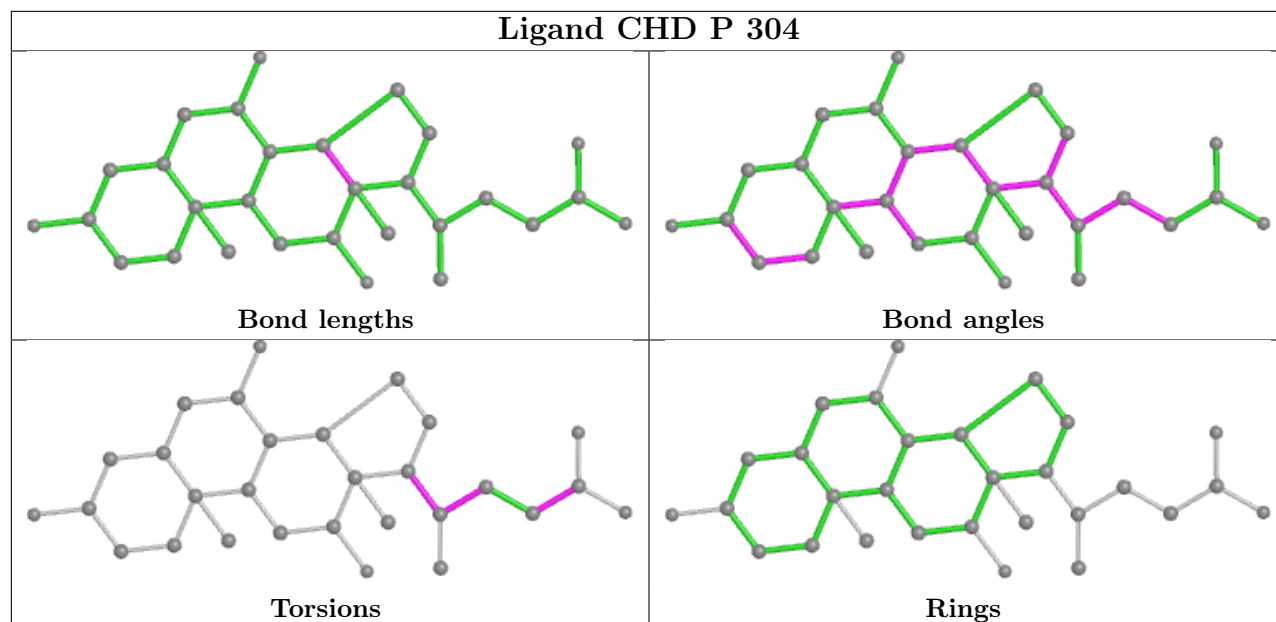
Ligand HEA A 601 (B)

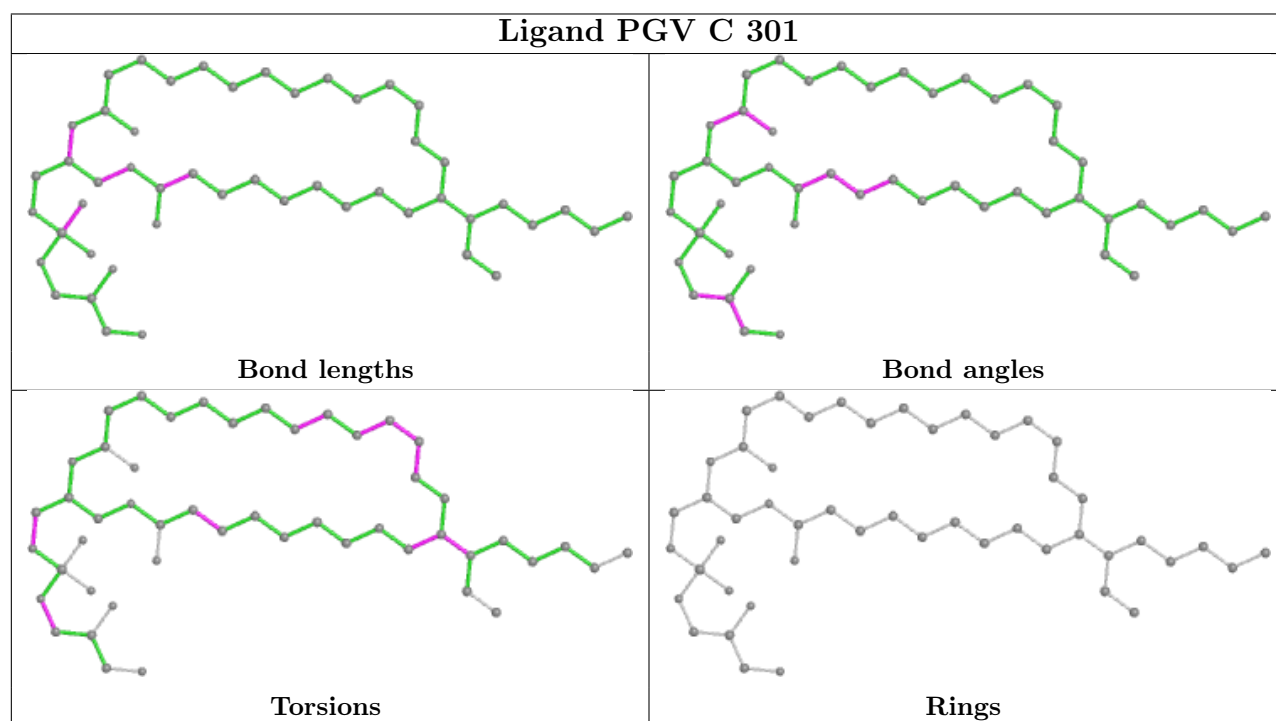
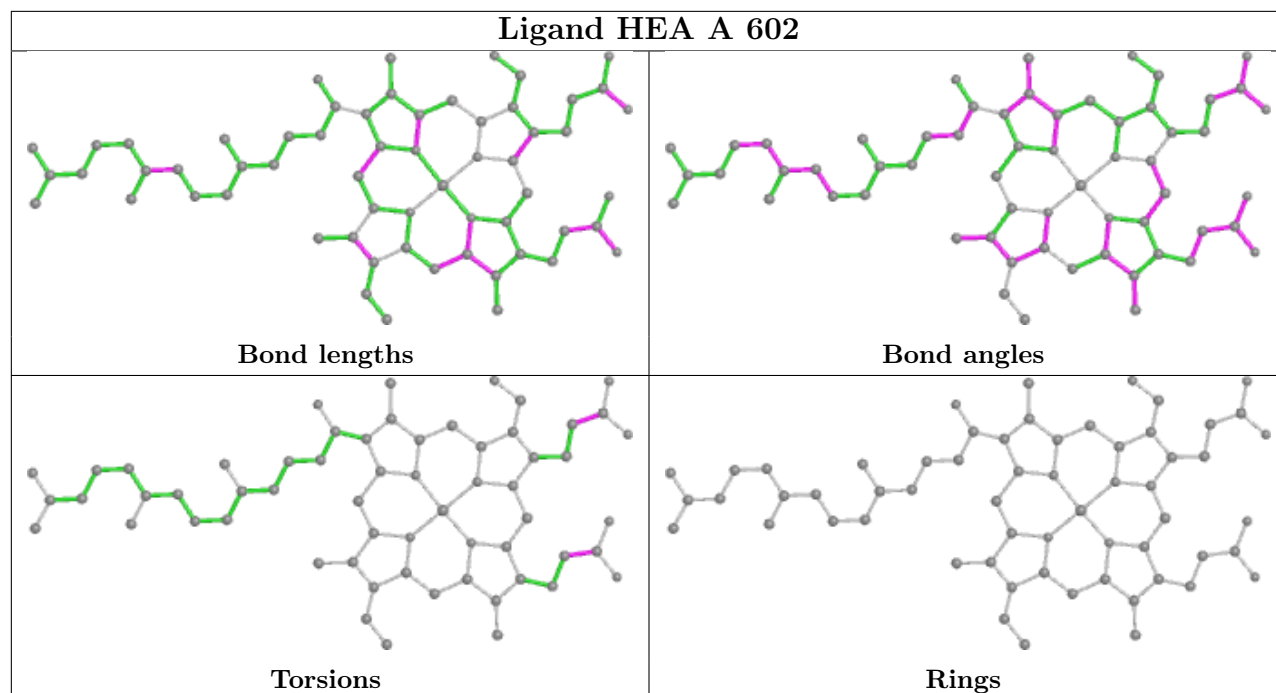


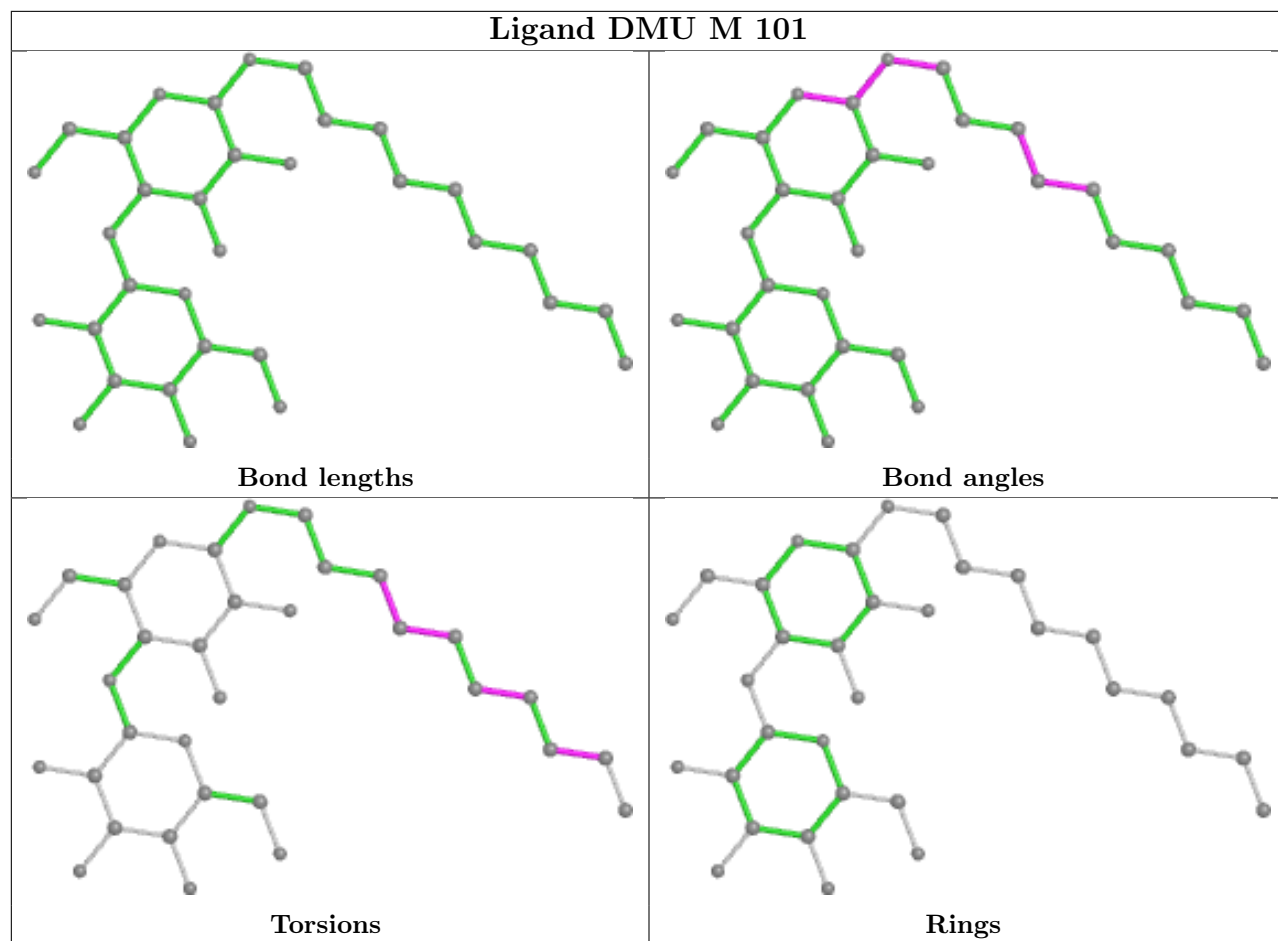
Ligand DMU K 101

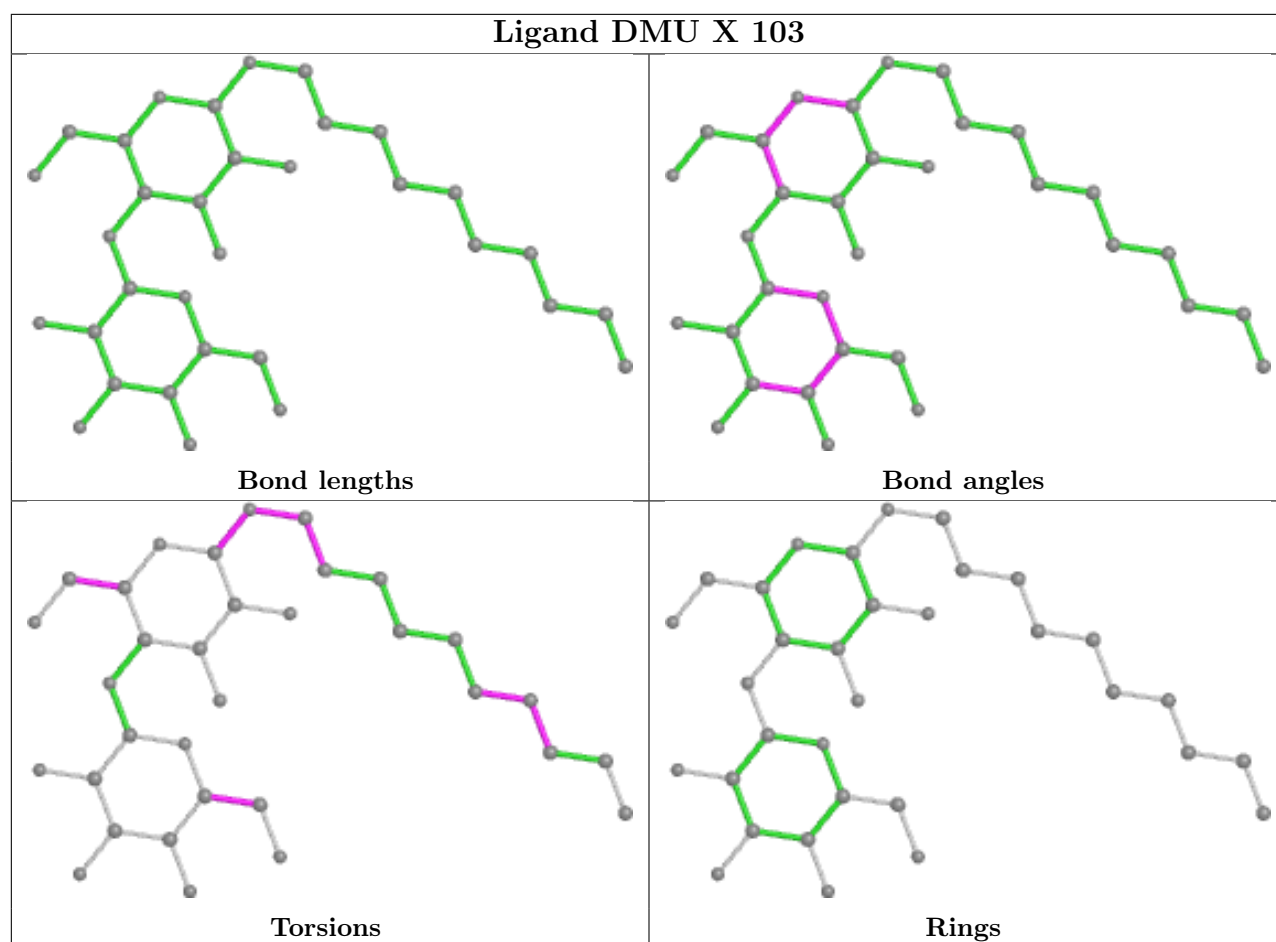


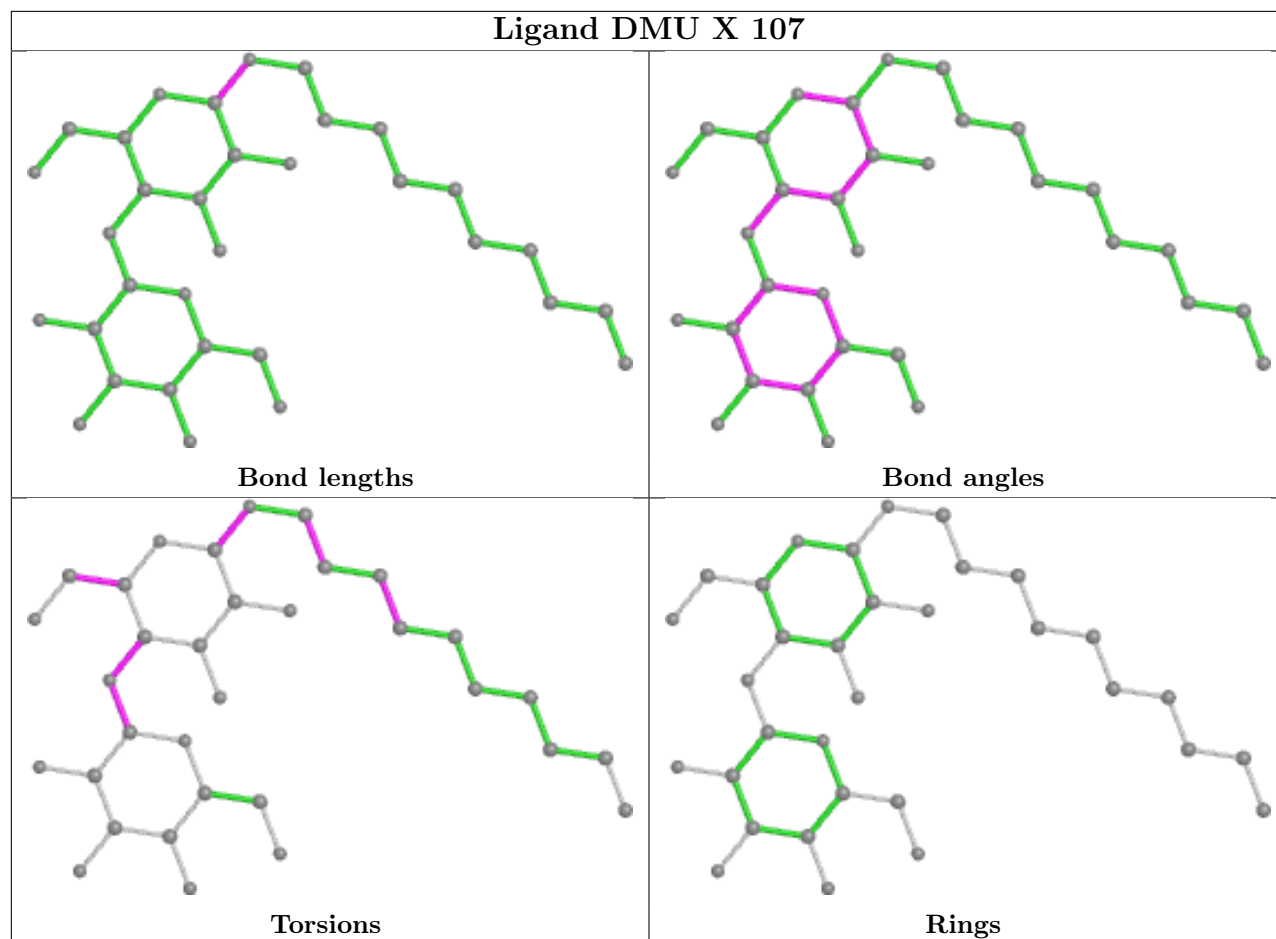


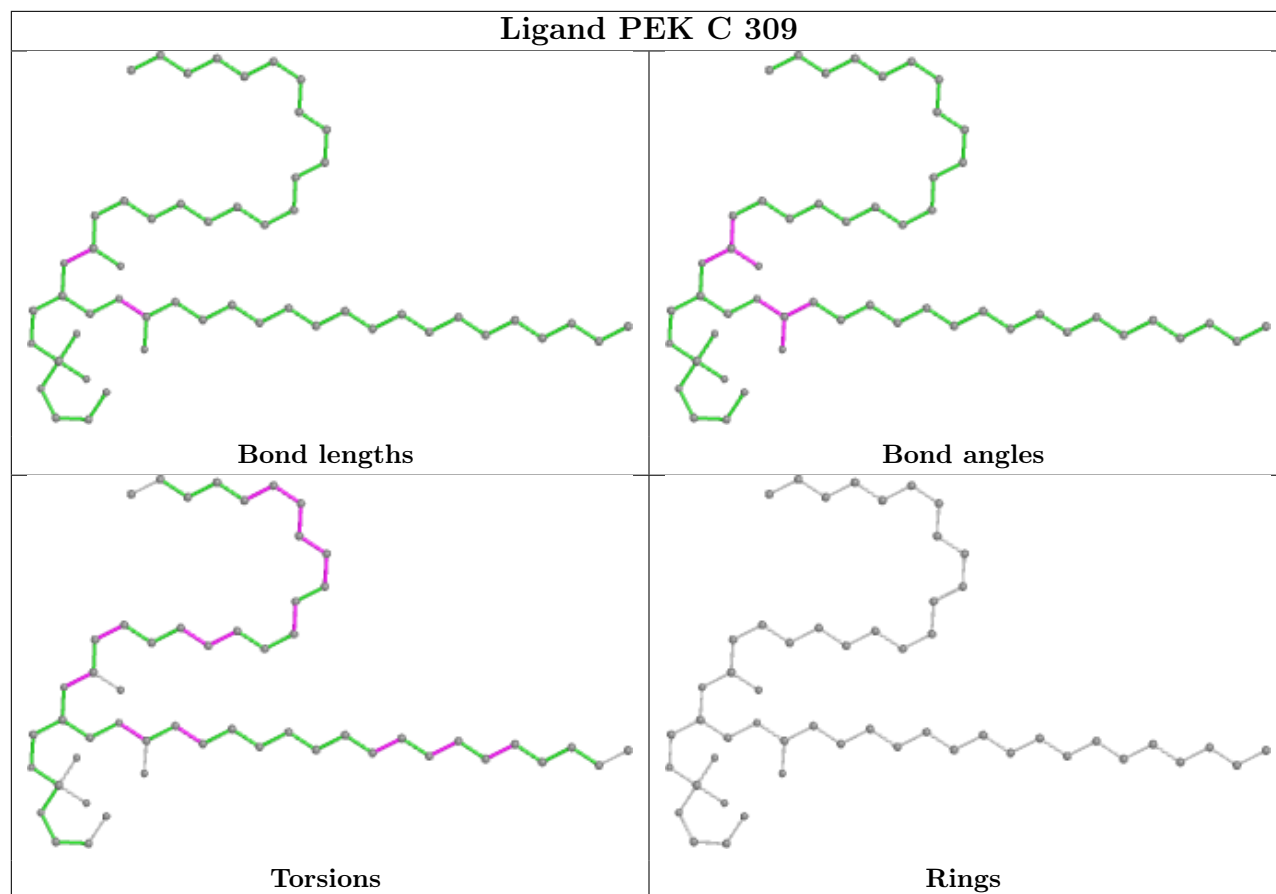


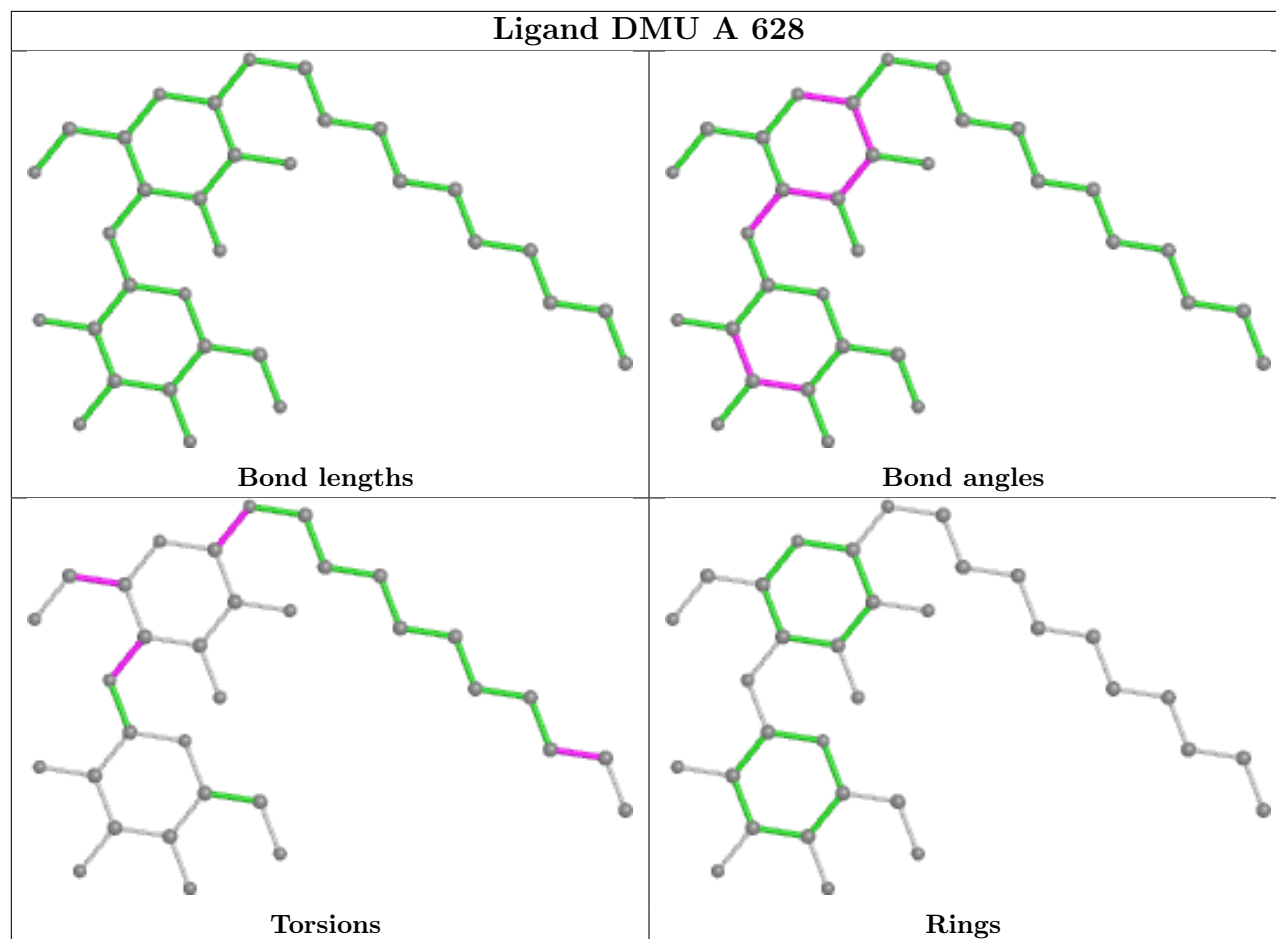


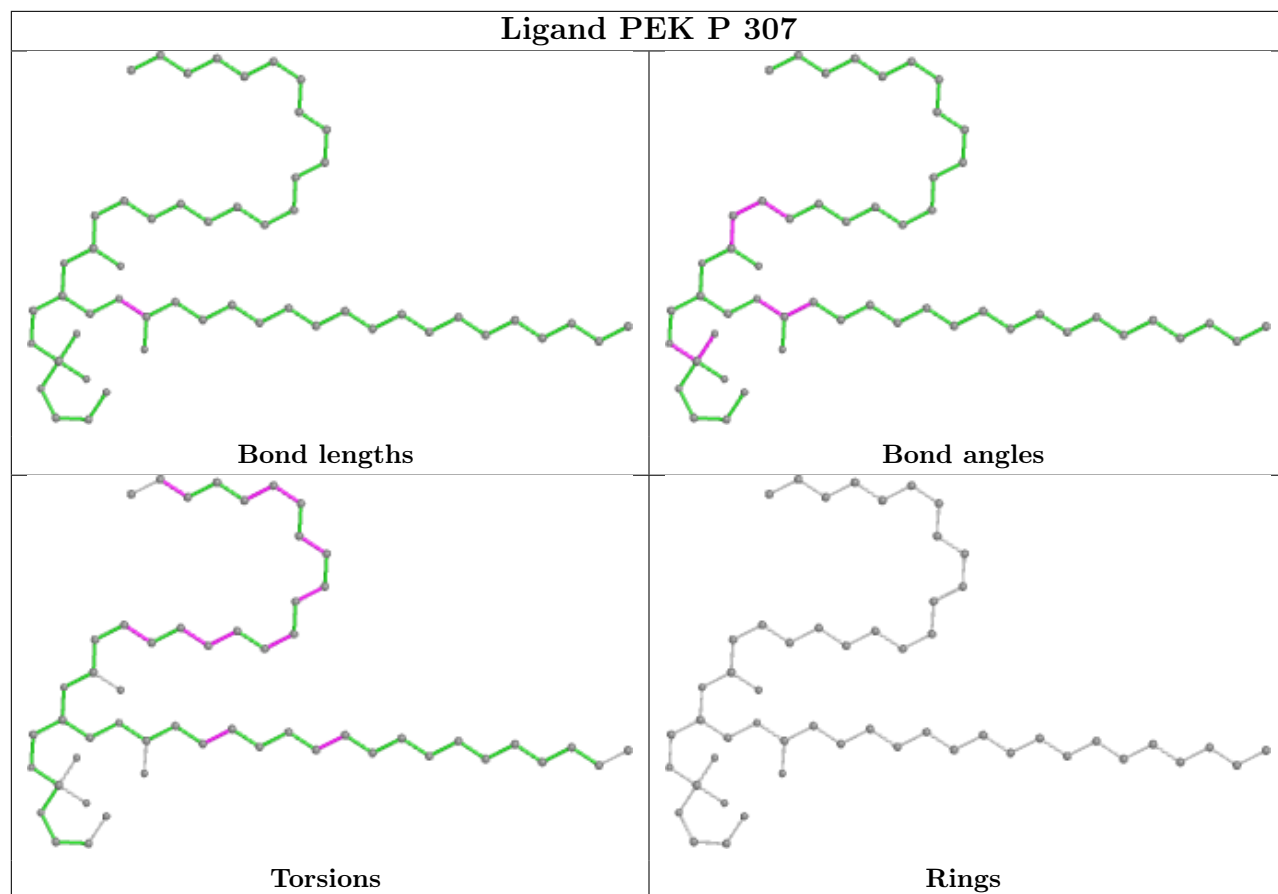


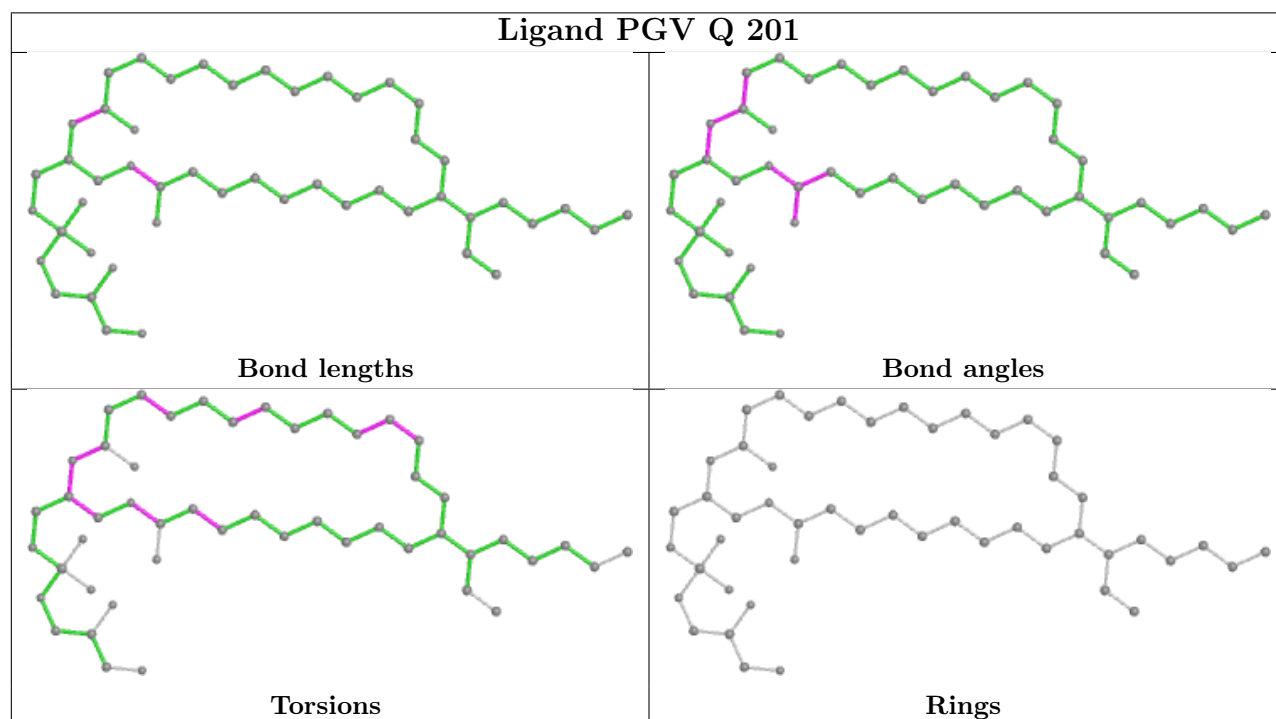
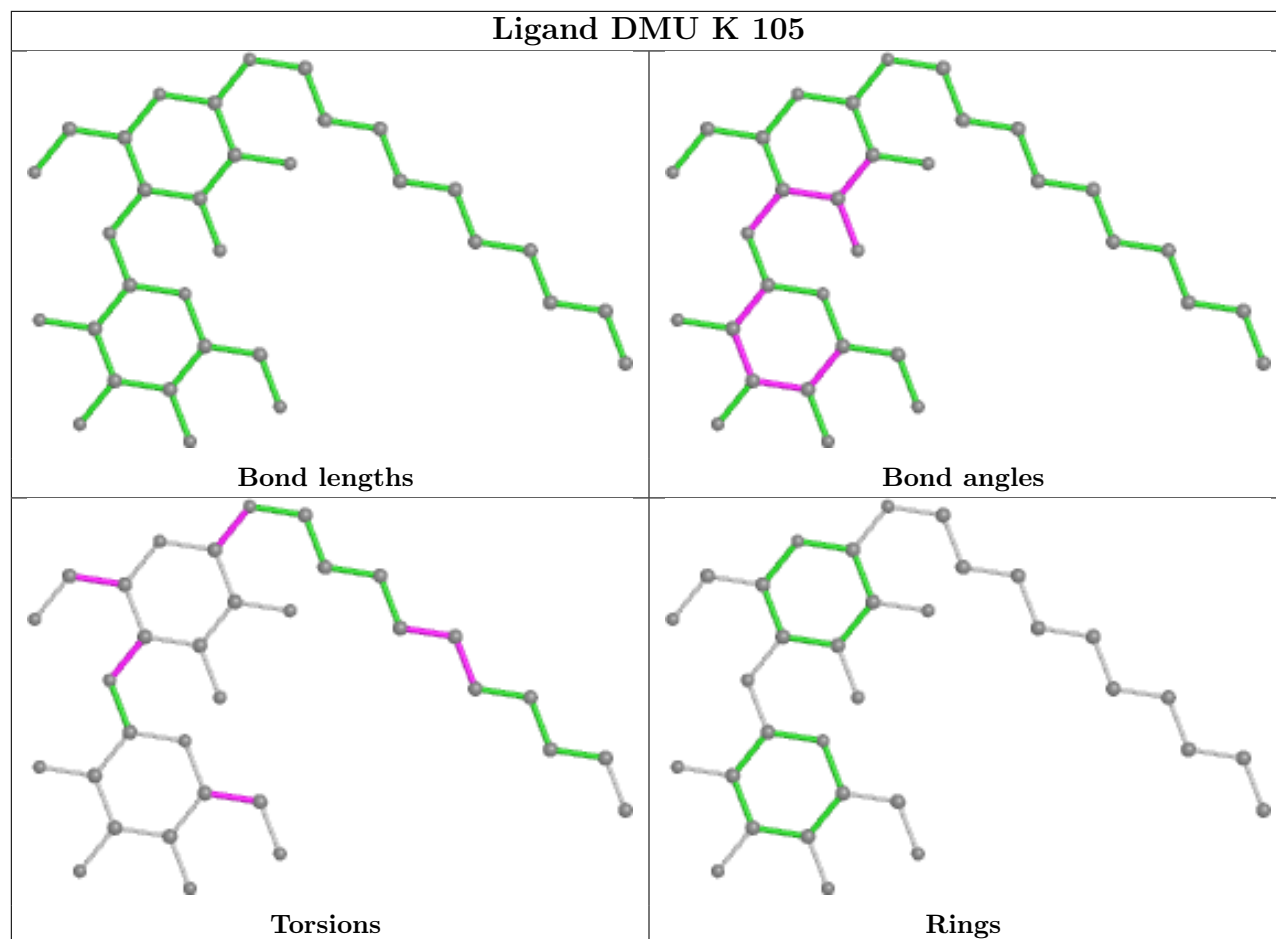


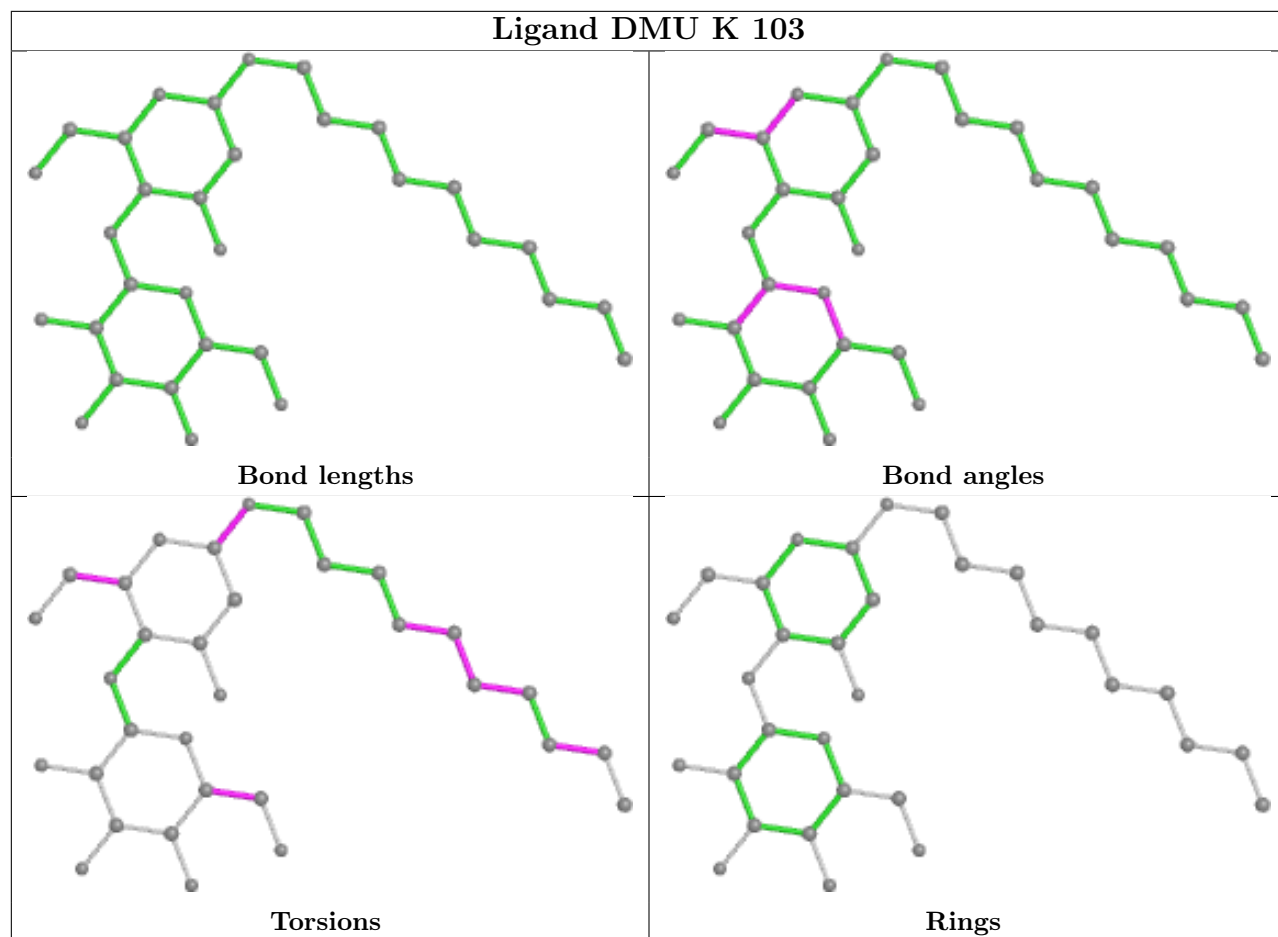




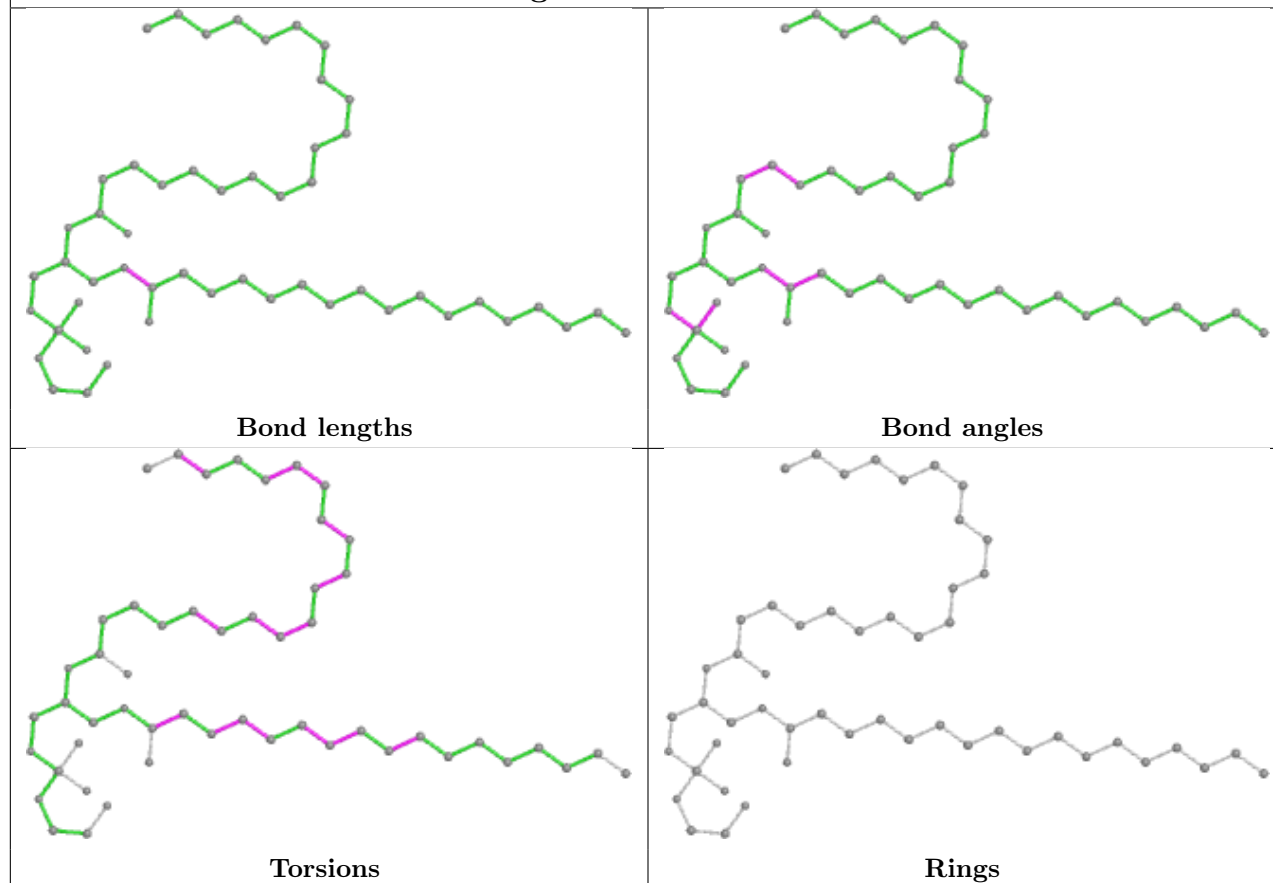




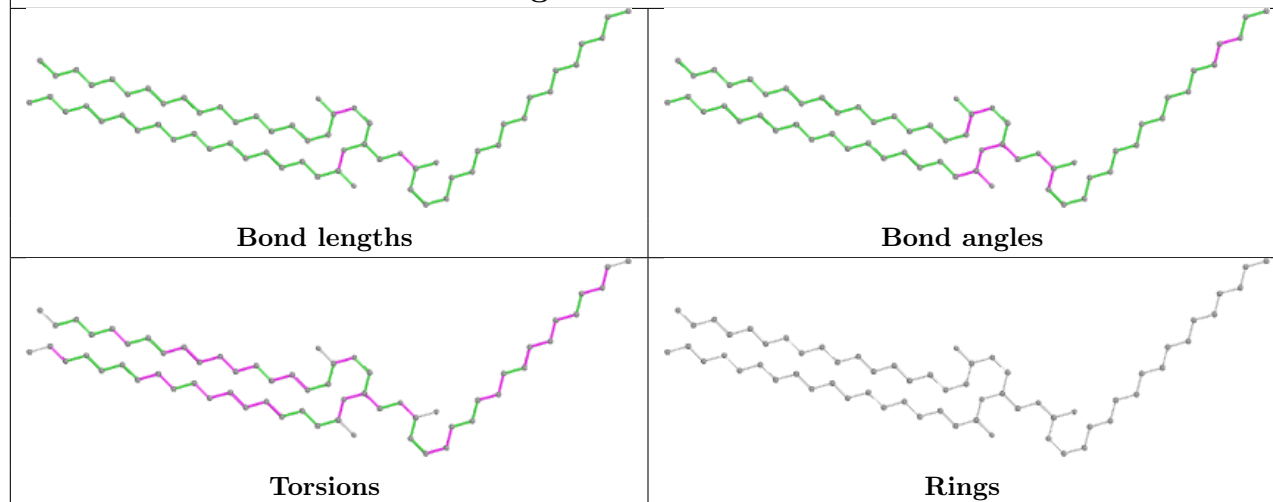


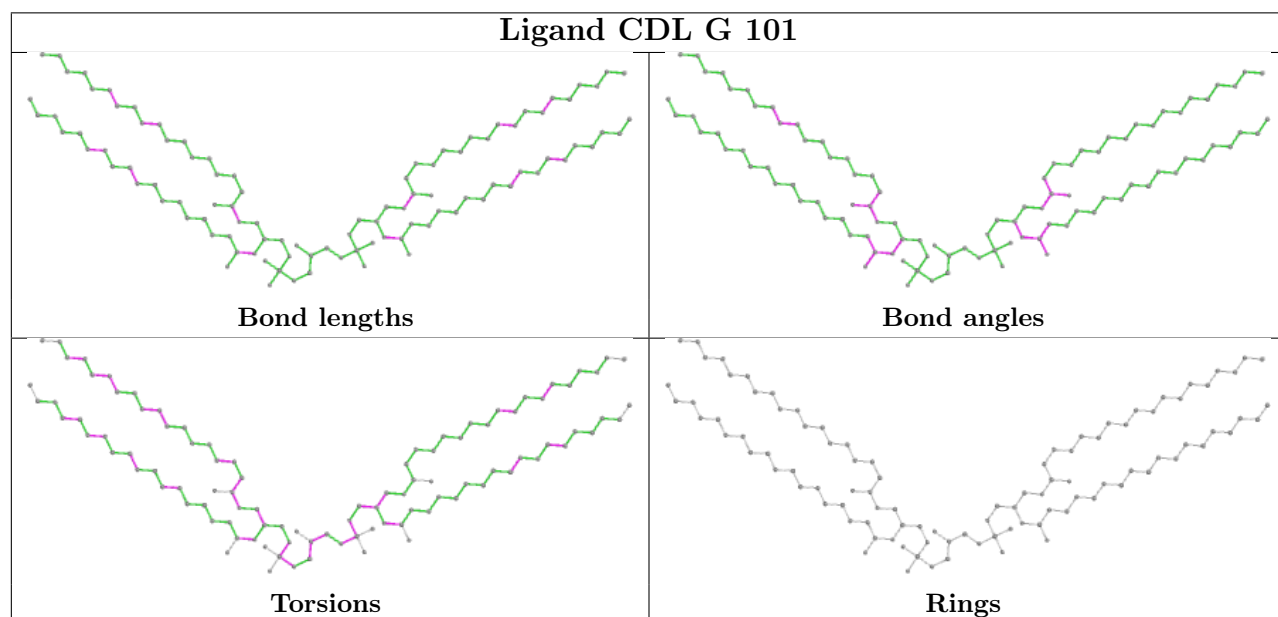
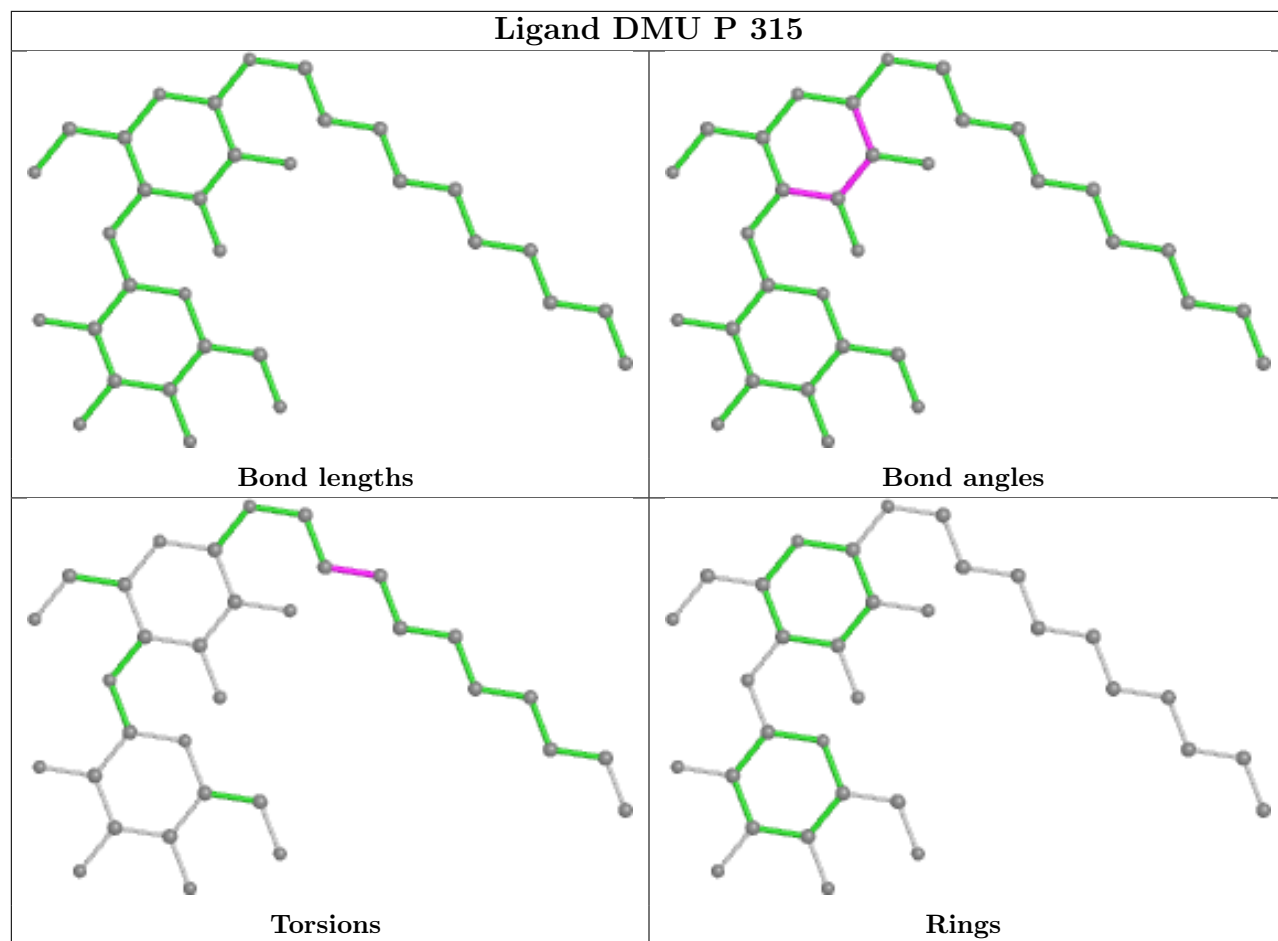


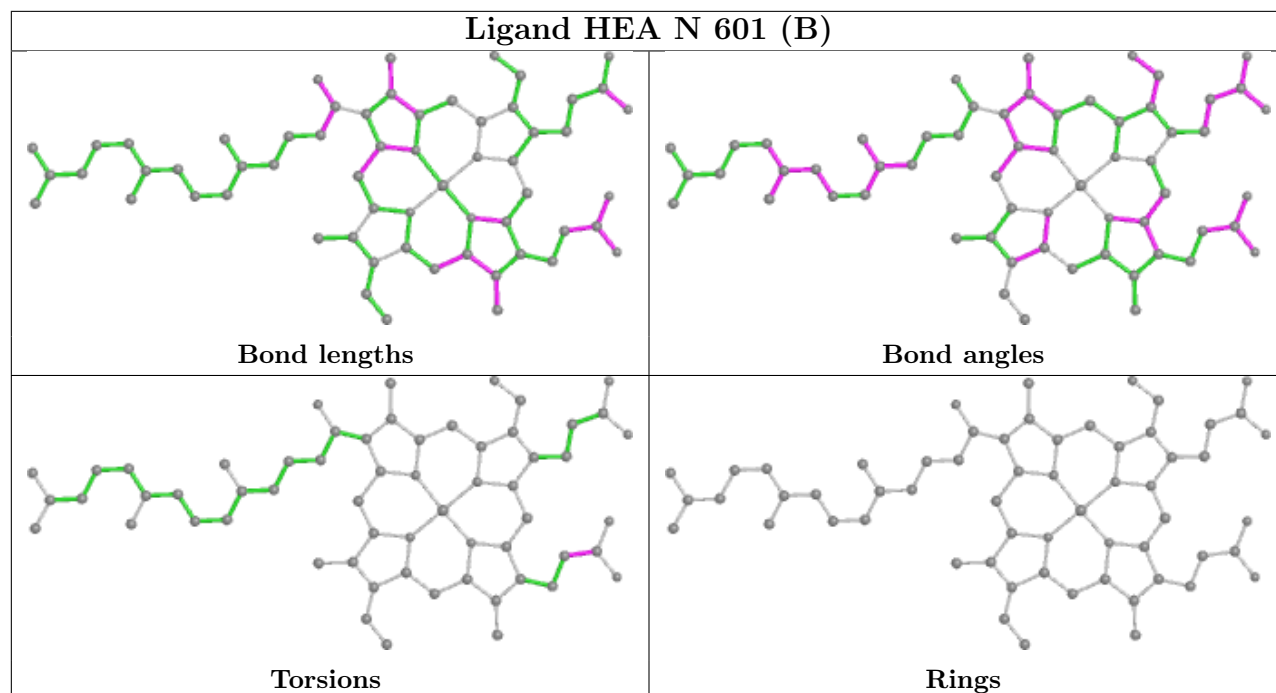
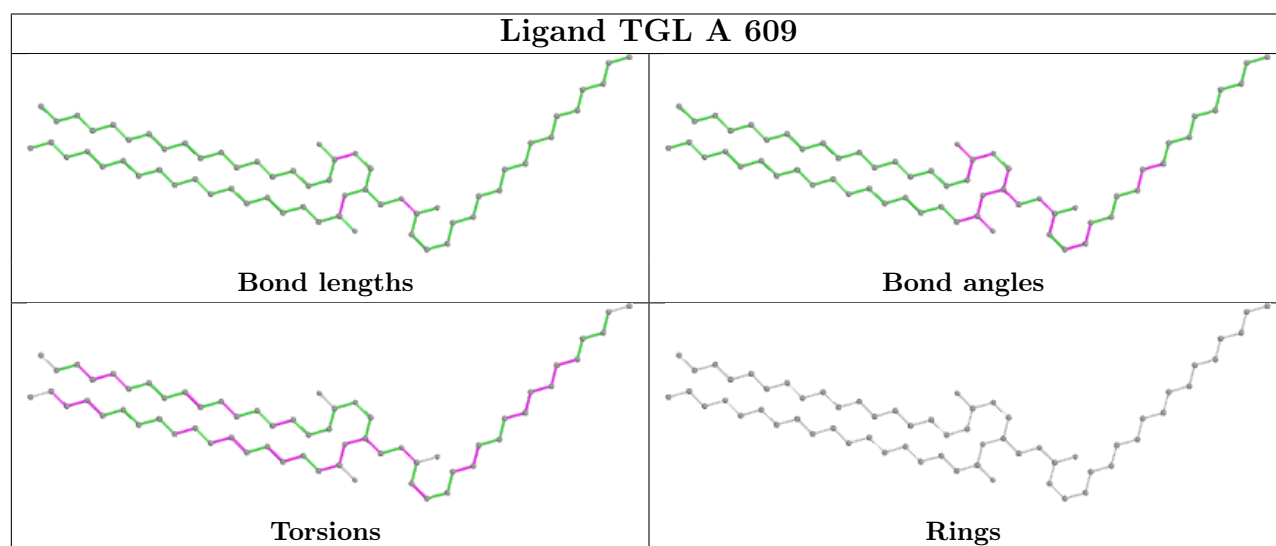
Ligand PEK C 307

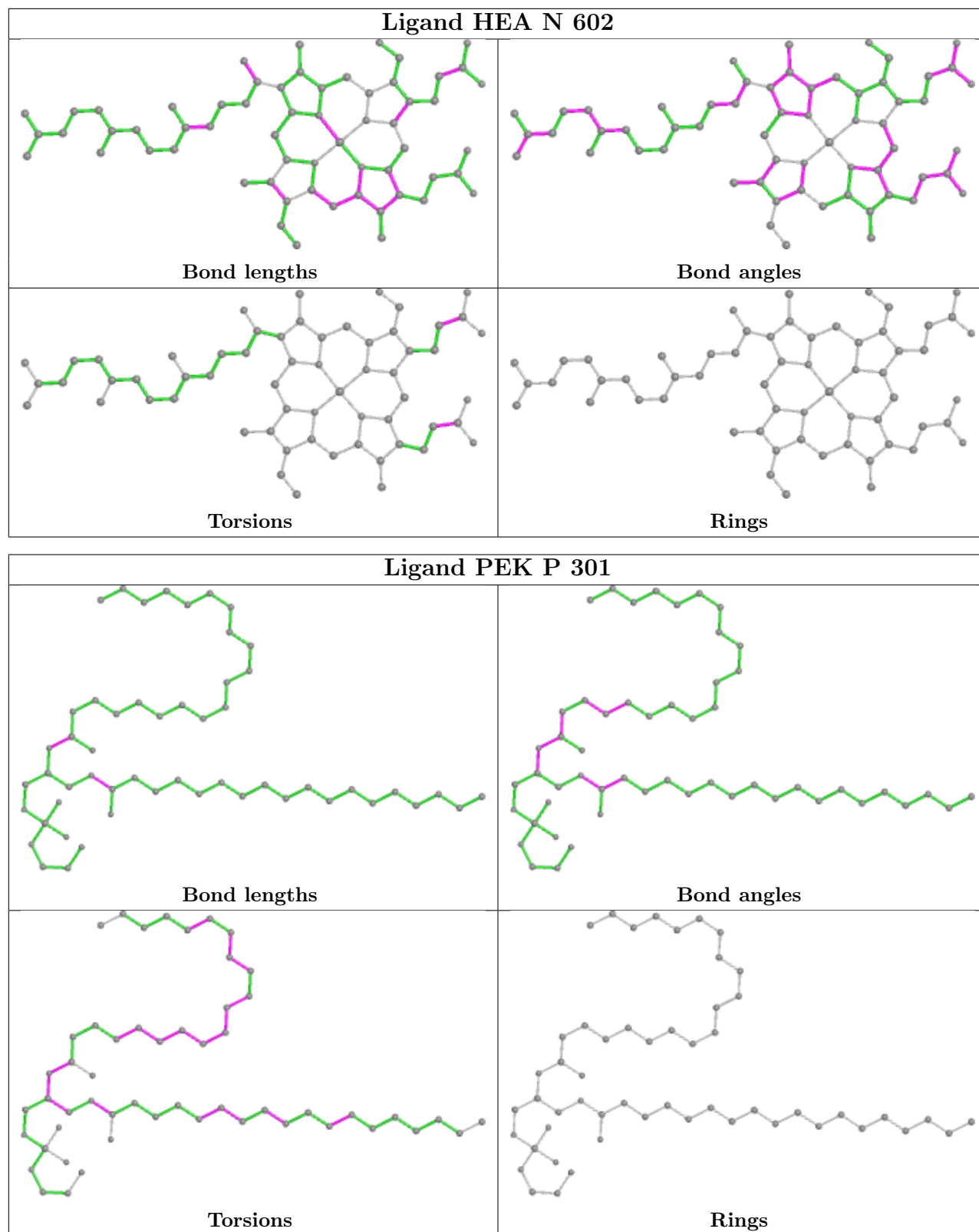


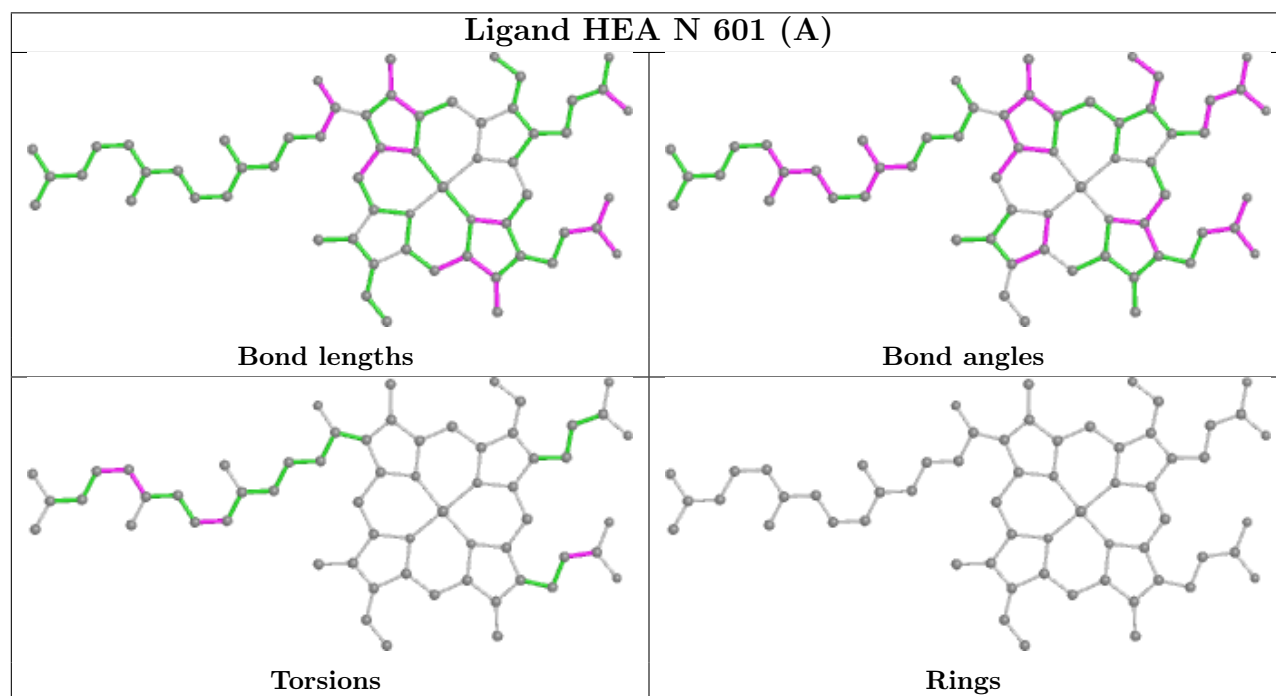
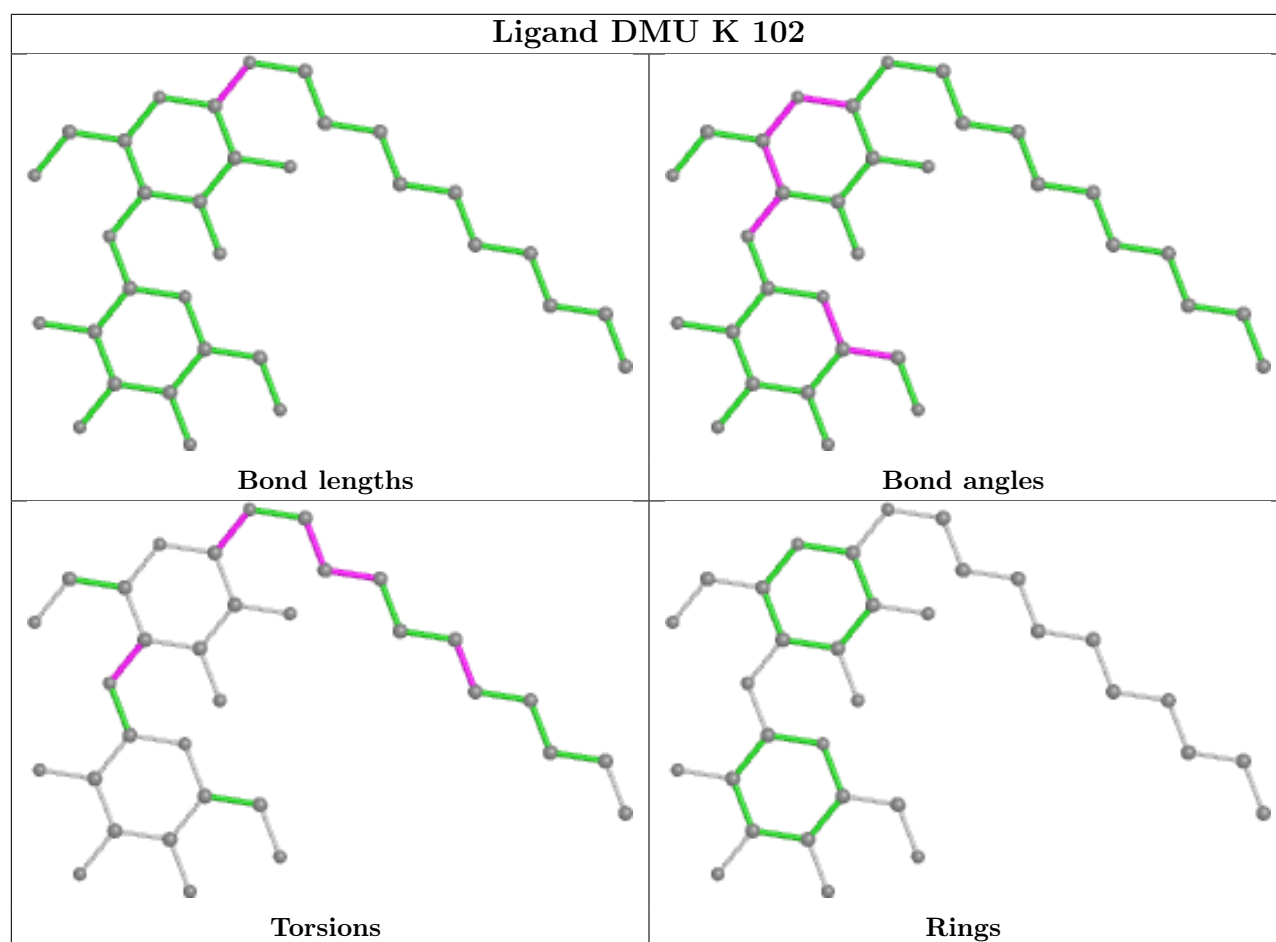
Ligand TGL Y 101

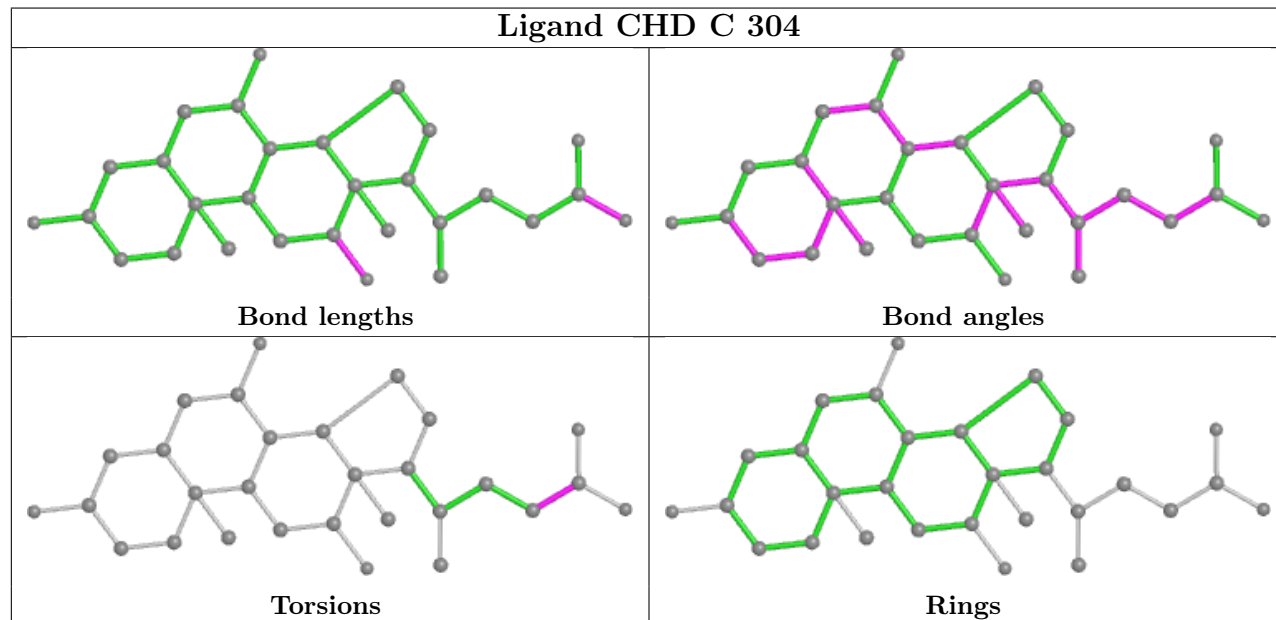
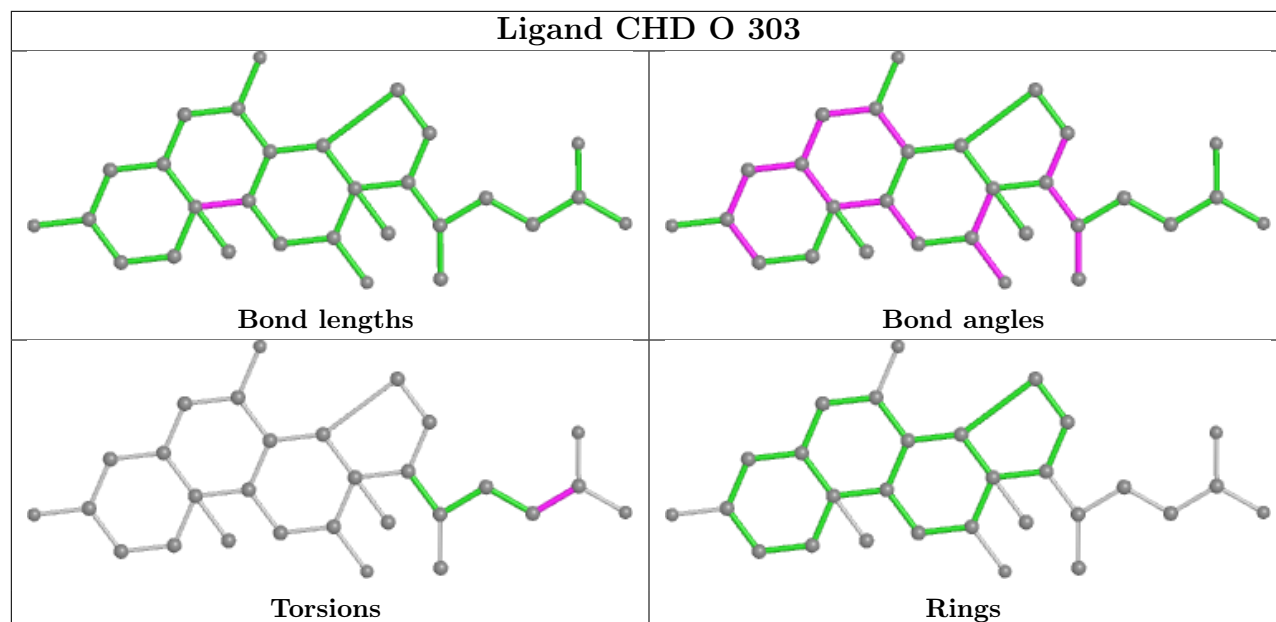


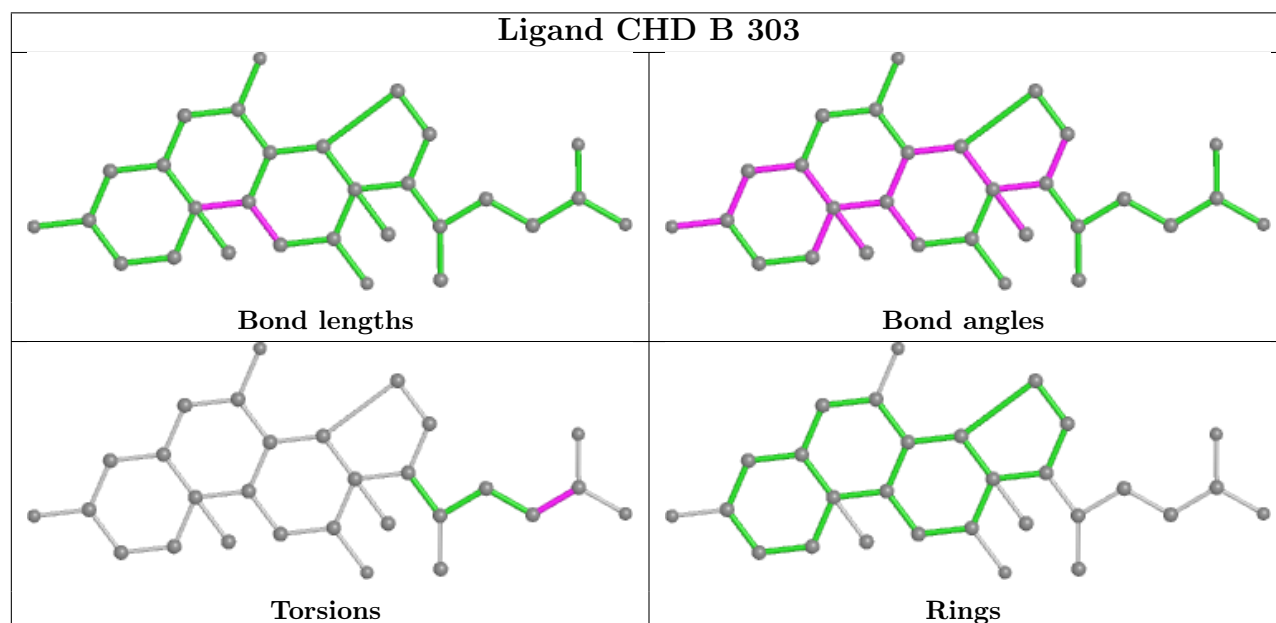
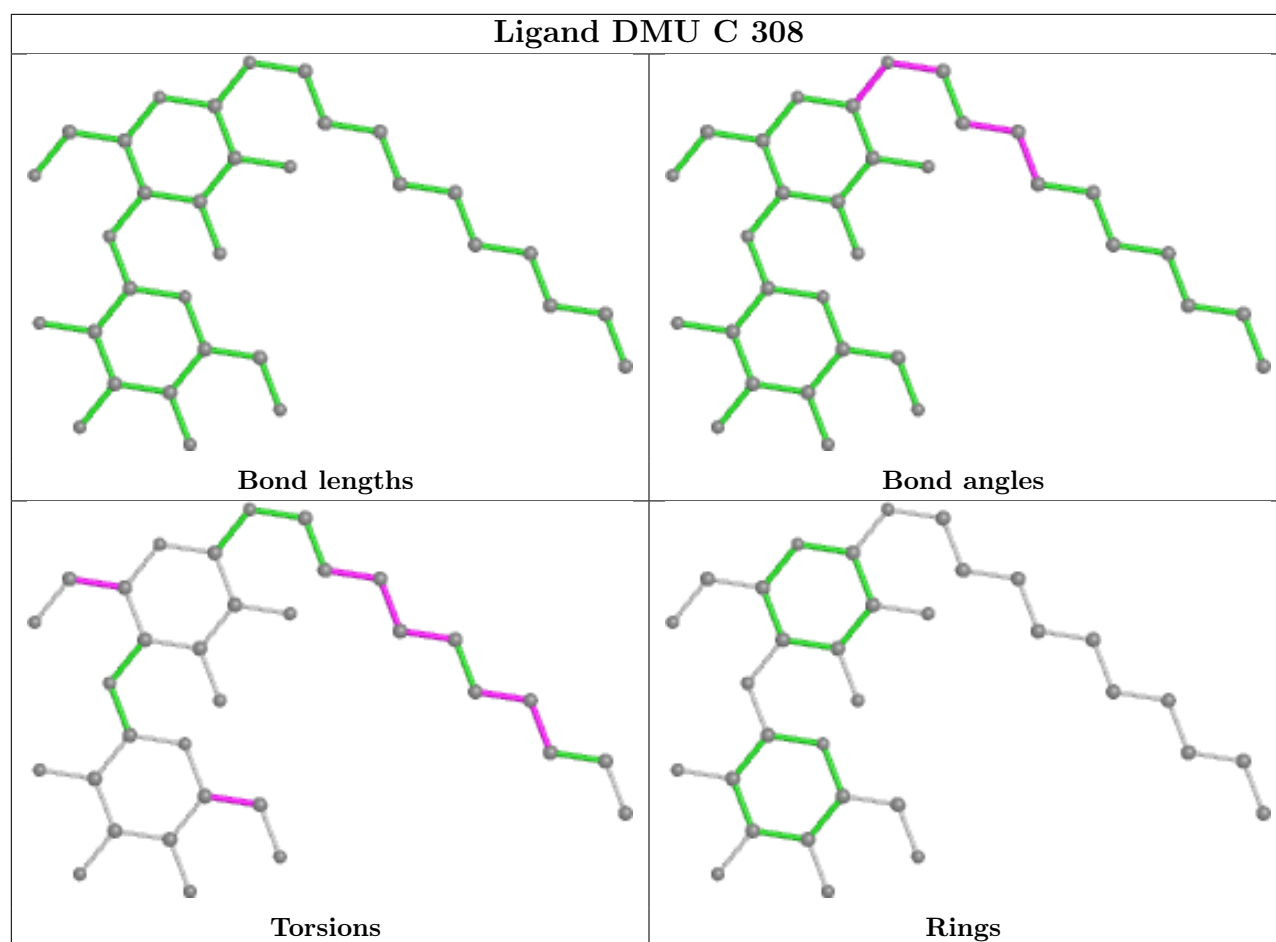


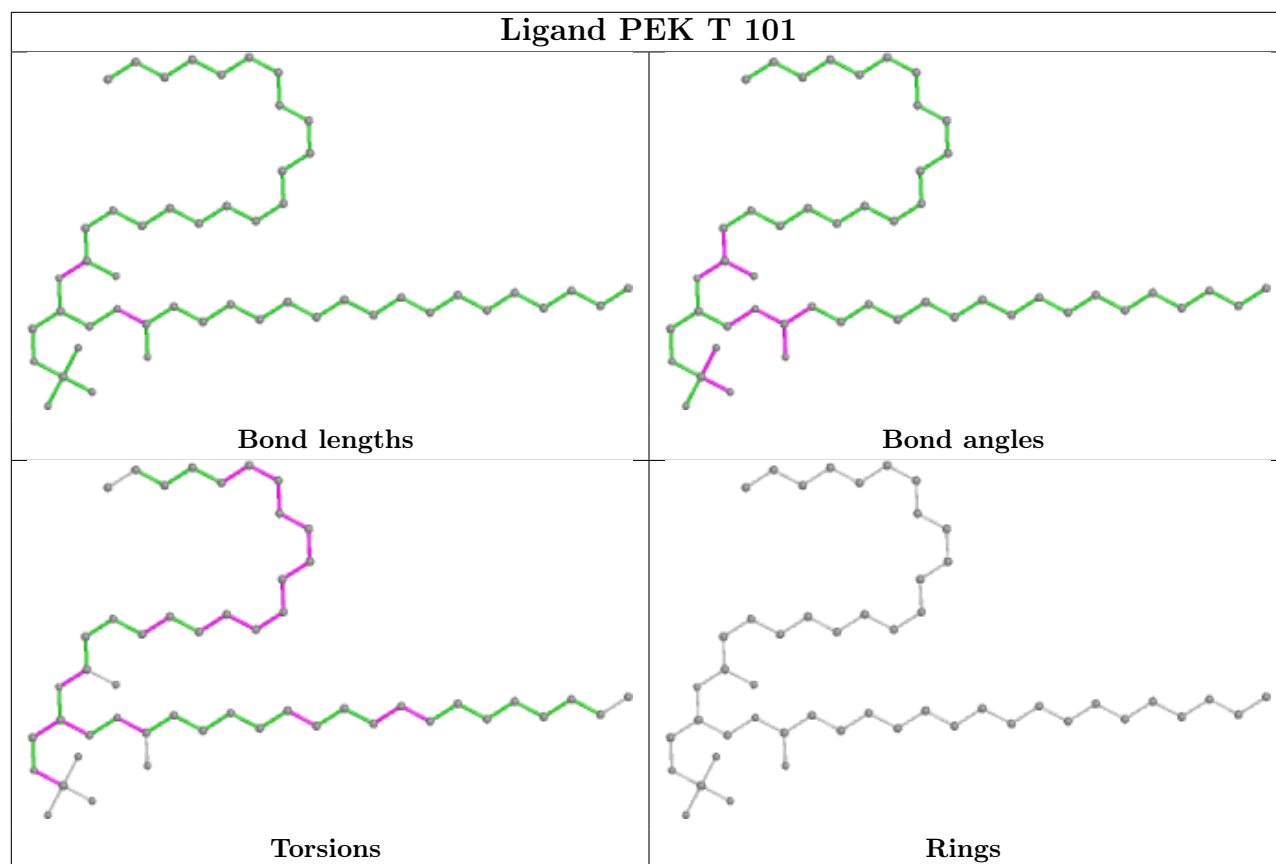
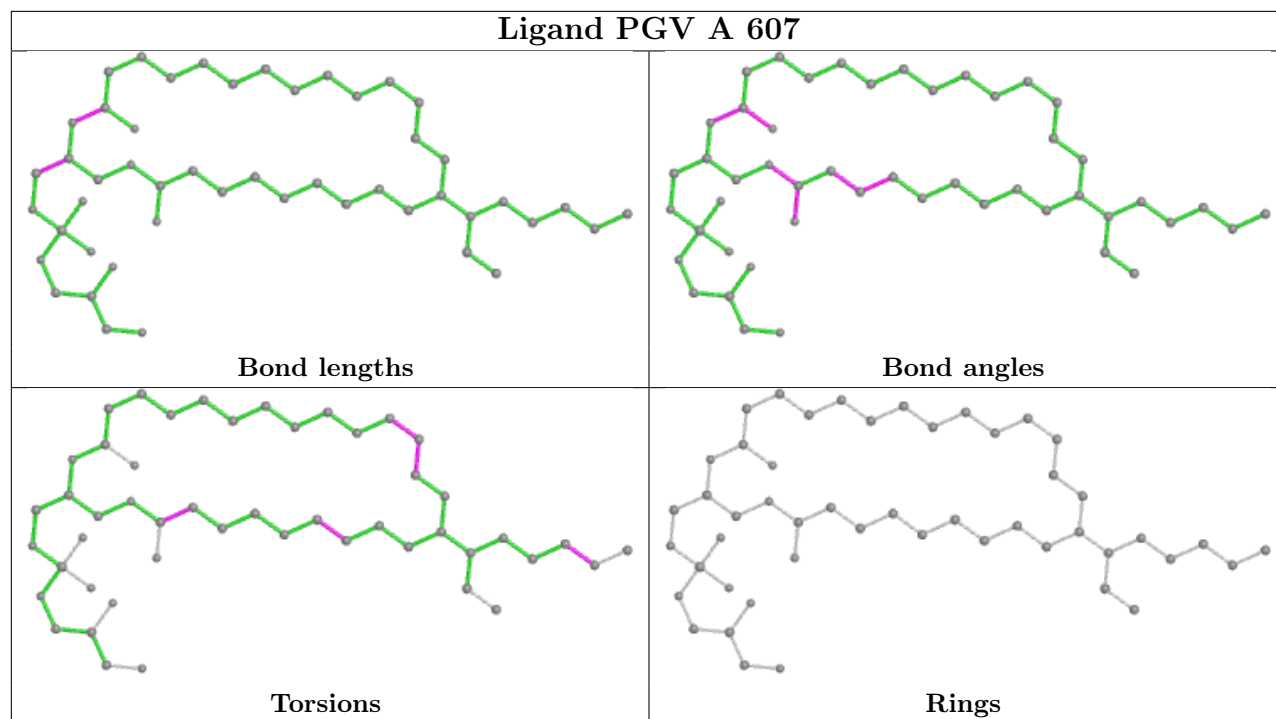
Ligand HEA N 601 (B)**Ligand TGL A 609**

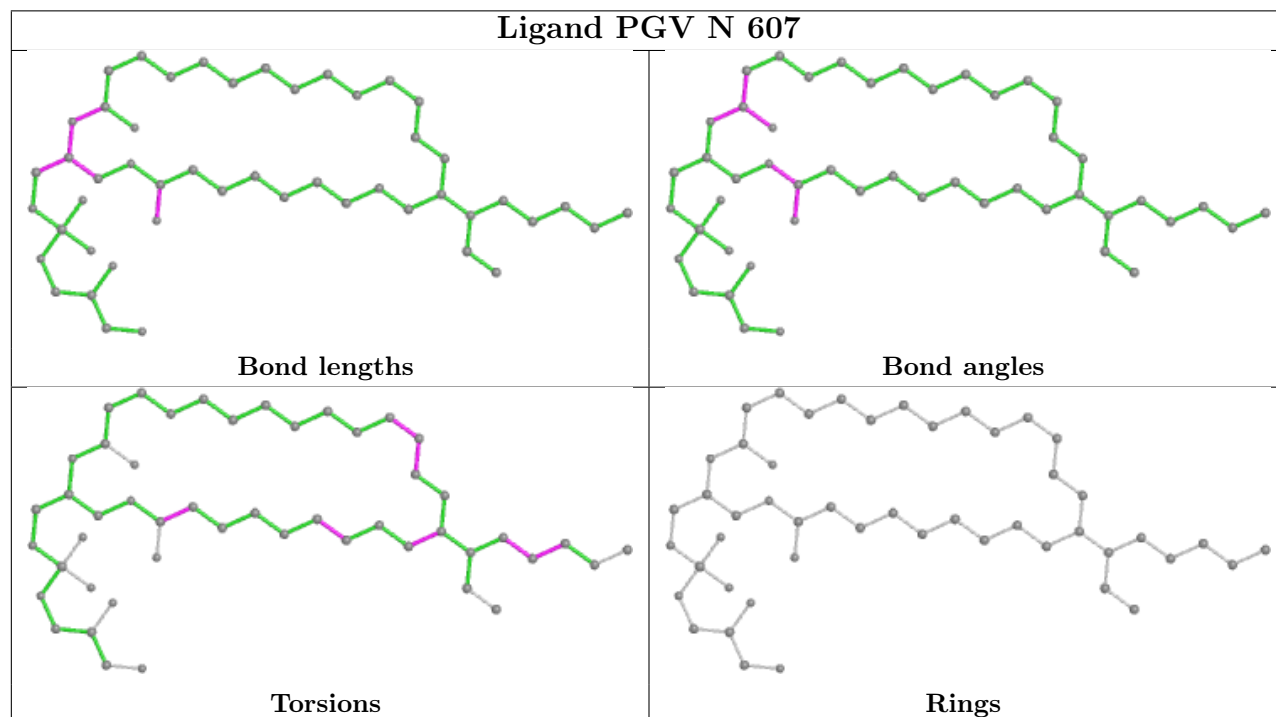
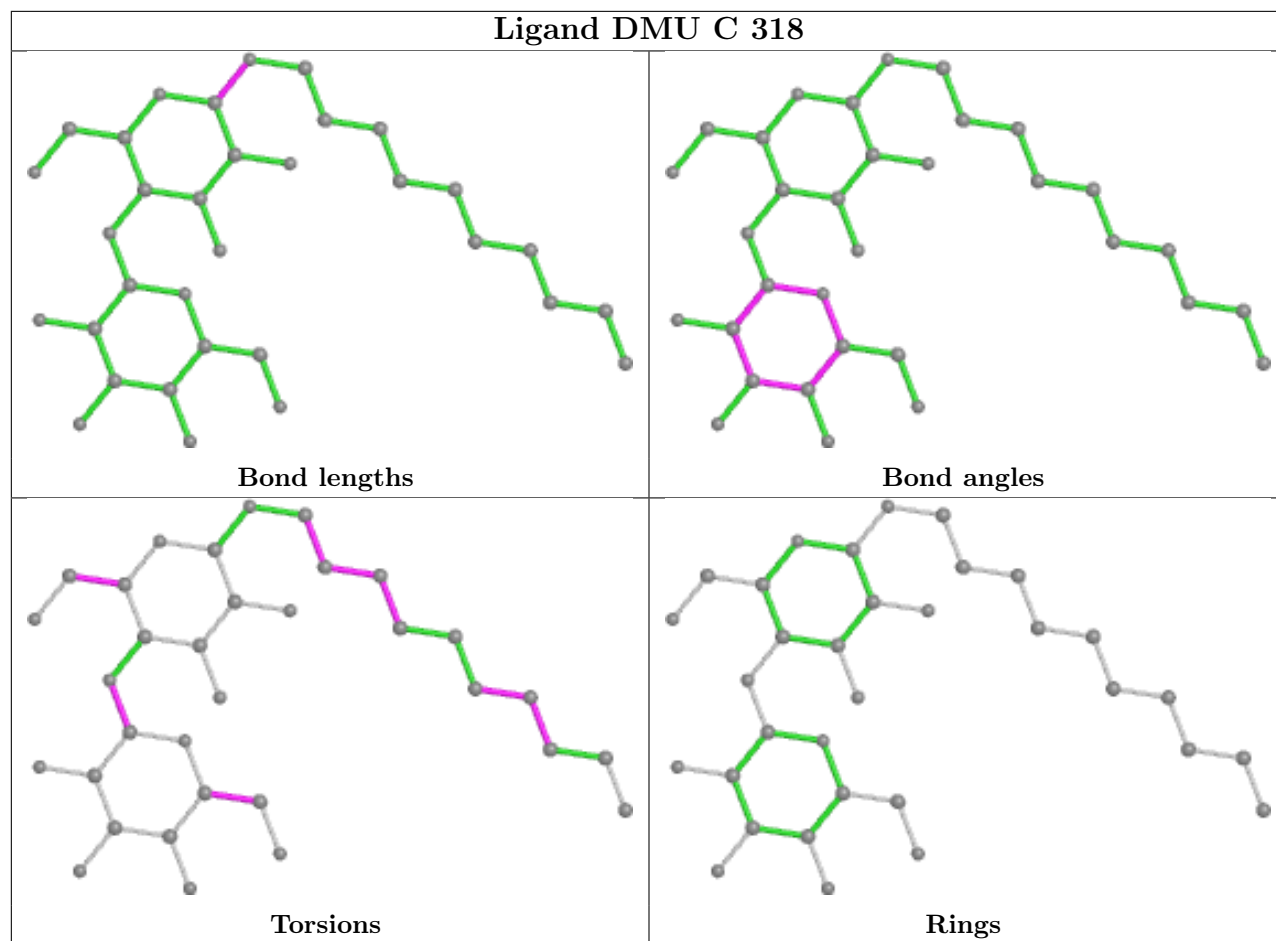


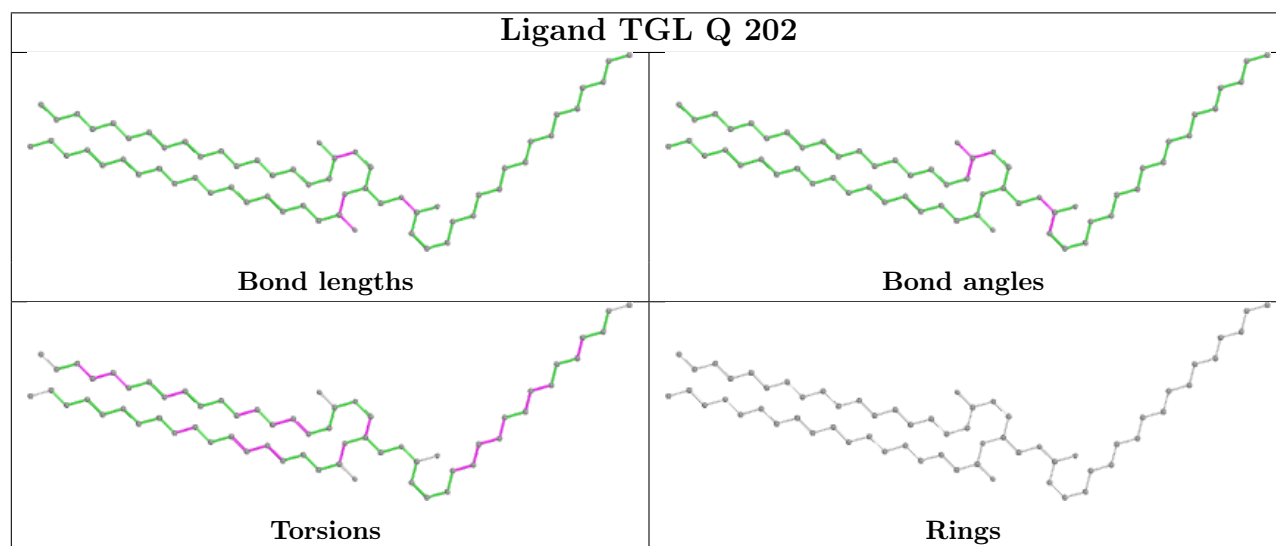
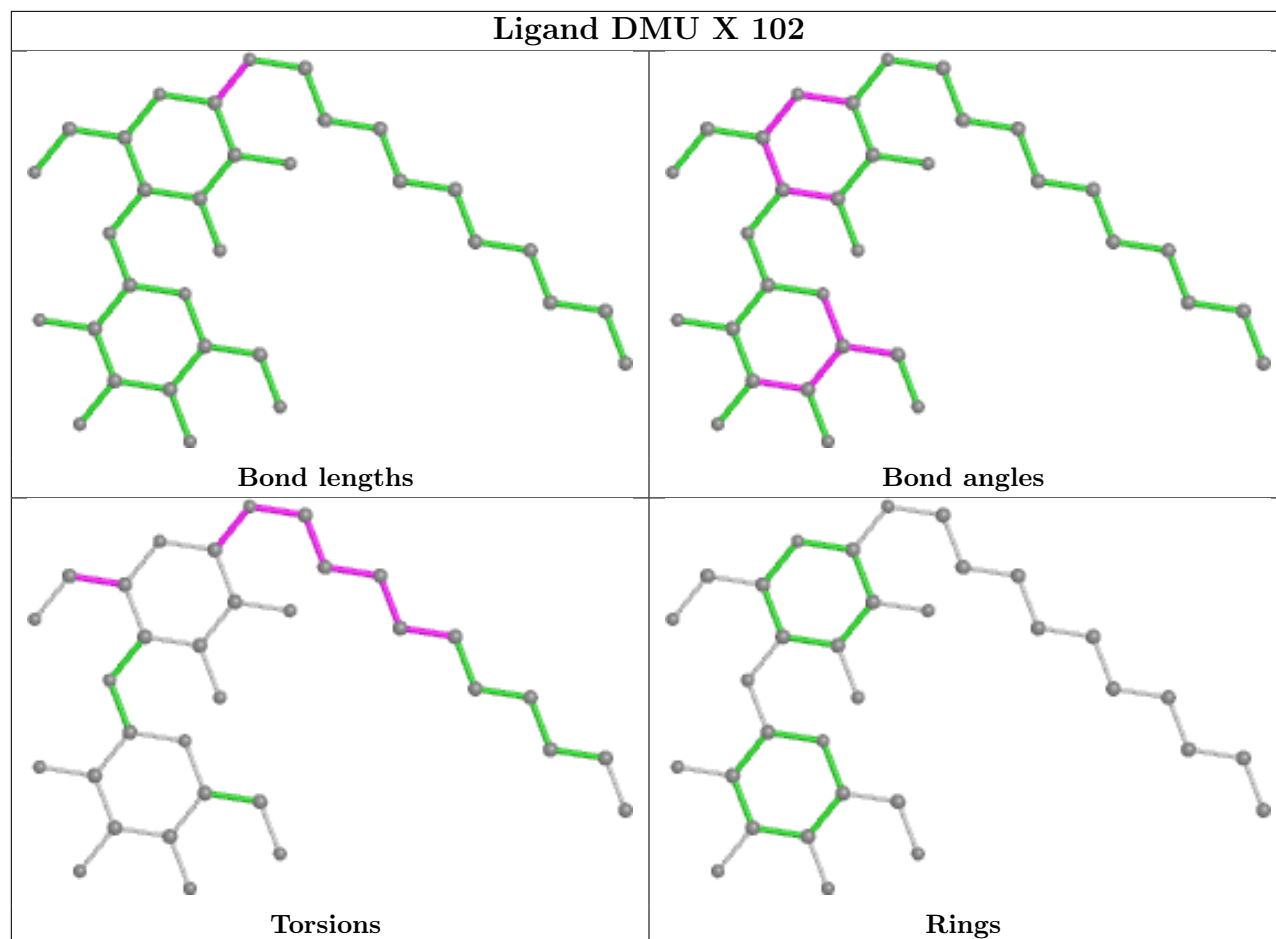


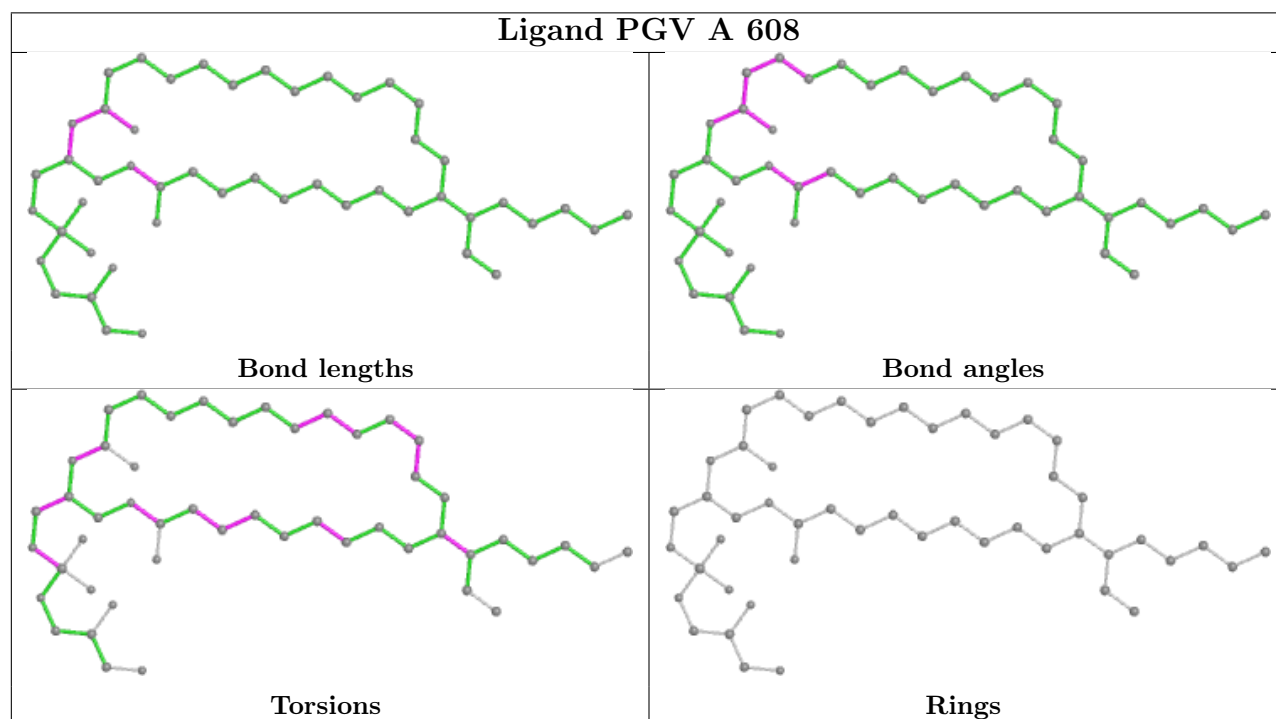
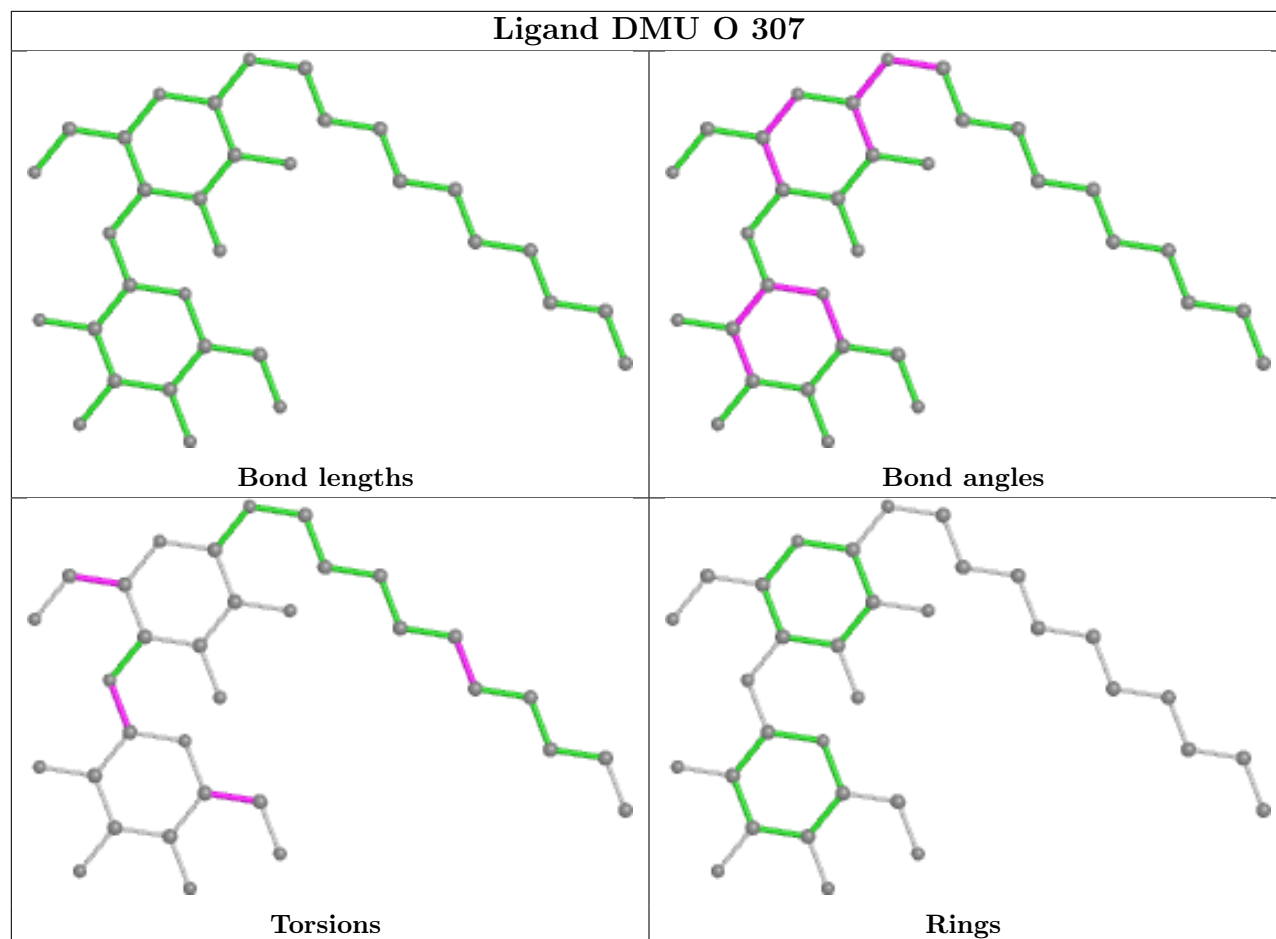


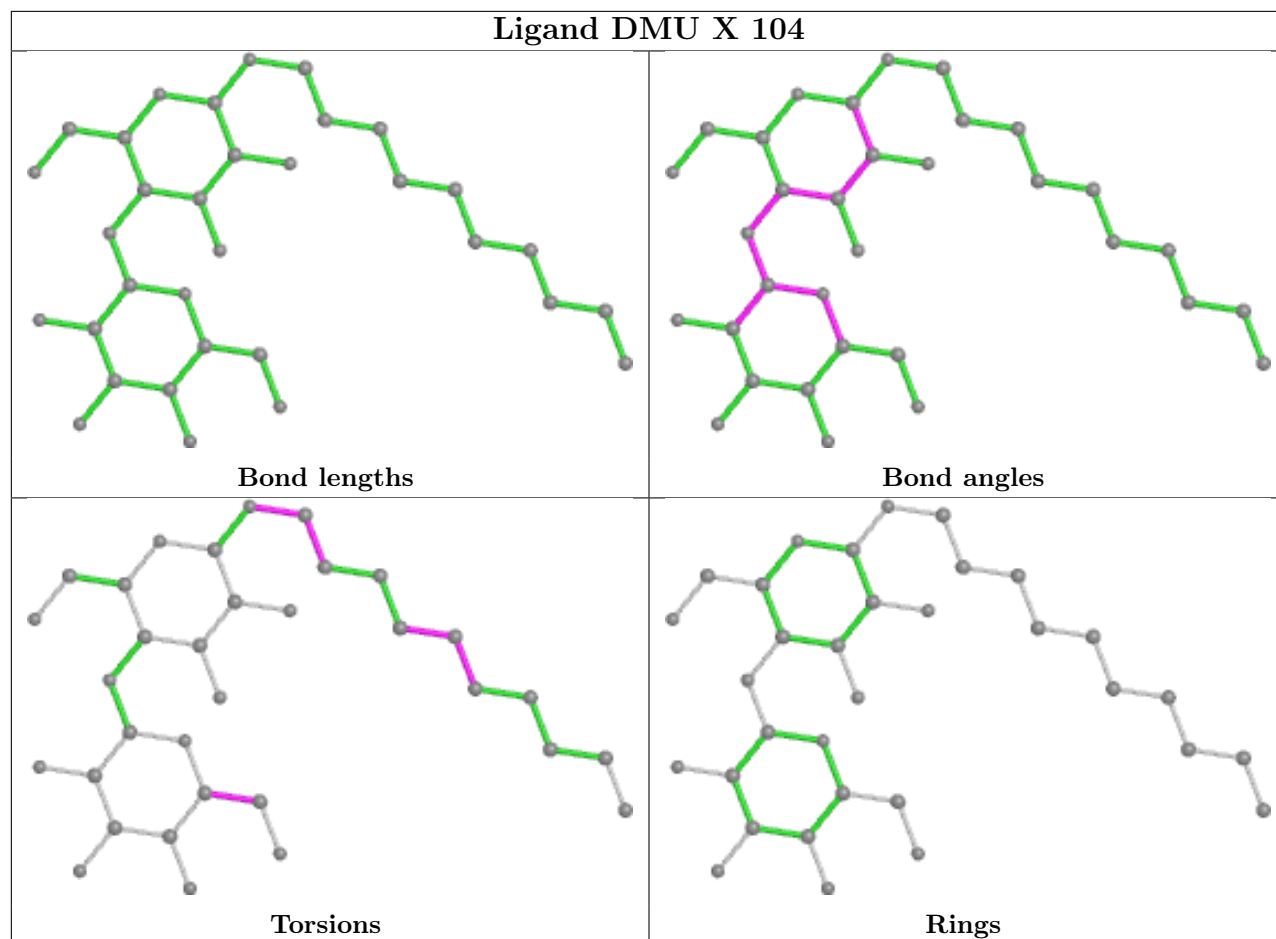


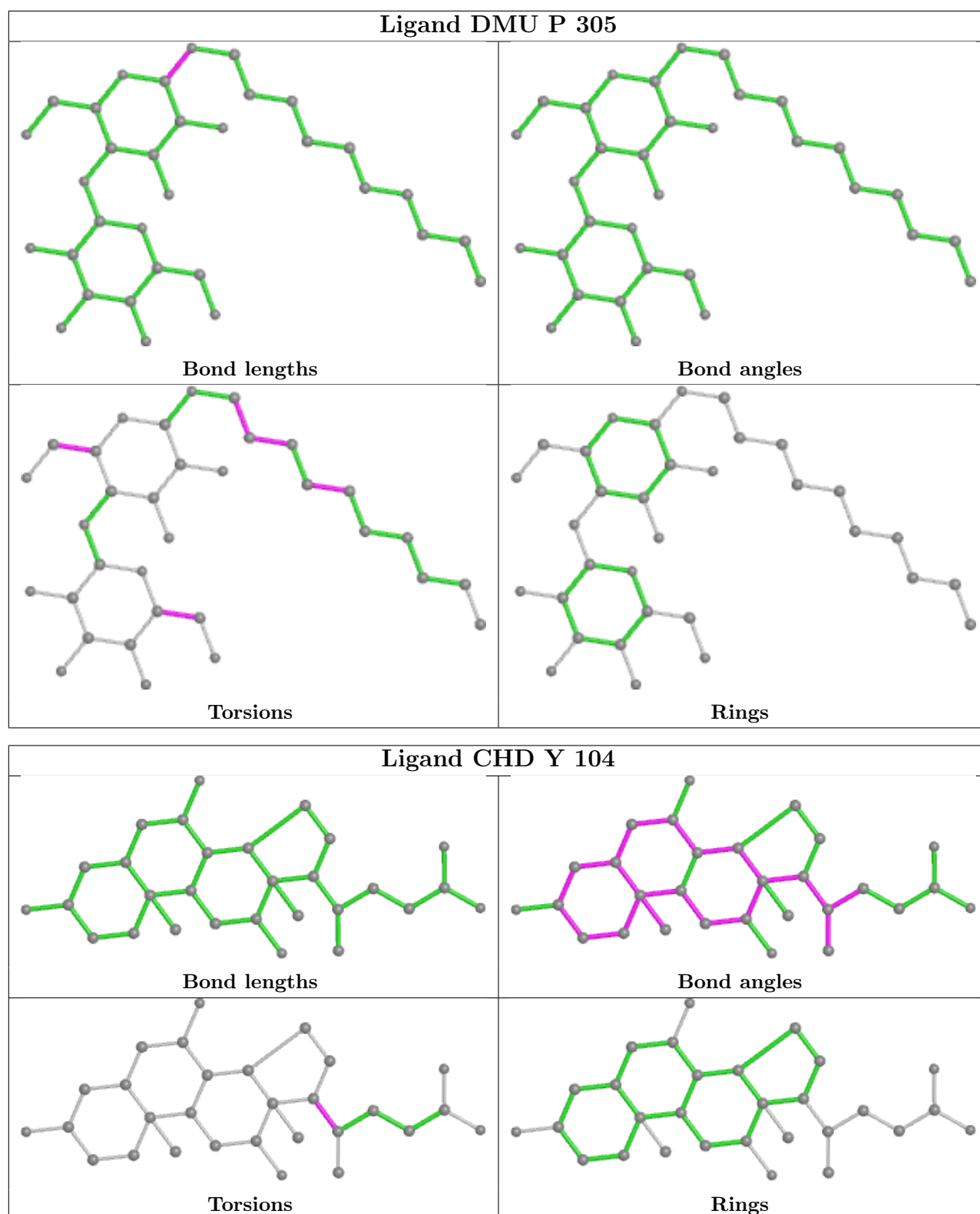


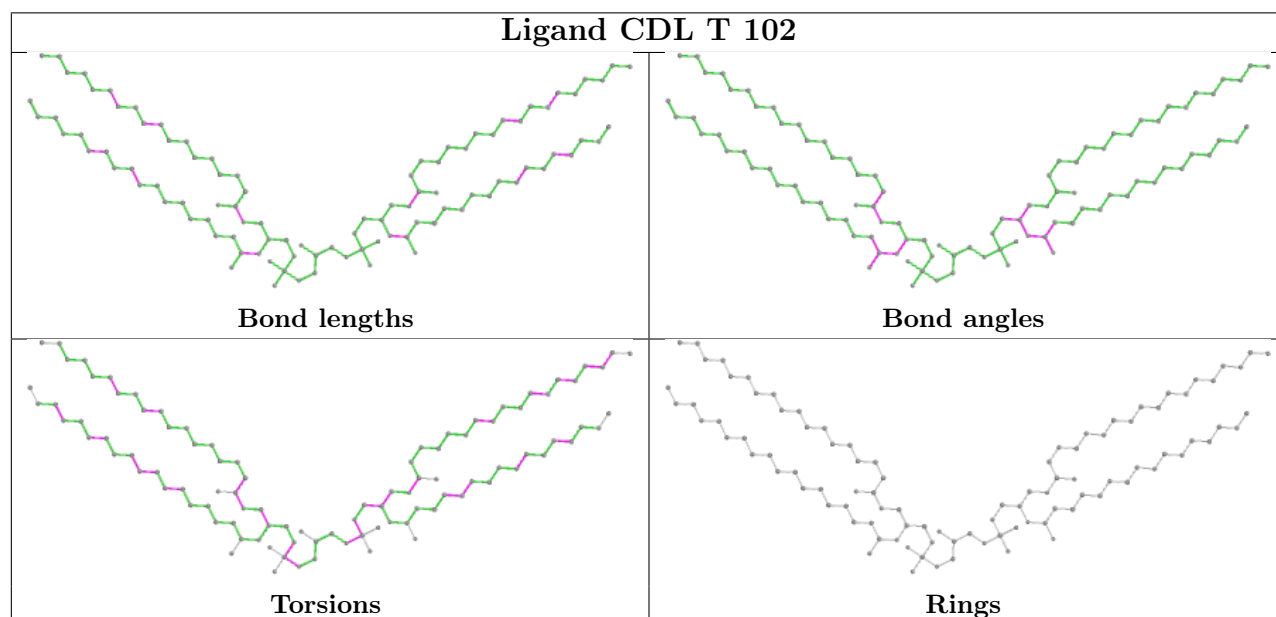
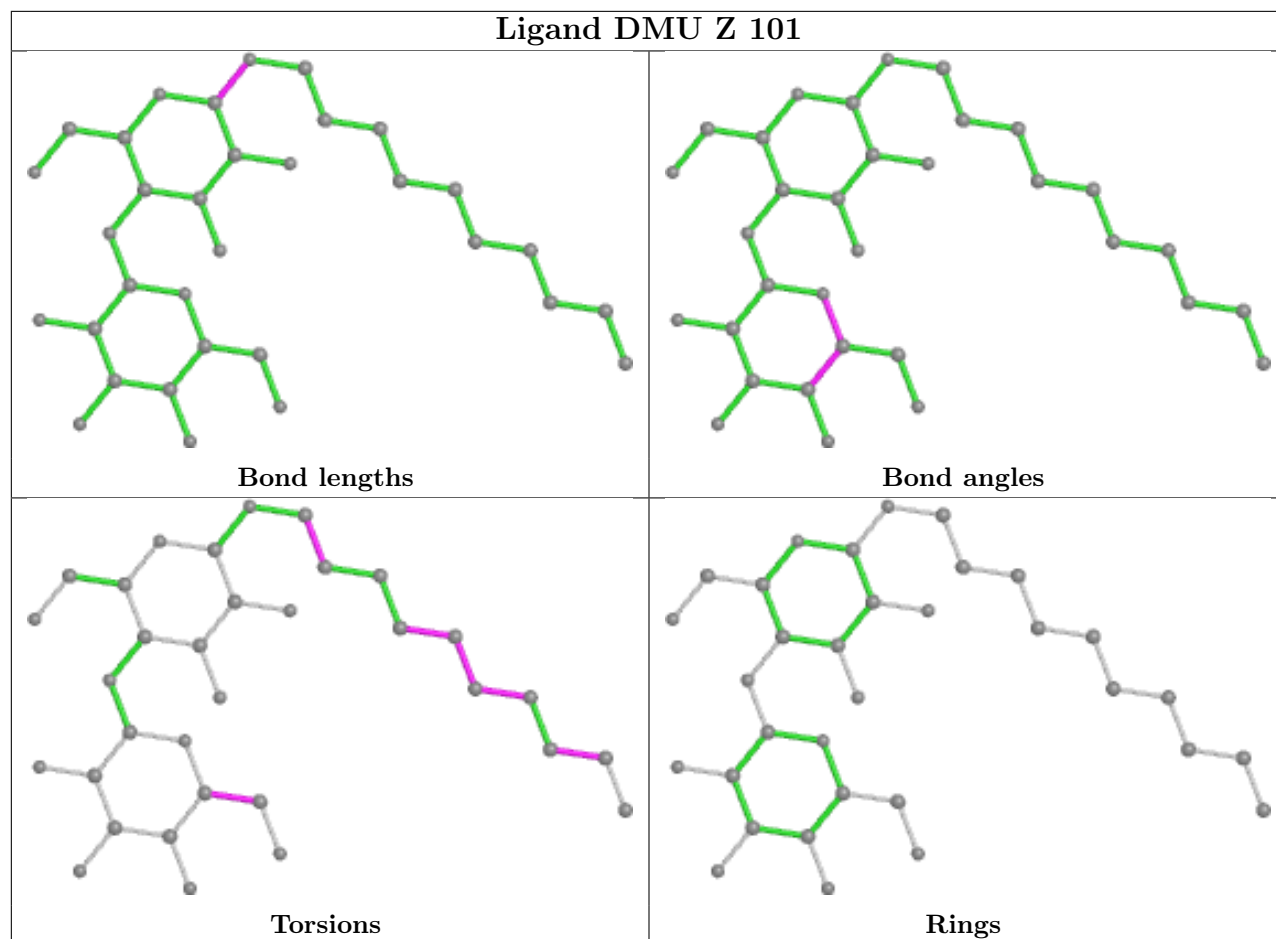


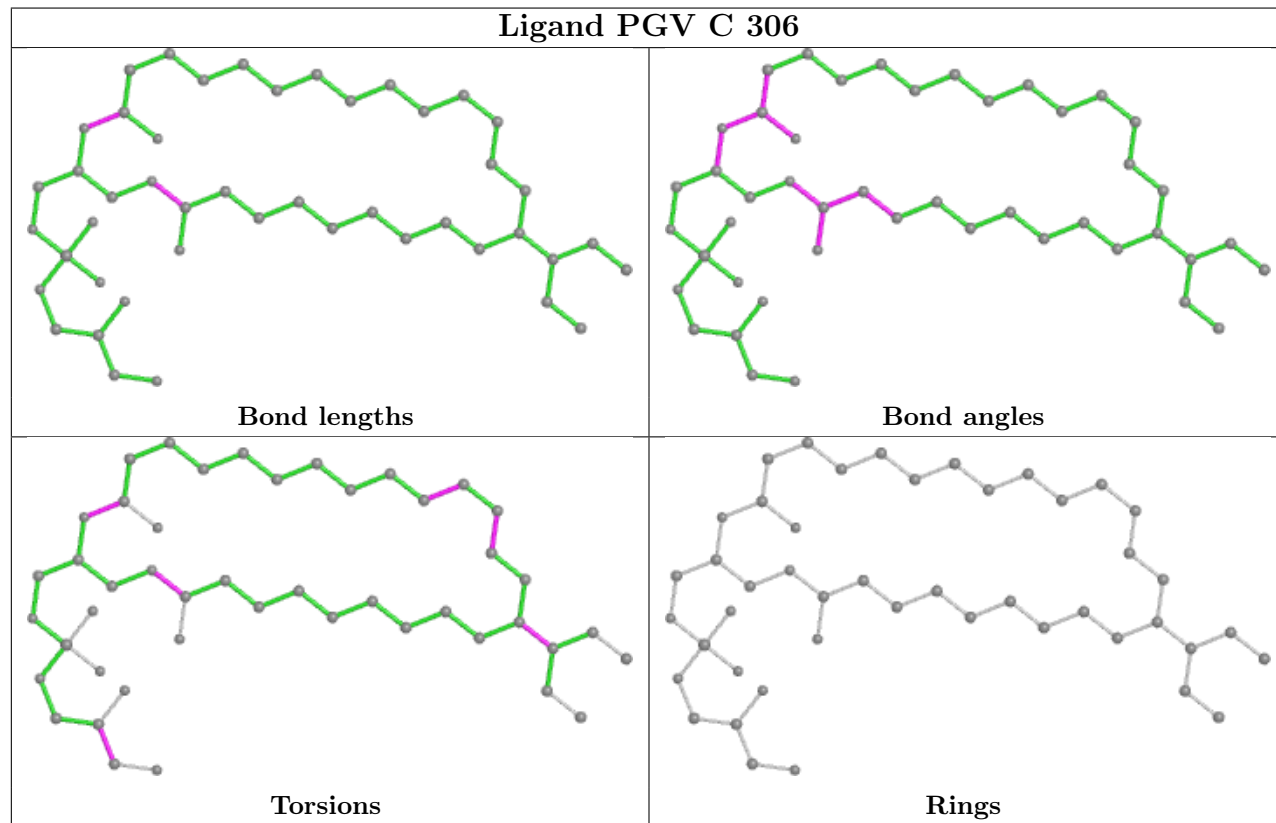
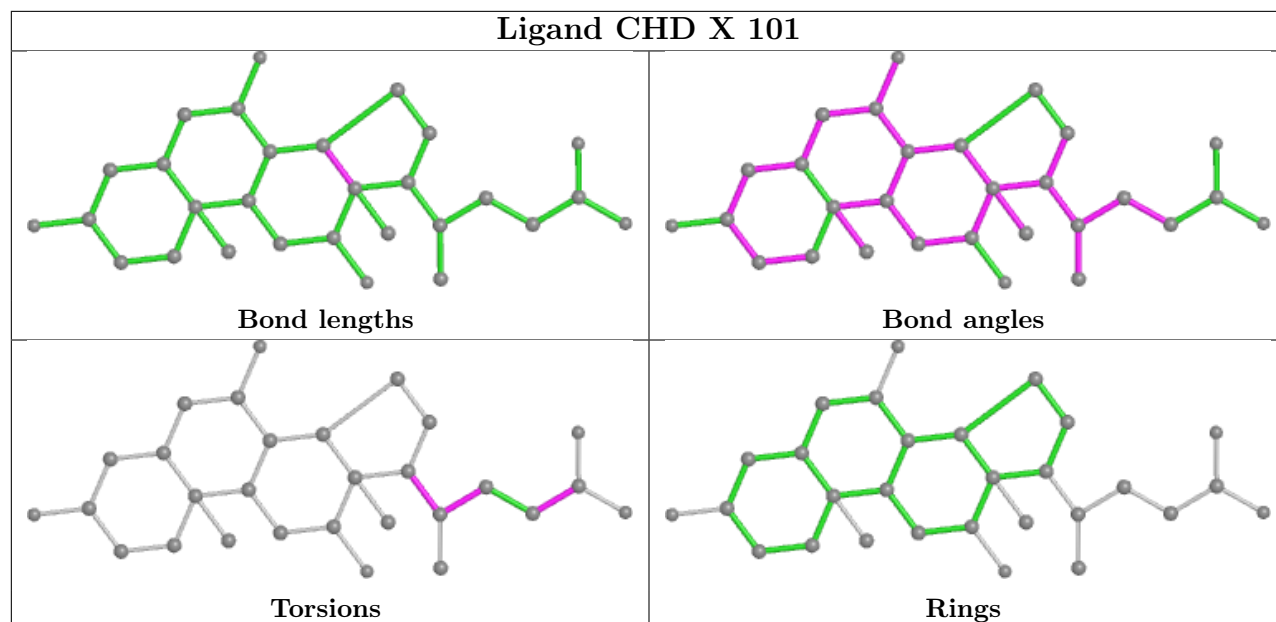




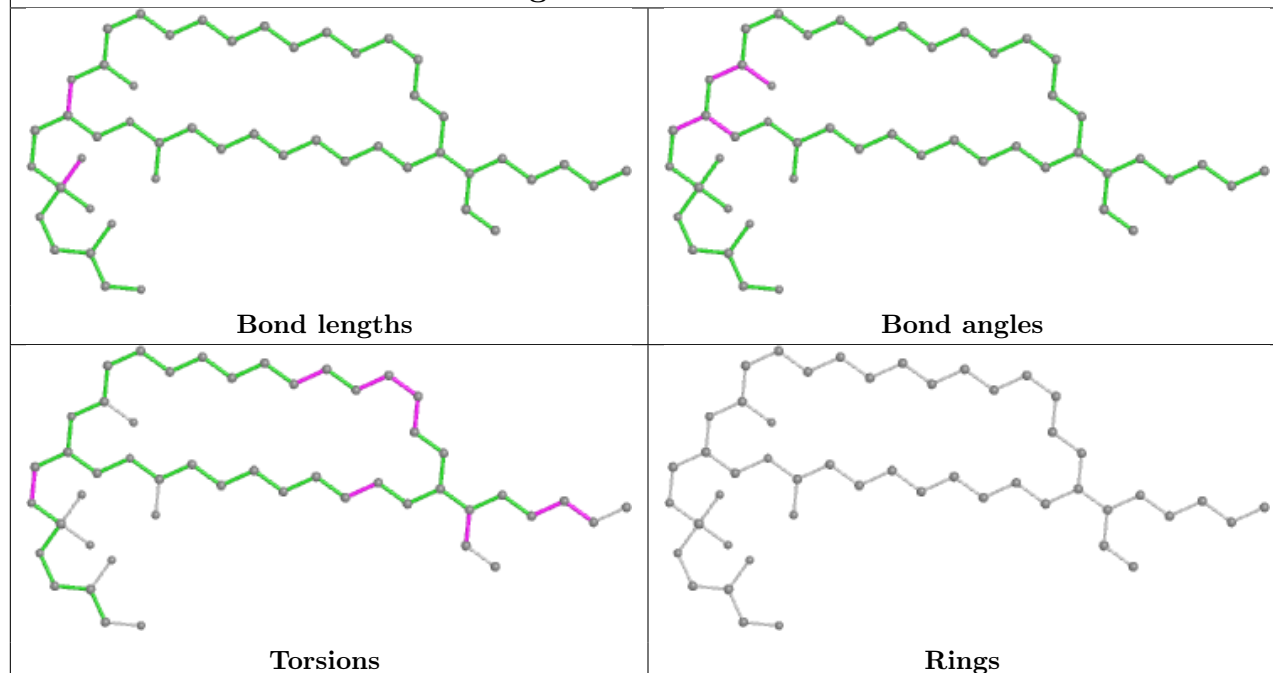




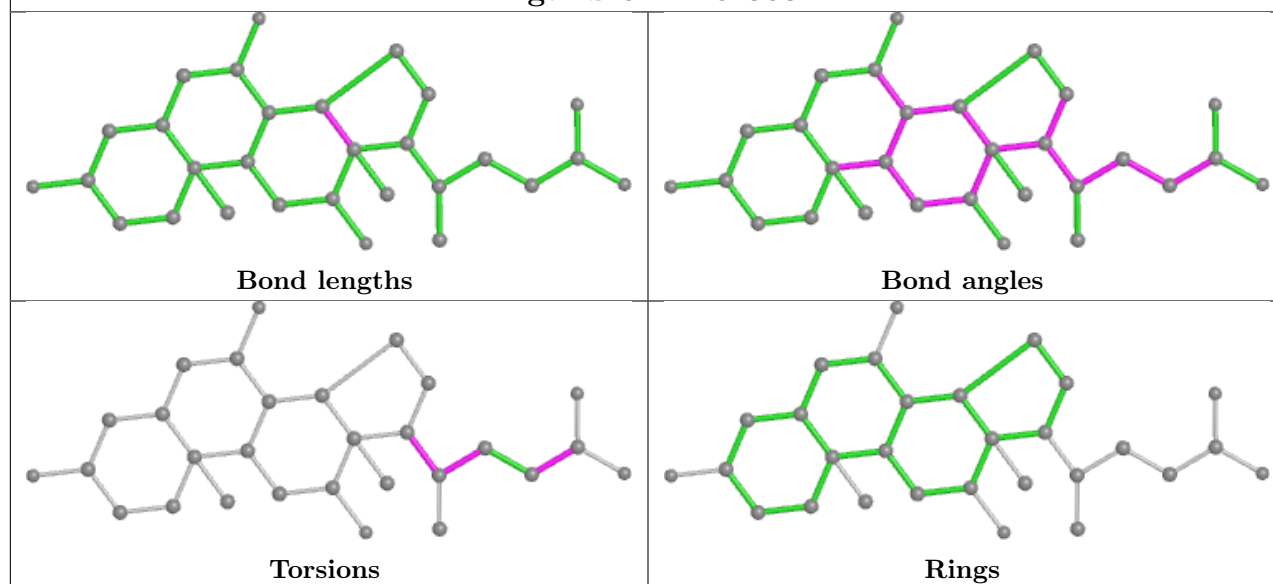


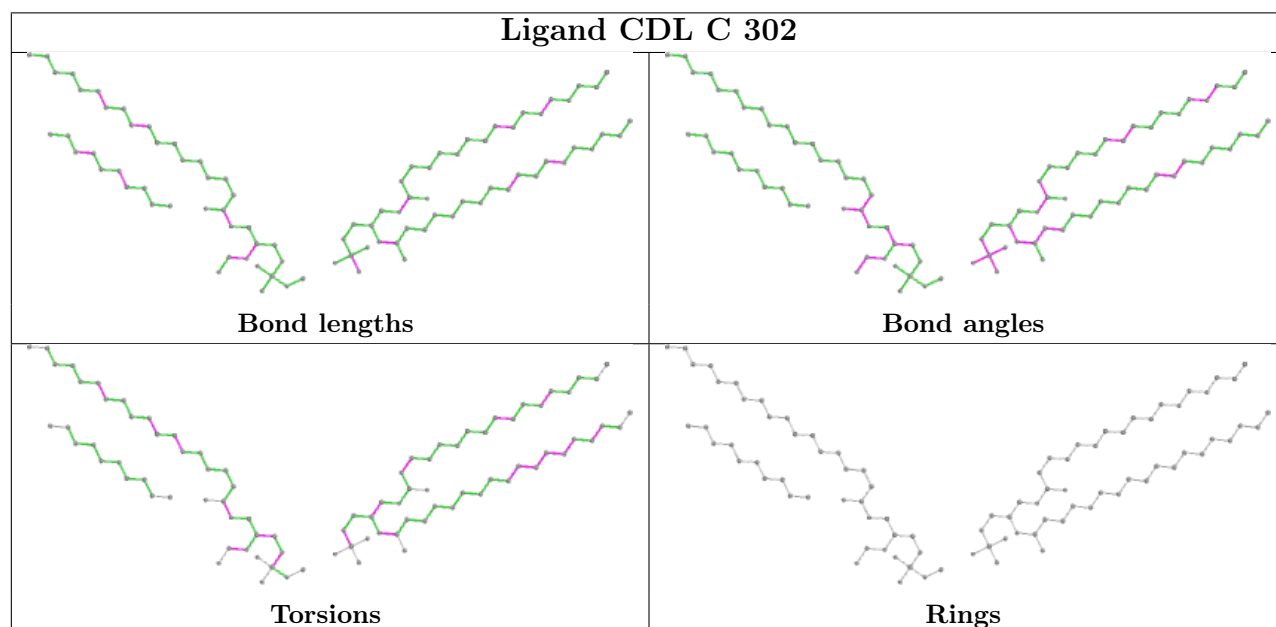
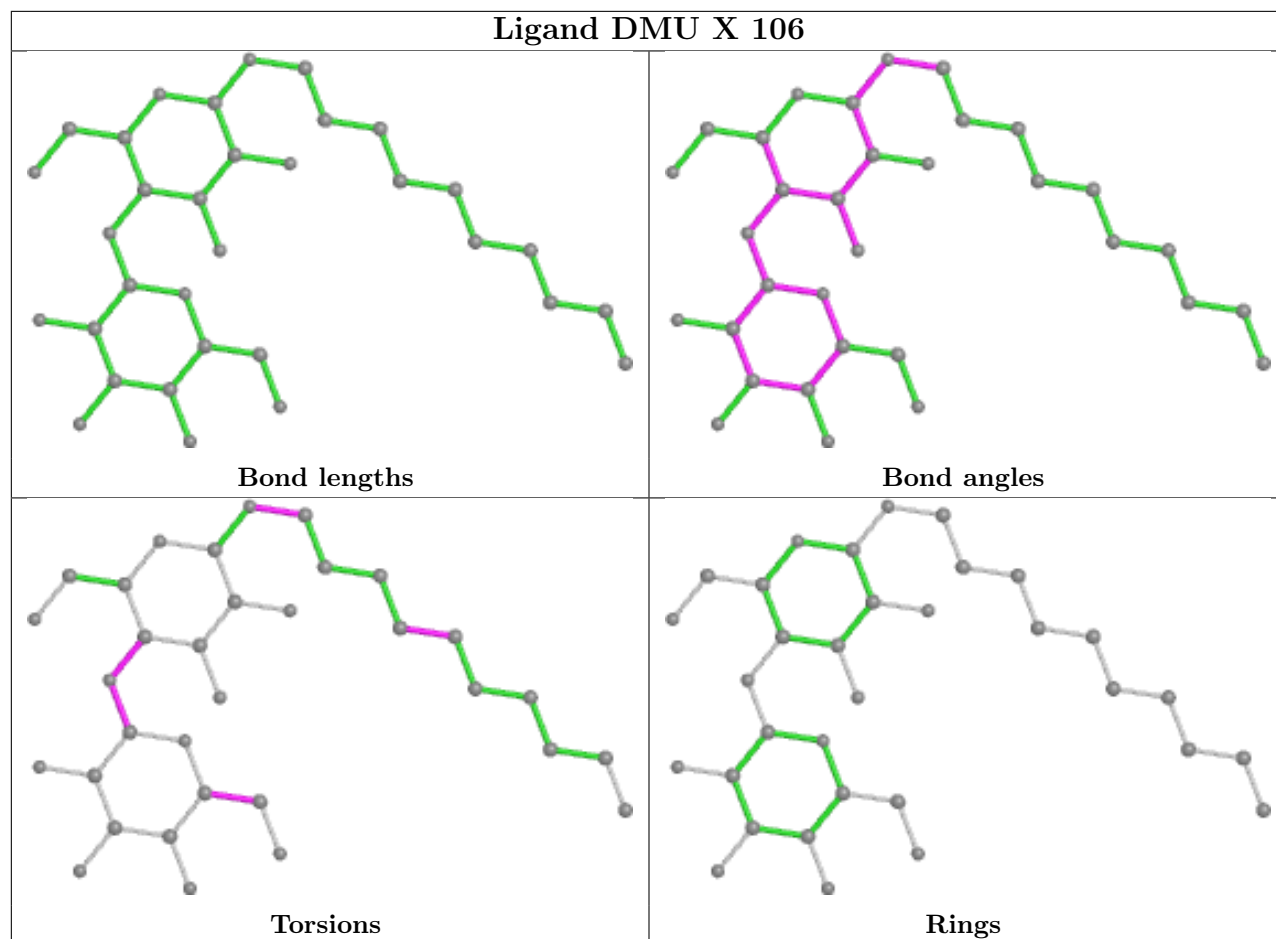


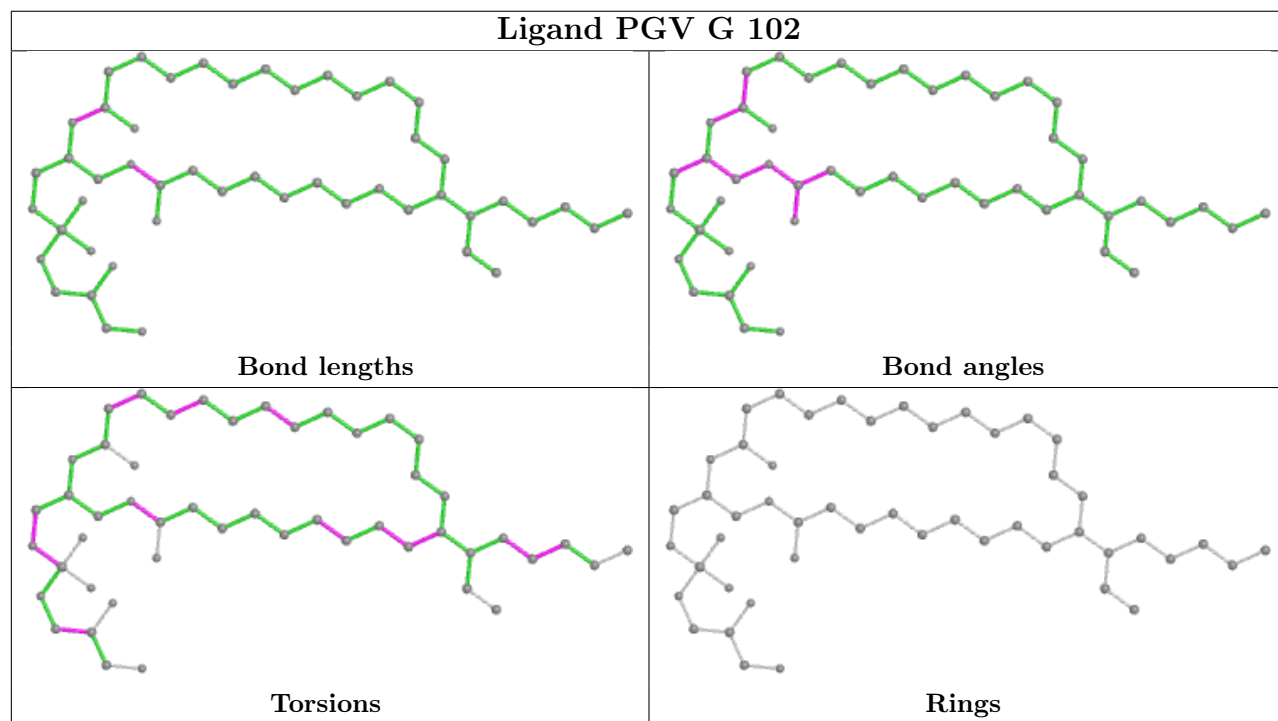
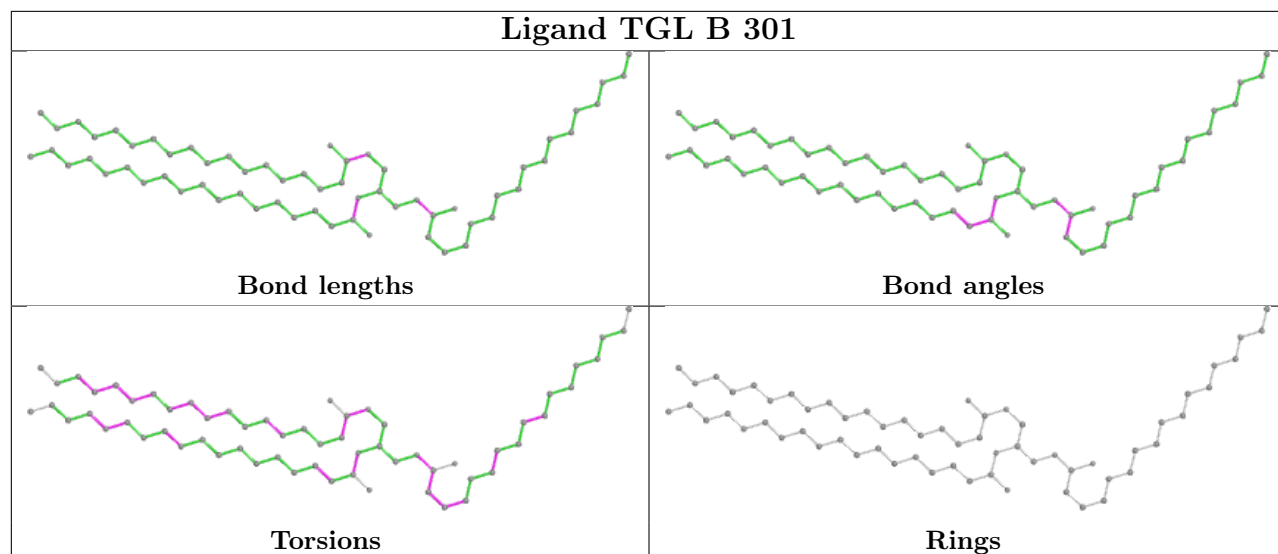
Ligand PGV P 302

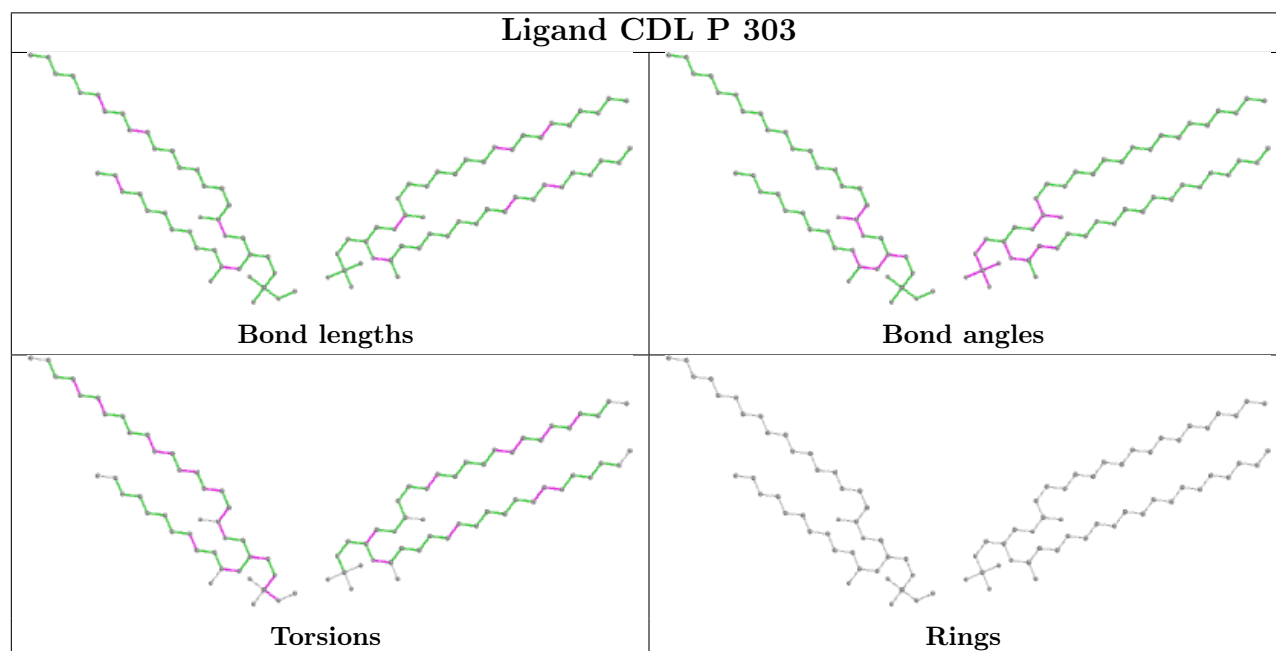
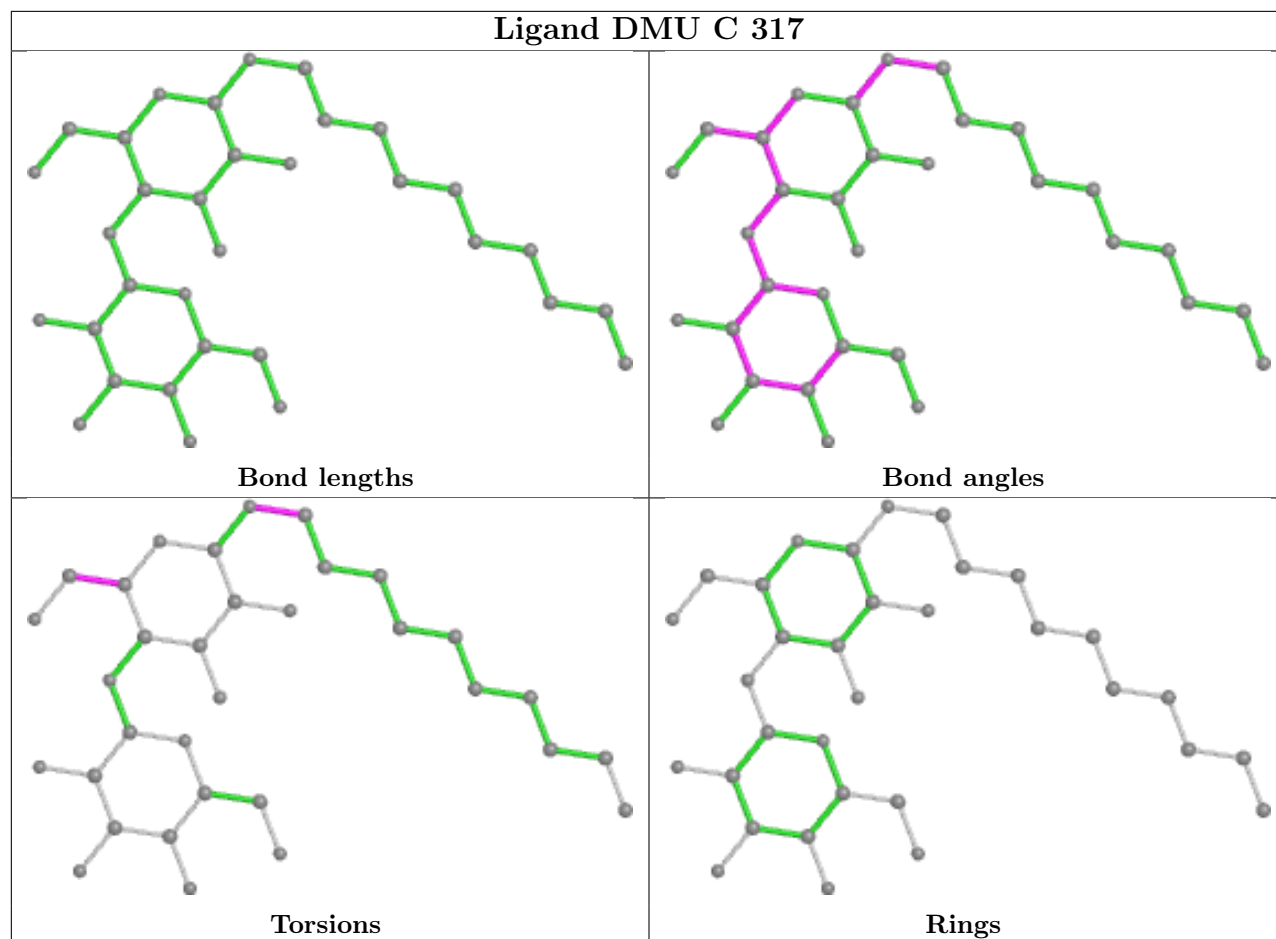


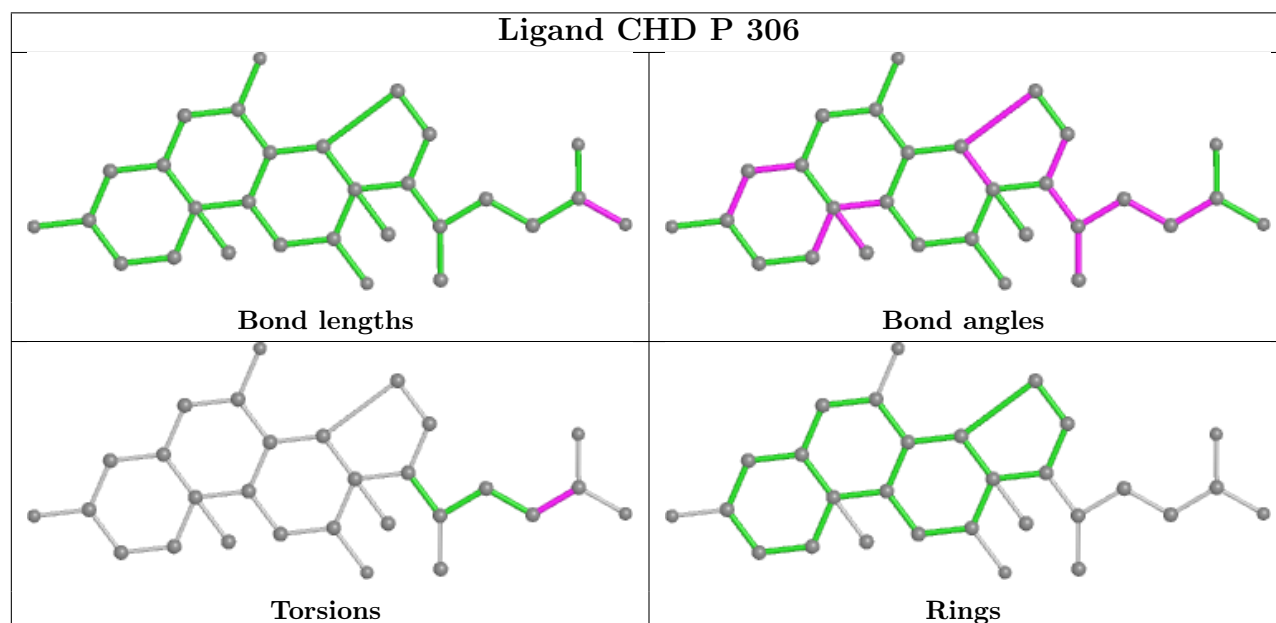
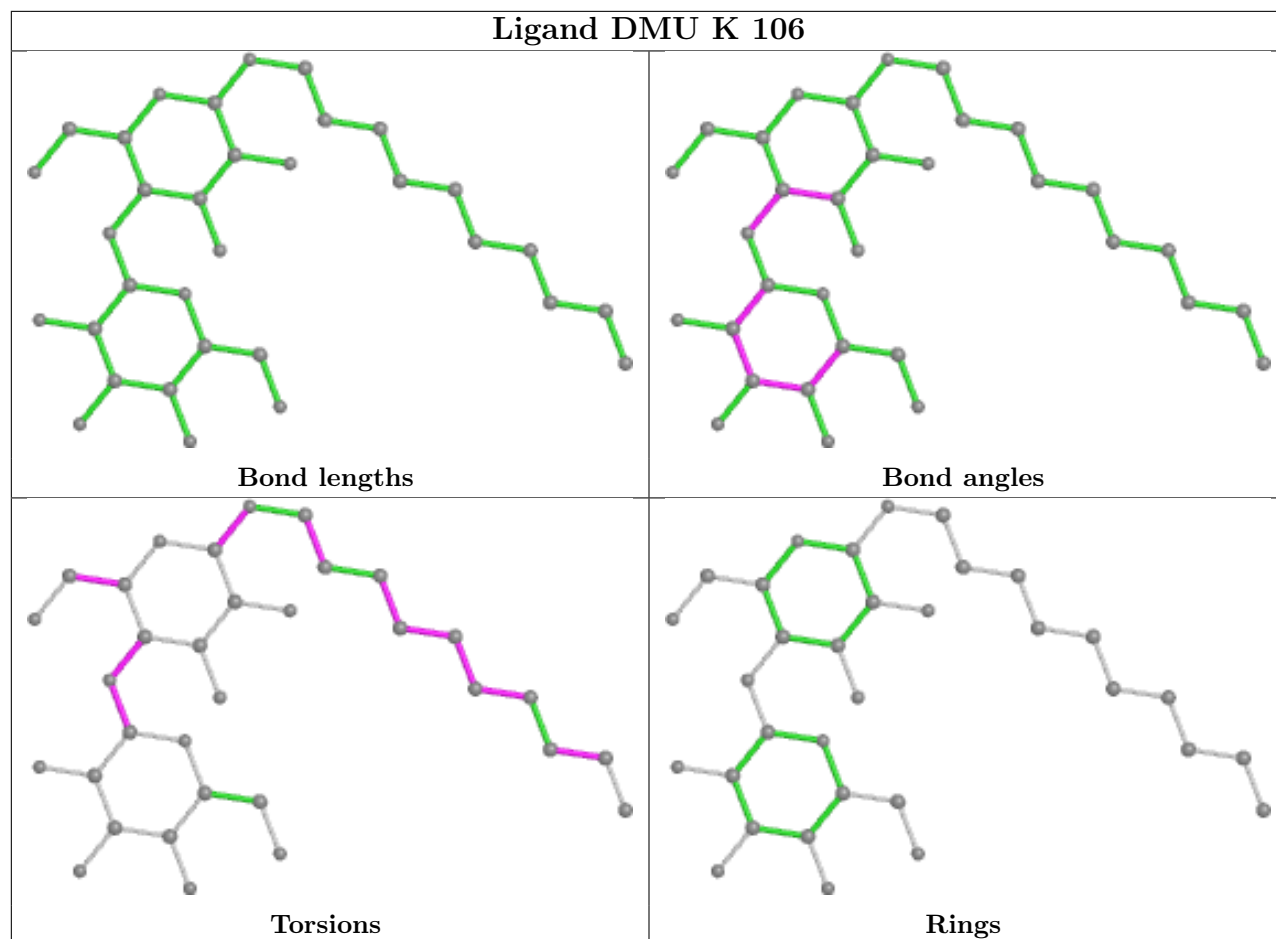
Ligand CHD C 303

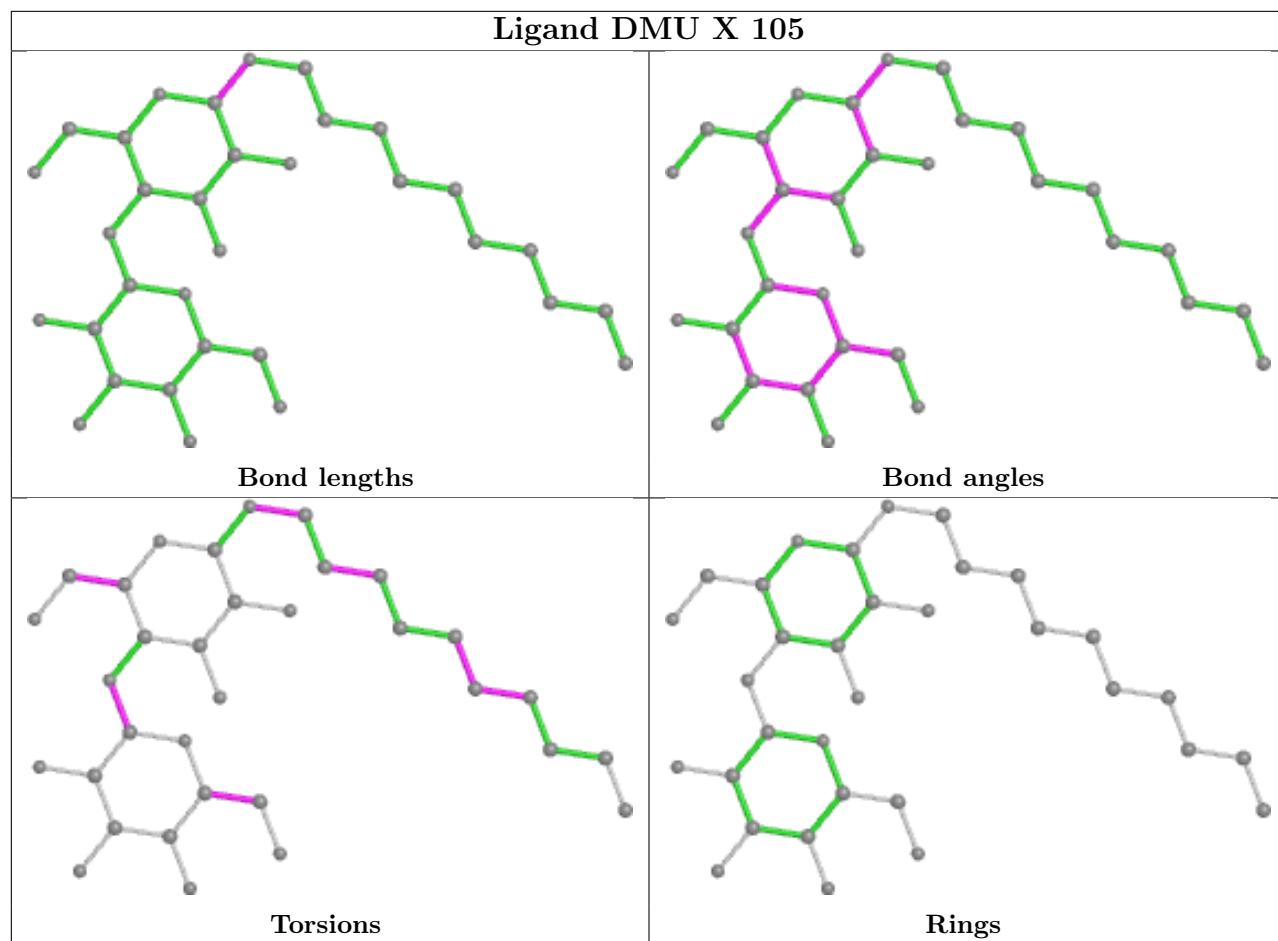


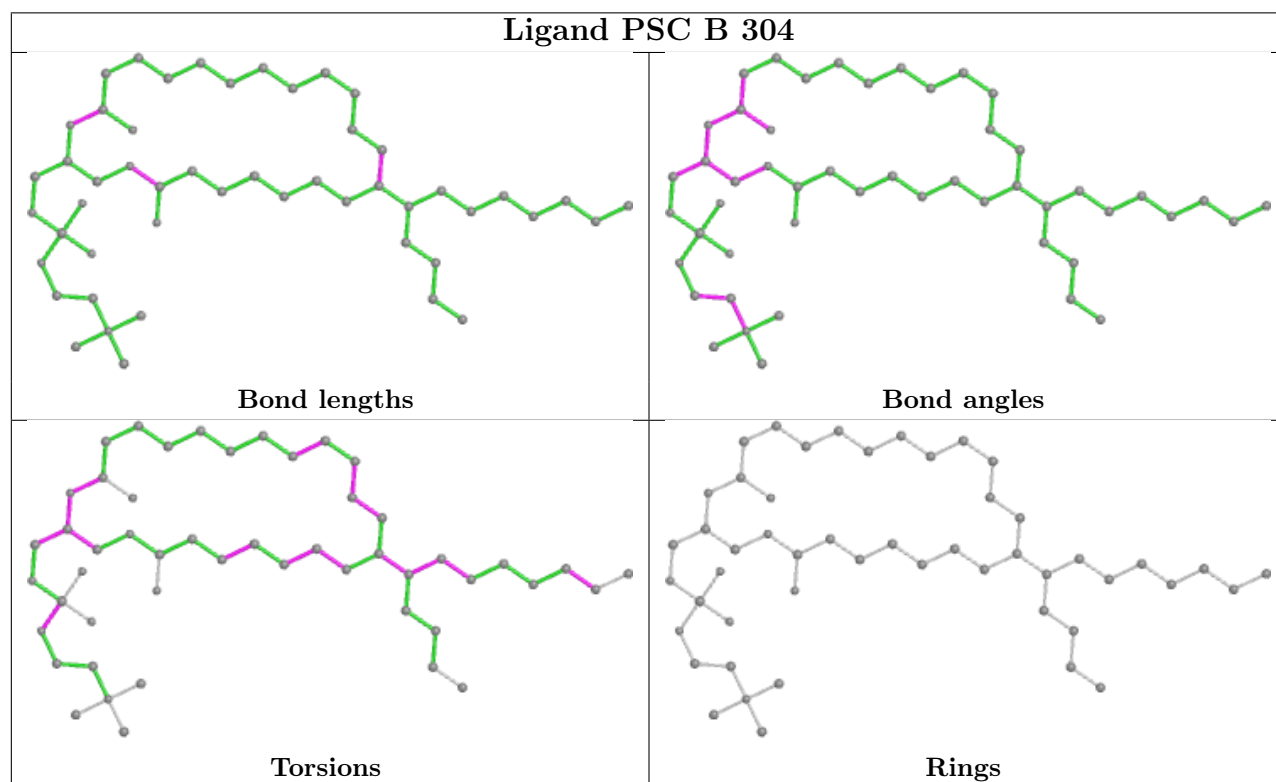
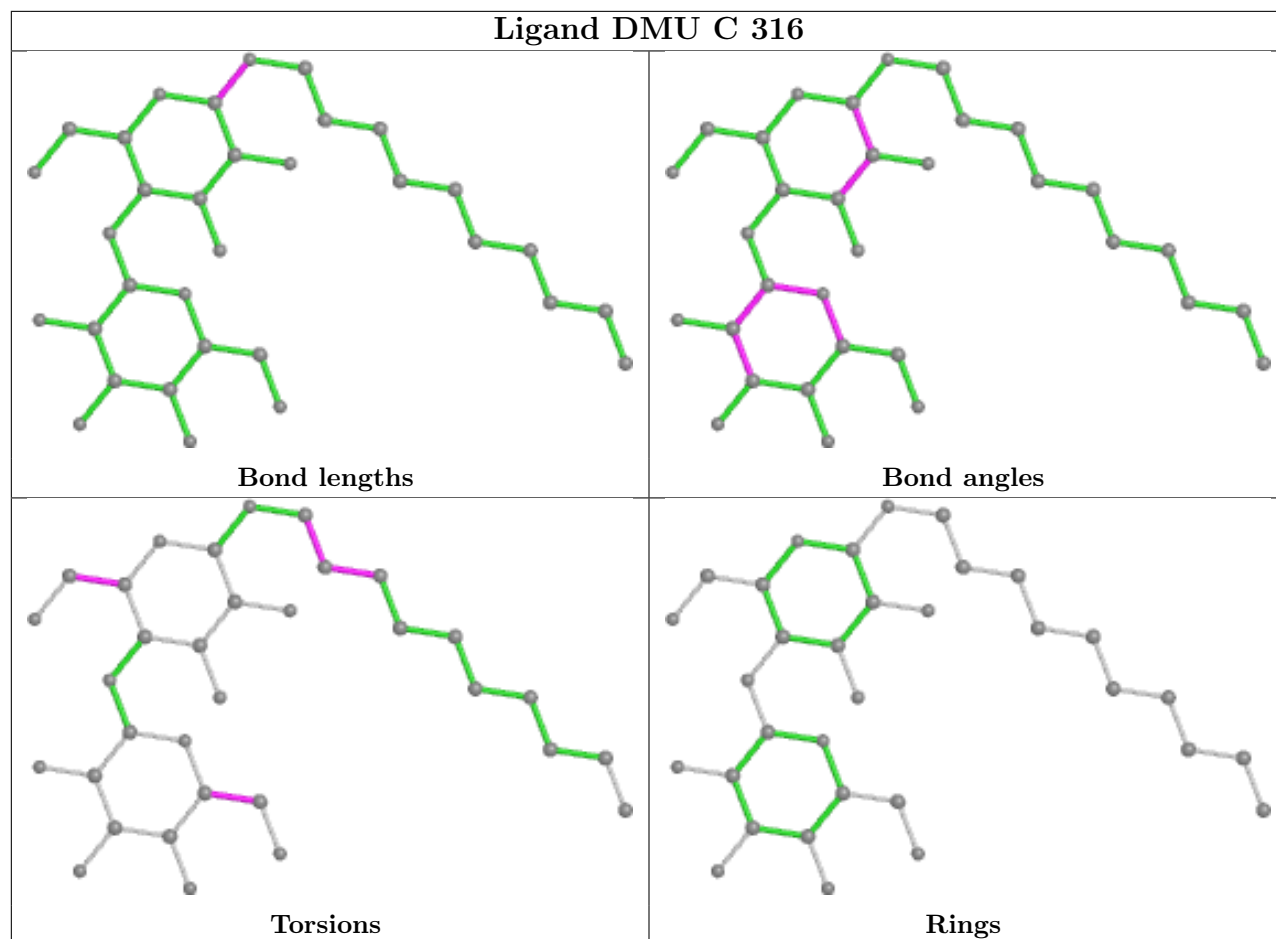












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.33	1 (0%) 95 95	17, 21, 28, 84	0
1	N	513/514 (99%)	-0.32	1 (0%) 95 95	18, 25, 34, 70	0
2	B	226/227 (99%)	-0.34	3 (1%) 77 81	20, 28, 62, 117	0
2	O	226/227 (99%)	-0.33	4 (1%) 68 73	25, 33, 76, 138	0
3	C	259/261 (99%)	-0.68	0 100 100	19, 25, 40, 80	0
3	P	259/261 (99%)	-0.59	0 100 100	20, 26, 43, 111	0
4	D	144/147 (97%)	-0.67	1 (0%) 87 90	24, 30, 63, 106	0
4	Q	144/147 (97%)	0.41	9 (6%) 20 21	30, 46, 115, 259	0
5	E	105/109 (96%)	-0.63	1 (0%) 82 85	23, 30, 72, 157	0
5	R	105/109 (96%)	-0.19	2 (1%) 66 71	26, 38, 81, 173	0
6	F	98/98 (100%)	-0.06	6 (6%) 21 23	21, 31, 118, 176	0
6	S	98/98 (100%)	-0.25	8 (8%) 11 12	22, 31, 114, 172	0
7	G	83/85 (97%)	0.75	17 (20%) 1 1	24, 32, 135, 176	0
8	H	79/85 (92%)	-0.24	6 (7%) 13 14	24, 35, 133, 157	0
8	U	79/85 (92%)	-0.27	4 (5%) 28 30	31, 41, 166, 191	0
9	I	72/73 (98%)	0.24	5 (6%) 16 17	27, 42, 93, 119	0
9	V	72/73 (98%)	0.48	7 (9%) 7 8	27, 54, 130, 251	0
10	J	58/59 (98%)	0.27	3 (5%) 27 30	25, 35, 95, 145	0
10	W	58/59 (98%)	-0.12	3 (5%) 27 30	27, 37, 100, 186	0
11	K	49/56 (87%)	-0.32	0 100 100	27, 34, 65, 92	0
11	X	49/56 (87%)	0.98	9 (18%) 1 1	35, 46, 126, 135	0
12	L	46/47 (97%)	-0.66	0 100 100	22, 26, 58, 119	0
12	Y	46/47 (97%)	-0.60	1 (2%) 62 67	28, 34, 88, 160	0
13	M	43/46 (93%)	-0.28	3 (6%) 16 17	23, 27, 91, 142	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	Z	43/46 (93%)	-0.05	2 (4%) 31 34	31, 37, 118, 255	0
14	T	84/85 (98%)	0.70	17 (20%) 1 1	23, 36, 145, 257	0
All	All	3551/3614 (98%)	-0.24	113 (3%) 47 52	17, 29, 86, 259	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	18.8
4	Q	5	VAL	15.7
14	T	8	HIS	14.4
4	Q	4	SER	13.2
7	G	3	ALA	10.9
6	F	96	LEU	9.7
10	J	1	PHE	9.6
14	T	9	GLY	9.4
4	Q	8	SER	8.9
10	J	58	LYS	8.9
7	G	8	HIS	8.5
4	Q	7	LYS	8.1
6	S	97	ALA	7.6
14	T	1	ALA	7.4
14	T	10	GLY	7.3
6	F	97	ALA	7.3
8	U	8	ILE	7.2
5	R	109	VAL	7.1
9	I	37	PHE	6.7
14	T	36	TRP	6.7
5	R	5	HIS	6.6
6	S	94	HIS	6.6
9	V	37	PHE	6.5
8	U	7	LYS	6.3
6	F	1	ALA	6.1
6	F	95	GLN	5.9
7	G	36	TRP	5.9
7	G	9	GLY	5.8
8	H	45	ALA	5.8
7	G	40	GLY	5.5
7	G	7	ASP	5.5
9	V	2	THR	5.4
11	X	6	ALA	5.1
6	F	98	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
6	S	96	LEU	4.9
10	W	1	PHE	4.9
7	G	1	ALA	4.9
2	O	227	LEU	4.9
13	Z	42	LYS	4.8
13	M	40	TYR	4.7
7	G	2	SER	4.7
4	Q	51	LEU	4.5
14	T	7	ASP	4.5
6	S	1	ALA	4.5
13	M	43	SER	4.3
13	M	42	LYS	4.3
5	E	5	HIS	4.1
6	S	98	HIS	4.1
14	T	2	SER	4.0
7	G	84	LYS	4.0
9	I	25	PHE	3.9
8	U	46	LYS	3.9
7	G	6	GLY	3.8
13	Z	43	SER	3.8
6	S	93	PRO	3.7
14	T	6	GLY	3.7
14	T	3	ALA	3.6
7	G	5	LYS	3.6
8	H	46	LYS	3.5
7	G	4	ALA	3.5
14	T	42	ARG	3.5
2	O	226	MET	3.4
9	V	25	PHE	3.4
9	V	34	PHE	3.4
6	S	95	GLN	3.3
2	O	90	ILE	3.3
11	X	13	TYR	3.3
14	T	39	SER	3.2
10	W	52	TRP	3.2
14	T	11	THR	3.1
12	Y	47	LYS	3.1
6	S	2	SER	3.1
7	G	41	HIS	3.0
9	I	29	LEU	3.0
7	G	42	ARG	3.0
4	Q	53	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	56[A]	MET	2.8
14	T	84	LYS	2.8
11	X	7	PRO	2.8
11	X	23	THR	2.8
14	T	5	LYS	2.7
10	W	58	LYS	2.6
4	Q	9	GLU	2.6
7	G	39	SER	2.5
14	T	40	GLY	2.5
6	F	2	SER	2.4
8	U	9	LYS	2.4
8	H	44	THR	2.4
8	H	8	ILE	2.4
1	A	195	LEU	2.3
14	T	37	LEU	2.3
1	N	195	LEU	2.3
4	Q	147	LYS	2.3
11	X	30	VAL	2.3
9	I	36	LYS	2.2
2	O	113	TYR	2.2
2	B	61	VAL	2.2
9	V	3	ALA	2.2
9	V	39	VAL	2.2
9	I	39	VAL	2.2
11	X	24	PHE	2.2
11	X	34	THR	2.2
7	G	35	SER	2.2
10	J	57	HIS	2.1
14	T	33	LEU	2.1
7	G	10	GLY	2.1
9	V	31	PHE	2.1
11	X	28[A]	VAL	2.1
4	D	147	LYS	2.1
8	H	7	LYS	2.0
8	H	48	GLY	2.0
2	B	55	THR	2.0
11	X	19	ALA	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
9	SAC	V	1	9/10	0.66	0.63	336,360,399,412	0
7	TPO	G	11	11/12	0.73	0.25	82,115,176,188	0
9	SAC	I	1	9/10	0.81	0.19	111,135,185,189	0
1	FME	N	1	10/11	0.94	0.11	34,39,109,122	0
1	FME	A	1	10/11	0.96	0.09	32,41,86,119	0
2	FME	B	1	10/11	0.96	0.06	25,26,35,139	0
2	FME	O	1	10/11	0.97	0.06	33,34,48,155	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
23	DMU	X	106	33/33	0.11	0.69	70,86,93,94	0
23	DMU	C	318	33/33	0.20	0.35	54,98,133,144	0
23	DMU	X	102	33/33	0.28	0.49	43,111,135,146	0
23	DMU	K	106	33/33	0.31	0.62	45,112,131,135	0
23	DMU	K	104	33/33	0.33	0.54	39,109,133,136	0
23	DMU	X	105	33/33	0.37	0.66	54,113,130,144	0
22	EDO	P	311	4/4	0.40	0.26	70,73,76,82	0
23	DMU	K	102	33/33	0.44	0.49	54,109,126,129	0
23	DMU	A	628	33/33	0.46	0.61	66,104,128,132	0
23	DMU	K	101	33/33	0.46	0.42	37,115,128,133	0
23	DMU	X	107	33/33	0.47	0.73	68,119,135,145	0
23	DMU	P	314	33/33	0.54	0.28	48,96,128,144	0
23	DMU	X	103	33/33	0.55	0.48	63,102,135,139	0
22	EDO	J	103	4/4	0.58	0.53	63,82,84,128	0
23	DMU	C	316	33/33	0.59	0.37	51,103,124,128	0
23	DMU	D	206	33/33	0.60	0.37	56,126,197,214	0
23	DMU	O	307	33/33	0.60	0.33	44,104,142,148	0
23	DMU	C	317	33/33	0.62	0.37	47,96,125,129	0
22	EDO	A	623	4/4	0.62	0.20	44,48,56,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	B	309	4/4	0.63	0.16	49,62,73,76	0
23	DMU	K	105	33/33	0.63	0.40	56,93,126,128	0
22	EDO	G	105	4/4	0.64	0.26	56,81,84,93	0
23	DMU	I	101	33/33	0.64	0.40	49,114,130,139	0
25	CHD	X	101	29/29	0.64	0.55	50,92,112,115	0
23	DMU	K	103	32/33	0.65	0.30	48,98,121,134	0
28	PEK	T	101	50/53	0.65	0.28	40,82,148,188	0
22	EDO	V	101	4/4	0.66	0.12	71,76,82,83	0
26	PSC	B	304	52/52	0.67	0.32	39,97,184,225	0
23	DMU	P	315	33/33	0.68	0.31	52,102,118,126	0
22	EDO	A	610	4/4	0.69	0.24	49,66,66,70	0
22	EDO	A	627	4/4	0.69	0.14	64,66,68,74	0
22	EDO	A	622	4/4	0.69	0.43	35,67,74,77	0
22	EDO	S	107	4/4	0.69	0.27	49,64,69,79	0
23	DMU	L	105	33/33	0.70	0.34	51,103,129,133	0
23	DMU	X	104	33/33	0.70	0.36	50,95,122,127	0
22	EDO	A	619	4/4	0.71	0.18	47,51,53,59	0
27	CDL	T	102	98/100	0.72	0.28	42,92,166,203	0
27	CDL	G	101	100/100	0.73	0.33	47,95,178,197	0
22	EDO	D	203	4/4	0.73	0.15	38,53,58,65	0
20	PGV	G	102	51/51	0.73	0.26	42,82,161,206	0
28	PEK	C	309	53/53	0.74	0.27	45,85,184,201	0
22	EDO	G	103	4/4	0.75	0.12	44,61,76,77	0
25	CHD	P	304	29/29	0.75	0.36	56,105,138,147	0
22	EDO	N	615	4/4	0.76	0.17	46,50,57,62	0
28	PEK	C	305	53/53	0.77	0.23	36,78,161,193	0
25	CHD	Y	104	29/29	0.77	0.35	62,82,119,131	0
22	EDO	P	313	4/4	0.77	0.17	45,52,65,81	0
23	DMU	P	305	33/33	0.78	0.23	36,92,151,168	0
21	TGL	Y	101	63/63	0.79	0.22	38,64,124,183	0
23	DMU	C	308	33/33	0.79	0.26	30,79,126,143	0
28	PEK	P	301	53/53	0.79	0.26	46,85,150,179	0
22	EDO	D	205	4/4	0.79	0.17	37,40,64,65	0
22	EDO	F	106	4/4	0.80	0.09	64,66,70,74	0
25	CHD	C	303	29/29	0.80	0.36	51,96,140,144	0
21	TGL	Q	202	63/63	0.80	0.18	43,73,114,139	0
20	PGV	A	608	51/51	0.81	0.23	29,85,159,205	0
22	EDO	N	622	4/4	0.81	0.16	29,44,59,66	0
22	EDO	O	305	4/4	0.81	0.16	70,74,76,81	0
21	TGL	D	201	62/63	0.81	0.17	30,64,107,130	0
25	CHD	L	104	29/29	0.81	0.32	53,80,105,110	0
22	EDO	C	315	4/4	0.82	0.12	30,37,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	C	313	4/4	0.83	0.24	30,75,75,75	0
22	EDO	Q	204	4/4	0.83	0.12	46,46,50,51	0
22	EDO	A	617	4/4	0.83	0.15	43,49,54,71	0
22	EDO	D	202	4/4	0.83	0.26	49,51,56,63	0
22	EDO	N	611	4/4	0.83	0.19	68,74,75,75	0
20	PGV	C	306	48/51	0.84	0.21	40,80,142,210	0
21	TGL	B	301	62/63	0.84	0.17	34,64,100,116	0
26	PSC	O	304	51/52	0.84	0.25	37,81,202,224	0
27	CDL	P	303	90/100	0.85	0.24	29,74,149,171	0
22	EDO	L	101	4/4	0.85	0.12	38,47,54,86	0
23	DMU	M	101	33/33	0.85	0.15	33,39,51,57	0
22	EDO	N	609	4/4	0.85	0.16	30,34,65,68	0
20	PGV	Q	201	51/51	0.85	0.28	43,84,152,180	0
21	TGL	A	609	63/63	0.85	0.20	29,58,121,168	0
22	EDO	P	309	4/4	0.86	0.12	53,53,68,78	0
23	DMU	Z	101	33/33	0.86	0.16	40,48,69,88	0
22	EDO	N	623	4/4	0.86	0.12	42,45,77,80	0
22	EDO	T	105	4/4	0.86	0.18	46,53,71,82	0
27	CDL	C	302	89/100	0.86	0.29	26,75,138,150	0
22	EDO	M	103	4/4	0.86	0.08	60,63,64,69	0
21	TGL	O	301	60/63	0.87	0.24	39,76,110,133	0
22	EDO	S	105	4/4	0.88	0.09	37,39,45,49	0
22	EDO	J	101	4/4	0.89	0.18	47,48,64,103	0
22	EDO	N	610	4/4	0.89	0.20	31,43,72,80	0
22	EDO	C	312	4/4	0.89	0.27	37,55,60,90	0
22	EDO	N	608	4/4	0.89	0.15	39,49,72,73	0
22	EDO	N	618	4/4	0.90	0.12	29,38,46,52	0
25	CHD	P	306	29/29	0.90	0.07	25,28,33,33	0
22	EDO	Z	102	4/4	0.90	0.14	56,70,88,122	0
22	EDO	N	620	4/4	0.90	0.25	69,70,73,82	0
22	EDO	A	611	4/4	0.90	0.11	31,35,41,74	0
22	EDO	E	203	4/4	0.90	0.08	41,44,47,49	0
22	EDO	T	106	4/4	0.90	0.19	49,59,61,88	0
22	EDO	D	204	4/4	0.91	0.09	40,40,52,55	0
22	EDO	F	107	4/4	0.91	0.11	31,33,47,51	0
22	EDO	H	101	4/4	0.91	0.17	35,36,66,67	0
22	EDO	L	103	4/4	0.91	0.09	51,55,61,62	0
22	EDO	Q	203	4/4	0.91	0.12	34,39,41,41	0
22	EDO	Y	102	4/4	0.91	0.12	46,57,75,94	0
22	EDO	M	102	4/4	0.91	0.15	52,63,72,77	0
25	CHD	C	304	29/29	0.92	0.07	25,27,33,35	0
22	EDO	S	108	4/4	0.92	0.17	38,42,52,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	EDO	A	615	4/4	0.92	0.16	31,32,72,74	0
22	EDO	S	104	4/4	0.92	0.12	29,35,37,39	0
22	EDO	A	612	4/4	0.93	0.12	29,29,65,67	0
22	EDO	W	101	4/4	0.93	0.15	47,52,83,100	0
22	EDO	A	625	4/4	0.93	0.21	29,38,43,93	0
22	EDO	Y	103	4/4	0.93	0.06	50,51,52,64	0
22	EDO	N	619	4/4	0.93	0.08	34,37,41,42	0
22	EDO	C	314	4/4	0.93	0.23	36,58,63,109	0
22	EDO	G	104	4/4	0.93	0.06	29,31,34,34	0
22	EDO	N	614	4/4	0.93	0.07	33,33,34,35	0
22	EDO	B	308	4/4	0.94	0.09	35,39,49,69	0
22	EDO	J	105	4/4	0.94	0.23	36,48,53,55	0
22	EDO	A	613	4/4	0.94	0.15	32,42,71,78	0
22	EDO	P	308	4/4	0.94	0.08	28,34,37,44	0
22	EDO	T	103	4/4	0.94	0.09	36,39,41,55	0
22	EDO	L	102	4/4	0.94	0.14	40,69,74,95	0
22	EDO	A	624	4/4	0.94	0.16	26,28,36,46	0
22	EDO	P	312	4/4	0.94	0.09	47,48,62,84	0
19	PER	A	606	2/2	0.94	0.17	16,16,16,23	0
22	EDO	A	616	4/4	0.94	0.10	36,38,40,42	0
22	EDO	B	306	4/4	0.94	0.07	27,34,37,45	0
30	PO4	U	101	5/5	0.94	0.11	52,54,131,144	0
22	EDO	S	103	4/4	0.95	0.11	36,49,74,79	0
22	EDO	A	618	4/4	0.95	0.07	23,25,25,26	0
22	EDO	A	626	4/4	0.95	0.14	30,34,48,89	0
22	EDO	C	310	4/4	0.95	0.06	28,28,31,32	0
22	EDO	C	311	4/4	0.95	0.10	28,30,37,50	0
19	PER	N	606	2/2	0.95	0.19	19,19,19,26	0
22	EDO	B	305	4/4	0.95	0.10	36,44,62,83	0
22	EDO	J	102	4/4	0.95	0.26	43,57,69,78	0
22	EDO	F	102	4/4	0.95	0.11	32,34,35,40	0
22	EDO	J	104	4/4	0.95	0.19	35,48,75,79	0
22	EDO	F	104	4/4	0.95	0.21	38,41,64,89	0
22	EDO	N	617	4/4	0.95	0.08	33,40,41,53	0
22	EDO	A	620	4/4	0.95	0.10	28,37,38,46	0
22	EDO	R	201	4/4	0.95	0.08	34,36,38,43	0
30	PO4	H	102	5/5	0.95	0.17	56,58,101,148	0
25	CHD	O	303	29/29	0.95	0.06	22,25,29,37	0
18	NA	N	605	1/1	0.96	0.05	28,28,28,28	0
22	EDO	N	616	4/4	0.96	0.06	27,34,59,72	0
22	EDO	N	621	4/4	0.96	0.10	29,32,39,77	0
28	PEK	C	307	52/53	0.96	0.10	25,41,93,123	0

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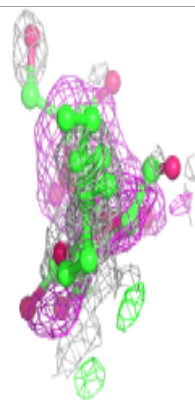
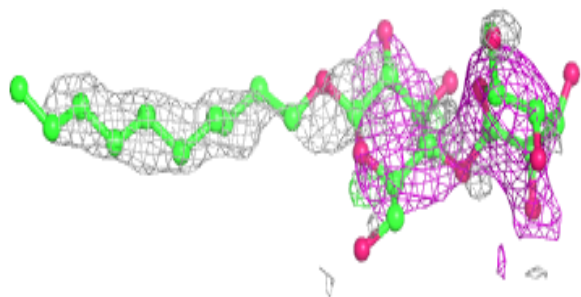
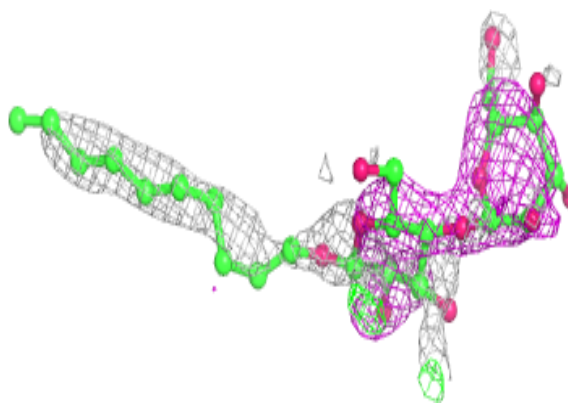
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	CHD	B	303	29/29	0.96	0.06	22,25,31,39	0
22	EDO	P	310	4/4	0.96	0.07	32,36,38,40	0
28	PEK	P	307	53/53	0.96	0.11	26,46,96,119	0
22	EDO	T	104	4/4	0.96	0.06	31,32,36,39	0
22	EDO	N	612	4/4	0.96	0.07	25,26,26,26	0
22	EDO	A	621	4/4	0.96	0.14	22,38,78,106	0
22	EDO	E	202	4/4	0.97	0.07	32,35,38,40	0
22	EDO	S	109	4/4	0.97	0.09	28,29,29,32	0
22	EDO	O	306	4/4	0.97	0.04	28,30,31,31	0
22	EDO	N	613	4/4	0.97	0.07	23,26,26,29	0
20	PGV	C	301	51/51	0.97	0.08	20,29,88,95	0
22	EDO	E	201	4/4	0.97	0.07	32,34,35,36	0
20	PGV	N	607	51/51	0.98	0.08	21,29,61,93	0
20	PGV	P	302	51/51	0.98	0.08	21,29,85,110	0
20	PGV	A	607	51/51	0.98	0.08	20,28,72,88	0
15	HEA	N	602	60/60	0.98	0.09	18,21,27,33	0
22	EDO	N	624	4/4	0.98	0.09	29,30,63,75	0
15	HEA	A	601[A]	60/60	0.98	0.08	16,19,32,41	9
22	EDO	S	102	4/4	0.98	0.06	22,22,22,23	0
15	HEA	A	601[B]	60/60	0.98	0.08	16,19,32,41	9
22	EDO	F	103	4/4	0.98	0.13	27,28,29,30	0
22	EDO	A	614	4/4	0.98	0.10	20,21,22,25	0
22	EDO	S	106	4/4	0.98	0.04	31,32,35,36	0
15	HEA	A	602	60/60	0.98	0.07	16,18,25,31	0
16	CU	N	603	1/1	0.99	0.08	21,21,21,21	0
17	MG	A	604	1/1	0.99	0.03	19,19,19,19	0
17	MG	N	604	1/1	0.99	0.02	22,22,22,22	0
24	CUA	O	302	2/2	0.99	0.07	26,26,26,26	0
22	EDO	F	105	4/4	0.99	0.06	21,21,22,22	0
18	NA	A	605	1/1	0.99	0.03	22,22,22,22	0
15	HEA	N	601[B]	60/60	0.99	0.08	20,23,32,35	9
22	EDO	B	307	4/4	0.99	0.05	23,23,23,27	0
15	HEA	N	601[A]	60/60	0.99	0.08	20,23,38,41	9
29	ZN	F	101	1/1	1.00	0.03	25,25,25,25	0
29	ZN	S	101	1/1	1.00	0.04	25,25,25,25	0
16	CU	A	603	1/1	1.00	0.08	19,19,19,19	0
24	CUA	B	302	2/2	1.00	0.08	20,20,20,21	0

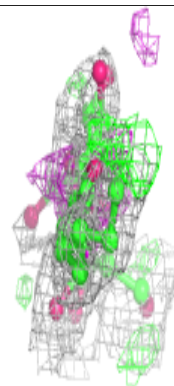
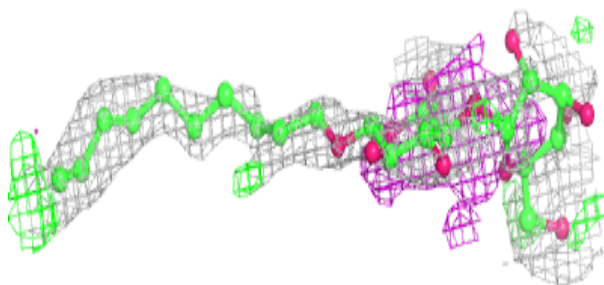
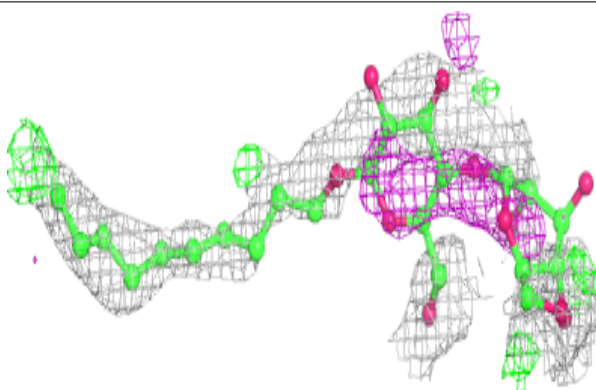
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU X 106:

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

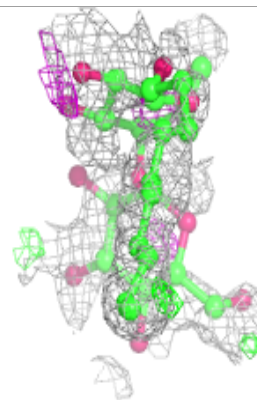
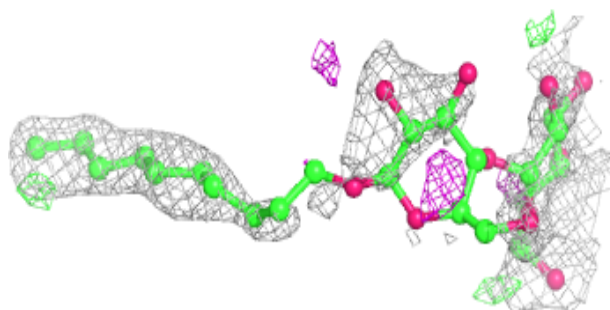
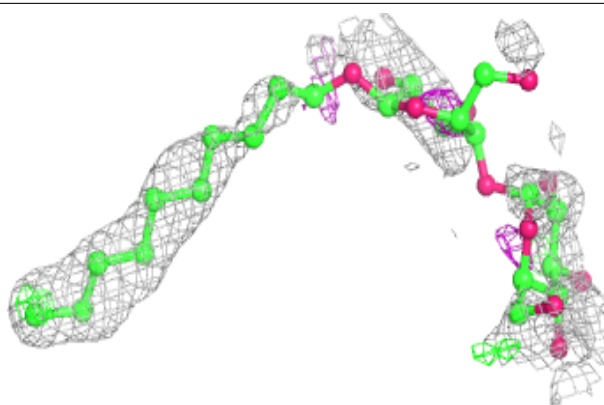
**Electron density around DMU C 318:**

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

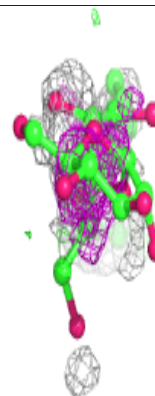
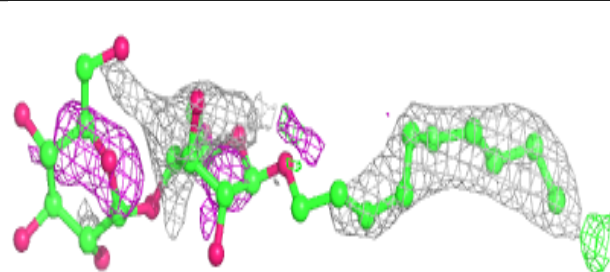
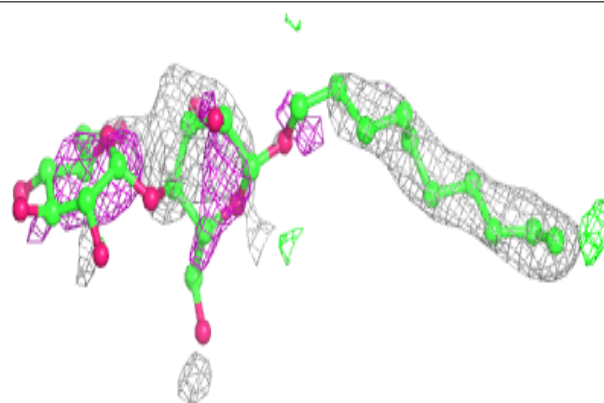


Electron density around DMU X 102:

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

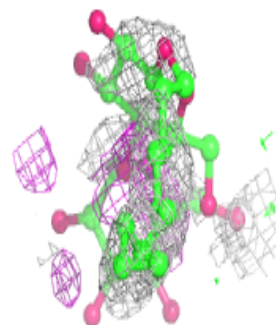
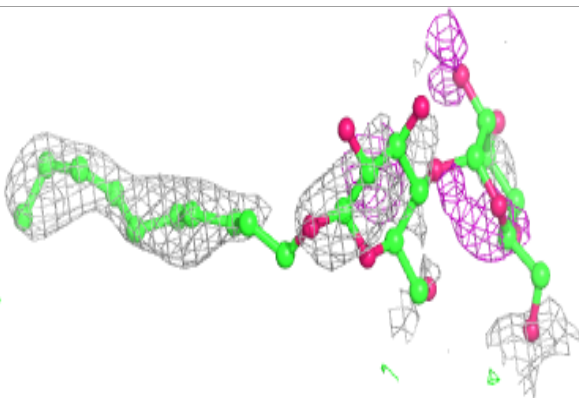
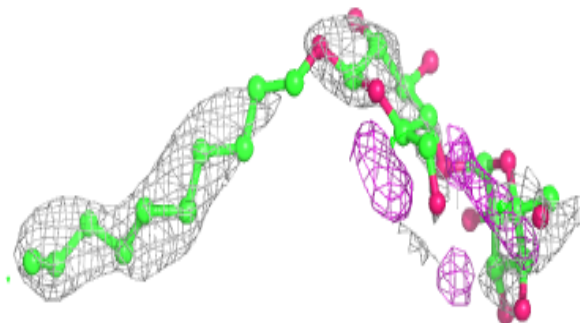
**Electron density around DMU K 106:**

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

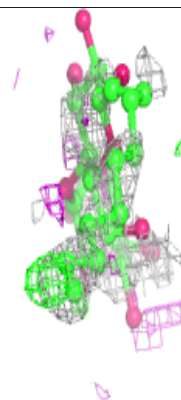
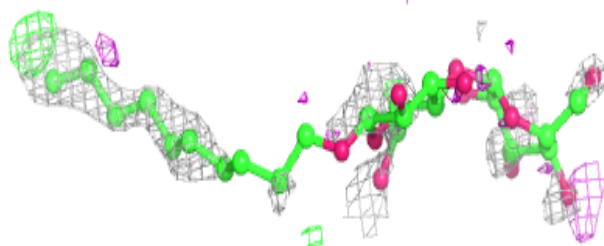
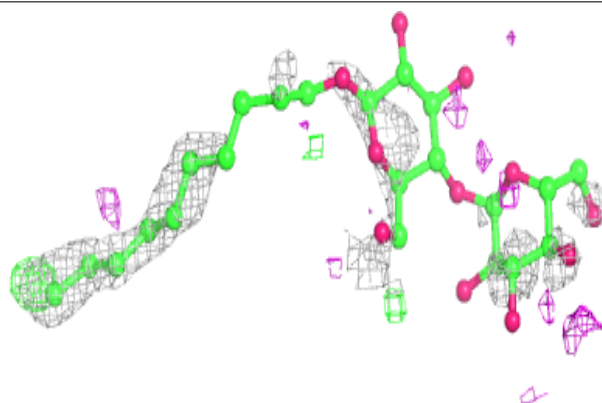


Electron density around DMU K 104:

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

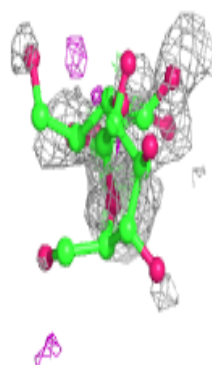
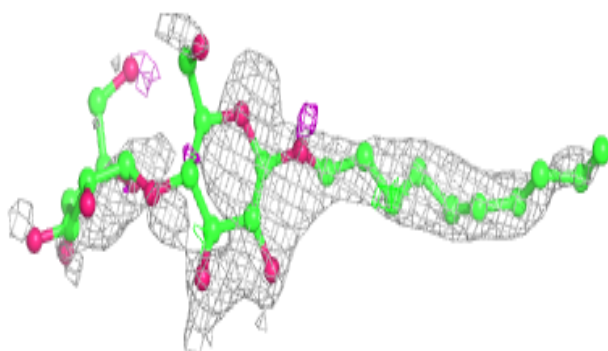
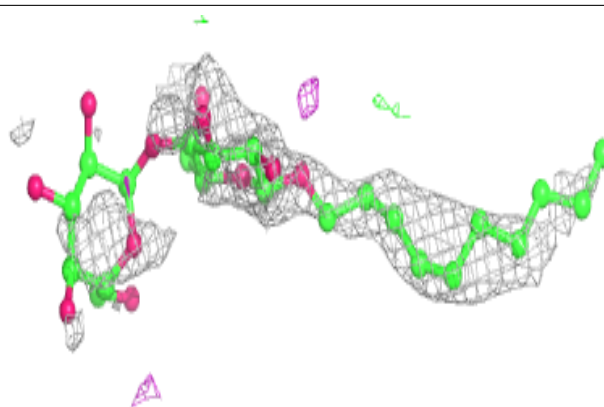
**Electron density around DMU X 105:**

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

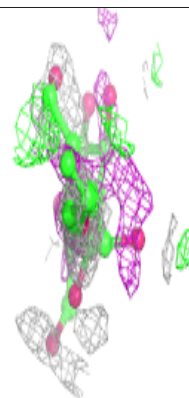
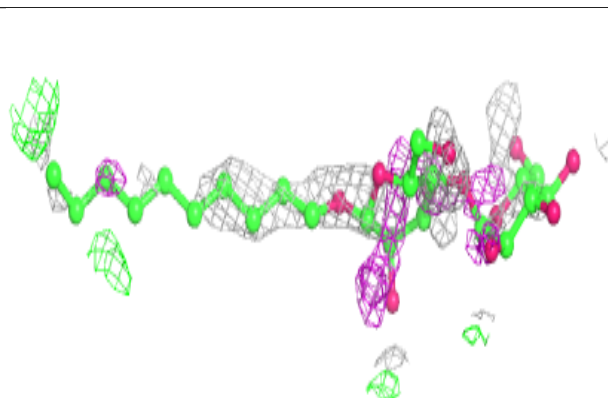
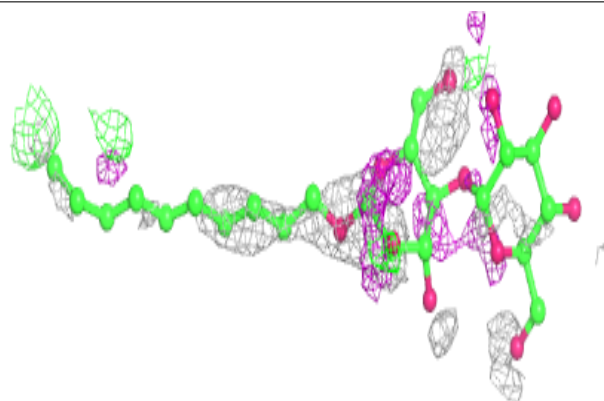


Electron density around DMU K 102:

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

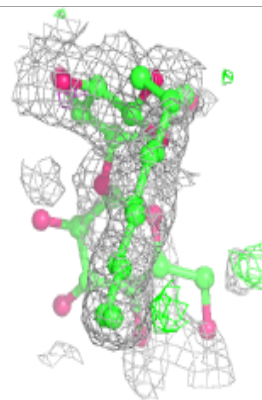
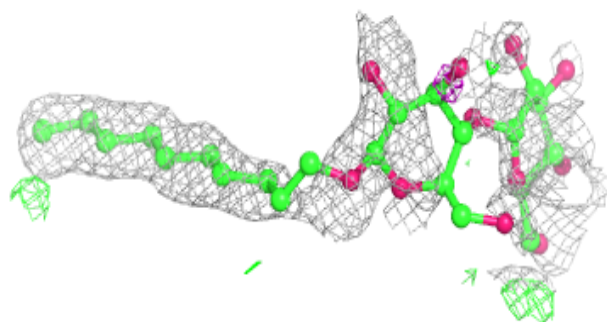
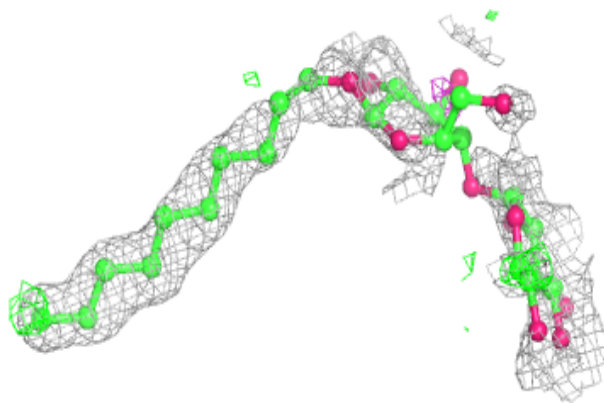
**Electron density around DMU A 628:**

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

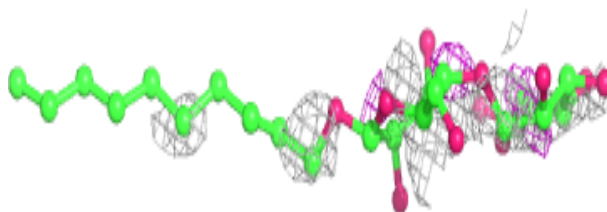
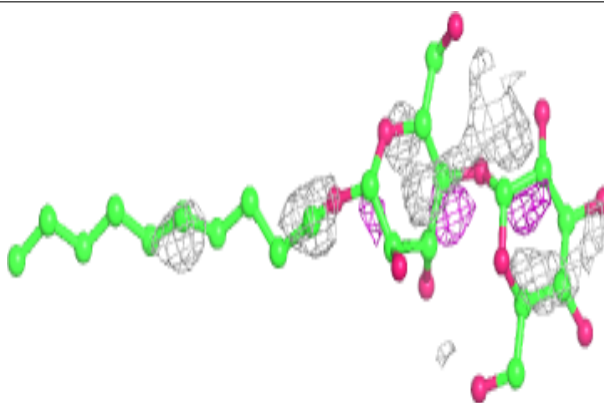


Electron density around DMU K 101:

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

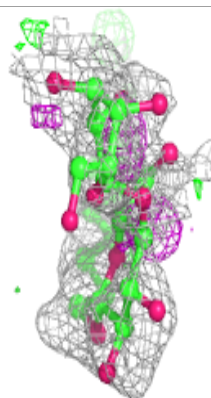
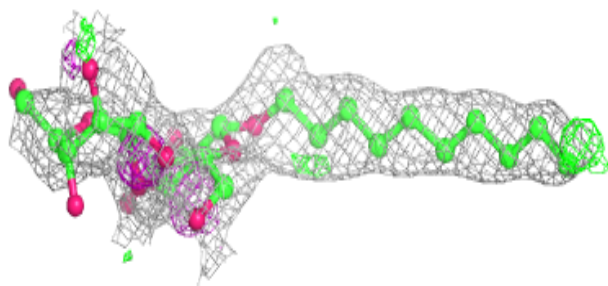
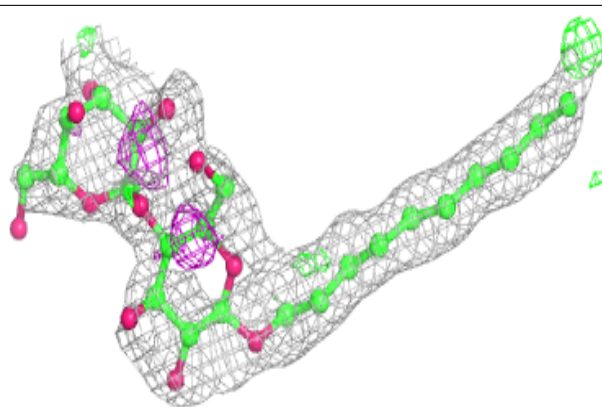
**Electron density around DMU X 107:**

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

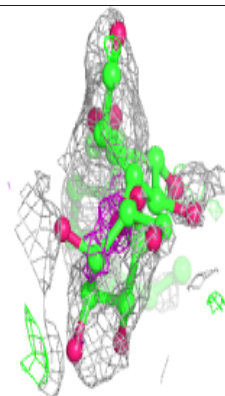
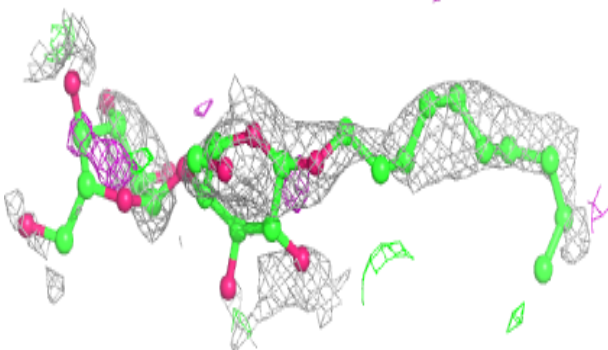
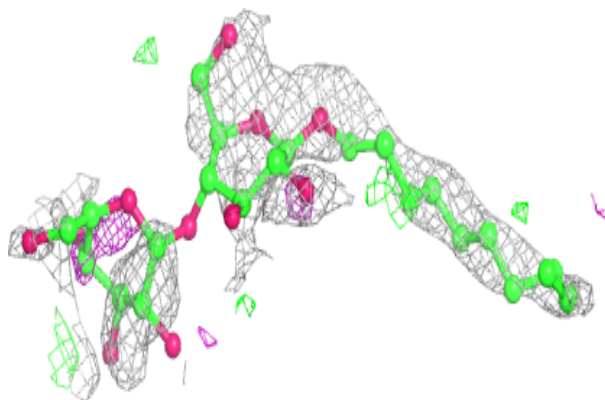


Electron density around DMU P 314:

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

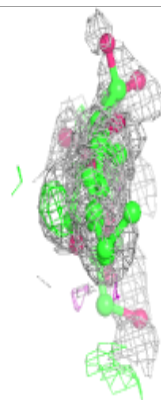
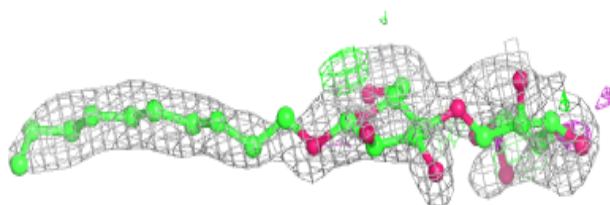
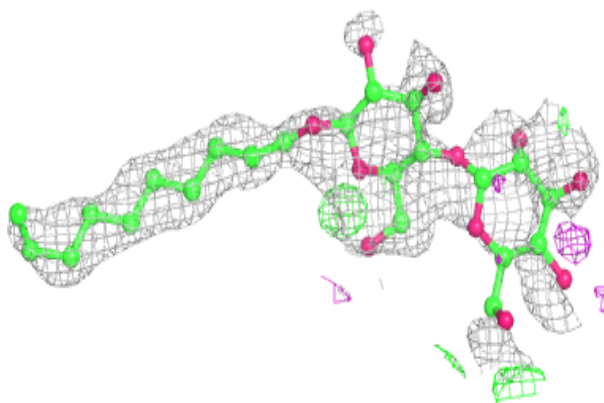
**Electron density around DMU X 103:**

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

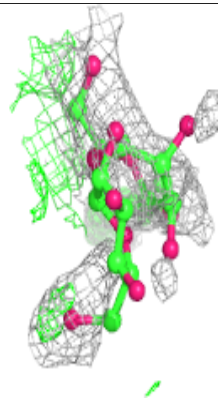
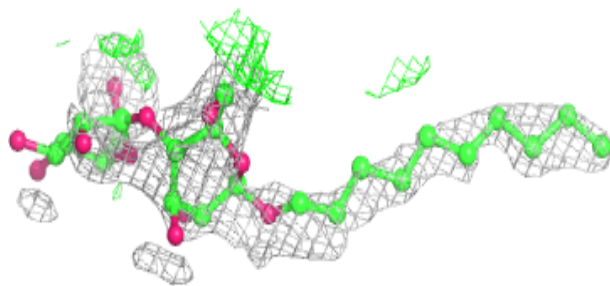
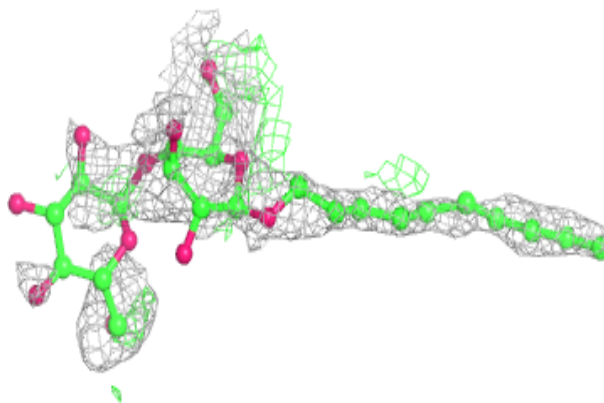


Electron density around DMU C 316:

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

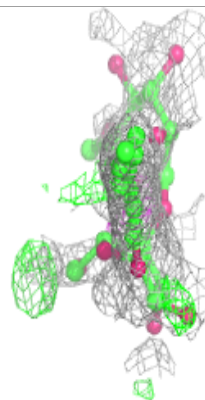
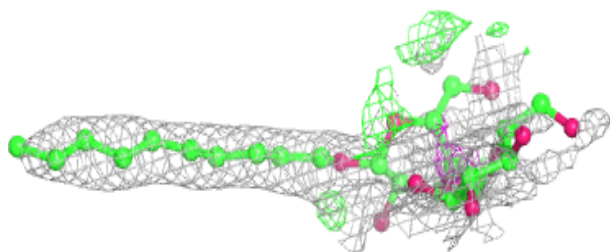
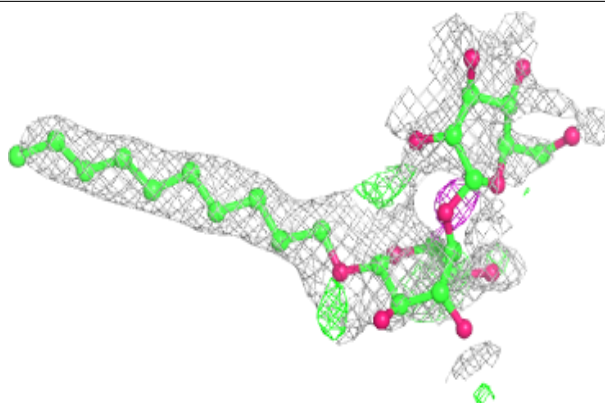
**Electron density around DMU D 206:**

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

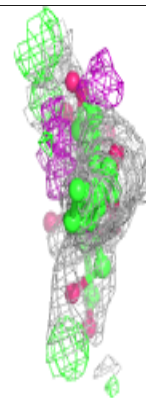
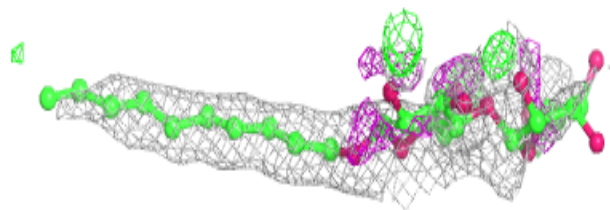
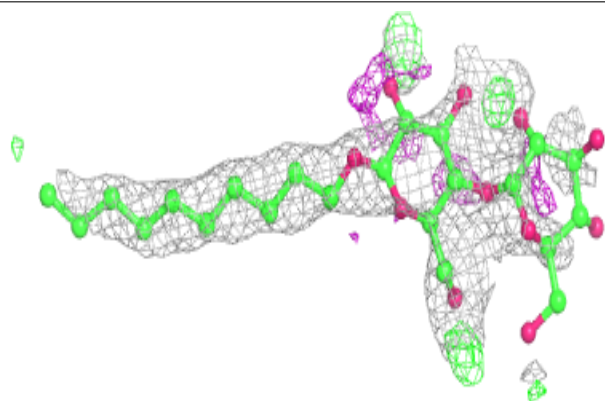


Electron density around DMU O 307:

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

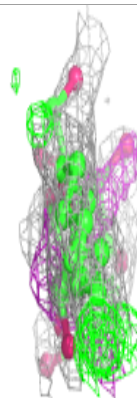
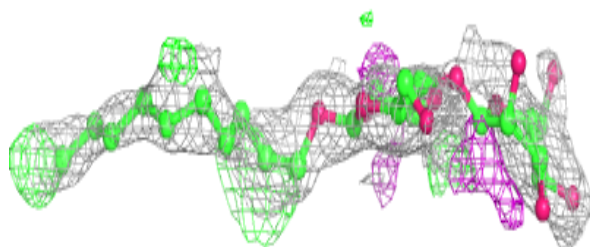
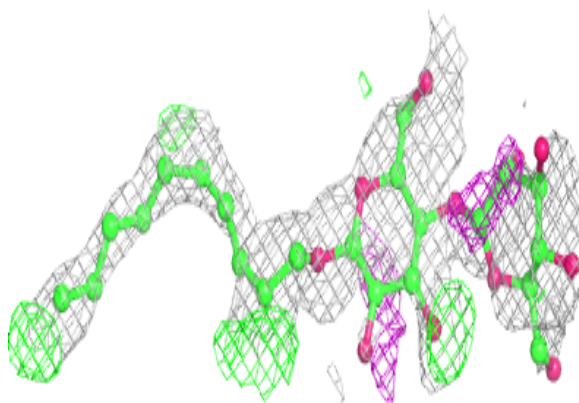
**Electron density around DMU C 317:**

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

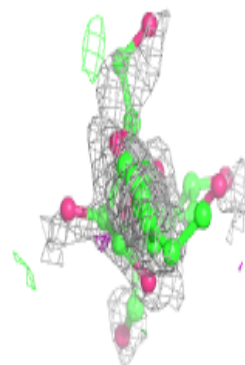
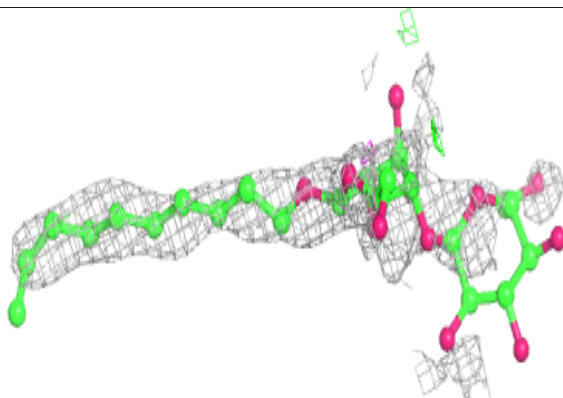
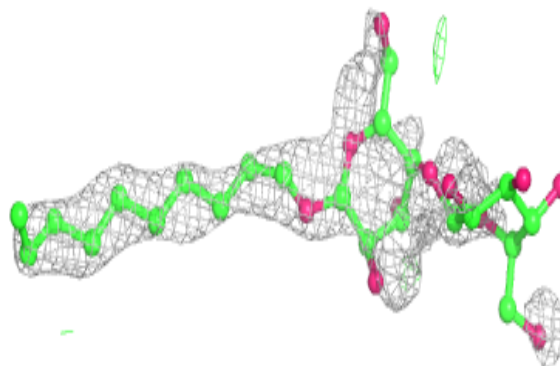


Electron density around DMU K 105:

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

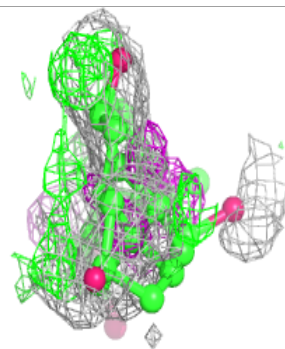
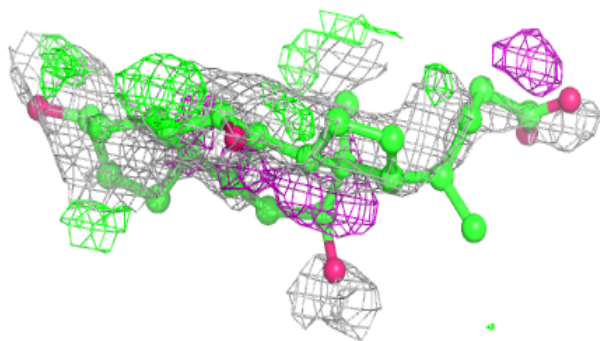
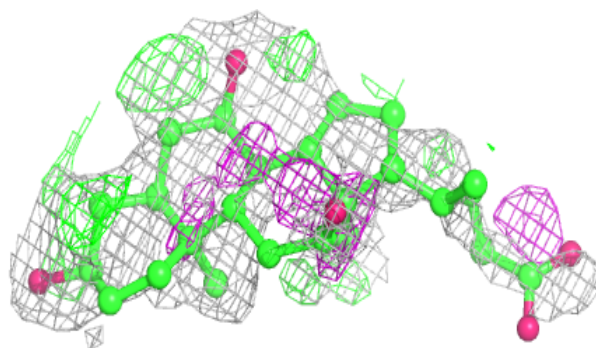
**Electron density around DMU I 101:**

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

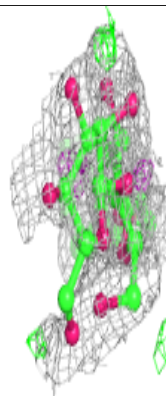
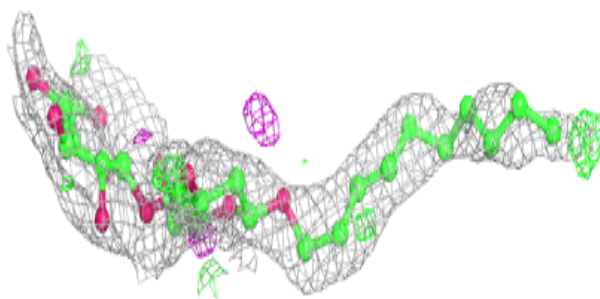
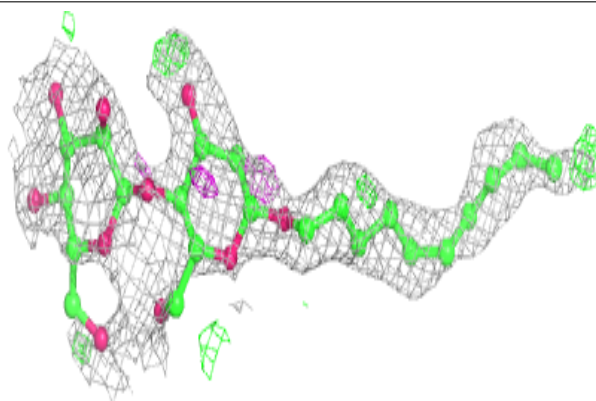


Electron density around CHD X 101:

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

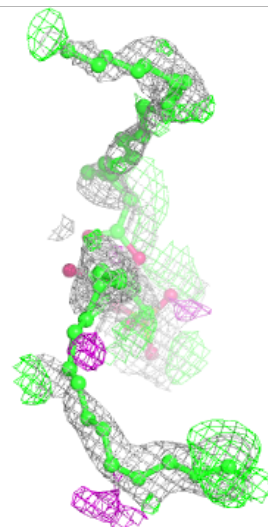
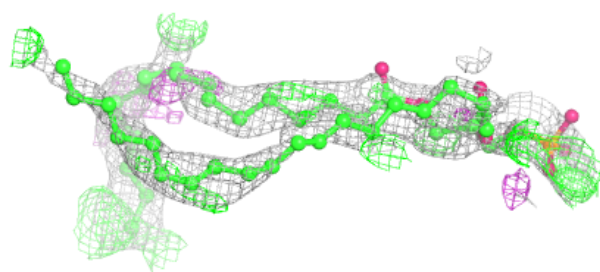
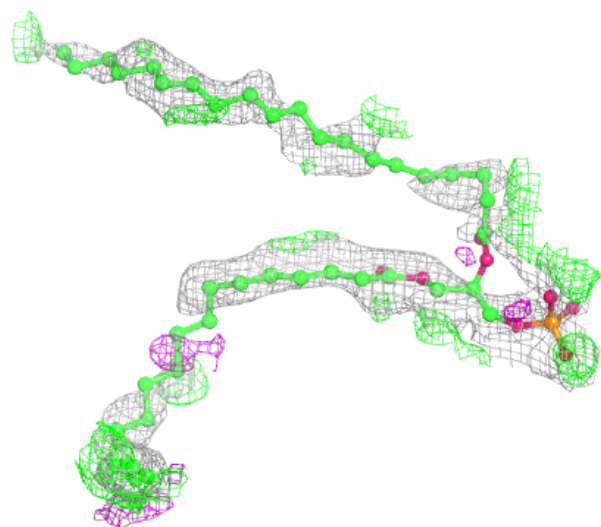
**Electron density around DMU K 103:**

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



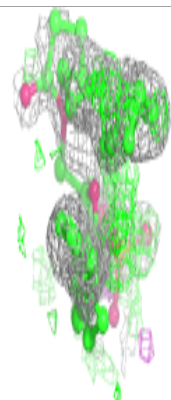
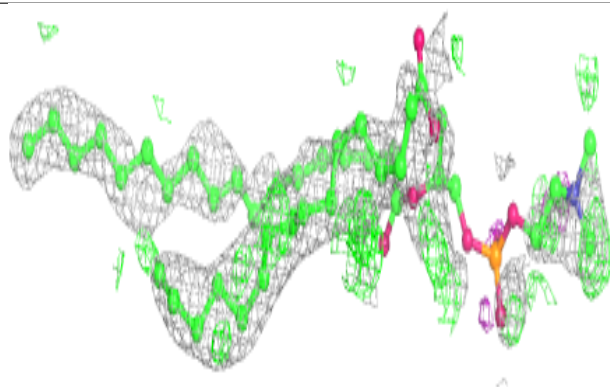
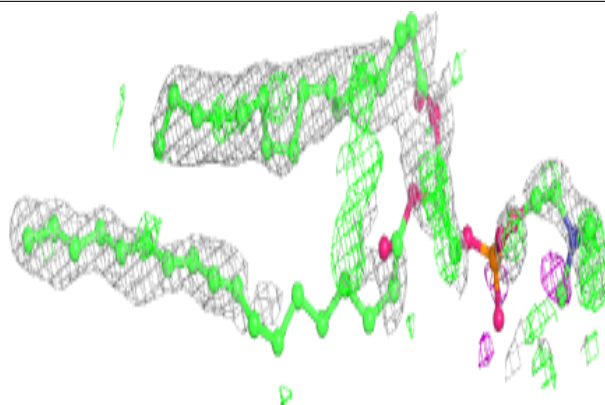
Electron density around PEK T 101:

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

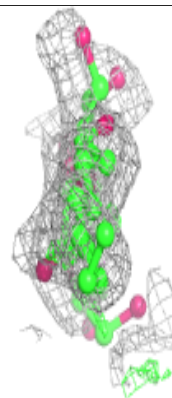
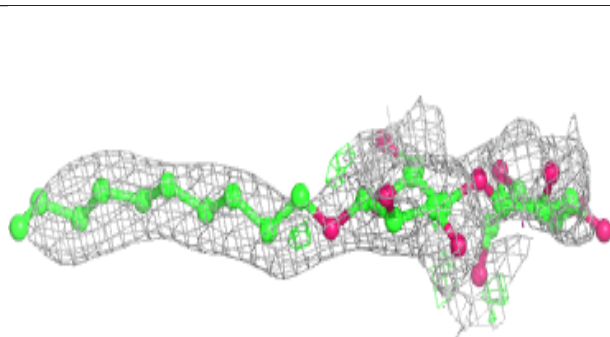
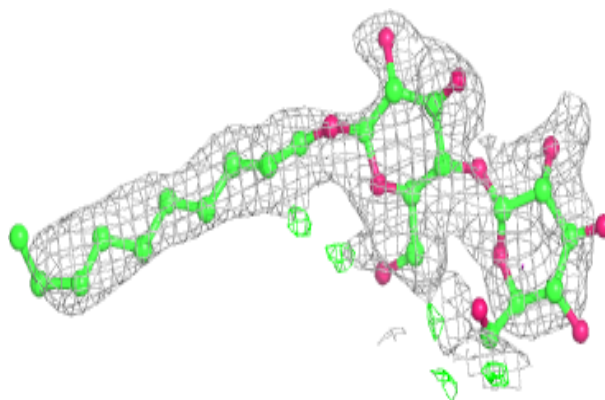


Electron density around PSC B 304:

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

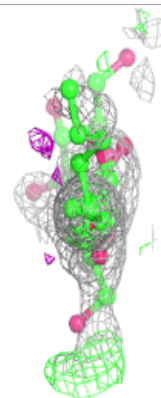
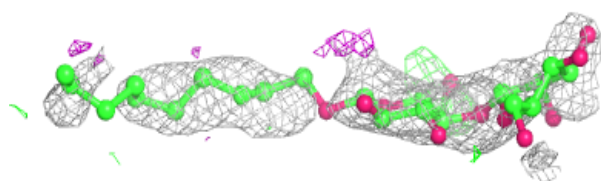
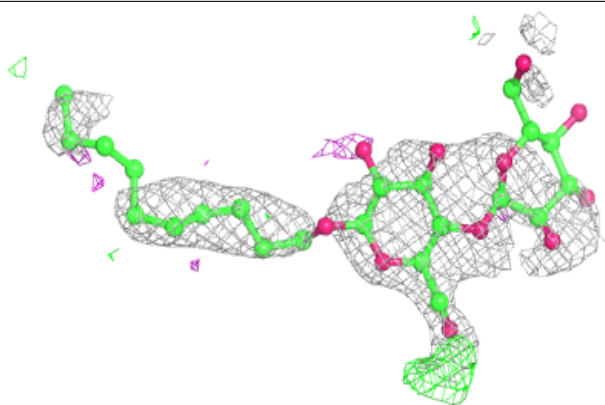
**Electron density around DMU P 315:**

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

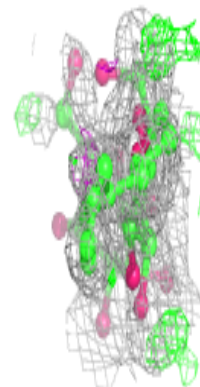
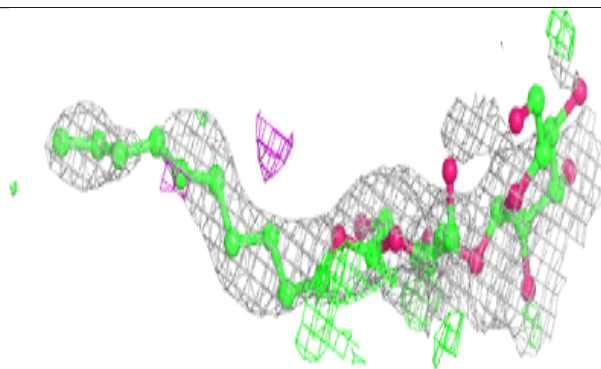
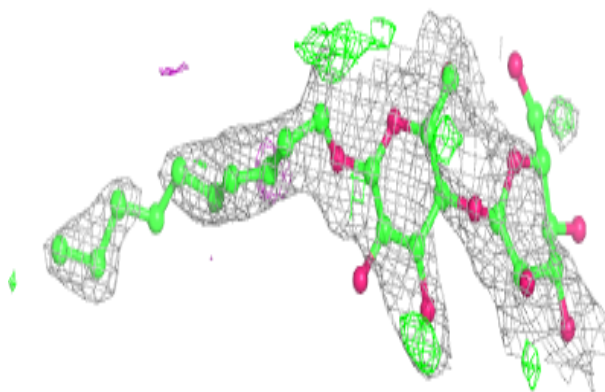


Electron density around DMU L 105:

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

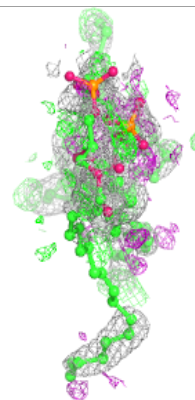
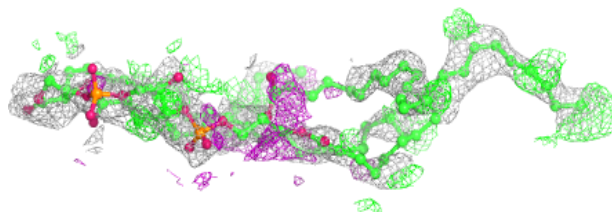
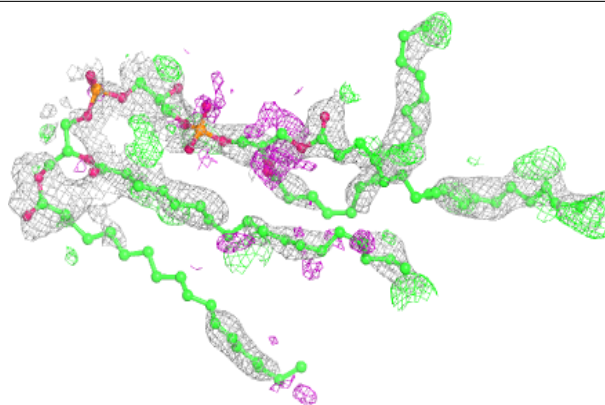
**Electron density around DMU X 104:**

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

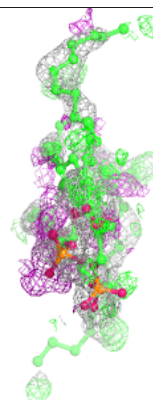
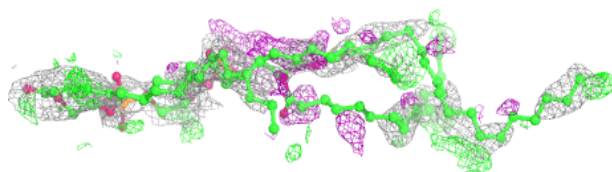
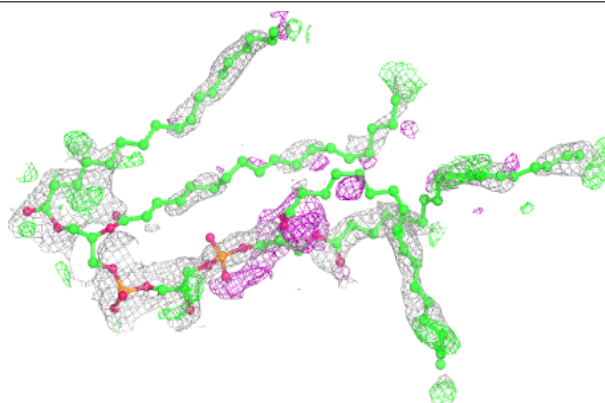


Electron density around CDL T 102:

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

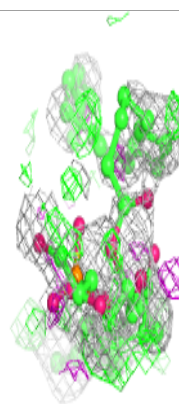
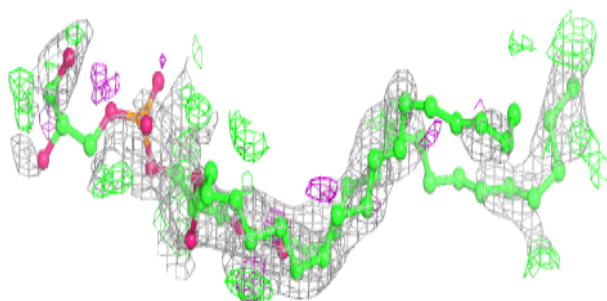
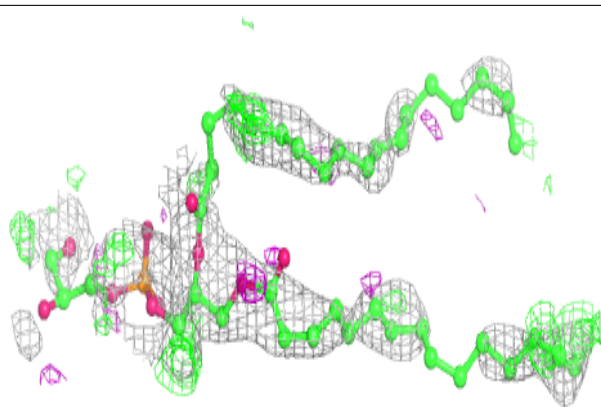
**Electron density around CDL G 101:**

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

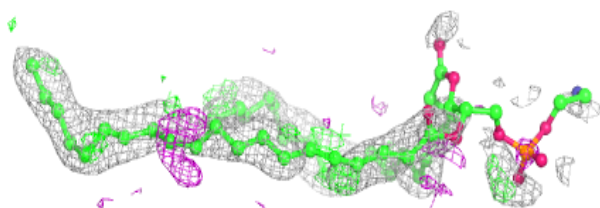
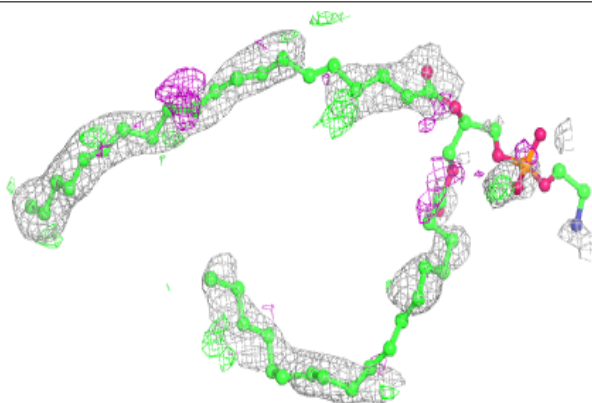


Electron density around PGV G 102:

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

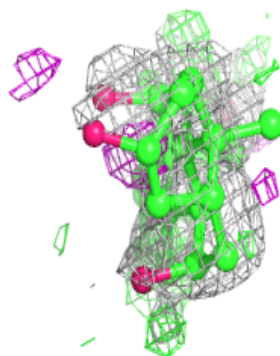
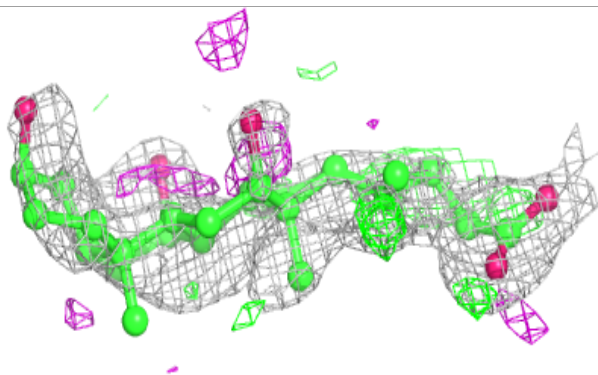
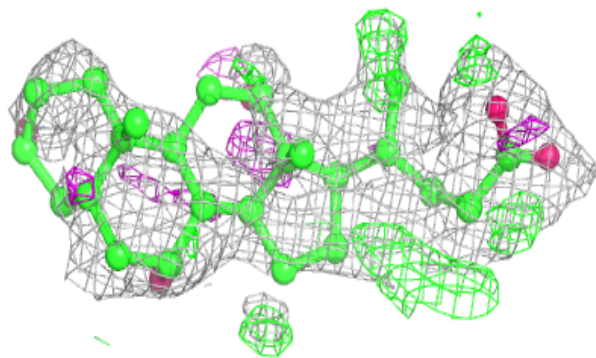
**Electron density around PEK C 309:**

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



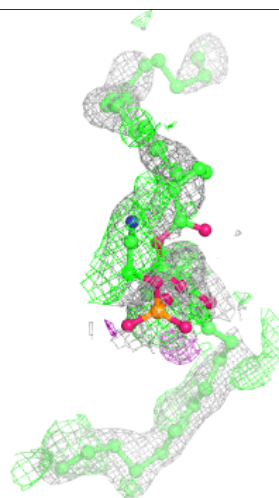
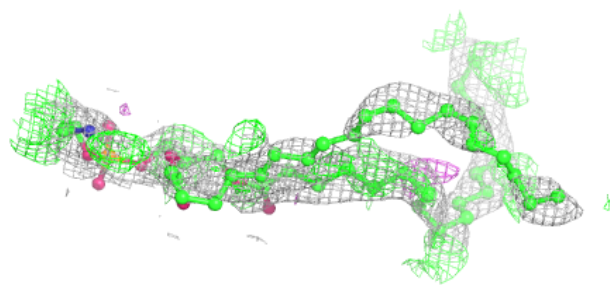
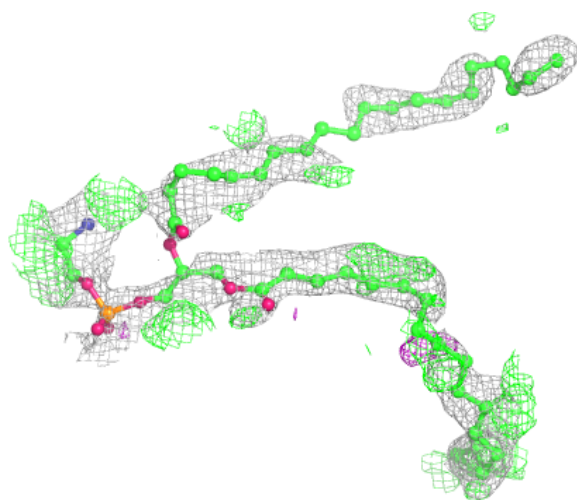
Electron density around CHD P 304:

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



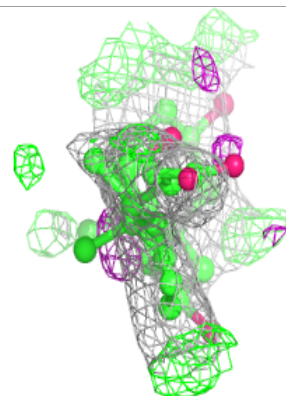
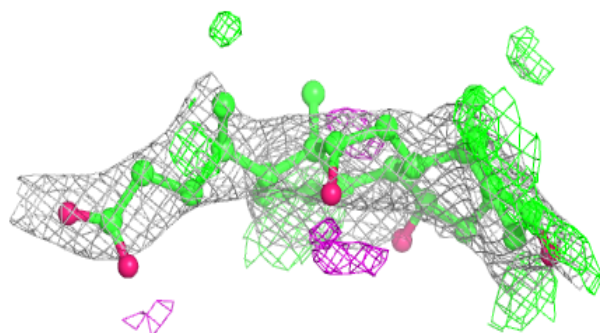
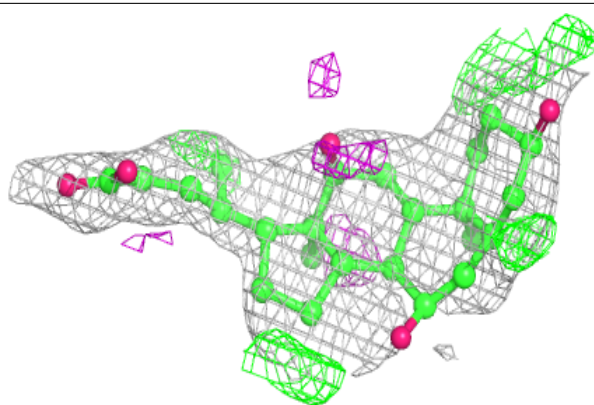
Electron density around PEK C 305:

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

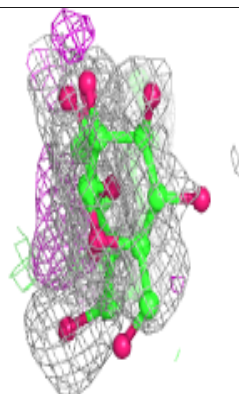
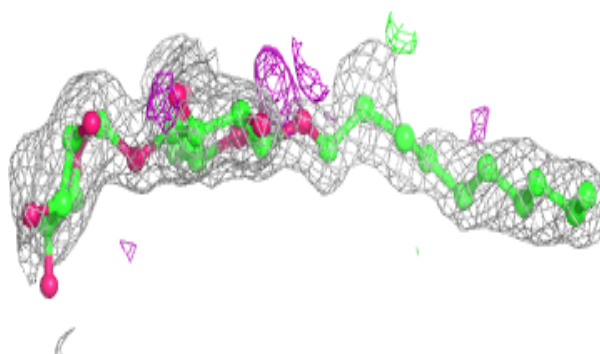
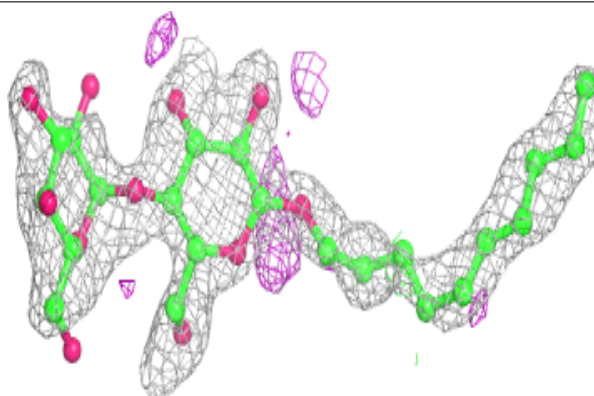


Electron density around CHD Y 104:

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

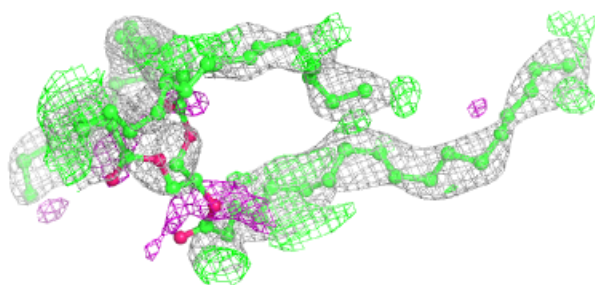
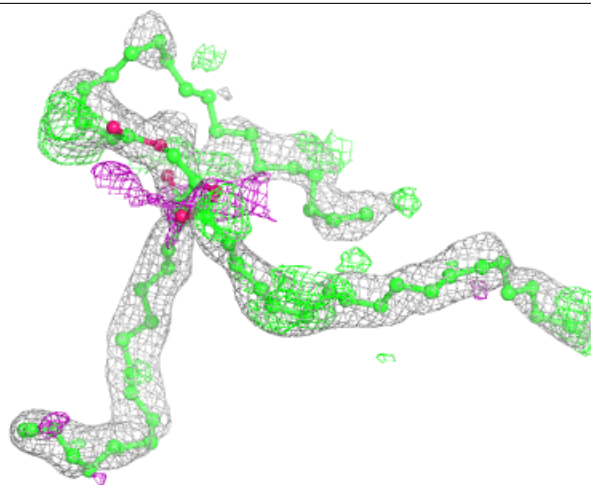
**Electron density around DMU P 305:**

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



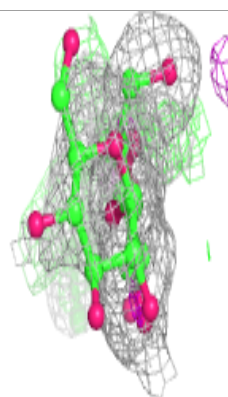
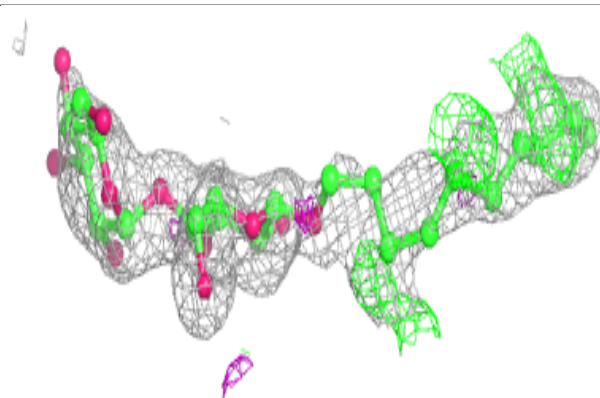
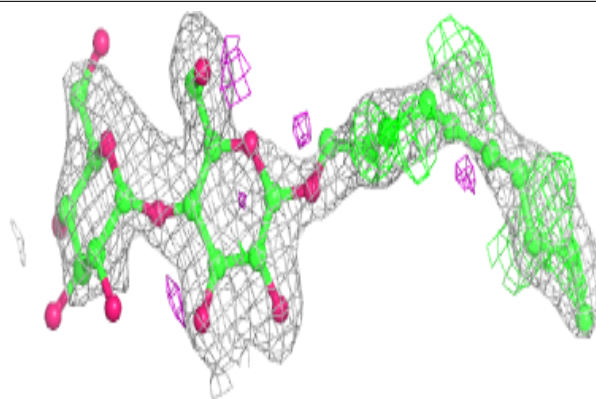
Electron density around TGL Y 101:

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

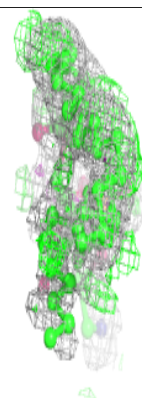
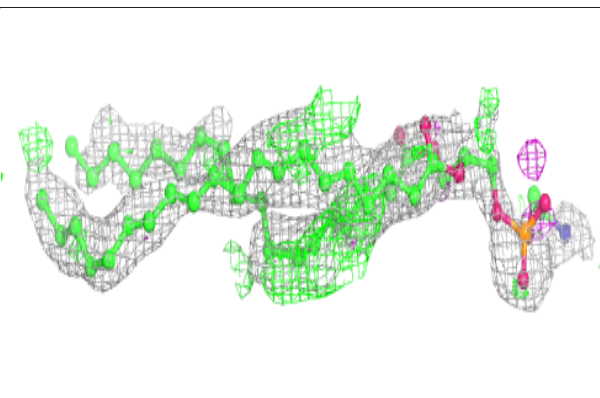
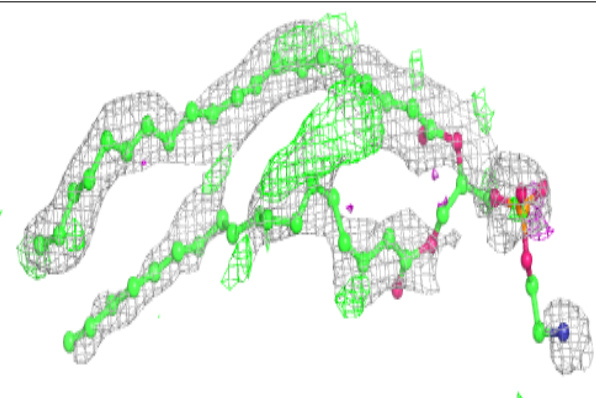


Electron density around DMU C 308:

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

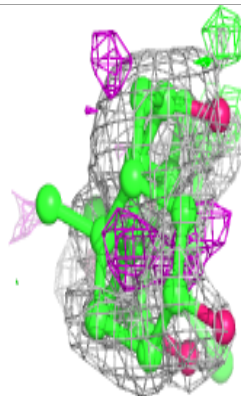
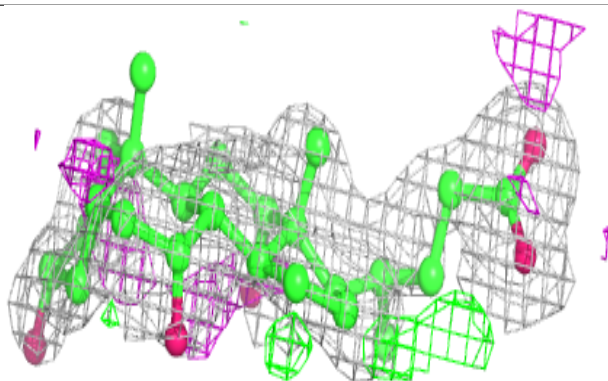
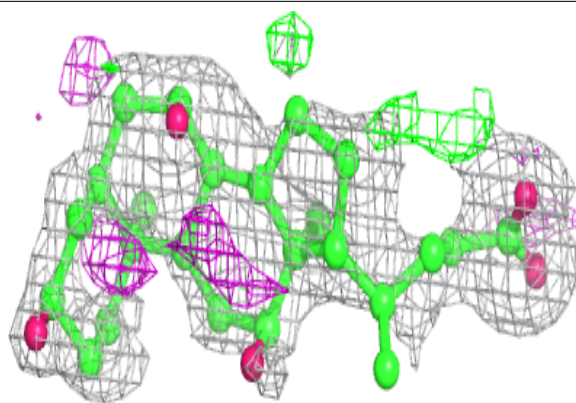
**Electron density around PEK P 301:**

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

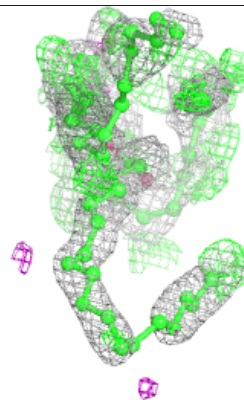
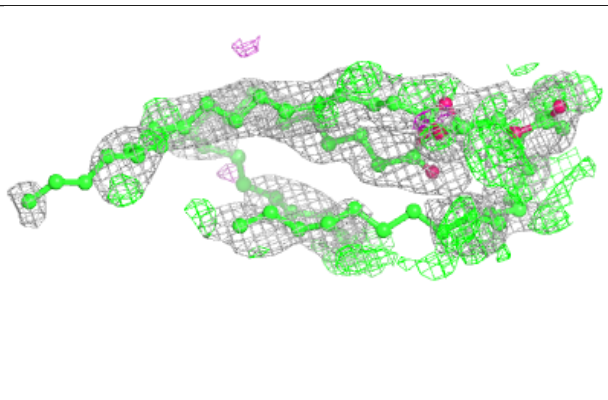
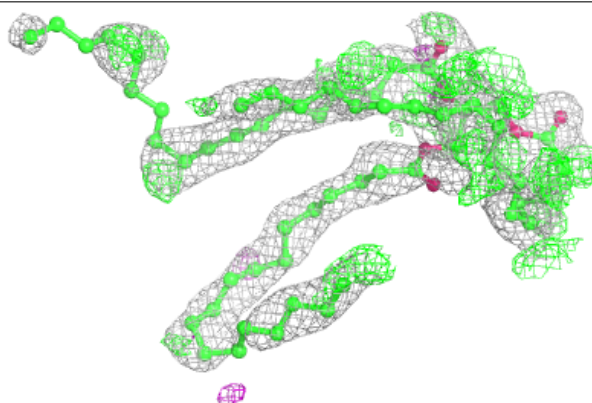


Electron density around CHD C 303:

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

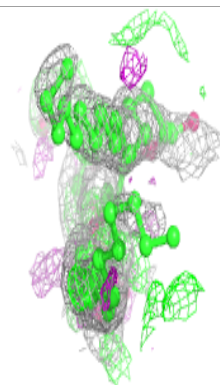
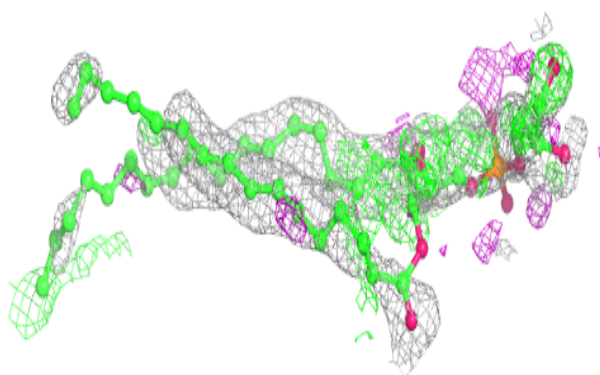
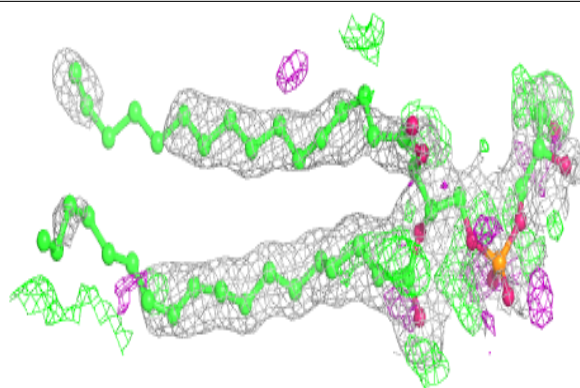
**Electron density around TGL Q 202:**

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

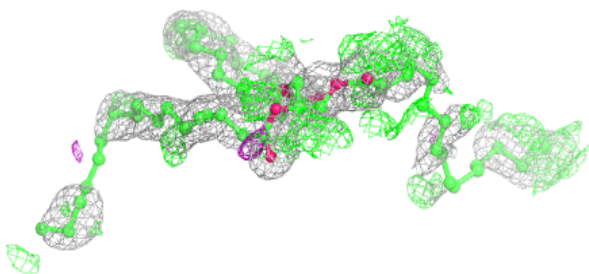
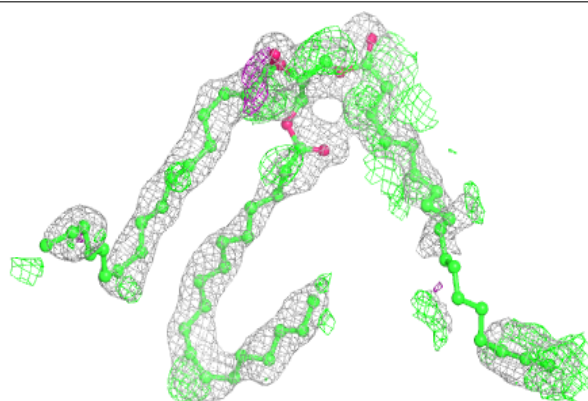


Electron density around PGV A 608:

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

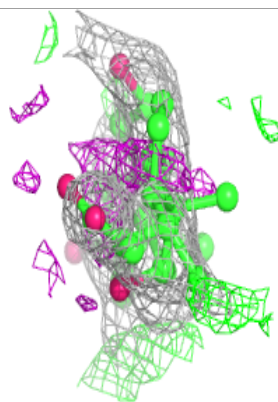
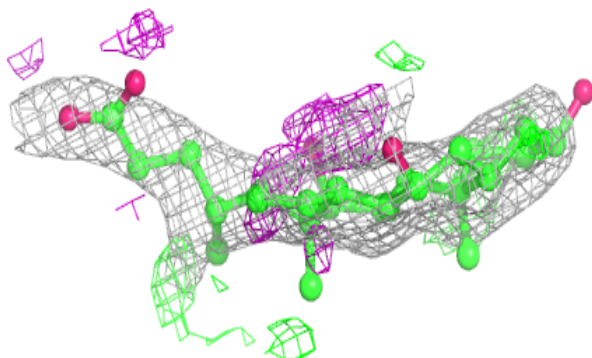
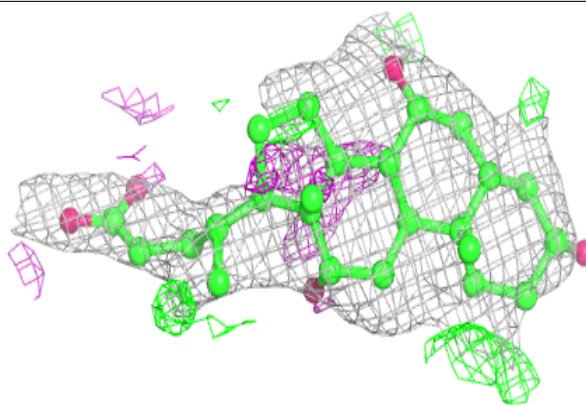
**Electron density around TGL D 201:**

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

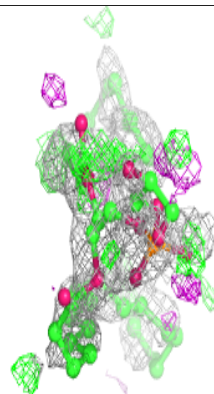
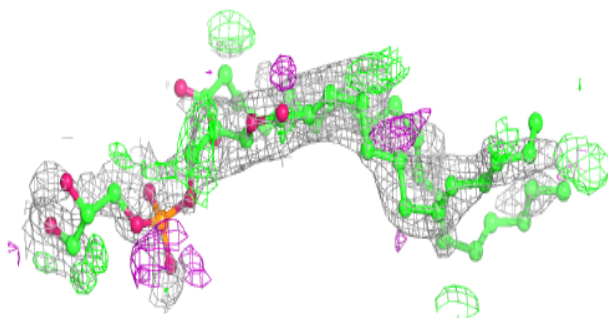
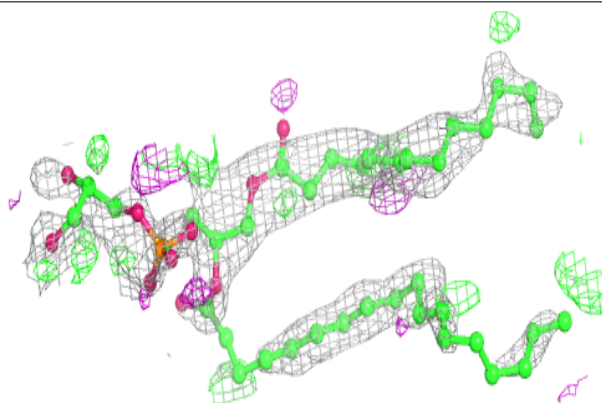


Electron density around CHD L 104:

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

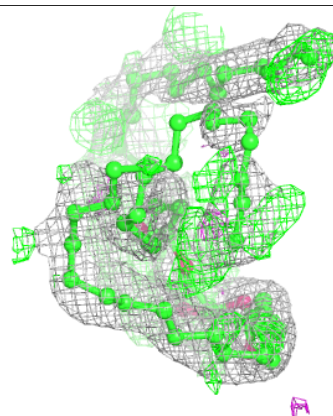
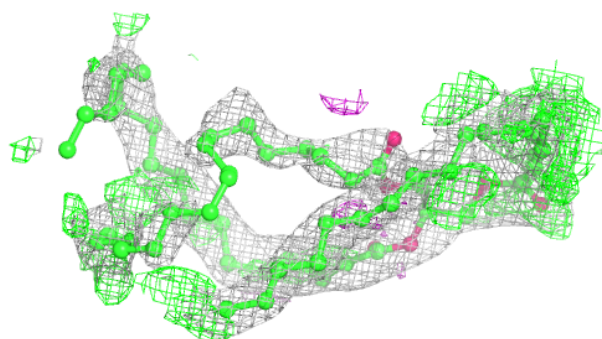
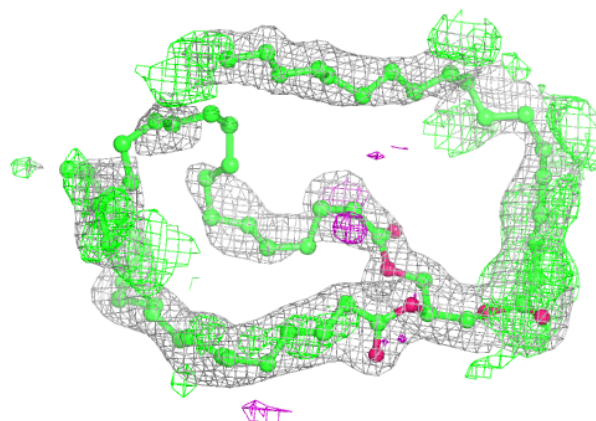
**Electron density around PGV C 306:**

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

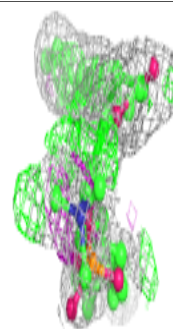
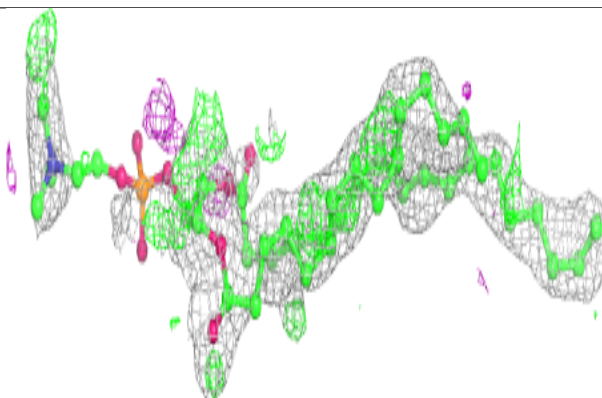
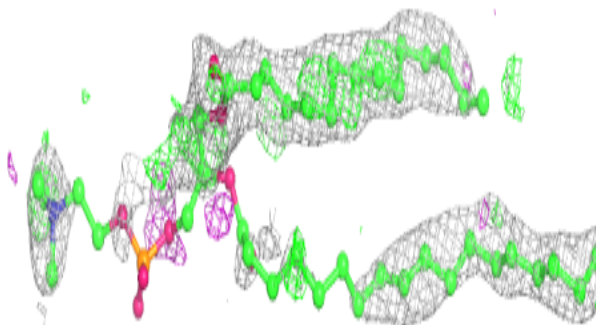


Electron density around TGL B 301:

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

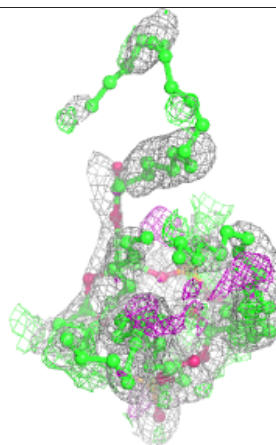
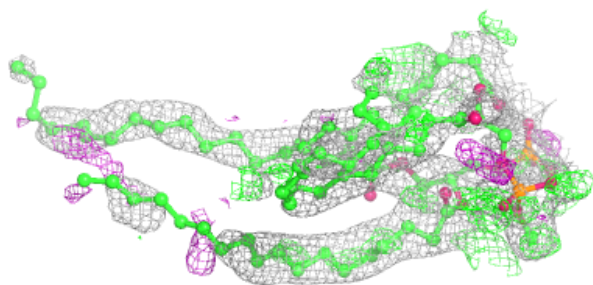
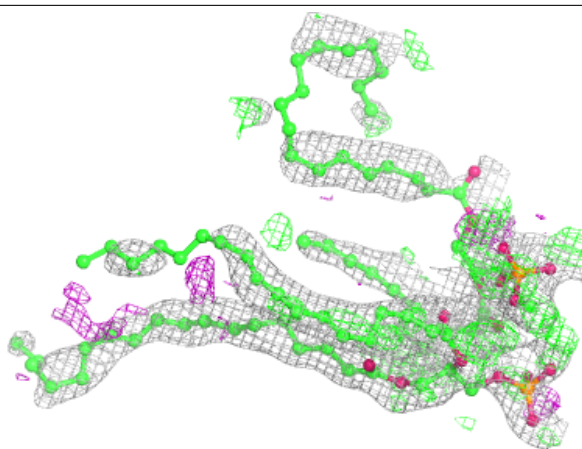
**Electron density around PSC O 304:**

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

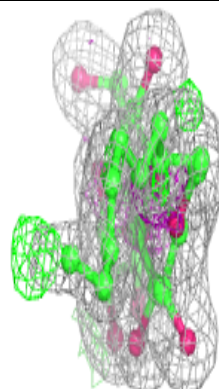
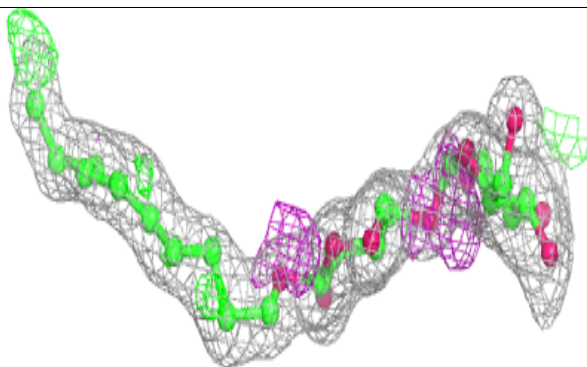
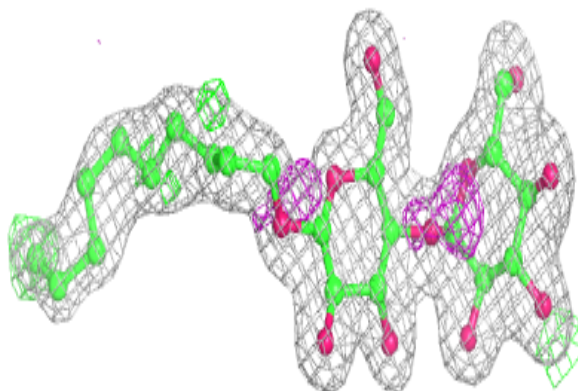


Electron density around CDL P 303:

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

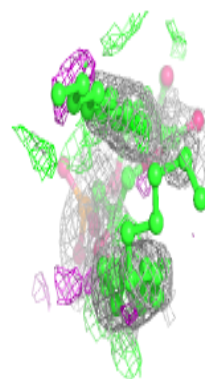
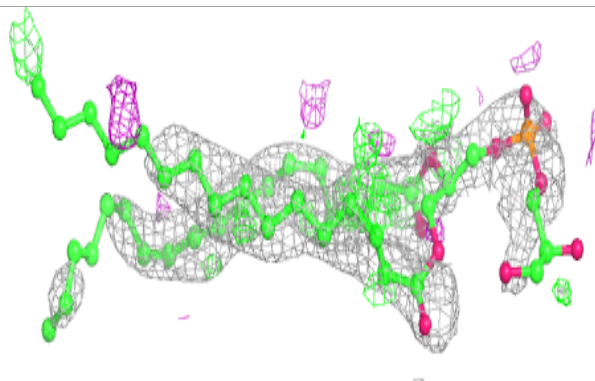
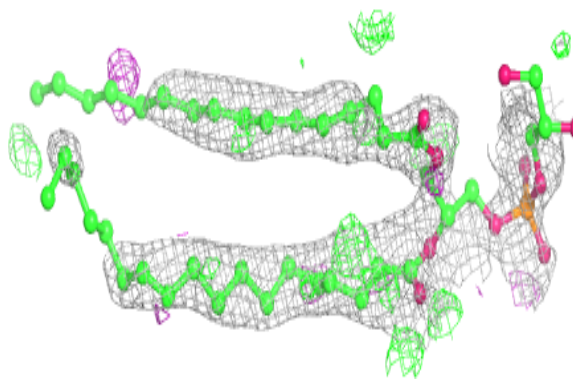
**Electron density around DMU M 101:**

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



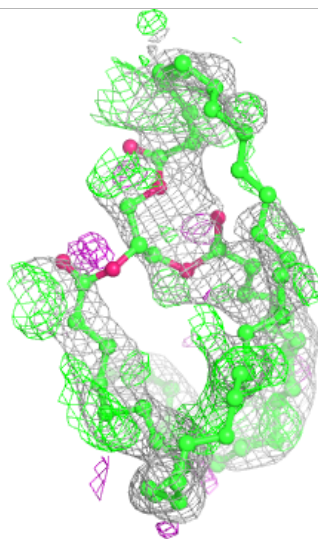
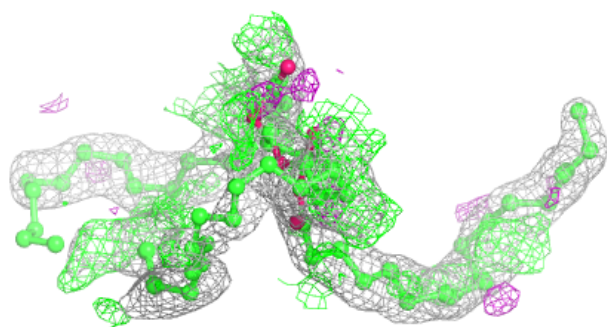
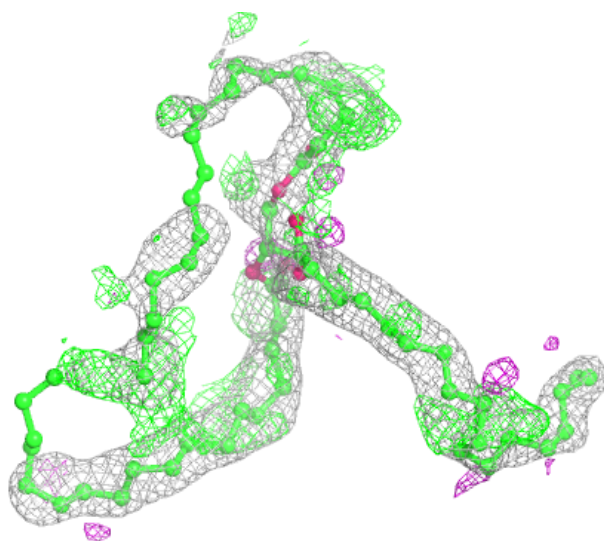
Electron density around PGV Q 201:

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



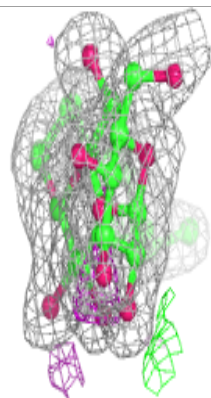
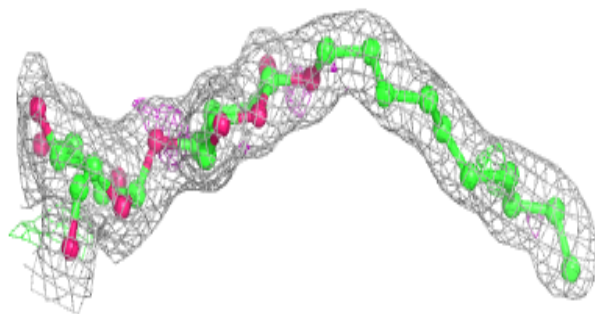
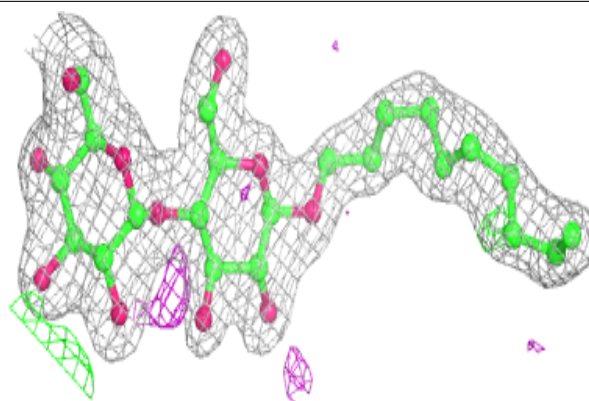
Electron density around TGL A 609:

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



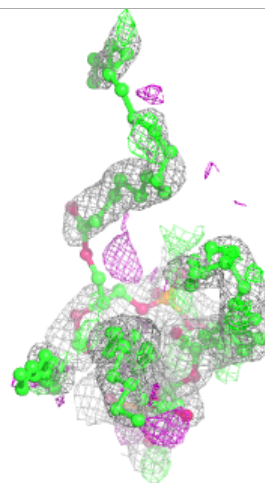
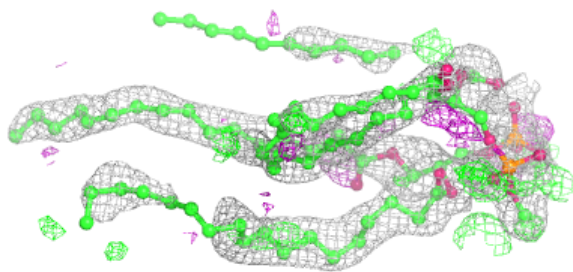
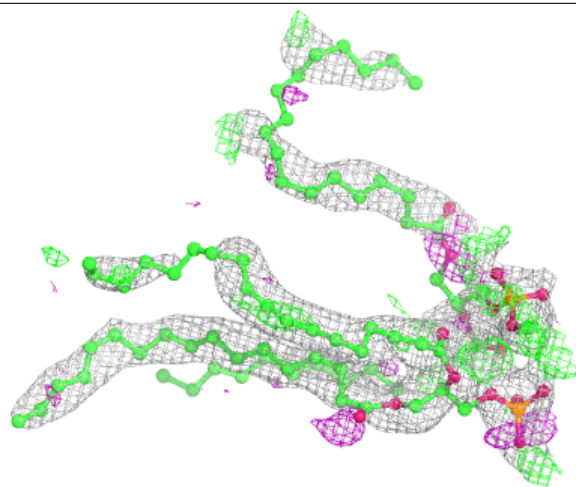
Electron density around DMU Z 101:

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



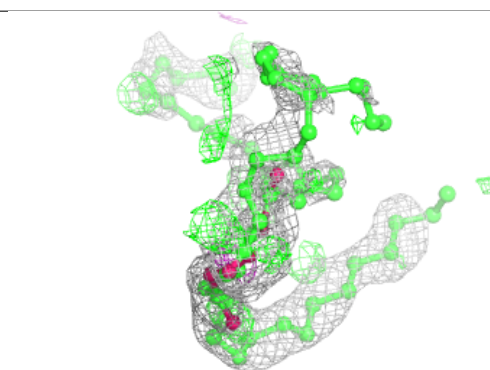
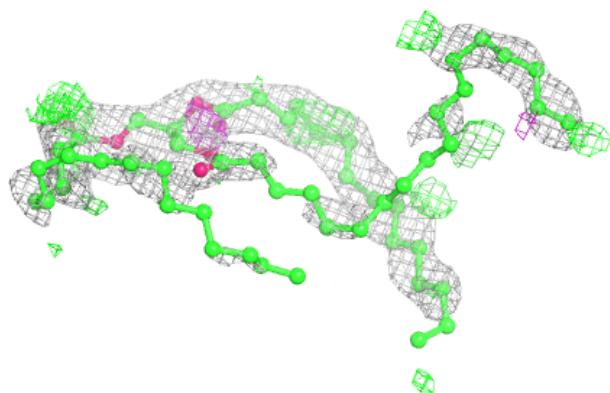
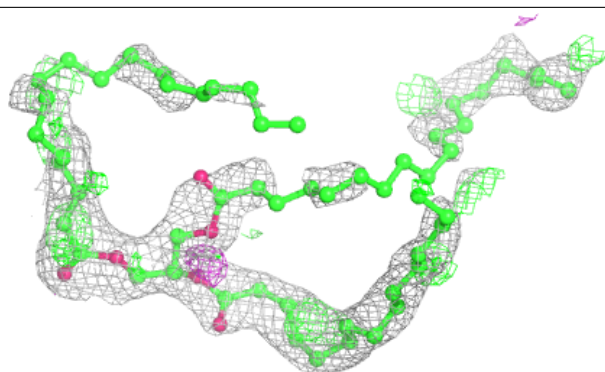
Electron density around CDL C 302:

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

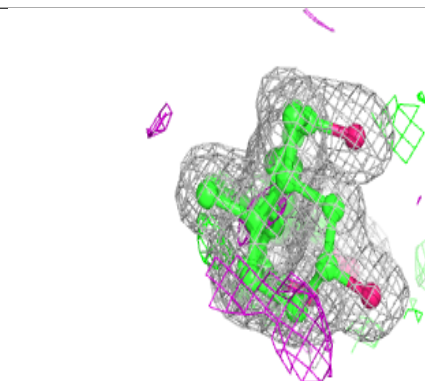
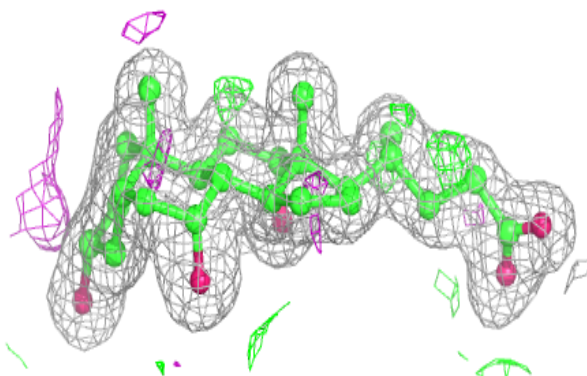
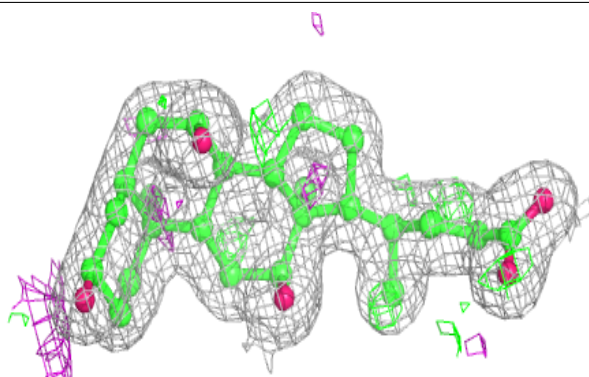


Electron density around TGL O 301:

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

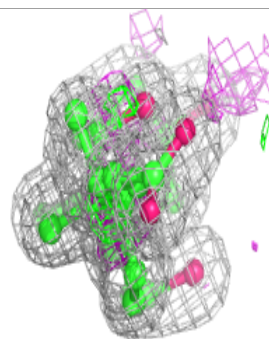
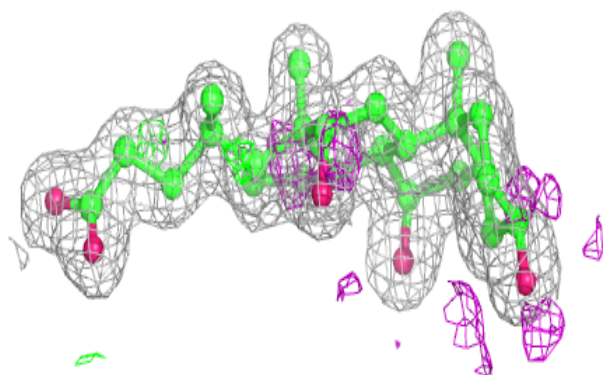
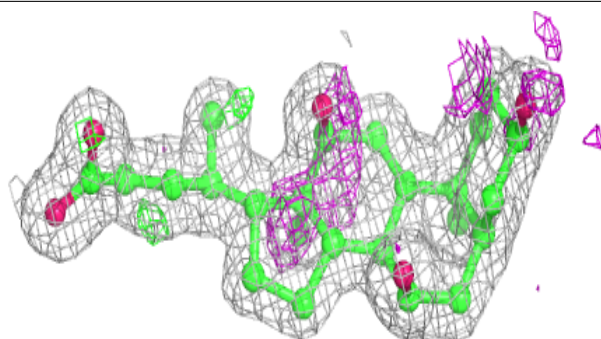
**Electron density around CHD P 306:**

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

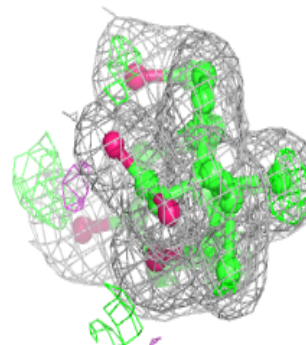
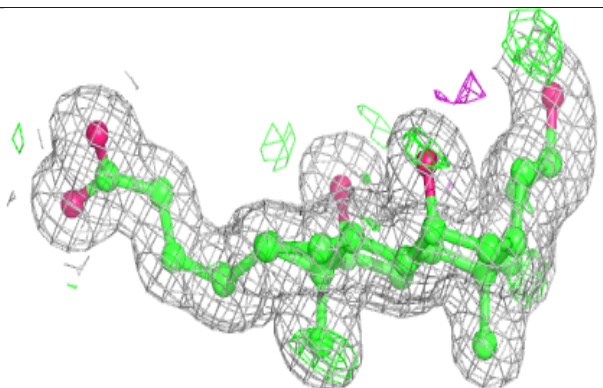
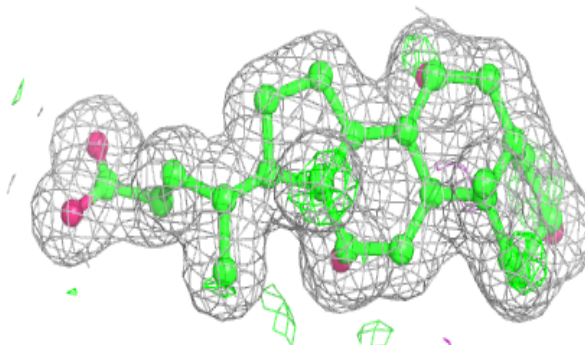


Electron density around CHD C 304:

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

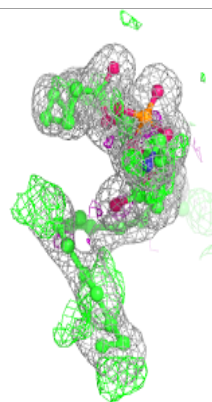
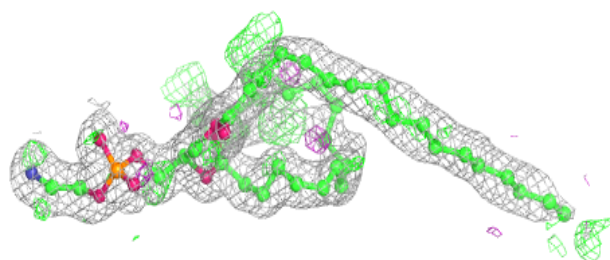
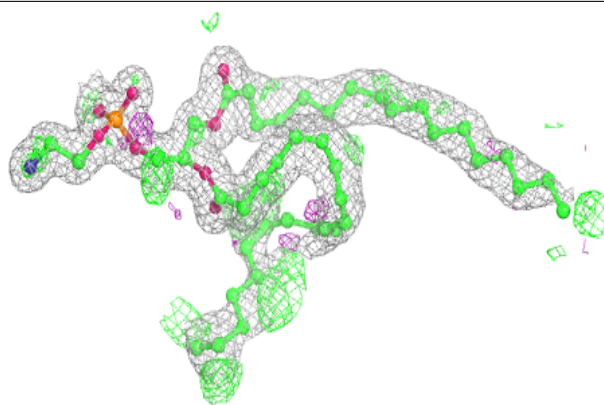
**Electron density around CHD O 303:**

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

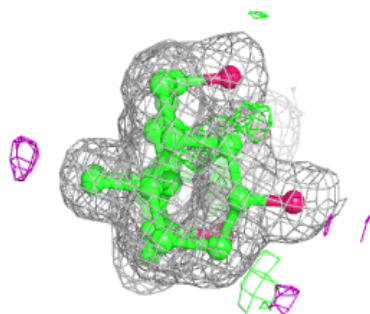
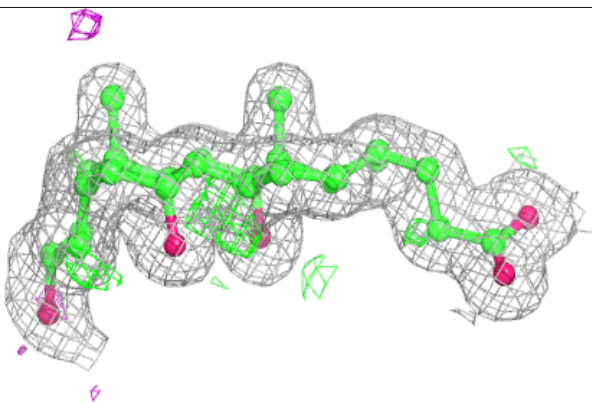
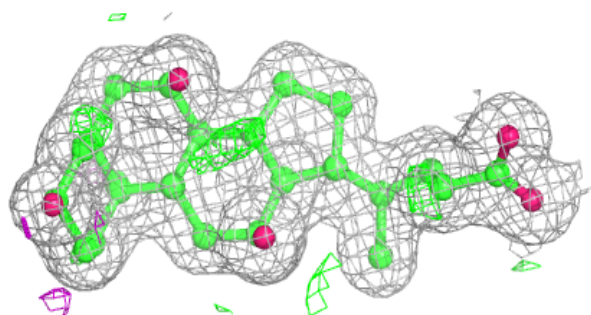


Electron density around PEK C 307:

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

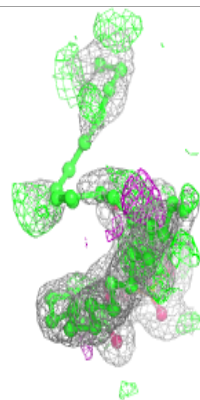
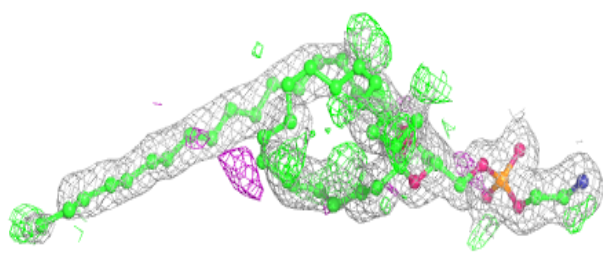
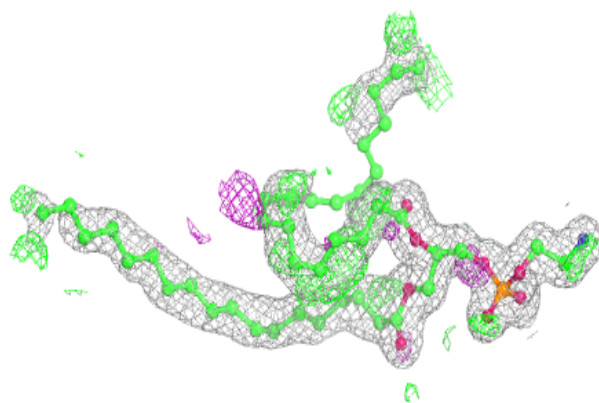
**Electron density around CHD B 303:**

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

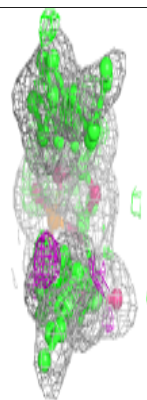
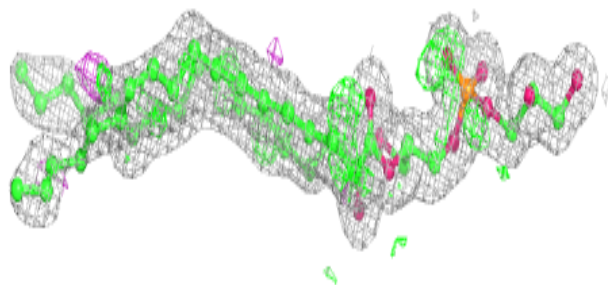
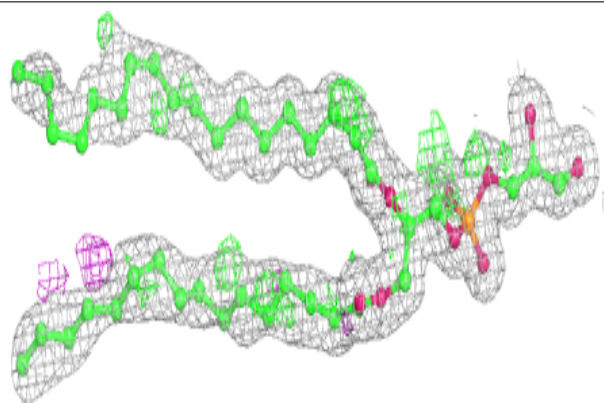


Electron density around PEK P 307:

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

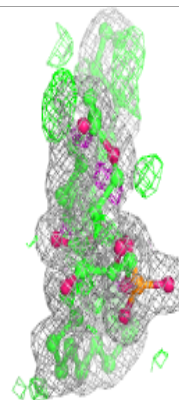
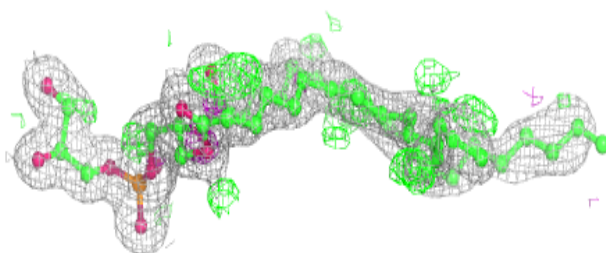
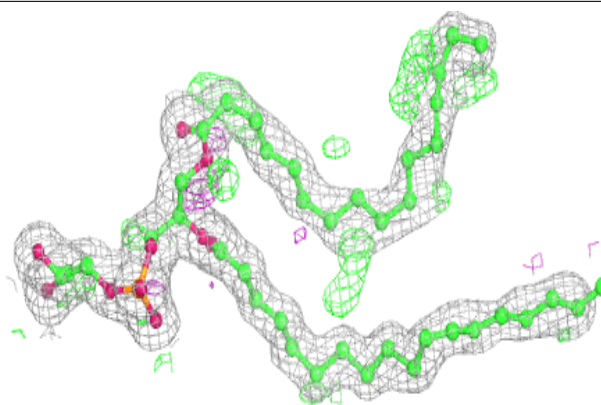
**Electron density around PGV C 301:**

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

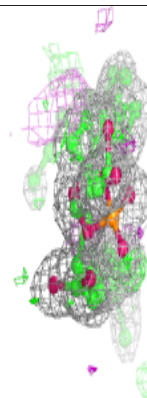
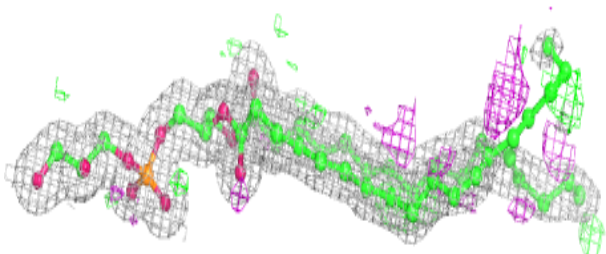
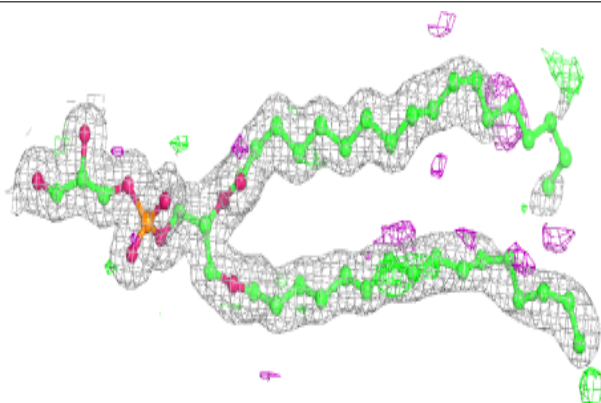


Electron density around PGV N 607:

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

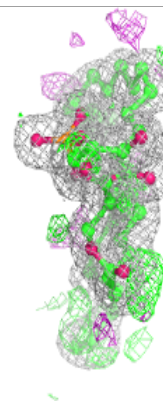
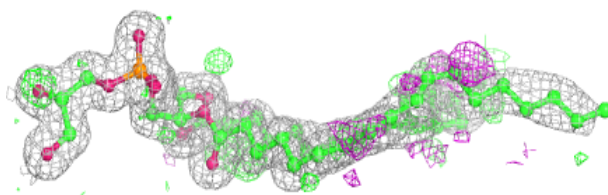
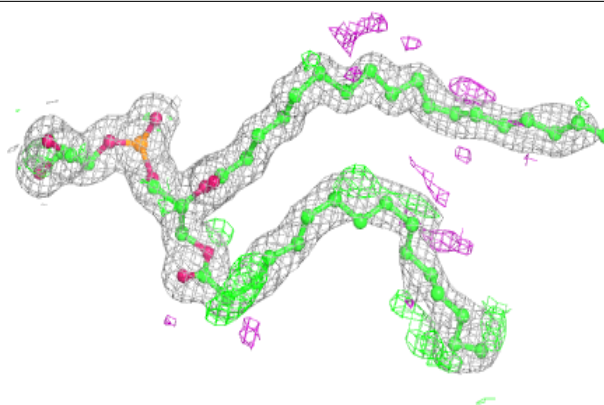
**Electron density around PGV P 302:**

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

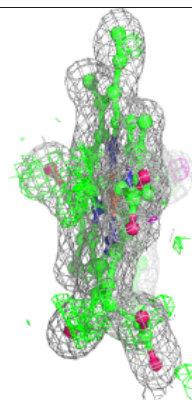
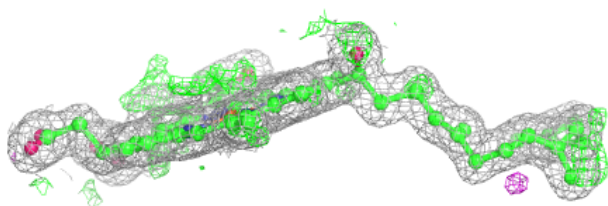
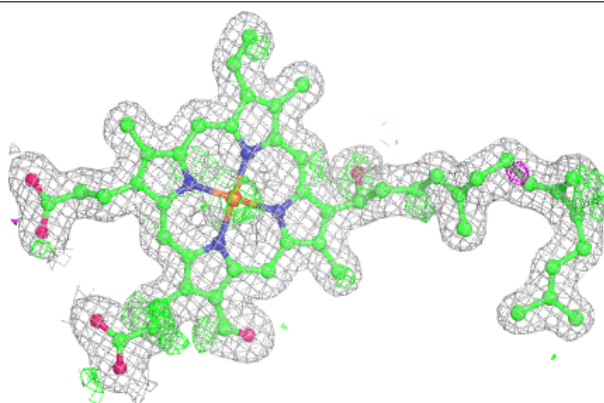


Electron density around PGV A 607:

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

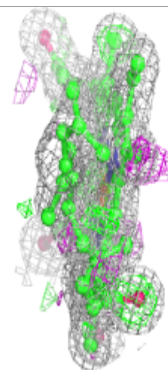
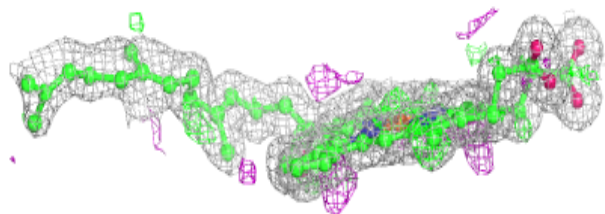
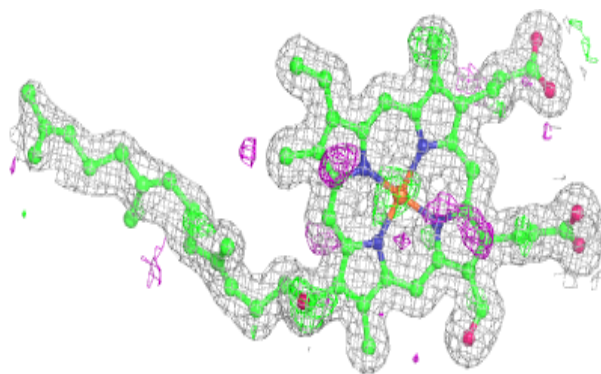
**Electron density around HEA N 602:**

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

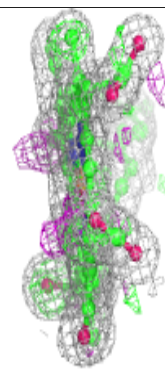
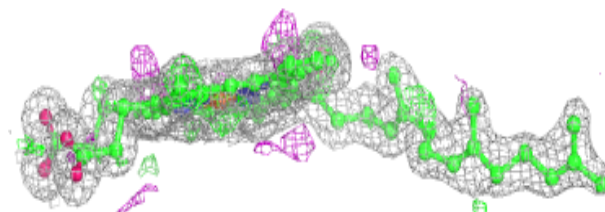
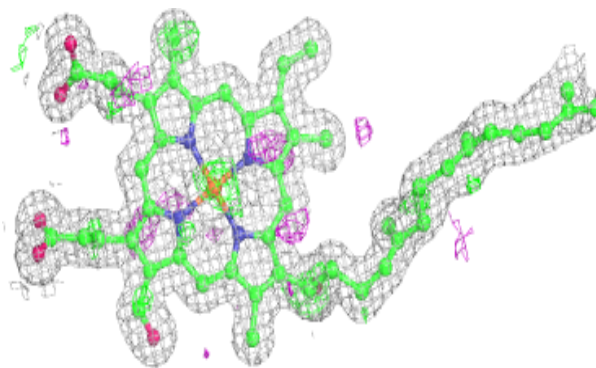


Electron density around HEA A 601 (A):

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

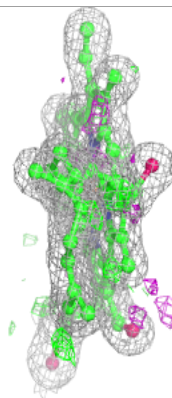
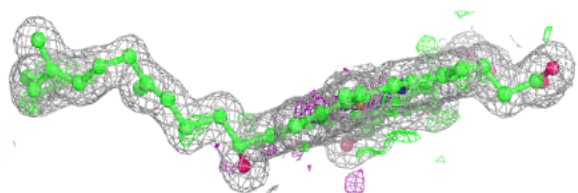
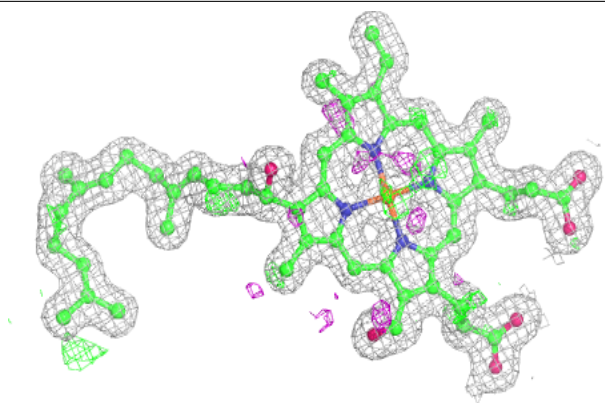
**Electron density around HEA A 601 (B):**

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

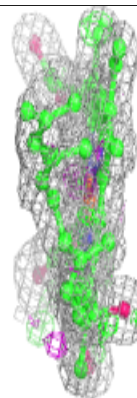
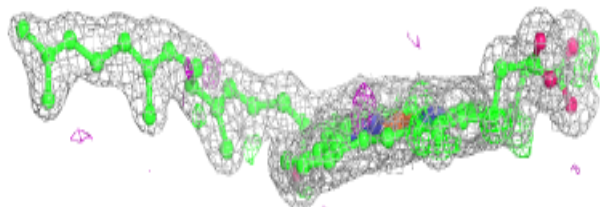
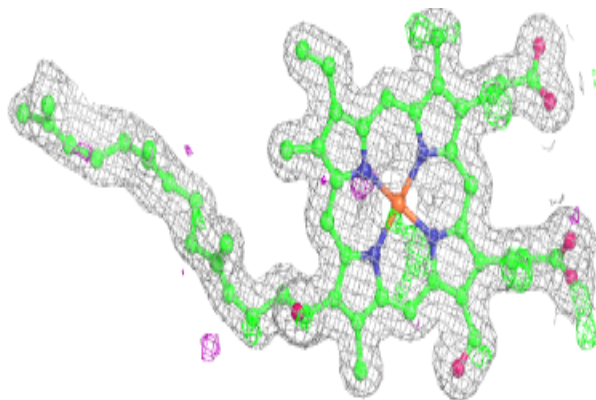


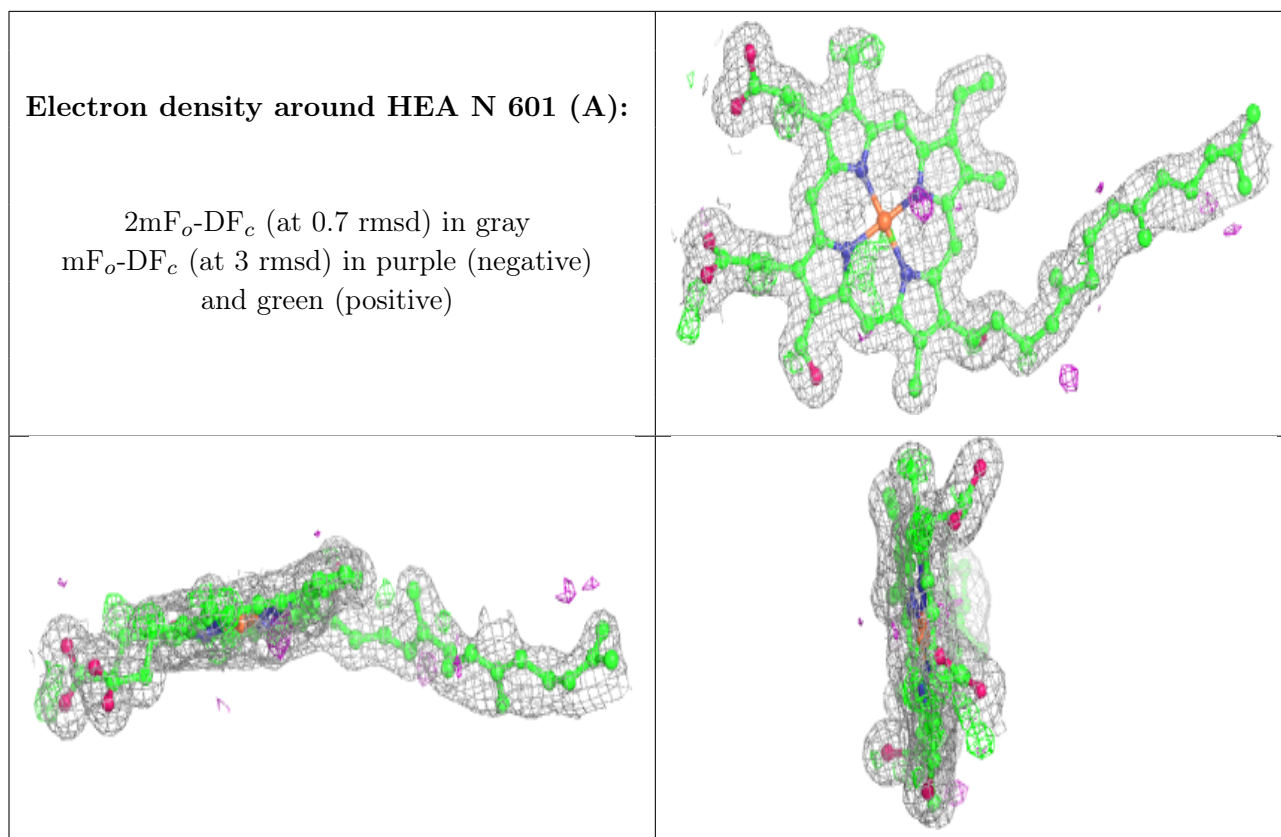
Electron density around HEA A 602:

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

**Electron density around HEA N 601 (B):**

$2mF_o-DF_c$ (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.