



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2022 – 01:08 PM JST

PDB ID : 5B3S
Title : Bovine heart cytochrome c oxidase in the carbon monoxide-bound mixed-valence state at 1.68 angstrom resolution (50 K)
Authors : Shimada, A.; Shinzawa-Ito, K.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2016-03-11
Resolution : 1.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
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)	:	2.26

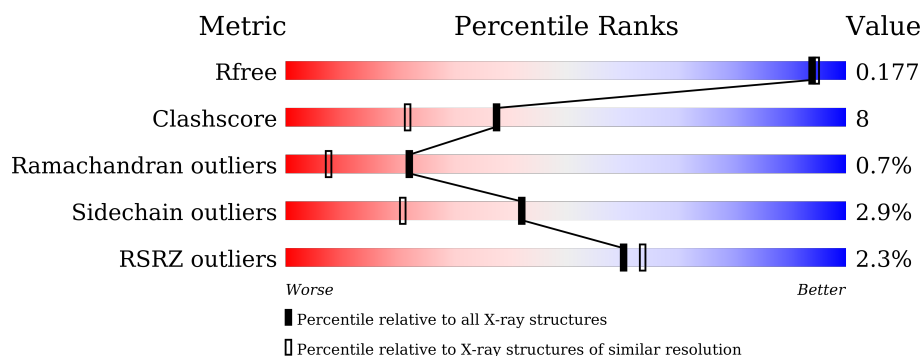
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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	 89% 10% .
1	N	514	 87% 13%
2	B	227	 82% 16% .
2	O	227	 81% 18% .
3	C	259	 92% 8%
3	P	259	 86% 14%

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	94	
6	S	94	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601[A]	X	-	-	-
14	HEA	A	601[B]	X	-	-	-
14	HEA	A	601[C]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602	X	-	-	-
14	HEA	N	601[A]	X	-	-	-
14	HEA	N	601[B]	X	-	-	-
14	HEA	N	601[C]	X	-	-	-
14	HEA	N	602	X	-	-	-
20	EDO	A	622	-	-	X	X
20	EDO	M	103	-	-	X	-
20	EDO	N	618	-	-	X	-
20	EDO	U	101	-	-	X	-
27	DMU	K	104	-	-	-	X
27	DMU	K	105	-	-	-	X
27	DMU	K	106	-	-	-	X
9	SAC	V	1	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34917 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	39	0
			4192	2793	644	712	43			
1	N	514	Total	C	N	O	S	0	36	0
			4182	2787	641	712	42			

- 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	12	0
			1858	1207	283	348	20			
2	O	227	Total	C	N	O	S	0	11	0
			1856	1205	286	346	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	7	0
			2124	1419	337	355	13			
3	P	259	Total	C	N	O	S	0	8	0
			2126	1420	337	355	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	2	0
			1207	786	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1201	780	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	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	2	0
			721	446	128	142	5			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 676	C 431	N 129	O 114	P 1	S 1	0	0	0
7	T	84	Total 676	C 431	N 129	O 114	P 1	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	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
			461	297	78	83	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			461	297	78	83	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

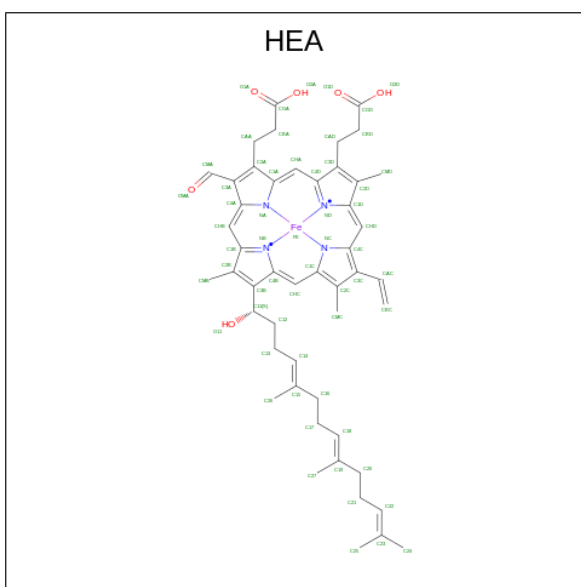
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	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
			336	223	53	60			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



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

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

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

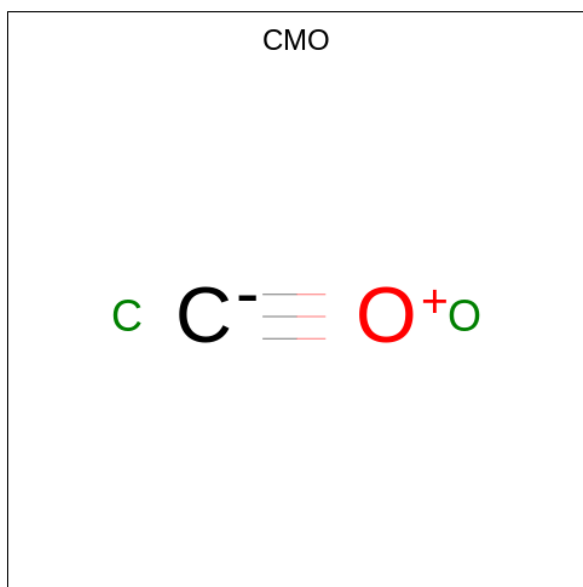
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

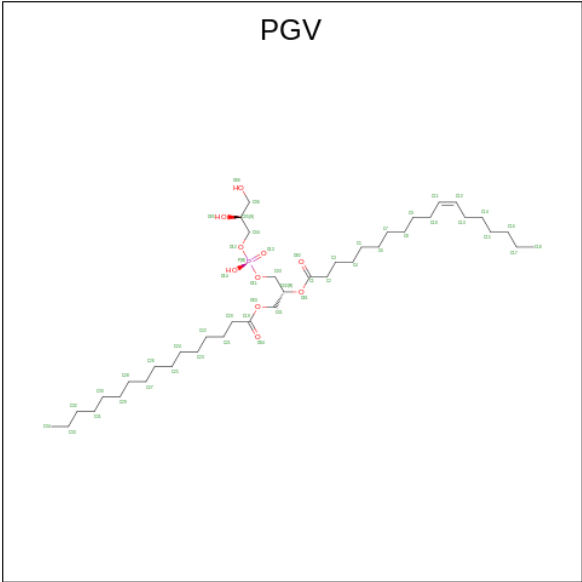
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO).



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

- Molecule 19 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			48	37	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			50	39	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	G	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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

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

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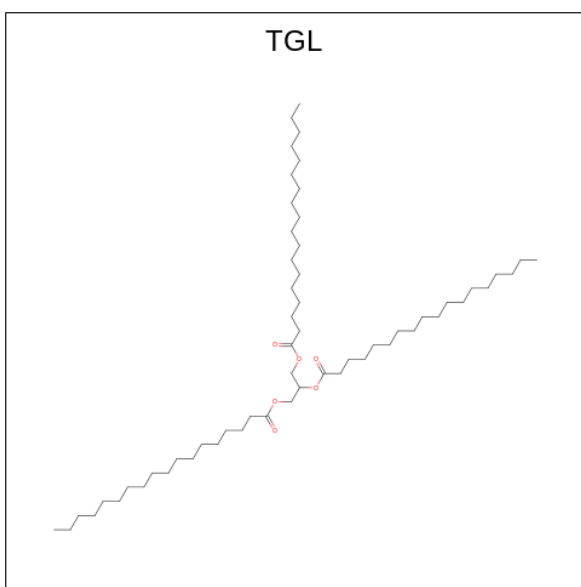
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4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

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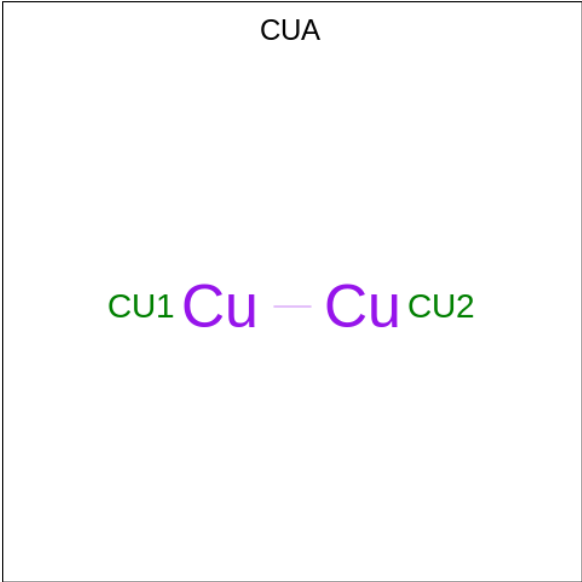
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	Q	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20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

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



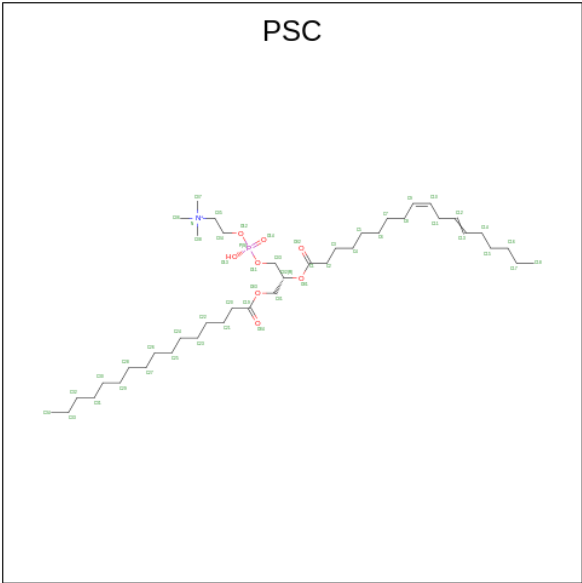
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	B	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			60	54	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



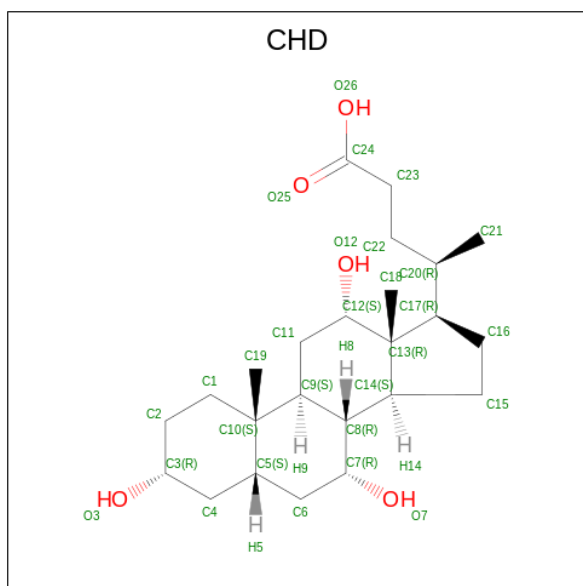
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	O	1	Total	C	O	P	0	0
			46	37	8	1		

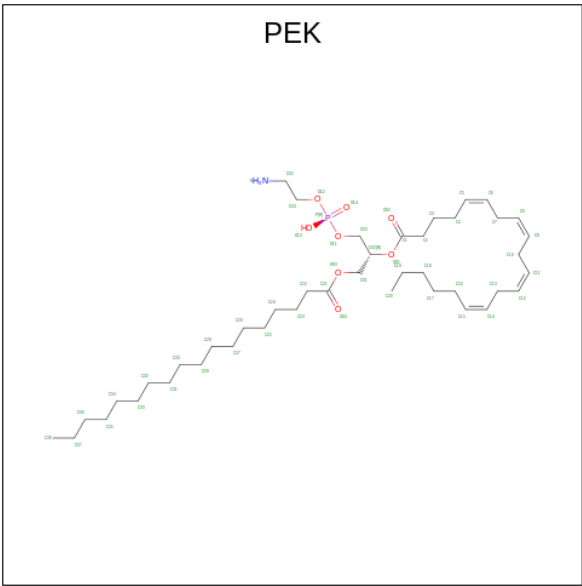
- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

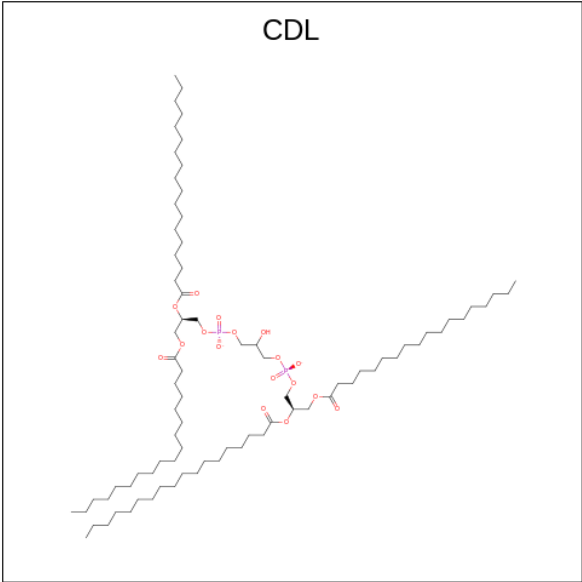
- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE

(three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



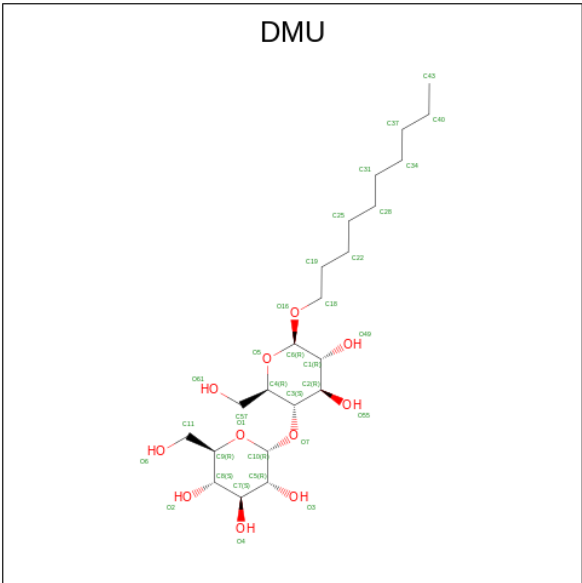
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			44	34	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			92	78	13	1		
26	G	1	Total	C	O	P	0	0
			99	80	17	2		
26	P	1	Total	C	O	P	0	0
			84	72	11	1		
26	T	1	Total	C	O	P	0	0
			96	77	17	2		

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 33 22 11	0	0
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	K	1	Total C O 21 16 5	0	0
27	K	1	Total C O 22 16 6	0	0
27	K	1	Total C O 33 22 11	0	0
27	K	1	Total C O 33 22 11	0	0
27	K	1	Total C O 33 22 11	0	0
27	K	1	Total C O 33 22 11	0	0
27	L	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	O	1	Total C O 32 21 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 22 16 6	0	0
27	X	1	Total C O 33 22 11	0	0
27	X	1	Total C O 33 22 11	0	0
27	X	1	Total C O 22 16 6	0	0
27	X	1	Total C O 33 22 11	0	0
27	X	1	Total C O 22 16 6	0	0

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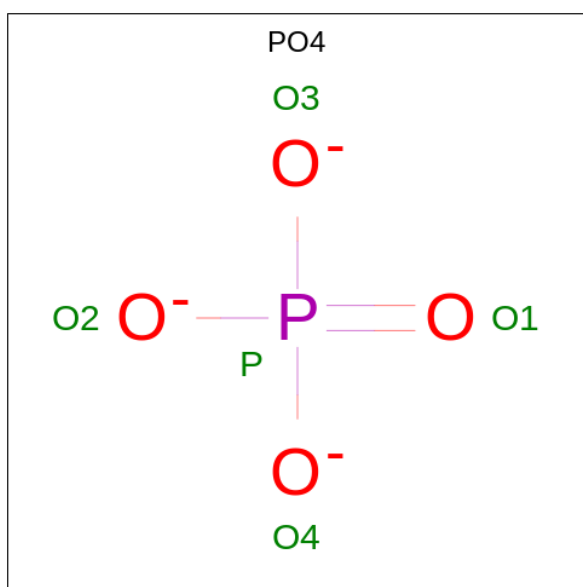
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	Z	1	Total	C	O	0	0
			33	22	11		

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	260	Total	O	0	4
			261	261		
30	B	220	Total	O	0	3
			222	222		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	C	154	Total 154	O 154	0	0
30	D	189	Total 189	O 189	0	0
30	E	145	Total 145	O 145	0	0
30	F	149	Total 149	O 149	0	0
30	G	93	Total 93	O 93	0	0
30	H	92	Total 92	O 92	0	0
30	I	67	Total 67	O 67	0	0
30	J	44	Total 44	O 44	0	0
30	K	41	Total 41	O 41	0	0
30	L	45	Total 45	O 45	0	1
30	M	28	Total 28	O 28	0	0
30	N	263	Total 264	O 264	0	4
30	O	181	Total 183	O 183	0	5
30	P	145	Total 145	O 145	0	0
30	Q	113	Total 113	O 113	0	0
30	R	100	Total 100	O 100	0	0
30	S	135	Total 135	O 135	0	0
30	T	77	Total 77	O 77	0	0
30	U	87	Total 87	O 87	0	0
30	V	62	Total 62	O 62	0	0
30	W	47	Total 47	O 47	0	1

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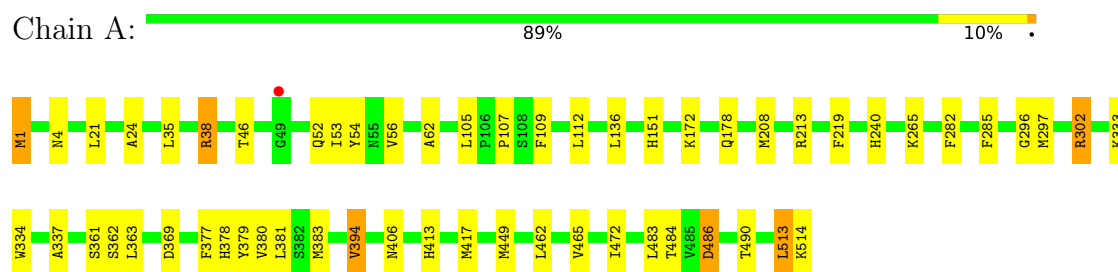
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	29	Total 29	O 29	0	0
30	Y	38	Total 38	O 38	0	1
30	Z	25	Total 25	O 25	0	2

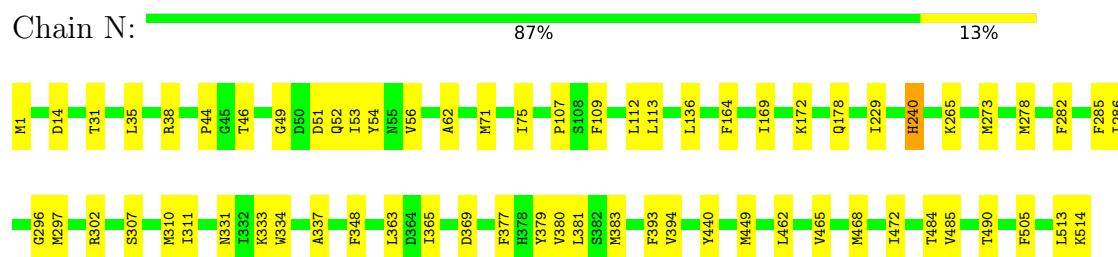
3 Residue-property plots

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.

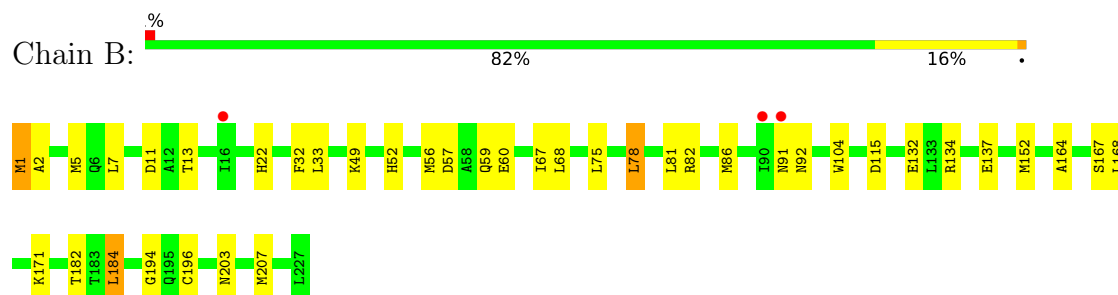
• Molecule 1: Cytochrome c oxidase subunit 1



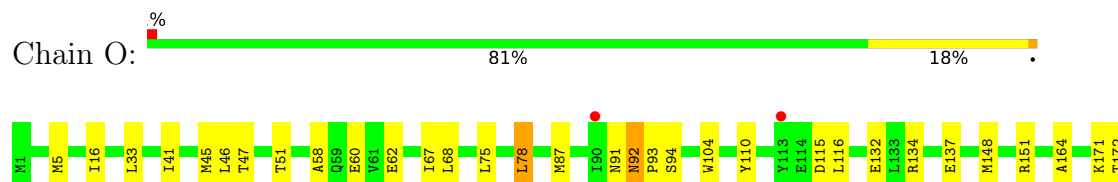
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

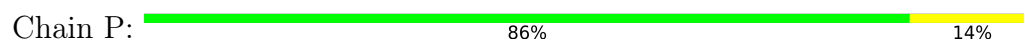




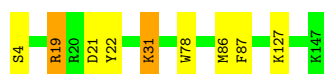
- Molecule 3: Cytochrome c oxidase subunit 3



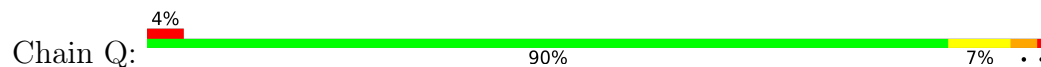
- Molecule 3: Cytochrome c oxidase subunit 3



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



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



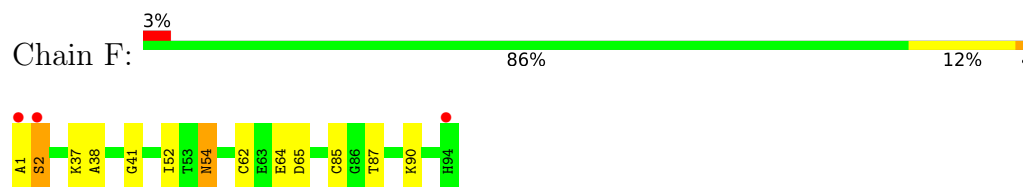
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



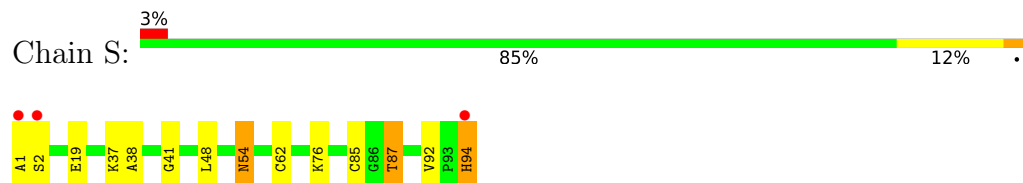
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



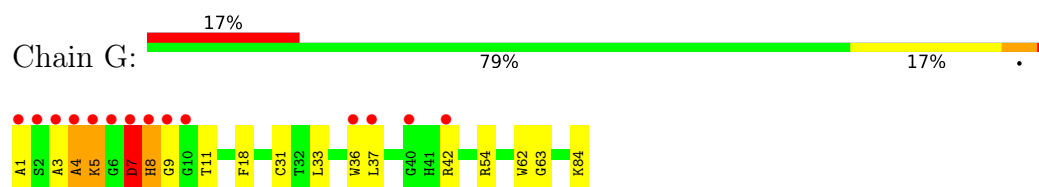
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



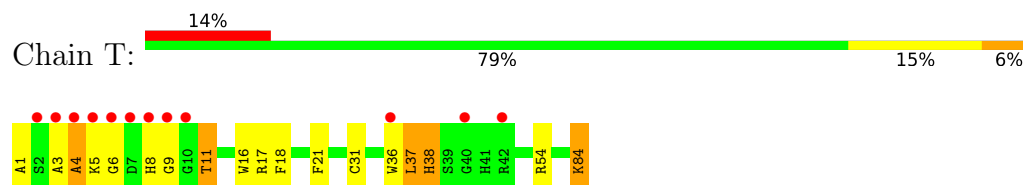
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



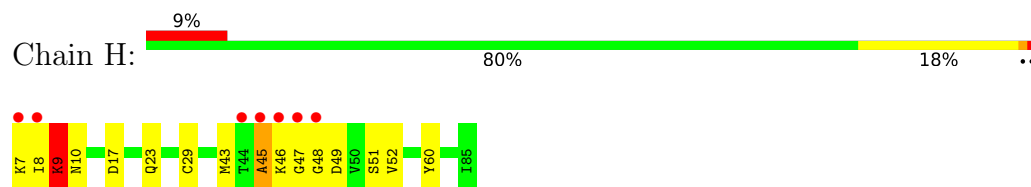
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



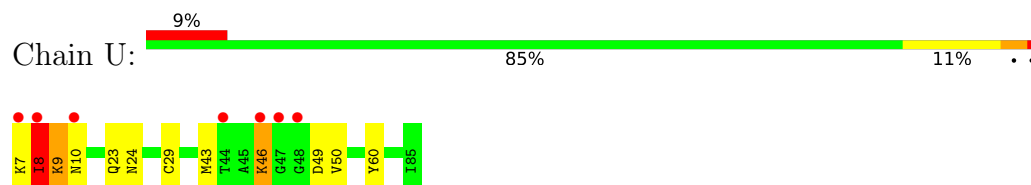
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



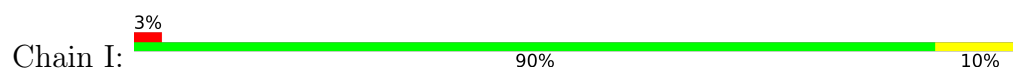
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 8: Cytochrome c oxidase subunit 6B1

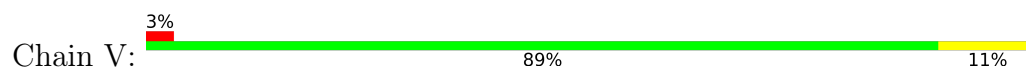


- Molecule 9: Cytochrome c oxidase subunit 6C

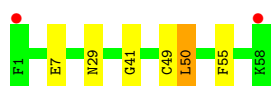




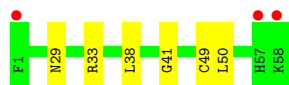
- Molecule 9: Cytochrome c oxidase subunit 6C



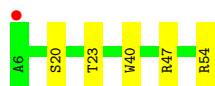
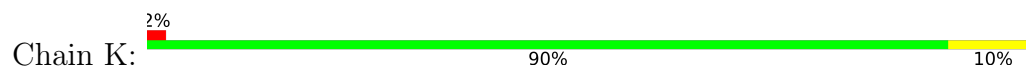
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



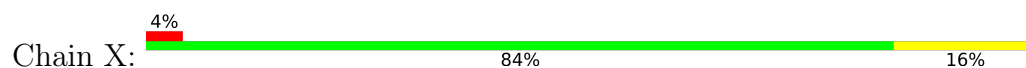
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



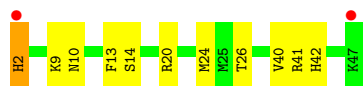
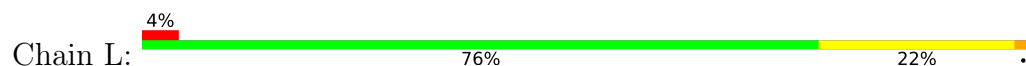
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



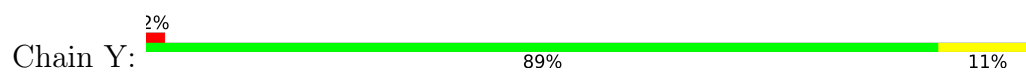
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



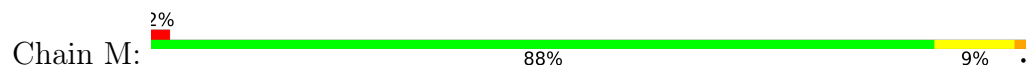
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



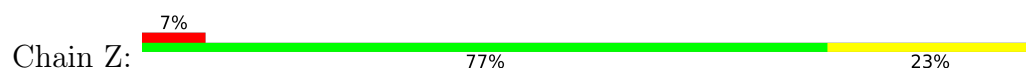
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.49Å 203.30Å 177.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 1.68 135.39 – 1.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.62-1.68) 99.9 (135.39-1.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 1.68Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.153 , 0.177 0.153 , 0.177	Depositor DCC
R_{free} test set	37040 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34917	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CU, PEK, FME, EDO, MG, CMO, CDL, PO4, TGL, TPO, DMU, CHD, PGV, ZN, CUA, PSC, SAC, HEA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.83	4/4460 (0.1%)	0.85	9/6086 (0.1%)
1	N	0.79	0/4433	0.81	3/6050 (0.0%)
2	B	0.75	0/1958	0.89	7/2667 (0.3%)
2	O	0.66	0/1953	0.79	1/2660 (0.0%)
3	C	0.73	0/2251	0.72	1/3077 (0.0%)
3	P	0.73	0/2259	0.73	0/3087
4	D	0.69	0/1252	0.71	0/1688
4	Q	0.54	0/1240	0.68	3/1672 (0.2%)
5	E	0.64	0/871	0.73	1/1182 (0.1%)
5	R	0.56	0/871	0.65	0/1182
6	F	0.68	0/747	0.75	0/1014
6	S	0.66	0/732	0.76	0/993
7	G	0.71	1/691 (0.1%)	0.77	0/937
7	T	0.62	1/691 (0.1%)	0.75	0/937
8	H	0.70	0/682	0.72	1/921 (0.1%)
8	U	0.67	0/682	0.71	0/921
9	I	0.59	0/605	0.68	0/802
9	V	0.55	0/605	0.65	0/802
10	J	0.54	0/472	0.64	0/636
10	W	0.49	0/472	0.63	0/636
11	K	0.58	0/399	0.65	0/546
11	X	0.57	0/399	0.62	0/546
12	L	0.75	0/401	0.70	0/536
12	Y	0.60	0/401	0.61	0/536
13	M	0.70	0/345	0.72	0/470
13	Z	0.56	0/346	0.63	0/470
All	All	0.71	6/30218 (0.0%)	0.76	26/41054 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
4	Q	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	36	TRP	CB-CG	6.33	1.61	1.50
1	A	394[A]	VAL	CB-CG2	-5.80	1.40	1.52
1	A	394[B]	VAL	CB-CG2	-5.80	1.40	1.52
1	A	362[A]	SER	CB-OG	-5.27	1.35	1.42
1	A	362[B]	SER	CB-OG	-5.27	1.35	1.42
7	T	36	TRP	CB-CG	5.01	1.59	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-11.62	81.61	100.20
1	N	310	MET	CG-SD-CE	-7.90	87.56	100.20
1	A	302[A]	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-7.58	116.51	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.79	116.90	120.30
4	Q	20	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	38	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	38	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	513	LEU	CA-CB-CG	-6.13	101.20	115.30
4	Q	51	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	213	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	B	184	LEU	CA-CB-CG	5.75	128.52	115.30
2	B	134	ARG	NE-CZ-NH1	5.72	123.16	120.30
5	E	30	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	B	134	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	N	38	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	B	152[A]	MET	CG-SD-CE	5.29	108.66	100.20
2	B	152[B]	MET	CG-SD-CE	5.29	108.66	100.20
2	B	11	ASP	CB-CG-OD1	5.28	123.05	118.30
2	B	184	LEU	CB-CG-CD1	-5.25	102.08	111.00
8	H	17	ASP	CB-CG-OD1	5.17	122.95	118.30
3	C	80	ARG	CG-CD-NE	-5.15	100.99	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	134	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	363[A]	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	363[B]	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	213	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
4	Q	8	SER	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	4192	0	4170	59	0
1	N	4182	0	4161	65	0
2	B	1858	0	1867	26	0
2	O	1856	0	1863	26	0
3	C	2124	0	2032	18	0
3	P	2126	0	2033	35	0
4	D	1207	0	1197	12	0
4	Q	1201	0	1192	14	0
5	E	852	0	845	2	0
5	R	852	0	845	5	0
6	F	721	0	702	11	0
6	S	716	0	697	15	0
7	G	676	0	644	12	0
7	T	676	0	643	18	0
8	H	662	0	623	12	0
8	U	662	0	623	10	0
9	I	601	0	613	9	0
9	V	601	0	613	3	0
10	J	461	0	459	9	0
10	W	461	0	459	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	385	0	366	4	0
11	X	385	0	366	7	0
12	L	382	0	381	19	0
12	Y	382	0	381	6	0
13	M	335	0	352	8	0
13	Z	336	0	352	8	0
14	A	139	0	111	8	0
14	N	139	0	111	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	4	0	0	0	0
18	N	4	0	0	0	0
19	A	99	0	143	4	0
19	C	101	0	147	5	0
19	G	51	0	76	6	0
19	N	102	0	152	6	0
19	P	51	0	76	3	0
20	A	56	0	84	10	0
20	B	24	0	36	2	0
20	C	36	0	54	1	0
20	D	20	0	30	1	0
20	E	12	0	18	0	0
20	F	20	0	30	1	0
20	G	8	0	12	0	0
20	I	4	0	6	0	0
20	J	8	0	12	1	0
20	L	4	0	6	3	0
20	M	16	0	24	6	0
20	N	68	0	102	15	0
20	O	16	0	24	0	0
20	P	24	0	36	0	0
20	Q	12	0	18	1	0
20	R	8	0	12	1	0
20	S	20	0	30	1	0
20	T	8	0	12	0	0
20	U	4	0	6	4	0
20	V	4	0	5	2	0
20	Y	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	126	0	220	18	0
21	L	60	0	101	13	0
21	N	63	0	110	2	0
21	Q	63	0	110	6	0
21	Y	63	0	110	9	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	51	0	75	13	0
23	O	46	0	62	4	0
24	C	29	0	39	0	0
24	G	29	0	39	0	0
24	J	58	0	78	3	0
24	P	58	0	78	2	0
24	T	29	0	39	0	0
24	W	29	0	38	1	0
24	Y	29	0	39	1	0
25	C	106	0	154	11	0
25	P	146	0	202	12	0
25	T	44	0	56	4	0
26	C	92	0	149	3	0
26	G	99	0	151	20	0
26	P	84	0	130	10	0
26	T	96	0	142	16	0
27	C	66	0	84	12	0
27	G	33	0	42	8	0
27	K	175	0	229	7	0
27	L	33	0	42	7	0
27	M	66	0	84	2	0
27	O	32	0	37	1	0
27	P	99	0	126	17	0
27	T	22	0	31	1	0
27	X	143	0	188	10	0
27	Z	33	0	42	3	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	261	0	0	17	0
30	B	222	0	0	3	0
30	C	154	0	0	4	0
30	D	189	0	0	2	0
30	E	145	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	149	0	0	6	0
30	G	93	0	0	2	0
30	H	92	0	0	2	0
30	I	67	0	0	4	0
30	J	44	0	0	1	0
30	K	41	0	0	0	0
30	L	45	0	0	4	0
30	M	28	0	0	0	0
30	N	264	0	0	11	0
30	O	183	0	0	6	0
30	P	145	0	0	4	0
30	Q	113	0	0	1	0
30	R	100	0	0	1	0
30	S	135	0	0	6	0
30	T	77	0	0	5	0
30	U	87	0	0	1	0
30	V	62	0	0	2	0
30	W	47	0	0	0	0
30	X	29	0	0	1	0
30	Y	38	0	0	1	0
30	Z	25	0	0	0	0
All	All	34917	0	32885	500	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 8.

All (500) 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)
30:N:911:HOH:O	2:O:87:MET:SD	2.25	0.94
8:U:24:ASN:HD21	20:U:101:EDO:H21	1.32	0.92
7:T:37:LEU:HD23	26:T:103:CDL:H371	1.56	0.87
12:L:20:ARG:HH22	21:L:101:TGL:HC61	1.39	0.85
23:B:303:PSC:H21	23:B:303:PSC:H212	1.60	0.81
7:G:62:TRP:HA	27:G:102:DMU:H29	1.63	0.80
10:W:33:ARG:HG2	24:W:101:CHD:H152	1.62	0.80
26:T:103:CDL:H561	26:T:103:CDL:H782	1.64	0.80
3:C:91:VAL:O	3:C:95[B]:THR:HG23	1.82	0.79
23:O:302:PSC:O01	23:O:302:PSC:H212	1.83	0.78
3:C:149:HIS:NE2	20:C:315:EDO:H21	2.00	0.77
30:O:553:HOH:O	21:Q:201:TGL:HC61	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD11	20:A:617:EDO:H11	1.67	0.76
3:P:33:MET:HB2	27:P:309:DMU:H11	1.67	0.75
20:A:617:EDO:H12	30:A:786:HOH:O	1.85	0.75
12:L:24[B]:MET:SD	30:L:225:HOH:O	2.46	0.74
7:T:84:LYS:OXT	30:T:201:HOH:O	2.07	0.73
11:X:34:THR:HG22	27:X:203:DMU:H7	1.71	0.73
27:P:307:DMU:H26	10:W:38:LEU:HA	1.72	0.71
1:N:297[B]:MET:HG2	30:N:772:HOH:O	1.90	0.71
1:N:505:PHE:H	20:N:618:EDO:H22	1.56	0.71
27:C:307:DMU:H42	27:G:102:DMU:H37	1.33	0.71
27:P:307:DMU:C43	10:W:38:LEU:HD23	2.21	0.70
3:C:33:MET:HE2	27:C:308:DMU:H8	1.74	0.70
9:V:20:HIS:HE1	20:V:101:EDO:H22	1.57	0.70
12:L:13:PHE:HA	21:L:101:TGL:HC21	1.73	0.69
27:K:102:DMU:H9	27:K:104:DMU:H29	1.73	0.69
1:A:472:ILE:HG21	21:L:101:TGL:HA91	1.75	0.69
26:C:306:CDL:H522	26:C:306:CDL:OB9	1.93	0.69
1:A:465:VAL:HG22	20:A:622:EDO:H12	1.75	0.69
27:P:307:DMU:H26	10:W:38:LEU:HD23	1.73	0.69
3:C:33:MET:CE	27:C:308:DMU:H8	2.23	0.68
1:N:465:VAL:HG22	20:N:626:EDO:H21	1.75	0.68
12:L:20:ARG:NH2	21:L:101:TGL:HC32	2.09	0.68
1:A:406:ASN:HD21	19:A:607:PGV:H22	1.58	0.67
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.76	0.67
11:X:34:THR:HA	27:X:203:DMU:H5	1.76	0.67
23:B:303:PSC:H071	9:I:10:ARG:HE	1.61	0.65
21:B:301:TGL:H242	21:B:301:TGL:HA91	1.78	0.65
7:T:8:HIS:HD2	25:T:102:PEK:H232	1.63	0.64
27:L:102:DMU:O1	27:L:102:DMU:O55	2.11	0.64
7:G:8:HIS:CG	7:G:9:GLY:H	2.16	0.64
1:A:178[B]:GLN:HE21	7:T:9:GLY:HA3	1.62	0.64
1:N:297[B]:MET:HG3	1:N:302:ARG:HG3	1.80	0.63
1:N:505:PHE:H	20:N:618:EDO:C2	2.12	0.63
13:M:42:LYS:HG2	13:M:42:LYS:O	1.98	0.63
11:K:20:SER:HB3	27:K:106:DMU:H30	1.82	0.62
19:C:305:PGV:H152	27:P:316:DMU:H23	1.81	0.62
27:X:202:DMU:O55	27:X:202:DMU:H35	1.99	0.62
25:P:304:PEK:H041	7:T:17:ARG:HH22	1.65	0.62
4:D:4:SER:HB2	30:D:380:HOH:O	1.99	0.61
1:N:164:PHE:HE2	20:N:617:EDO:H22	1.64	0.61
26:G:101:CDL:H222	26:G:101:CDL:H531	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:607:PGV:H032	30:N:928:HOH:O	2.00	0.61
1:A:282:PHE:HA	7:T:4:ALA:CB	2.30	0.61
1:A:417:MET:SD	20:A:622:EDO:O1	2.59	0.60
19:A:607:PGV:H012	30:A:930:HOH:O	2.01	0.60
26:G:101:CDL:H171	1:N:307:SER:HB3	1.82	0.60
20:L:103:EDO:H11	30:L:231:HOH:O	2.00	0.60
27:X:202:DMU:O49	27:X:204:DMU:H29	2.02	0.60
12:L:20:ARG:HH22	21:L:101:TGL:HC32	1.67	0.60
21:B:304:TGL:H332	30:I:238:HOH:O	2.02	0.60
26:G:101:CDL:H241	26:G:101:CDL:H542	1.84	0.59
1:N:53[B]:ILE:HG12	30:N:876:HOH:O	2.01	0.59
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.68	0.59
26:G:101:CDL:H712	26:G:101:CDL:H541	1.84	0.58
6:F:41:GLY:HA3	6:F:87[B]:THR:HG23	1.84	0.58
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.86	0.58
13:M:14:GLU:OE1	27:M:106:DMU:H32	2.04	0.58
19:N:607:PGV:H152	19:N:607:PGV:H312	1.84	0.58
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.86	0.58
6:S:19:GLU:HG2	30:S:300:HOH:O	2.03	0.58
1:A:417:MET:HE1	14:A:601[A]:HEA:H263	1.86	0.57
3:C:210:ILE:HG12	19:C:304:PGV:H132	1.85	0.57
11:K:23:THR:HG21	27:K:106:DMU:H32	1.85	0.57
1:N:514:LYS:HD3	30:S:254:HOH:O	2.05	0.57
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.85	0.57
8:U:43:MET:HE3	8:U:49:ASP:N	2.19	0.57
27:C:308:DMU:H11	10:J:49:CYS:HB3	1.85	0.57
26:T:103:CDL:H761	26:T:103:CDL:H242	1.87	0.57
1:A:514:LYS:HD2	30:F:221:HOH:O	2.04	0.57
12:Y:24[B]:MET:SD	21:Y:102:TGL:HC32	2.45	0.57
23:B:303:PSC:H071	9:I:10:ARG:HH21	1.70	0.56
7:T:8:HIS:CD2	25:T:102:PEK:H232	2.40	0.56
1:N:449[A]:MET:SD	2:O:5:MET:HG2	2.44	0.56
1:A:46[B]:THR:HG23	30:A:708:HOH:O	2.05	0.56
3:C:3:HIS:N	30:C:403:HOH:O	2.39	0.56
1:N:505:PHE:N	20:N:618:EDO:H22	2.19	0.56
1:A:413:HIS:NE2	20:A:622:EDO:H11	2.21	0.56
4:Q:98:TRP:CE3	27:Z:101:DMU:H12	2.41	0.56
2:B:81:LEU:HD12	26:T:103:CDL:H362	1.86	0.56
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.87	0.56
19:C:305:PGV:H172	27:P:316:DMU:H24	1.86	0.56
19:A:607:PGV:H031	30:A:930:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:54[B]:TYR:HB2	30:N:752:HOH:O	2.05	0.56
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.88	0.56
26:T:103:CDL:H181	26:T:103:CDL:OB6	2.06	0.56
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.87	0.55
3:C:161[A]:GLN:HE22	25:C:303:PEK:H22	1.70	0.55
5:E:90:ARG:HD2	30:E:385:HOH:O	2.06	0.55
6:S:85:CYS:SG	6:S:87:THR:OG1	2.63	0.55
23:B:303:PSC:C07	9:I:10:ARG:HH21	2.19	0.55
12:L:24[A]:MET:SD	21:L:101:TGL:H162	2.45	0.55
2:O:172:THR:HG1	2:O:182[B]:THR:HG1	1.53	0.55
2:B:57:ASP:H	23:B:303:PSC:H202	1.72	0.55
12:L:20:ARG:HH22	21:L:101:TGL:CC6	2.15	0.55
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.89	0.55
8:H:52:VAL:HA	8:U:46:LYS:HD2	1.89	0.55
21:B:301:TGL:HC51	30:B:607:HOH:O	2.06	0.55
1:N:468:MET:SD	20:N:626:EDO:H11	2.47	0.54
25:C:303:PEK:H383	26:G:101:CDL:H271	1.89	0.54
1:N:472:ILE:HG21	21:Y:102:TGL:H201	1.89	0.54
20:N:625:EDO:H22	12:Y:10:ASN:HD22	1.71	0.54
3:P:156:ARG:HE	24:P:308:CHD:C24	2.21	0.54
27:G:102:DMU:O6	30:G:202:HOH:O	2.19	0.54
20:N:612:EDO:H12	13:Z:2:THR:HG23	1.88	0.54
3:C:161[A]:GLN:NE2	25:C:303:PEK:H22	2.23	0.54
6:S:87:THR:HG21	30:S:274:HOH:O	2.07	0.54
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.88	0.54
2:B:56:MET:HB3	23:B:303:PSC:H221	1.90	0.54
12:L:42:HIS:ND1	27:L:102:DMU:H29	2.22	0.53
3:P:261:SER:OXT	27:P:316:DMU:H33	2.08	0.53
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.89	0.53
19:C:305:PGV:H152	27:P:316:DMU:C40	2.39	0.53
1:N:365:ILE:HD11	30:N:907:HOH:O	2.08	0.53
4:Q:81:VAL:HG11	21:Q:201:TGL:HB62	1.90	0.53
1:A:465:VAL:CG2	20:A:622:EDO:H12	2.38	0.53
21:B:304:TGL:HB22	4:D:78:TRP:HB3	1.89	0.53
8:H:43:MET:HE1	8:H:48:GLY:HA3	1.91	0.53
27:M:106:DMU:O55	27:M:106:DMU:O6	2.26	0.53
30:A:708:HOH:O	20:B:309:EDO:H11	2.08	0.53
8:H:47:GLY:HA2	30:H:269:HOH:O	2.08	0.53
3:P:224:LYS:HE2	26:P:306:CDL:H131	1.89	0.53
30:N:899:HOH:O	4:Q:20:ARG:HG2	2.08	0.53
3:C:165:ILE:HG12	25:C:303:PEK:H9	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:333:LYS:NZ	30:N:704:HOH:O	2.42	0.52
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.90	0.52
8:H:45:ALA:O	8:H:47:GLY:N	2.42	0.52
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.91	0.52
12:Y:20:ARG:HH22	21:Y:102:TGL:HC62	1.74	0.52
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.09	0.52
27:P:307:DMU:H22	10:W:41:GLY:HA3	1.91	0.52
6:S:1:ALA:HB2	20:S:104:EDO:O2	2.10	0.52
20:A:611:EDO:H11	12:L:10:ASN:HD22	1.74	0.52
26:G:101:CDL:H512	26:G:101:CDL:C20	2.40	0.52
8:H:43:MET:CE	8:H:48:GLY:HA3	2.41	0.51
20:N:616:EDO:H22	20:N:617:EDO:O2	2.10	0.51
2:O:41:ILE:HD13	23:O:302:PSC:H321	1.92	0.51
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.46	0.51
12:Y:13:PHE:HA	21:Y:102:TGL:HC31	1.91	0.51
27:X:202:DMU:C9	27:X:202:DMU:H28	2.22	0.51
21:L:101:TGL:H231	21:L:101:TGL:HA92	1.92	0.51
3:P:164:PHE:CD1	24:P:308:CHD:H192	2.46	0.51
1:N:136[B]:LEU:HD11	30:T:269:HOH:O	2.10	0.51
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.11	0.51
3:P:213:THR:HG23	26:P:306:CDL:H771	1.92	0.51
3:P:258:TRP:CZ3	27:P:316:DMU:H10	2.45	0.51
19:G:104:PGV:H331	25:P:302:PEK:H182	1.91	0.51
8:H:9:LYS:HG3	8:H:10:ASN:H	1.75	0.51
25:T:102:PEK:O04	30:T:202:HOH:O	2.19	0.51
30:C:406:HOH:O	6:F:52:ILE:HD11	2.11	0.50
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.11	0.50
3:P:3:HIS:HA	30:P:520:HOH:O	2.11	0.50
3:P:168:THR:HG22	25:P:304:PEK:H12	1.92	0.50
19:G:104:PGV:H061	8:U:24:ASN:HB3	1.94	0.50
10:J:55:PHE:HE1	27:L:102:DMU:C57	2.25	0.50
3:P:98:PHE:CD2	25:P:302:PEK:H172	2.46	0.50
27:P:316:DMU:H30	27:P:316:DMU:O3	2.12	0.50
21:B:304:TGL:HG12	21:B:304:TGL:HC31	1.94	0.50
27:G:102:DMU:H40	30:G:210:HOH:O	2.10	0.50
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.50
21:B:304:TGL:H342	30:B:429:HOH:O	2.11	0.50
19:N:607:PGV:H142	4:Q:87:PHE:CD2	2.46	0.50
2:O:41:ILE:O	2:O:45:MET:HG2	2.12	0.50
26:T:103:CDL:H541	26:T:103:CDL:H741	1.94	0.50
1:A:334:TRP:HZ3	21:B:304:TGL:HA62	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:63:GLY:H	27:G:102:DMU:H3	1.77	0.50
3:P:247:VAL:HB	25:P:302:PEK:H11	1.93	0.50
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.92	0.50
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.12	0.50
6:S:1:ALA:HA	7:T:17:ARG:NH1	2.27	0.49
12:L:9:LYS:HD3	20:L:103:EDO:H12	1.93	0.49
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.95	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.49
13:Z:43:SER:OXT	13:Z:43:SER:OG	2.29	0.49
1:A:417:MET:CE	14:A:601[A]:HEA:H263	2.42	0.49
8:U:50:VAL:HG23	30:U:226:HOH:O	2.12	0.49
11:X:24:PHE:HE1	27:X:205:DMU:H15	1.78	0.49
30:A:903:HOH:O	6:F:37:LYS:HE2	2.13	0.49
19:N:607:PGV:H011	19:N:607:PGV:H31	1.95	0.49
2:O:92:ASN:HB2	30:O:543:HOH:O	2.12	0.49
7:G:31:CYS:SG	26:G:101:CDL:H522	2.53	0.49
3:P:33:MET:HG2	3:P:39:SER:O	2.12	0.49
12:L:14:SER:H	21:L:101:TGL:HC31	1.78	0.49
3:P:33:MET:HB2	27:P:309:DMU:C22	2.37	0.49
30:A:781:HOH:O	23:B:303:PSC:H22	2.12	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.48	0.48
13:M:32:TRP:CZ2	20:M:103:EDO:H11	2.48	0.48
1:N:348:PHE:CE1	1:N:380[B]:VAL:HG23	2.48	0.48
25:P:304:PEK:H383	26:T:103:CDL:C26	2.44	0.48
2:B:13:THR:OG1	2:B:167:SER:HB3	2.14	0.48
1:A:35[B]:LEU:HD11	1:A:462:LEU:HD13	1.94	0.48
2:B:7:LEU:HD11	21:B:301:TGL:H152	1.96	0.48
27:C:307:DMU:O6	27:C:307:DMU:O2	2.25	0.48
3:P:226:HIS:HE1	26:P:306:CDL:HB32	1.77	0.48
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD2	2.14	0.48
3:C:160:LEU:HD13	24:J:101:CHD:H181	1.96	0.48
9:I:6:LYS:NZ	30:I:201:HOH:O	2.39	0.48
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.43	0.48
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.94	0.48
26:G:101:CDL:H542	26:G:101:CDL:C24	2.43	0.48
1:N:113:LEU:HB2	21:Y:102:TGL:C30	2.43	0.48
3:P:259:TRP:HD1	27:P:316:DMU:H1	1.78	0.48
26:G:101:CDL:H552	26:G:101:CDL:H582	1.57	0.48
27:G:102:DMU:H30	27:G:102:DMU:O1	2.14	0.48
10:J:55:PHE:HE1	27:L:102:DMU:H30	1.79	0.48
1:N:113:LEU:HB2	21:Y:102:TGL:H301	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:172:TYR:CE2	25:P:304:PEK:H15	2.49	0.48
8:U:7:LYS:O	8:U:8:ILE:HB	2.14	0.48
1:A:282:PHE:HA	7:T:4:ALA:HB1	1.94	0.48
13:M:32:TRP:CH2	20:M:103:EDO:H22	2.49	0.48
1:N:112:LEU:HD23	1:N:112:LEU:C	2.35	0.48
3:P:55:TYR:OH	26:P:306:CDL:HA62	2.14	0.48
6:F:54[A]:ASN:ND2	30:F:202:HOH:O	2.47	0.47
7:T:1:ALA:N	30:T:205:HOH:O	2.47	0.47
1:A:513:LEU:O	1:A:514:LYS:HB2	2.13	0.47
4:D:127:LYS:HD2	30:I:246:HOH:O	2.14	0.47
11:X:24:PHE:O	11:X:28:VAL:HG12	2.14	0.47
1:A:46[B]:THR:HG22	30:A:702:HOH:O	2.13	0.47
12:L:9:LYS:HA	20:L:103:EDO:H12	1.96	0.47
13:M:32:TRP:HH2	20:M:103:EDO:HO2	1.63	0.47
1:N:273:MET:HE2	30:N:750:HOH:O	2.14	0.47
12:Y:20:ARG:HH12	21:Y:102:TGL:HC42	1.78	0.47
26:G:101:CDL:H771	26:G:101:CDL:H571	1.97	0.47
3:P:247:VAL:HG12	25:P:302:PEK:H132	1.97	0.47
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.55	0.47
27:O:303:DMU:H9	27:O:303:DMU:O5	2.14	0.47
30:P:543:HOH:O	27:T:104:DMU:H22	2.13	0.47
10:W:29:ASN:HD22	10:W:29:ASN:H	1.62	0.47
19:G:104:PGV:H101	19:G:104:PGV:H131	1.44	0.47
7:T:38:HIS:CE1	26:T:103:CDL:H122	2.50	0.47
1:A:35[B]:LEU:HD11	1:A:462:LEU:HB2	1.95	0.47
3:P:226:HIS:CE1	26:P:306:CDL:HB32	2.49	0.47
26:P:306:CDL:HB62	26:P:306:CDL:H521	1.97	0.47
4:Q:5:VAL:HG22	13:Z:5:PRO:HD2	1.97	0.47
5:R:90:ARG:NH2	30:R:301:HOH:O	2.32	0.47
26:G:101:CDL:H512	26:G:101:CDL:C21	2.45	0.47
1:N:381[B]:LEU:HB2	14:N:602:HEA:CAC	2.45	0.47
20:Q:202:EDO:C2	20:Q:204:EDO:H22	2.45	0.47
25:C:302:PEK:H131	25:C:302:PEK:H262	1.97	0.47
30:N:760:HOH:O	20:U:101:EDO:H11	2.15	0.47
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.47
12:L:41:ARG:HH12	27:L:102:DMU:H2	1.80	0.47
2:B:57:ASP:N	23:B:303:PSC:H202	2.30	0.46
26:C:306:CDL:H232	30:C:554:HOH:O	2.16	0.46
21:N:608:TGL:HC22	30:V:250:HOH:O	2.14	0.46
1:A:379:TYR:O	1:A:383[B]:MET:HB2	2.15	0.46
8:H:7:LYS:O	30:H:201:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:14:ASP:OD1	20:N:625:EDO:H11	2.16	0.46
6:F:90:LYS:HD2	30:F:324:HOH:O	2.15	0.46
1:N:331[B]:ASN:ND2	2:O:51:THR:HG21	2.30	0.46
26:P:306:CDL:H232	30:P:541:HOH:O	2.16	0.46
12:L:24[B]:MET:HE1	21:L:101:TGL:HC22	1.96	0.46
1:N:35[A]:LEU:HD11	1:N:462:LEU:HB2	1.97	0.46
4:Q:98:TRP:CD2	27:Z:101:DMU:H12	2.51	0.46
24:Y:101:CHD:H112	24:Y:101:CHD:H12A	1.57	0.46
1:A:208[B]:MET:HG2	1:A:219:PHE:CE2	2.50	0.46
2:O:16[B]:ILE:HG23	30:O:511:HOH:O	2.14	0.46
27:L:102:DMU:H5	30:L:208:HOH:O	2.15	0.46
4:Q:121:LYS:NZ	30:Q:301:HOH:O	2.48	0.46
2:B:52:HIS:HE1	23:B:303:PSC:H02	1.80	0.46
26:G:101:CDL:H512	26:G:101:CDL:H211	1.98	0.46
10:J:55:PHE:CE1	27:L:102:DMU:H29	2.51	0.46
1:A:334:TRP:CZ3	21:B:304:TGL:HA62	2.51	0.46
6:F:87[A]:THR:HG21	30:F:294:HOH:O	2.15	0.46
10:J:29:ASN:HD22	10:J:29:ASN:H	1.62	0.46
19:N:607:PGV:H301	13:Z:19:LEU:HD23	1.98	0.46
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.16	0.46
19:A:607:PGV:H31	19:A:607:PGV:H011	1.98	0.46
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.50	0.46
3:P:251:PHE:CD2	25:P:302:PEK:H203	2.51	0.46
1:A:172:LYS:NZ	1:A:178[B]:GLN:HE22	2.14	0.45
4:D:19[A]:ARG:NE	4:D:21:ASP:OD1	2.44	0.45
19:G:104:PGV:H031	3:P:107:ALA:HB2	1.98	0.45
3:P:161[A]:GLN:HE22	25:P:304:PEK:H21	1.81	0.45
6:S:41:GLY:HA3	6:S:87:THR:HG22	1.97	0.45
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.57	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.45
21:B:304:TGL:H312	4:D:86:MET:HG2	1.97	0.45
2:O:58:ALA:O	2:O:62:GLU:HG3	2.17	0.45
26:G:101:CDL:H232	1:N:286:ILE:CD1	2.45	0.45
7:G:1:ALA:H2	19:G:104:PGV:H292	1.82	0.45
21:L:101:TGL:HC72	30:L:243:HOH:O	2.17	0.45
3:P:91:VAL:HG22	25:P:302:PEK:H12	1.97	0.45
3:P:158:HIS:HD2	3:P:161[B]:GLN:OE1	1.98	0.45
26:T:103:CDL:H322	26:T:103:CDL:H351	1.78	0.45
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.97	0.45
3:C:172:TYR:CZ	25:C:303:PEK:H171	2.51	0.45
10:J:7:GLU:HG3	30:J:228:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.45
3:P:155:ASP:OD2	6:S:2:SER:HA	2.16	0.45
26:P:306:CDL:H112	30:P:535:HOH:O	2.17	0.45
2:O:148[B]:MET:CE	2:O:216:LEU:HD22	2.46	0.45
3:P:259:TRP:CD1	27:P:316:DMU:H1	2.51	0.45
1:A:297[A]:MET:HG2	30:A:918:HOH:O	2.15	0.45
4:D:87[B]:PHE:CE1	27:K:106:DMU:H29	2.51	0.45
14:N:602:HEA:HMC1	14:N:602:HEA:CBC	2.46	0.45
3:P:210:ILE:HG23	19:P:305:PGV:H91	1.98	0.45
6:S:41:GLY:HA3	6:S:87:THR:CG2	2.47	0.45
1:A:151:HIS:CD2	25:C:302:PEK:H382	2.52	0.45
21:B:304:TGL:HB22	4:D:78:TRP:CA	2.47	0.45
27:C:307:DMU:O6	27:G:102:DMU:O2	2.08	0.45
26:G:101:CDL:H541	26:G:101:CDL:H511	1.38	0.45
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.72	0.45
4:Q:114:GLU:CD	11:X:51:LYS:HE2	2.37	0.45
1:A:112:LEU:HG	30:A:924:HOH:O	2.16	0.44
26:P:306:CDL:H162	26:P:306:CDL:H132	1.57	0.44
21:Q:201:TGL:HC32	21:Q:201:TGL:HG12	1.98	0.44
27:C:307:DMU:H23	10:J:41:GLY:HA3	1.98	0.44
26:G:101:CDL:H441	1:N:311:ILE:CD1	2.47	0.44
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.52	0.44
2:B:81:LEU:CD1	26:T:103:CDL:H362	2.47	0.44
11:K:20:SER:HB3	27:K:106:DMU:C57	2.45	0.44
4:D:19[A]:ARG:HG2	4:D:22:TYR:HB3	1.99	0.44
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.44
1:N:381[B]:LEU:HD13	14:N:602:HEA:HBC2	1.99	0.44
7:T:8:HIS:HD2	25:T:102:PEK:C23	2.29	0.44
2:B:49:LYS:HE3	21:B:304:TGL:HC72	1.98	0.44
27:P:309:DMU:H10	10:W:49:CYS:HB3	1.99	0.44
4:Q:7:LYS:H	4:Q:7:LYS:HG2	1.59	0.44
2:B:1:FME:HE2	2:B:2:ALA:O	2.17	0.44
23:B:303:PSC:H081	5:E:8:ASP:HA	1.99	0.44
27:C:308:DMU:C22	10:J:49:CYS:HB3	2.47	0.44
7:G:8:HIS:CG	7:G:9:GLY:N	2.83	0.44
6:S:92:VAL:O	6:S:92:VAL:HG23	2.18	0.44
21:B:304:TGL:HB22	4:D:78:TRP:CB	2.47	0.44
26:G:101:CDL:H441	1:N:311:ILE:HD13	2.00	0.44
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.53	0.44
6:S:54:ASN:HD22	6:S:54:ASN:C	2.20	0.44
7:T:31:CYS:SG	26:T:103:CDL:H532	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:306:CDL:H852	26:P:306:CDL:H822	1.76	0.44
2:B:32[A]:PHE:CE1	21:B:301:TGL:HA52	2.53	0.43
3:C:37:PHE:CD2	27:C:308:DMU:H13	2.53	0.43
26:G:101:CDL:H352	2:O:78:LEU:HD12	2.00	0.43
1:N:31:THR:O	1:N:35[B]:LEU:HD23	2.17	0.43
8:U:9:LYS:HB3	8:U:10:ASN:H	1.56	0.43
23:B:303:PSC:H12	23:B:303:PSC:H322	1.99	0.43
8:H:9:LYS:O	8:H:10:ASN:HB2	2.18	0.43
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.54	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
3:C:33:MET:HE3	27:C:308:DMU:H8	2.00	0.43
27:K:105:DMU:O61	27:K:106:DMU:O49	2.23	0.43
13:M:32:TRP:CH2	20:M:103:EDO:C2	3.00	0.43
1:N:505:PHE:CA	20:N:618:EDO:H22	2.48	0.43
1:A:514:LYS:HE2	30:F:222:HOH:O	2.18	0.43
3:C:39:SER:OG	27:C:307:DMU:H30	2.19	0.43
7:G:5:LYS:HD3	1:N:278[B]:MET:HE3	1.98	0.43
24:J:102:CHD:H111	24:J:102:CHD:H193	1.51	0.43
2:O:116:LEU:HD13	2:O:226:MET:HG2	2.00	0.43
8:U:24:ASN:HD21	20:U:101:EDO:C2	2.15	0.43
1:A:484[B]:THR:HG22	30:A:883:HOH:O	2.17	0.43
25:C:302:PEK:H101	25:C:302:PEK:H132	1.76	0.43
7:T:38:HIS:HE1	26:T:103:CDL:H122	1.84	0.43
1:A:302[B]:ARG:HE	1:A:361:SER:HB2	1.84	0.43
12:L:9:LYS:HD3	12:L:9:LYS:HA	1.77	0.43
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.00	0.43
25:C:303:PEK:H051	6:F:1:ALA:N	2.34	0.43
26:G:101:CDL:H571	26:G:101:CDL:C77	2.47	0.43
2:O:92:ASN:ND2	30:O:405:HOH:O	2.42	0.43
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.93	0.43
2:B:22[B]:HIS:CE1	9:I:44:LYS:HE3	2.53	0.43
3:C:128:GLU:OE1	7:G:42:ARG:NH2	2.52	0.43
2:O:67:ILE:HD11	30:O:572:HOH:O	2.18	0.43
11:X:40:TRP:CD1	27:X:203:DMU:H11	2.54	0.43
12:Y:20:ARG:HH22	21:Y:102:TGL:HC82	1.84	0.43
14:N:601[B]:HEA:H122	30:N:818:HOH:O	2.18	0.43
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	2.00	0.43
1:A:112:LEU:C	1:A:112:LEU:HD23	2.38	0.42
27:C:308:DMU:H20	10:J:50:LEU:HG	2.01	0.42
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.81	0.42
1:N:484[B]:THR:HG22	13:Z:2:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:102:TGL:H202	21:Y:102:TGL:H232	1.60	0.42
1:A:54[B]:TYR:HB2	30:A:836:HOH:O	2.19	0.42
20:A:617:EDO:H22	30:A:788:HOH:O	2.19	0.42
1:A:381[B]:LEU:HD13	14:A:602:HEA:HBC2	2.01	0.42
26:C:306:CDL:H631	26:C:306:CDL:H661	1.72	0.42
14:N:601[B]:HEA:H172	14:N:601[B]:HEA:H261	1.78	0.42
26:T:103:CDL:H511	26:T:103:CDL:H202	2.01	0.42
2:B:182[B]:THR:HG21	30:B:517:HOH:O	2.18	0.42
8:H:49:ASP:O	8:H:52:VAL:HG22	2.19	0.42
1:N:505:PHE:HA	20:N:618:EDO:H22	2.01	0.42
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.19	0.42
27:P:309:DMU:H32	27:P:309:DMU:H29	2.02	0.42
26:T:103:CDL:H541	26:T:103:CDL:H762	2.02	0.42
20:A:613:EDO:H22	21:L:101:TGL:HC51	2.01	0.42
26:G:101:CDL:H372	26:G:101:CDL:H141	2.01	0.42
4:Q:6:VAL:HG12	4:Q:7:LYS:HG2	2.01	0.42
30:A:914:HOH:O	20:D:202:EDO:H21	2.20	0.42
2:B:22[B]:HIS:ND1	9:I:44:LYS:HE3	2.35	0.42
14:A:601[B]:HEA:H122	30:A:841:HOH:O	2.20	0.42
2:B:203:ASN:ND2	20:B:310:EDO:O2	2.47	0.42
25:C:302:PEK:H101	25:C:302:PEK:H42	2.00	0.42
21:Q:201:TGL:H122	21:Q:201:TGL:HB91	1.93	0.42
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.02	0.42
6:S:94:HIS:HA	30:S:292:HOH:O	2.19	0.42
24:J:102:CHD:H212	24:J:102:CHD:H12	2.01	0.42
1:N:513:LEU:O	1:N:514:LYS:HB2	2.19	0.42
3:P:38:ASN:O	27:P:307:DMU:H35	2.20	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.02	0.42
20:V:101:EDO:H12	30:V:202:HOH:O	2.20	0.42
1:A:21:LEU:HD23	21:L:101:TGL:H211	2.00	0.42
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.20	0.42
30:A:771:HOH:O	20:M:105:EDO:H12	2.19	0.42
9:I:73:LYS:HA	9:I:73:LYS:HD3	1.68	0.42
19:P:305:PGV:H172	19:P:305:PGV:H141	1.78	0.42
30:Y:230:HOH:O	13:Z:32:TRP:HH2	2.03	0.42
1:N:49[B]:GLY:HA3	13:Z:41:LYS:HE3	2.02	0.41
1:N:51[B]:ASP:OD2	2:O:206:PHE:HE2	2.02	0.41
1:N:393:PHE:CG	14:N:601[A]:HEA:H241	2.55	0.41
5:R:14:ARG:HH11	20:R:201:EDO:C1	2.32	0.41
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.08	0.41
21:B:301:TGL:H342	21:B:301:TGL:H212	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:101:HIS:CG	27:X:201:DMU:H6	2.55	0.41
27:X:202:DMU:H9	27:X:202:DMU:H5	1.81	0.41
8:U:24:ASN:ND2	20:U:101:EDO:H21	2.16	0.41
12:L:2:HIS:CD2	12:L:2:HIS:N	2.88	0.41
1:N:52[B]:GLN:O	1:N:56:VAL:HG23	2.20	0.41
7:G:62:TRP:CA	27:G:102:DMU:H29	2.44	0.41
26:G:101:CDL:H542	26:G:101:CDL:H231	2.02	0.41
2:B:78:LEU:HD12	26:T:103:CDL:H352	2.01	0.41
7:G:7:ASP:HB3	7:G:8:HIS:H	1.45	0.41
13:M:32:TRP:HH2	20:M:103:EDO:C2	2.34	0.41
1:N:75:ILE:CG2	20:N:616:EDO:H21	2.50	0.41
1:N:164:PHE:CE2	20:N:617:EDO:H22	2.51	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.03	0.41
21:B:304:TGL:HA92	21:B:304:TGL:H241	2.03	0.41
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.19	0.41
1:N:240:HIS:CD2	1:N:240:HIS:C	2.94	0.41
1:N:334:TRP:CE3	21:Q:201:TGL:HA31	2.56	0.41
2:O:47:THR:HA	21:Q:201:TGL:HC81	2.03	0.41
2:O:172:THR:HG1	2:O:182[A]:THR:HB	1.85	0.41
4:D:31:LYS:HE2	30:D:442:HOH:O	2.21	0.41
20:N:612:EDO:C1	13:Z:2:THR:HG23	2.51	0.41
6:S:92:VAL:HG23	30:S:203:HOH:O	2.21	0.41
27:X:201:DMU:O61	30:X:301:HOH:O	2.22	0.41
1:A:1:FME:CE	1:A:4:ASN:HD22	2.34	0.41
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.55	0.41
3:C:107:ALA:HB2	19:C:305:PGV:H031	2.01	0.41
30:F:213:HOH:O	20:J:104:EDO:H11	2.20	0.41
11:K:40:TRP:NE1	27:K:103:DMU:H10	2.36	0.41
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.20	0.41
3:P:86:PHE:CZ	19:P:305:PGV:H281	2.55	0.41
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.04	0.41
5:R:77:PRO:O	5:R:79:LYS:HD2	2.21	0.41
21:B:301:TGL:HC81	21:B:301:TGL:HC52	1.91	0.41
2:O:93:PRO:HG3	2:O:151:ARG:HB2	2.03	0.41
23:O:302:PSC:H201	23:O:302:PSC:H231	1.61	0.41
5:R:23:ASP:OD1	5:R:23:ASP:N	2.52	0.41
1:A:136[B]:LEU:HD11	30:A:951:HOH:O	2.20	0.40
4:D:19[A]:ARG:HE	4:D:21:ASP:CG	2.24	0.40
19:G:104:PGV:H232	3:P:99:TRP:CE2	2.56	0.40
1:N:46[B]:THR:HG21	30:O:563:HOH:O	2.21	0.40
20:A:621:EDO:H11	20:F:106:EDO:H11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:GLU:HG3	30:C:401:HOH:O	2.21	0.40
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.03	0.40
19:N:607:PGV:H142	4:Q:87:PHE:CE2	2.57	0.40
21:N:608:TGL:HC81	21:N:608:TGL:HC52	1.74	0.40
23:O:302:PSC:H62	23:O:302:PSC:H241	2.03	0.40
27:Z:101:DMU:H9	27:Z:101:DMU:H15	1.81	0.40
21:B:301:TGL:H272	21:B:301:TGL:H241	1.86	0.40
23:B:303:PSC:H282	23:B:303:PSC:H311	1.97	0.40
23:B:303:PSC:H51	30:I:225:HOH:O	2.20	0.40
1:A:24:ALA:HB2	14:A:601[C]:HEA:H253	2.04	0.40
1:A:378:HIS:O	1:A:383[B]:MET:HG3	2.21	0.40
25:C:302:PEK:H271	25:C:302:PEK:H302	1.87	0.40
6:F:64:GLU:O	6:F:65:ASP:HB2	2.21	0.40
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.20	0.40
25:P:304:PEK:H222	7:T:21:PHE:CD1	2.57	0.40
6:S:76:LYS:HE2	30:S:312:HOH:O	2.21	0.40
26:T:103:CDL:H762	26:T:103:CDL:C54	2.52	0.40
2:B:67:ILE:HD11	30:T:266:HOH:O	2.21	0.40
2:B:86:MET:HE2	2:B:86:MET:HB2	1.97	0.40
8:H:9:LYS:HG3	8:H:10:ASN:N	2.36	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%)	539 (98%)	13 (2%)	0	100	100
1	N	549/514 (107%)	535 (97%)	14 (3%)	0	100	100
2	B	237/227 (104%)	232 (98%)	4 (2%)	1 (0%)	34	17
2	O	236/227 (104%)	229 (97%)	6 (2%)	1 (0%)	34	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	264/259 (102%)	259 (98%)	5 (2%)	0	100	100
3	P	265/259 (102%)	260 (98%)	5 (2%)	0	100	100
4	D	144/144 (100%)	140 (97%)	4 (3%)	0	100	100
4	Q	143/144 (99%)	136 (95%)	5 (4%)	2 (1%)	11	2
5	E	103/105 (98%)	102 (99%)	0	1 (1%)	15	3
5	R	103/105 (98%)	102 (99%)	0	1 (1%)	15	3
6	F	94/94 (100%)	92 (98%)	1 (1%)	1 (1%)	14	3
6	S	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
7	G	81/84 (96%)	72 (89%)	4 (5%)	5 (6%)	1	0
7	T	81/84 (96%)	72 (89%)	5 (6%)	4 (5%)	2	0
8	H	77/79 (98%)	71 (92%)	2 (3%)	4 (5%)	2	0
8	U	77/79 (98%)	69 (90%)	6 (8%)	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	2
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3618/3550 (102%)	3513 (97%)	82 (2%)	23 (1%)	22	10

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
7	G	4	ALA
7	G	8	HIS
7	T	5	LYS
8	U	8	ILE
8	U	46	LYS
9	V	2	THR

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Mol	Chain	Res	Type
7	G	3	ALA
7	G	7	ASP
8	H	8	ILE
8	H	45	ALA
7	T	3	ALA
7	T	6	GLY
7	G	5	LYS
8	H	46	LYS
7	T	4	ALA
8	H	9	LYS
5	E	6	GLU
2	O	92	ASN
4	Q	5	VAL
4	Q	10	ASP
5	R	6	GLU
2	B	92	ASN

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	463/426 (109%)	457 (99%)	6 (1%)	69	54
1	N	460/426 (108%)	455 (99%)	5 (1%)	73	61
2	B	222/210 (106%)	210 (95%)	12 (5%)	22	6
2	O	221/210 (105%)	209 (95%)	12 (5%)	22	6
3	C	231/224 (103%)	227 (98%)	4 (2%)	60	43
3	P	232/224 (104%)	229 (99%)	3 (1%)	69	54
4	D	130/128 (102%)	127 (98%)	3 (2%)	50	30
4	Q	129/128 (101%)	125 (97%)	4 (3%)	40	18
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	61
5	R	92/92 (100%)	90 (98%)	2 (2%)	52	32
6	F	80/78 (103%)	77 (96%)	3 (4%)	33	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	78/78 (100%)	73 (94%)	5 (6%)	17	4
7	G	67/67 (100%)	61 (91%)	6 (9%)	9	1
7	T	67/67 (100%)	62 (92%)	5 (8%)	13	2
8	H	71/71 (100%)	67 (94%)	4 (6%)	21	6
8	U	71/71 (100%)	67 (94%)	4 (6%)	21	6
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	40
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	15
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	36
10	W	49/49 (100%)	48 (98%)	1 (2%)	55	36
11	K	39/39 (100%)	37 (95%)	2 (5%)	24	7
11	X	39/39 (100%)	37 (95%)	2 (5%)	24	7
12	L	40/39 (103%)	39 (98%)	1 (2%)	47	26
12	Y	40/39 (103%)	39 (98%)	1 (2%)	47	26
13	M	37/37 (100%)	35 (95%)	2 (5%)	22	6
13	Z	37/37 (100%)	33 (89%)	4 (11%)	6	1
All	All	3150/3034 (104%)	3054 (97%)	96 (3%)	42	20

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	333	LYS
1	A	369	ASP
1	A	486[A]	ASP
1	A	486[B]	ASP
2	B	33	LEU
2	B	59	GLN
2	B	60	GLU
2	B	68[A]	LEU
2	B	68[B]	LEU
2	B	75	LEU
2	B	78	LEU
2	B	82	ARG
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP

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Mol	Chain	Res	Type
2	B	171	LYS
3	C	40	MET
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	19[A]	ARG
4	D	19[B]	ARG
4	D	31	LYS
5	E	90	ARG
6	F	2	SER
6	F	54[A]	ASN
6	F	54[B]	ASN
7	G	7	ASP
7	G	18	PHE
7	G	33	LEU
7	G	37	LEU
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	29	CYS
8	H	51	SER
8	H	60	TYR
9	I	2	THR
10	J	50	LEU
11	K	47	ARG
11	K	54	ARG
12	L	2	HIS
13	M	38	ASP
13	M	42	LYS
1	N	109	PHE
1	N	363[A]	LEU
1	N	363[B]	LEU
1	N	369	ASP
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	68[A]	LEU
2	O	68[B]	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER

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Mol	Chain	Res	Type
2	O	110	TYR
2	O	115	ASP
2	O	171	LYS
2	O	226	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	6	VAL
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
5	R	46	LYS
5	R	79	LYS
6	S	37	LYS
6	S	48	LEU
6	S	54	ASN
6	S	87	THR
6	S	94	HIS
7	T	18	PHE
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	65	LYS
10	W	50	LEU
11	X	39	GLU
11	X	54	ARG
12	Y	47	LYS
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN

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Mol	Chain	Res	Type
2	B	59	GLN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
2	B	203	ASN
3	C	68	GLN
4	D	101	HIS
5	E	94	ASN
8	H	37	HIS
10	J	29	ASN
11	K	35	GLN
12	L	2	HIS
2	O	10	GLN
2	O	103	GLN
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
4	Q	109	HIS
5	R	78	HIS
5	R	94	ASN
6	S	54	ASN
7	T	8	HIS
8	U	37	HIS
9	V	8	GLN
10	W	29	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	0.51	0	7,9,11	1.47	2 (28%)
7	TPO	G	11	7	8,10,11	1.32	1 (12%)	10,14,16	1.04	0
2	FME	B	1	2	8,9,10	0.90	0	7,9,11	1.68	1 (14%)
9	SAC	V	1	9	7,8,9	0.55	0	8,9,11	1.23	2 (25%)
7	TPO	T	11	7	8,10,11	1.34	1 (12%)	10,14,16	1.08	2 (20%)
1	FME	A	1	1	8,9,10	0.57	0	7,9,11	1.86	3 (42%)
2	FME	O	1	2	8,9,10	0.85	0	7,9,11	1.12	0
9	SAC	I	1	9	7,8,9	0.64	0	8,9,11	1.06	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
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	V	1	9	-	2/7/8/10	-
7	TPO	T	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	2/7/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.75	1.59	1.50
7	G	11	TPO	P-O1P	2.70	1.59	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.19	104.08	112.95
1	A	1	FME	CE-SD-CG	3.12	111.10	100.40
1	N	1	FME	CE-SD-CG	2.80	110.03	100.40
7	T	11	TPO	CG2-CB-CA	2.34	117.78	113.16
9	V	1	SAC	O-C-CA	-2.28	118.81	124.78
9	V	1	SAC	C-CA-N	2.25	113.79	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.08	119.34	124.78
1	A	1	FME	O-C-CA	-2.05	119.41	124.78
1	A	1	FME	C-CA-N	2.05	113.42	109.73
7	T	11	TPO	O3P-P-OG1	2.04	115.15	105.99

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	O1-CN-N-CA
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 176 ligands modelled in this entry, 8 are monoatomic - leaving 168 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
20	EDO	S	102	-	3,3,3	0.80	0	2,2,2	0.49	0
20	EDO	B	305	-	3,3,3	0.66	0	2,2,2	0.27	0
20	EDO	O	306	-	3,3,3	0.55	0	2,2,2	0.23	0
27	DMU	X	204	-	34,34,34	0.59	1 (2%)	45,45,45	0.99	2 (4%)
20	EDO	C	315	-	3,3,3	0.60	0	2,2,2	0.19	0
19	PGV	C	305	-	50,50,50	1.26	2 (4%)	53,56,56	1.77	9 (16%)
20	EDO	B	306	-	3,3,3	0.81	0	2,2,2	0.13	0
20	EDO	E	203	-	3,3,3	0.54	0	2,2,2	0.61	0
21	TGL	N	608	-	62,62,62	1.04	3 (4%)	65,65,65	1.25	5 (7%)
24	CHD	W	101	-	29,32,32	0.78	0	48,51,51	3.66	24 (50%)
20	EDO	N	622	-	3,3,3	0.63	0	2,2,2	0.12	0
20	EDO	R	202	-	3,3,3	0.59	0	2,2,2	0.47	0
20	EDO	O	304	-	3,3,3	0.84	0	2,2,2	0.57	0
20	EDO	M	105	-	3,3,3	0.72	0	2,2,2	0.29	0
20	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.56	0
20	EDO	C	316	-	3,3,3	0.49	0	2,2,2	0.17	0
20	EDO	S	105	-	3,3,3	0.68	0	2,2,2	0.10	0
27	DMU	Z	101	-	34,34,34	0.49	0	45,45,45	1.62	9 (20%)
20	EDO	C	313	-	3,3,3	0.55	0	2,2,2	0.56	0
20	EDO	C	317	-	3,3,3	0.51	0	2,2,2	0.39	0
20	EDO	S	103	-	3,3,3	0.86	0	2,2,2	0.60	0
27	DMU	X	205	-	22,22,34	0.70	1 (4%)	27,27,45	0.67	0
21	TGL	B	301	-	62,62,62	1.10	3 (4%)	65,65,65	1.40	6 (9%)
23	PSC	B	303	-	50,50,51	1.20	3 (6%)	56,58,59	1.46	7 (12%)
14	HEA	N	601[C]	-	44,57,67	1.52	3 (6%)	37,89,103	2.76	18 (48%)
27	DMU	P	307	-	34,34,34	0.65	1 (2%)	45,45,45	1.61	11 (24%)
20	EDO	N	620	-	3,3,3	0.85	0	2,2,2	0.20	0
25	PEK	T	102	-	43,43,52	1.18	2 (4%)	46,48,57	1.56	5 (10%)
20	EDO	S	106	-	3,3,3	0.40	0	2,2,2	0.76	0
20	EDO	O	307	-	3,3,3	0.60	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	K	101	-	21,21,34	0.51	0	24,25,45	1.26	4 (16%)
20	EDO	T	105	-	3,3,3	0.75	0	2,2,2	0.83	0
20	EDO	G	105	-	3,3,3	0.75	0	2,2,2	0.57	0
20	EDO	N	611	-	3,3,3	0.79	0	2,2,2	0.52	0
25	PEK	P	304	-	52,52,52	1.07	2 (3%)	55,57,57	1.49	8 (14%)
19	PGV	A	608	-	50,50,50	0.85	3 (6%)	53,56,56	1.13	3 (5%)
14	HEA	A	601[C]	-	44,57,67	1.76	2 (4%)	37,89,103	2.86	16 (43%)
20	EDO	C	312	-	3,3,3	0.80	0	2,2,2	0.16	0
24	CHD	T	101	-	29,32,32	0.86	0	48,51,51	1.43	9 (18%)
20	EDO	U	101	-	3,3,3	0.64	0	2,2,2	0.37	0
19	PGV	G	104	-	50,50,50	1.14	2 (4%)	53,56,56	1.34	5 (9%)
27	DMU	X	201	-	34,34,34	0.62	0	45,45,45	1.38	6 (13%)
27	DMU	M	106	-	34,34,34	0.86	1 (2%)	45,45,45	1.90	13 (28%)
27	DMU	C	307	-	34,34,34	0.47	0	45,45,45	0.92	2 (4%)
20	EDO	C	310	-	3,3,3	0.34	0	2,2,2	1.17	0
20	EDO	S	104	-	3,3,3	0.61	0	2,2,2	0.12	0
20	EDO	N	626	-	3,3,3	0.49	0	2,2,2	0.31	0
27	DMU	M	101	-	34,34,34	0.59	1 (2%)	45,45,45	1.12	3 (6%)
27	DMU	X	202	-	34,34,34	0.64	1 (2%)	45,45,45	2.36	15 (33%)
20	EDO	D	205	-	3,3,3	0.54	0	2,2,2	0.13	0
20	EDO	A	612	-	3,3,3	0.42	0	2,2,2	0.45	0
25	PEK	P	302	-	47,47,52	1.18	2 (4%)	50,52,57	1.44	5 (10%)
20	EDO	N	619	-	3,3,3	0.29	0	2,2,2	0.90	0
25	PEK	P	303	-	44,44,52	0.77	1 (2%)	47,49,57	1.30	5 (10%)
20	EDO	A	618	-	3,3,3	0.81	0	2,2,2	0.74	0
18	CMO	N	606[B]	15	0,1,1	-	-	-	-	-
27	DMU	T	104	-	22,22,34	0.51	0	27,27,45	1.12	3 (11%)
26	CDL	C	306	-	90,90,99	1.52	15 (16%)	96,97,111	1.93	17 (17%)
19	PGV	N	609	-	50,50,50	0.97	3 (6%)	53,56,56	1.10	4 (7%)
25	PEK	C	303	-	52,52,52	1.12	2 (3%)	55,57,57	1.44	5 (9%)
20	EDO	F	102	-	3,3,3	0.74	0	2,2,2	0.42	0
24	CHD	J	101	-	29,32,32	0.54	0	48,51,51	1.50	11 (22%)
24	CHD	C	301	-	29,32,32	0.80	1 (3%)	48,51,51	1.37	5 (10%)
24	CHD	J	102	-	29,32,32	0.61	0	48,51,51	1.89	12 (25%)
20	EDO	A	615	-	3,3,3	0.56	0	2,2,2	0.11	0
20	EDO	E	202	-	3,3,3	0.55	0	2,2,2	0.32	0
20	EDO	M	102	-	3,3,3	0.46	0	2,2,2	0.69	0
20	EDO	A	610	-	3,3,3	0.99	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	A	611	-	3,3,3	0.73	0	2,2,2	0.56	0
23	PSC	O	302	-	45,45,51	1.23	3 (6%)	48,50,59	1.85	8 (16%)
19	PGV	N	607	-	50,50,50	1.01	2 (4%)	53,56,56	1.24	8 (15%)
24	CHD	P	308	-	29,32,32	0.74	0	48,51,51	1.95	13 (27%)
20	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.50	0
20	EDO	C	309	-	3,3,3	0.74	0	2,2,2	0.11	0
20	EDO	N	610	-	3,3,3	0.48	0	2,2,2	0.49	0
18	CMO	N	606[A]	-	0,1,1	-	-	-	-	-
20	EDO	P	313	-	3,3,3	0.43	0	2,2,2	1.14	0
20	EDO	P	310	-	3,3,3	0.90	0	2,2,2	0.23	0
18	CMO	A	606[B]	15	0,1,1	-	-	-	-	-
20	EDO	B	307	-	3,3,3	0.77	0	2,2,2	0.08	0
20	EDO	G	106	-	3,3,3	0.76	0	2,2,2	0.87	0
20	EDO	N	613	-	3,3,3	0.80	0	2,2,2	0.45	0
25	PEK	C	302	-	52,52,52	0.85	2 (3%)	55,57,57	1.18	3 (5%)
20	EDO	B	310	-	3,3,3	0.35	0	2,2,2	0.40	0
20	EDO	N	612	-	3,3,3	0.58	0	2,2,2	0.11	0
20	EDO	N	623	-	3,3,3	0.65	0	2,2,2	0.24	0
20	EDO	Q	204	-	3,3,3	0.47	0	2,2,2	0.67	0
27	DMU	O	303	-	31,31,34	0.54	0	36,38,45	2.92	16 (44%)
19	PGV	A	607	-	47,47,50	1.06	2 (4%)	50,53,56	1.08	4 (8%)
20	EDO	C	314	-	3,3,3	0.59	0	2,2,2	0.24	0
19	PGV	C	304	-	49,49,50	0.70	1 (2%)	52,55,56	0.87	2 (3%)
29	PO4	H	101	-	4,4,4	0.77	0	6,6,6	0.53	0
27	DMU	C	308	-	34,34,34	0.65	1 (2%)	45,45,45	1.78	7 (15%)
18	CMO	A	606[A]	-	0,1,1	-	-	-	-	-
20	EDO	N	615	-	3,3,3	0.62	0	2,2,2	0.49	0
20	EDO	P	314	-	3,3,3	0.89	0	2,2,2	0.31	0
21	TGL	Y	102	-	62,62,62	1.08	3 (4%)	65,65,65	1.24	6 (9%)
20	EDO	Q	203	-	3,3,3	0.69	0	2,2,2	0.14	0
20	EDO	P	315	-	3,3,3	0.50	0	2,2,2	0.39	0
20	EDO	J	103	-	3,3,3	0.64	0	2,2,2	0.15	0
24	CHD	P	301	-	29,32,32	0.87	1 (3%)	48,51,51	1.31	6 (12%)
20	EDO	A	609	-	3,3,3	0.74	0	2,2,2	0.47	0
20	EDO	N	624	-	3,3,3	0.80	0	2,2,2	0.31	0
20	EDO	T	106	-	3,3,3	0.53	0	2,2,2	0.20	0
20	EDO	E	201	-	3,3,3	0.43	0	2,2,2	0.36	0
27	DMU	K	106	-	34,34,34	1.06	2 (5%)	45,45,45	1.71	14 (31%)
19	PGV	P	305	-	50,50,50	0.65	1 (2%)	53,56,56	1.18	5 (9%)
27	DMU	X	203	-	22,22,34	0.63	0	27,27,45	1.30	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	A	621	-	3,3,3	0.72	0	2,2,2	0.40	0
20	EDO	N	616	-	3,3,3	0.34	0	2,2,2	0.11	0
29	PO4	U	102	-	4,4,4	0.70	0	6,6,6	0.56	0
24	CHD	G	103	-	29,32,32	0.83	0	48,51,51	1.42	11 (22%)
14	HEA	N	601[A]	-	44,67,67	1.01	3 (6%)	37,103,103	2.03	9 (24%)
27	DMU	L	102	-	34,34,34	0.66	0	45,45,45	2.23	21 (46%)
20	EDO	I	101	-	3,3,3	0.56	0	2,2,2	1.02	0
20	EDO	Y	103	-	3,3,3	0.60	0	2,2,2	0.26	0
27	DMU	K	102	-	22,22,34	0.49	0	27,27,45	1.40	5 (18%)
20	EDO	R	201	-	3,3,3	0.33	0	2,2,2	1.08	0
26	CDL	P	306	-	79,82,99	1.49	12 (15%)	82,87,111	1.58	11 (13%)
20	EDO	B	309	-	3,3,3	0.72	0	2,2,2	0.73	0
20	EDO	B	308	-	3,3,3	0.77	0	2,2,2	0.39	0
27	DMU	P	316	-	34,34,34	1.20	3 (8%)	45,45,45	2.29	12 (26%)
27	DMU	K	103	-	34,34,34	0.53	0	45,45,45	1.12	3 (6%)
24	CHD	Y	101	-	29,32,32	0.65	0	48,51,51	2.21	16 (33%)
27	DMU	K	104	-	34,34,34	0.66	1 (2%)	45,45,45	1.29	5 (11%)
20	EDO	D	201	-	3,3,3	0.53	0	2,2,2	0.70	0
20	EDO	A	619	-	3,3,3	0.60	0	2,2,2	0.28	0
20	EDO	M	103	-	3,3,3	0.41	0	2,2,2	0.68	0
27	DMU	P	309	-	34,34,34	0.80	1 (2%)	45,45,45	2.07	16 (35%)
20	EDO	F	106	-	3,3,3	0.63	0	2,2,2	0.16	0
20	EDO	N	621	-	3,3,3	0.65	0	2,2,2	0.28	0
20	EDO	J	104	-	3,3,3	0.41	0	2,2,2	0.31	0
21	TGL	B	304	-	62,62,62	1.05	3 (4%)	65,65,65	1.25	10 (15%)
20	EDO	A	616	-	3,3,3	0.50	0	2,2,2	0.51	0
20	EDO	D	203	-	3,3,3	0.64	0	2,2,2	0.34	0
20	EDO	A	622	-	3,3,3	0.76	0	2,2,2	0.42	0
14	HEA	A	601[A]	-	44,67,67	0.94	0	37,103,103	1.83	10 (27%)
27	DMU	K	105	-	34,34,34	0.60	0	45,45,45	1.73	10 (22%)
14	HEA	N	602	1	44,67,67	1.28	5 (11%)	37,103,103	1.61	9 (24%)
20	EDO	Q	202	-	3,3,3	0.42	0	2,2,2	0.27	0
20	EDO	L	103	-	3,3,3	0.67	0	2,2,2	0.42	0
22	CUA	O	301	2	0,1,1	-	-	-	-	-
20	EDO	P	311	-	3,3,3	0.50	0	2,2,2	0.25	0
20	EDO	A	620	-	3,3,3	0.70	0	2,2,2	0.12	0
20	EDO	D	204	-	3,3,3	0.78	0	2,2,2	0.41	0
20	EDO	C	311	-	3,3,3	0.42	0	2,2,2	0.65	0
20	EDO	F	104	-	3,3,3	0.71	0	2,2,2	0.19	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	614	-	3,3,3	0.56	0	2,2,2	0.06	0
27	DMU	G	102	-	34,34,34	0.77	0	45,45,45	2.08	14 (31%)
26	CDL	T	103	-	95,95,99	1.39	12 (12%)	101,107,111	1.61	19 (18%)
20	EDO	A	617	-	3,3,3	0.22	0	2,2,2	1.08	0
20	EDO	M	104	-	3,3,3	0.35	0	2,2,2	0.45	0
20	EDO	V	101	-	3,3,3	0.61	0	2,2,2	1.25	0
20	EDO	N	617	-	3,3,3	0.53	0	2,2,2	0.85	0
20	EDO	O	305	-	3,3,3	0.62	0	2,2,2	0.51	0
20	EDO	N	618	-	3,3,3	0.78	0	2,2,2	0.52	0
20	EDO	P	312	-	3,3,3	0.56	0	2,2,2	0.14	0
20	EDO	D	202	-	3,3,3	0.49	0	2,2,2	0.29	0
20	EDO	F	105	-	3,3,3	0.80	0	2,2,2	0.31	0
26	CDL	G	101	-	98,98,99	1.38	12 (12%)	104,110,111	1.42	10 (9%)
14	HEA	A	602	1	44,67,67	1.09	4 (9%)	37,103,103	1.87	10 (27%)
20	EDO	F	103	-	3,3,3	0.69	0	2,2,2	0.62	0
21	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.18	5 (7%)
20	EDO	N	625	-	3,3,3	0.62	0	2,2,2	0.54	0
21	TGL	L	101	-	59,59,62	1.17	3 (5%)	62,62,65	1.44	9 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	O	306	-	-	0/1/1/1	-
27	DMU	X	204	-	-	11/19/59/59	0/2/2/2
20	EDO	C	315	-	-	0/1/1/1	-
19	PGV	C	305	-	-	15/55/55/55	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
21	TGL	N	608	-	-	20/65/65/65	-
24	CHD	W	101	-	-	7/7/74/74	0/4/4/4
20	EDO	N	622	-	-	0/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	M	105	-	-	1/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
27	DMU	X	205	-	-	3/13/33/59	0/1/1/2
21	TGL	B	301	-	-	18/65/65/65	-
23	PSC	B	303	-	-	28/54/54/55	-
14	HEA	N	601[C]	-	3/3/5/16	4/24/60/76	-
27	DMU	P	307	-	-	5/19/59/59	0/2/2/2
20	EDO	N	620	-	-	1/1/1/1	-
25	PEK	T	102	-	-	25/47/47/56	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	O	307	-	-	0/1/1/1	-
27	DMU	K	101	-	-	10/13/29/59	0/1/1/2
20	EDO	T	105	-	-	0/1/1/1	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
25	PEK	P	304	-	-	23/56/56/56	-
19	PGV	A	608	-	-	10/55/55/55	-
14	HEA	A	601[C]	-	3/3/5/16	3/24/60/76	-
20	EDO	C	312	-	-	0/1/1/1	-
24	CHD	T	101	-	-	0/7/74/74	0/4/4/4
20	EDO	U	101	-	-	1/1/1/1	-
19	PGV	G	104	-	-	17/55/55/55	-
27	DMU	X	201	-	-	12/19/59/59	0/2/2/2
27	DMU	M	106	-	-	9/19/59/59	0/2/2/2
27	DMU	C	307	-	-	6/19/59/59	0/2/2/2
20	EDO	C	310	-	-	1/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	N	626	-	-	0/1/1/1	-
27	DMU	M	101	-	-	5/19/59/59	0/2/2/2
27	DMU	X	202	-	-	13/19/59/59	0/2/2/2
20	EDO	D	205	-	-	0/1/1/1	-
20	EDO	A	612	-	-	1/1/1/1	-
25	PEK	P	302	-	-	19/51/51/56	-
20	EDO	N	619	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	P	303	-	-	7/48/48/56	-
20	EDO	A	618	-	-	0/1/1/1	-
27	DMU	T	104	-	-	10/13/33/59	0/1/1/2
26	CDL	C	306	-	-	54/94/94/110	-
19	PGV	N	609	-	-	6/55/55/55	-
25	PEK	C	303	-	-	22/56/56/56	-
20	EDO	F	102	-	-	0/1/1/1	-
24	CHD	J	101	-	-	3/7/74/74	0/4/4/4
24	CHD	C	301	-	-	0/7/74/74	0/4/4/4
24	CHD	J	102	-	-	3/7/74/74	0/4/4/4
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	E	202	-	-	1/1/1/1	-
20	EDO	M	102	-	-	1/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	A	611	-	-	1/1/1/1	-
23	PSC	O	302	-	-	17/49/49/55	-
19	PGV	N	607	-	-	24/55/55/55	-
24	CHD	P	308	-	-	3/7/74/74	0/4/4/4
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	C	309	-	-	0/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	P	313	-	-	1/1/1/1	-
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	G	106	-	-	0/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
25	PEK	C	302	-	-	13/56/56/56	-
20	EDO	B	310	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
20	EDO	N	623	-	-	0/1/1/1	-
20	EDO	Q	204	-	-	1/1/1/1	-
27	DMU	O	303	-	-	12/27/47/59	0/1/1/2
19	PGV	A	607	-	-	23/52/52/55	-
20	EDO	C	314	-	-	1/1/1/1	-
19	PGV	C	304	-	-	10/54/54/55	-
27	DMU	C	308	-	-	8/19/59/59	0/2/2/2
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	Y	102	-	-	35/65/65/65	-
20	EDO	Q	203	-	-	1/1/1/1	-
20	EDO	P	315	-	-	1/1/1/1	-
20	EDO	J	103	-	-	0/1/1/1	-
14	HEA	N	601[B]	-	3/3/5/16	-	-
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
20	EDO	A	609	-	-	0/1/1/1	-
20	EDO	N	624	-	-	0/1/1/1	-
20	EDO	T	106	-	-	0/1/1/1	-
20	EDO	E	201	-	-	0/1/1/1	-
27	DMU	K	106	-	-	9/19/59/59	0/2/2/2
19	PGV	P	305	-	-	10/55/55/55	-
27	DMU	X	203	-	-	8/13/33/59	0/1/1/2
20	EDO	A	621	-	-	0/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
24	CHD	G	103	-	-	0/7/74/74	0/4/4/4
14	HEA	N	601[A]	-	3/3/7/16	1/24/76/76	-
27	DMU	L	102	-	-	14/19/59/59	0/2/2/2
20	EDO	I	101	-	-	1/1/1/1	-
14	HEA	A	601[B]	-	3/3/5/16	-	-
20	EDO	Y	103	-	-	1/1/1/1	-
27	DMU	K	102	-	-	7/13/33/59	0/1/1/2
20	EDO	R	201	-	-	0/1/1/1	-
26	CDL	P	306	-	-	30/83/85/110	-
20	EDO	B	309	-	-	1/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
27	DMU	P	316	-	-	10/19/59/59	0/2/2/2
27	DMU	K	103	-	-	10/19/59/59	0/2/2/2
24	CHD	Y	101	-	-	3/7/74/74	0/4/4/4
27	DMU	K	104	-	-	6/19/59/59	0/2/2/2
20	EDO	D	201	-	-	1/1/1/1	-
20	EDO	A	619	-	-	0/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
27	DMU	P	309	-	-	10/19/59/59	0/2/2/2
20	EDO	F	106	-	-	1/1/1/1	-
20	EDO	N	621	-	-	0/1/1/1	-
20	EDO	J	104	-	-	1/1/1/1	-
21	TGL	B	304	-	-	25/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	D	203	-	-	0/1/1/1	-
20	EDO	A	622	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	3/3/7/16	1/24/76/76	-
27	DMU	K	105	-	-	7/19/59/59	0/2/2/2
14	HEA	N	602	1	3/3/7/16	0/24/76/76	-
20	EDO	Q	202	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-
20	EDO	D	204	-	-	0/1/1/1	-
20	EDO	C	311	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
27	DMU	G	102	-	-	12/19/59/59	0/2/2/2
26	CDL	T	103	-	-	41/106/106/110	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	M	104	-	-	0/1/1/1	-
20	EDO	V	101	-	-	1/1/1/1	-
20	EDO	N	617	-	-	1/1/1/1	-
20	EDO	O	305	-	-	1/1/1/1	-
20	EDO	N	618	-	-	0/1/1/1	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	D	202	-	-	0/1/1/1	-
20	EDO	F	105	-	-	1/1/1/1	-
26	CDL	G	101	-	-	39/109/109/110	-
14	HEA	A	602	1	3/3/7/16	0/24/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
21	TGL	Q	201	-	-	23/65/65/65	-
20	EDO	N	625	-	-	1/1/1/1	-
21	TGL	L	101	-	-	33/62/62/65	-

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[C]	HEA	C18-C19	9.76	1.56	1.33
14	N	601[C]	HEA	C18-C19	7.95	1.52	1.33
19	C	305	PGV	O03-C19	5.86	1.50	1.33
25	C	303	PEK	O03-C21	5.46	1.49	1.33
26	C	306	CDL	OA8-CA7	5.41	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	302	PEK	O03-C21	5.28	1.48	1.33
26	P	306	CDL	OA8-CA7	5.23	1.48	1.33
19	G	104	PGV	O03-C19	5.13	1.48	1.33
21	L	101	TGL	OG2-CB1	5.06	1.48	1.34
25	P	304	PEK	O01-C1	5.04	1.48	1.34
26	C	306	CDL	OB8-CB7	5.03	1.48	1.33
25	T	102	PEK	O01-C1	4.99	1.48	1.34
26	C	306	CDL	OA6-CA5	4.95	1.48	1.34
23	O	302	PSC	O01-C1	4.94	1.48	1.34
21	L	101	TGL	OG3-CC1	4.91	1.47	1.33
26	G	101	CDL	OB8-CB7	4.89	1.47	1.33
26	T	103	CDL	OB8-CB7	4.86	1.47	1.33
21	Y	102	TGL	OG1-CA1	4.82	1.47	1.33
21	B	301	TGL	OG1-CA1	4.75	1.47	1.33
19	G	104	PGV	O01-C1	4.72	1.47	1.34
25	P	302	PEK	O01-C1	4.72	1.47	1.34
19	A	607	PGV	O03-C19	4.70	1.47	1.33
21	N	608	TGL	OG2-CB1	4.68	1.47	1.34
21	Y	102	TGL	OG2-CB1	4.68	1.47	1.34
26	T	103	CDL	OB6-CB5	4.66	1.47	1.34
21	B	301	TGL	OG3-CC1	4.65	1.46	1.33
23	B	303	PSC	O01-C1	4.64	1.47	1.34
26	G	101	CDL	OA6-CA5	4.64	1.47	1.34
19	N	607	PGV	O03-C19	4.64	1.46	1.33
26	G	101	CDL	OB6-CB5	4.63	1.47	1.34
25	P	304	PEK	O03-C21	4.61	1.46	1.33
19	C	305	PGV	O01-C1	4.61	1.47	1.34
25	T	102	PEK	O03-C21	4.59	1.46	1.33
26	T	103	CDL	OA6-CA5	4.58	1.47	1.34
26	P	306	CDL	OB8-CB7	4.57	1.46	1.33
21	B	301	TGL	OG2-CB1	4.51	1.47	1.34
25	C	303	PEK	O01-C1	4.51	1.47	1.34
21	N	608	TGL	OG3-CC1	4.45	1.46	1.33
26	G	101	CDL	OA8-CA7	4.41	1.46	1.33
21	Y	102	TGL	OG3-CC1	4.34	1.46	1.33
21	B	304	TGL	OG2-CB1	4.30	1.46	1.34
21	Q	201	TGL	OG2-CB1	4.30	1.46	1.34
21	Q	201	TGL	OG1-CA1	4.30	1.45	1.33
26	P	306	CDL	OA6-CA5	4.29	1.46	1.34
26	P	306	CDL	OB6-CB5	4.28	1.46	1.34
21	N	608	TGL	OG1-CA1	4.20	1.45	1.33
21	L	101	TGL	OG1-CA1	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	103	CDL	OA8-CA7	4.19	1.45	1.33
21	Q	201	TGL	OG3-CC1	4.18	1.45	1.33
19	N	607	PGV	O01-C1	4.09	1.45	1.34
19	A	607	PGV	O01-C1	4.02	1.45	1.34
26	C	306	CDL	OB6-CB5	4.01	1.45	1.34
23	B	303	PSC	C13-C12	3.99	1.54	1.31
23	O	302	PSC	C13-C12	3.97	1.54	1.31
21	B	304	TGL	OG1-CA1	3.96	1.44	1.33
21	B	304	TGL	OG3-CC1	3.95	1.44	1.33
23	O	302	PSC	O03-C19	3.73	1.44	1.33
25	C	302	PEK	O03-C21	3.73	1.44	1.33
23	B	303	PSC	O03-C19	3.68	1.44	1.33
26	C	306	CDL	C59-C58	-3.58	1.31	1.51
26	T	103	CDL	C62-C61	-3.49	1.32	1.51
26	G	101	CDL	C59-C58	-3.49	1.32	1.51
14	N	602	HEA	CAD-C3D	3.47	1.57	1.52
19	A	608	PGV	O01-C1	3.46	1.44	1.34
26	P	306	CDL	C82-C81	-3.38	1.32	1.51
26	G	101	CDL	C62-C61	-3.37	1.32	1.51
26	P	306	CDL	C79-C78	-3.35	1.32	1.51
27	K	106	DMU	O16-C6	3.35	1.45	1.40
26	T	103	CDL	C79-C78	-3.33	1.32	1.51
26	P	306	CDL	C59-C58	-3.31	1.33	1.51
26	T	103	CDL	C59-C58	-3.30	1.33	1.51
14	N	602	HEA	C3B-C11	-3.29	1.50	1.52
26	T	103	CDL	C82-C81	-3.28	1.33	1.51
25	P	303	PEK	O03-C21	3.24	1.42	1.33
26	P	306	CDL	C19-C18	-3.21	1.33	1.51
26	C	306	CDL	C62-C61	-3.18	1.33	1.51
26	C	306	CDL	C82-C81	-3.16	1.33	1.51
26	C	306	CDL	C79-C78	-3.10	1.34	1.51
26	G	101	CDL	C82-C81	-3.08	1.34	1.51
26	G	101	CDL	C79-C78	-3.08	1.34	1.51
27	P	316	DMU	O16-C6	3.07	1.45	1.40
26	P	306	CDL	C22-C21	-3.07	1.34	1.51
19	N	609	PGV	O01-C1	3.06	1.42	1.34
19	N	609	PGV	O03-C19	3.05	1.42	1.33
26	T	103	CDL	C42-C41	-3.05	1.34	1.51
26	T	103	CDL	C39-C38	-3.02	1.34	1.51
26	C	306	CDL	C19-C18	-3.01	1.34	1.51
26	C	306	CDL	C22-C21	-3.01	1.34	1.51
14	N	601[C]	HEA	C3B-C11	-3.00	1.50	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601[A]	HEA	C3B-C11	-2.99	1.50	1.52
26	P	306	CDL	C39-C38	-2.97	1.34	1.51
26	G	101	CDL	C19-C18	-2.97	1.34	1.51
25	C	302	PEK	O01-C1	2.97	1.42	1.34
26	C	306	CDL	C39-C38	-2.93	1.35	1.51
26	G	101	CDL	C22-C21	-2.91	1.35	1.51
26	G	101	CDL	C42-C41	-2.91	1.35	1.51
26	P	306	CDL	C42-C41	-2.90	1.35	1.51
26	C	306	CDL	C42-C41	-2.87	1.35	1.51
26	T	103	CDL	C22-C21	-2.80	1.35	1.51
26	T	103	CDL	C19-C18	-2.76	1.36	1.51
26	G	101	CDL	C39-C38	-2.76	1.36	1.51
19	N	609	PGV	O01-C02	-2.75	1.39	1.46
26	C	306	CDL	CA3-CA4	2.57	1.57	1.51
27	X	205	DMU	O16-C6	2.57	1.44	1.40
27	C	308	DMU	O16-C6	2.48	1.44	1.40
14	A	602	HEA	CAD-C3D	2.48	1.55	1.52
19	C	304	PGV	O01-C1	2.48	1.41	1.34
27	P	309	DMU	O16-C6	2.47	1.44	1.40
26	C	306	CDL	PB2-OB3	2.46	1.58	1.50
14	A	602	HEA	CMC-C2C	2.44	1.56	1.51
14	A	601[C]	HEA	C3B-C11	-2.44	1.51	1.52
27	P	316	DMU	C2-C1	2.30	1.58	1.52
14	A	602	HEA	C3C-C2C	-2.30	1.37	1.40
27	P	307	DMU	O16-C6	2.28	1.44	1.40
14	N	602	HEA	C3C-C2C	-2.27	1.37	1.40
14	N	601[A]	HEA	O11-C11	2.26	1.48	1.42
14	A	602	HEA	C14-C15	2.25	1.38	1.33
27	M	101	DMU	O16-C6	2.24	1.44	1.40
26	C	306	CDL	PB2-OB2	2.21	1.63	1.54
24	P	301	CHD	C11-C9	2.21	1.57	1.53
14	N	602	HEA	CMC-C2C	2.20	1.56	1.51
26	P	306	CDL	OA6-CA4	-2.19	1.43	1.47
14	N	601[A]	HEA	C3C-C2C	-2.17	1.37	1.40
14	N	601[C]	HEA	C3C-C2C	-2.17	1.37	1.40
19	A	608	PGV	O03-C19	2.17	1.39	1.33
27	K	106	DMU	O1-C10	2.16	1.47	1.41
19	P	305	PGV	O03-C19	2.12	1.39	1.33
27	X	204	DMU	O16-C6	2.12	1.43	1.40
24	C	301	CHD	O12-C12	2.10	1.47	1.43
14	N	602	HEA	C1C-NC	2.09	1.40	1.36
27	M	106	DMU	O16-C6	2.04	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	316	DMU	C6-C1	2.03	1.58	1.52
27	K	104	DMU	O16-C6	2.02	1.43	1.40
19	A	608	PGV	O01-C02	-2.01	1.41	1.46
27	X	202	DMU	O16-C6	2.01	1.43	1.40

All (558) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[C]	HEA	C13-C12-C11	-9.28	100.41	114.35
24	W	101	CHD	C14-C8-C9	-8.95	97.43	109.71
24	W	101	CHD	C10-C9-C8	8.73	121.20	111.82
26	C	306	CDL	OA8-CA6-CA4	8.43	132.98	108.43
24	W	101	CHD	C11-C12-C13	7.47	118.92	111.24
14	N	601[C]	HEA	C13-C12-C11	-7.41	103.21	114.35
23	O	302	PSC	O01-C1-C2	7.25	127.12	111.50
14	A	601[C]	HEA	C17-C18-C19	7.22	145.05	127.66
24	W	101	CHD	C13-C17-C20	7.10	127.97	119.50
27	G	102	DMU	C7-C8-C9	-6.91	97.91	110.24
27	P	309	DMU	C7-C8-C9	-6.91	97.92	110.24
21	B	301	TGL	OG2-CB1-CB2	6.80	126.15	111.50
27	P	316	DMU	C8-C7-C5	-6.71	99.12	110.82
24	W	101	CHD	C14-C8-C7	6.66	120.64	111.81
19	C	305	PGV	O03-C19-C20	6.39	131.95	111.91
26	G	101	CDL	OA6-CA5-C11	6.29	125.05	111.50
27	X	202	DMU	O1-C9-C8	6.25	121.05	109.69
26	T	103	CDL	OA6-CA5-C11	6.16	124.77	111.50
26	C	306	CDL	CA4-OA6-CA5	-6.10	102.77	117.79
27	O	303	DMU	O1-C9-C8	6.04	120.66	109.69
25	T	102	PEK	O01-C1-C2	5.98	124.39	111.50
24	W	101	CHD	C13-C14-C8	-5.92	107.18	114.74
24	W	101	CHD	C9-C8-C7	5.74	118.75	111.88
19	C	305	PGV	O01-C1-C2	5.67	123.73	111.50
27	P	316	DMU	O1-C9-C8	5.52	119.72	109.69
26	T	103	CDL	OB6-CB5-C51	5.50	123.36	111.50
24	Y	101	CHD	C1-C10-C5	5.47	115.86	107.77
23	B	303	PSC	O01-C1-C2	5.40	123.15	111.50
25	P	302	PEK	O01-C1-C2	5.39	123.11	111.50
27	X	202	DMU	O2-C8-C9	-5.37	95.96	109.30
27	X	202	DMU	O7-C10-C5	5.36	121.99	108.10
24	Y	101	CHD	C14-C8-C7	5.33	118.88	111.81
27	L	102	DMU	O4-C7-C5	-5.22	98.28	110.35
24	W	101	CHD	C6-C5-C4	-5.22	105.18	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	608	TGL	OG2-CB1-CB2	5.22	122.75	111.50
27	O	303	DMU	C10-O1-C9	5.18	123.85	113.69
24	W	101	CHD	C17-C13-C12	5.17	122.39	117.67
26	C	306	CDL	OA5-CA3-CA4	5.16	125.48	111.78
25	C	303	PEK	O03-C21-C22	5.11	127.95	111.91
27	C	308	DMU	C8-C7-C5	-5.11	101.90	110.82
14	A	602	HEA	C1B-C2B-C3B	-5.07	103.47	107.00
26	C	306	CDL	CA6-CA4-CA3	5.05	123.63	111.80
27	O	303	DMU	O4-C7-C5	-5.03	98.71	110.35
27	O	303	DMU	O16-C6-O5	-5.03	102.08	112.51
14	A	601[C]	HEA	C27-C19-C18	-5.03	110.78	123.68
26	P	306	CDL	OB6-CB5-C51	5.01	122.30	111.50
24	W	101	CHD	C1-C2-C3	5.01	116.89	110.47
27	K	106	DMU	O16-C6-C1	5.00	116.12	108.30
27	G	102	DMU	C8-C7-C5	-4.96	102.16	110.82
27	O	303	DMU	O5-C4-C3	4.96	116.43	106.21
27	O	303	DMU	O2-C8-C9	-4.96	96.99	109.30
26	P	306	CDL	OB8-CB7-C71	4.95	127.45	111.91
19	G	104	PGV	O03-C19-C20	4.93	127.39	111.91
14	N	601[C]	HEA	C27-C19-C18	-4.85	111.22	123.68
27	C	308	DMU	O1-C9-C8	4.82	118.44	109.69
14	N	601[A]	HEA	C13-C12-C11	-4.81	107.12	114.35
26	C	306	CDL	OB8-CB7-C71	4.81	127.01	111.91
19	C	305	PGV	C01-O03-C19	4.79	134.86	117.12
24	P	308	CHD	C15-C14-C13	4.77	108.23	103.55
24	J	102	CHD	C11-C9-C10	-4.75	108.82	113.73
25	P	304	PEK	O03-C21-C22	4.74	126.79	111.91
27	O	303	DMU	C6-O5-C4	4.67	123.34	115.09
23	B	303	PSC	C03-C02-C01	-4.66	100.75	111.79
25	P	304	PEK	C2-C3-C4	-4.66	104.92	113.23
27	L	102	DMU	C10-O1-C9	4.65	122.82	113.69
24	Y	101	CHD	C21-C20-C17	4.64	120.03	112.92
25	T	102	PEK	C03-C02-C01	-4.64	100.81	111.79
24	W	101	CHD	C1-C10-C9	-4.63	104.07	111.35
25	P	302	PEK	O03-C21-C22	4.63	126.44	111.91
27	X	202	DMU	O55-C2-C1	-4.63	99.65	110.35
27	X	202	DMU	O1-C10-C5	-4.61	100.59	110.35
14	N	601[A]	HEA	CMB-C2B-C3B	4.61	133.71	124.69
14	N	601[C]	HEA	CMB-C2B-C3B	4.61	133.71	124.69
24	J	102	CHD	C19-C10-C9	-4.59	104.86	111.18
27	L	102	DMU	O2-C8-C9	-4.57	97.94	109.30
24	Y	101	CHD	C6-C5-C4	-4.57	105.93	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	308	DMU	O2-C8-C9	-4.48	98.18	109.30
14	N	601[A]	HEA	C1B-C2B-C3B	-4.45	103.90	107.00
14	N	601[C]	HEA	C1B-C2B-C3B	-4.45	103.90	107.00
27	K	105	DMU	C10-O1-C9	-4.45	104.95	113.69
27	K	105	DMU	O7-C10-C5	4.45	119.62	108.10
27	L	102	DMU	O7-C3-C2	4.40	118.98	107.28
27	G	102	DMU	C10-O1-C9	4.37	122.26	113.69
23	O	302	PSC	C02-O01-C1	4.34	128.47	117.79
24	W	101	CHD	C9-C10-C5	4.33	114.67	108.58
21	L	101	TGL	OG2-CB1-CB2	4.33	120.83	111.50
25	C	303	PEK	O01-C1-C2	4.32	120.81	111.50
26	C	306	CDL	OA6-CA5-C11	4.26	120.68	111.50
24	W	101	CHD	C14-C13-C12	4.26	111.37	107.40
21	B	304	TGL	CG3-OG3-CC1	4.25	132.86	117.12
27	M	106	DMU	O7-C3-C2	4.22	118.52	107.28
27	P	316	DMU	O7-C10-C5	4.22	119.03	108.10
27	O	303	DMU	C10-C5-C7	4.21	118.76	110.00
21	Y	102	TGL	OG2-CB1-CB2	4.20	120.55	111.50
27	O	303	DMU	O7-C10-C5	4.18	118.94	108.10
21	Q	201	TGL	OG2-CB1-CB2	4.18	120.51	111.50
21	B	301	TGL	OG1-CA1-CA2	4.14	124.91	111.91
14	A	601[C]	HEA	C20-C19-C18	4.14	129.50	121.12
24	W	101	CHD	C18-C13-C14	-4.13	104.74	111.21
27	P	316	DMU	O5-C6-C1	4.13	119.09	110.35
24	W	101	CHD	C11-C9-C8	-4.11	104.86	110.88
26	P	306	CDL	OA8-CA7-C31	4.07	124.69	111.91
24	Y	101	CHD	C19-C10-C1	-4.06	101.72	108.26
27	K	105	DMU	C1-C2-C3	4.05	118.93	109.68
27	L	102	DMU	O1-C9-C8	4.04	117.03	109.69
14	N	601[A]	HEA	C3C-C4C-NC	4.04	114.43	109.21
14	N	601[C]	HEA	C3C-C4C-NC	4.04	114.43	109.21
14	N	601[C]	HEA	C12-C11-C3B	4.03	123.15	112.56
27	O	303	DMU	C7-C8-C9	4.03	117.43	110.24
24	C	301	CHD	C18-C13-C12	4.03	113.17	109.07
27	M	106	DMU	C6-O5-C4	4.00	121.54	113.69
27	O	303	DMU	C8-C7-C5	3.98	117.78	110.82
24	P	308	CHD	C22-C23-C24	-3.98	105.03	113.59
14	N	601[C]	HEA	C21-C20-C19	-3.97	99.91	112.98
27	G	102	DMU	O1-C9-C11	3.97	116.31	106.44
19	G	104	PGV	O01-C1-C2	3.96	120.04	111.50
14	N	601[A]	HEA	CMB-C2B-C1B	-3.95	122.39	128.46
14	N	601[C]	HEA	CMB-C2B-C1B	-3.95	122.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	304	PEK	O03-C21-O04	-3.95	113.63	123.59
26	G	101	CDL	OB6-CB5-C51	3.90	119.90	111.50
21	Q	201	TGL	CG2-OG2-CB1	-3.87	108.26	117.79
14	A	602	HEA	CAD-CBD-CGD	-3.85	106.20	112.67
27	Z	101	DMU	C8-C7-C5	-3.83	104.13	110.82
24	J	102	CHD	C6-C5-C4	-3.82	106.79	111.19
21	B	304	TGL	OG2-CB1-CB2	3.81	119.70	111.50
14	A	601[A]	HEA	CAA-CBA-CGA	-3.80	106.30	112.67
14	A	601[C]	HEA	CAA-CBA-CGA	-3.80	106.30	112.67
14	N	601[C]	HEA	C17-C18-C19	3.78	136.77	127.66
14	A	601[A]	HEA	C1B-C2B-C3B	-3.78	104.37	107.00
14	A	601[C]	HEA	C1B-C2B-C3B	-3.78	104.37	107.00
27	P	316	DMU	O55-C2-C1	3.76	119.05	110.35
27	P	309	DMU	O4-C7-C5	-3.76	101.67	110.35
27	M	106	DMU	O16-C6-C1	3.75	114.16	108.30
23	O	302	PSC	C03-C02-C01	-3.75	102.92	111.79
14	A	601[A]	HEA	CMB-C2B-C3B	3.75	132.03	124.69
14	A	601[C]	HEA	CMB-C2B-C3B	3.75	132.03	124.69
27	P	316	DMU	O3-C5-C7	3.74	119.01	110.35
19	N	607	PGV	O03-C01-C02	3.74	119.32	108.43
25	P	302	PEK	C01-O03-C21	3.70	130.84	117.12
27	O	303	DMU	O6-C11-C9	-3.70	98.59	111.29
26	C	306	CDL	OB6-CB5-C51	3.70	119.48	111.50
27	X	201	DMU	C7-C8-C9	-3.70	103.64	110.24
14	A	601[C]	HEA	C12-C11-C3B	3.69	122.25	112.56
27	Z	101	DMU	O7-C10-C5	3.69	117.65	108.10
19	C	305	PGV	O03-C19-O04	-3.69	114.29	123.59
26	P	306	CDL	OA8-CA6-CA4	3.69	119.00	108.38
21	Q	201	TGL	OG1-CA1-CA2	3.68	123.46	111.91
24	W	101	CHD	C22-C20-C17	3.68	117.88	110.28
14	A	602	HEA	C27-C19-C20	3.67	121.45	115.27
27	Z	101	DMU	C10-O1-C9	-3.64	106.54	113.69
26	C	306	CDL	OA8-CA7-C31	3.62	123.26	111.91
24	T	101	CHD	C11-C9-C10	-3.61	110.01	113.73
25	C	302	PEK	O03-C21-C22	3.61	123.23	111.91
26	C	306	CDL	OA6-CA4-CA3	3.60	121.28	108.36
25	T	102	PEK	O03-C01-C02	3.60	118.91	108.43
25	C	303	PEK	C01-O03-C21	3.60	130.45	117.12
19	P	305	PGV	O01-C1-O02	-3.60	115.01	123.70
27	P	309	DMU	O1-C10-C5	3.60	117.96	110.35
27	K	102	DMU	C2-C3-C4	3.59	116.64	110.24
27	P	309	DMU	C6-O5-C4	3.59	120.73	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	106	DMU	C7-C8-C9	-3.59	103.84	110.24
27	C	308	DMU	O7-C10-C5	3.58	117.38	108.10
27	P	316	DMU	O4-C7-C5	3.57	118.61	110.35
27	X	202	DMU	C7-C8-C9	3.57	116.60	110.24
24	J	102	CHD	C14-C8-C9	3.56	114.59	109.71
24	W	101	CHD	C15-C14-C8	3.56	123.31	118.33
27	L	102	DMU	O6-C11-C9	-3.55	99.11	111.29
21	L	101	TGL	OG1-CA1-CA2	3.54	123.01	111.91
21	L	101	TGL	OG3-CC1-OC1	-3.53	114.68	123.59
19	N	609	PGV	O03-C19-O04	-3.53	114.69	123.59
26	T	103	CDL	OA6-CA5-OA7	-3.51	115.22	123.70
27	P	309	DMU	O3-C5-C10	3.48	118.49	110.05
14	N	602	HEA	CBD-CAD-C3D	3.47	118.89	112.49
27	K	104	DMU	C6-C1-C2	3.46	117.19	110.00
27	K	104	DMU	C10-O1-C9	3.46	120.47	113.69
14	N	601[A]	HEA	CAA-CBA-CGA	-3.45	106.88	112.67
14	N	601[C]	HEA	CAA-CBA-CGA	-3.45	106.88	112.67
24	P	308	CHD	C14-C8-C9	-3.44	105.00	109.71
24	Y	101	CHD	C4-C3-C2	-3.43	106.45	110.55
27	K	105	DMU	C8-C7-C5	3.42	116.80	110.82
21	L	101	TGL	CG3-CG2-CG1	-3.42	103.70	111.79
27	M	106	DMU	C6-C1-C2	-3.41	102.89	110.00
19	A	608	PGV	O03-C19-C20	3.41	122.61	111.91
24	C	301	CHD	C22-C20-C17	-3.40	103.27	110.28
26	P	306	CDL	CB4-OB6-CB5	-3.38	109.47	117.79
27	P	307	DMU	C10-C5-C7	3.38	117.03	110.00
27	Z	101	DMU	O1-C10-C5	-3.37	103.22	110.35
27	M	106	DMU	O5-C4-C3	3.36	116.84	109.75
27	P	307	DMU	O16-C6-C1	3.34	113.51	108.30
27	K	104	DMU	C1-C2-C3	3.33	117.29	109.68
21	L	101	TGL	CC3-CC2-CC1	3.33	125.72	113.62
27	L	102	DMU	O61-C57-C4	3.33	122.70	111.29
27	X	202	DMU	C10-O1-C9	3.32	120.21	113.69
24	T	101	CHD	C4-C5-C10	-3.32	109.13	112.66
26	P	306	CDL	OB8-CB7-OB9	-3.32	115.22	123.59
23	B	303	PSC	O01-C1-O02	-3.31	115.70	123.70
27	X	202	DMU	O1-C9-C11	3.31	114.66	106.44
26	T	103	CDL	CB2-C1-CA2	-3.30	103.06	112.79
26	G	101	CDL	OA6-CA5-OA7	-3.30	115.72	123.70
14	N	602	HEA	CAD-CBD-CGD	-3.30	107.13	112.67
27	M	106	DMU	O5-C4-C57	3.30	114.64	106.44
24	Y	101	CHD	C4-C5-C10	3.29	116.15	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601[C]	HEA	C27-C19-C20	3.28	120.80	115.27
27	X	202	DMU	O7-C3-C2	3.28	116.00	107.28
14	A	602	HEA	C3C-C4C-NC	3.27	113.44	109.21
27	P	316	DMU	O1-C9-C11	3.24	114.50	106.44
25	C	303	PEK	O03-C21-O04	-3.24	115.41	123.59
23	O	302	PSC	O01-C1-O02	-3.23	115.89	123.70
25	P	304	PEK	C01-O03-C21	3.23	129.08	117.12
26	G	101	CDL	CA4-OA6-CA5	-3.22	109.86	117.79
27	G	102	DMU	O7-C10-C5	3.22	116.44	108.10
21	Q	201	TGL	OG1-CA1-OA1	-3.21	115.49	123.59
27	L	102	DMU	O1-C9-C11	3.20	114.39	106.44
24	P	308	CHD	C19-C10-C9	-3.19	106.78	111.18
27	X	203	DMU	O16-C6-C1	-3.18	103.34	108.30
27	K	106	DMU	O5-C4-C3	3.17	116.44	109.75
14	A	601[A]	HEA	CMB-C2B-C1B	-3.17	123.59	128.46
14	A	601[C]	HEA	CMB-C2B-C1B	-3.17	123.59	128.46
24	J	101	CHD	C14-C8-C9	-3.14	105.41	109.71
27	P	307	DMU	C7-C8-C9	3.13	115.82	110.24
27	G	102	DMU	O5-C4-C3	3.12	116.34	109.75
24	P	301	CHD	O12-C12-C13	-3.12	105.75	111.03
14	A	601[A]	HEA	C26-C15-C16	3.08	120.45	115.27
21	B	304	TGL	OG3-CG3-CG2	-3.08	99.48	108.43
27	M	106	DMU	O49-C1-C6	3.07	117.51	110.05
25	P	303	PEK	O03-C21-C22	3.06	121.52	111.91
26	P	306	CDL	CA4-OA6-CA5	-3.06	113.94	117.88
27	M	106	DMU	O7-C3-C4	-3.05	101.09	109.45
25	T	102	PEK	O01-C1-O02	-3.04	116.34	123.70
19	P	305	PGV	C30-C29-C28	-3.04	98.98	114.42
27	K	105	DMU	C6-C1-C2	3.03	116.31	110.00
21	N	608	TGL	OG1-CA1-CA2	3.03	121.40	111.91
27	G	102	DMU	O6-C11-C9	-3.03	100.91	111.29
27	K	102	DMU	O5-C4-C3	3.02	115.18	109.69
24	J	102	CHD	C10-C9-C8	-3.02	108.58	111.82
27	M	106	DMU	C10-O1-C9	3.01	119.59	113.69
26	T	103	CDL	OB8-CB6-CB4	3.00	117.17	108.43
14	N	601[C]	HEA	C20-C19-C18	3.00	127.18	121.12
27	X	201	DMU	C10-O1-C9	3.00	119.57	113.69
19	A	608	PGV	O03-C19-O04	-2.99	116.04	123.59
24	J	102	CHD	C1-C10-C5	2.99	112.19	107.77
27	K	104	DMU	O7-C3-C2	2.98	115.22	107.28
24	W	101	CHD	C17-C13-C14	-2.98	97.09	100.09
27	K	106	DMU	C1-C2-C3	2.97	116.45	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	101	CHD	C6-C5-C4	-2.96	107.78	111.19
26	G	101	CDL	CB6-OB8-CB7	2.96	128.08	117.12
24	Y	101	CHD	C10-C9-C8	2.95	114.98	111.82
27	K	106	DMU	C10-O1-C9	2.94	119.47	113.69
26	T	103	CDL	CB6-CB4-CB3	-2.94	104.83	111.79
23	O	302	PSC	O01-C02-C03	2.94	119.04	108.40
19	N	609	PGV	O01-C1-O02	-2.93	116.61	123.70
24	P	308	CHD	C11-C12-C13	-2.93	108.24	111.24
14	N	602	HEA	C1B-C2B-C3B	-2.93	104.96	107.00
27	P	316	DMU	O6-C11-C9	-2.93	101.25	111.29
19	C	305	PGV	C03-C02-C01	2.92	118.70	111.79
24	P	301	CHD	C22-C20-C17	-2.92	104.26	110.28
26	T	103	CDL	OB8-CB7-C71	2.91	121.05	111.91
25	P	302	PEK	O03-C21-O04	-2.91	116.24	123.59
27	P	307	DMU	C6-C1-C2	2.90	116.04	110.00
25	P	303	PEK	C3-C2-C1	-2.90	103.07	113.62
24	W	101	CHD	C11-C9-C10	2.90	116.71	113.73
19	N	609	PGV	O03-C19-C20	2.88	120.96	111.91
27	M	106	DMU	O1-C10-C5	2.87	116.43	110.35
26	C	306	CDL	OB8-CB7-OB9	-2.87	116.35	123.59
27	P	316	DMU	C6-C1-C2	2.87	115.96	110.00
14	A	602	HEA	CMC-C2C-C3C	2.86	130.04	124.68
25	P	303	PEK	O01-C1-O02	-2.86	116.80	123.70
21	Y	102	TGL	OG1-CA1-CA2	2.85	120.86	111.91
14	N	601[C]	HEA	C26-C15-C16	2.85	120.07	115.27
27	C	308	DMU	O6-C11-C9	-2.85	101.51	111.29
24	J	102	CHD	C4-C3-C2	-2.85	107.15	110.55
27	M	101	DMU	O16-C6-C1	2.84	112.74	108.30
14	A	601[A]	HEA	C27-C19-C20	2.84	120.04	115.27
26	T	103	CDL	C19-C18-C17	2.83	128.81	114.42
27	T	104	DMU	C2-C3-C4	2.83	115.29	110.24
19	C	305	PGV	O01-C1-O02	-2.82	116.88	123.70
27	P	309	DMU	C1-C2-C3	-2.82	103.24	109.68
21	B	304	TGL	CG2-OG2-CB1	-2.82	110.86	117.79
19	G	104	PGV	C01-O03-C19	2.81	127.54	117.12
27	T	104	DMU	C6-C1-C2	2.81	115.85	110.00
27	P	309	DMU	C11-C9-C8	2.81	119.59	113.00
27	K	106	DMU	O1-C10-C5	2.81	116.29	110.35
26	C	306	CDL	CB4-OB6-CB5	-2.81	110.88	117.79
27	K	105	DMU	C10-C5-C7	2.81	115.84	110.00
26	C	306	CDL	C42-C41-C40	2.80	128.66	114.42
27	X	201	DMU	C6-O5-C4	-2.80	108.19	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	302	PEK	O01-C1-O02	-2.80	116.93	123.70
14	A	601[A]	HEA	C13-C12-C11	-2.80	110.15	114.35
23	O	302	PSC	C23-C22-C21	-2.79	100.26	114.42
24	Y	101	CHD	C14-C13-C12	2.78	109.99	107.40
24	Y	101	CHD	C15-C14-C8	2.77	122.21	118.33
14	N	602	HEA	C27-C19-C20	2.77	119.93	115.27
26	C	306	CDL	OB5-PB2-OB3	2.77	114.23	106.47
27	P	309	DMU	O7-C3-C2	2.76	114.64	107.28
25	T	102	PEK	O03-C21-C22	2.76	120.56	111.91
21	Y	102	TGL	OG3-CC1-CC2	2.76	120.56	111.91
24	P	301	CHD	C11-C9-C10	-2.75	110.89	113.73
27	L	102	DMU	C10-C5-C7	2.75	115.72	110.00
24	J	101	CHD	C16-C17-C13	2.74	106.25	103.55
27	O	303	DMU	O1-C10-C5	2.74	116.16	110.35
27	K	101	DMU	O16-C6-C1	2.74	112.58	108.30
27	P	309	DMU	C18-O16-C6	2.74	118.39	113.84
21	Y	102	TGL	CG3-CG2-CG1	-2.74	105.31	111.79
21	L	101	TGL	OG1-CA1-OA1	-2.74	116.68	123.59
24	J	101	CHD	C19-C10-C9	-2.73	107.42	111.18
19	N	607	PGV	O03-C19-C20	2.73	120.48	111.91
27	P	307	DMU	C1-C2-C3	2.73	115.91	109.68
24	P	301	CHD	C19-C10-C1	-2.73	103.87	108.26
24	P	308	CHD	C17-C13-C12	-2.73	115.18	117.67
27	P	307	DMU	C8-C7-C5	2.72	115.57	110.82
26	G	101	CDL	C61-C60-C59	-2.72	100.62	114.42
24	J	102	CHD	C1-C2-C3	2.72	113.95	110.47
21	B	304	TGL	OG1-CA1-CA2	2.71	120.42	111.91
24	C	301	CHD	C6-C5-C10	-2.71	109.78	112.66
26	G	101	CDL	OA8-CA7-C31	2.71	120.40	111.91
26	G	101	CDL	OA8-CA7-OA9	-2.70	116.77	123.59
14	N	601[C]	HEA	C13-C14-C15	-2.70	121.16	127.66
25	C	302	PEK	C24-C23-C22	-2.70	103.50	113.19
27	P	307	DMU	O1-C10-C5	2.68	116.03	110.35
24	C	301	CHD	C5-C6-C7	2.67	117.41	114.46
24	G	103	CHD	C19-C10-C5	-2.67	105.83	110.36
14	A	601[C]	HEA	C13-C14-C15	-2.67	121.23	127.66
27	C	308	DMU	O16-C6-C1	2.67	112.47	108.30
26	P	306	CDL	OA8-CA7-OA9	-2.66	116.87	123.59
19	N	607	PGV	C6-C5-C4	-2.66	100.91	114.42
23	O	302	PSC	C26-C25-C24	-2.66	100.92	114.42
19	N	607	PGV	C4-C3-C2	-2.66	103.64	113.19
24	P	308	CHD	C18-C13-C12	-2.65	106.37	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	202	DMU	C8-C7-C5	-2.64	106.21	110.82
27	Z	101	DMU	C10-O7-C3	-2.64	111.42	117.96
19	C	305	PGV	O04-C19-C20	-2.64	113.43	123.73
27	K	105	DMU	O7-C10-O1	-2.64	103.30	110.67
24	G	103	CHD	C6-C5-C4	-2.64	108.15	111.19
24	Y	101	CHD	C13-C17-C20	2.62	122.62	119.50
24	G	103	CHD	C11-C9-C10	-2.62	111.03	113.73
24	P	308	CHD	C5-C6-C7	2.62	117.35	114.46
14	A	601[A]	HEA	C20-C19-C18	-2.62	115.82	121.12
24	J	101	CHD	C10-C9-C8	2.61	114.63	111.82
27	X	202	DMU	C10-C5-C7	2.60	115.42	110.00
14	A	601[C]	HEA	C26-C15-C16	2.60	119.64	115.27
27	M	101	DMU	C18-O16-C6	-2.59	109.54	113.84
19	A	607	PGV	C03-C02-C01	2.59	117.92	111.79
24	P	301	CHD	C22-C23-C24	-2.59	108.02	113.59
19	A	607	PGV	O03-C19-C20	2.59	120.03	111.91
25	P	303	PEK	C28-C27-C26	-2.58	101.31	114.42
27	X	203	DMU	O5-C6-C1	2.58	115.82	110.35
14	A	602	HEA	C20-C19-C18	-2.58	115.89	121.12
27	L	102	DMU	O5-C4-C57	2.58	112.85	106.44
27	X	202	DMU	O7-C10-O1	2.57	117.84	110.67
14	A	601[C]	HEA	C27-C19-C20	2.56	119.58	115.27
27	Z	101	DMU	O1-C9-C8	2.56	114.35	109.69
27	P	309	DMU	C10-C5-C7	2.56	115.34	110.00
26	T	103	CDL	C20-C19-C18	2.56	127.40	114.42
19	C	305	PGV	O06-C06-C05	2.55	122.44	110.20
21	N	608	TGL	CG3-CG2-CG1	-2.55	105.75	111.79
27	K	102	DMU	C18-O16-C6	-2.55	109.61	113.84
24	Y	101	CHD	O7-C7-C8	2.55	115.12	109.43
27	L	102	DMU	O7-C10-C5	2.55	114.70	108.10
21	B	304	TGL	CC3-CC2-CC1	-2.54	104.37	113.62
24	T	101	CHD	O12-C12-C11	2.54	114.30	109.12
24	W	101	CHD	C2-C1-C10	2.54	117.13	112.78
14	A	602	HEA	CBA-CAA-C2A	-2.54	107.81	112.48
24	Y	101	CHD	C2-C1-C10	2.53	117.12	112.78
27	P	309	DMU	O7-C3-C4	2.53	116.38	109.45
26	T	103	CDL	OB6-CB4-CB3	2.53	117.56	108.40
14	N	602	HEA	C3C-C4C-NC	2.52	112.47	109.21
19	G	104	PGV	O04-C19-C20	-2.52	113.88	123.73
26	C	306	CDL	OB4-PB2-OB3	2.51	120.53	110.68
25	P	304	PEK	O01-C1-C2	2.51	116.91	111.50
19	C	304	PGV	C21-C20-C19	-2.50	104.54	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	103	CDL	CB4-OB6-CB5	-2.49	111.65	117.79
19	A	607	PGV	O12-P-O13	2.49	118.81	109.07
21	B	301	TGL	OG1-CA1-OA1	-2.49	117.30	123.59
27	G	102	DMU	O3-C5-C10	2.49	116.10	110.05
27	X	204	DMU	O1-C9-C11	2.49	112.63	106.44
26	T	103	CDL	OB6-CB5-OB7	-2.49	117.70	123.70
24	J	101	CHD	C4-C5-C10	2.48	115.30	112.66
27	K	106	DMU	O1-C9-C11	2.48	112.61	106.44
26	P	306	CDL	OA6-CA5-C11	2.48	116.85	111.50
27	L	102	DMU	O55-C2-C1	-2.48	104.62	110.35
27	K	106	DMU	O49-C1-C6	2.47	116.06	110.05
21	B	301	TGL	CB3-CB2-CB1	-2.47	104.63	113.62
14	N	602	HEA	C26-C15-C16	2.46	119.42	115.27
24	P	308	CHD	C16-C17-C13	2.46	105.97	103.55
27	G	102	DMU	C1-C2-C3	2.46	115.30	109.68
24	P	308	CHD	C21-C20-C17	2.46	116.69	112.92
27	P	307	DMU	O1-C9-C11	2.46	112.55	106.44
14	N	602	HEA	C20-C19-C18	-2.45	116.15	121.12
27	C	308	DMU	O5-C4-C57	2.45	112.53	106.44
19	N	607	PGV	O01-C1-C2	2.45	116.78	111.50
27	O	303	DMU	O3-C5-C10	2.45	115.99	110.05
23	O	302	PSC	C3-C2-C1	2.44	122.50	113.62
27	K	105	DMU	C10-O7-C3	2.44	124.01	117.96
21	B	301	TGL	OB1-CB1-CB2	-2.44	114.21	123.73
27	L	102	DMU	C18-O16-C6	-2.44	109.79	113.84
27	X	201	DMU	O1-C10-C5	2.44	115.52	110.35
27	L	102	DMU	C6-O5-C4	2.44	118.48	113.69
27	P	316	DMU	O4-C7-C8	2.44	115.99	110.35
26	C	306	CDL	OA8-CA7-OA9	-2.43	117.45	123.59
26	C	306	CDL	C24-C23-C22	-2.41	102.21	114.42
21	N	608	TGL	OG3-CC1-CC2	2.41	119.46	111.91
27	K	103	DMU	C10-O1-C9	2.39	118.37	113.69
27	M	106	DMU	C57-C4-C3	-2.39	106.38	113.33
27	X	203	DMU	O49-C1-C6	2.39	115.84	110.05
21	B	301	TGL	OG3-CC1-CC2	2.38	119.39	111.91
19	P	305	PGV	C03-C02-C01	-2.37	106.18	111.79
27	T	104	DMU	C3-C2-C1	2.37	114.96	110.82
24	Y	101	CHD	C16-C17-C13	-2.37	101.23	103.55
27	G	102	DMU	C11-C9-C8	-2.37	107.46	113.00
27	O	303	DMU	O5-C4-C57	-2.37	104.47	110.45
24	T	101	CHD	C6-C5-C4	-2.36	108.47	111.19
27	O	303	DMU	O1-C9-C11	2.36	112.31	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	T	101	CHD	C19-C10-C1	-2.36	104.47	108.26
27	L	102	DMU	O3-C5-C10	2.36	115.77	110.05
24	C	301	CHD	C22-C23-C24	-2.35	108.54	113.59
27	P	307	DMU	C6-O5-C4	-2.35	109.08	113.69
27	G	102	DMU	C10-O7-C3	2.34	123.75	117.96
27	K	101	DMU	O5-C4-C3	2.34	113.77	110.04
19	P	305	PGV	C22-C21-C20	-2.33	104.81	113.19
27	Z	101	DMU	O1-C9-C11	2.33	112.23	106.44
14	A	602	HEA	C21-C20-C19	2.33	120.64	112.98
24	J	102	CHD	C11-C9-C8	2.33	114.29	110.88
24	T	101	CHD	C5-C6-C7	2.33	117.03	114.46
25	C	303	PEK	C24-C23-C22	2.33	121.55	113.19
24	G	103	CHD	O12-C12-C13	-2.32	107.10	111.03
27	P	309	DMU	O1-C9-C11	2.32	112.21	106.44
27	G	102	DMU	O7-C3-C4	2.32	115.81	109.45
25	P	303	PEK	O03-C21-O04	-2.32	117.74	123.59
24	W	101	CHD	C1-C10-C5	2.31	111.19	107.77
27	P	316	DMU	O7-C10-O1	2.31	117.13	110.67
24	G	103	CHD	C19-C10-C1	-2.31	104.54	108.26
27	K	103	DMU	O55-C2-C3	2.31	116.06	109.94
26	T	103	CDL	C23-C22-C21	2.30	126.12	114.42
21	B	304	TGL	OG1-CA1-OA1	-2.30	117.78	123.59
24	Y	101	CHD	C21-C20-C22	-2.30	106.75	110.36
27	P	307	DMU	C10-O1-C9	2.30	118.20	113.69
24	G	103	CHD	C13-C14-C8	-2.30	111.80	114.74
24	G	103	CHD	C13-C17-C20	-2.30	116.75	119.50
27	K	102	DMU	O16-C6-C1	2.29	111.88	108.30
27	P	309	DMU	C10-O7-C3	-2.29	112.29	117.96
27	X	203	DMU	C2-C3-C4	2.29	114.33	110.24
24	P	308	CHD	C11-C9-C8	2.29	114.23	110.88
26	T	103	CDL	PB2-OB2-CB2	-2.28	108.32	121.68
27	M	106	DMU	O1-C9-C8	2.27	113.83	109.69
24	P	308	CHD	C6-C7-C8	2.27	113.90	111.48
14	N	602	HEA	C16-C15-C14	-2.27	116.53	121.12
24	J	101	CHD	C18-C13-C12	-2.27	106.76	109.07
27	X	204	DMU	C1-C2-C3	2.27	114.85	109.68
25	C	302	PEK	C03-C02-C01	-2.25	106.46	111.79
27	G	102	DMU	O5-C6-C1	-2.25	105.59	110.35
27	P	307	DMU	C2-C3-C4	-2.25	105.77	110.93
24	T	101	CHD	C17-C13-C12	2.25	119.72	117.67
24	J	101	CHD	C4-C3-C2	-2.25	107.87	110.55
27	K	105	DMU	O1-C9-C11	2.24	112.01	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	DMU	O1-C9-C8	2.24	113.76	109.69
14	A	602	HEA	CMC-C2C-C1C	-2.24	125.03	128.46
21	L	101	TGL	OG2-CB1-OB1	-2.24	118.30	123.70
27	L	102	DMU	C57-C4-C3	-2.23	106.83	113.33
25	P	304	PEK	C3-C2-C1	2.23	121.73	113.62
24	J	102	CHD	C16-C17-C20	2.23	115.60	112.15
19	C	305	PGV	C21-C20-C19	-2.23	105.51	113.62
26	C	306	CDL	OB2-PB2-OB5	-2.23	100.81	106.73
14	A	601[C]	HEA	C21-C22-C23	-2.22	120.16	127.75
27	X	202	DMU	O55-C2-C3	2.22	115.82	109.94
24	J	102	CHD	C9-C8-C7	-2.21	109.23	111.88
14	A	602	HEA	C13-C14-C15	-2.21	122.34	127.66
24	P	308	CHD	C17-C13-C14	2.21	102.32	100.09
21	Y	102	TGL	C26-C25-C24	-2.21	103.21	114.42
27	K	106	DMU	C2-C3-C4	2.21	115.99	110.93
21	B	304	TGL	C36-C35-C34	2.20	130.16	113.42
19	A	607	PGV	C4-C3-C2	-2.20	105.27	113.19
19	N	607	PGV	O03-C19-O04	-2.19	118.06	123.59
26	P	306	CDL	C59-C58-C57	2.18	125.51	114.42
14	A	601[C]	HEA	C26-C15-C14	-2.18	118.08	123.68
27	P	309	DMU	O55-C2-C3	2.18	115.72	109.94
27	L	102	DMU	O1-C10-C5	2.18	114.96	110.35
14	N	601[A]	HEA	CMD-C2D-C3D	2.17	129.04	124.94
14	N	601[C]	HEA	CMD-C2D-C3D	2.17	129.04	124.94
27	L	102	DMU	C6-C1-C2	-2.17	105.47	110.00
19	N	607	PGV	O14-P-O13	2.17	122.97	112.24
14	N	602	HEA	C21-C20-C19	2.17	120.11	112.98
27	K	106	DMU	O3-C5-C10	2.17	115.31	110.05
24	W	101	CHD	C6-C7-C8	-2.17	109.17	111.48
24	J	102	CHD	C22-C20-C17	2.16	114.76	110.28
21	Y	102	TGL	CG1-OG1-CA1	2.16	125.13	117.12
24	J	101	CHD	C17-C13-C14	2.16	102.27	100.09
24	J	101	CHD	C14-C13-C12	2.16	109.41	107.40
27	K	102	DMU	C6-C1-C2	-2.16	105.50	110.00
14	N	601[C]	HEA	C21-C22-C23	-2.16	120.38	127.75
26	T	103	CDL	OA8-CA7-C31	2.15	118.67	111.91
24	T	101	CHD	O12-C12-C13	-2.15	107.40	111.03
26	T	103	CDL	C60-C59-C58	2.15	125.33	114.42
24	W	101	CHD	O7-C7-C8	2.15	114.22	109.43
25	P	304	PEK	O11-P-O14	-2.15	100.68	109.07
14	A	601[C]	HEA	C21-C20-C19	-2.14	105.92	112.98
19	P	305	PGV	O01-C1-C2	2.14	116.11	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	304	PEK	C24-C23-C22	2.14	120.88	113.19
27	L	102	DMU	O16-C6-C1	-2.14	104.97	108.30
27	C	307	DMU	O5-C4-C3	2.14	114.25	109.75
27	X	201	DMU	C11-C9-C8	2.13	117.99	113.00
26	T	103	CDL	C40-C39-C38	2.13	125.23	114.42
27	K	106	DMU	C11-C9-C8	2.12	117.97	113.00
24	G	103	CHD	C4-C3-C2	-2.12	108.02	110.55
24	T	101	CHD	C1-C10-C5	2.12	110.90	107.77
27	K	106	DMU	C18-O16-C6	2.12	117.36	113.84
24	Y	101	CHD	C11-C9-C10	-2.12	111.54	113.73
26	G	101	CDL	C62-C61-C60	2.11	125.15	114.42
14	N	601[C]	HEA	C26-C15-C14	-2.11	118.26	123.68
26	T	103	CDL	C83-C82-C81	2.11	125.14	114.42
24	G	103	CHD	O3-C3-C4	-2.10	105.66	109.85
24	W	101	CHD	C22-C23-C24	-2.10	109.07	113.59
27	X	202	DMU	O3-C5-C10	2.10	115.14	110.05
14	N	601[A]	HEA	OMA-CMA-C3A	-2.10	120.34	124.91
14	N	601[C]	HEA	OMA-CMA-C3A	-2.10	120.34	124.91
27	K	105	DMU	C7-C8-C9	2.09	113.97	110.24
19	G	104	PGV	O03-C19-O04	-2.09	118.31	123.59
26	T	103	CDL	CA4-OA6-CA5	-2.09	112.64	117.79
21	L	101	TGL	OG1-CG1-CG2	2.09	114.51	108.43
27	K	106	DMU	O7-C10-C5	2.09	113.50	108.10
27	C	307	DMU	C57-C4-C3	-2.08	107.26	113.33
27	K	106	DMU	O5-C6-C1	-2.08	105.95	110.35
27	L	102	DMU	O55-C2-C3	2.08	115.45	109.94
24	J	101	CHD	C15-C14-C13	2.08	105.59	103.55
19	A	608	PGV	O01-C1-O02	-2.08	118.69	123.70
21	B	304	TGL	CG3-CG2-CG1	-2.07	106.88	111.79
24	P	301	CHD	C6-C7-C8	-2.07	109.27	111.48
21	B	304	TGL	OG2-CB1-OB1	-2.07	118.71	123.70
23	B	303	PSC	C23-C22-C21	-2.06	103.94	114.42
21	N	608	TGL	OG1-CA1-OA1	-2.06	118.39	123.59
26	P	306	CDL	C43-C42-C41	2.05	124.85	114.42
14	N	601[A]	HEA	C27-C19-C20	2.05	118.72	115.27
14	A	601[A]	HEA	C13-C14-C15	-2.05	122.73	127.66
27	K	101	DMU	C18-O16-C6	-2.05	110.45	113.84
24	G	103	CHD	C1-C10-C9	2.04	114.57	111.35
19	C	304	PGV	C22-C21-C20	-2.04	105.84	113.19
23	B	303	PSC	C26-C25-C24	-2.04	104.06	114.42
27	X	202	DMU	O3-C5-C7	2.04	115.07	110.35
27	L	102	DMU	C1-C2-C3	-2.04	105.02	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	201	TGL	OG3-CC1-CC2	2.04	118.31	111.91
27	M	106	DMU	C18-O16-C6	-2.04	110.46	113.84
26	G	101	CDL	C19-C18-C17	2.03	124.75	114.42
19	N	607	PGV	C3-C2-C1	-2.03	106.22	113.62
24	G	103	CHD	C17-C13-C12	2.03	119.52	117.67
27	M	101	DMU	C22-C19-C18	-2.03	104.48	113.49
14	A	601[A]	HEA	OMA-CMA-C3A	-2.03	120.49	124.91
14	A	601[C]	HEA	OMA-CMA-C3A	-2.03	120.49	124.91
27	P	309	DMU	C57-C4-C3	2.03	119.23	113.33
27	X	201	DMU	O3-C5-C10	2.03	114.97	110.05
27	Z	101	DMU	C34-C31-C28	-2.03	104.14	114.42
27	G	102	DMU	C10-C5-C7	2.02	114.21	110.00
23	B	303	PSC	O03-C01-C02	-2.02	102.55	108.43
27	K	104	DMU	C8-C7-C5	-2.02	107.30	110.82
21	L	101	TGL	OG3-CC1-CC2	2.01	118.22	111.91
23	B	303	PSC	C04-C05-N	-2.01	109.06	115.78
27	Z	101	DMU	O61-C57-C4	-2.01	104.40	111.29
27	P	309	DMU	O7-C10-C5	2.01	113.30	108.10
27	K	101	DMU	O61-C57-C4	-2.01	106.46	111.78
19	N	609	PGV	O01-C1-C2	2.01	115.82	111.50

All (24) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
14	N	601[C]	HEA	ND
14	N	601[C]	HEA	NA
14	N	601[C]	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB

All (846) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[C]	HEA	C17-C18-C19-C20
14	A	601[C]	HEA	C17-C18-C19-C27
19	A	607	PGV	C03-O11-P-O12
19	A	607	PGV	C03-O11-P-O13
19	A	607	PGV	C03-O11-P-O14
19	A	607	PGV	O02-C1-O01-C02
19	A	607	PGV	C2-C1-O01-C02
19	A	607	PGV	O04-C19-O03-C01
19	A	607	PGV	C20-C19-O03-C01
19	C	305	PGV	C04-O12-P-O13
19	G	104	PGV	C04-O12-P-O13
19	G	104	PGV	C2-C1-O01-C02
19	N	607	PGV	O12-C04-C05-C06
19	N	607	PGV	O04-C19-O03-C01
19	N	607	PGV	C20-C19-O03-C01
21	L	101	TGL	OB1-CB1-OG2-CG2
21	Y	102	TGL	CB2-CB1-OG2-CG2
23	B	303	PSC	C03-O11-P-O12
23	B	303	PSC	C03-O11-P-O13
23	B	303	PSC	C03-O11-P-O14
23	B	303	PSC	C04-O12-P-O13
23	B	303	PSC	O12-C04-C05-N
23	B	303	PSC	O02-C1-O01-C02
23	B	303	PSC	C2-C1-O01-C02
23	O	302	PSC	C04-O12-P-O13
23	O	302	PSC	C2-C1-O01-C02
24	P	308	CHD	C20-C22-C23-C24
24	W	101	CHD	C13-C17-C20-C21
24	W	101	CHD	C13-C17-C20-C22
24	W	101	CHD	C16-C17-C20-C21
24	W	101	CHD	C16-C17-C20-C22
25	C	303	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
25	C	303	PEK	C04-O12-P-O13
25	C	303	PEK	C04-O12-P-O14
25	C	303	PEK	C13-C14-C15-C16
25	P	302	PEK	O02-C1-O01-C02
25	P	302	PEK	O04-C21-O03-C01
25	P	302	PEK	C22-C21-O03-C01
25	P	304	PEK	C04-O12-P-O13
25	P	304	PEK	C2-C1-O01-C02
25	T	102	PEK	C03-O11-P-O13
25	T	102	PEK	C03-O11-P-O14
25	T	102	PEK	O04-C21-O03-C01
25	T	102	PEK	C22-C21-O03-C01
25	T	102	PEK	C11-C10-C9-C8
26	C	306	CDL	OA7-CA5-OA6-CA4
26	C	306	CDL	C11-CA5-OA6-CA4
26	C	306	CDL	OA9-CA7-OA8-CA6
26	C	306	CDL	C31-CA7-OA8-CA6
26	G	101	CDL	CA2-OA2-PA1-OA4
26	G	101	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	C31-CA7-OA8-CA6
26	G	101	CDL	CB2-OB2-PB2-OB5
26	G	101	CDL	CB3-OB5-PB2-OB4
26	P	306	CDL	OA9-CA7-OA8-CA6
26	P	306	CDL	C31-CA7-OA8-CA6
26	T	103	CDL	CA3-OA5-PA1-OA2
26	T	103	CDL	OA5-CA3-CA4-OA6
26	T	103	CDL	OA9-CA7-OA8-CA6
26	T	103	CDL	C31-CA7-OA8-CA6
26	T	103	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	OB6-CB4-CB6-OB8
27	G	102	DMU	O5-C6-O16-C18
27	K	101	DMU	C3-C4-C57-O61
27	K	101	DMU	O5-C4-C57-O61
27	K	101	DMU	C1-C6-O16-C18
27	K	101	DMU	O5-C6-O16-C18
27	K	102	DMU	C19-C18-O16-C6
27	K	103	DMU	C1-C6-O16-C18
27	K	103	DMU	O5-C6-O16-C18
27	K	104	DMU	C2-C3-O7-C10
27	K	106	DMU	C1-C6-O16-C18
27	K	106	DMU	O5-C6-O16-C18
27	O	303	DMU	C3-C4-O5-C6

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Mol	Chain	Res	Type	Atoms
27	O	303	DMU	C57-C4-O5-C6
27	P	316	DMU	C1-C6-O16-C18
27	T	104	DMU	C1-C6-O16-C18
27	T	104	DMU	O5-C6-O16-C18
27	X	201	DMU	C1-C6-O16-C18
27	X	201	DMU	O5-C6-O16-C18
27	X	202	DMU	C19-C18-O16-C6
27	X	204	DMU	O5-C6-O16-C18
27	K	105	DMU	O1-C10-O7-C3
27	K	105	DMU	C5-C10-O7-C3
25	C	303	PEK	O04-C21-O03-C01
27	L	102	DMU	C2-C3-O7-C10
27	T	104	DMU	C3-C4-C57-O61
27	M	106	DMU	C2-C3-O7-C10
27	X	202	DMU	O1-C10-O7-C3
27	X	204	DMU	O1-C10-O7-C3
19	C	305	PGV	C20-C19-O03-C01
25	C	303	PEK	C22-C21-O03-C01
25	P	304	PEK	C22-C21-O03-C01
27	X	201	DMU	O6-C11-C9-C8
19	C	305	PGV	O04-C19-O03-C01
19	G	104	PGV	O04-C19-O03-C01
25	P	304	PEK	O04-C21-O03-C01
19	G	104	PGV	O02-C1-O01-C02
21	Y	102	TGL	OB1-CB1-OG2-CG2
25	T	102	PEK	O02-C1-O01-C02
19	G	104	PGV	C20-C19-O03-C01
21	L	101	TGL	CB2-CB1-OG2-CG2
27	G	102	DMU	C4-C3-O7-C10
27	L	102	DMU	O6-C11-C9-O1
27	T	104	DMU	O5-C4-C57-O61
19	A	607	PGV	C10-C11-C12-C13
23	B	303	PSC	C11-C10-C9-C8
23	O	302	PSC	C11-C12-C13-C14
25	C	302	PEK	C7-C8-C9-C10
25	C	302	PEK	C13-C14-C15-C16
25	P	304	PEK	C4-C5-C6-C7
25	T	102	PEK	C4-C5-C6-C7
23	O	302	PSC	O02-C1-O01-C02
25	P	304	PEK	O02-C1-O01-C02
27	X	204	DMU	O6-C11-C9-C8
27	M	106	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
25	P	302	PEK	C2-C1-O01-C02
25	T	102	PEK	C2-C1-O01-C02
27	G	102	DMU	O6-C11-C9-O1
27	L	102	DMU	O5-C4-C57-O61
27	X	203	DMU	O5-C4-C57-O61
27	O	303	DMU	O6-C11-C9-C8
21	L	101	TGL	CC3-CC4-CC5-CC6
26	P	306	CDL	C17-C18-C19-C20
27	X	201	DMU	O6-C11-C9-O1
27	X	204	DMU	O5-C4-C57-O61
27	L	102	DMU	C3-C4-C57-O61
26	C	306	CDL	C20-C21-C22-C23
26	P	306	CDL	C80-C81-C82-C83
27	K	105	DMU	O6-C11-C9-O1
27	P	316	DMU	O6-C11-C9-O1
27	X	204	DMU	O6-C11-C9-O1
21	L	101	TGL	CC1-CC2-CC3-CC4
27	O	303	DMU	C5-C10-O7-C3
24	W	101	CHD	C21-C20-C22-C23
14	A	601[A]	HEA	C19-C20-C21-C22
14	A	601[C]	HEA	C19-C20-C21-C22
27	K	106	DMU	O6-C11-C9-O1
24	P	308	CHD	C17-C20-C22-C23
24	W	101	CHD	C17-C20-C22-C23
26	G	101	CDL	C51-CB5-OB6-CB4
27	M	106	DMU	O1-C10-O7-C3
26	T	103	CDL	C71-C72-C73-C74
26	T	103	CDL	CA2-C1-CB2-OB2
26	C	306	CDL	OB7-CB5-OB6-CB4
26	G	101	CDL	OB7-CB5-OB6-CB4
27	L	102	DMU	O6-C11-C9-C8
26	C	306	CDL	C63-C64-C65-C66
26	G	101	CDL	C55-C56-C57-C58
26	C	306	CDL	OB5-CB3-CB4-OB6
27	Z	101	DMU	C19-C22-C25-C28
27	M	106	DMU	O6-C11-C9-C8
27	X	204	DMU	C3-C4-C57-O61
19	N	607	PGV	O12-C04-C05-O05
27	P	309	DMU	O6-C11-C9-O1
26	C	306	CDL	C51-CB5-OB6-CB4
19	A	607	PGV	C19-C20-C21-C22
27	X	202	DMU	O6-C11-C9-O1

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Mol	Chain	Res	Type	Atoms
24	J	102	CHD	C21-C20-C22-C23
24	P	308	CHD	C21-C20-C22-C23
19	N	607	PGV	C1-C2-C3-C4
21	B	301	TGL	CB1-CB2-CB3-CB4
23	O	302	PSC	C11-C10-C9-C8
25	P	303	PEK	C7-C8-C9-C10
25	P	304	PEK	C13-C14-C15-C16
19	N	607	PGV	C19-C20-C21-C22
21	N	608	TGL	CB1-CB2-CB3-CB4
27	X	204	DMU	O16-C18-C19-C22
27	K	104	DMU	O5-C4-C57-O61
27	P	307	DMU	O6-C11-C9-O1
23	O	302	PSC	C20-C21-C22-C23
27	P	316	DMU	C2-C3-O7-C10
21	Y	102	TGL	CC1-CC2-CC3-CC4
27	X	201	DMU	O1-C10-O7-C3
27	G	102	DMU	O16-C18-C19-C22
27	P	316	DMU	O5-C6-O16-C18
14	N	601[A]	HEA	C19-C20-C21-C22
14	N	601[C]	HEA	C19-C20-C21-C22
27	K	101	DMU	O16-C18-C19-C22
19	C	305	PGV	O12-C04-C05-O05
26	T	103	CDL	O1-C1-CB2-OB2
27	C	308	DMU	O16-C18-C19-C22
27	P	309	DMU	O16-C18-C19-C22
27	T	104	DMU	O16-C18-C19-C22
27	Z	101	DMU	O16-C18-C19-C22
19	C	304	PGV	C10-C11-C12-C13
25	P	302	PEK	C4-C5-C6-C7
25	P	302	PEK	C10-C11-C12-C13
26	P	306	CDL	C51-CB5-OB6-CB4
19	C	305	PGV	C04-O12-P-O11
19	G	104	PGV	C04-O12-P-O11
19	N	607	PGV	C04-O12-P-O11
23	B	303	PSC	C04-O12-P-O11
25	C	303	PEK	C03-O11-P-O12
25	C	303	PEK	C04-O12-P-O11
25	P	304	PEK	C04-O12-P-O11
25	T	102	PEK	C03-O11-P-O12
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CB3-OB5-PB2-OB2
27	L	102	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
19	C	305	PGV	O12-C04-C05-C06
26	P	306	CDL	OB7-CB5-OB6-CB4
21	Y	102	TGL	CA2-CA1-OG1-CG1
27	X	201	DMU	C4-C3-O7-C10
27	P	309	DMU	O6-C11-C9-C8
27	Z	101	DMU	O6-C11-C9-C8
21	L	101	TGL	C11-C10-CB9-CB8
21	N	608	TGL	CB3-CB4-CB5-CB6
21	N	608	TGL	C10-C11-C12-C13
26	C	306	CDL	C40-C41-C42-C43
27	T	104	DMU	C28-C31-C34-C37
24	J	101	CHD	C17-C20-C22-C23
19	A	608	PGV	C21-C22-C23-C24
21	B	304	TGL	CC4-CC5-CC6-CC7
21	B	304	TGL	CA9-C20-C21-C22
21	Y	102	TGL	C24-C25-C26-C27
27	P	309	DMU	C22-C25-C28-C31
27	X	201	DMU	C19-C22-C25-C28
23	B	303	PSC	C20-C19-O03-C01
21	L	101	TGL	CA3-CA4-CA5-CA6
21	Q	201	TGL	CC5-CC6-CC7-CC8
21	Y	102	TGL	CC3-CC4-CC5-CC6
26	C	306	CDL	C12-C13-C14-C15
26	C	306	CDL	C43-C44-C45-C46
26	C	306	CDL	C81-C82-C83-C84
26	P	306	CDL	C20-C21-C22-C23
27	M	101	DMU	C19-C22-C25-C28
27	T	104	DMU	C31-C34-C37-C40
19	A	607	PGV	C03-C02-O01-C1
19	N	607	PGV	O02-C1-O01-C02
21	Y	102	TGL	CB2-CB3-CB4-CB5
26	C	306	CDL	C36-C37-C38-C39
26	P	306	CDL	C11-C12-C13-C14
26	T	103	CDL	C60-C61-C62-C63
21	Y	102	TGL	OA1-CA1-OG1-CG1
19	N	607	PGV	C10-C11-C12-C13
25	P	304	PEK	C10-C11-C12-C13
21	Q	201	TGL	C21-C22-C23-C24
27	G	102	DMU	C1-C6-O16-C18
27	X	202	DMU	C1-C6-O16-C18
21	B	304	TGL	C19-C33-C34-C35
21	N	608	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	C17-C18-C19-C20
26	T	103	CDL	C77-C78-C79-C80
27	P	309	DMU	C2-C3-O7-C10
27	X	201	DMU	C25-C28-C31-C34
27	X	203	DMU	C19-C22-C25-C28
19	A	608	PGV	C29-C30-C31-C32
21	Y	102	TGL	CC4-CC5-CC6-CC7
21	Y	102	TGL	CC5-CC6-CC7-CC8
26	P	306	CDL	C77-C78-C79-C80
21	B	304	TGL	CA6-CA7-CA8-CA9
21	Y	102	TGL	CB7-CB8-CB9-C10
27	C	308	DMU	C31-C34-C37-C40
21	L	101	TGL	C22-C23-C24-C25
21	Q	201	TGL	C16-C17-C18-C19
14	N	601[C]	HEA	C17-C18-C19-C20
23	O	302	PSC	C1-C2-C3-C4
19	G	104	PGV	C26-C27-C28-C29
21	L	101	TGL	CA9-C20-C21-C22
21	Y	102	TGL	C15-C16-C17-C18
21	Y	102	TGL	C21-C22-C23-C24
26	C	306	CDL	C62-C63-C64-C65
26	P	306	CDL	C40-C41-C42-C43
27	K	101	DMU	C28-C31-C34-C37
27	K	105	DMU	O16-C18-C19-C22
27	L	102	DMU	C19-C22-C25-C28
27	P	307	DMU	O16-C18-C19-C22
27	P	316	DMU	C22-C25-C28-C31
27	X	201	DMU	C2-C3-O7-C10
27	X	202	DMU	O5-C6-O16-C18
21	B	301	TGL	C20-C21-C22-C23
27	L	102	DMU	C25-C28-C31-C34
21	B	301	TGL	C21-C22-C23-C24
21	B	304	TGL	CA3-CA4-CA5-CA6
21	B	304	TGL	CC7-CC8-CC9-C15
21	L	101	TGL	C23-C24-C25-C26
21	B	304	TGL	C11-C10-CB9-CB8
24	J	101	CHD	C21-C20-C22-C23
27	C	308	DMU	C5-C10-O7-C3
27	G	102	DMU	C19-C18-O16-C6
27	K	105	DMU	C19-C18-O16-C6
27	K	106	DMU	C19-C18-O16-C6
19	C	304	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	C11-C12-C13-C14
21	Q	201	TGL	C18-C19-C33-C34
25	T	102	PEK	C23-C24-C25-C26
21	Y	102	TGL	CA3-CA4-CA5-CA6
21	Y	102	TGL	CB9-C10-C11-C12
26	G	101	CDL	OA7-CA5-OA6-CA4
19	C	304	PGV	C7-C8-C9-C10
21	Q	201	TGL	CC2-CC1-OG3-CG3
19	N	607	PGV	C2-C1-O01-C02
21	B	301	TGL	CB2-CB1-OG2-CG2
26	G	101	CDL	C11-CA5-OA6-CA4
21	Y	102	TGL	C13-C14-C29-C30
27	P	309	DMU	C4-C3-O7-C10
26	C	306	CDL	C15-C16-C17-C18
26	C	306	CDL	C52-C53-C54-C55
26	T	103	CDL	C17-C18-C19-C20
27	P	316	DMU	C4-C3-O7-C10
27	P	307	DMU	C18-C19-C22-C25
19	G	104	PGV	C3-C4-C5-C6
19	A	607	PGV	C1-C2-C3-C4
27	K	102	DMU	O5-C4-C57-O61
21	Q	201	TGL	C20-C21-C22-C23
26	G	101	CDL	C51-C52-C53-C54
26	G	101	CDL	C60-C61-C62-C63
27	K	101	DMU	C31-C34-C37-C40
27	K	103	DMU	C28-C31-C34-C37
21	B	301	TGL	OB1-CB1-OG2-CG2
21	N	608	TGL	OB1-CB1-OG2-CG2
27	L	102	DMU	C18-C19-C22-C25
26	T	103	CDL	C34-C35-C36-C37
26	T	103	CDL	C37-C38-C39-C40
27	K	103	DMU	C31-C34-C37-C40
27	C	308	DMU	C18-C19-C22-C25
27	M	106	DMU	C18-C19-C22-C25
21	Q	201	TGL	CC4-CC5-CC6-CC7
20	A	620	EDO	O1-C1-C2-O2
20	B	309	EDO	O1-C1-C2-O2
20	E	202	EDO	O1-C1-C2-O2
20	I	101	EDO	O1-C1-C2-O2
20	M	105	EDO	O1-C1-C2-O2
20	N	612	EDO	O1-C1-C2-O2
20	N	620	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	P	313	EDO	O1-C1-C2-O2
20	Y	103	EDO	O1-C1-C2-O2
27	C	308	DMU	O6-C11-C9-O1
21	L	101	TGL	CC2-CC3-CC4-CC5
21	Q	201	TGL	C11-C10-CB9-CB8
19	P	305	PGV	C14-C15-C16-C17
21	Q	201	TGL	CA9-C20-C21-C22
26	C	306	CDL	CA5-C11-C12-C13
27	P	316	DMU	C25-C28-C31-C34
27	O	303	DMU	O1-C10-O7-C3
25	P	302	PEK	C7-C8-C9-C10
23	B	303	PSC	O04-C19-O03-C01
25	P	302	PEK	C15-C16-C17-C18
26	T	103	CDL	OA7-CA5-OA6-CA4
26	T	103	CDL	OB7-CB5-OB6-CB4
23	O	302	PSC	C20-C19-O03-C01
23	B	303	PSC	C4-C5-C6-C7
26	C	306	CDL	C58-C59-C60-C61
25	P	304	PEK	C29-C30-C31-C32
27	M	101	DMU	O6-C11-C9-C8
21	L	101	TGL	C11-C12-C13-C14
26	G	101	CDL	C52-C53-C54-C55
26	P	306	CDL	C38-C39-C40-C41
27	X	202	DMU	C4-C3-O7-C10
26	C	306	CDL	C38-C39-C40-C41
27	X	205	DMU	C25-C28-C31-C34
27	O	303	DMU	C18-C19-C22-C25
19	C	305	PGV	C2-C1-O01-C02
21	B	304	TGL	CB2-CB1-OG2-CG2
21	N	608	TGL	CB2-CB1-OG2-CG2
21	Q	201	TGL	CB2-CB1-OG2-CG2
26	T	103	CDL	C11-CA5-OA6-CA4
26	T	103	CDL	C51-CB5-OB6-CB4
27	M	106	DMU	C19-C22-C25-C28
27	X	202	DMU	C5-C10-O7-C3
19	A	608	PGV	C22-C23-C24-C25
19	C	305	PGV	O02-C1-O01-C02
21	Q	201	TGL	OB1-CB1-OG2-CG2
21	B	304	TGL	CB5-CB6-CB7-CB8
21	L	101	TGL	CB3-CB4-CB5-CB6
27	T	104	DMU	C25-C28-C31-C34
27	X	203	DMU	C1-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
21	Y	102	TGL	OG2-CG2-CG3-OG3
26	G	101	CDL	OB6-CB4-CB6-OB8
27	C	307	DMU	O6-C11-C9-O1
26	T	103	CDL	C35-C36-C37-C38
27	X	203	DMU	C3-C4-C57-O61
21	N	608	TGL	CA9-C20-C21-C22
14	N	601[C]	HEA	C26-C15-C16-C17
27	P	309	DMU	C18-C19-C22-C25
27	X	202	DMU	C2-C3-O7-C10
27	X	201	DMU	C3-C4-C57-O61
21	B	304	TGL	OB1-CB1-OG2-CG2
23	B	303	PSC	C20-C21-C22-C23
26	C	306	CDL	C19-C20-C21-C22
26	T	103	CDL	C36-C37-C38-C39
27	G	102	DMU	O1-C10-O7-C3
27	G	102	DMU	C18-C19-C22-C25
19	N	607	PGV	C13-C14-C15-C16
26	C	306	CDL	C55-C56-C57-C58
19	G	104	PGV	C2-C3-C4-C5
21	B	304	TGL	CC6-CC7-CC8-CC9
26	P	306	CDL	C13-C14-C15-C16
21	Q	201	TGL	OC1-CC1-OG3-CG3
27	Z	101	DMU	C18-C19-C22-C25
19	N	607	PGV	C01-C02-C03-O11
26	C	306	CDL	OB5-CB3-CB4-CB6
26	T	103	CDL	OA5-CA3-CA4-CA6
26	P	306	CDL	C55-C56-C57-C58
26	T	103	CDL	C79-C80-C81-C82
27	C	308	DMU	O1-C10-O7-C3
21	Y	102	TGL	CB3-CB4-CB5-CB6
26	C	306	CDL	C75-C76-C77-C78
27	K	105	DMU	C28-C31-C34-C37
19	G	104	PGV	C11-C10-C9-C8
19	G	104	PGV	C1-C2-C3-C4
21	Q	201	TGL	C33-C34-C35-C36
21	Y	102	TGL	CC7-CC8-CC9-C15
25	P	302	PEK	C27-C28-C29-C30
26	C	306	CDL	C42-C43-C44-C45
27	L	102	DMU	C28-C31-C34-C37
21	Q	201	TGL	CB2-CB3-CB4-CB5
19	A	607	PGV	O03-C01-C02-C03
19	C	304	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	C	303	PEK	O03-C01-C02-C03
25	P	304	PEK	O03-C01-C02-C03
26	G	101	CDL	CB3-CB4-CB6-OB8
26	T	103	CDL	CA3-CA4-CA6-OA8
25	C	302	PEK	C10-C11-C12-C13
25	C	303	PEK	C10-C11-C12-C13
21	B	304	TGL	C18-C19-C33-C34
26	T	103	CDL	C53-C54-C55-C56
27	K	104	DMU	O16-C18-C19-C22
24	Y	101	CHD	C21-C20-C22-C23
21	Q	201	TGL	CA1-CA2-CA3-CA4
27	C	307	DMU	C3-C4-C57-O61
21	B	301	TGL	C25-C26-C27-C28
26	C	306	CDL	C21-C22-C23-C24
19	P	305	PGV	C11-C10-C9-C8
21	N	608	TGL	CA4-CA5-CA6-CA7
27	X	202	DMU	C22-C25-C28-C31
21	L	101	TGL	CC2-CC1-OG3-CG3
21	B	304	TGL	C20-C21-C22-C23
26	C	306	CDL	C57-C58-C59-C60
23	O	302	PSC	C03-C02-O01-C1
21	N	608	TGL	CC5-CC6-CC7-CC8
26	C	306	CDL	C11-C12-C13-C14
27	L	102	DMU	C34-C37-C40-C43
26	C	306	CDL	CB3-OB5-PB2-OB3
19	A	607	PGV	O01-C02-C03-O11
19	C	305	PGV	O01-C02-C03-O11
26	G	101	CDL	OA5-CA3-CA4-OA6
23	O	302	PSC	O01-C1-C2-C3
21	N	608	TGL	C20-C21-C22-C23
27	T	104	DMU	C22-C25-C28-C31
27	K	101	DMU	C18-C19-C22-C25
20	A	611	EDO	O1-C1-C2-O2
20	C	311	EDO	O1-C1-C2-O2
25	P	302	PEK	C30-C31-C32-C33
26	C	306	CDL	CB7-C71-C72-C73
23	O	302	PSC	O03-C01-C02-O01
26	C	306	CDL	OB6-CB4-CB6-OB8
19	P	305	PGV	C13-C14-C15-C16
27	X	203	DMU	O16-C18-C19-C22
27	M	106	DMU	O5-C4-C57-O61
21	N	608	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	K	102	DMU	C34-C37-C40-C43
21	B	301	TGL	CA5-CA6-CA7-CA8
27	X	203	DMU	C25-C28-C31-C34
19	N	609	PGV	C26-C27-C28-C29
27	K	102	DMU	C3-C4-C57-O61
26	C	306	CDL	C24-C25-C26-C27
26	P	306	CDL	C36-C37-C38-C39
27	M	101	DMU	C22-C25-C28-C31
21	Q	201	TGL	CA4-CA5-CA6-CA7
21	N	608	TGL	CB9-C10-C11-C12
26	C	306	CDL	C37-C38-C39-C40
19	A	608	PGV	C10-C11-C12-C13
25	C	303	PEK	C4-C5-C6-C7
27	O	303	DMU	C19-C18-O16-C6
19	C	305	PGV	C01-C02-C03-O11
27	X	203	DMU	C22-C25-C28-C31
26	T	103	CDL	C74-C75-C76-C77
19	N	607	PGV	C4-C5-C6-C7
21	B	301	TGL	C12-C13-C14-C29
27	X	205	DMU	O16-C18-C19-C22
21	Y	102	TGL	C23-C24-C25-C26
27	G	102	DMU	C2-C3-O7-C10
27	X	202	DMU	C28-C31-C34-C37
21	B	304	TGL	CB1-CB2-CB3-CB4
27	X	202	DMU	C19-C22-C25-C28
27	K	101	DMU	C19-C18-O16-C6
27	K	103	DMU	C19-C22-C25-C28
21	N	608	TGL	CA5-CA6-CA7-CA8
27	C	307	DMU	O5-C4-C57-O61
26	P	306	CDL	C71-CB7-OB8-CB6
27	K	103	DMU	O16-C18-C19-C22
21	Y	102	TGL	OG1-CG1-CG2-CG3
23	B	303	PSC	O03-C01-C02-C03
26	T	103	CDL	CB3-CB4-CB6-OB8
23	O	302	PSC	O04-C19-O03-C01
26	C	306	CDL	C84-C85-C86-C87
26	T	103	CDL	C80-C81-C82-C83
19	A	608	PGV	C20-C21-C22-C23
25	P	303	PEK	C27-C28-C29-C30
19	C	305	PGV	C30-C31-C32-C33
21	B	304	TGL	C15-C16-C17-C18
27	C	307	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C41-C42-C43-C44
23	B	303	PSC	C9-C10-C11-C12
23	B	303	PSC	C10-C11-C12-C13
23	O	302	PSC	C9-C10-C11-C12
25	C	302	PEK	C6-C7-C8-C9
25	C	302	PEK	C9-C10-C11-C12
25	C	302	PEK	C11-C12-C13-C14
25	C	303	PEK	C6-C7-C8-C9
25	C	303	PEK	C9-C10-C11-C12
25	C	303	PEK	C11-C12-C13-C14
25	C	303	PEK	C12-C13-C14-C15
25	P	302	PEK	C5-C6-C7-C8
25	P	302	PEK	C6-C7-C8-C9
25	P	302	PEK	C11-C10-C9-C8
25	P	302	PEK	C9-C10-C11-C12
25	P	302	PEK	C12-C13-C14-C15
25	P	304	PEK	C5-C6-C7-C8
25	P	304	PEK	C6-C7-C8-C9
25	P	304	PEK	C11-C10-C9-C8
25	P	304	PEK	C11-C12-C13-C14
25	P	304	PEK	C12-C13-C14-C15
25	T	102	PEK	C5-C6-C7-C8
25	T	102	PEK	C9-C10-C11-C12
25	T	102	PEK	C11-C12-C13-C14
25	T	102	PEK	C12-C13-C14-C15
26	C	306	CDL	CA7-C31-C32-C33
27	G	102	DMU	O6-C11-C9-C8
26	G	101	CDL	C57-C58-C59-C60
19	G	104	PGV	O01-C02-C03-O11
25	T	102	PEK	O01-C02-C03-O11
26	P	306	CDL	OB9-CB7-OB8-CB6
21	L	101	TGL	CC6-CC7-CC8-CC9
26	P	306	CDL	C58-C59-C60-C61
21	L	101	TGL	OC1-CC1-OG3-CG3
26	C	306	CDL	C23-C24-C25-C26
21	L	101	TGL	OG1-CG1-CG2-OG2
26	C	306	CDL	OA6-CA4-CA6-OA8
21	L	101	TGL	CA2-CA1-OG1-CG1
19	N	609	PGV	C27-C28-C29-C30
21	Y	102	TGL	C22-C23-C24-C25
19	P	305	PGV	C02-C03-O11-P
25	T	102	PEK	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
27	X	202	DMU	C25-C28-C31-C34
26	G	101	CDL	C17-C18-C19-C20
27	K	105	DMU	O6-C11-C9-C8
20	A	617	EDO	O1-C1-C2-O2
20	J	104	EDO	O1-C1-C2-O2
20	N	625	EDO	O1-C1-C2-O2
26	C	306	CDL	C53-C54-C55-C56
27	P	316	DMU	C18-C19-C22-C25
19	A	607	PGV	C20-C21-C22-C23
24	Y	101	CHD	C13-C17-C20-C21
19	N	607	PGV	C30-C31-C32-C33
27	M	106	DMU	C4-C3-O7-C10
24	W	101	CHD	C20-C22-C23-C24
21	N	608	TGL	C29-C30-C31-C32
19	A	607	PGV	C01-C02-C03-O11
25	P	304	PEK	C01-C02-C03-O11
21	Q	201	TGL	CB3-CB4-CB5-CB6
19	N	607	PGV	C21-C22-C23-C24
19	P	305	PGV	C24-C25-C26-C27
27	M	101	DMU	C25-C28-C31-C34
23	B	303	PSC	C3-C4-C5-C6
27	P	309	DMU	C19-C22-C25-C28
21	L	101	TGL	C17-C18-C19-C33
26	C	306	CDL	C41-C42-C43-C44
27	O	303	DMU	O16-C6-O5-C4
21	B	301	TGL	CC2-CC1-OG3-CG3
21	N	608	TGL	CC2-CC1-OG3-CG3
21	L	101	TGL	CC7-CC8-CC9-C15
27	K	103	DMU	C4-C3-O7-C10
19	C	304	PGV	C12-C13-C14-C15
19	C	304	PGV	C02-C03-O11-P
21	L	101	TGL	OG1-CG1-CG2-CG3
25	P	302	PEK	O03-C01-C02-C03
27	O	303	DMU	C2-C3-O7-C10
19	N	607	PGV	O01-C02-C03-O11
25	P	304	PEK	O01-C02-C03-O11
25	P	303	PEK	C9-C10-C11-C12
27	K	102	DMU	C18-C19-C22-C25
21	B	301	TGL	CB4-CB5-CB6-CB7
21	Y	102	TGL	CC6-CC7-CC8-CC9
21	L	101	TGL	OA1-CA1-OG1-CG1
21	N	608	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	CC9-C15-C16-C17
27	C	307	DMU	C18-C19-C22-C25
19	N	607	PGV	O03-C01-C02-O01
21	L	101	TGL	OG2-CG2-CG3-OG3
21	Y	102	TGL	OG1-CG1-CG2-OG2
25	C	303	PEK	O03-C01-C02-O01
21	L	101	TGL	CB2-CB3-CB4-CB5
21	Q	201	TGL	CB9-C10-C11-C12
26	C	306	CDL	C73-C74-C75-C76
27	P	309	DMU	C25-C28-C31-C34
27	T	104	DMU	C19-C22-C25-C28
19	C	304	PGV	C24-C25-C26-C27
26	C	306	CDL	C13-C14-C15-C16
27	K	103	DMU	C2-C3-O7-C10
27	P	316	DMU	C34-C37-C40-C43
19	G	104	PGV	C02-C03-O11-P
14	N	601[C]	HEA	C14-C15-C16-C17
21	N	608	TGL	C12-C13-C14-C29
19	C	305	PGV	C04-O12-P-O14
19	G	104	PGV	C04-O12-P-O14
19	N	607	PGV	C04-O12-P-O13
23	B	303	PSC	C04-O12-P-O14
25	C	303	PEK	C03-O11-P-O14
25	P	304	PEK	C04-O12-P-O14
26	G	101	CDL	CB2-OB2-PB2-OB4
26	T	103	CDL	CA3-OA5-PA1-OA4
26	T	103	CDL	CB3-OB5-PB2-OB4
27	X	203	DMU	O5-C6-O16-C18
25	T	102	PEK	C01-C02-C03-O11
26	P	306	CDL	OB5-CB3-CB4-CB6
25	P	303	PEK	C24-C25-C26-C27
26	G	101	CDL	C18-C19-C20-C21
27	C	308	DMU	C34-C37-C40-C43
20	C	317	EDO	O1-C1-C2-O2
20	F	106	EDO	O1-C1-C2-O2
19	C	305	PGV	C10-C11-C12-C13
23	B	303	PSC	C05-C04-O12-P
21	L	101	TGL	CC4-CC5-CC6-CC7
21	Y	102	TGL	CA6-CA7-CA8-CA9
26	P	306	CDL	C44-C45-C46-C47
21	Y	102	TGL	CB1-CB2-CB3-CB4
27	P	316	DMU	O6-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
21	B	304	TGL	OG3-CC1-CC2-CC3
21	B	301	TGL	C16-C15-CC9-CC8
21	Q	201	TGL	C12-C13-C14-C29
21	Q	201	TGL	CC7-CC8-CC9-C15
21	B	301	TGL	OC1-CC1-OG3-CG3
21	L	101	TGL	CG1-CG2-CG3-OG3
21	Y	102	TGL	CG1-CG2-CG3-OG3
23	B	303	PSC	C22-C23-C24-C25
23	B	303	PSC	O03-C01-C02-O01
25	P	302	PEK	O03-C01-C02-O01
25	C	302	PEK	C4-C5-C6-C7
25	C	302	PEK	C16-C17-C18-C19
27	K	104	DMU	O1-C10-O7-C3
19	N	607	PGV	C02-C03-O11-P
26	T	103	CDL	C1-CB2-OB2-PB2
24	J	102	CHD	C20-C22-C23-C24
26	T	103	CDL	C18-C19-C20-C21
19	N	607	PGV	C27-C28-C29-C30
27	K	103	DMU	O6-C11-C9-C8
26	P	306	CDL	C57-C58-C59-C60
27	K	102	DMU	C31-C34-C37-C40
25	C	302	PEK	O03-C21-C22-C23
24	J	101	CHD	C20-C22-C23-C24
27	K	106	DMU	O5-C4-C57-O61
26	C	306	CDL	C44-C45-C46-C47
19	A	607	PGV	C02-C03-O11-P
26	G	101	CDL	C1-CB2-OB2-PB2
25	T	102	PEK	C7-C8-C9-C10
26	G	101	CDL	C22-C23-C24-C25
27	X	204	DMU	C31-C34-C37-C40
19	C	304	PGV	C1-C2-C3-C4
20	A	622	EDO	O1-C1-C2-O2
20	N	617	EDO	O1-C1-C2-O2
20	Q	203	EDO	O1-C1-C2-O2
19	N	607	PGV	C9-C10-C11-C12
26	T	103	CDL	OA6-CA4-CA6-OA8
19	A	607	PGV	C04-O12-P-O11
26	G	101	CDL	CA3-OA5-PA1-OA2
26	T	103	CDL	CB2-OB2-PB2-OB5
19	G	104	PGV	C31-C32-C33-C34
27	C	308	DMU	C28-C31-C34-C37
19	N	607	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	CB3-CB4-CB6-OB8
21	L	101	TGL	C24-C25-C26-C27
19	A	607	PGV	O01-C1-C2-C3
19	A	608	PGV	C26-C27-C28-C29
21	L	101	TGL	C21-C22-C23-C24
26	G	101	CDL	C71-CB7-OB8-CB6
19	A	607	PGV	C05-C04-O12-P
26	G	101	CDL	C43-C44-C45-C46
19	C	304	PGV	C11-C12-C13-C14
27	K	106	DMU	O6-C11-C9-C8
23	B	303	PSC	C2-C3-C4-C5
26	C	306	CDL	C22-C23-C24-C25
27	C	307	DMU	O16-C18-C19-C22
26	P	306	CDL	C82-C83-C84-C85
27	X	201	DMU	C5-C10-O7-C3
21	B	301	TGL	CA9-C20-C21-C22
27	P	307	DMU	C31-C34-C37-C40
27	K	102	DMU	C25-C28-C31-C34
19	A	607	PGV	C23-C24-C25-C26
27	G	102	DMU	C22-C25-C28-C31
21	L	101	TGL	CA5-CA6-CA7-CA8
25	C	303	PEK	C29-C30-C31-C32
26	P	306	CDL	C43-C44-C45-C46
21	L	101	TGL	CA1-CA2-CA3-CA4
21	B	304	TGL	C10-C11-C12-C13
25	C	302	PEK	C15-C16-C17-C18
26	C	306	CDL	C77-C78-C79-C80
26	G	101	CDL	OB9-CB7-OB8-CB6
25	P	303	PEK	C23-C24-C25-C26
19	A	608	PGV	C23-C24-C25-C26
26	P	306	CDL	OB6-CB4-CB6-OB8
27	M	101	DMU	C28-C31-C34-C37
26	P	306	CDL	C12-C13-C14-C15
23	B	303	PSC	C12-C13-C14-C15
26	G	101	CDL	C20-C21-C22-C23
19	P	305	PGV	C12-C13-C14-C15
20	M	102	EDO	O1-C1-C2-O2
20	V	101	EDO	O1-C1-C2-O2
27	K	106	DMU	C19-C22-C25-C28
21	Y	102	TGL	C20-C21-C22-C23
23	O	302	PSC	O03-C01-C02-C03
19	A	608	PGV	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	C15-C16-C17-C18
25	P	303	PEK	C4-C5-C6-C7
21	B	304	TGL	C11-C12-C13-C14
19	N	607	PGV	C7-C8-C9-C10
27	O	303	DMU	C22-C25-C28-C31
25	P	302	PEK	C14-C15-C16-C17
26	T	103	CDL	C11-C12-C13-C14
25	C	303	PEK	C11-C10-C9-C8
25	P	302	PEK	C11-C12-C13-C14
25	P	304	PEK	C9-C10-C11-C12
25	T	102	PEK	C6-C7-C8-C9
19	C	305	PGV	C20-C21-C22-C23
21	Y	102	TGL	C12-C13-C14-C29
26	T	103	CDL	C38-C39-C40-C41
27	O	303	DMU	O5-C4-C57-O61
26	G	101	CDL	C77-C78-C79-C80
27	X	204	DMU	C34-C37-C40-C43
26	G	101	CDL	OA5-CA3-CA4-CA6
19	A	608	PGV	C11-C12-C13-C14
26	G	101	CDL	C32-C33-C34-C35
19	N	609	PGV	C30-C31-C32-C33
26	G	101	CDL	C35-C36-C37-C38
21	B	301	TGL	OG1-CG1-CG2-OG2
25	P	304	PEK	O03-C01-C02-O01
21	B	301	TGL	C15-C16-C17-C18
25	C	303	PEK	C32-C33-C34-C35
25	T	102	PEK	C13-C14-C15-C16
21	L	101	TGL	C16-C17-C18-C19
27	K	104	DMU	C4-C3-O7-C10
27	X	201	DMU	O5-C4-C57-O61
27	L	102	DMU	O1-C10-O7-C3
25	P	304	PEK	C14-C15-C16-C17
21	Q	201	TGL	C16-C15-CC9-CC8
24	J	102	CHD	C16-C17-C20-C22
21	B	304	TGL	OC1-CC1-OG3-CG3
20	D	201	EDO	O1-C1-C2-O2
20	F	105	EDO	O1-C1-C2-O2
27	P	309	DMU	C5-C10-O7-C3
21	B	304	TGL	C17-C18-C19-C33
25	P	304	PEK	C3-C4-C5-C6
25	T	102	PEK	C3-C4-C5-C6
26	P	306	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	C43-C44-C45-C46
27	K	106	DMU	C2-C3-O7-C10
19	G	104	PGV	C01-C02-C03-O11
19	P	305	PGV	C1-C2-C3-C4
19	G	104	PGV	C22-C23-C24-C25
26	P	306	CDL	C74-C75-C76-C77
21	B	301	TGL	C21-C20-CA9-CA8
26	C	306	CDL	OA5-CA3-CA4-OA6
23	O	302	PSC	O03-C19-C20-C21
21	N	608	TGL	C15-C16-C17-C18
19	N	609	PGV	C11-C12-C13-C14
23	B	303	PSC	C7-C8-C9-C10
25	T	102	PEK	O03-C21-C22-C23
27	X	204	DMU	C18-C19-C22-C25
23	B	303	PSC	C19-C20-C21-C22
21	N	608	TGL	OG3-CC1-CC2-CC3
27	K	106	DMU	C5-C10-O7-C3
27	L	102	DMU	C22-C25-C28-C31
19	P	305	PGV	C9-C10-C11-C12
23	O	302	PSC	C7-C8-C9-C10
25	C	302	PEK	C24-C25-C26-C27
27	K	104	DMU	C3-C4-C57-O61
26	T	103	CDL	C20-C21-C22-C23
26	G	101	CDL	C16-C17-C18-C19
21	Y	102	TGL	CC2-CC3-CC4-CC5
21	Q	201	TGL	CA5-CA6-CA7-CA8
26	T	103	CDL	C33-C34-C35-C36
23	B	303	PSC	O01-C1-C2-C3
25	T	102	PEK	O01-C1-C2-C3
19	N	607	PGV	C11-C12-C13-C14
23	O	302	PSC	C12-C13-C14-C15
25	C	303	PEK	C3-C4-C5-C6
26	P	306	CDL	CB3-CB4-CB6-OB8
27	O	303	DMU	C4-C3-O7-C10
21	Q	201	TGL	C11-C12-C13-C14
24	Y	101	CHD	C16-C17-C20-C22
26	C	306	CDL	C52-C51-CB5-OB6
26	T	103	CDL	C32-C31-CA7-OA8
20	C	310	EDO	O1-C1-C2-O2
20	O	305	EDO	O1-C1-C2-O2
20	P	315	EDO	O1-C1-C2-O2
20	Q	204	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	A	607	PGV	C11-C12-C13-C14
19	C	304	PGV	C9-C10-C11-C12
21	L	101	TGL	C12-C13-C14-C29
21	L	101	TGL	C19-C33-C34-C35
25	C	302	PEK	C25-C26-C27-C28
26	G	101	CDL	OA6-CA4-CA6-OA8
19	N	609	PGV	C10-C11-C12-C13
26	P	306	CDL	C78-C79-C80-C81
21	B	304	TGL	CC3-CC4-CC5-CC6
27	X	204	DMU	C28-C31-C34-C37
26	P	306	CDL	OA7-CA5-OA6-CA4
19	N	609	PGV	O03-C19-C20-C21
21	Y	102	TGL	CB4-CB5-CB6-CB7
21	Y	102	TGL	OG3-CC1-CC2-CC3
25	T	102	PEK	O04-C21-C22-C23
23	B	303	PSC	C29-C30-C31-C32
26	C	306	CDL	C14-C15-C16-C17
26	G	101	CDL	C56-C57-C58-C59
25	C	303	PEK	C14-C15-C16-C17
27	M	106	DMU	C5-C10-O7-C3
26	T	103	CDL	C32-C31-CA7-OA9
19	A	607	PGV	C04-O12-P-O13
26	G	101	CDL	CA3-OA5-PA1-OA3
26	G	101	CDL	C54-C55-C56-C57
25	C	302	PEK	O12-C04-C05-N
21	N	608	TGL	OC1-CC1-CC2-CC3
21	Y	102	TGL	OC1-CC1-CC2-CC3
23	B	303	PSC	O02-C1-C2-C3
25	T	102	PEK	O02-C1-C2-C3
20	A	612	EDO	O1-C1-C2-O2
20	C	314	EDO	O1-C1-C2-O2
20	U	101	EDO	O1-C1-C2-O2
19	C	305	PGV	C24-C25-C26-C27
21	B	301	TGL	C11-C10-CB9-CB8
26	C	306	CDL	C52-C51-CB5-OB7
25	P	303	PEK	C28-C29-C30-C31
26	C	306	CDL	C60-C61-C62-C63
19	A	608	PGV	O04-C19-C20-C21
19	P	305	PGV	C7-C8-C9-C10
26	C	306	CDL	C12-C11-CA5-OA6
27	X	202	DMU	C18-C19-C22-C25
27	X	205	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	C32-C31-CA7-OA8
26	G	101	CDL	C12-C11-CA5-OA6
21	B	304	TGL	OC1-CC1-CC2-CC3
27	K	101	DMU	C22-C25-C28-C31
27	L	102	DMU	C19-C18-O16-C6
21	Y	102	TGL	C21-C20-CA9-CA8
27	P	307	DMU	C34-C37-C40-C43
26	C	306	CDL	C12-C11-CA5-OA7
19	P	305	PGV	C20-C21-C22-C23
21	Y	102	TGL	CA5-CA6-CA7-CA8
19	A	607	PGV	C9-C10-C11-C12
27	K	103	DMU	C18-C19-C22-C25
27	G	102	DMU	C5-C10-O7-C3
21	B	304	TGL	CC2-CC3-CC4-CC5
21	B	304	TGL	OG1-CA1-CA2-CA3
21	B	304	TGL	OG2-CB1-CB2-CB3

There are no ring outliers.

82 monomers are involved in 295 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	204	DMU	1	0
20	C	315	EDO	1	0
19	C	305	PGV	4	0
21	N	608	TGL	2	0
24	W	101	CHD	1	0
20	M	105	EDO	1	0
20	A	613	EDO	1	0
27	Z	101	DMU	3	0
27	X	205	DMU	1	0
21	B	301	TGL	7	0
23	B	303	PSC	13	0
27	P	307	DMU	5	0
25	T	102	PEK	4	0
25	P	304	PEK	6	0
14	A	601[C]	HEA	1	0
20	U	101	EDO	4	0
19	G	104	PGV	6	0
27	X	201	DMU	2	0
27	M	106	DMU	2	0
27	C	307	DMU	5	0
20	S	104	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	626	EDO	2	0
27	X	202	DMU	4	0
25	P	302	PEK	6	0
27	T	104	DMU	1	0
26	C	306	CDL	3	0
25	C	303	PEK	6	0
24	J	101	CHD	1	0
24	J	102	CHD	2	0
20	A	611	EDO	1	0
23	O	302	PSC	4	0
19	N	607	PGV	6	0
24	P	308	CHD	2	0
25	C	302	PEK	5	0
20	B	310	EDO	1	0
20	N	612	EDO	2	0
20	Q	204	EDO	1	0
27	O	303	DMU	1	0
19	A	607	PGV	4	0
19	C	304	PGV	1	0
27	C	308	DMU	7	0
21	Y	102	TGL	9	0
14	N	601[B]	HEA	2	0
27	K	106	DMU	5	0
19	P	305	PGV	3	0
27	X	203	DMU	3	0
20	A	621	EDO	1	0
20	N	616	EDO	2	0
14	N	601[A]	HEA	2	0
27	L	102	DMU	7	0
14	A	601[B]	HEA	1	0
27	K	102	DMU	1	0
20	R	201	EDO	1	0
26	P	306	CDL	10	0
20	B	309	EDO	1	0
27	P	316	DMU	8	0
27	K	103	DMU	1	0
24	Y	101	CHD	1	0
27	K	104	DMU	1	0
20	M	103	EDO	5	0
27	P	309	DMU	4	0
20	F	106	EDO	1	0
20	J	104	EDO	1	0

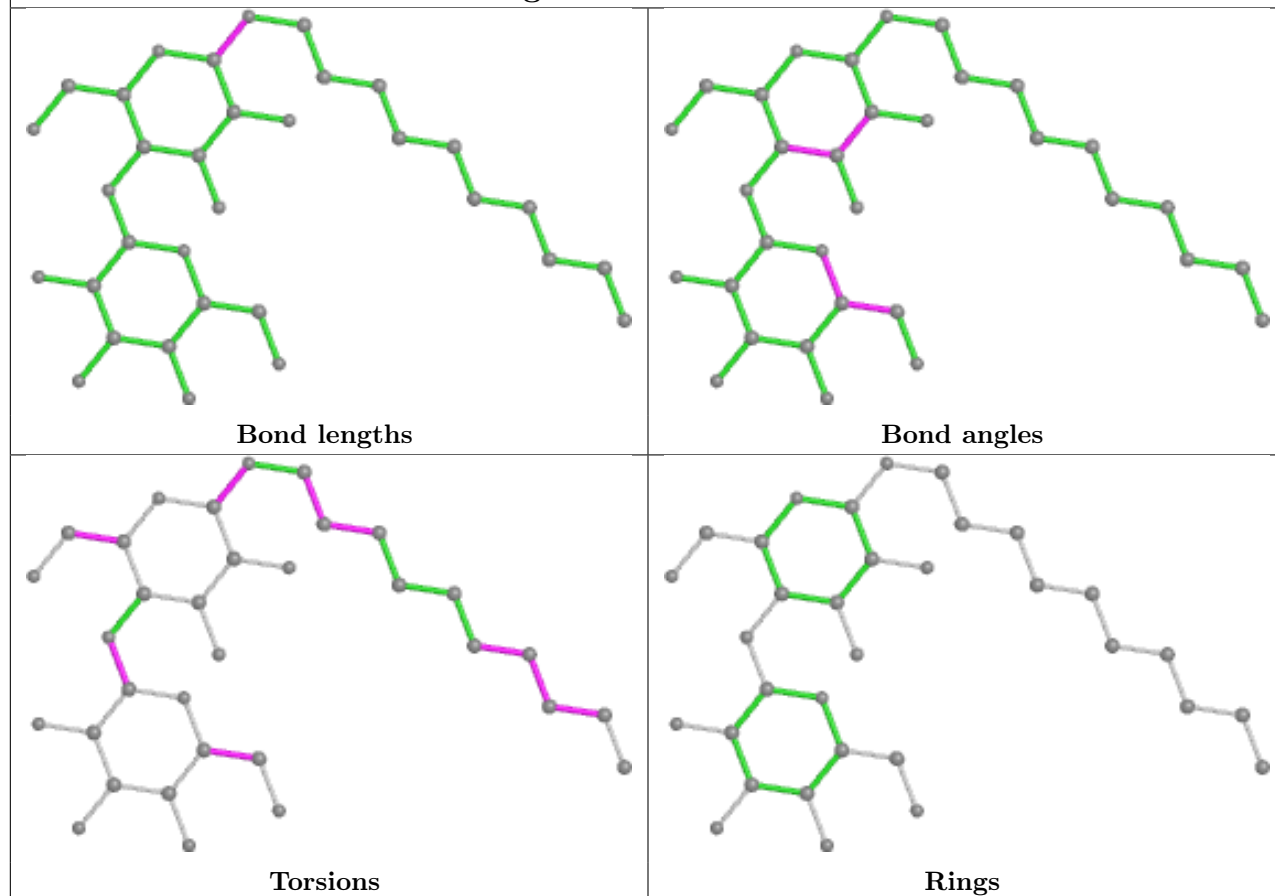
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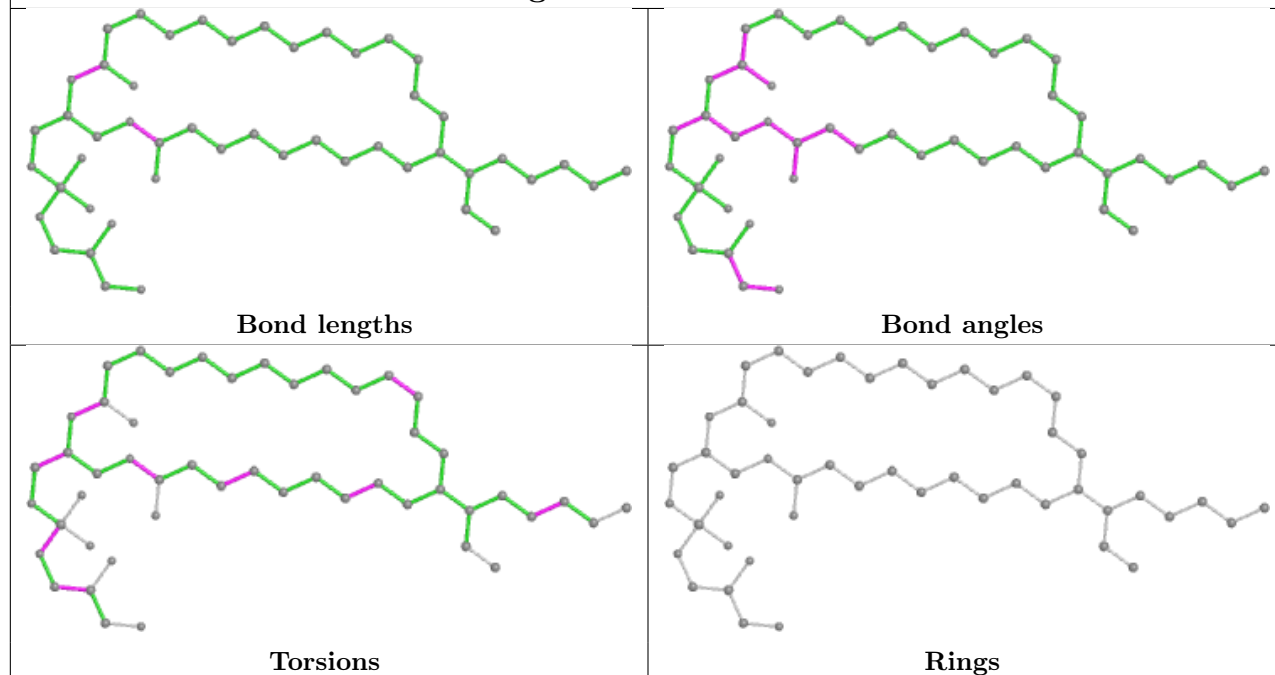
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	B	304	TGL	11	0
20	A	622	EDO	4	0
14	A	601[A]	HEA	3	0
27	K	105	DMU	1	0
14	N	602	HEA	4	0
20	Q	202	EDO	1	0
20	L	103	EDO	3	0
27	G	102	DMU	8	0
26	T	103	CDL	16	0
20	A	617	EDO	3	0
20	V	101	EDO	2	0
20	N	617	EDO	3	0
20	N	618	EDO	5	0
20	D	202	EDO	1	0
26	G	101	CDL	20	0
14	A	602	HEA	3	0
21	Q	201	TGL	6	0
20	N	625	EDO	2	0
21	L	101	TGL	13	0

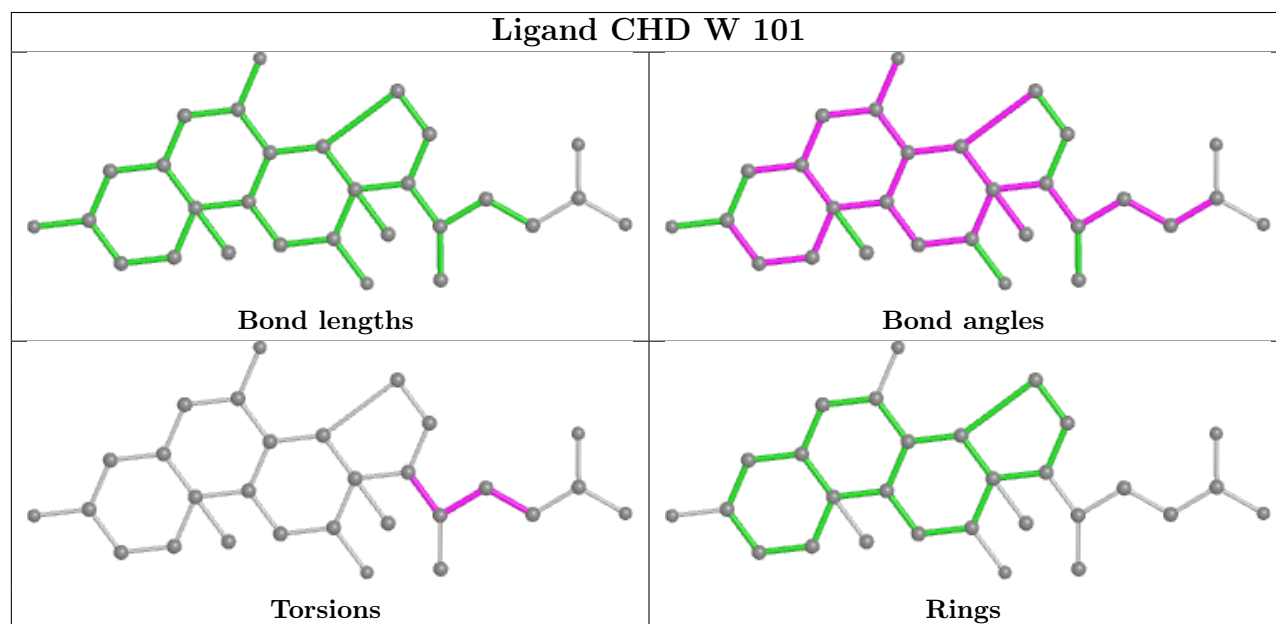
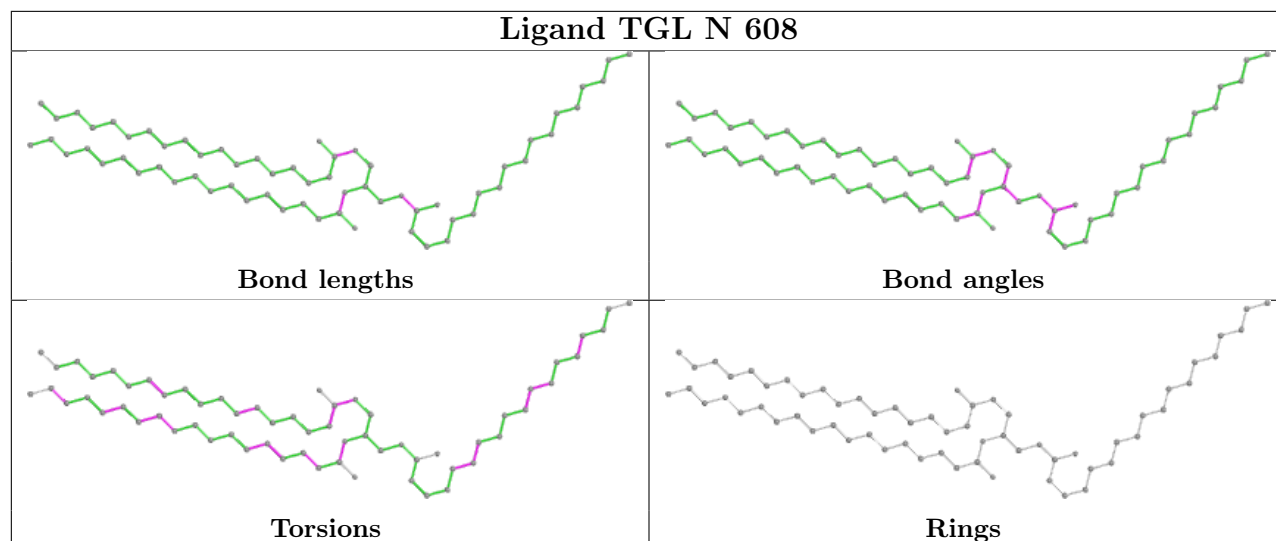
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

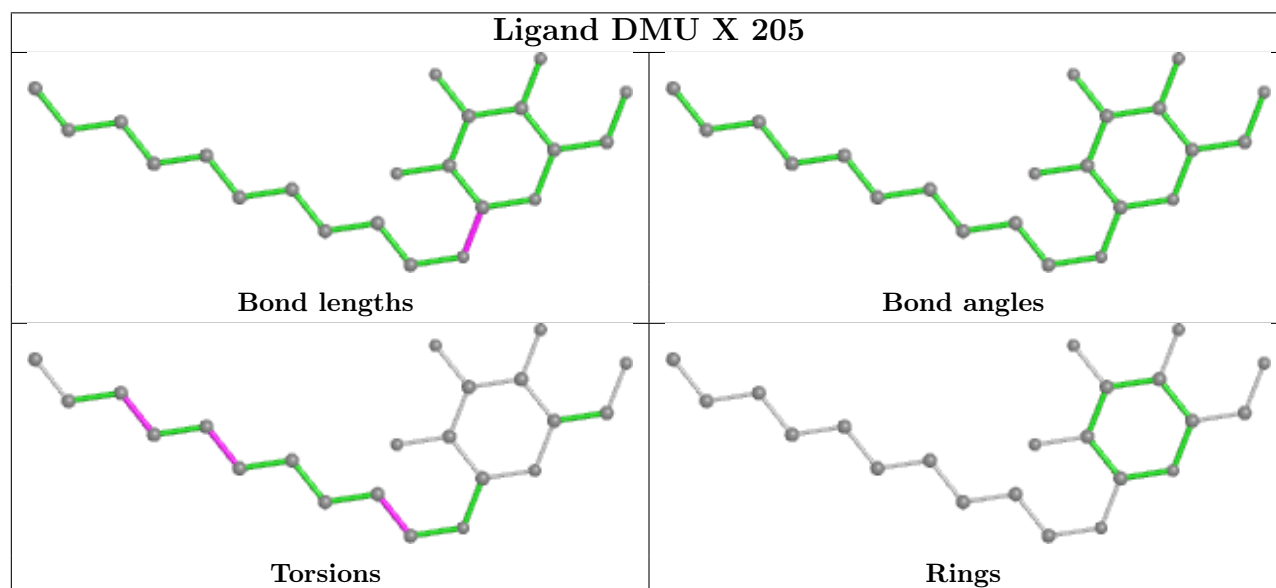
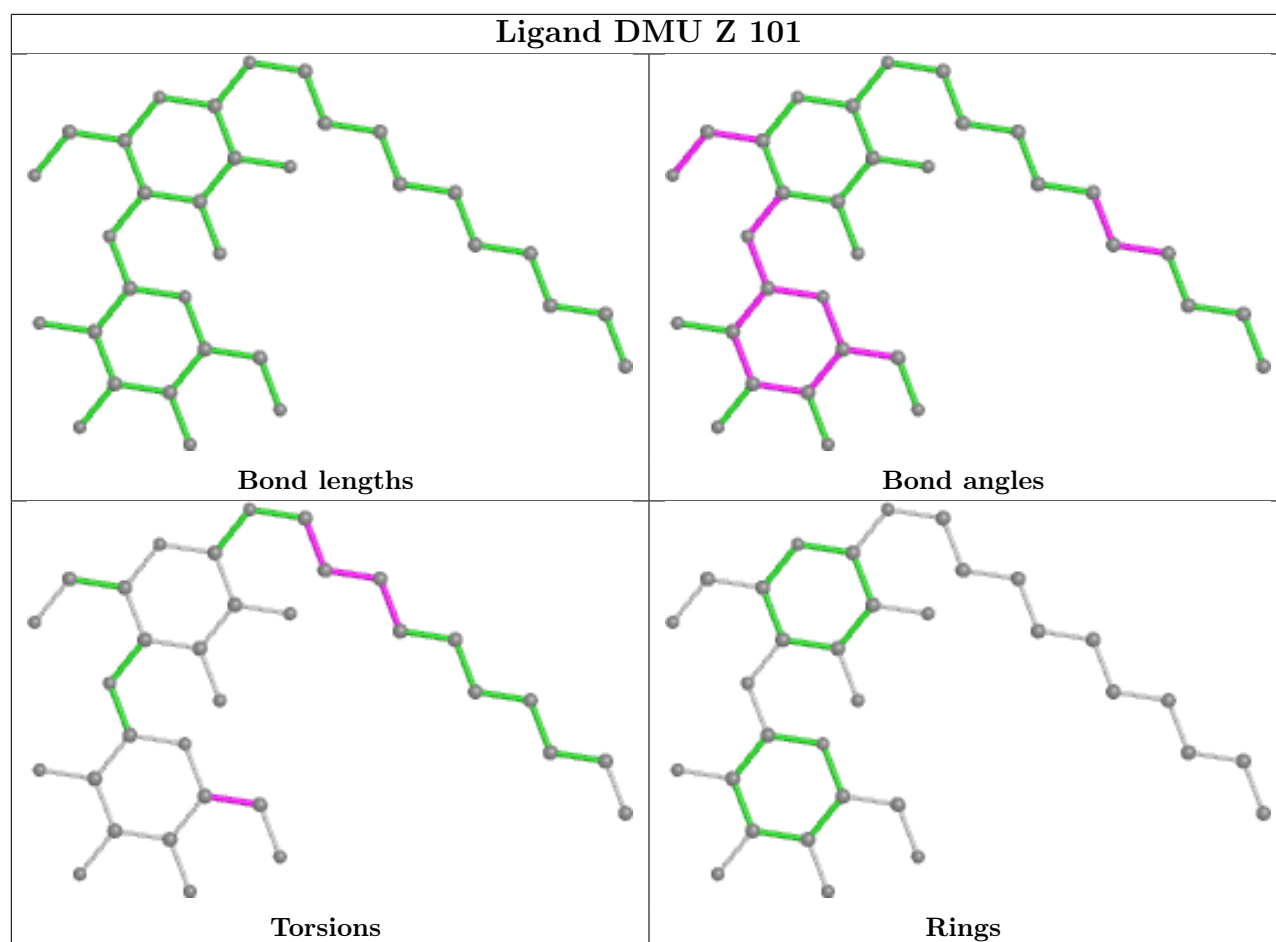
Ligand DMU X 204

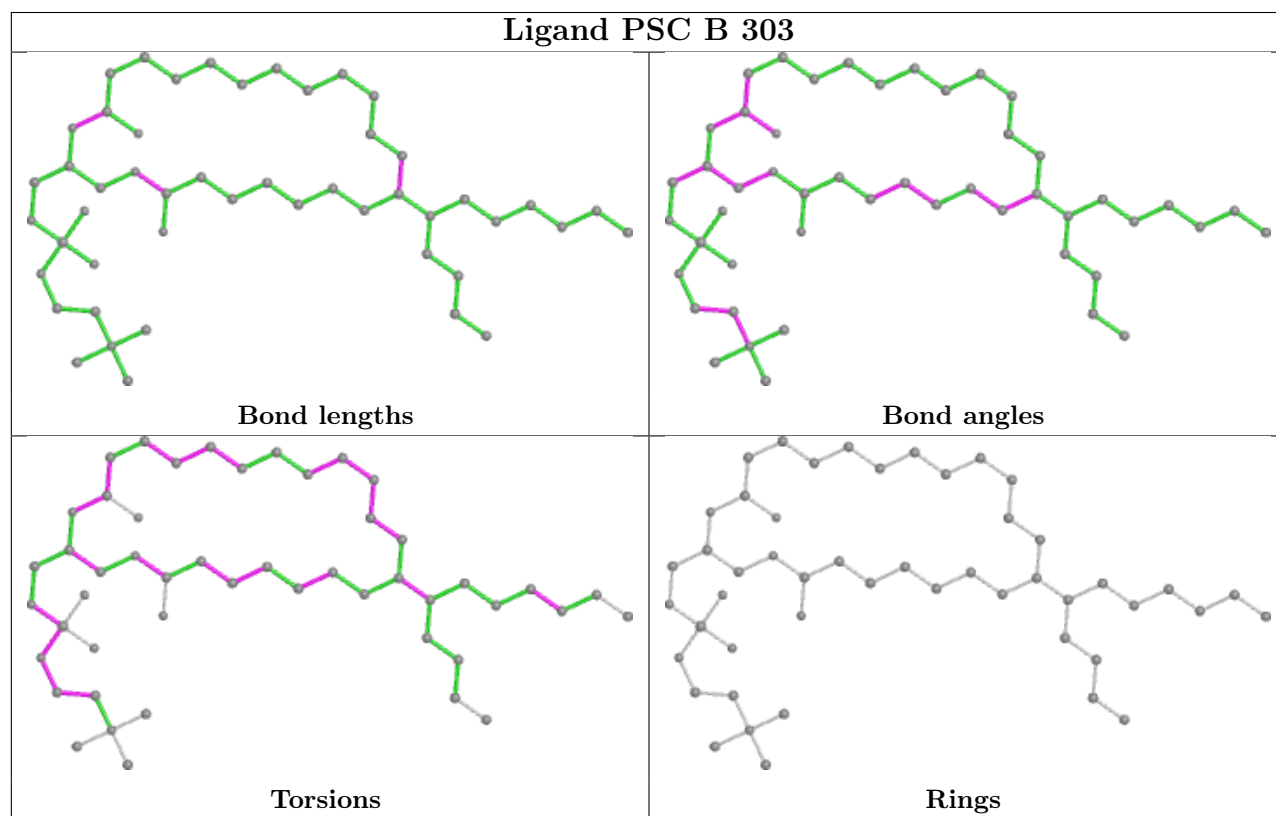
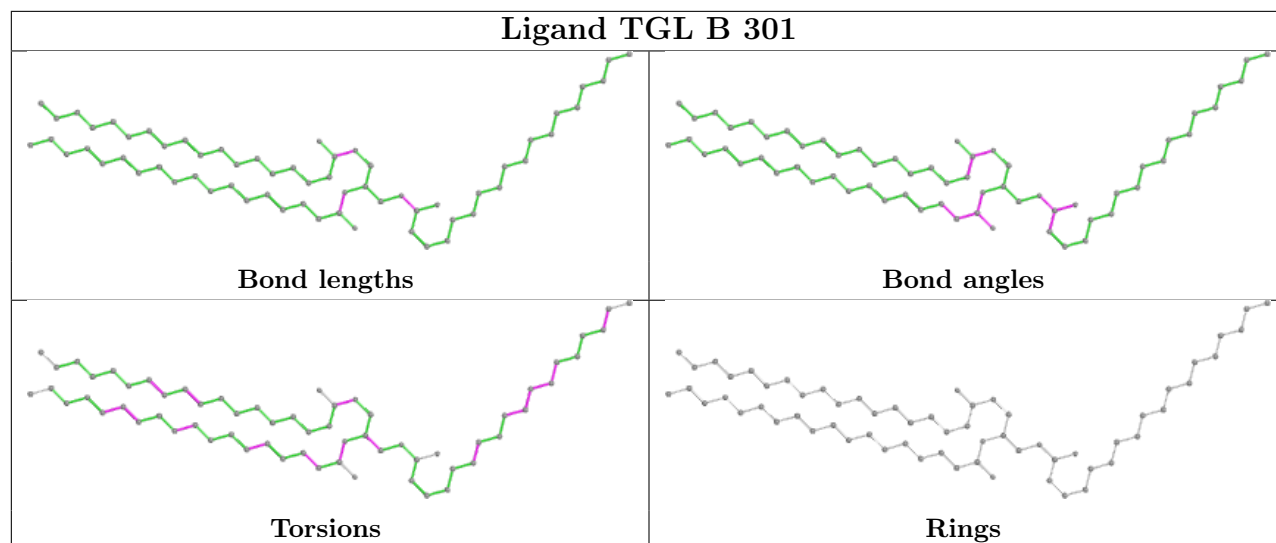


Ligand PGV C 305

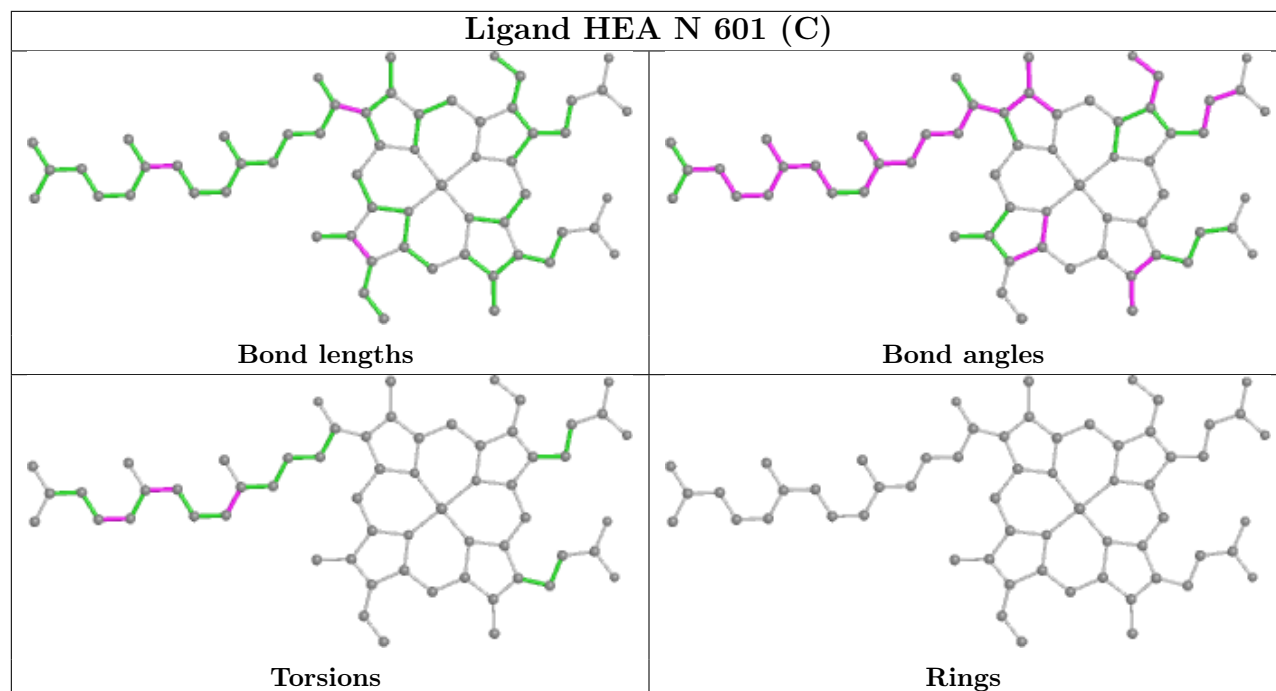




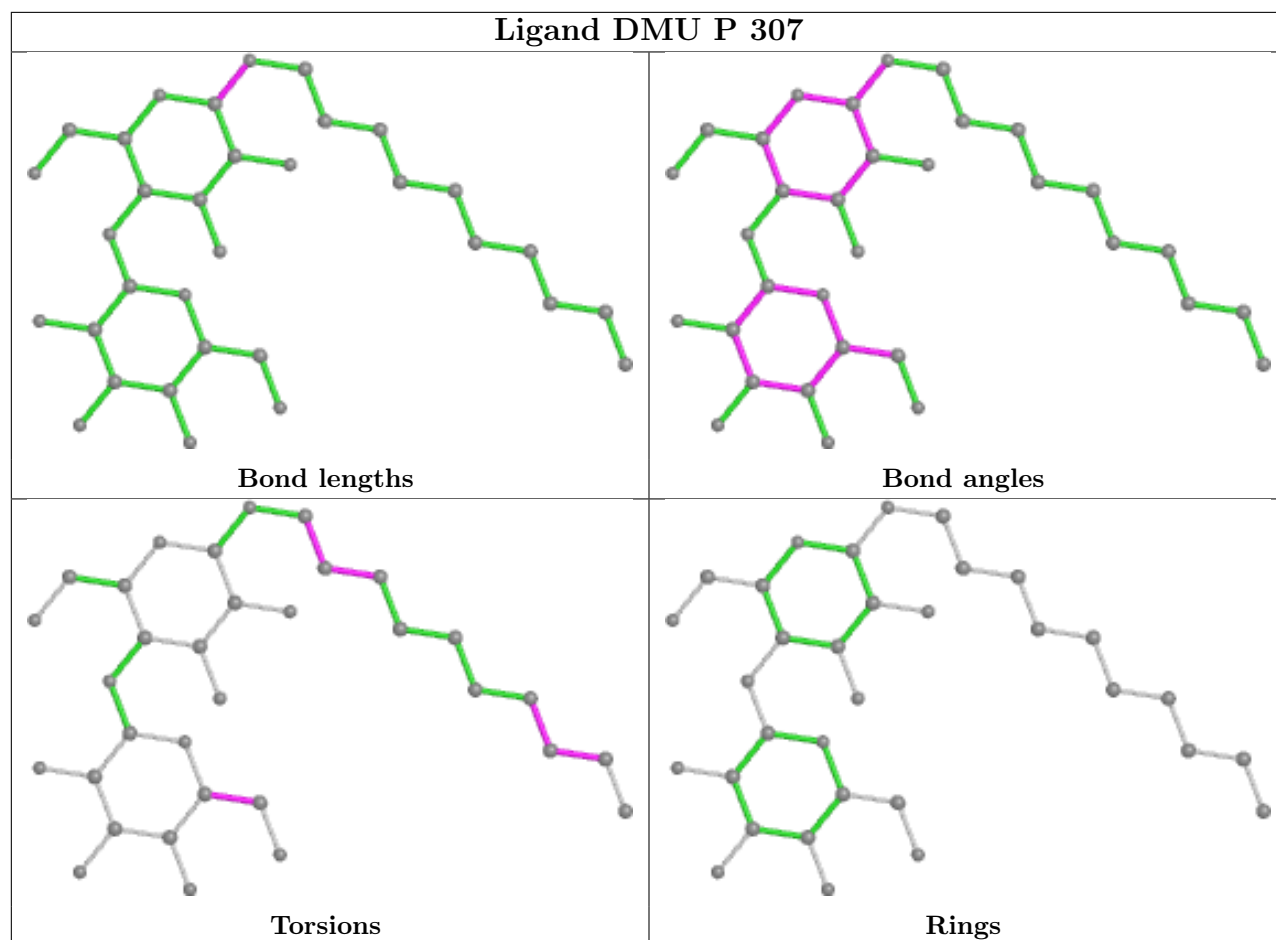


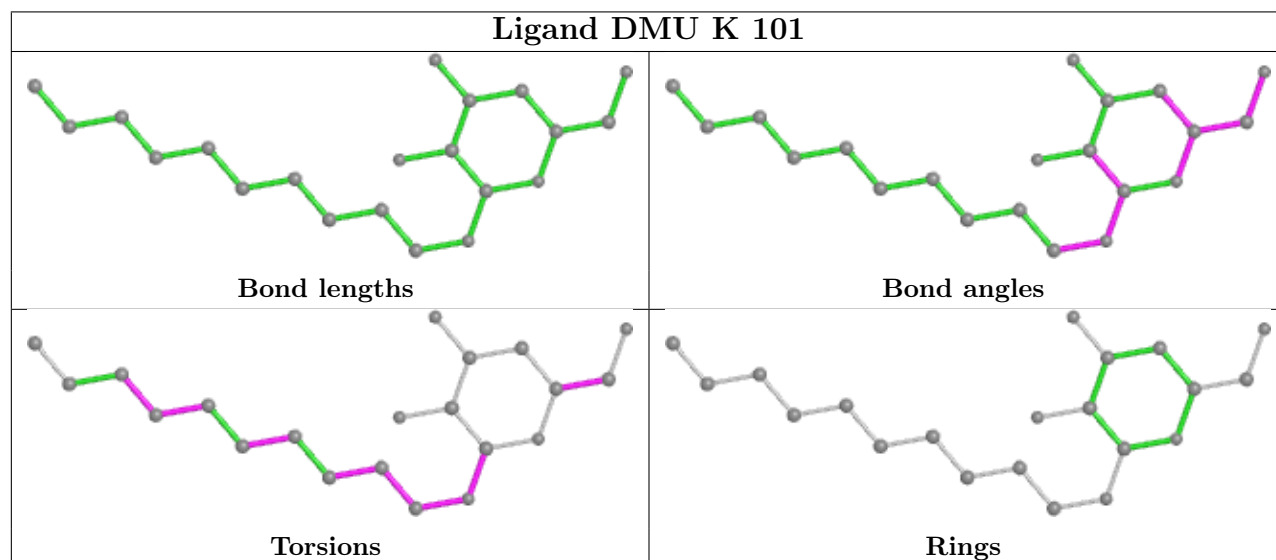
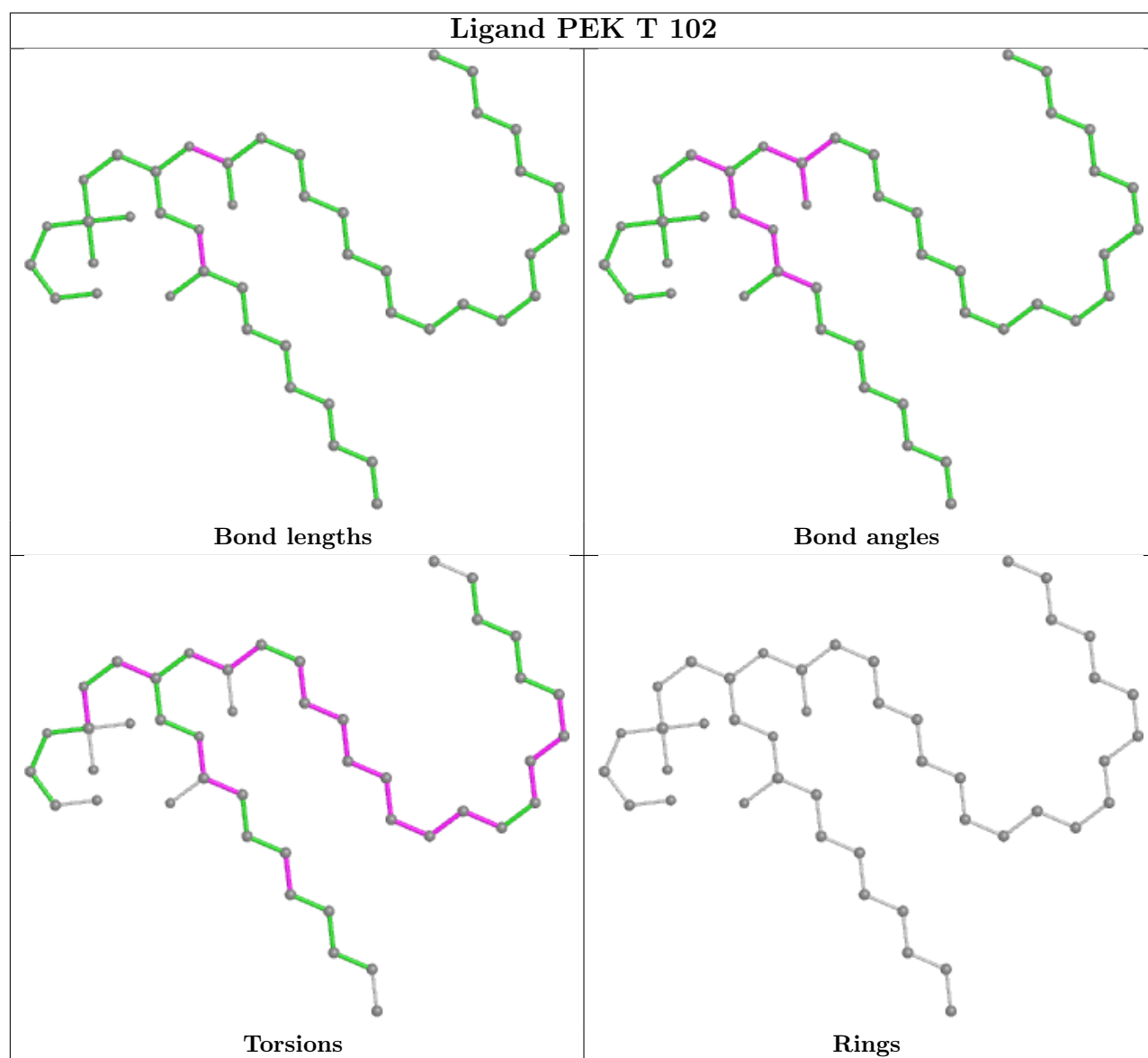


Ligand HEA N 601 (C)

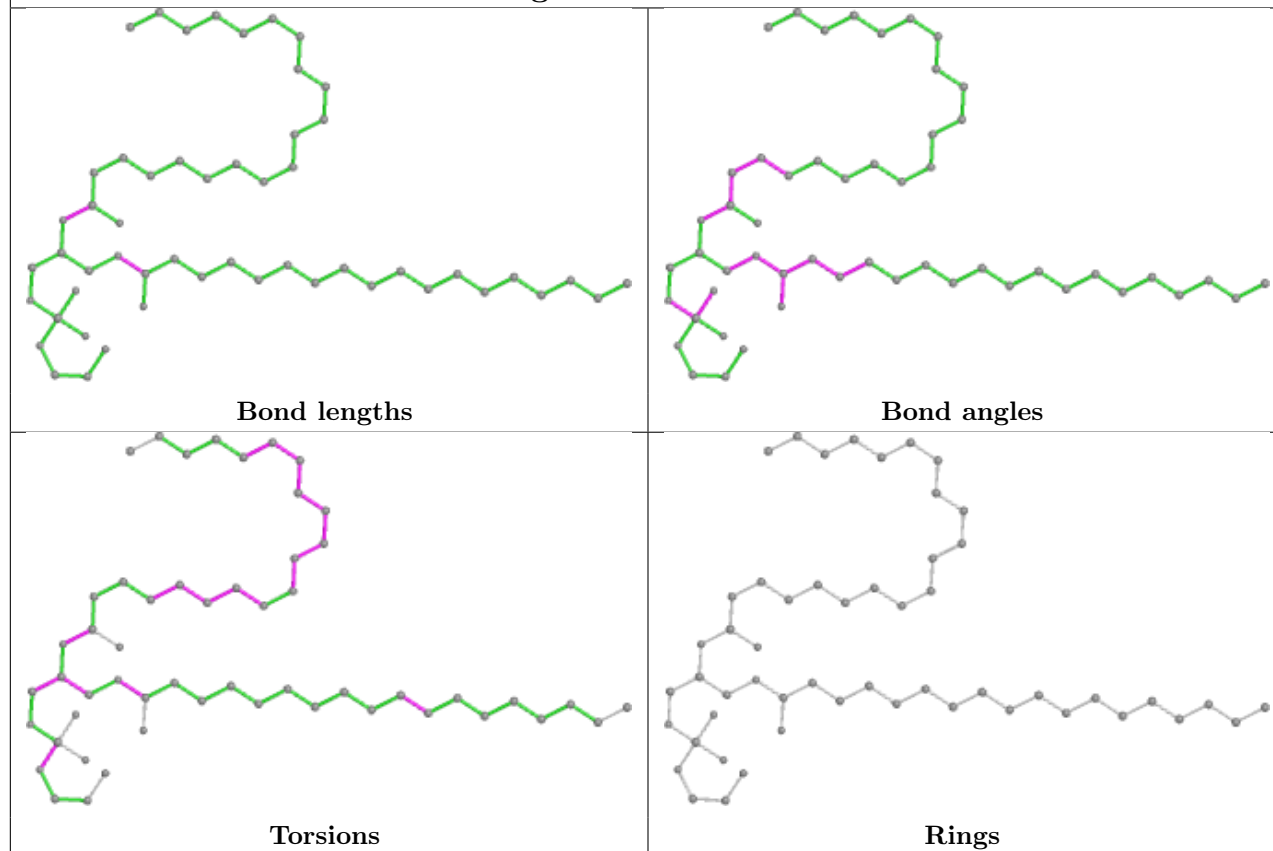


Ligand DMU P 307

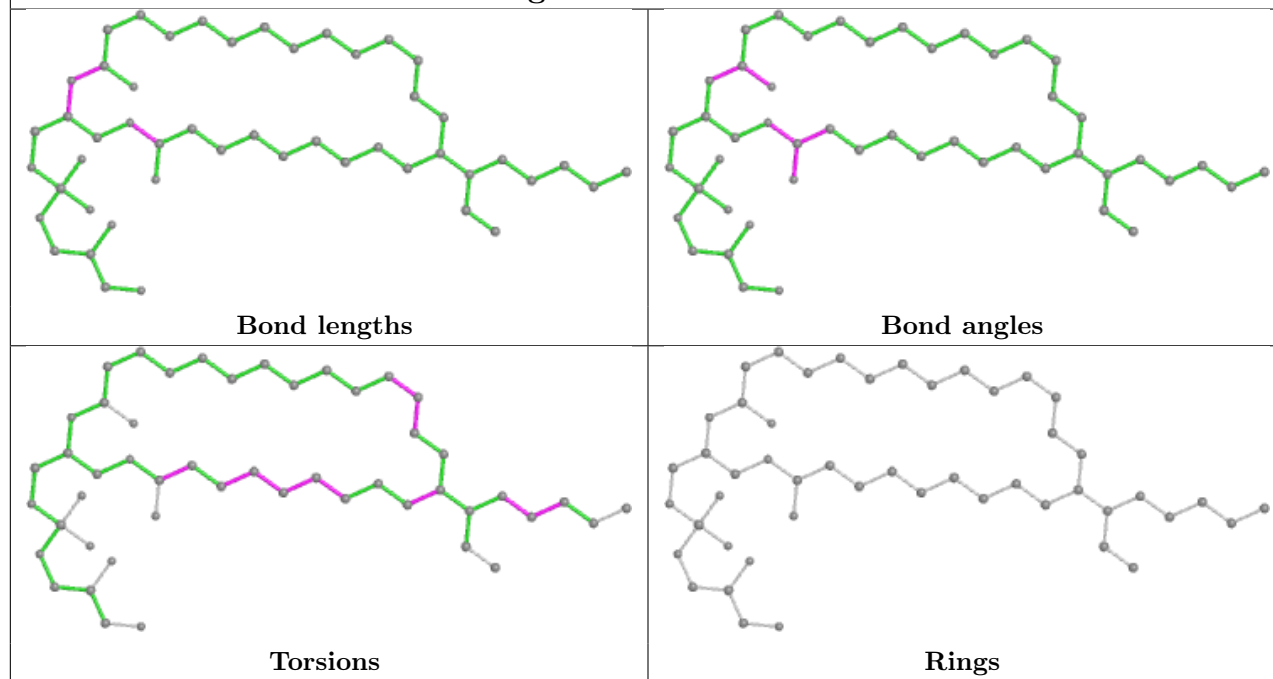




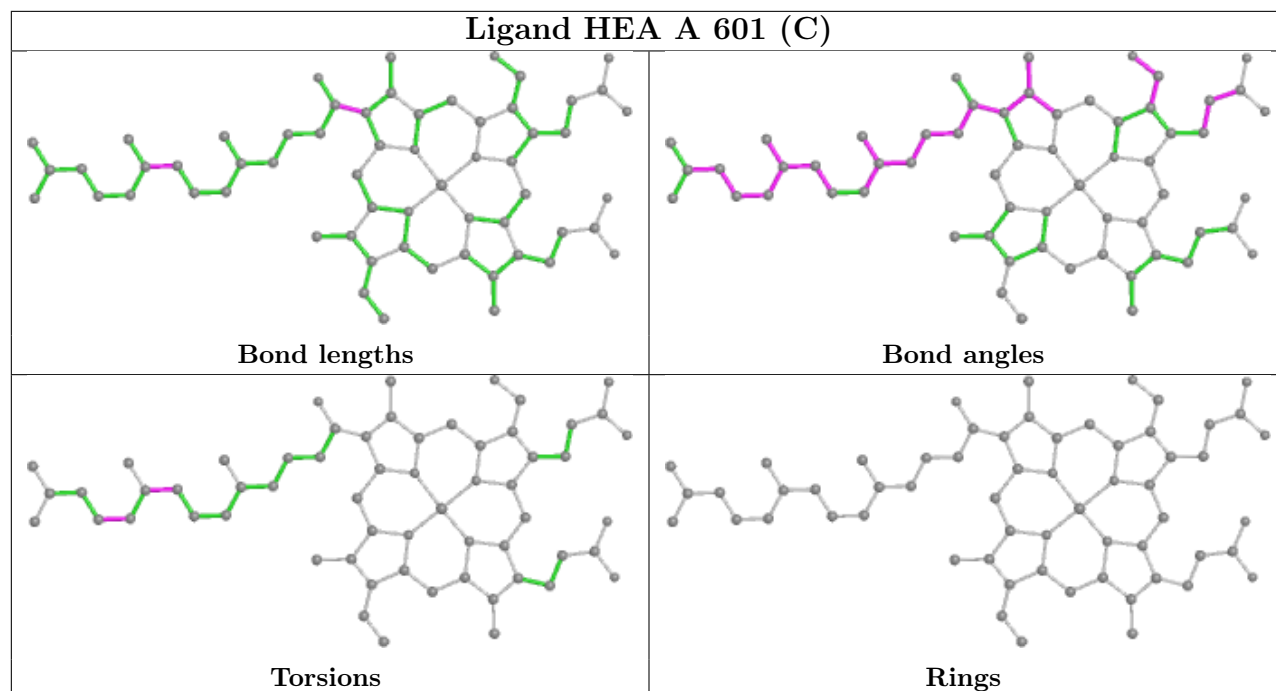
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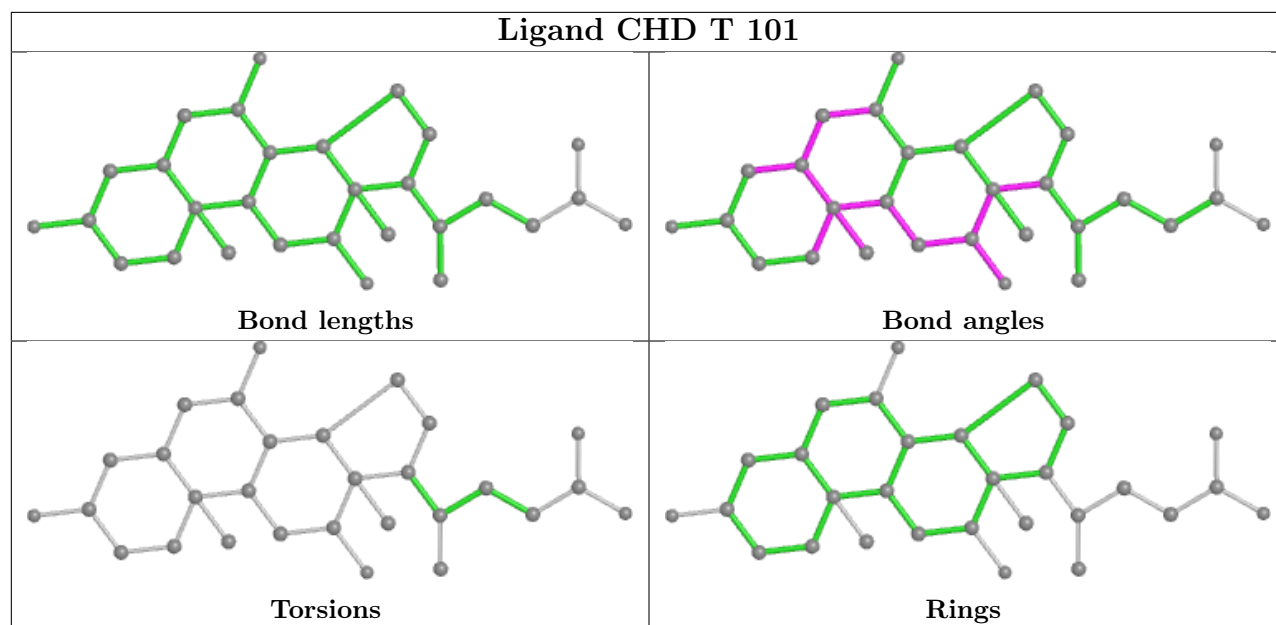
Ligand PGV A 608

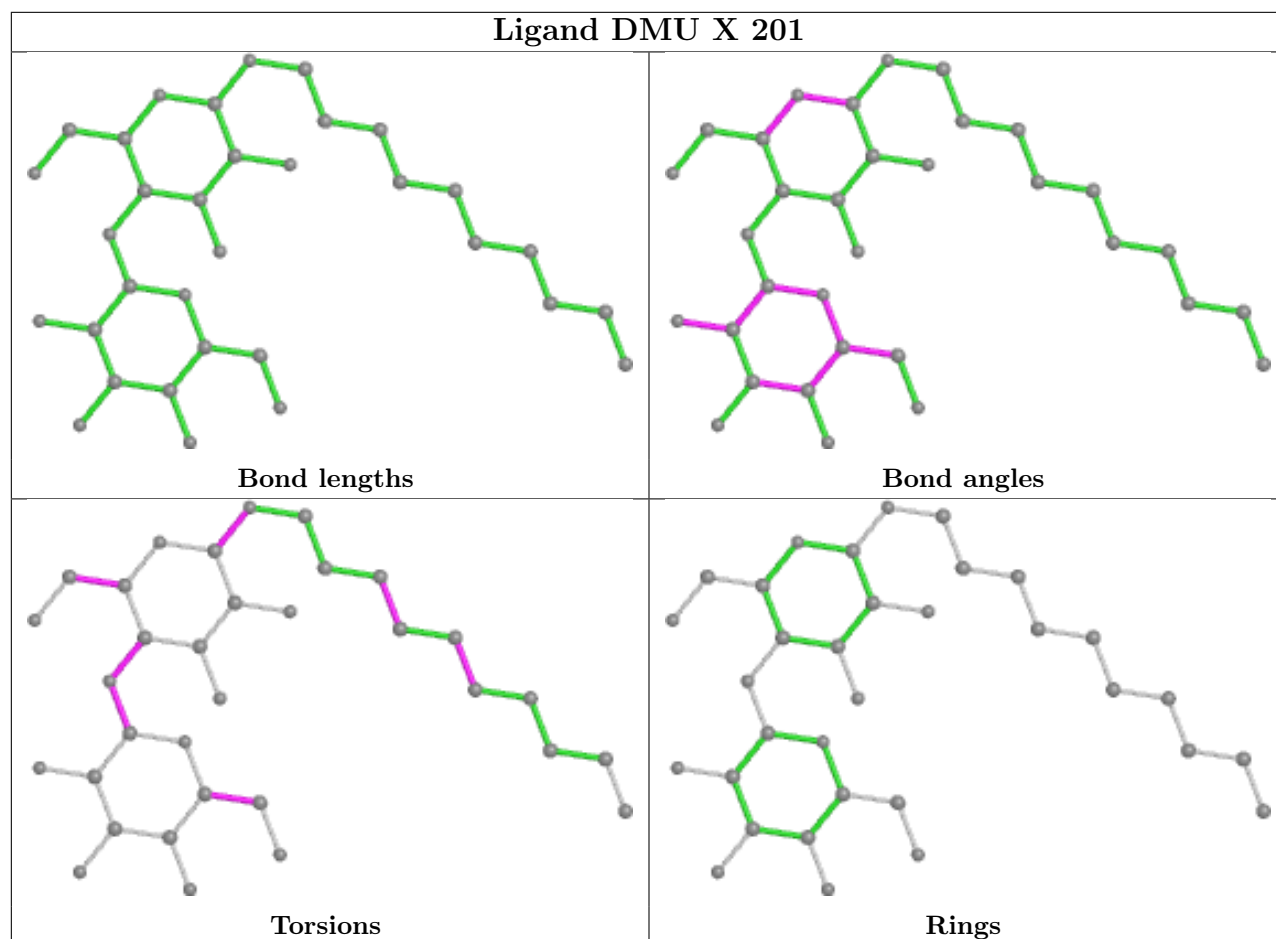
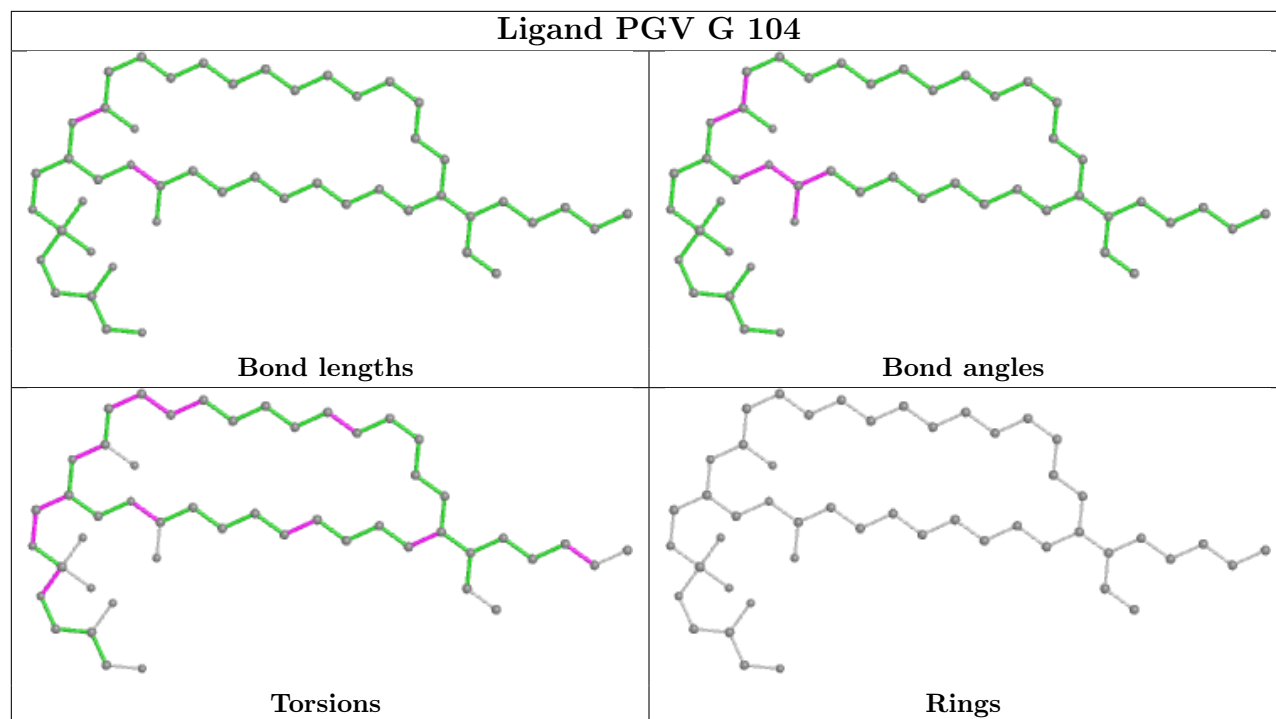


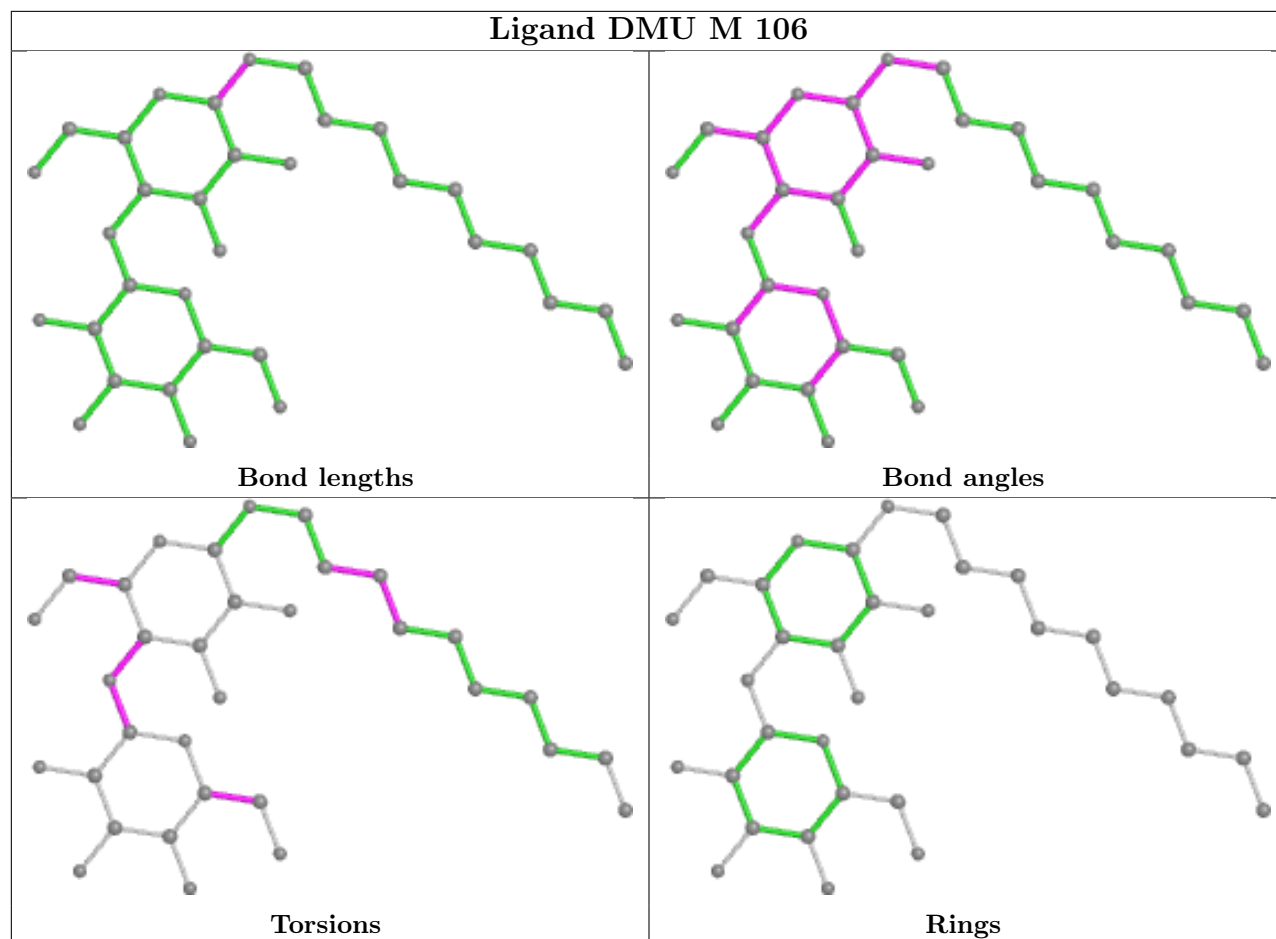
Ligand HEA A 601 (C)

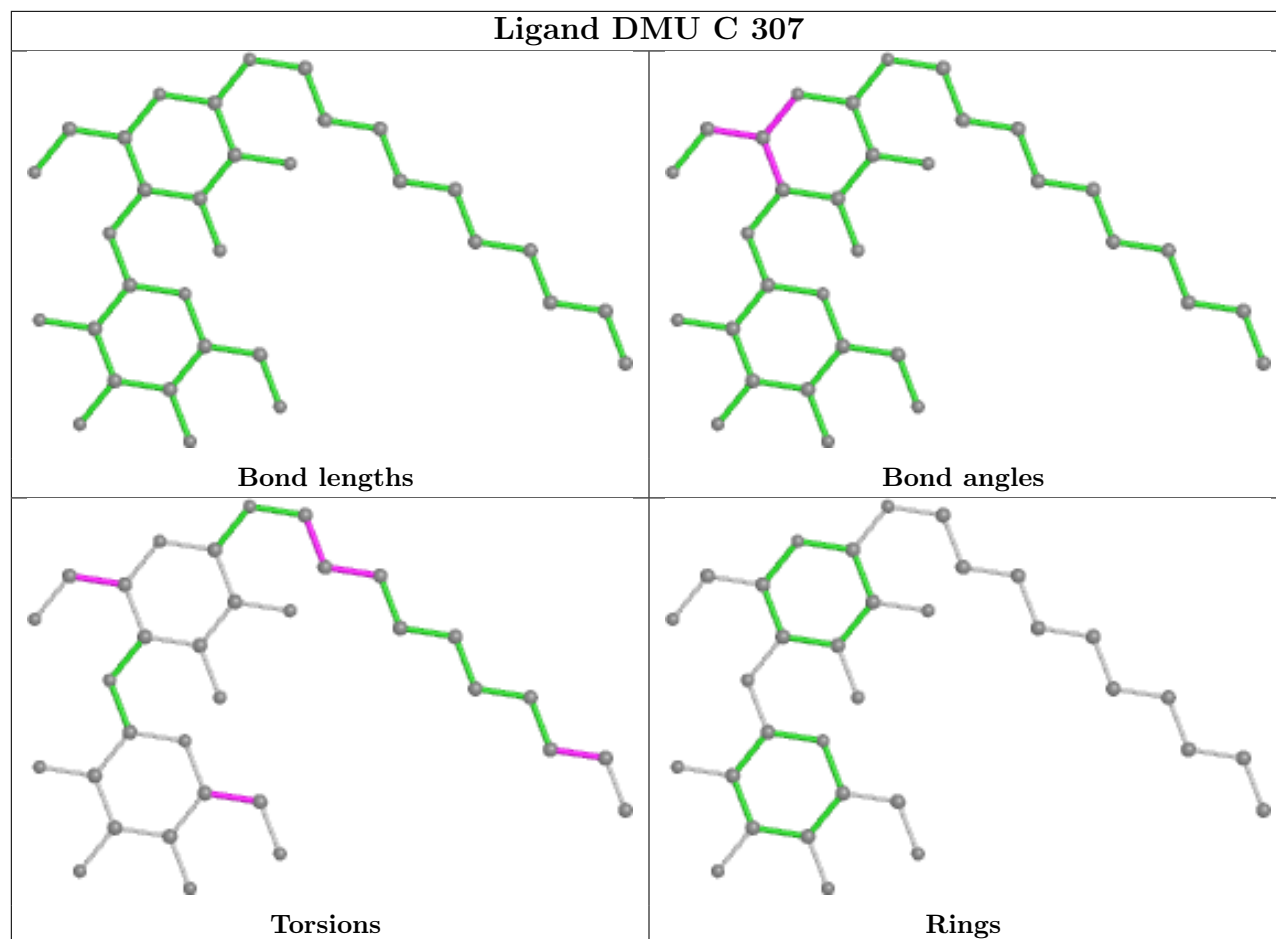


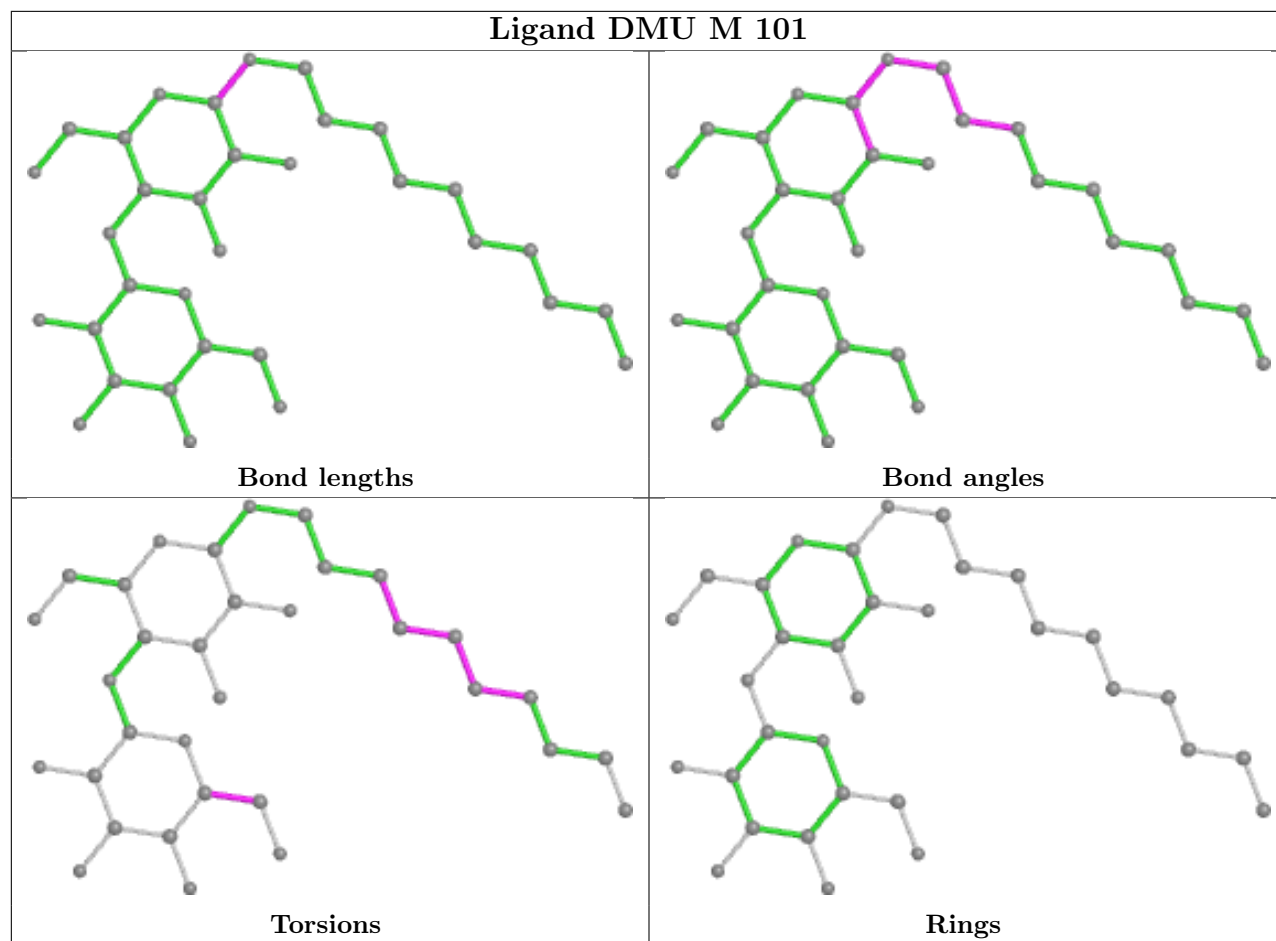
Ligand CHD T 101

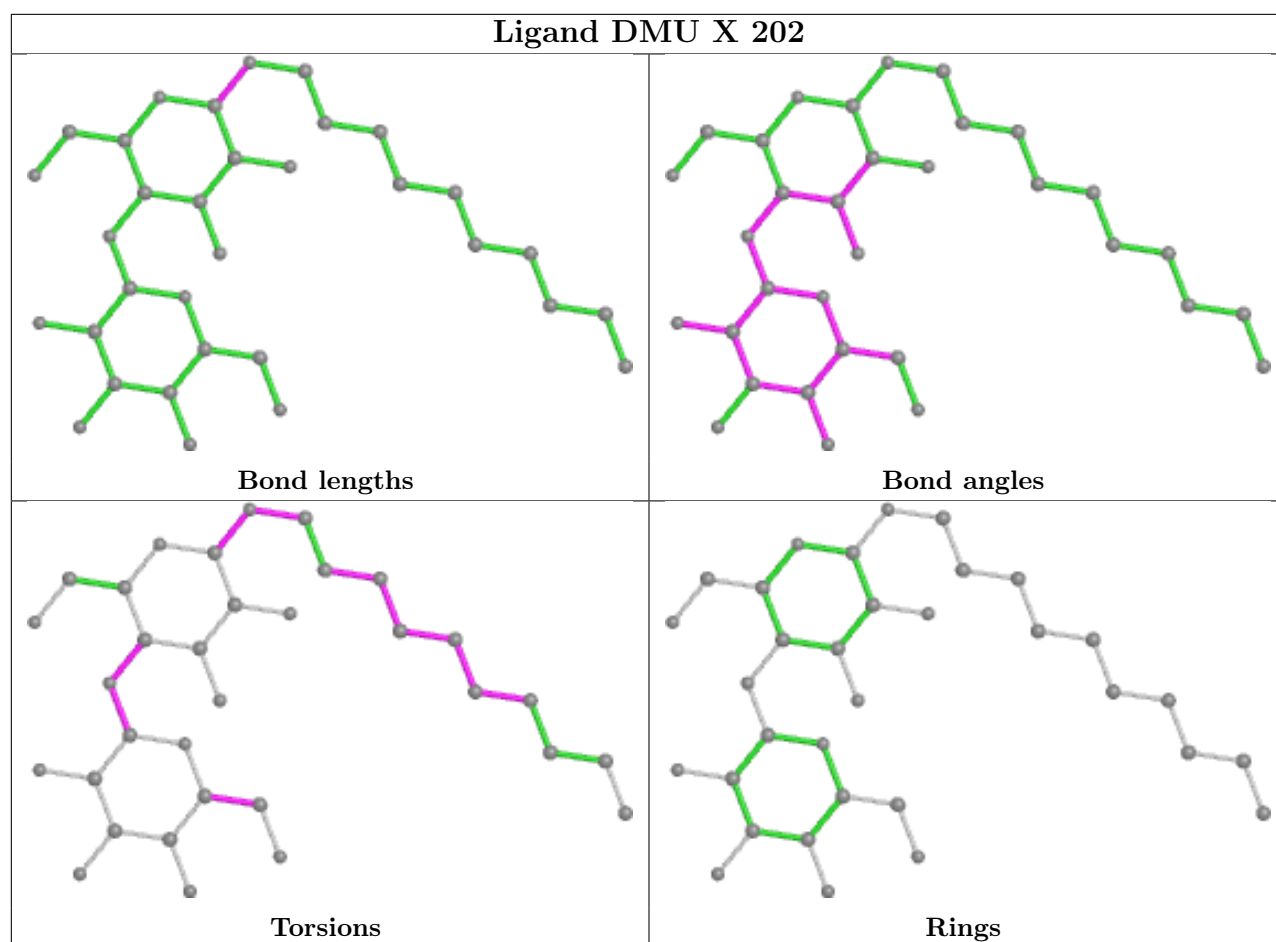


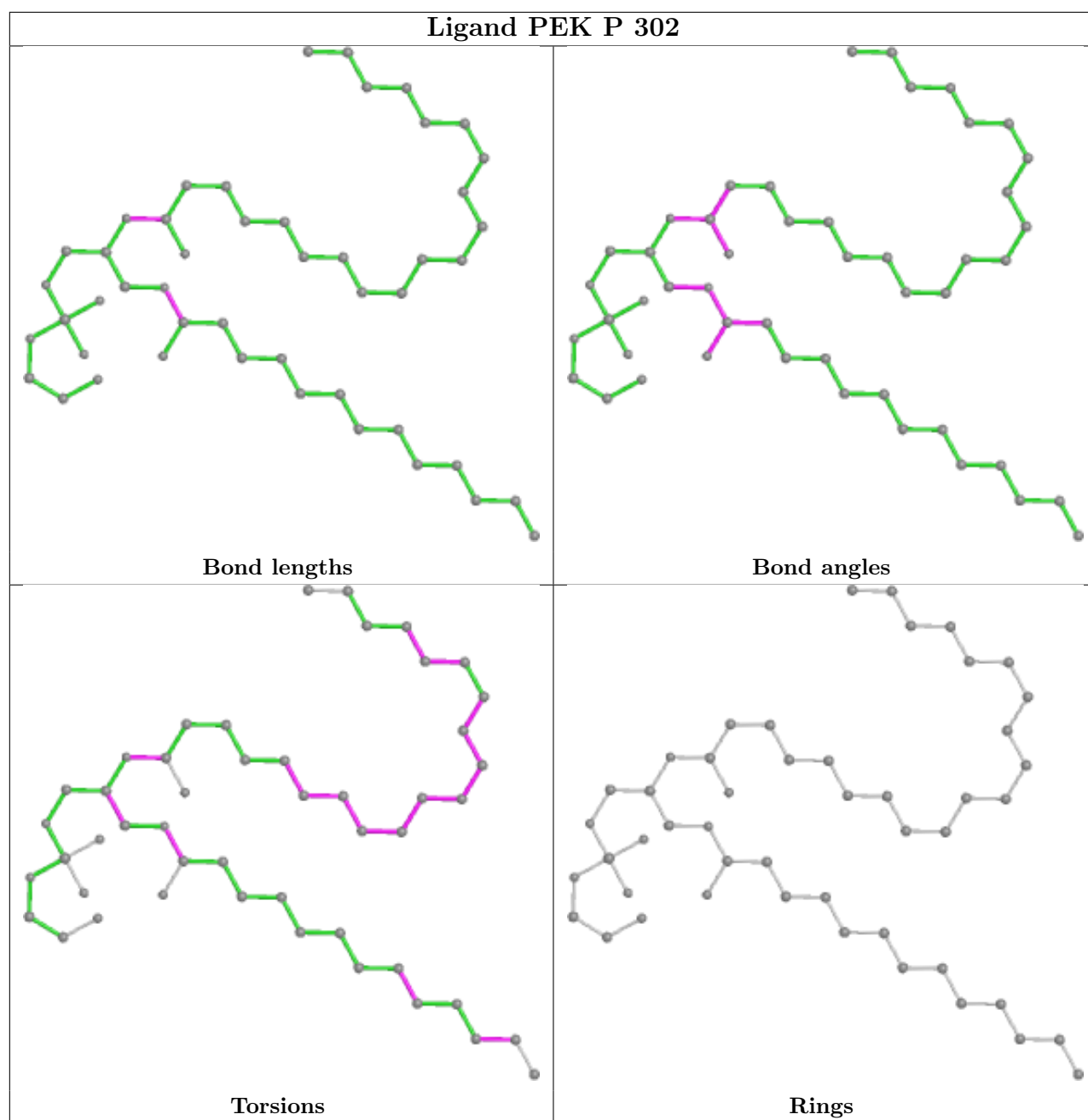




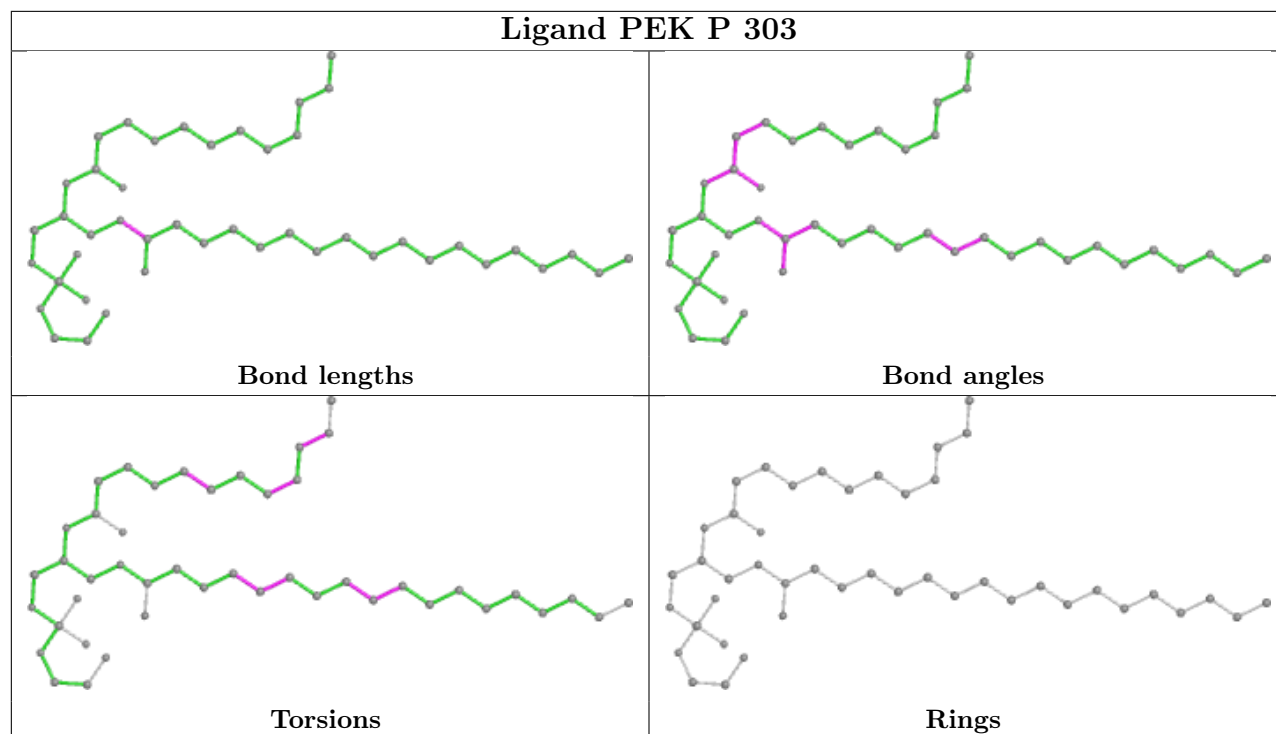




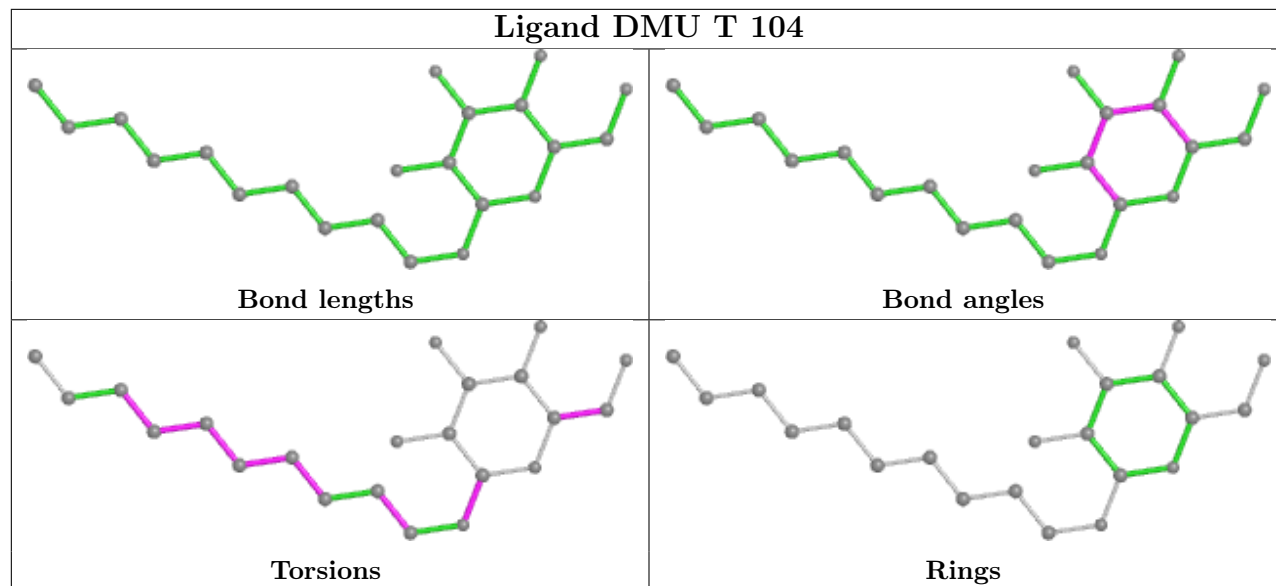


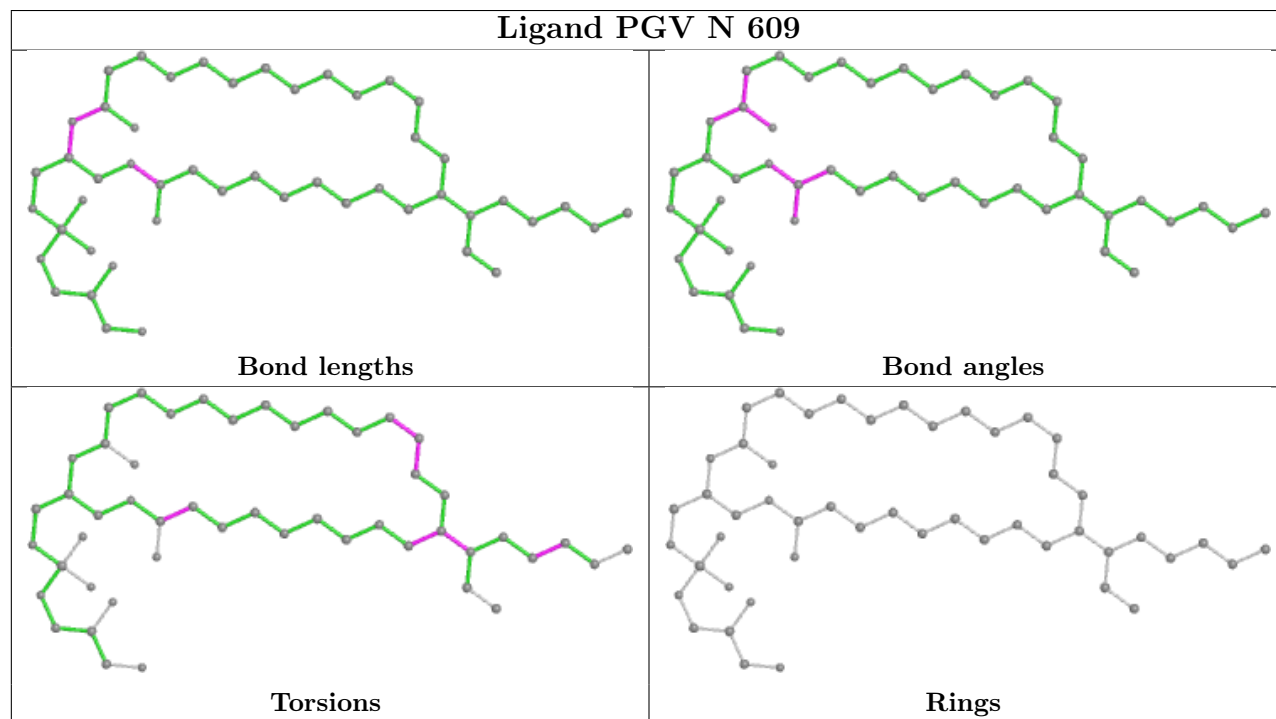
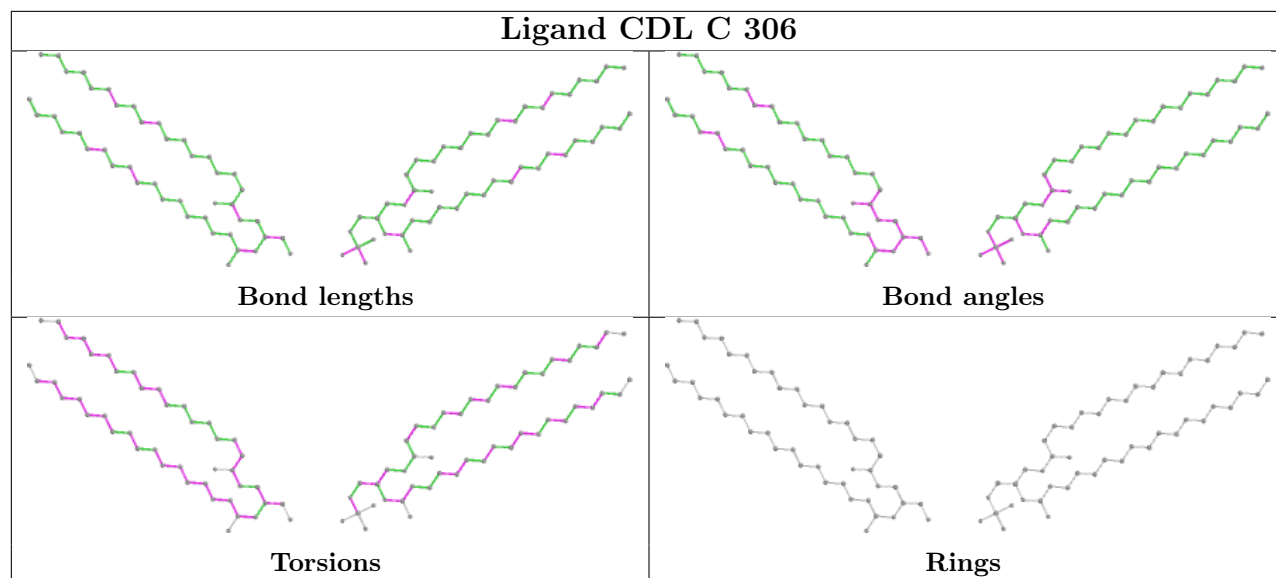


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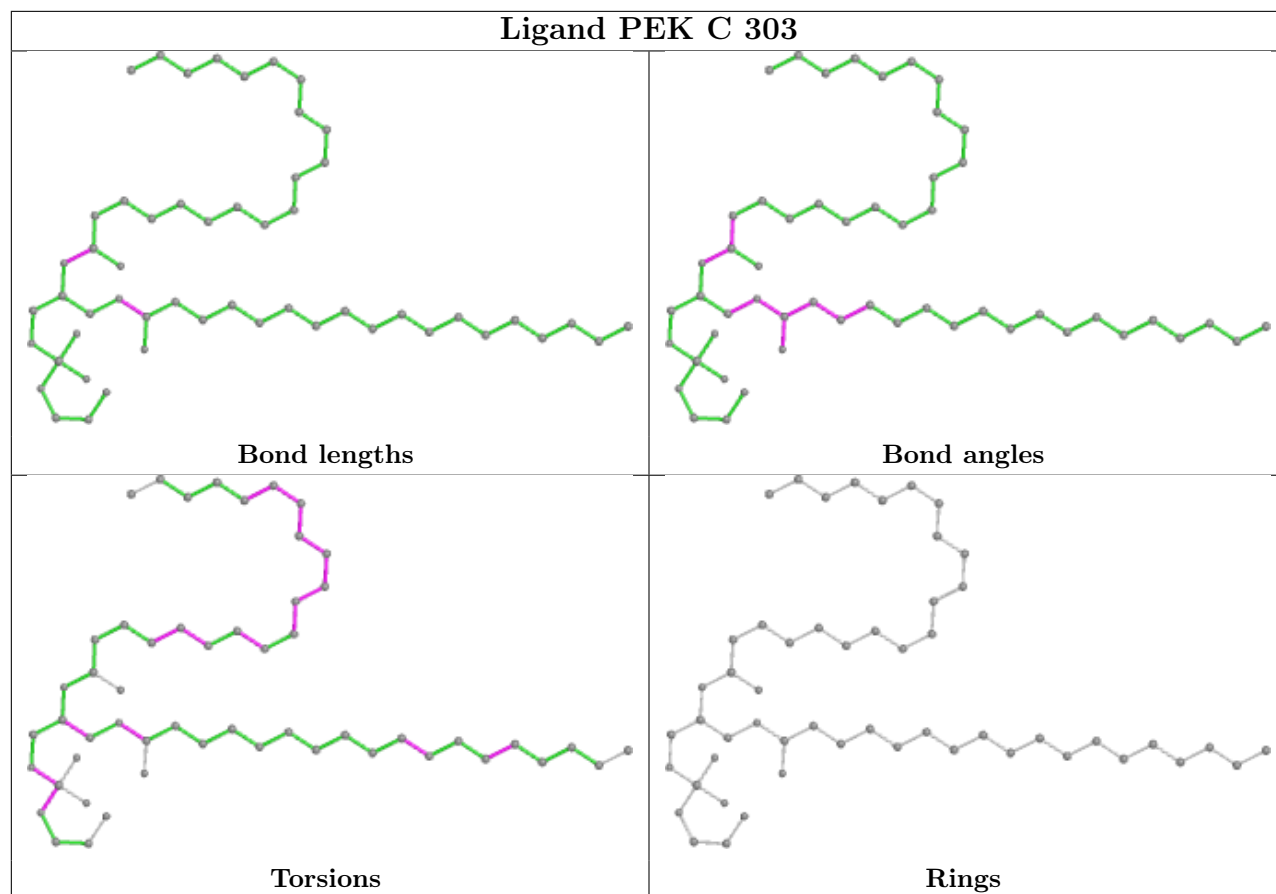


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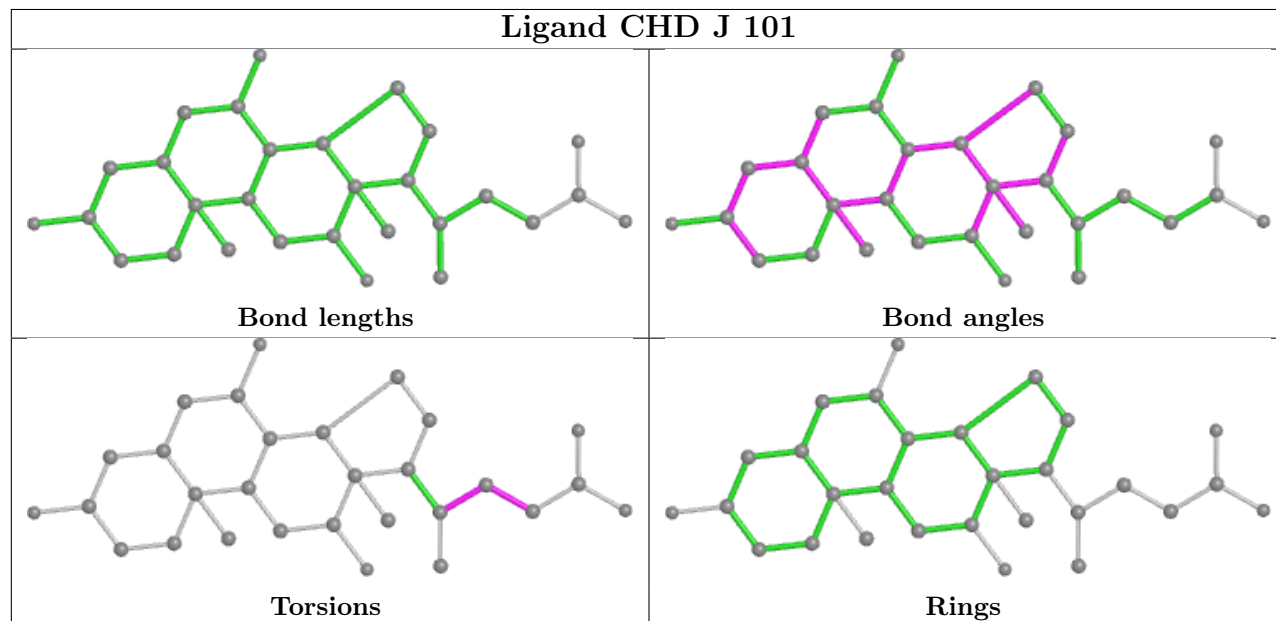


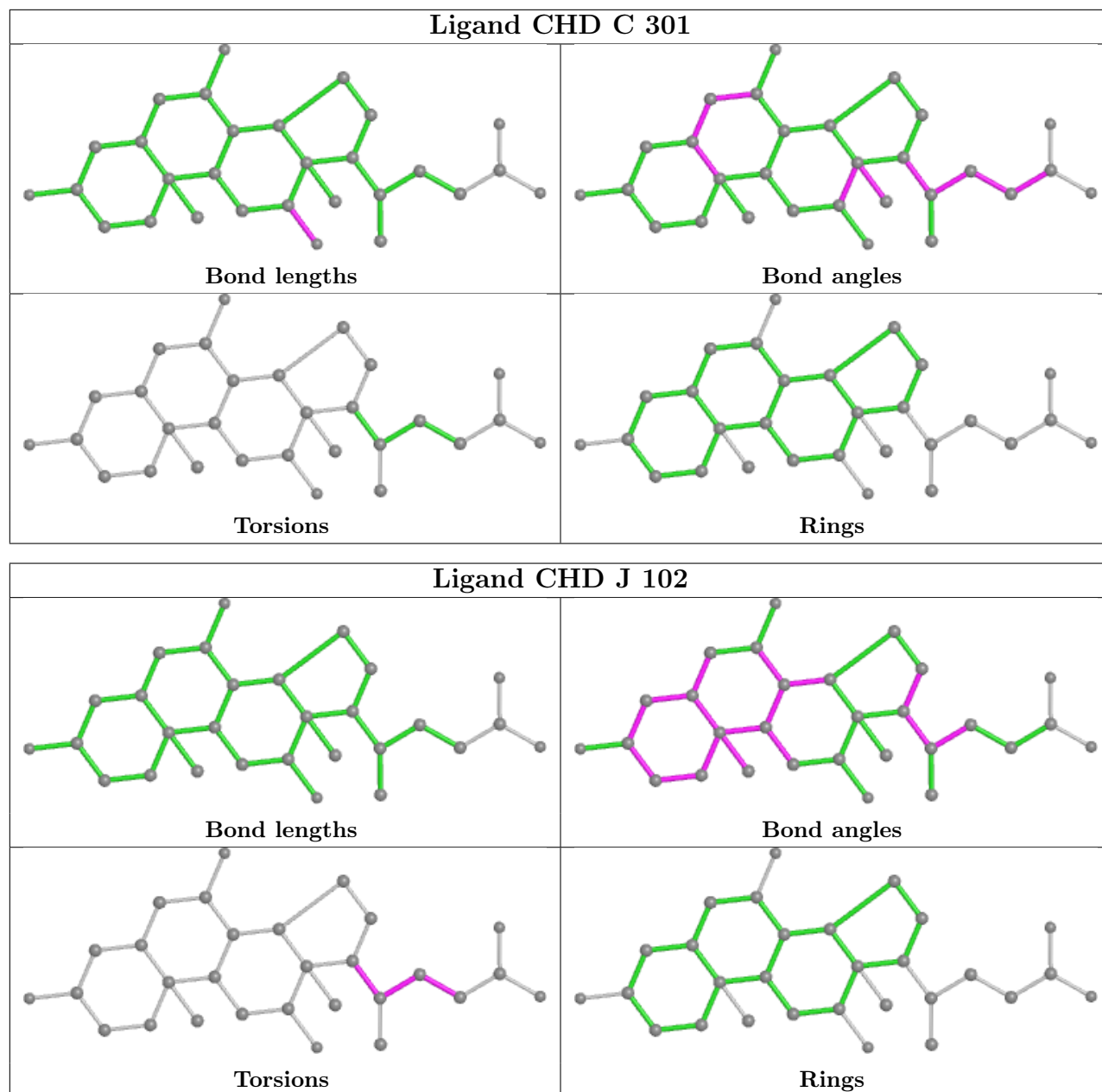


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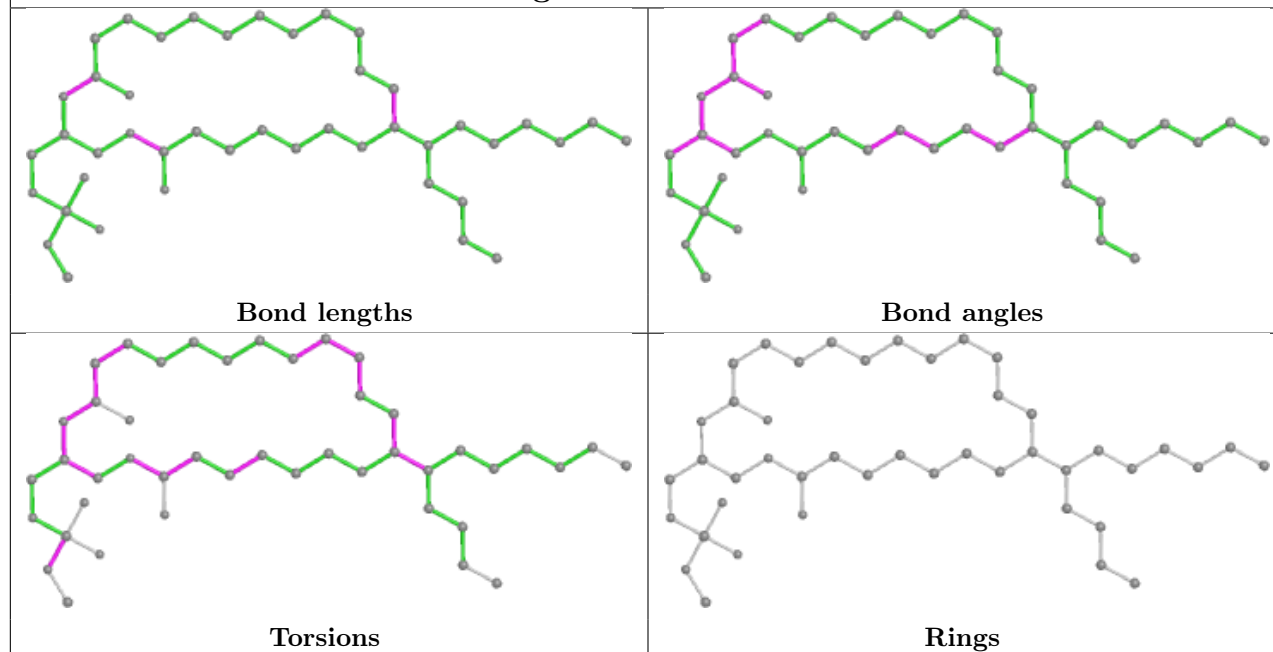


Ligand CHD J 101

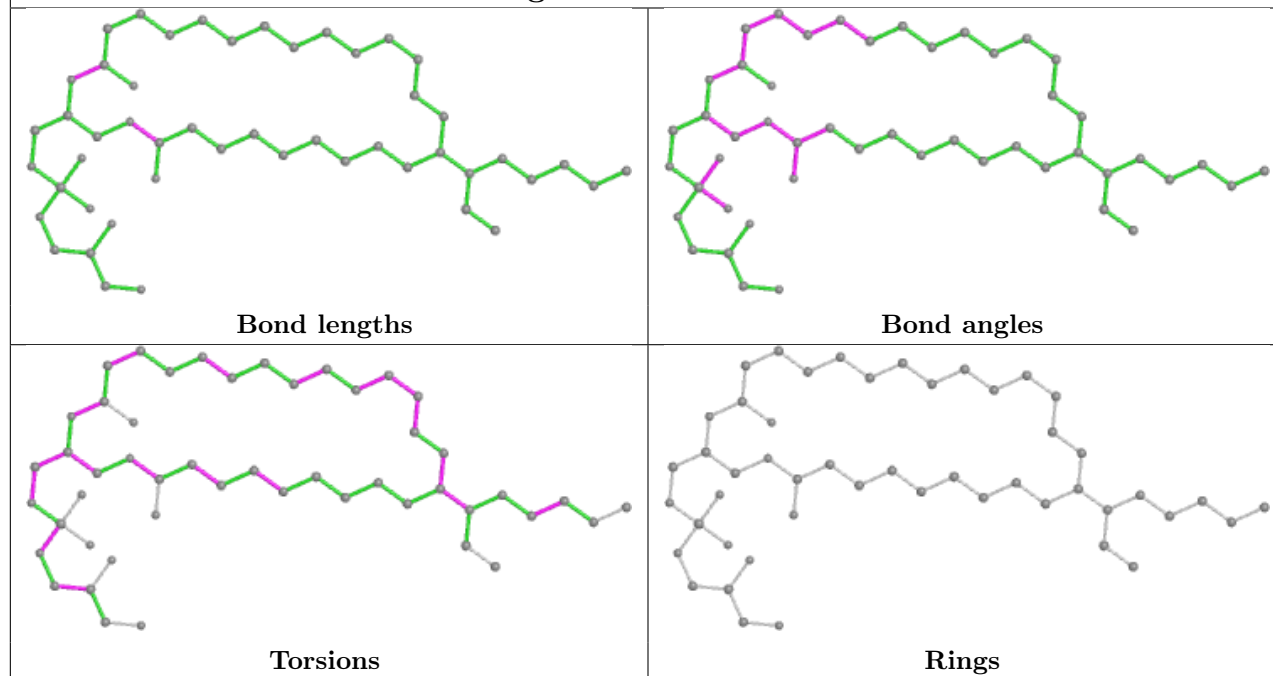


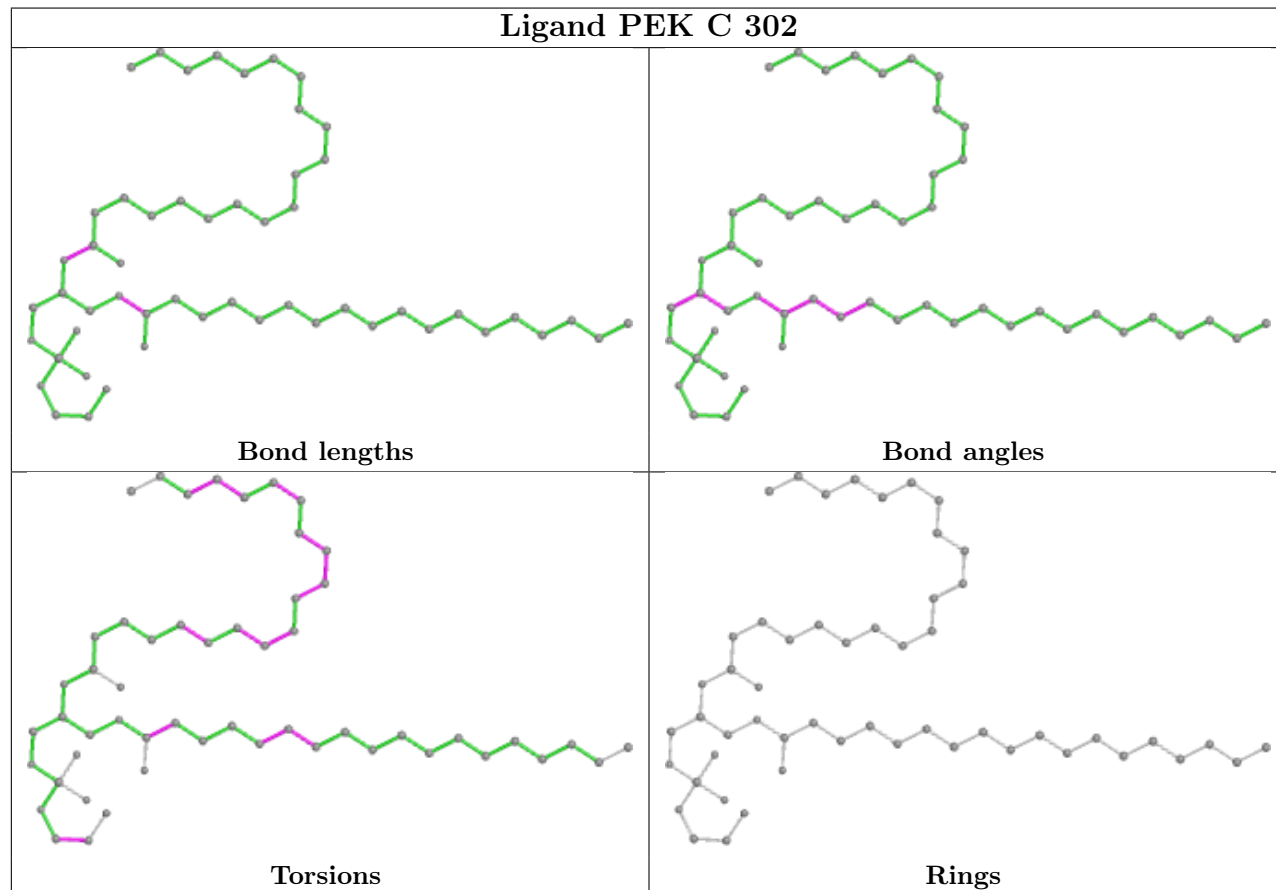
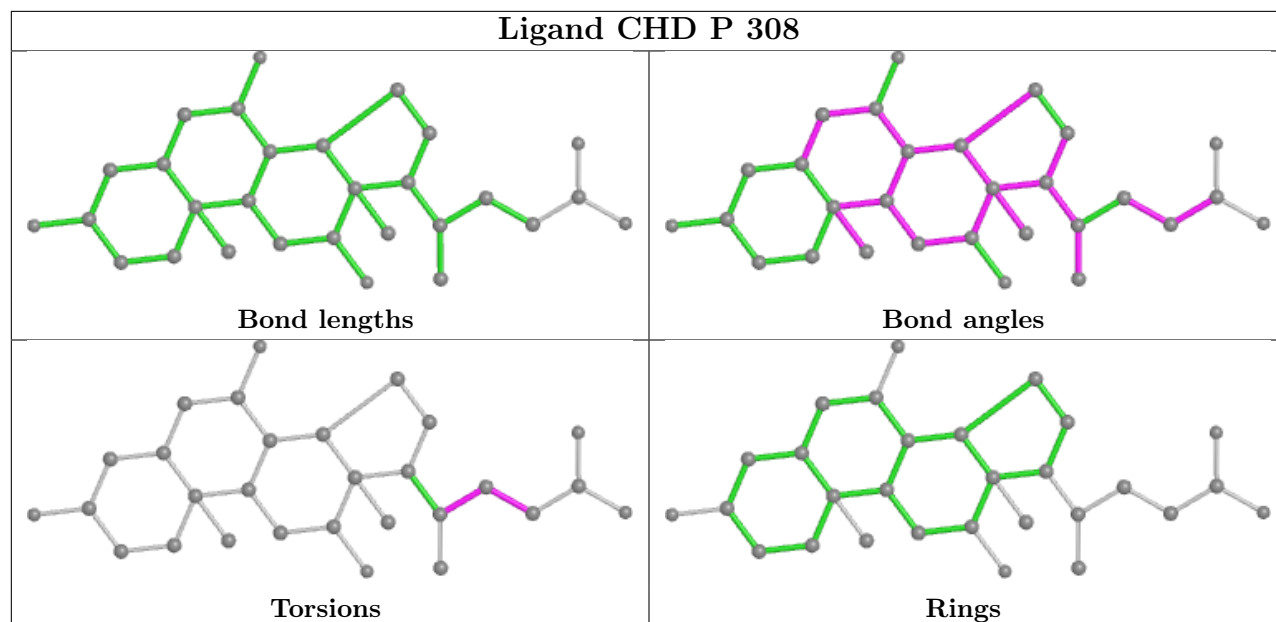


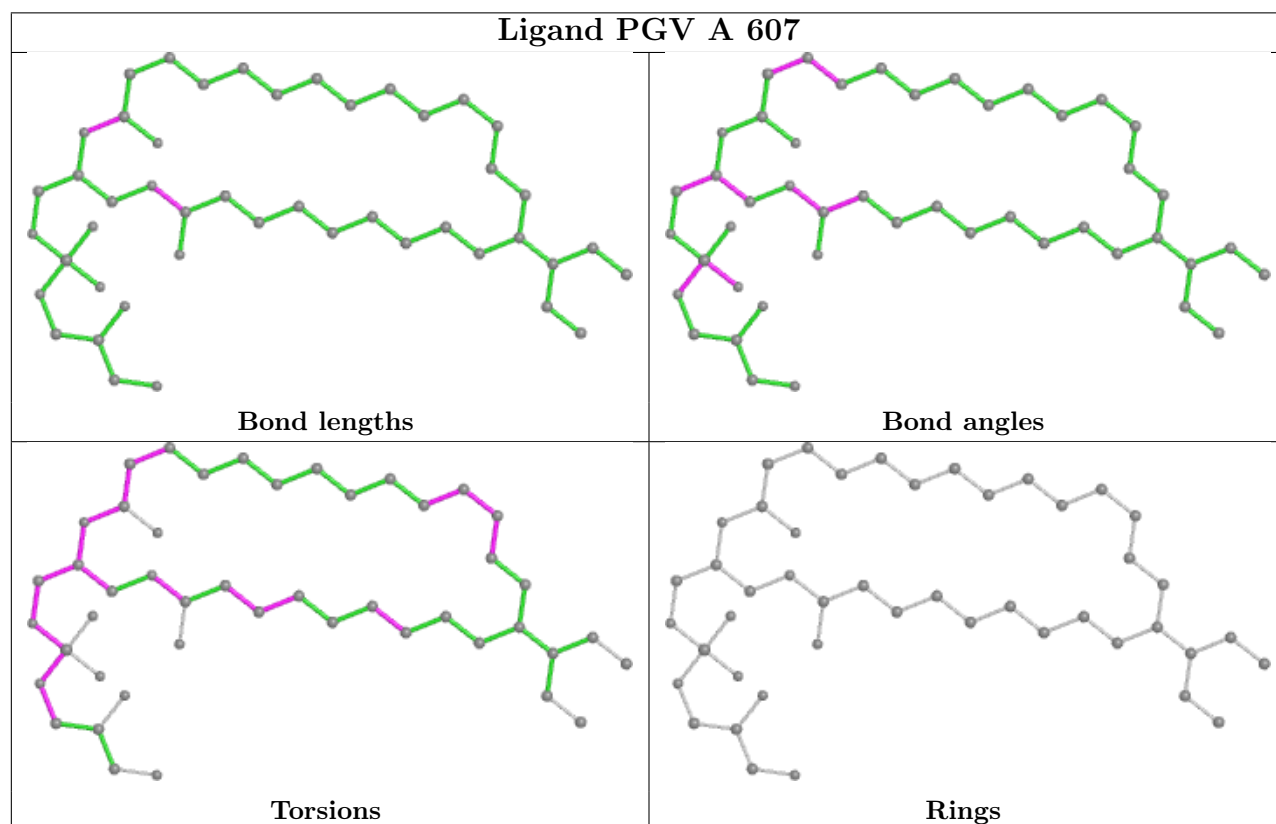
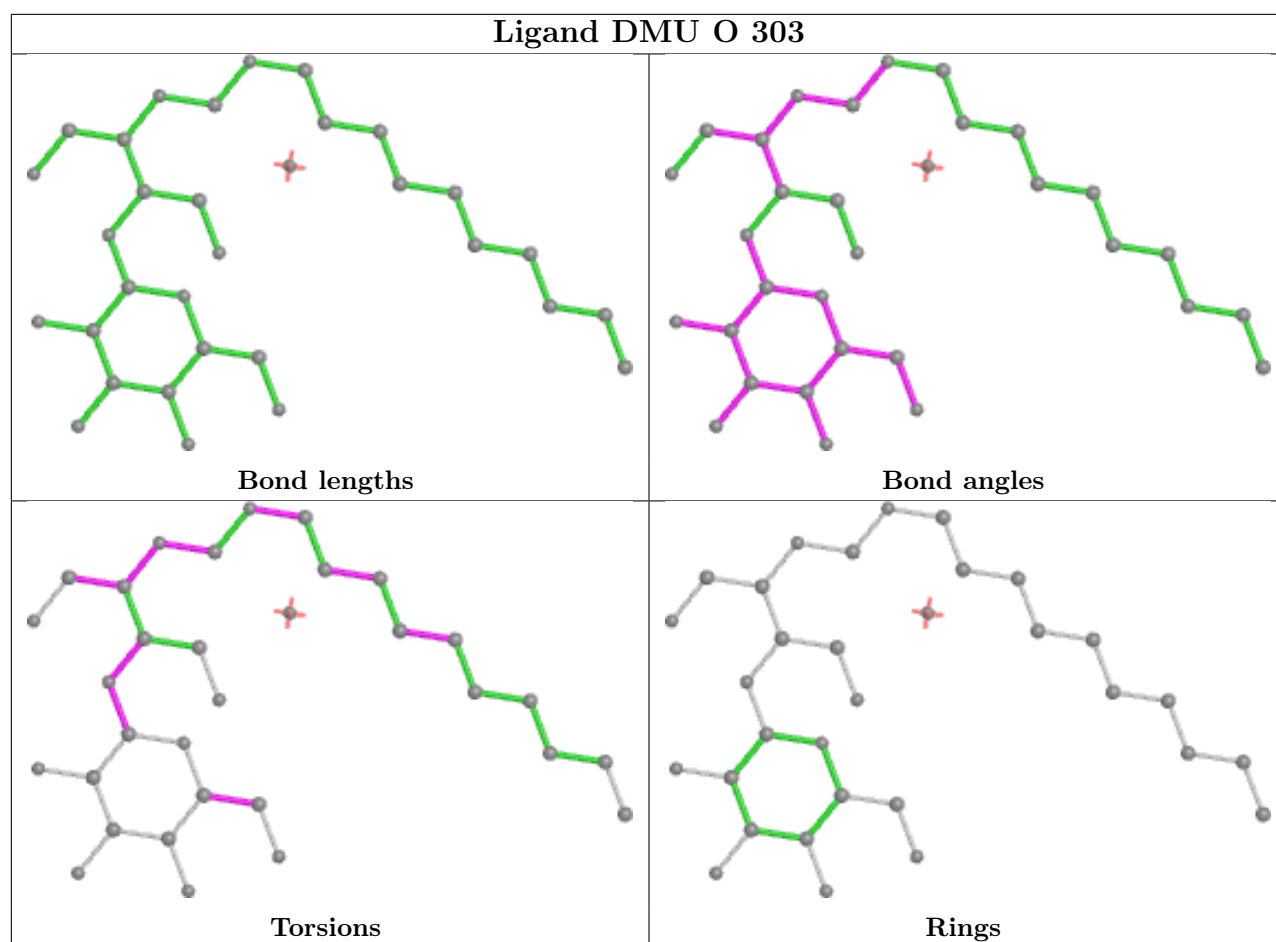
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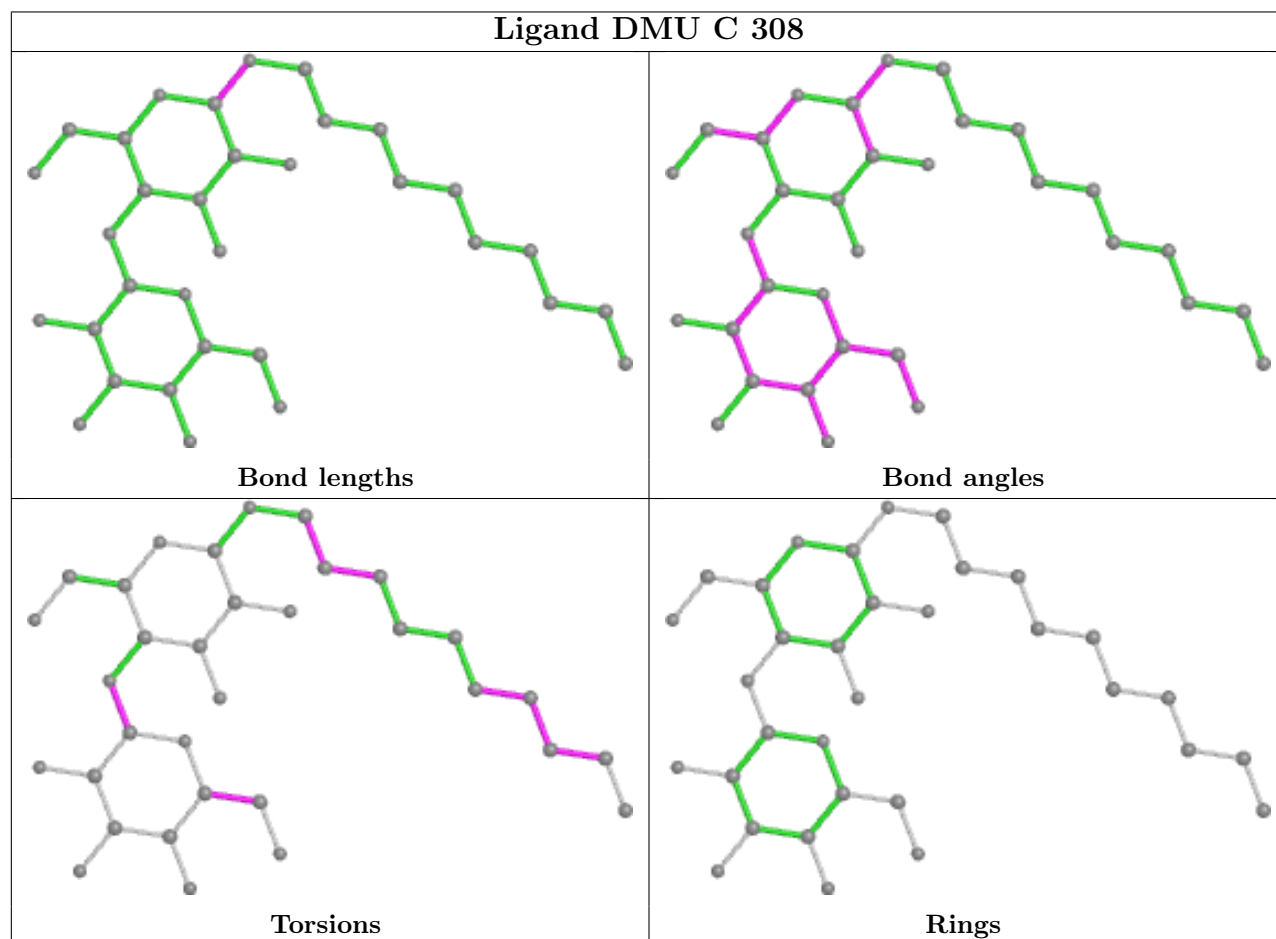
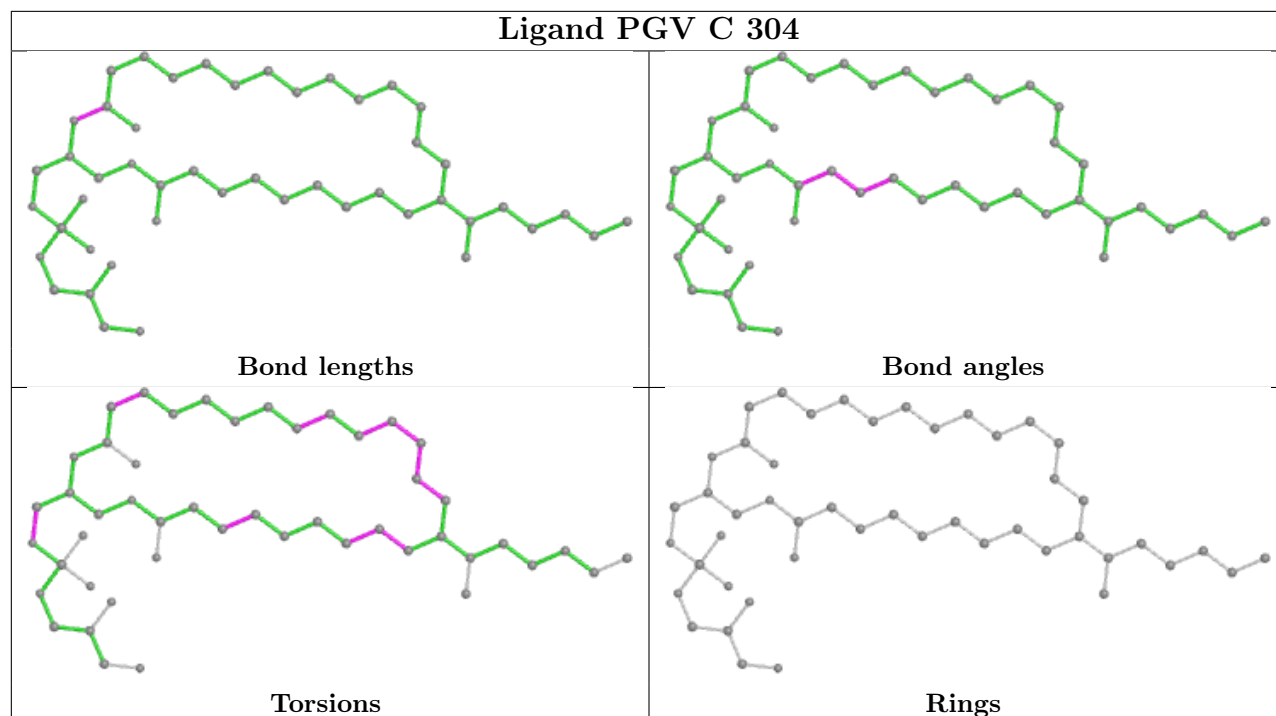


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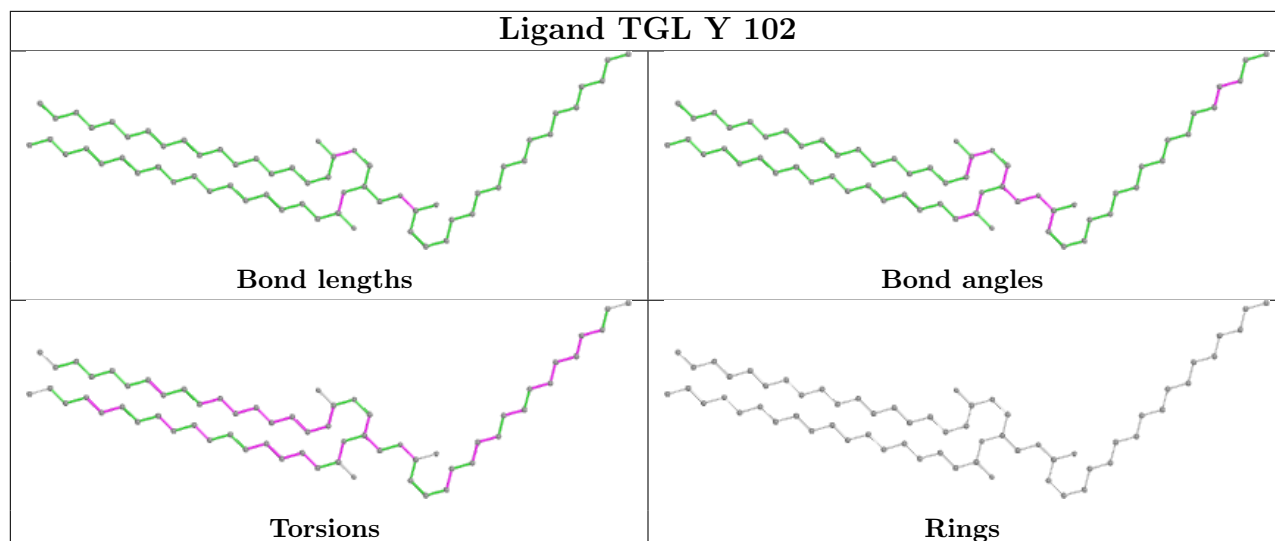




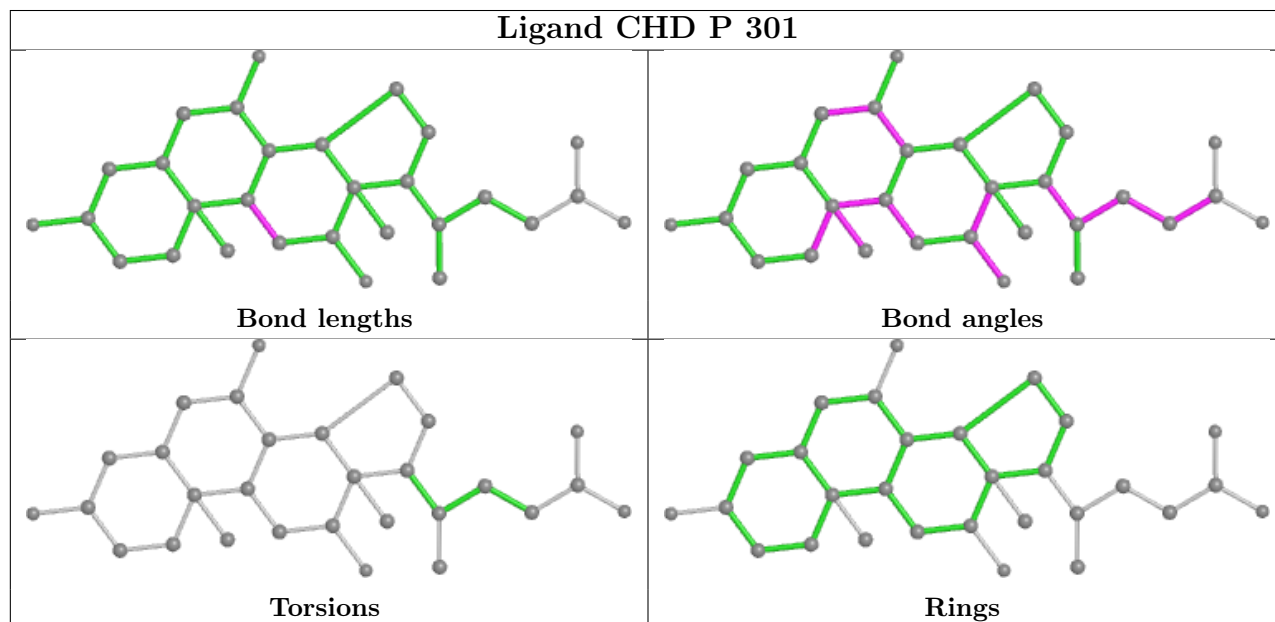




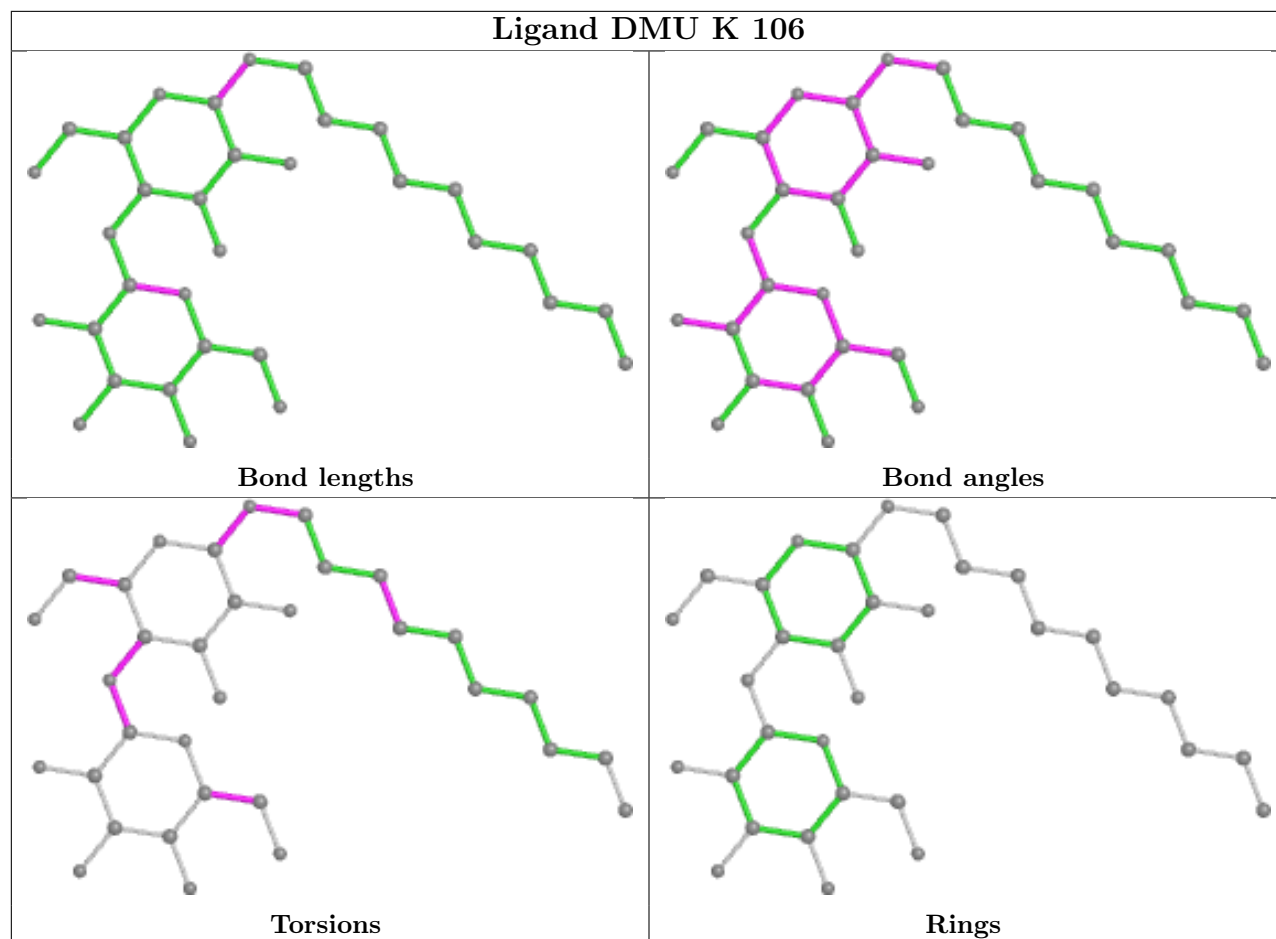
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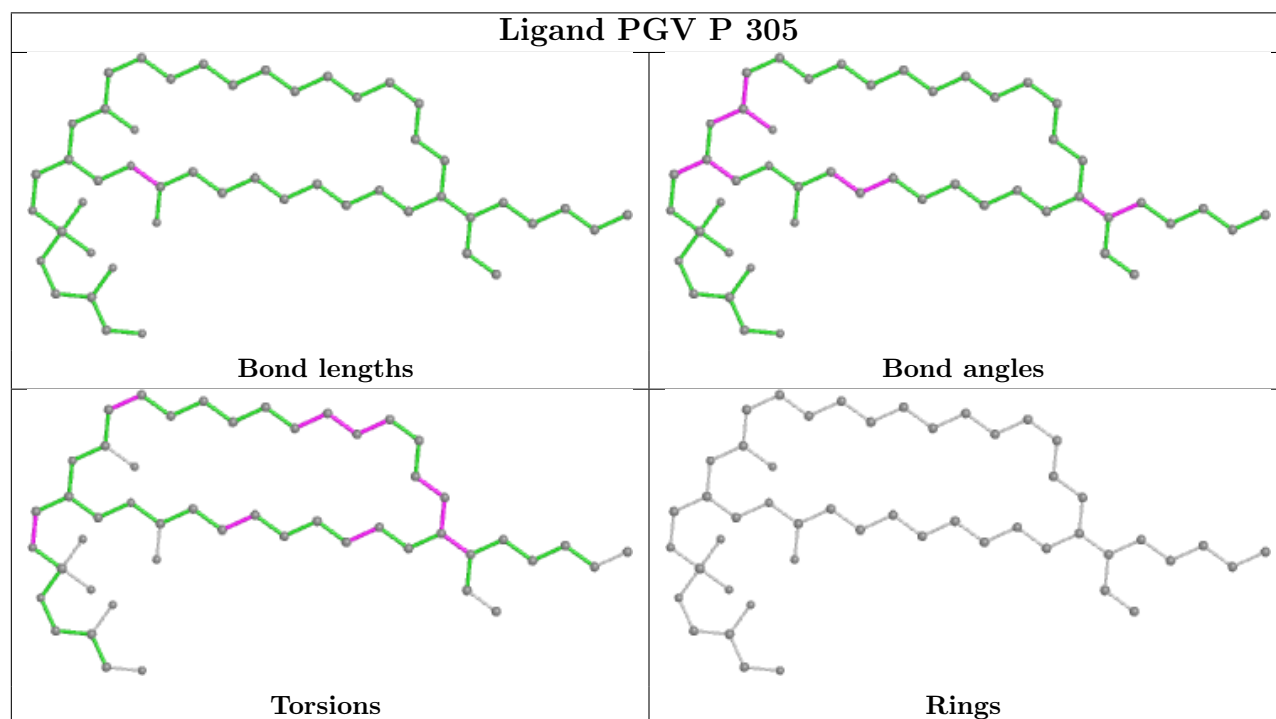
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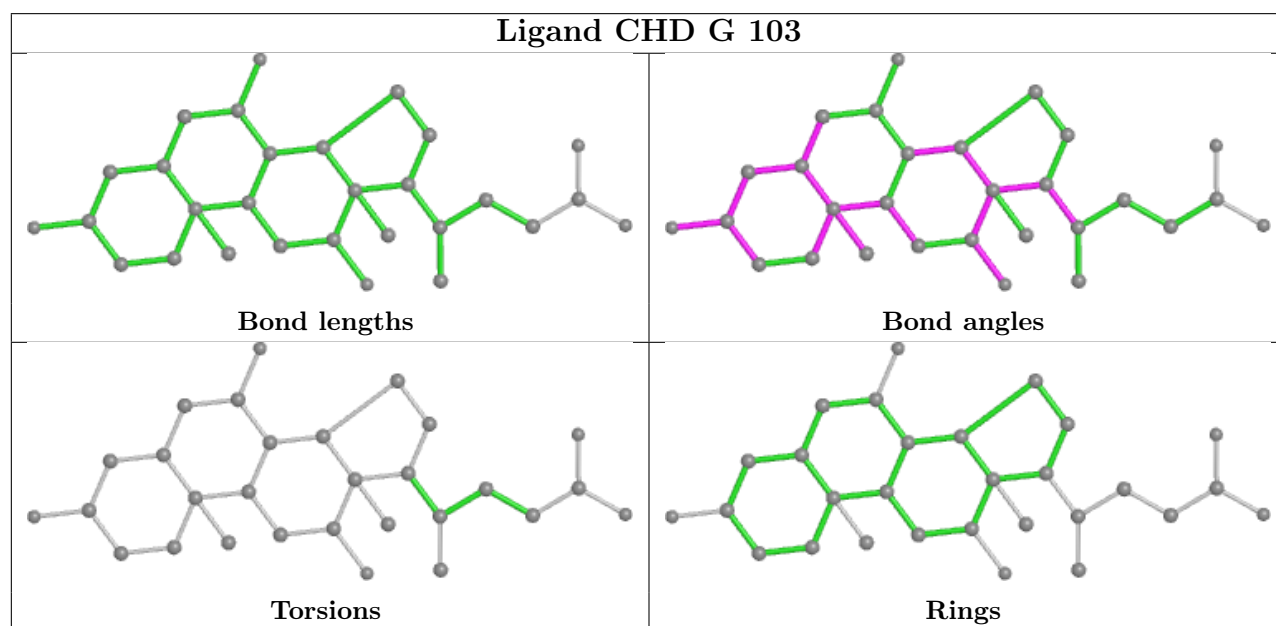
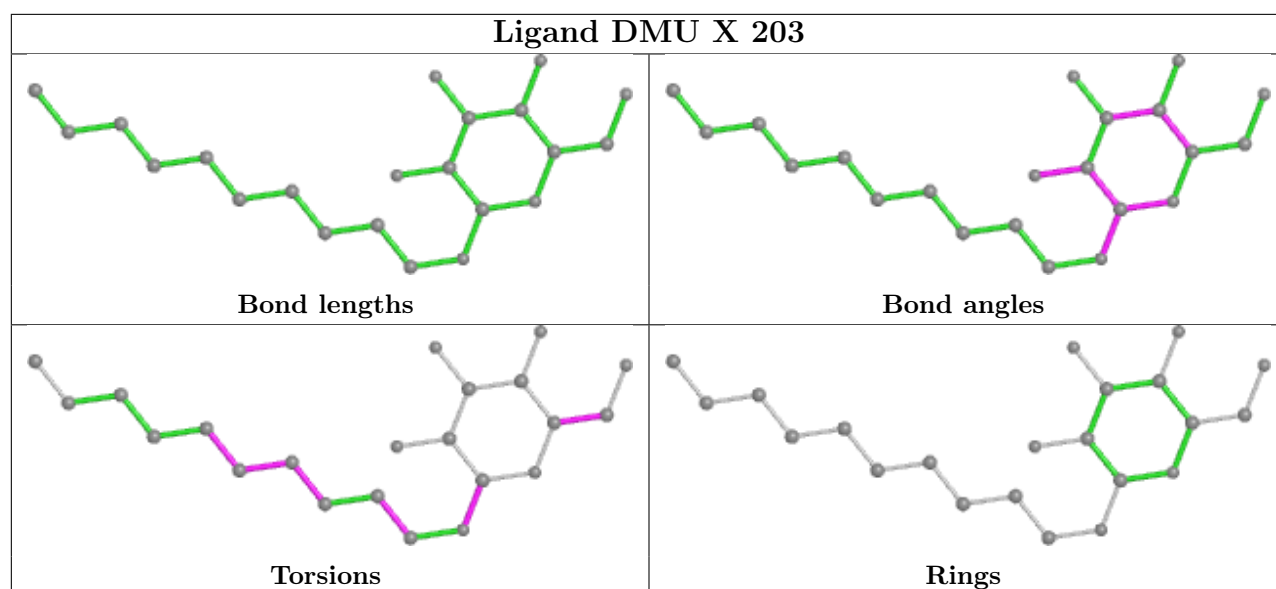


Ligand DMU K 106

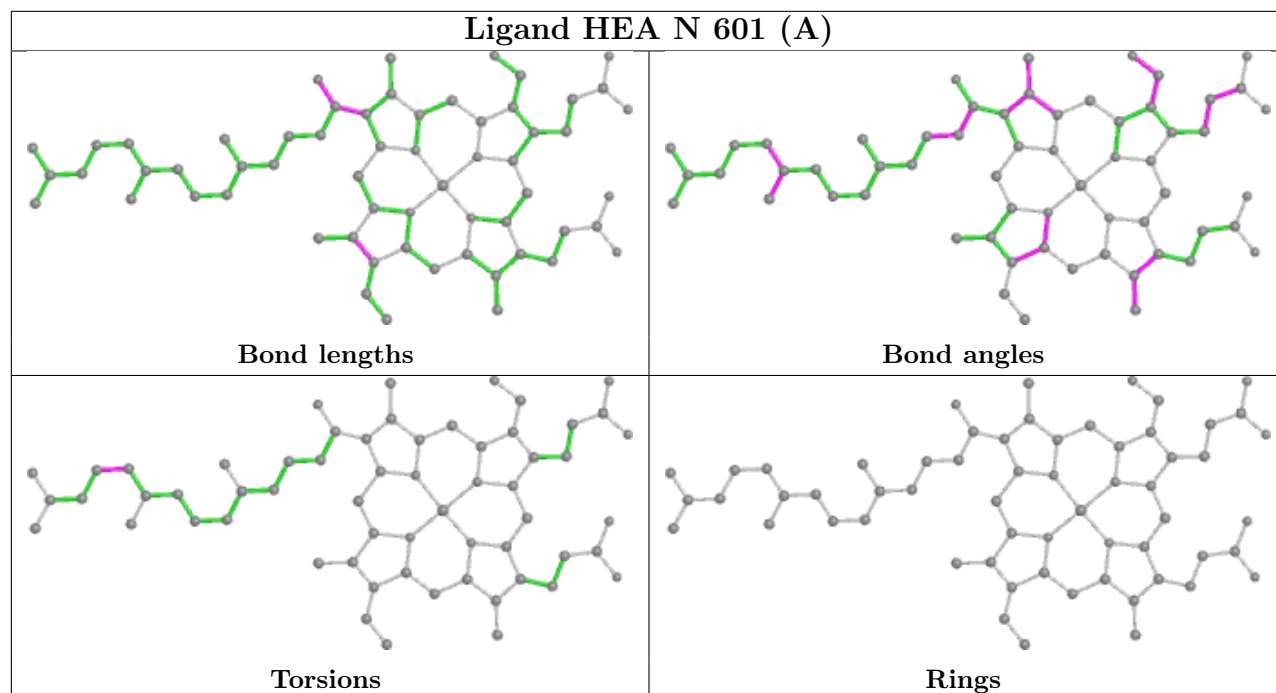


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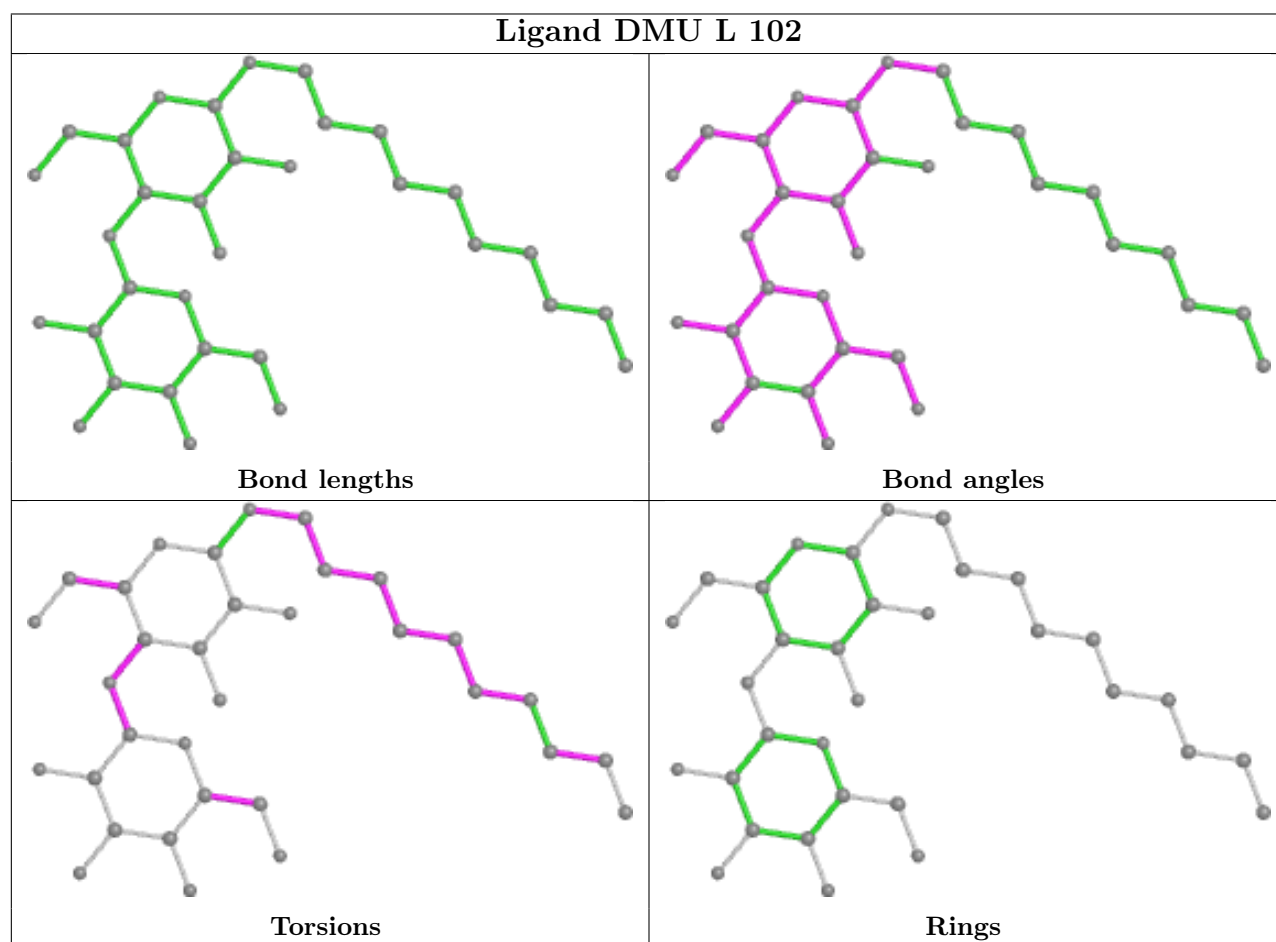


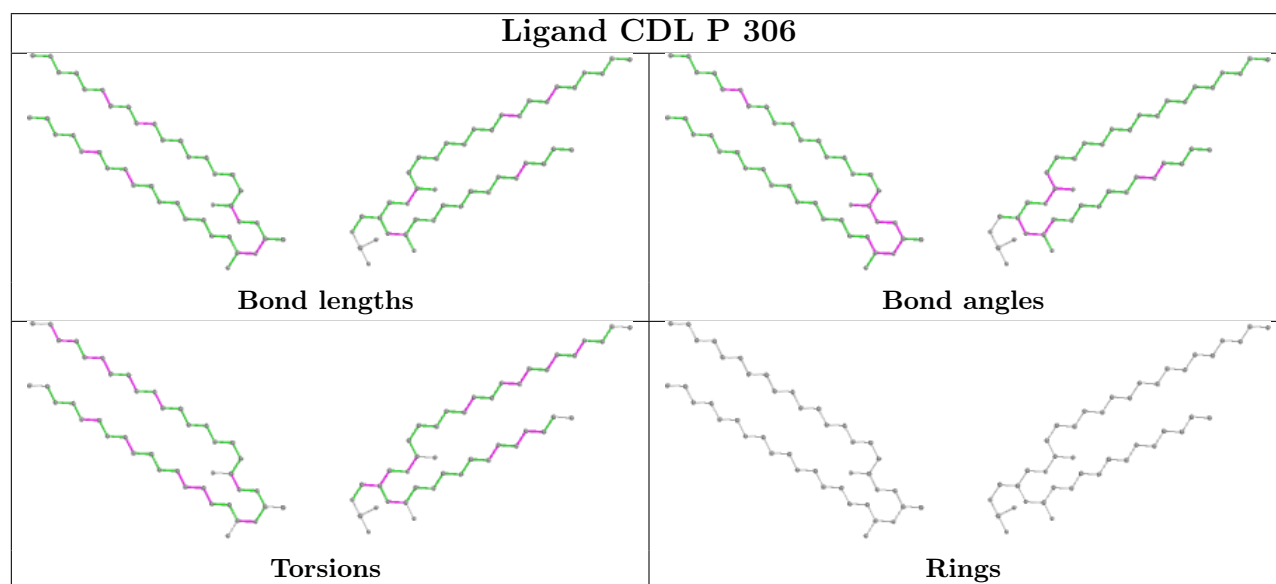
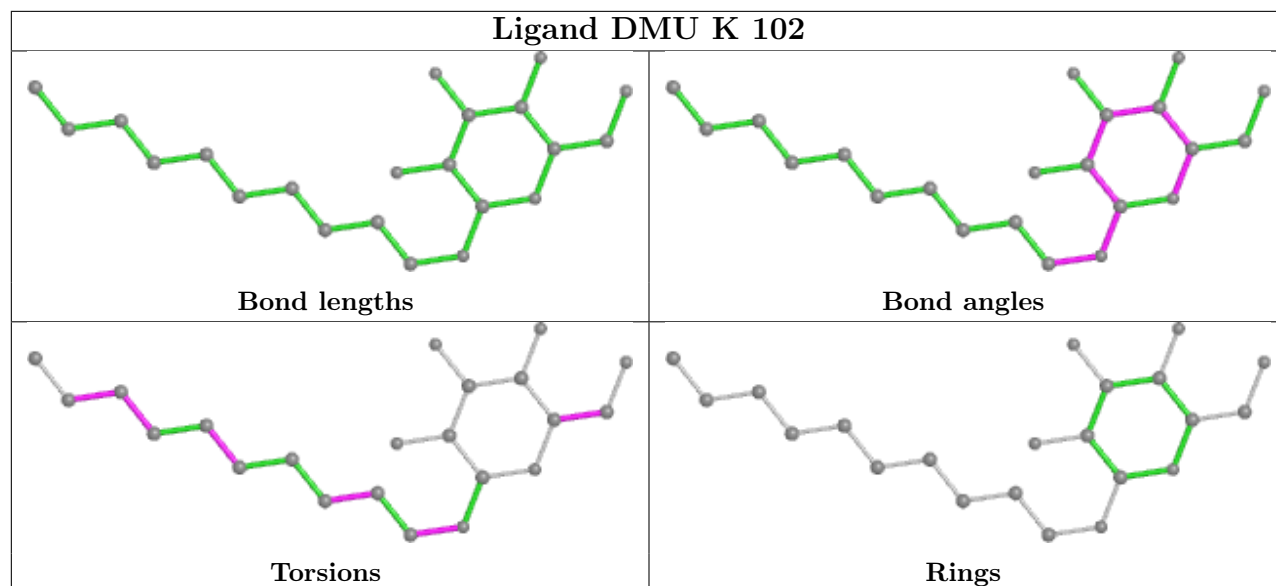


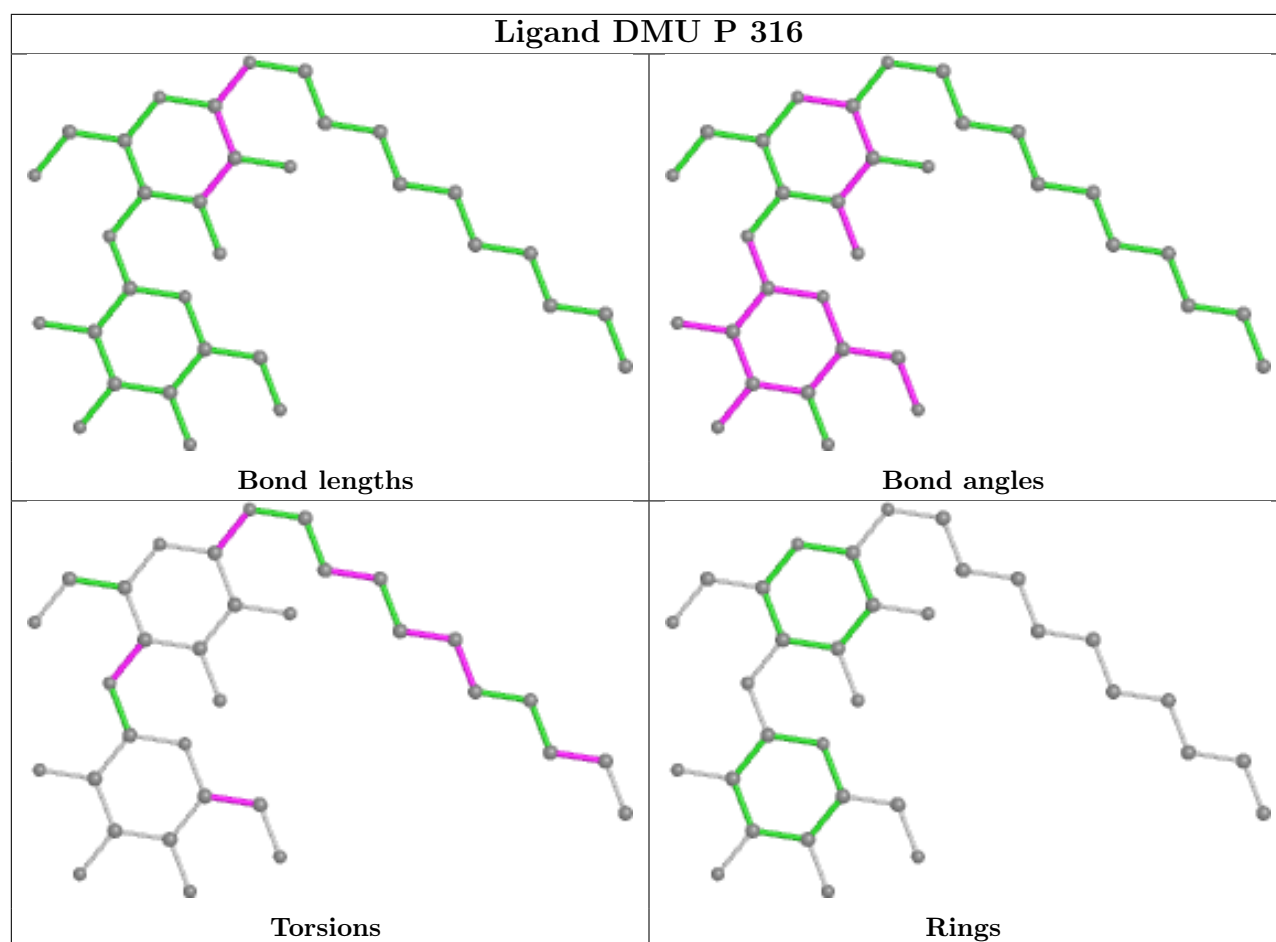
Ligand HEA N 601 (A)



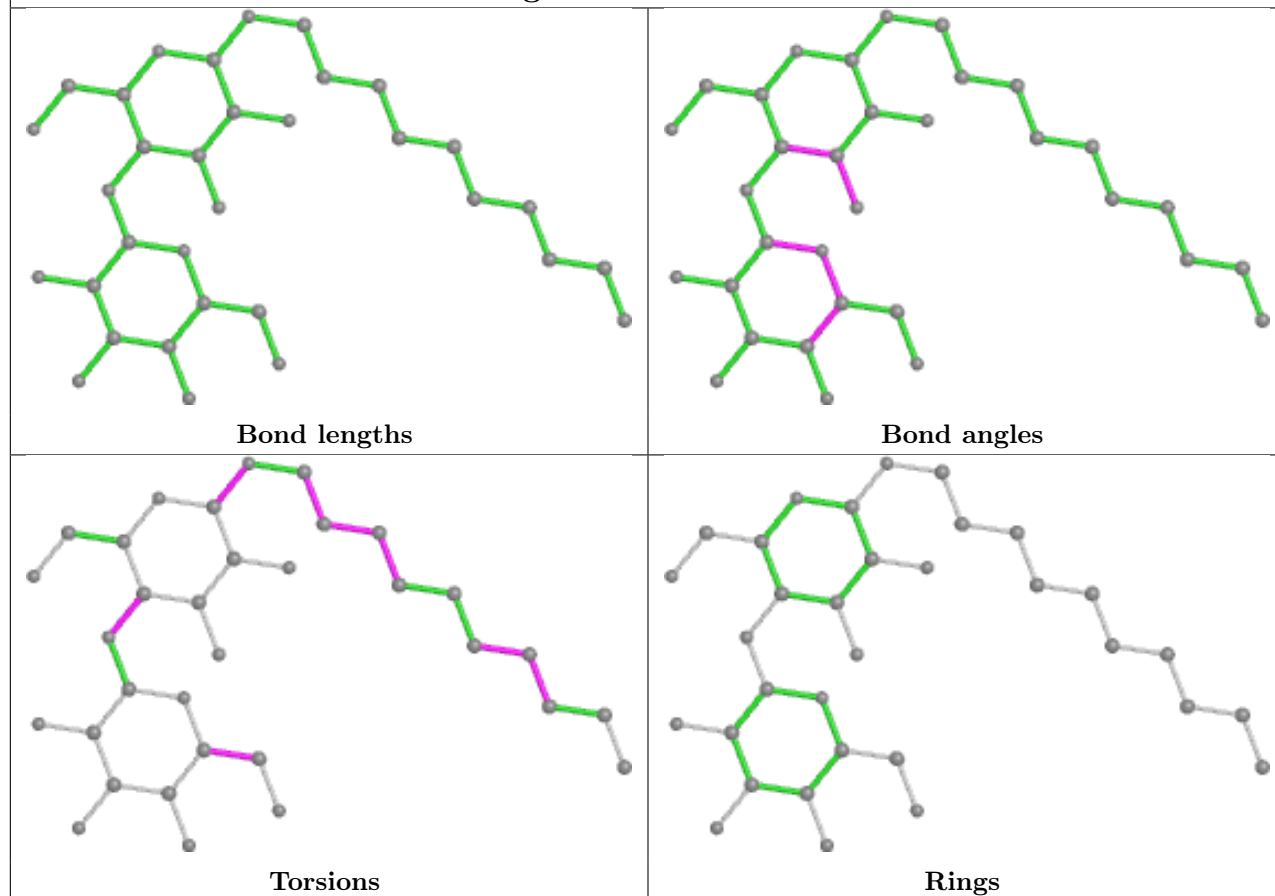
Ligand DMU L 102



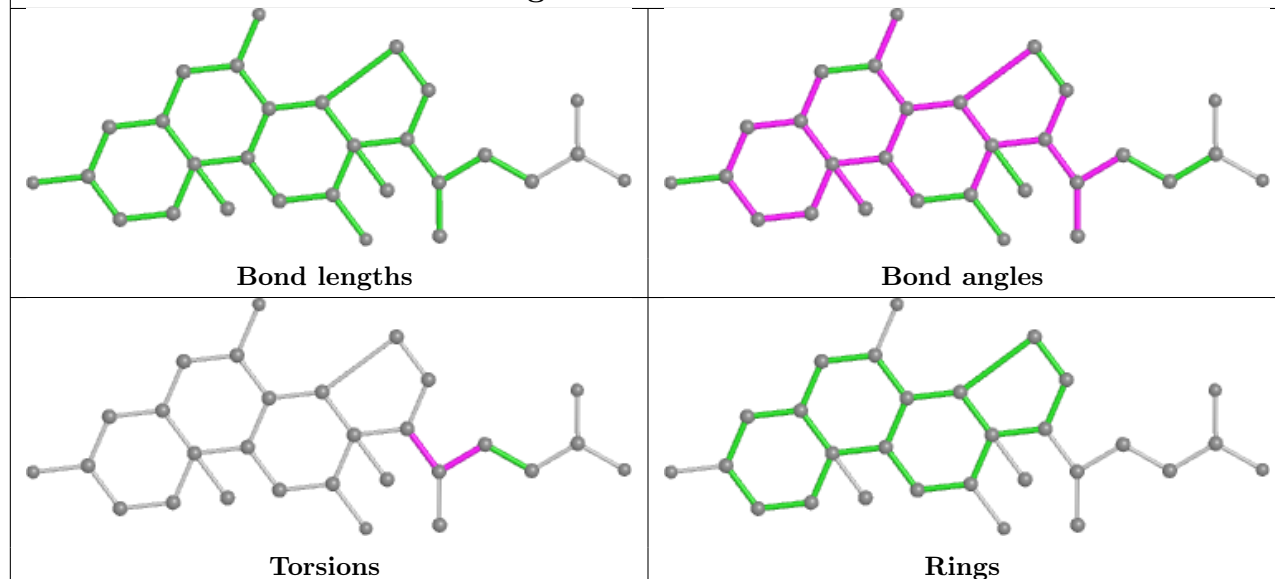


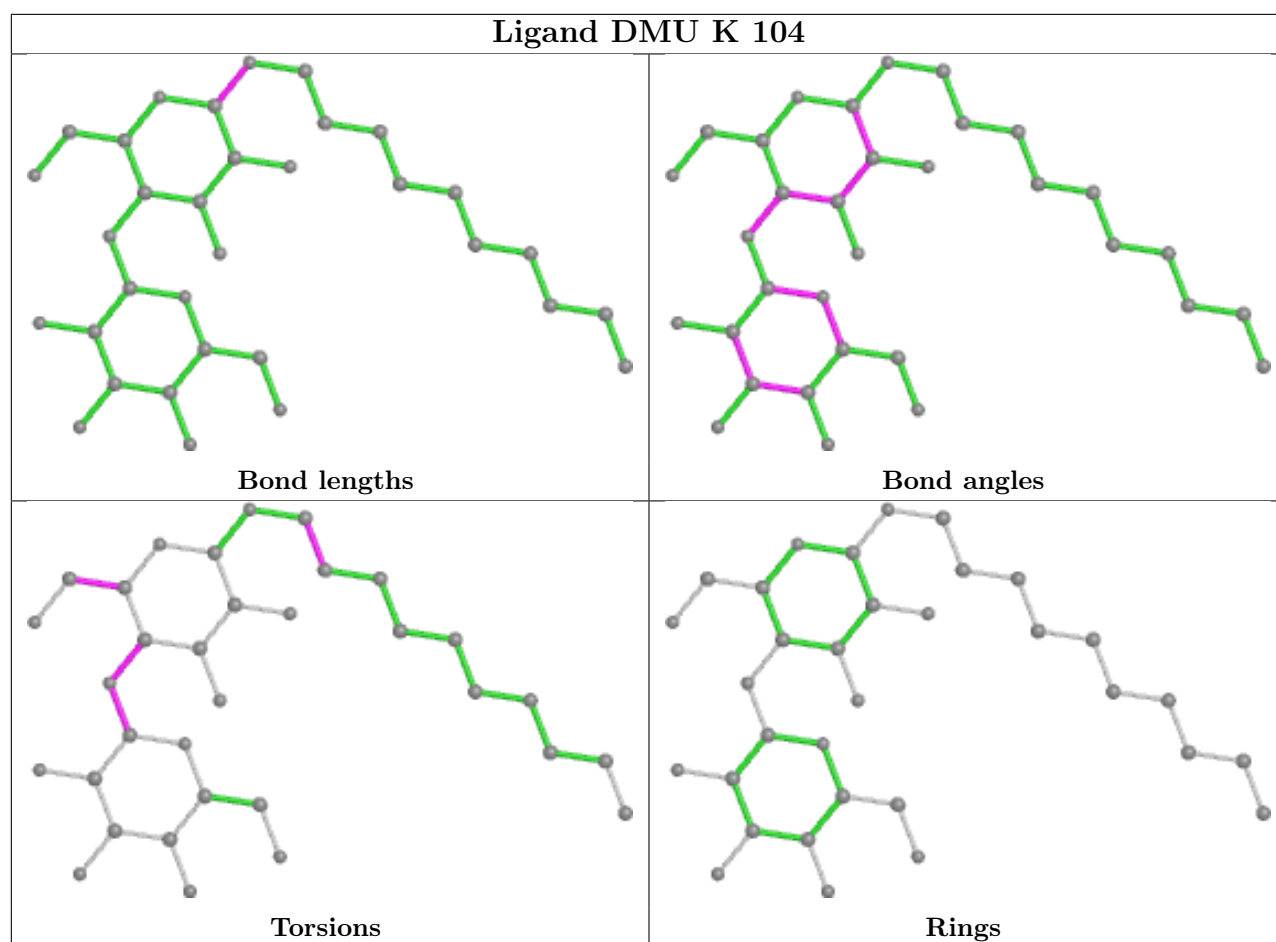


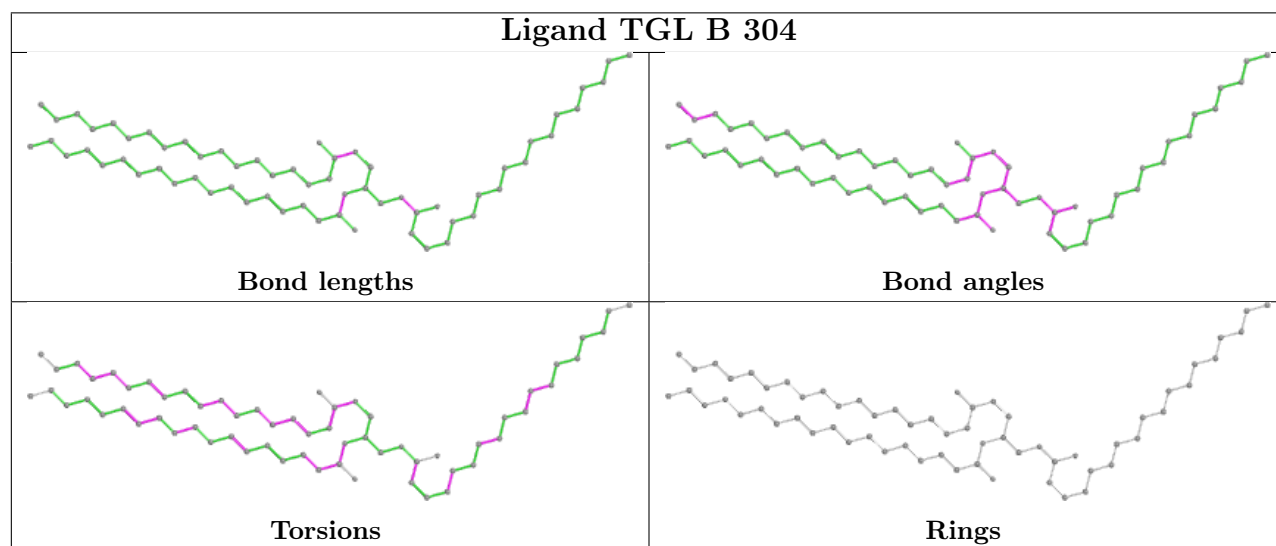
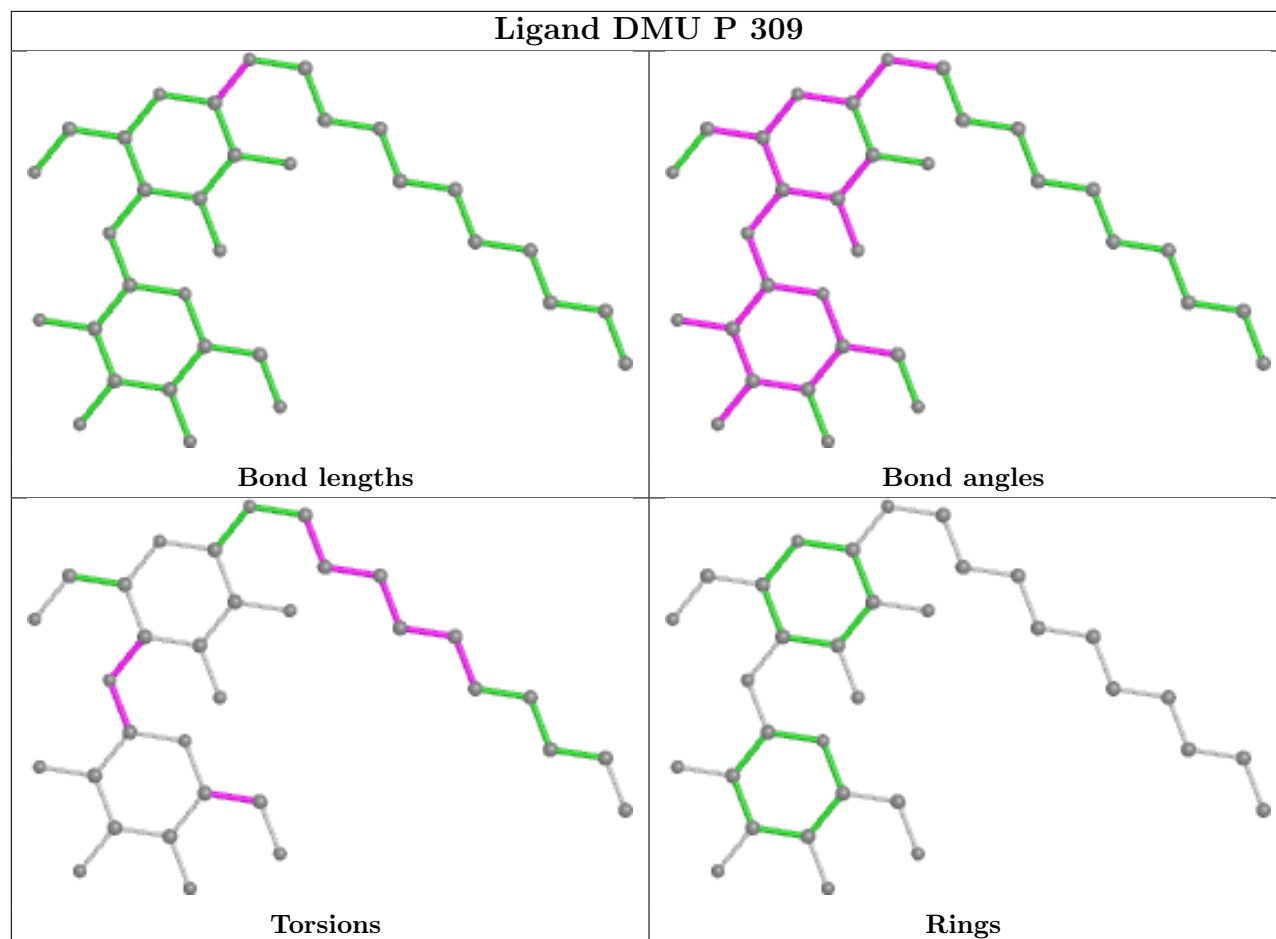
Ligand DMU K 103



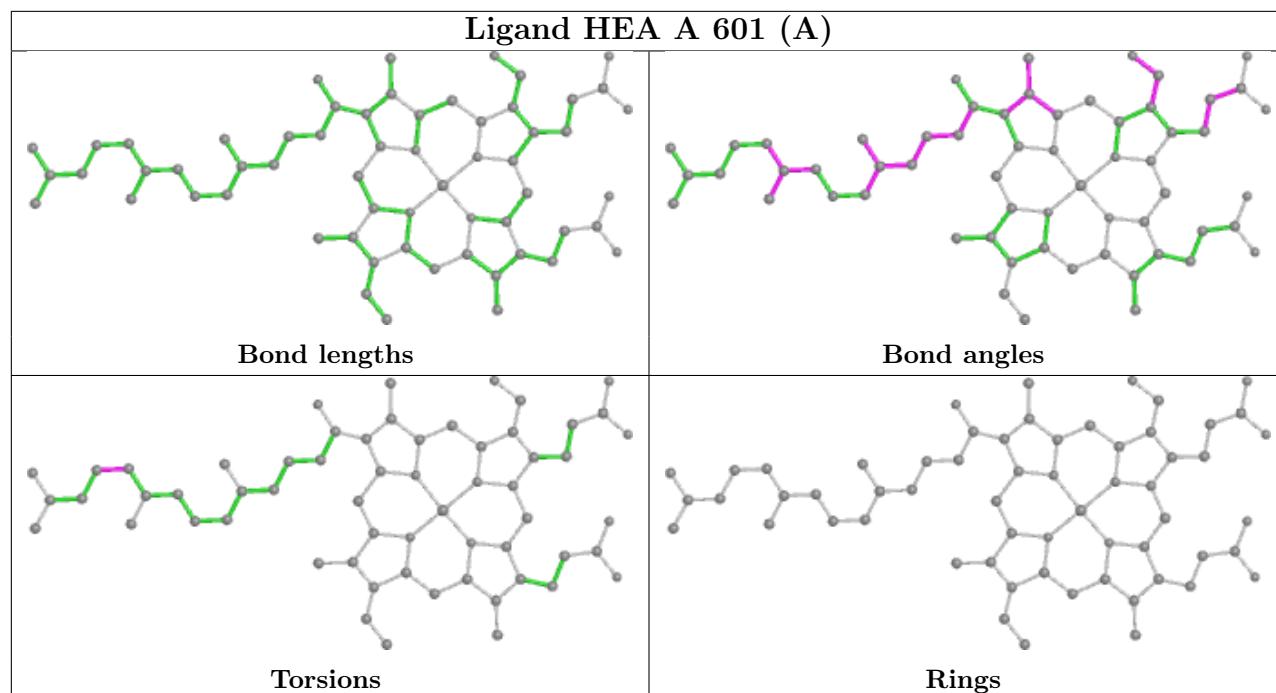
Ligand CHD Y 101



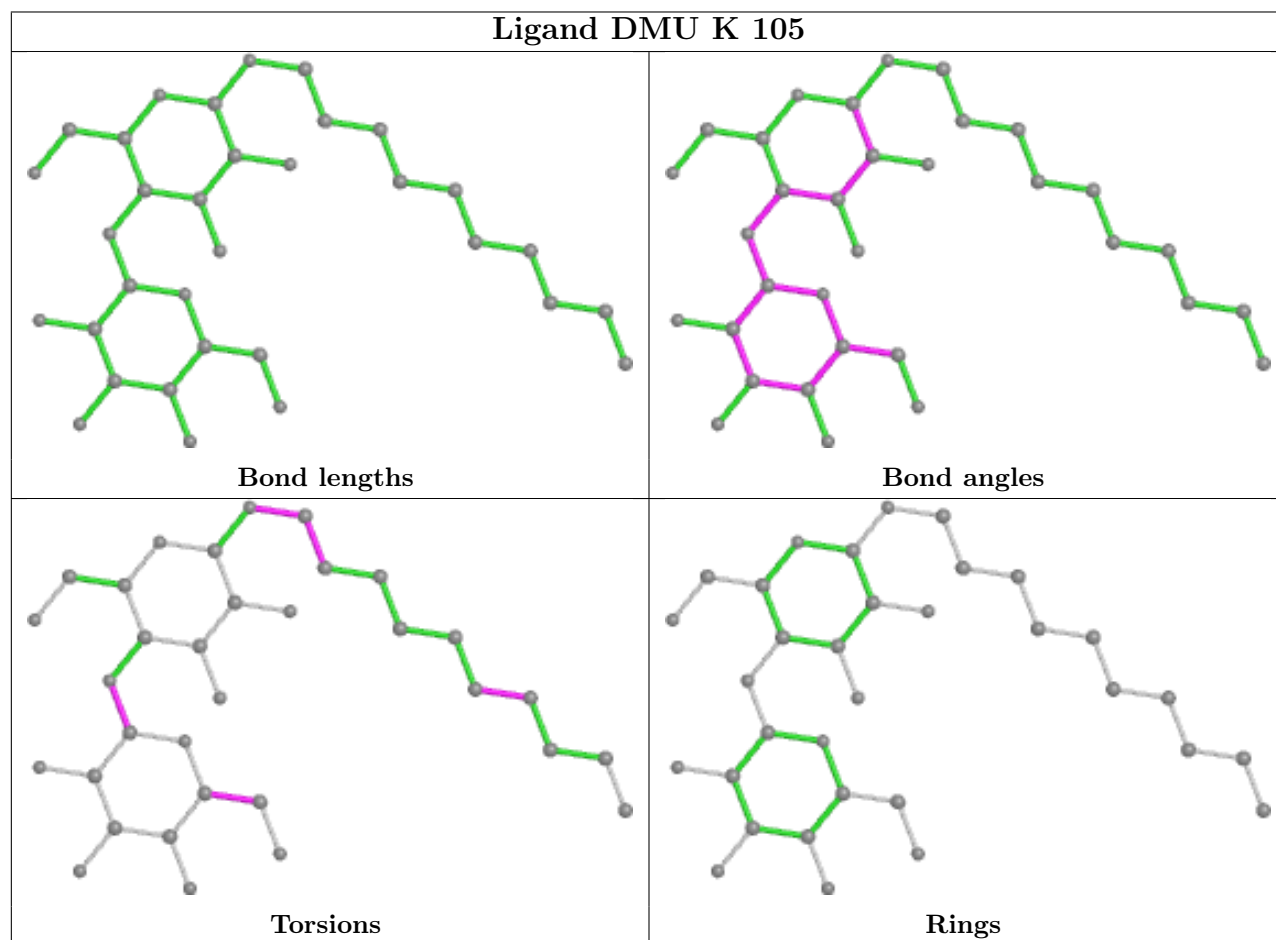


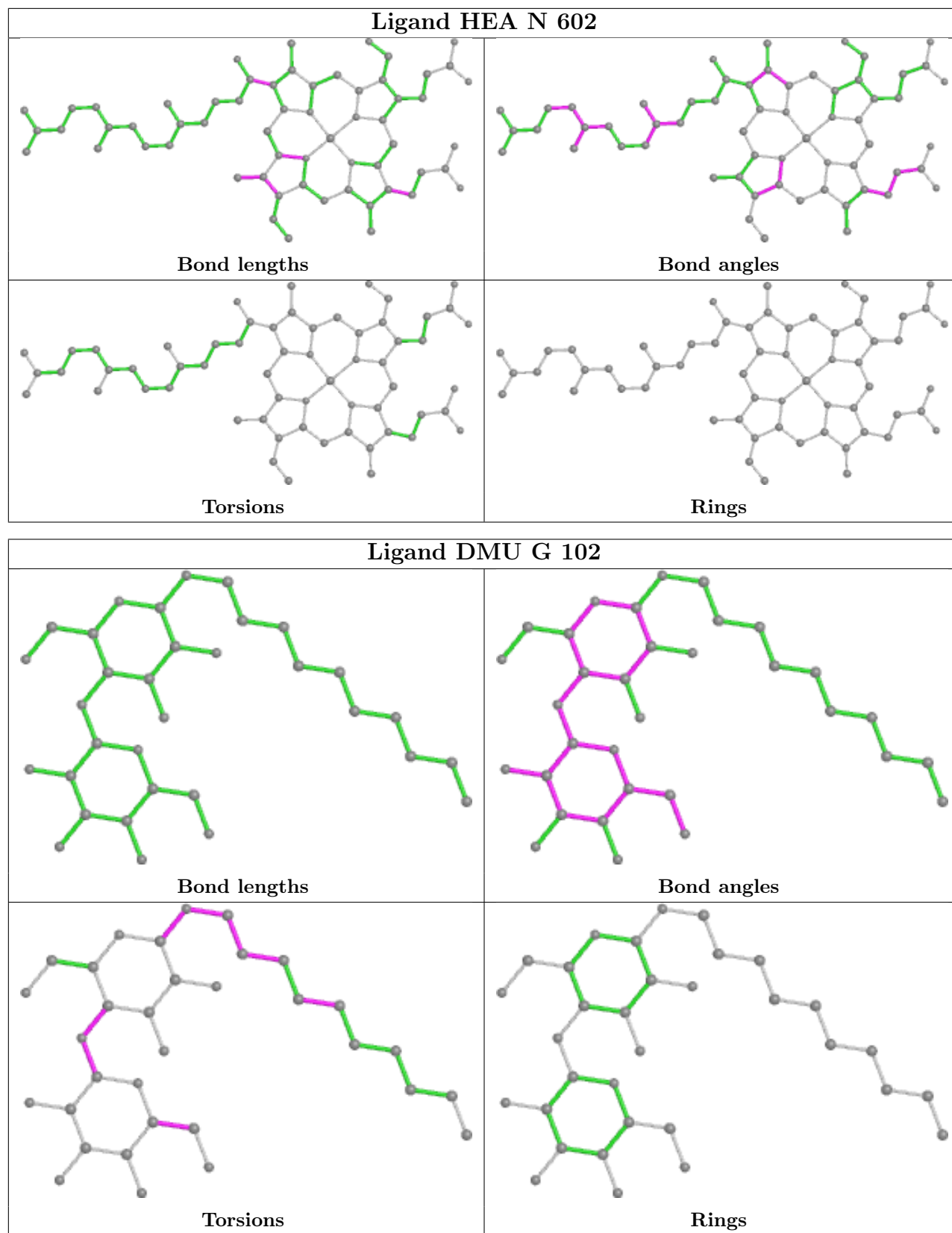


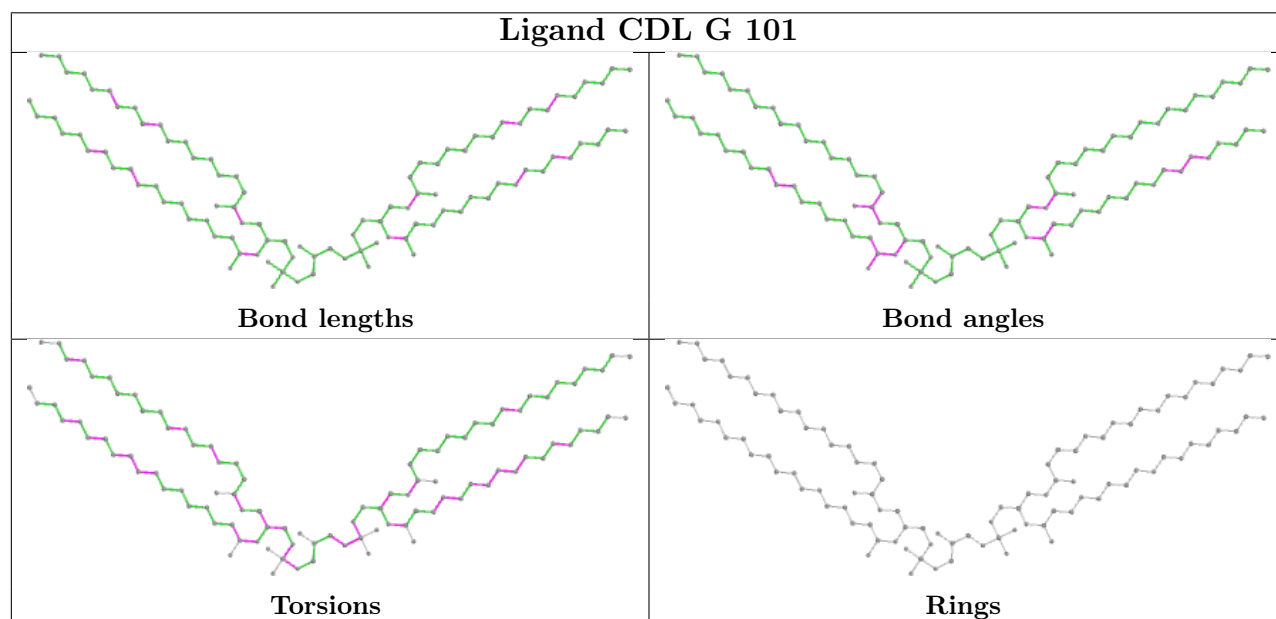
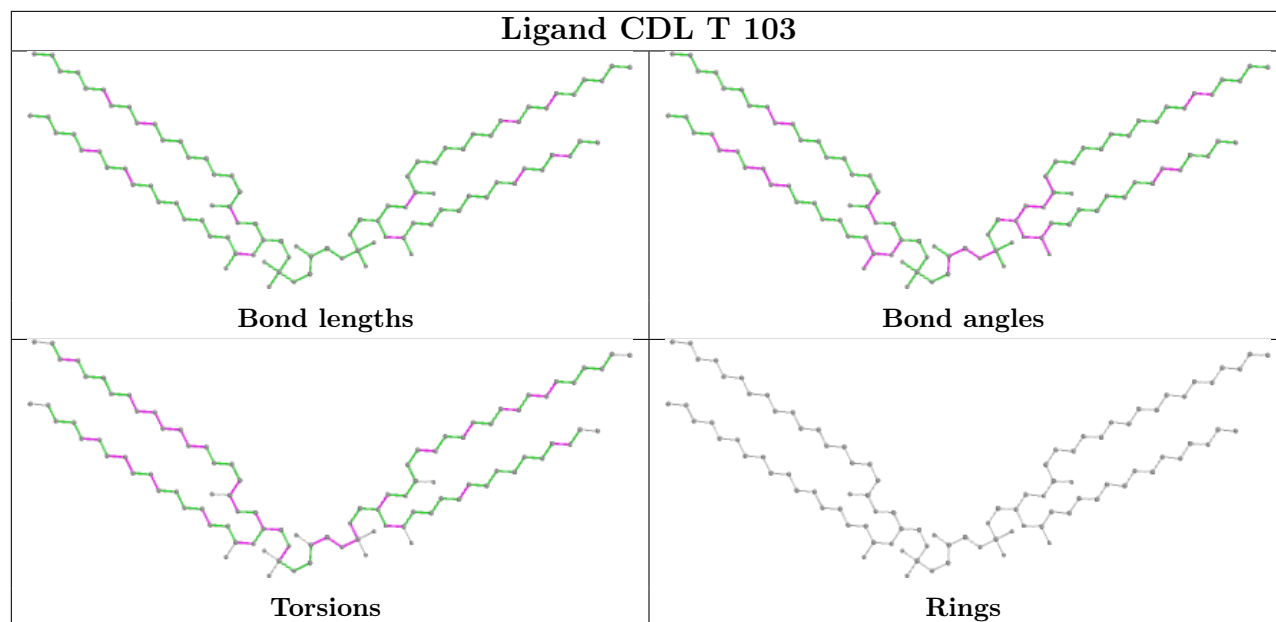
Ligand HEA A 601 (A)

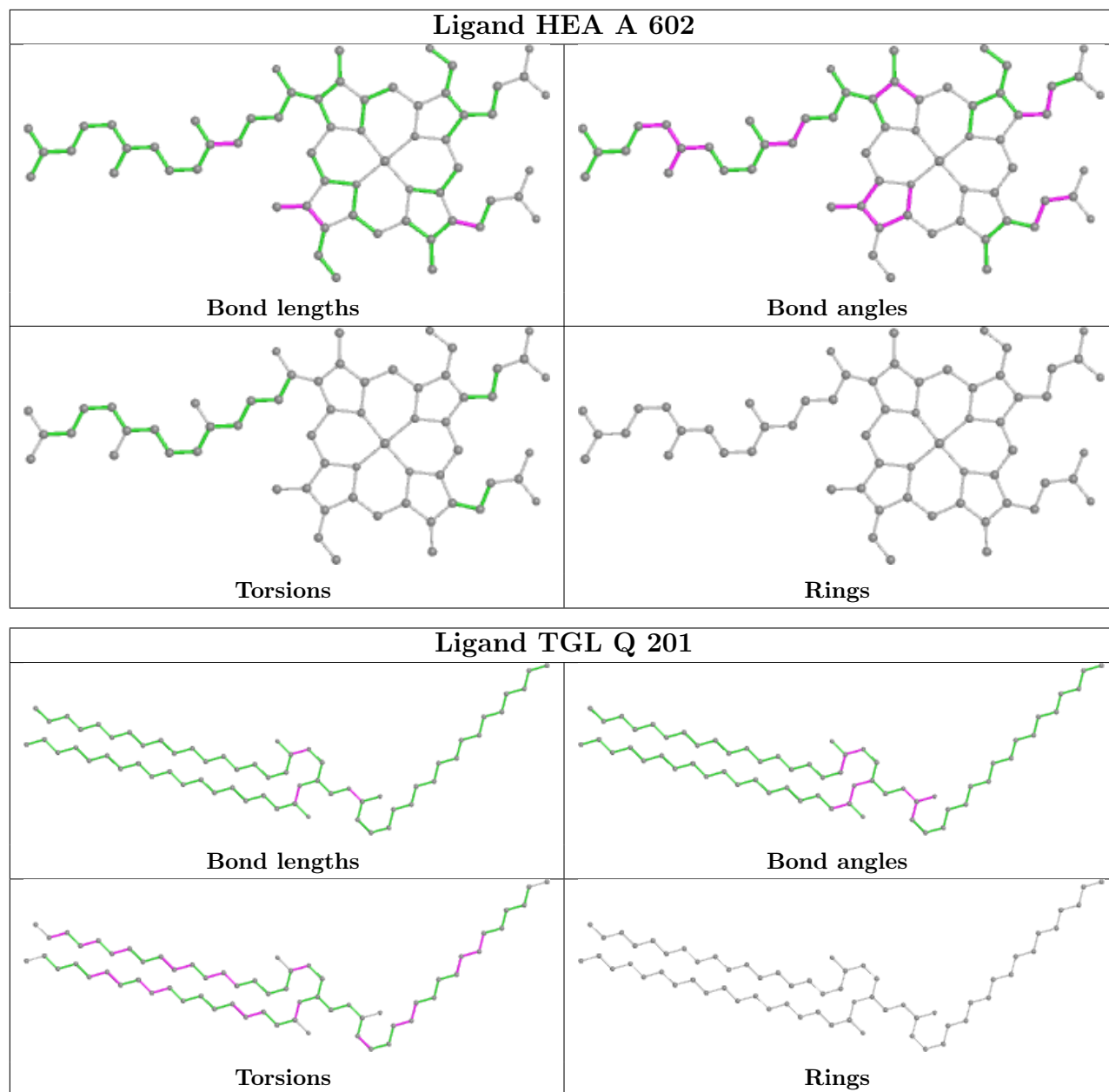


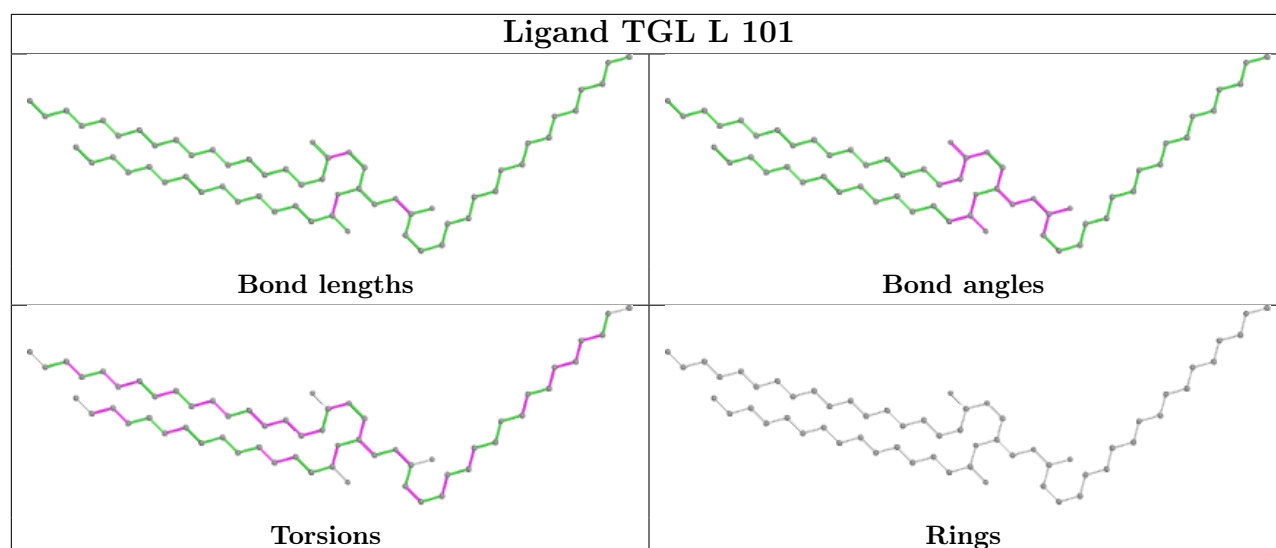
Ligand DMU K 105











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%)	-0.22	1 (0%) 95 95	19, 23, 31, 89	0
1	N	513/514 (99%)	-0.28	0 100 100	19, 26, 34, 78	0
2	B	226/227 (99%)	-0.25	3 (1%) 77 80	22, 30, 53, 128	0
2	O	226/227 (99%)	-0.28	2 (0%) 84 87	25, 33, 70, 109	0
3	C	259/259 (100%)	-0.28	0 100 100	21, 26, 41, 102	0
3	P	259/259 (100%)	-0.32	1 (0%) 92 93	21, 27, 41, 93	0
4	D	144/144 (100%)	-0.41	0 100 100	25, 33, 54, 97	0
4	Q	144/144 (100%)	0.20	6 (4%) 36 38	30, 46, 96, 266	0
5	E	105/105 (100%)	-0.41	1 (0%) 82 85	26, 32, 64, 139	0
5	R	105/105 (100%)	-0.28	2 (1%) 66 70	27, 38, 76, 133	0
6	F	94/94 (100%)	-0.14	3 (3%) 47 50	22, 34, 64, 125	0
6	S	94/94 (100%)	-0.05	3 (3%) 47 50	22, 32, 63, 150	0
7	G	83/84 (98%)	0.74	14 (16%) 1 1	25, 35, 135, 234	0
7	T	83/84 (98%)	0.57	12 (14%) 2 2	24, 36, 122, 189	0
8	H	79/79 (100%)	0.10	7 (8%) 9 10	26, 37, 112, 126	0
8	U	79/79 (100%)	0.15	7 (8%) 9 10	30, 39, 111, 141	0
9	I	72/73 (98%)	-0.14	2 (2%) 53 55	29, 43, 76, 96	0
9	V	72/73 (98%)	0.05	2 (2%) 53 55	28, 50, 89, 234	0
10	J	58/58 (100%)	-0.08	2 (3%) 45 48	27, 38, 87, 134	0
10	W	58/58 (100%)	-0.10	3 (5%) 27 28	28, 39, 98, 181	0
11	K	49/49 (100%)	-0.24	1 (2%) 65 69	29, 37, 57, 67	0
11	X	49/49 (100%)	-0.03	2 (4%) 37 39	35, 45, 79, 82	0
12	L	46/46 (100%)	-0.25	2 (4%) 35 37	24, 29, 53, 124	0
12	Y	46/46 (100%)	-0.24	1 (2%) 62 65	28, 35, 61, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	-0.09	1 (2%) 60 64	25, 29, 70, 121	0
13	Z	43/43 (100%)	0.02	3 (6%) 16 17	32, 38, 81, 170	0
All	All	3542/3550 (99%)	-0.16	81 (2%) 60 64	19, 30, 72, 266	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	14.3
7	G	3	ALA	13.4
4	Q	6	VAL	12.9
6	S	2	SER	11.4
4	Q	5	VAL	10.5
6	S	1	ALA	10.4
7	T	3	ALA	8.9
7	T	10	GLY	8.1
7	G	2	SER	8.1
4	Q	7	LYS	7.2
6	F	1	ALA	6.7
7	T	36	TRP	6.6
4	Q	8	SER	6.5
8	U	46	LYS	6.4
7	G	7	ASP	6.1
6	F	94	HIS	6.0
7	T	40	GLY	5.4
9	V	2	THR	5.3
8	H	8	ILE	5.3
7	G	8	HIS	5.0
8	U	7	LYS	4.9
7	T	8	HIS	4.9
8	U	8	ILE	4.8
8	H	46	LYS	4.8
7	G	6	GLY	4.8
7	G	9	GLY	4.6
7	G	10	GLY	4.6
5	R	5	HIS	4.5
5	R	109	VAL	4.4
7	G	36	TRP	4.3
13	Z	42	LYS	4.3
10	J	1	PHE	4.2
2	O	90	ILE	4.1
7	G	42	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
13	M	43	SER	4.1
6	F	2	SER	4.0
11	X	6	ALA	4.0
7	T	42	ARG	3.8
8	H	47	GLY	3.8
4	Q	10	ASP	3.8
7	G	5	LYS	3.7
8	H	44	THR	3.7
7	T	2	SER	3.6
7	T	7	ASP	3.5
9	V	37	PHE	3.5
7	T	5	LYS	3.4
8	U	48	GLY	3.4
10	J	58	LYS	3.4
10	W	58	LYS	3.4
13	Z	40	TYR	3.3
9	I	37	PHE	3.1
7	G	1	ALA	3.1
2	O	113	TYR	3.0
2	B	90	ILE	3.0
6	S	94	HIS	3.0
3	P	3	HIS	2.9
7	T	9	GLY	2.9
7	T	6	GLY	2.9
7	T	4	ALA	2.8
7	G	40	GLY	2.8
8	U	44	THR	2.7
8	U	10	ASN	2.7
10	W	1	PHE	2.7
11	X	7	PRO	2.7
12	L	2	HIS	2.6
8	U	47	GLY	2.6
10	W	57	HIS	2.6
8	H	7	LYS	2.5
2	B	91	ASN	2.5
12	L	47	LYS	2.4
13	Z	43	SER	2.4
8	H	48	GLY	2.4
7	G	4	ALA	2.3
7	G	37	LEU	2.3
11	K	6	ALA	2.3
5	E	5	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
8	H	45	ALA	2.2
2	B	16[A]	ILE	2.2
9	I	25	PHE	2.1
1	A	49[A]	GLY	2.0
12	Y	47	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.27	0.35	139,175,198,204	0
9	SAC	V	1	9/10	0.49	0.54	167,216,240,253	0
9	SAC	I	1	9/10	0.62	0.29	113,144,171,199	0
7	TPO	T	11	11/12	0.67	0.28	55,128,192,194	0
1	FME	N	1	10/11	0.95	0.09	35,41,72,108	0
1	FME	A	1	10/11	0.97	0.07	34,44,63,88	0
2	FME	O	1	10/11	0.97	0.09	32,34,39,104	0
2	FME	B	1	10/11	0.98	0.10	28,29,36,113	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	DMU	K	104	33/33	0.47	0.46	74,126,182,201	0
27	DMU	X	204	33/33	0.51	0.37	63,144,182,202	0
27	DMU	P	316	33/33	0.60	0.31	53,60,74,79	0
27	DMU	K	106	33/33	0.63	0.45	43,88,108,118	0
27	DMU	K	103	33/33	0.64	0.27	55,114,190,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	N	620	4/4	0.66	0.22	46,53,64,68	0
27	DMU	M	106	33/33	0.66	0.32	49,76,103,112	0
27	DMU	X	203	22/33	0.67	0.24	64,96,171,186	0
20	EDO	B	308	4/4	0.68	0.15	45,45,66,70	0
25	PEK	P	304	53/53	0.69	0.29	42,77,136,186	0
27	DMU	G	102	33/33	0.69	0.22	54,105,156,157	0
20	EDO	F	106	4/4	0.69	0.13	44,52,65,74	0
27	DMU	X	205	22/33	0.70	0.32	65,104,160,162	0
20	EDO	G	106	4/4	0.71	0.17	35,45,83,104	0
19	PGV	G	104	51/51	0.71	0.23	40,82,127,155	0
27	DMU	X	201	33/33	0.72	0.34	53,106,180,192	0
27	DMU	X	202	33/33	0.72	0.30	43,142,216,227	0
27	DMU	K	101	21/33	0.72	0.30	41,110,189,196	0
27	DMU	P	309	33/33	0.72	0.25	31,78,157,181	0
24	CHD	J	102	29/29	0.72	0.33	52,94,162,199	0
20	EDO	A	622	4/4	0.73	0.52	46,55,59,71	0
25	PEK	T	102	44/53	0.73	0.29	43,96,157,183	0
24	CHD	P	308	29/29	0.73	0.30	56,77,138,177	0
26	CDL	T	103	96/100	0.74	0.25	45,82,125,176	0
24	CHD	W	101	29/29	0.74	0.35	46,119,204,206	0
26	CDL	G	101	99/100	0.75	0.28	36,85,129,181	0
20	EDO	C	315	4/4	0.75	0.13	42,65,69,70	0
27	DMU	K	105	33/33	0.75	0.43	47,125,201,217	0
20	EDO	A	610	4/4	0.76	0.17	34,47,71,82	0
25	PEK	P	302	48/53	0.76	0.24	43,76,148,161	0
27	DMU	K	102	22/33	0.76	0.29	53,109,188,214	0
20	EDO	A	615	4/4	0.77	0.18	50,58,69,100	0
25	PEK	C	303	53/53	0.77	0.28	40,78,139,158	0
27	DMU	O	303	32/33	0.78	0.20	42,102,173,202	0
20	EDO	Q	203	4/4	0.78	0.21	53,60,62,90	0
19	PGV	C	305	51/51	0.78	0.23	42,80,129,135	0
19	PGV	N	607	51/51	0.78	0.27	43,79,130,161	0
27	DMU	L	102	33/33	0.79	0.21	54,103,152,159	0
21	TGL	B	304	63/63	0.79	0.20	26,66,132,168	0
27	DMU	C	307	33/33	0.80	0.23	48,109,157,171	0
27	DMU	P	307	33/33	0.80	0.22	52,103,149,183	0
20	EDO	N	612	4/4	0.80	0.19	45,59,71,81	0
20	EDO	T	106	4/4	0.81	0.23	44,62,75,86	0
20	EDO	L	103	4/4	0.81	0.29	33,64,68,80	0
21	TGL	Q	201	63/63	0.81	0.19	44,74,134,171	0
24	CHD	J	101	29/29	0.81	0.28	56,80,126,169	0
23	PSC	O	302	46/52	0.82	0.25	32,76,132,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CHD	Y	101	29/29	0.82	0.28	67,92,145,156	0
23	PSC	B	303	51/52	0.82	0.28	39,79,158,184	0
20	EDO	D	203	4/4	0.83	0.14	45,56,56,60	0
20	EDO	C	316	4/4	0.83	0.13	51,55,65,78	0
27	DMU	C	308	33/33	0.83	0.26	28,76,162,192	0
20	EDO	O	306	4/4	0.84	0.11	43,54,61,70	0
20	EDO	A	616	4/4	0.84	0.20	45,51,54,55	0
20	EDO	S	104	4/4	0.84	0.43	59,108,114,122	0
20	EDO	N	626	4/4	0.85	0.40	60,67,68,69	0
26	CDL	C	306	92/100	0.85	0.21	40,77,112,123	0
21	TGL	Y	102	63/63	0.85	0.21	40,73,135,230	0
26	CDL	P	306	84/100	0.85	0.23	37,79,134,142	0
20	EDO	M	105	4/4	0.85	0.35	41,50,55,99	0
20	EDO	I	101	4/4	0.86	0.18	39,49,57,69	0
20	EDO	C	317	4/4	0.86	0.12	48,65,69,69	0
19	PGV	A	607	48/51	0.86	0.21	31,60,116,157	0
20	EDO	P	312	4/4	0.87	0.15	49,63,65,77	0
20	EDO	P	315	4/4	0.87	0.13	57,59,84,96	0
21	TGL	L	101	60/63	0.87	0.20	31,62,180,229	0
20	EDO	N	615	4/4	0.87	0.26	56,57,58,67	0
20	EDO	A	620	4/4	0.87	0.17	43,54,56,84	0
20	EDO	P	311	4/4	0.88	0.12	54,71,82,98	0
20	EDO	D	202	4/4	0.88	0.18	54,67,104,106	0
27	DMU	T	104	22/33	0.88	0.15	50,84,149,169	0
21	TGL	N	608	63/63	0.88	0.17	40,76,128,162	0
27	DMU	Z	101	33/33	0.88	0.13	36,50,67,70	0
20	EDO	M	103	4/4	0.89	0.19	40,72,86,94	0
20	EDO	P	314	4/4	0.89	0.14	34,40,42,42	0
20	EDO	J	103	4/4	0.89	0.26	49,51,69,73	0
27	DMU	M	101	33/33	0.89	0.11	33,43,61,83	0
20	EDO	E	203	4/4	0.90	0.09	40,55,56,65	0
20	EDO	Q	204	4/4	0.90	0.19	45,50,55,56	0
20	EDO	O	307	4/4	0.90	0.14	44,51,62,77	0
20	EDO	C	312	4/4	0.90	0.10	31,40,46,69	0
21	TGL	B	301	63/63	0.90	0.15	37,65,131,160	0
20	EDO	N	618	4/4	0.90	0.16	30,37,43,48	0
20	EDO	B	306	4/4	0.90	0.11	29,42,43,56	0
20	EDO	A	613	4/4	0.90	0.23	60,63,78,80	0
20	EDO	R	201	4/4	0.91	0.13	62,63,82,93	0
20	EDO	B	309	4/4	0.91	0.11	32,55,55,70	0
20	EDO	J	104	4/4	0.91	0.22	42,61,62,75	0
20	EDO	U	101	4/4	0.91	0.25	38,44,54,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	PO4	U	102	5/5	0.91	0.22	52,53,95,97	0
20	EDO	D	201	4/4	0.92	0.10	47,47,59,72	0
20	EDO	D	204	4/4	0.92	0.24	36,41,53,81	0
20	EDO	M	102	4/4	0.92	0.06	52,58,71,72	0
20	EDO	A	614	4/4	0.92	0.13	46,67,71,71	0
20	EDO	N	622	4/4	0.92	0.13	44,52,53,58	0
20	EDO	M	104	4/4	0.92	0.16	50,65,66,70	0
20	EDO	F	105	4/4	0.92	0.20	42,43,47,68	0
20	EDO	N	614	4/4	0.93	0.10	46,48,63,86	0
20	EDO	C	311	4/4	0.93	0.10	71,76,87,88	0
20	EDO	V	101	4/4	0.93	0.28	19,38,52,86	0
20	EDO	C	313	4/4	0.93	0.11	39,62,68,79	0
20	EDO	P	313	4/4	0.93	0.18	52,62,63,68	0
20	EDO	N	619	4/4	0.93	0.17	39,48,54,63	0
24	CHD	C	301	29/29	0.94	0.08	24,27,35,38	0
20	EDO	Y	103	4/4	0.94	0.21	48,52,65,81	0
20	EDO	S	106	4/4	0.94	0.13	36,51,71,84	0
20	EDO	A	621	4/4	0.94	0.15	39,39,48,49	0
25	PEK	P	303	45/53	0.94	0.12	26,42,78,93	0
20	EDO	N	624	4/4	0.95	0.14	32,33,47,92	0
20	EDO	N	613	4/4	0.95	0.11	36,38,42,44	0
20	EDO	N	617	4/4	0.95	0.20	32,38,48,75	0
20	EDO	F	104	4/4	0.95	0.07	33,36,44,57	0
20	EDO	P	310	4/4	0.95	0.12	33,36,37,40	0
24	CHD	P	301	29/29	0.95	0.07	23,29,34,36	0
24	CHD	G	103	29/29	0.96	0.08	21,24,30,37	0
20	EDO	T	105	4/4	0.96	0.09	28,31,36,38	0
20	EDO	O	304	4/4	0.96	0.09	29,29,30,31	0
20	EDO	O	305	4/4	0.96	0.13	37,48,52,54	0
20	EDO	B	307	4/4	0.96	0.10	34,45,48,48	0
20	EDO	R	202	4/4	0.96	0.10	40,42,43,45	0
20	EDO	C	314	4/4	0.96	0.23	43,62,63,92	0
20	EDO	C	309	4/4	0.96	0.09	30,33,33,35	0
20	EDO	N	625	4/4	0.97	0.27	33,44,48,82	0
20	EDO	B	305	4/4	0.97	0.09	22,26,27,29	0
20	EDO	A	611	4/4	0.97	0.13	30,38,39,68	0
20	EDO	S	103	4/4	0.97	0.12	29,30,30,35	0
20	EDO	A	618	4/4	0.97	0.12	26,28,30,34	0
19	PGV	N	609	51/51	0.97	0.11	22,29,65,89	0
20	EDO	N	616	4/4	0.97	0.18	33,35,55,74	0
20	EDO	D	205	4/4	0.97	0.11	35,40,61,70	0
20	EDO	E	202	4/4	0.97	0.08	36,40,42,43	0

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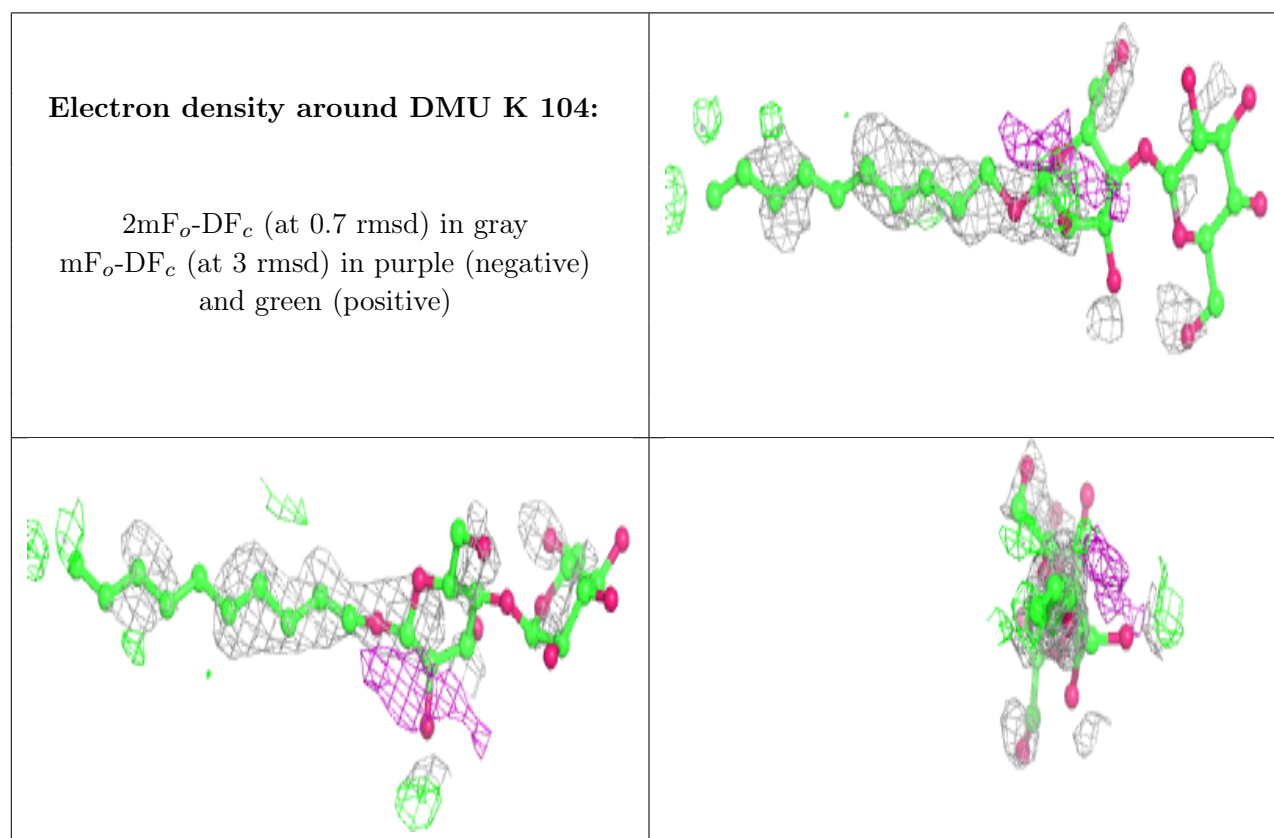
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	PGV	P	305	51/51	0.97	0.11	22,31,85,100	0
20	EDO	F	103	4/4	0.97	0.12	27,29,33,35	0
24	CHD	T	101	29/29	0.97	0.07	22,25,30,40	0
20	EDO	N	621	4/4	0.97	0.12	31,40,41,43	0
20	EDO	B	310	4/4	0.97	0.20	41,47,47,55	0
25	PEK	C	302	53/53	0.97	0.12	25,40,84,114	0
29	PO4	H	101	5/5	0.97	0.20	52,61,77,97	0
19	PGV	C	304	50/51	0.97	0.10	22,30,86,98	0
20	EDO	A	609	4/4	0.98	0.09	22,23,24,27	0
14	HEA	N	602	60/60	0.98	0.09	18,22,27,30	0
14	HEA	A	601[A]	60/60	0.98	0.10	17,20,33,36	18
20	EDO	N	623	4/4	0.98	0.11	35,39,42,48	0
20	EDO	S	105	4/4	0.98	0.08	33,37,41,44	0
20	EDO	A	612	4/4	0.98	0.10	28,38,78,85	0
19	PGV	A	608	51/51	0.98	0.10	22,28,69,77	0
14	HEA	A	601[B]	52/60	0.98	0.10	17,20,26,34	10
14	HEA	A	601[C]	51/60	0.98	0.10	17,20,32,33	9
20	EDO	E	201	4/4	0.98	0.08	39,40,42,43	0
20	EDO	N	610	4/4	0.98	0.11	22,27,28,30	0
20	EDO	N	611	4/4	0.98	0.07	25,26,28,30	0
14	HEA	A	602	60/60	0.98	0.08	18,20,26,31	0
20	EDO	C	310	4/4	0.98	0.10	27,32,44,57	0
20	EDO	A	617	4/4	0.98	0.14	29,36,37,88	0
14	HEA	N	601[A]	60/60	0.98	0.10	21,24,34,40	18
20	EDO	A	619	4/4	0.98	0.19	27,38,40,46	0
14	HEA	N	601[B]	52/60	0.98	0.10	20,23,30,36	10
20	EDO	Q	202	4/4	0.98	0.10	28,46,50,69	0
20	EDO	G	105	4/4	0.98	0.07	27,30,34,34	0
14	HEA	N	601[C]	51/60	0.98	0.10	20,23,29,37	9
18	CMO	N	606[B]	2/2	0.99	0.20	17,17,17,20	2
16	MG	A	604	1/1	0.99	0.05	20,20,20,20	0
16	MG	N	604	1/1	0.99	0.05	21,21,21,21	0
17	NA	A	605	1/1	0.99	0.09	24,24,24,24	0
17	NA	N	605	1/1	0.99	0.07	29,29,29,29	0
18	CMO	A	606[A]	2/2	0.99	0.20	17,17,17,18	2
20	EDO	F	102	4/4	0.99	0.09	22,23,24,25	0
18	CMO	A	606[B]	2/2	0.99	0.20	16,16,16,16	2
28	ZN	S	101	1/1	0.99	0.11	26,26,26,26	0
20	EDO	S	102	4/4	0.99	0.08	22,23,24,24	0
18	CMO	N	606[A]	2/2	0.99	0.20	19,19,19,19	2
22	CUA	O	301	2/2	1.00	0.11	25,25,25,26	0
28	ZN	F	101	1/1	1.00	0.10	26,26,26,26	0

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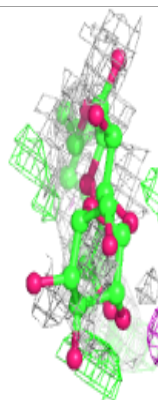
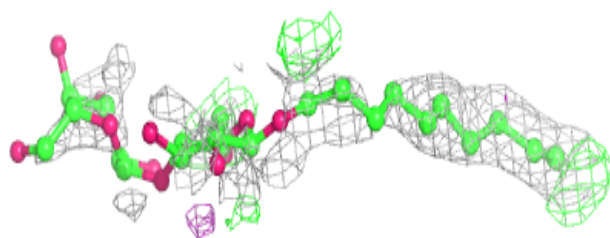
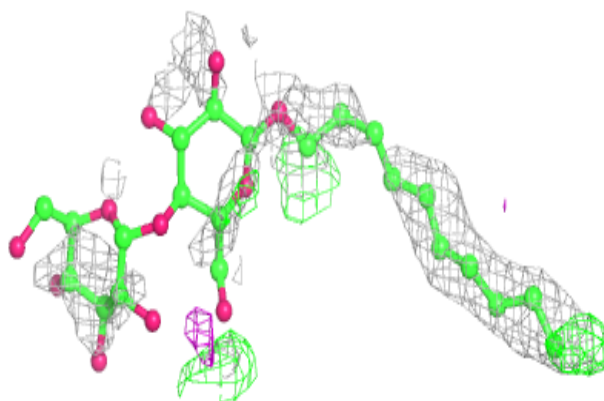
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	CU	A	603	1/1	1.00	0.13	21,21,21,21	0
15	CU	N	603	1/1	1.00	0.14	22,22,22,22	0
22	CUA	B	302	2/2	1.00	0.12	22,22,22,23	0

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.

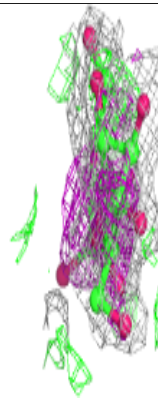
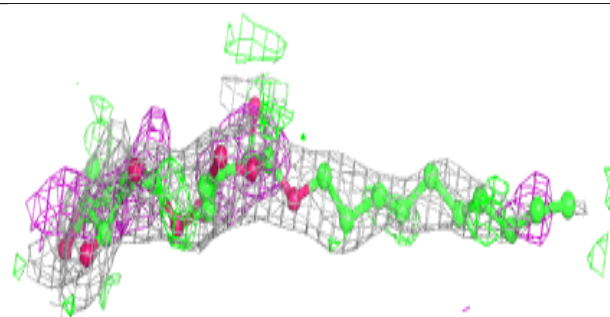
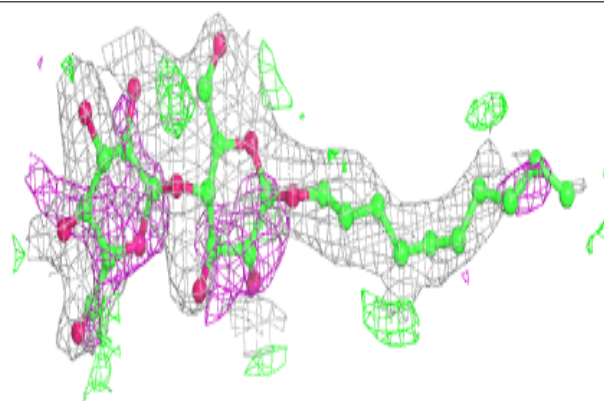


Electron density around DMU X 204:

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

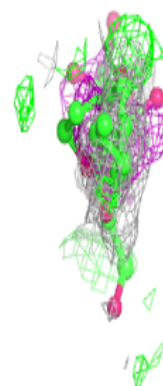
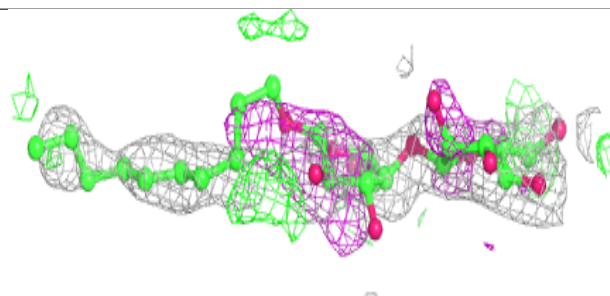
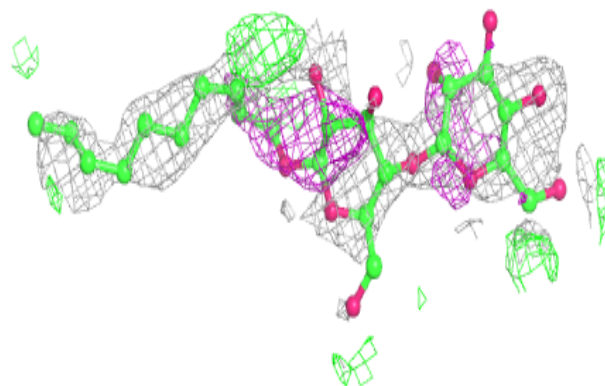
**Electron density around DMU P 316:**

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

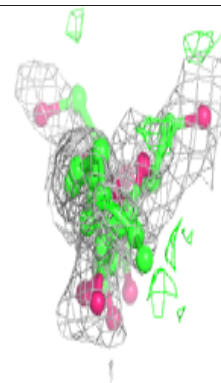
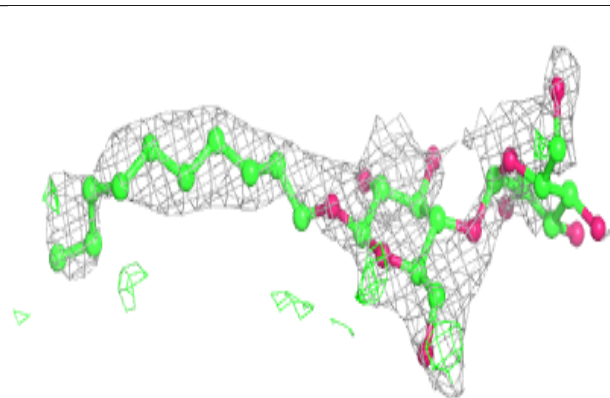
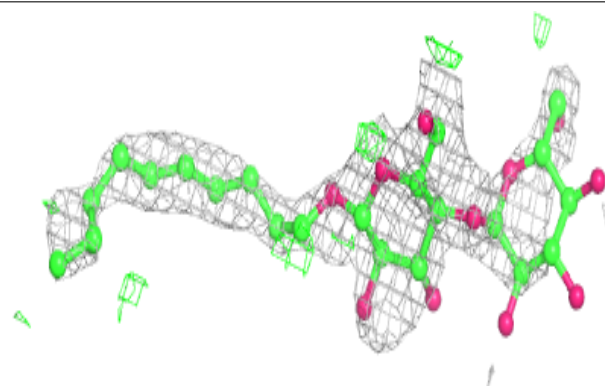


Electron density around DMU K 106:

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

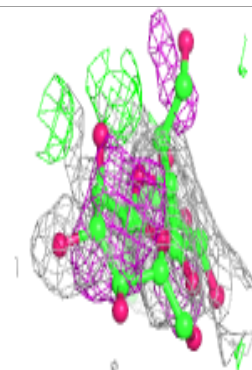
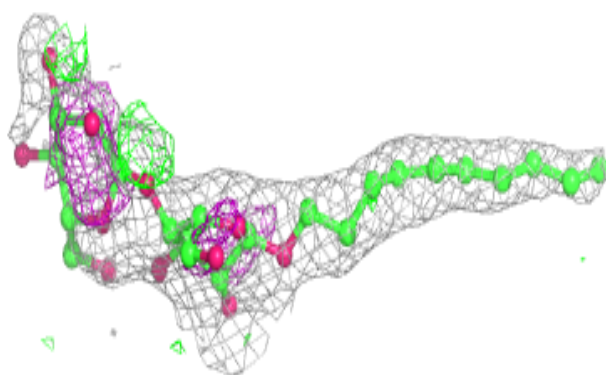
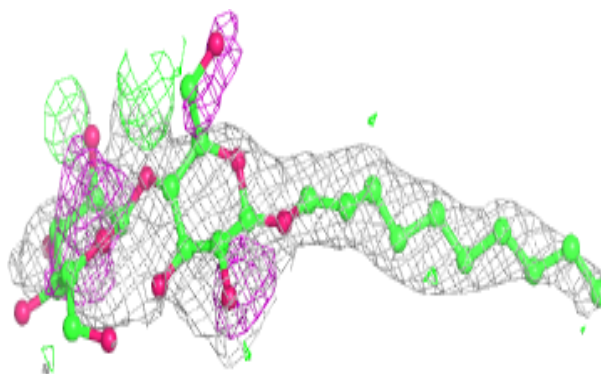
**Electron density around DMU K 103:**

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

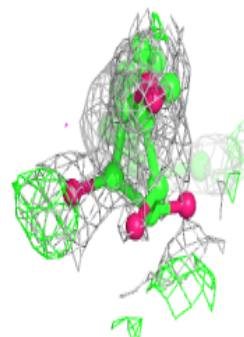
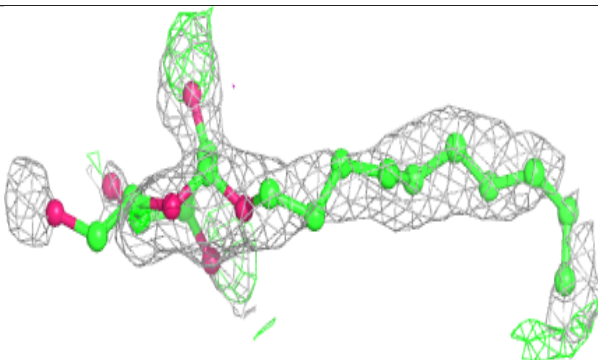
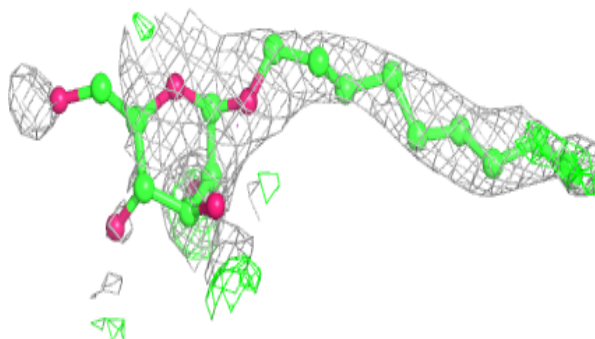


Electron density around DMU M 106:

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

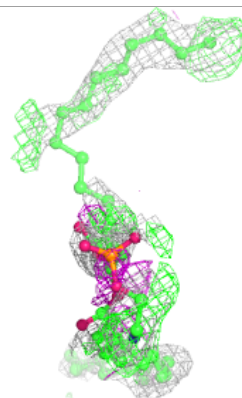
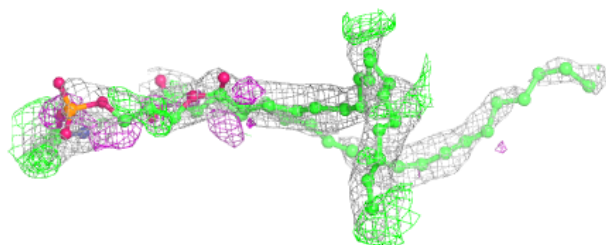
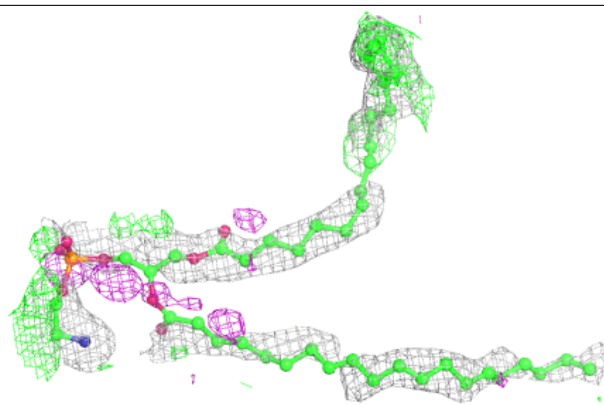
**Electron density around DMU X 203:**

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

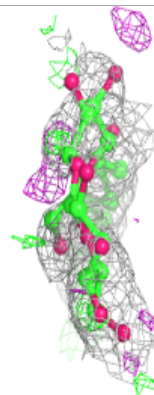
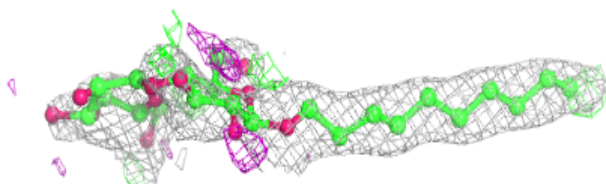
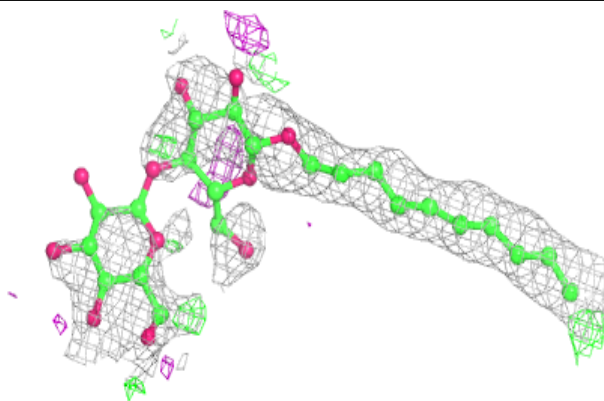


Electron density around PEK P 304:

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

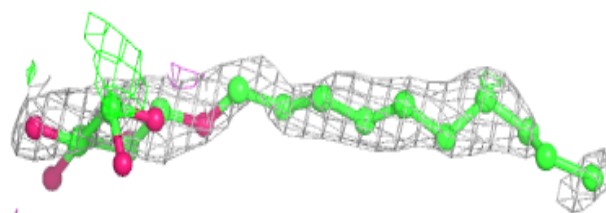
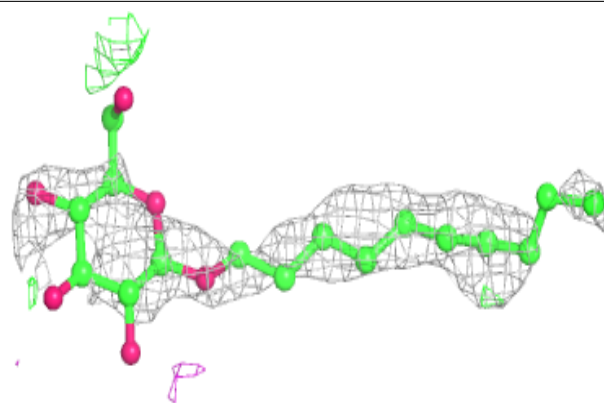
**Electron density around DMU G 102:**

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

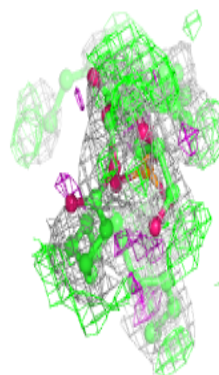
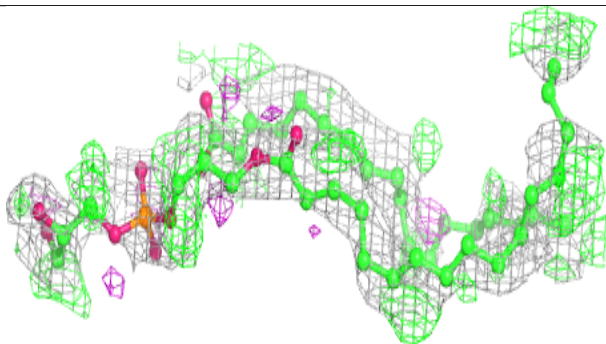
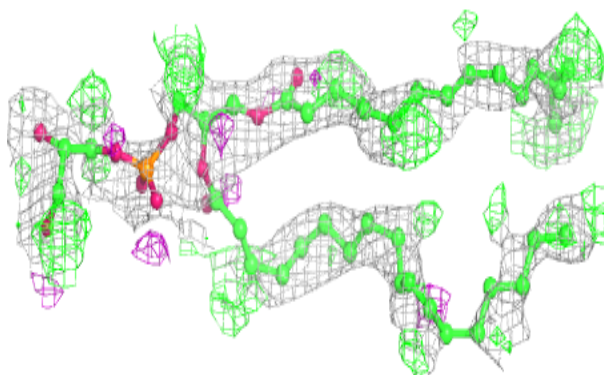


Electron density around DMU X 205:

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

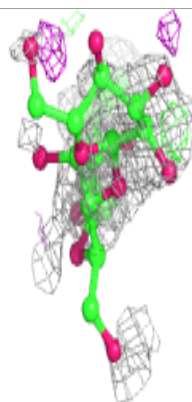
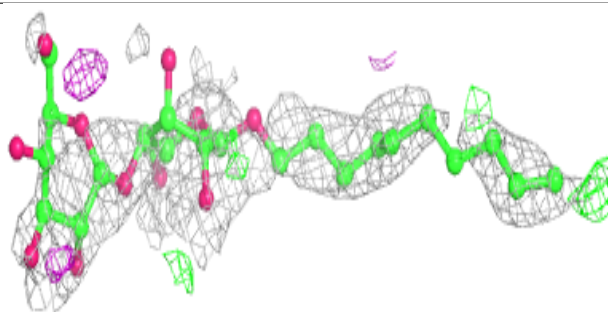
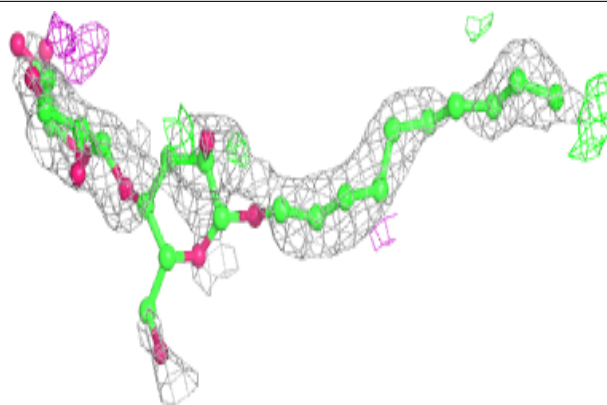
**Electron density around PGV G 104:**

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

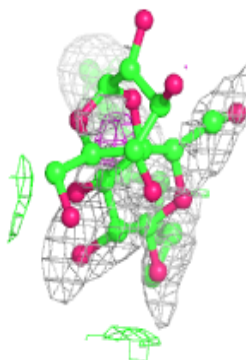
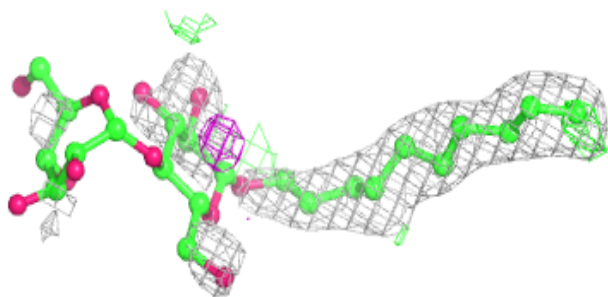
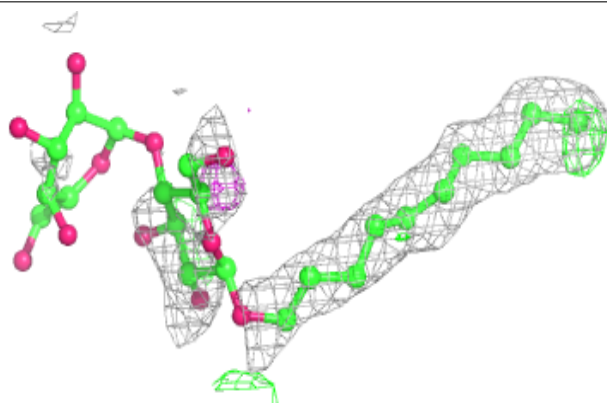


Electron density around DMU X 201:

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

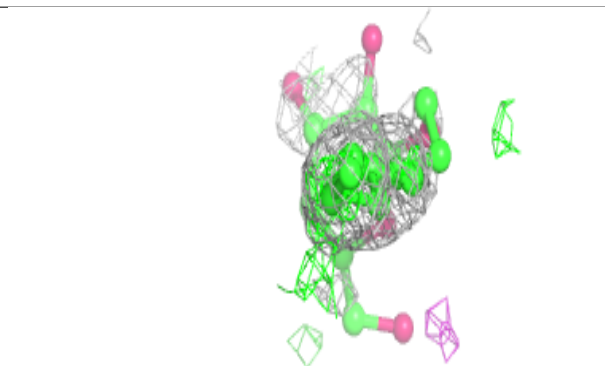
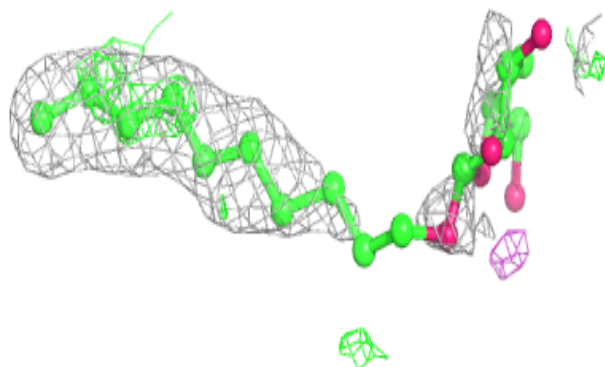
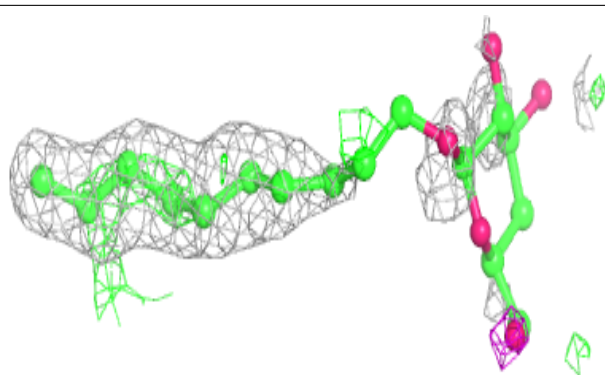
**Electron density around DMU X 202:**

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

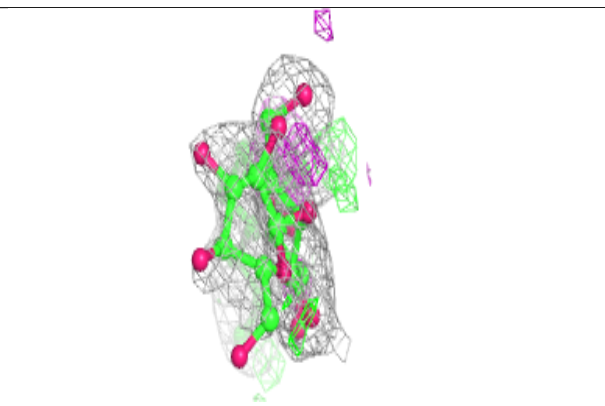
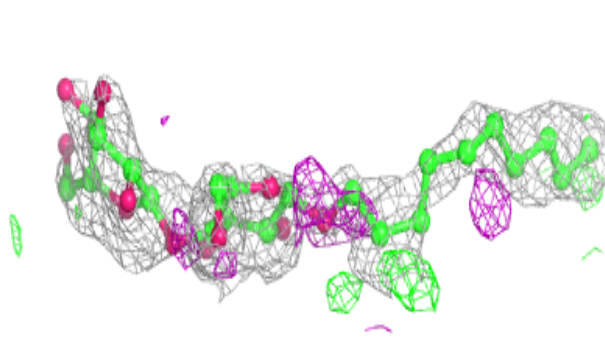
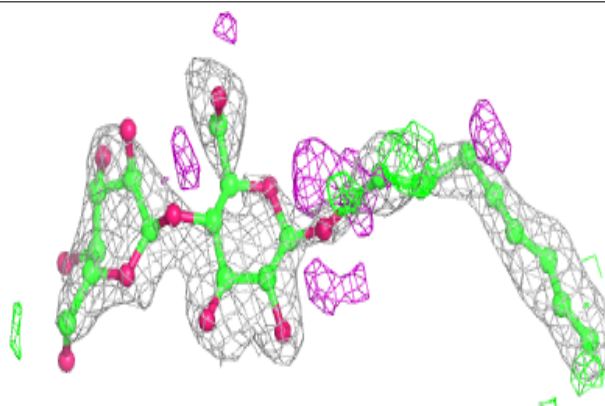


Electron density around DMU K 101:

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

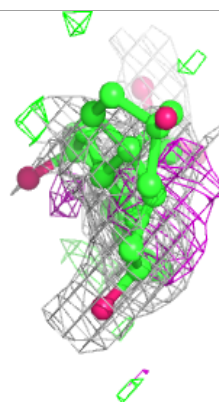
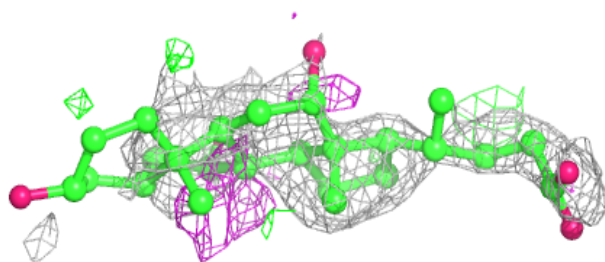
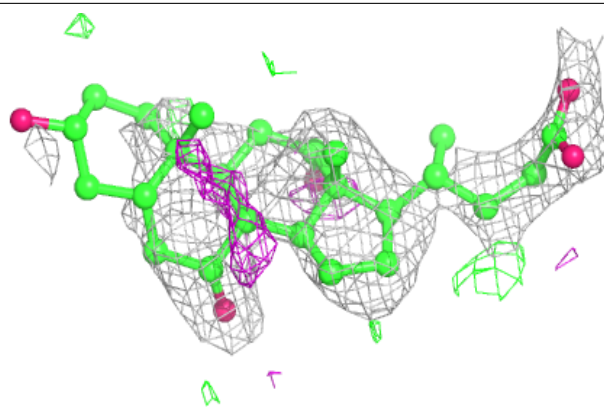
**Electron density around DMU P 309:**

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

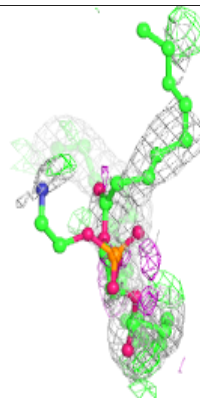
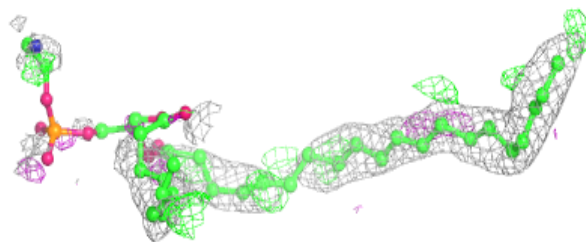
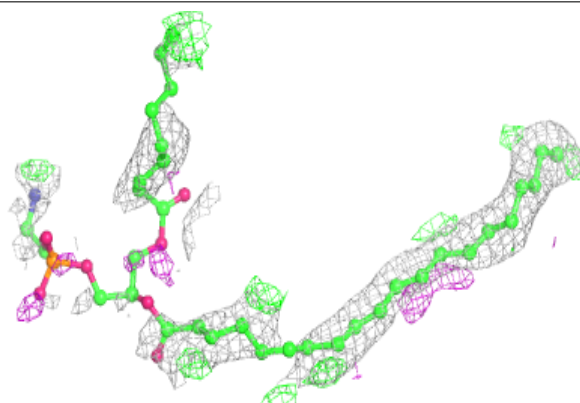


Electron density around CHD J 102:

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

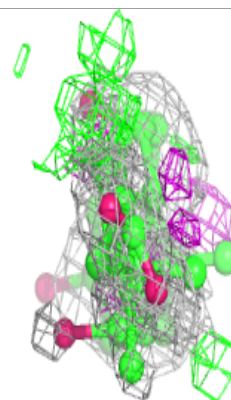
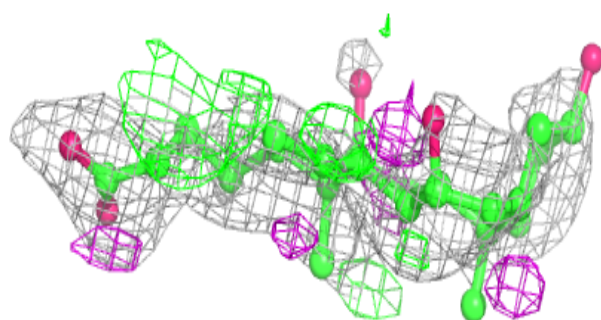
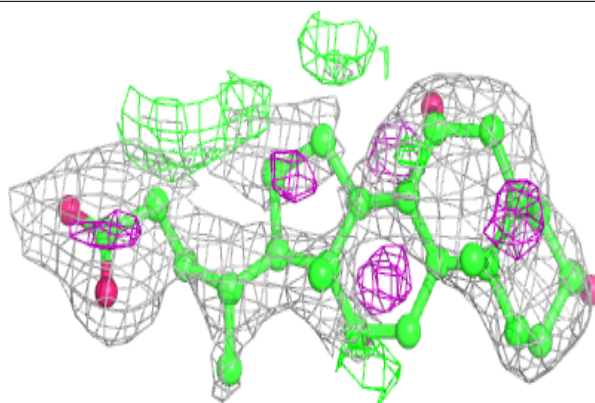
**Electron density around PEK T 102:**

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

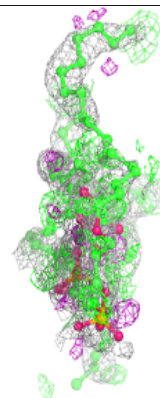
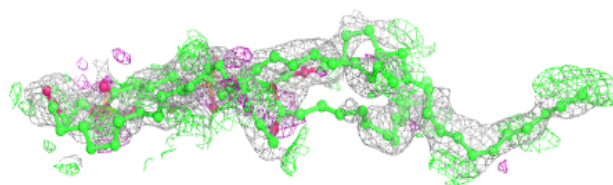
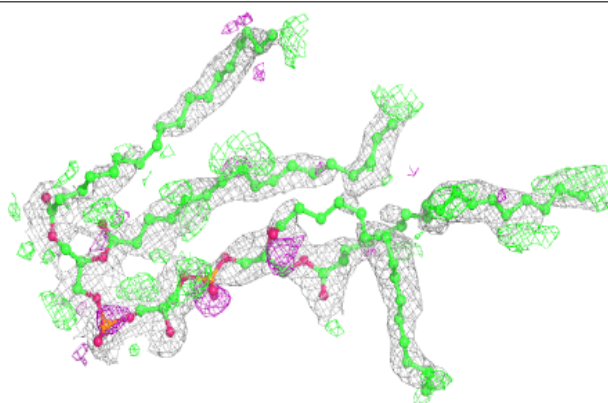


Electron density around CHD P 308:

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

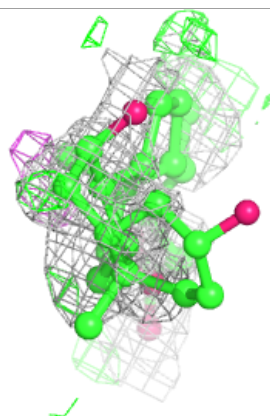
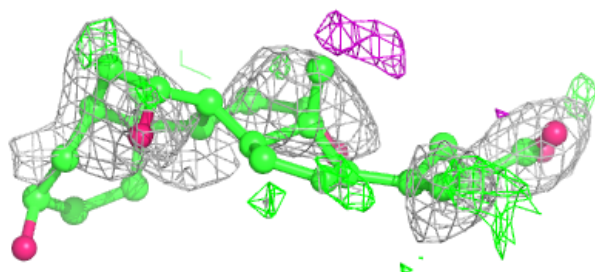
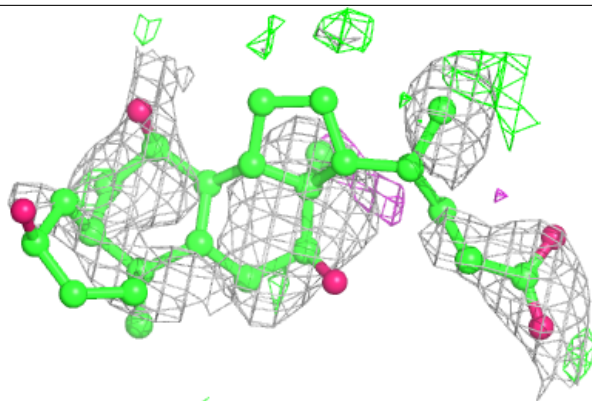
**Electron density around CDL T 103:**

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

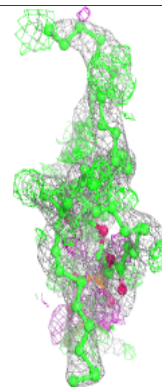
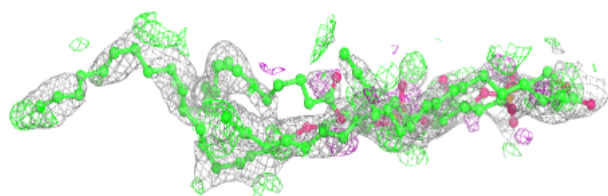
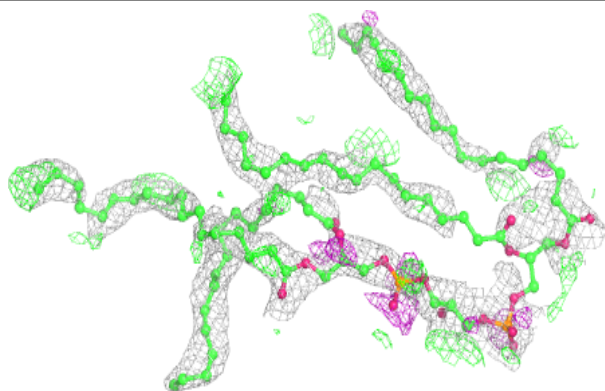


Electron density around CHD W 101:

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

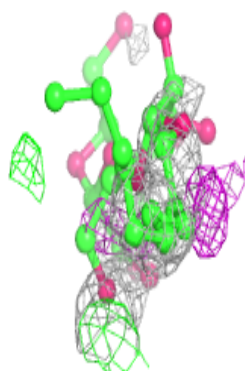
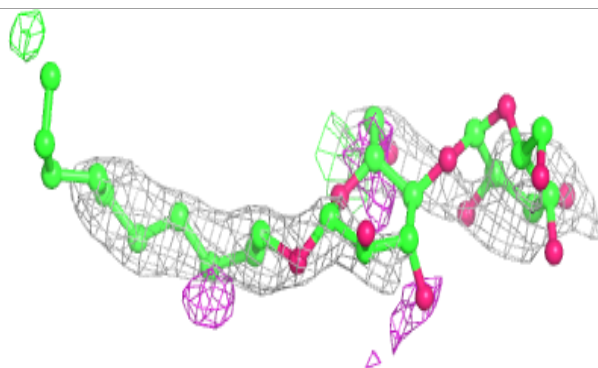
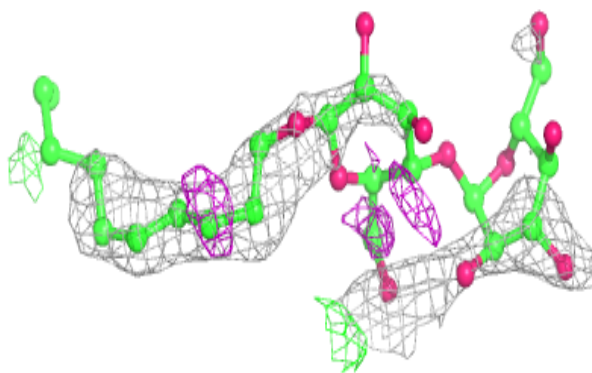
**Electron density around CDL G 101:**

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

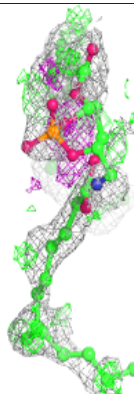
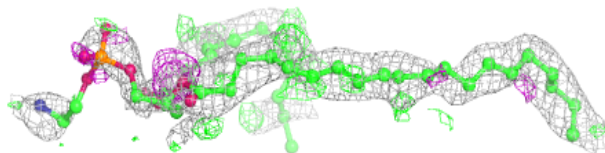
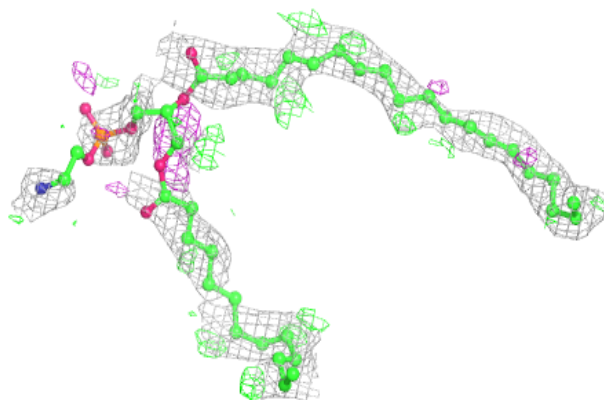


Electron density around DMU K 105:

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

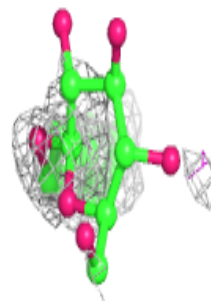
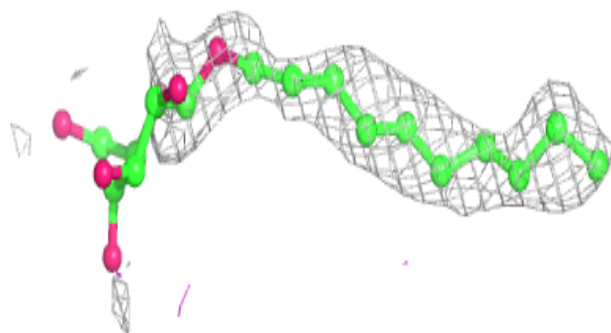
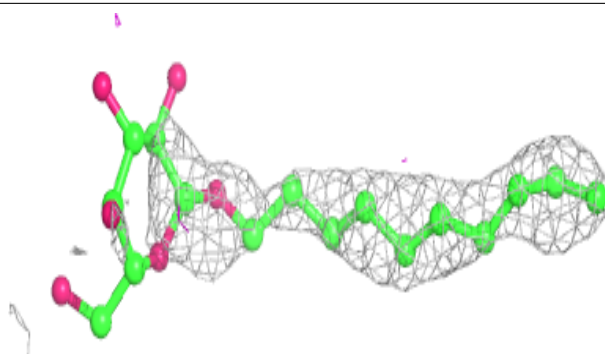
**Electron density around PEK P 302:**

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



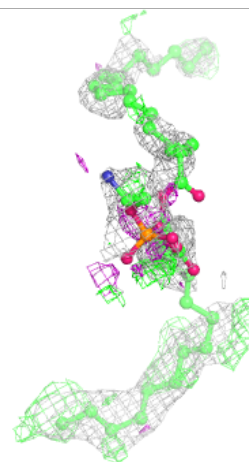
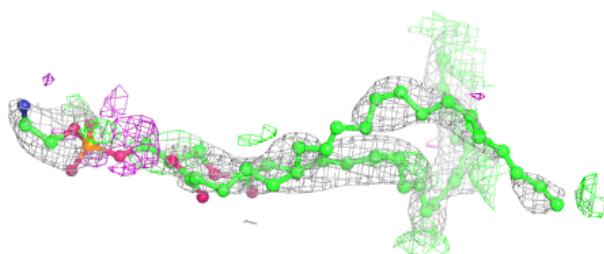
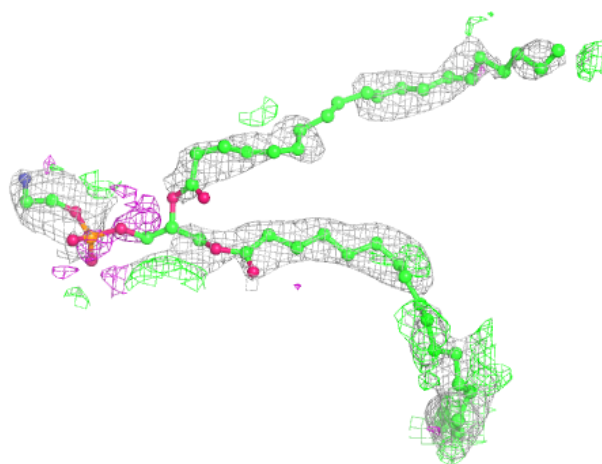
Electron density around DMU K 102:

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



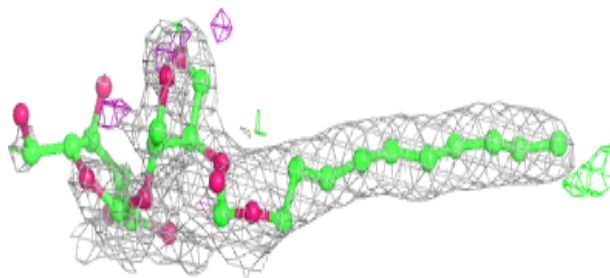
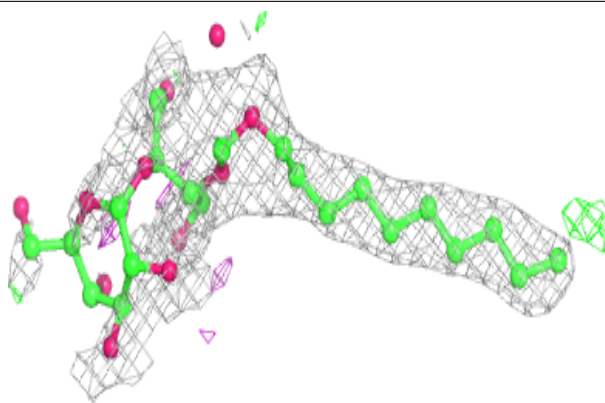
Electron density around PEK C 303:

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

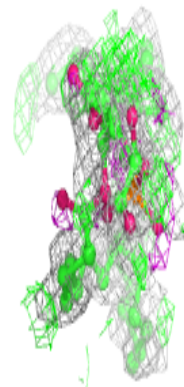
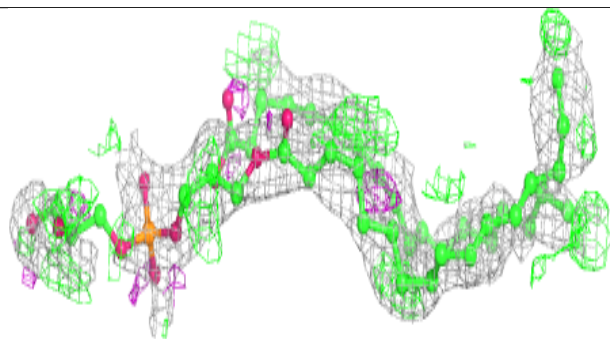
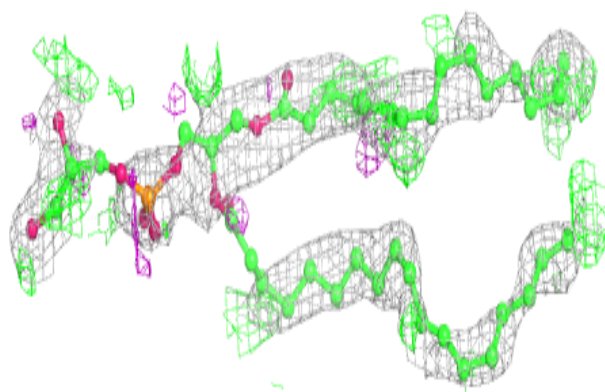


Electron density around DMU O 303:

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

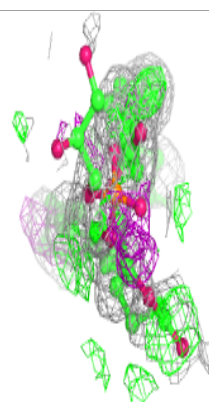
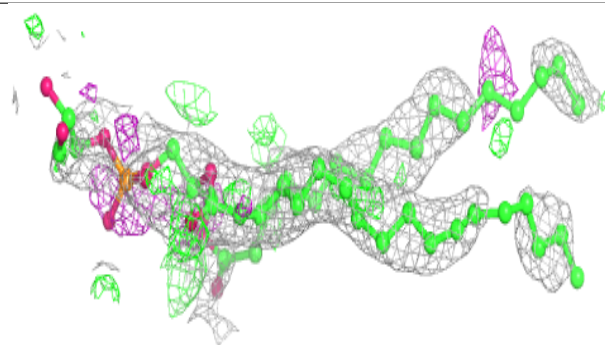
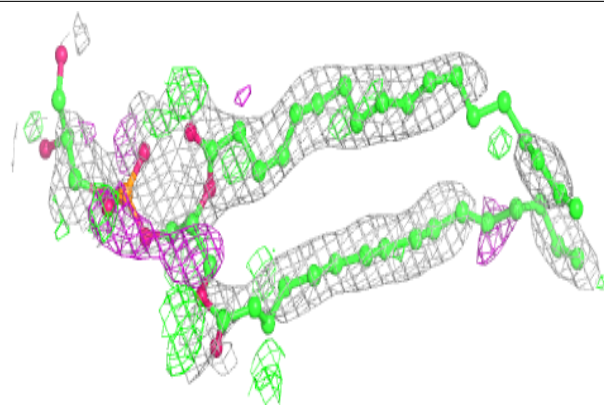
**Electron density around PGV C 305:**

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

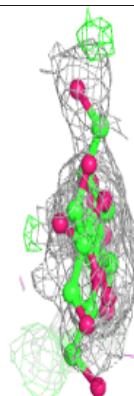
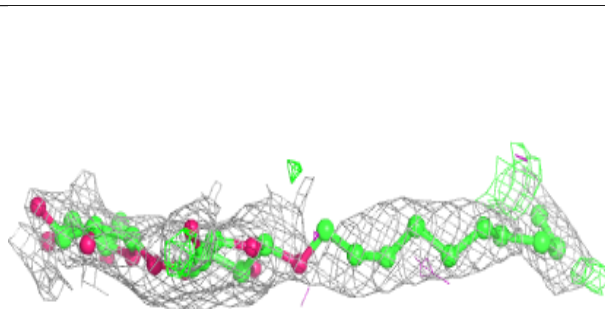
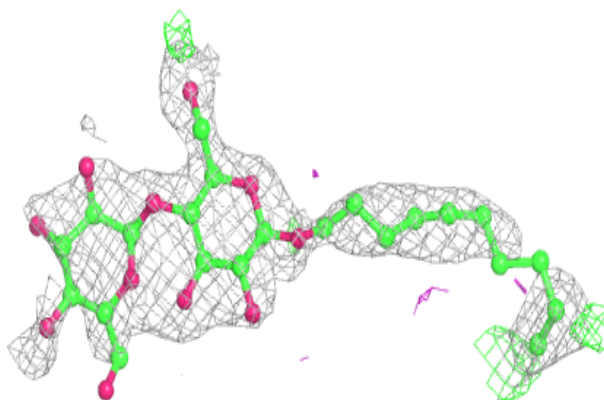


Electron density around PGV N 607:

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

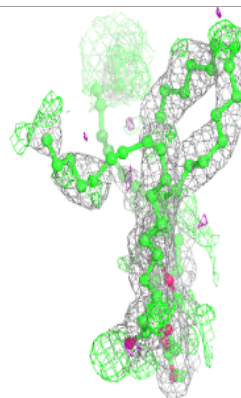
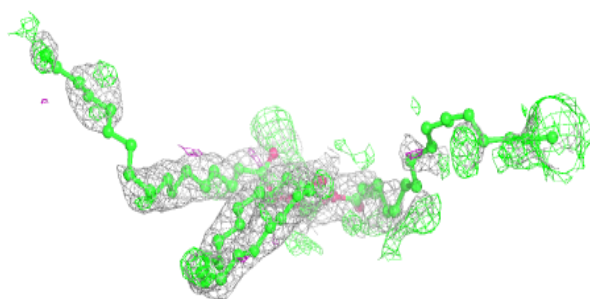
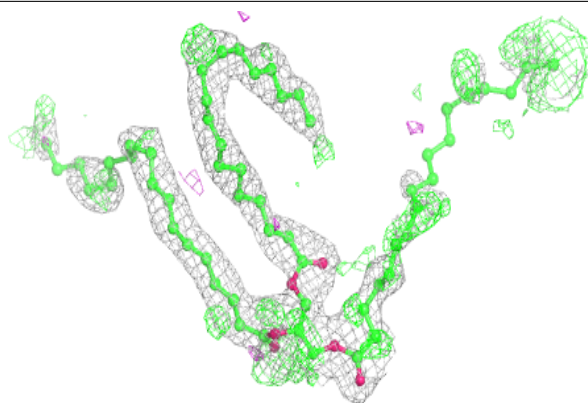
**Electron density around DMU L 102:**

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

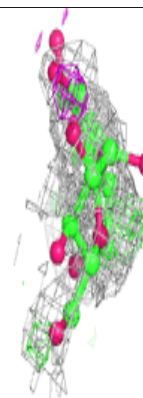
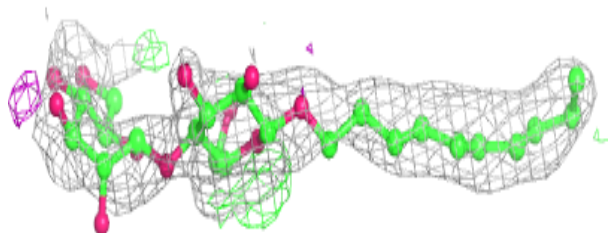
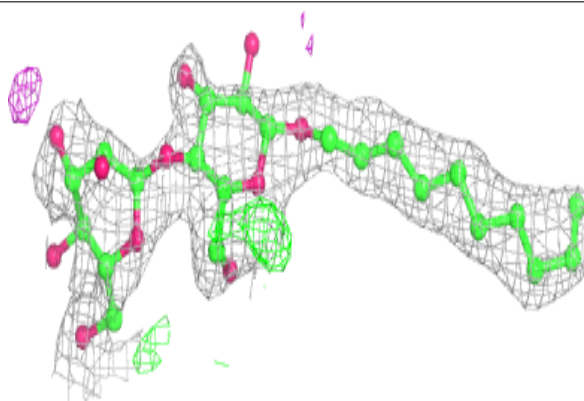


Electron density around TGL B 304:

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

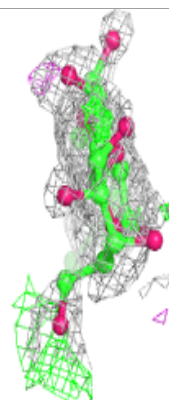
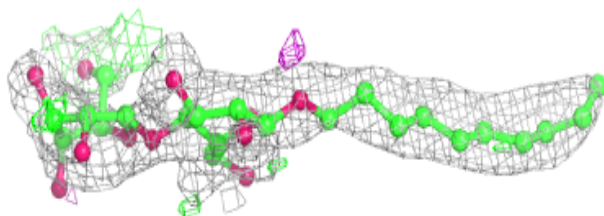
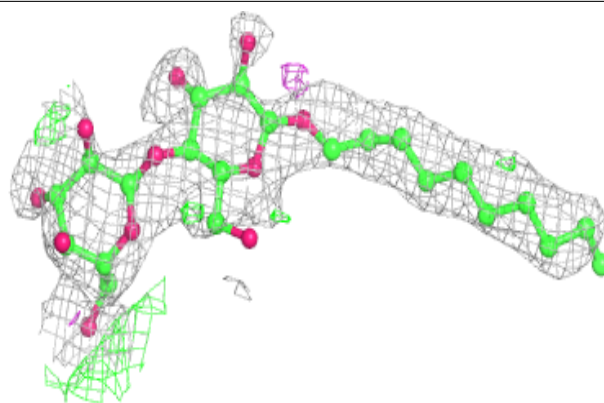
**Electron density around DMU C 307:**

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

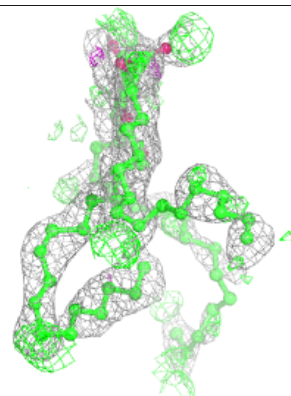
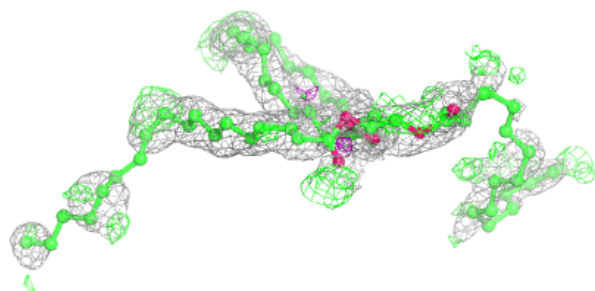
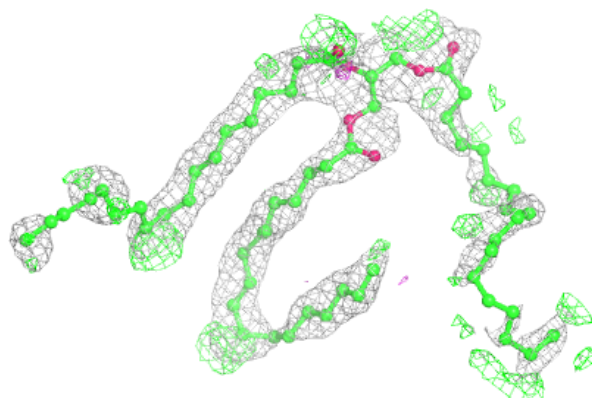


Electron density around DMU P 307:

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

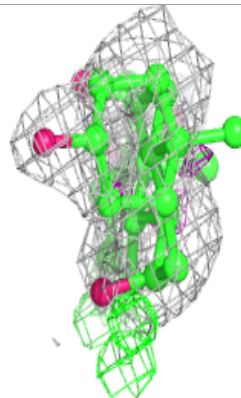
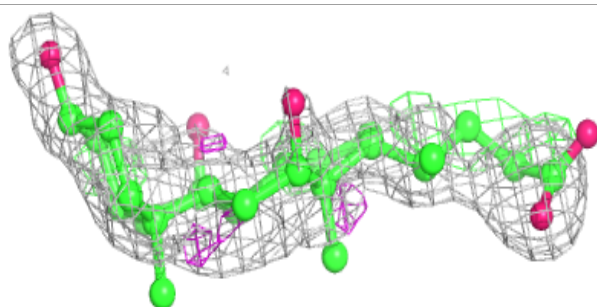
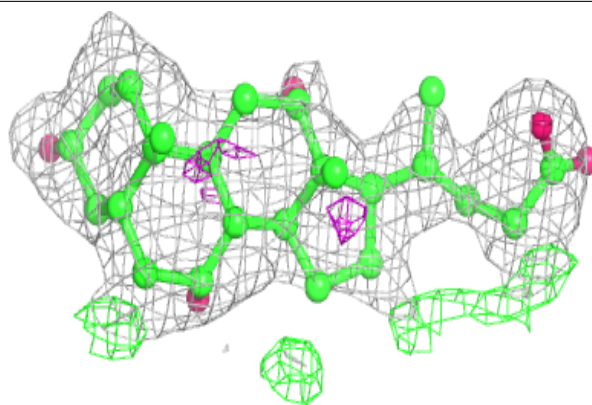
**Electron density around TGL Q 201:**

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

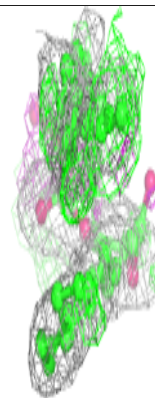
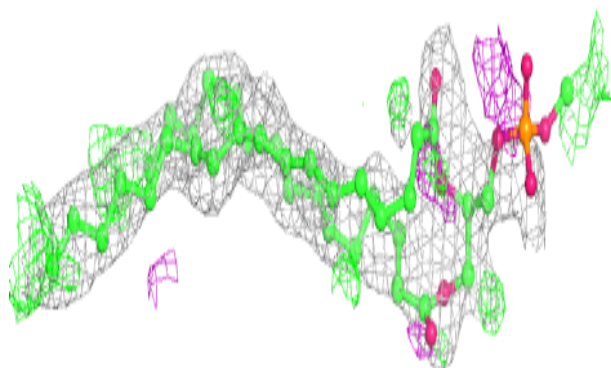
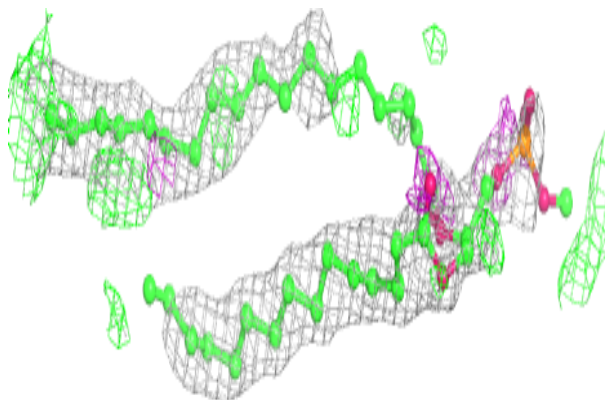


Electron density around CHD J 101:

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

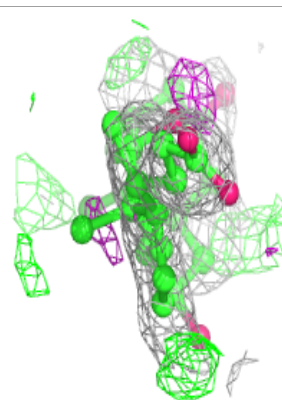
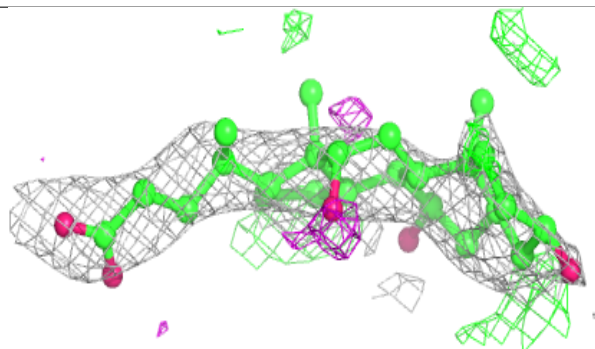
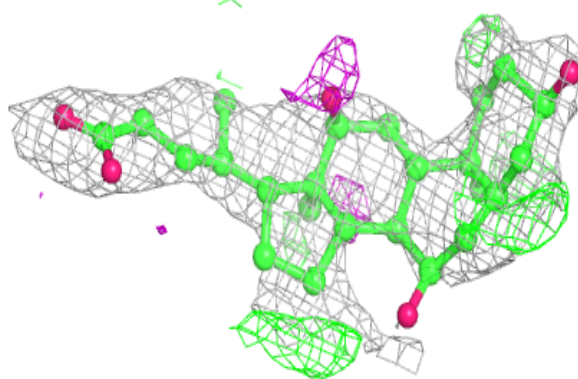
**Electron density around PSC O 302:**

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

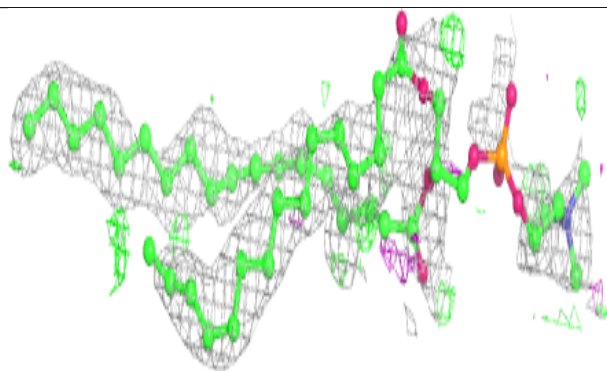
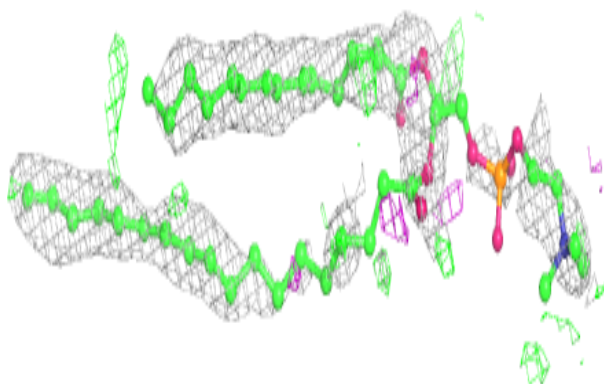


Electron density around CHD Y 101:

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

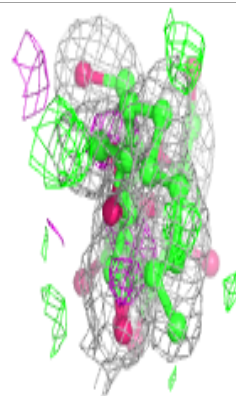
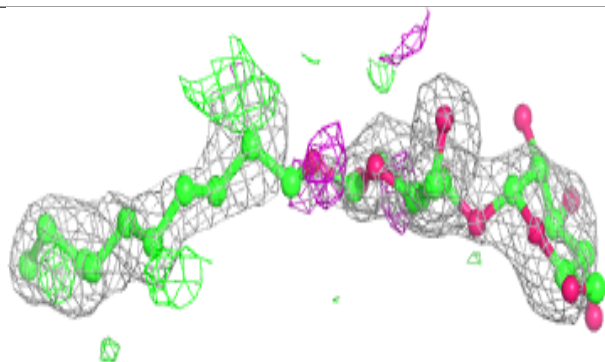
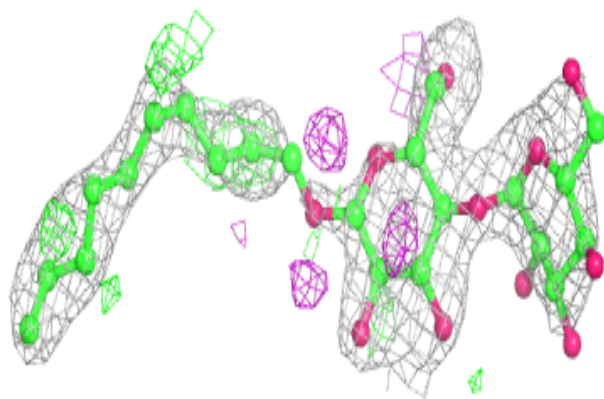
**Electron density around PSC B 303:**

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



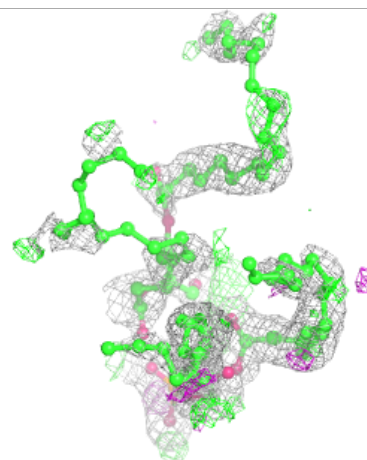
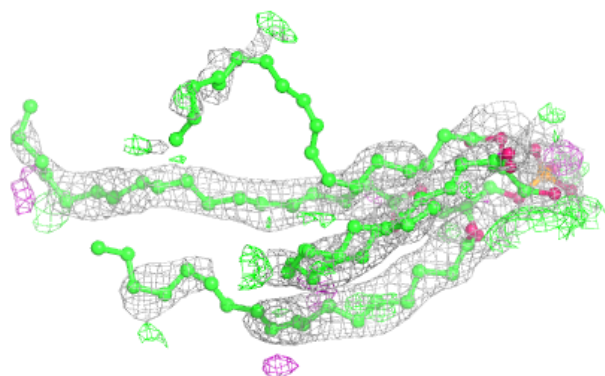
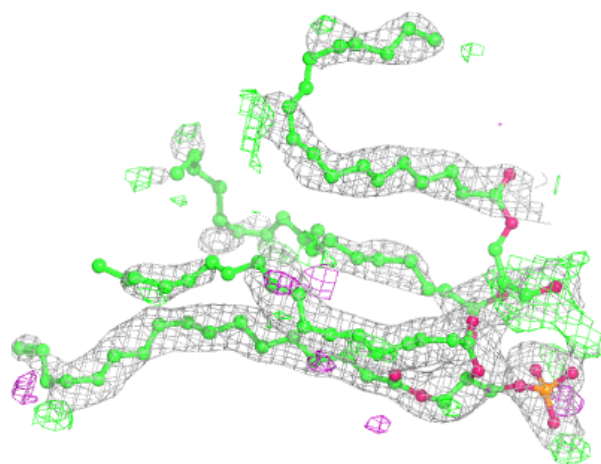
Electron density around DMU C 308:

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



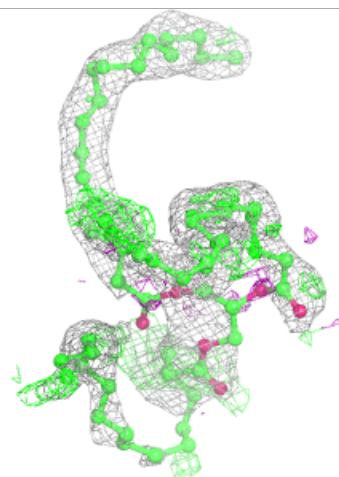
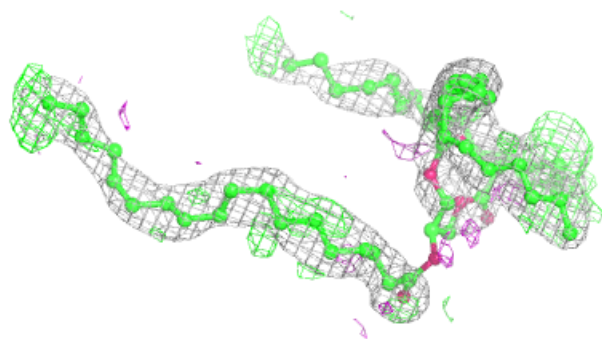
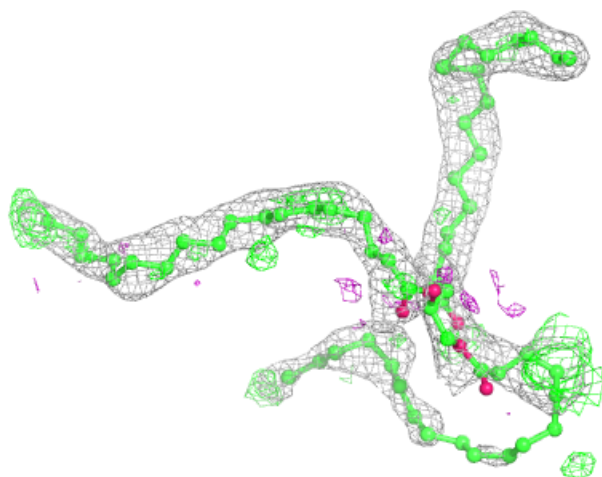
Electron density around CDL C 306:

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



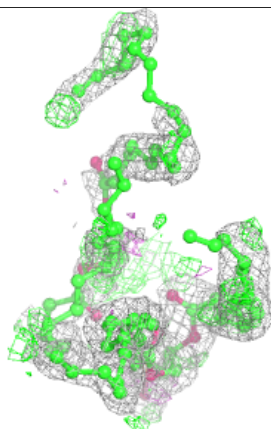
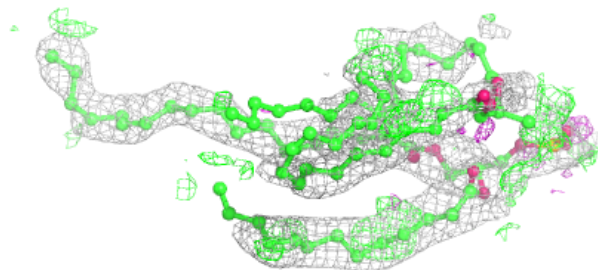
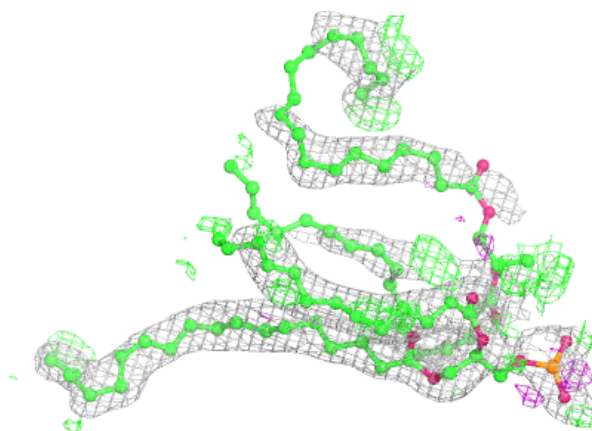
Electron density around TGL Y 102:

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

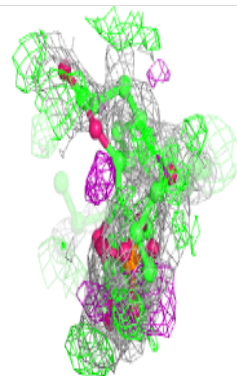
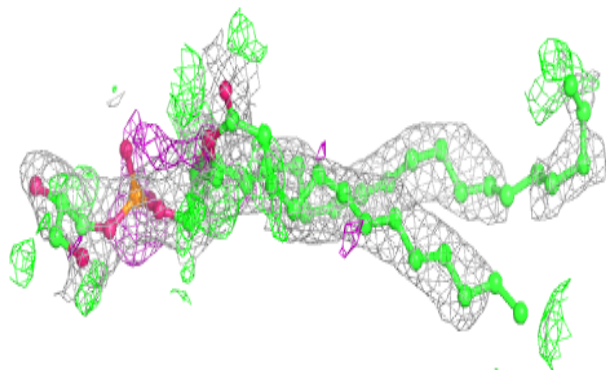
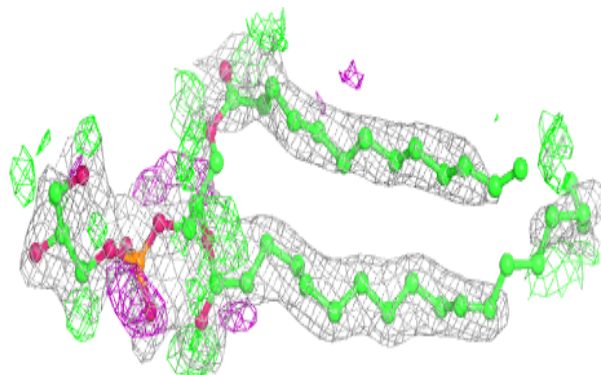


Electron density around CDL P 306:

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

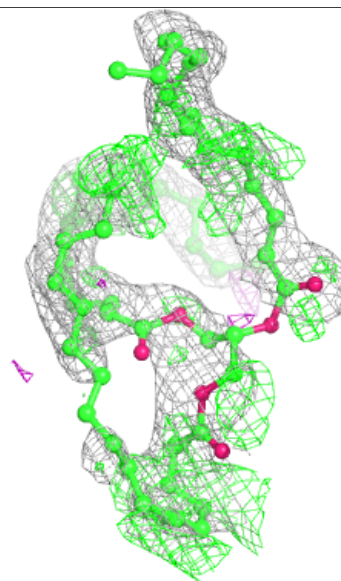
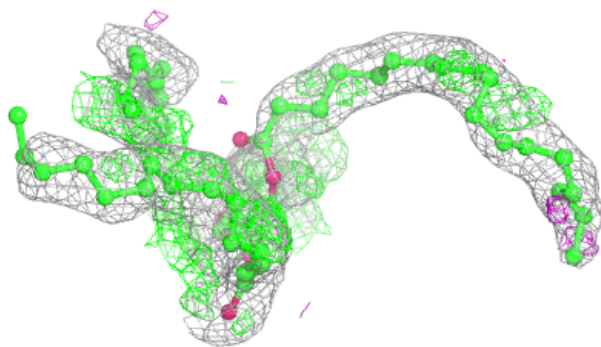
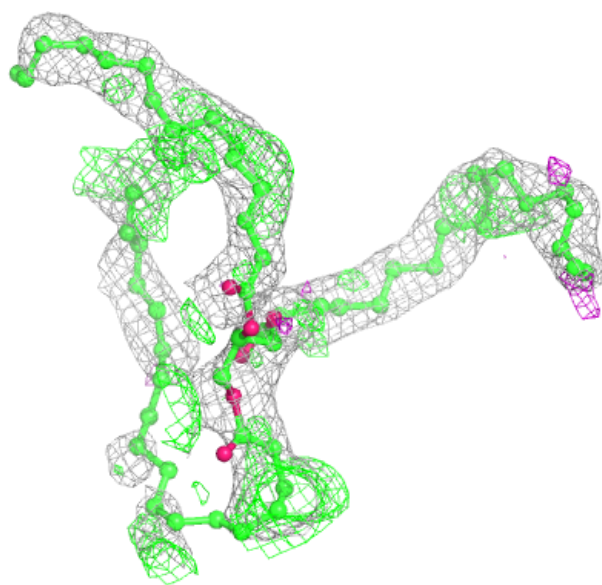
**Electron density around PGV A 607:**

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



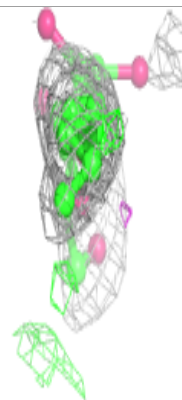
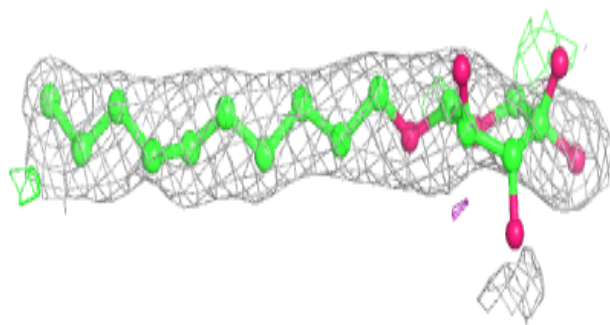
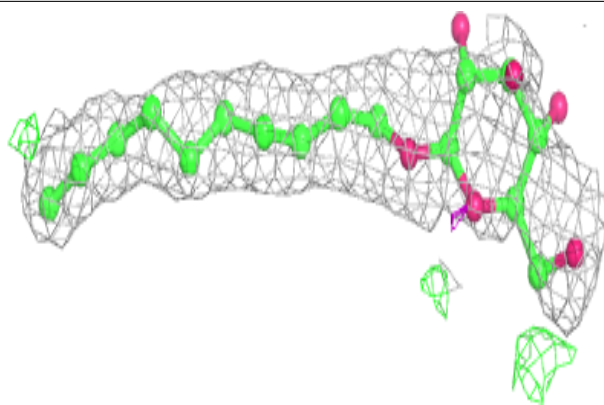
Electron density around TGL L 101:

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

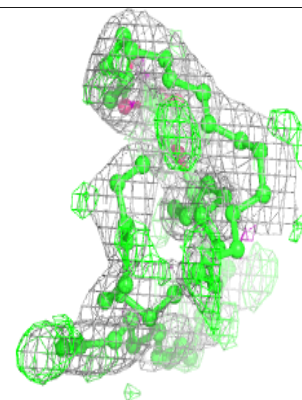
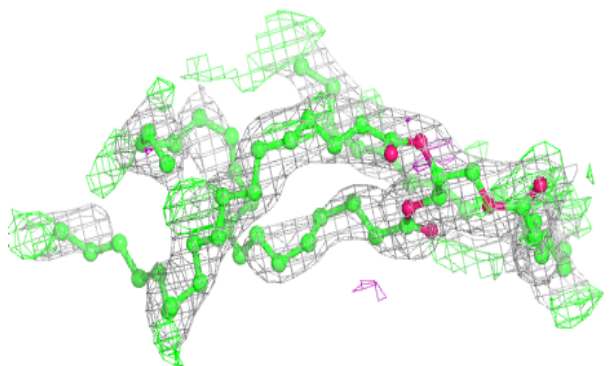
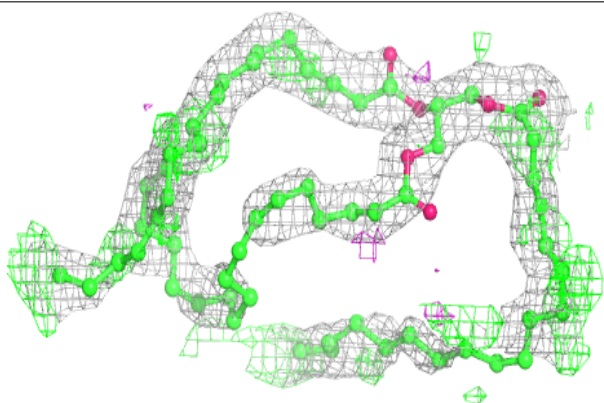


Electron density around DMU T 104:

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

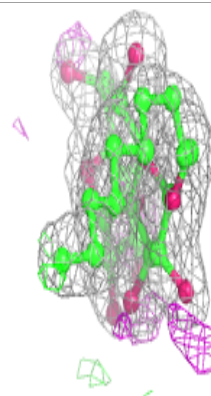
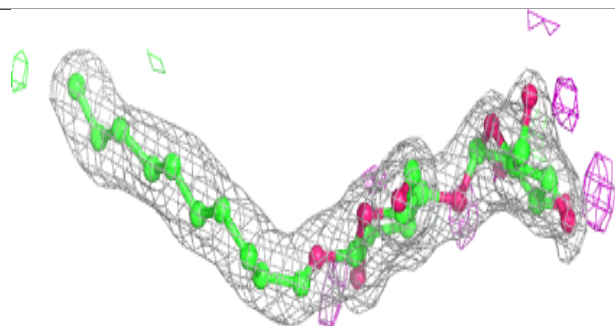
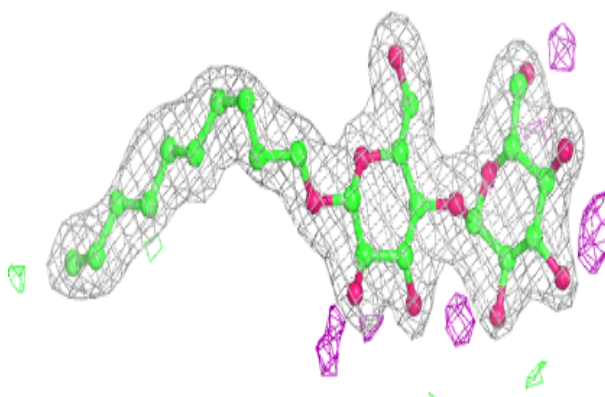
**Electron density around TGL N 608:**

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

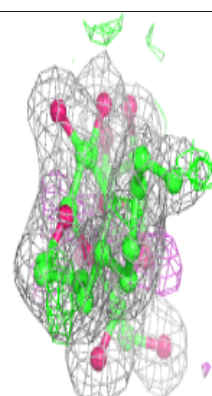
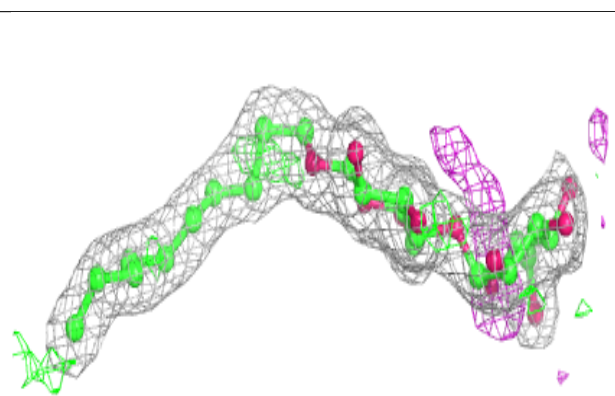
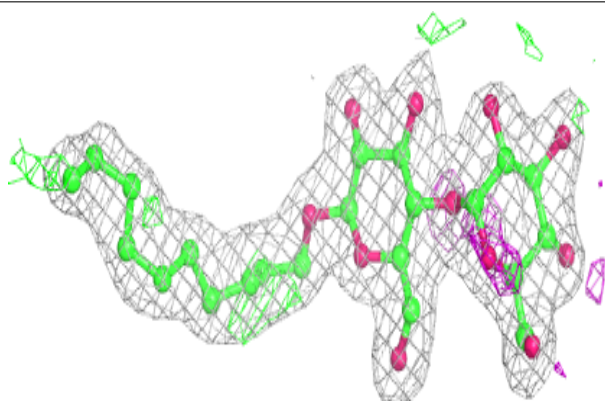


Electron density around DMU Z 101:

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

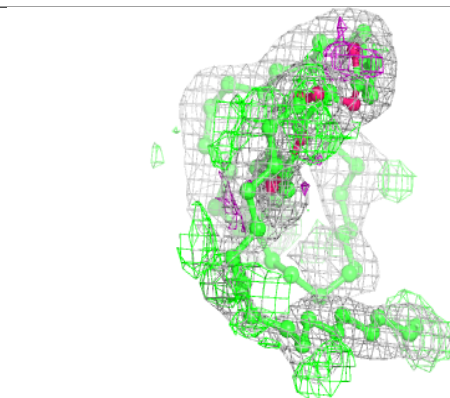
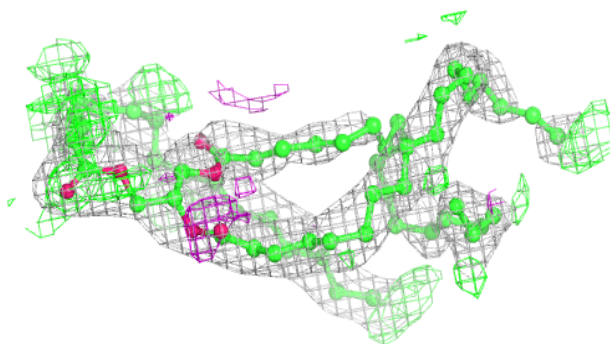
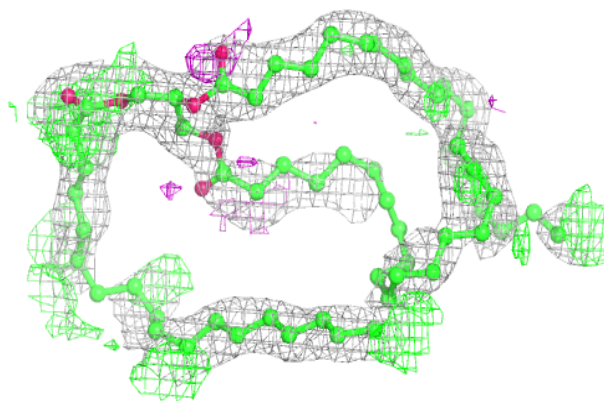
**Electron density around DMU M 101:**

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

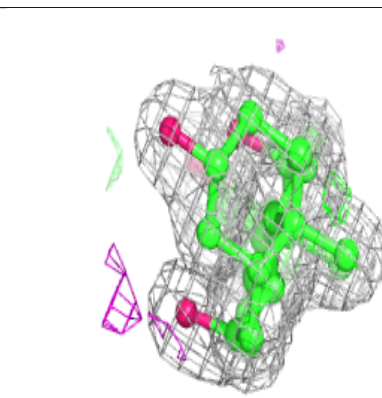
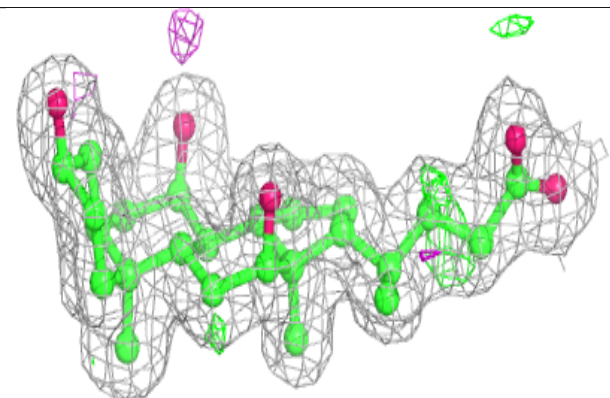
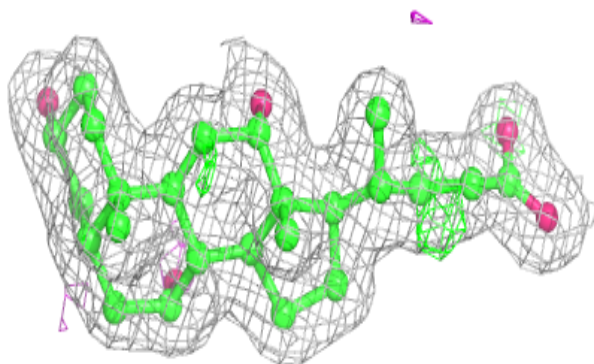


Electron density around TGL B 301:

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

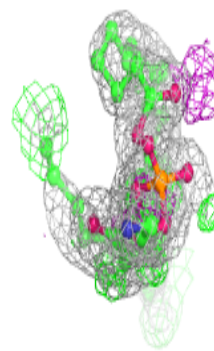
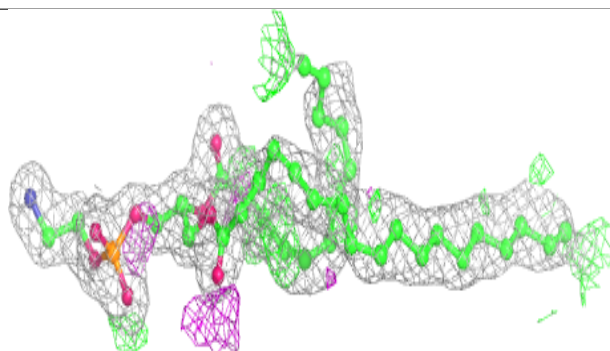
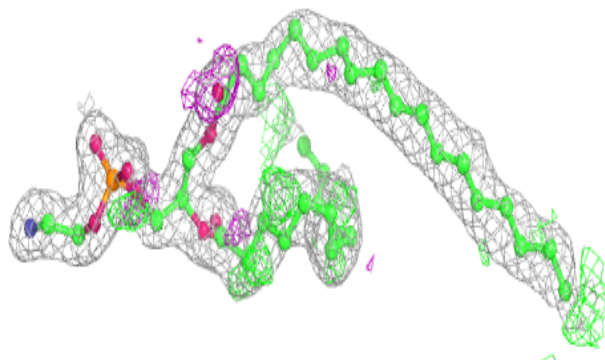
**Electron density around CHD C 301:**

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

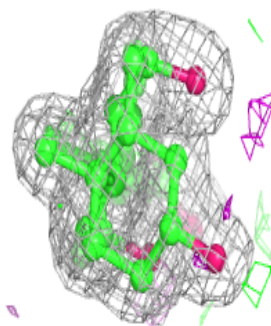
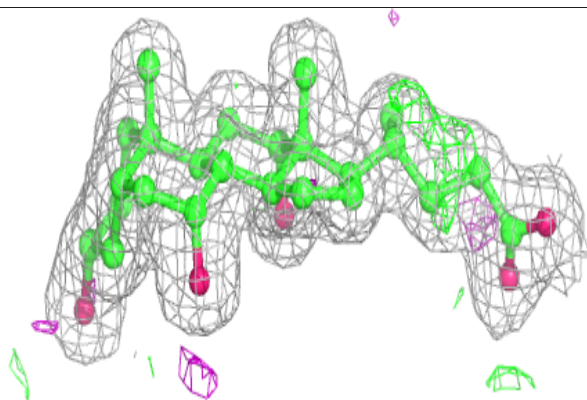
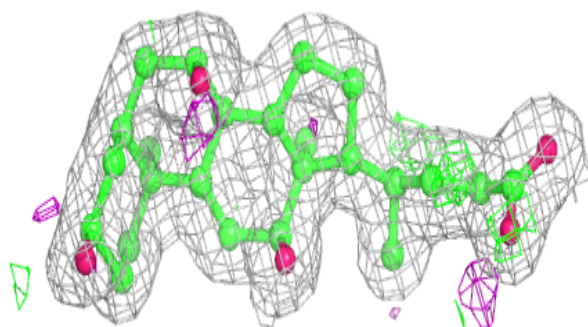


Electron density around PEK P 303:

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

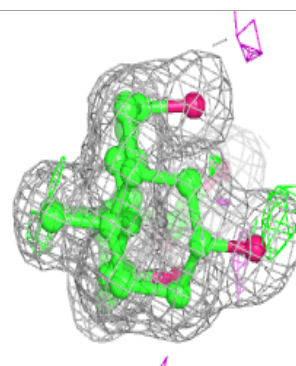
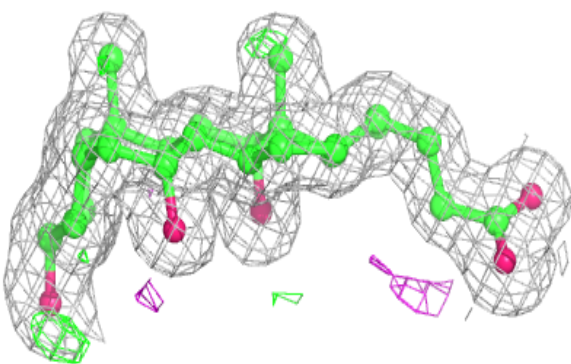
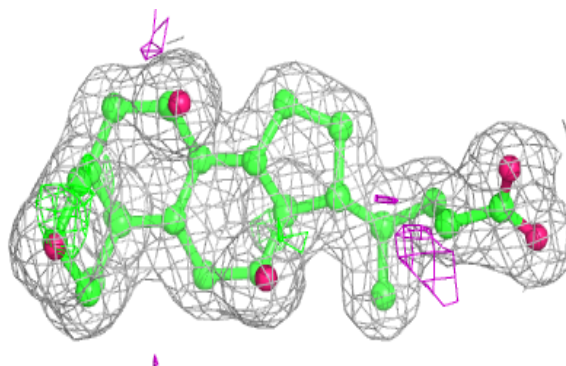
**Electron density around CHD P 301:**

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

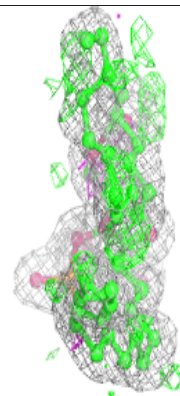
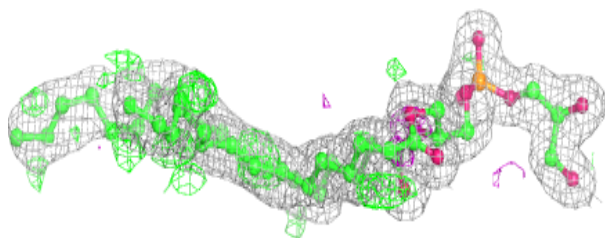
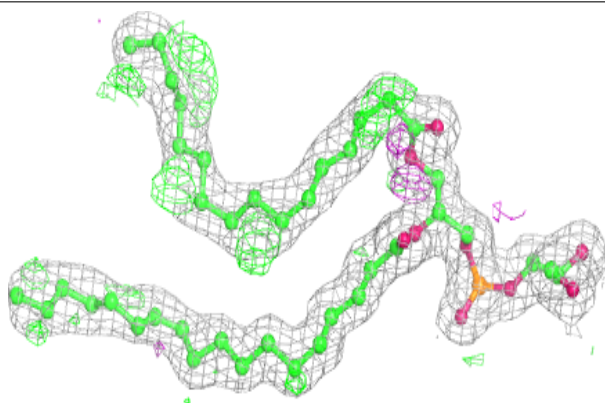


Electron density around CHD G 103:

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

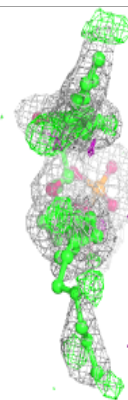
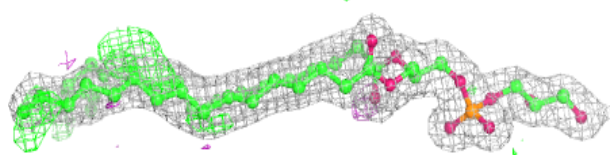
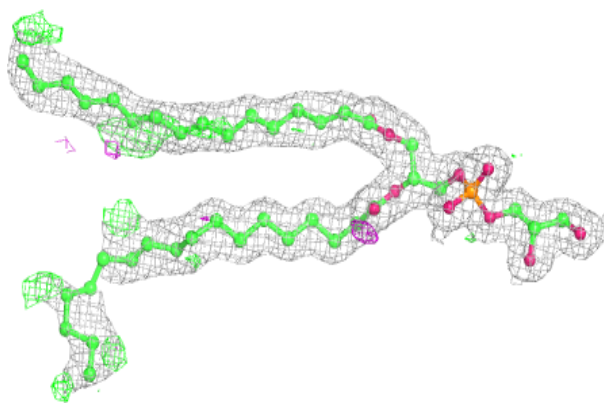
**Electron density around PGV N 609:**

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

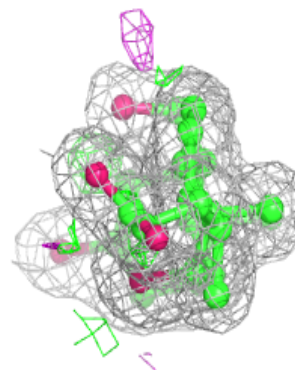
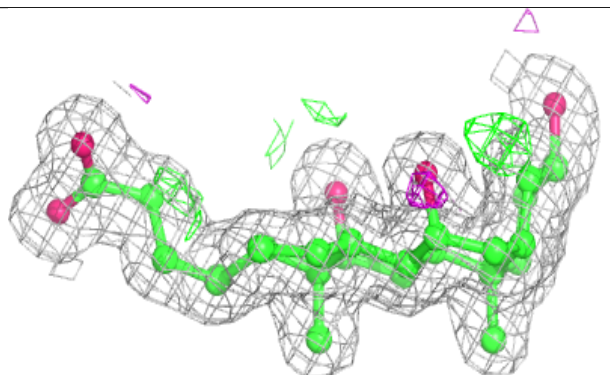
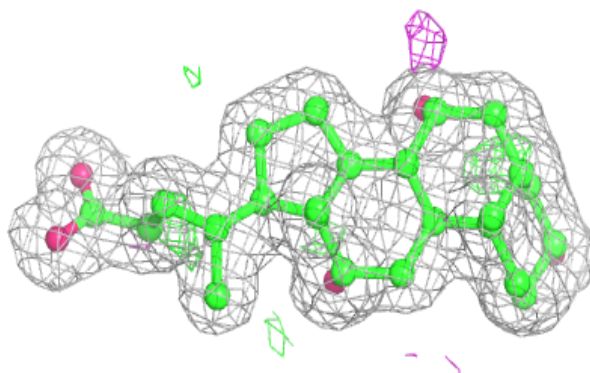


Electron density around PGV P 305:

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

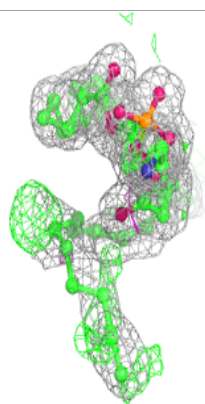
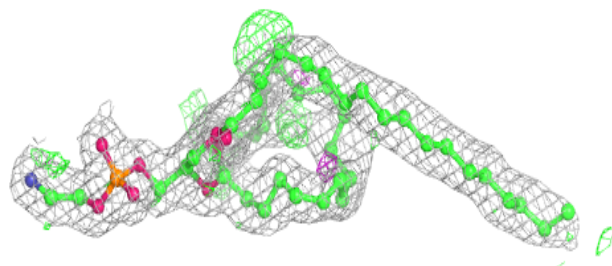
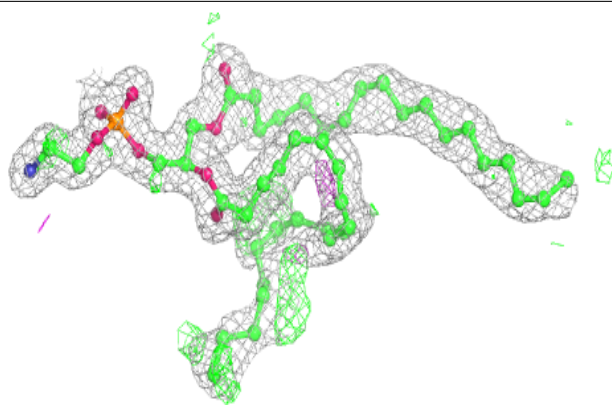
**Electron density around CHD T 101:**

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

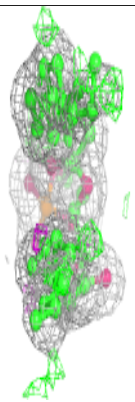
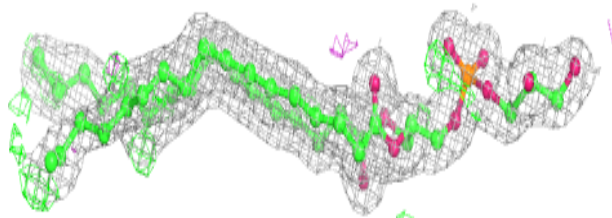
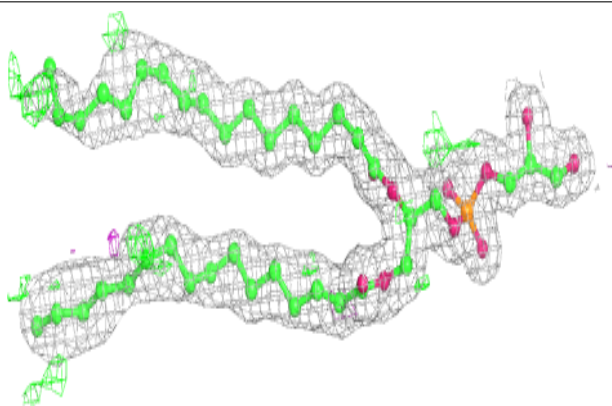


Electron density around PEK C 302:

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

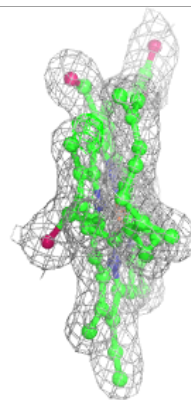
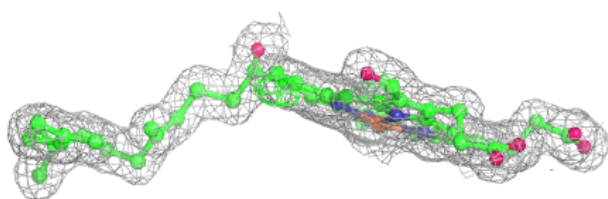
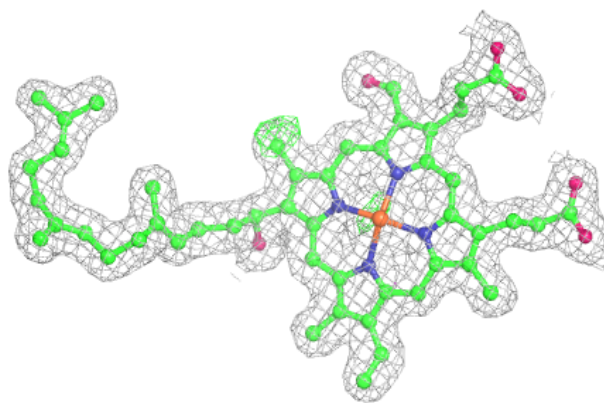
**Electron density around PGV C 304:**

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

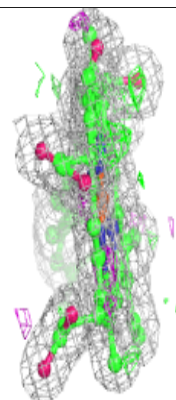
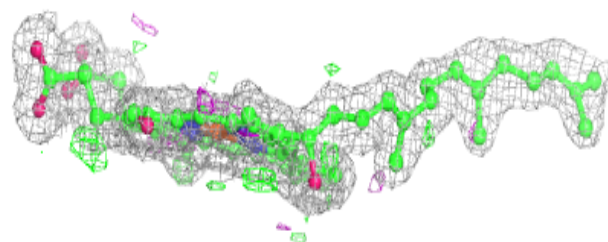
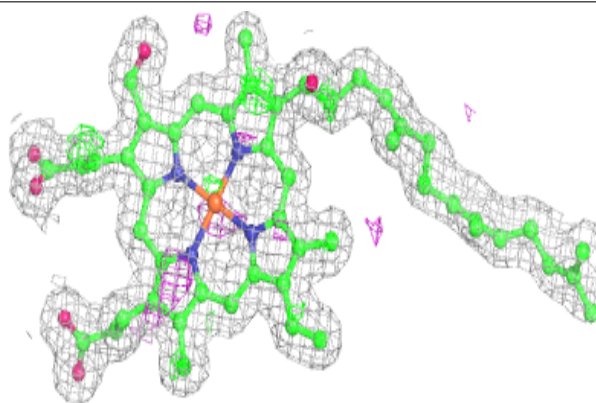


Electron density around HEA N 602:

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

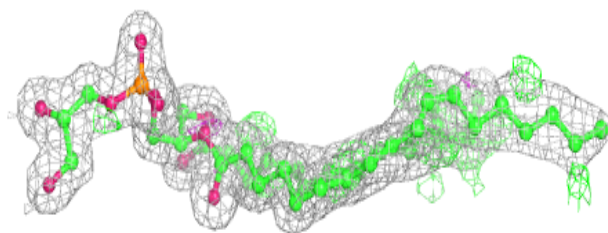
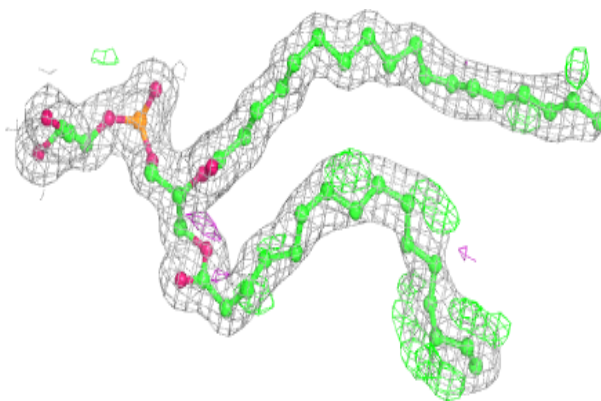
**Electron density around HEA A 601 (A):**

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

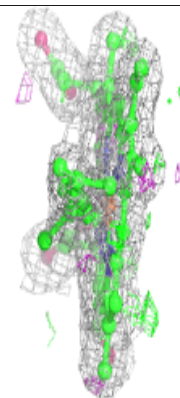
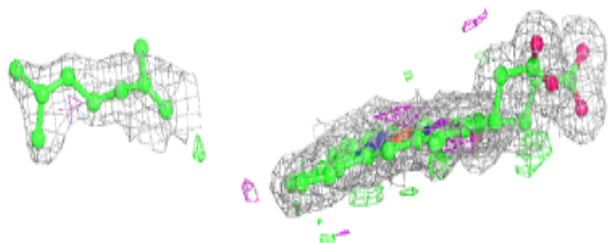
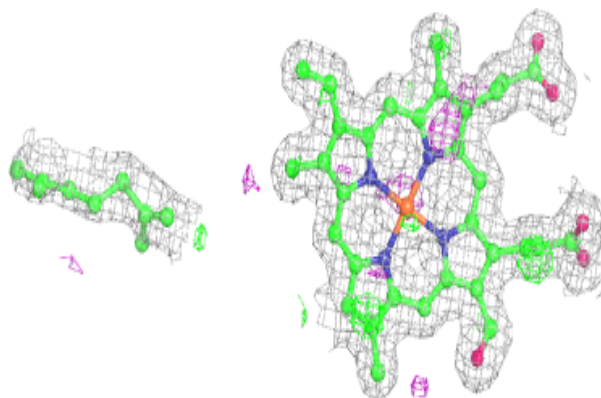


Electron density around PGV A 608:

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

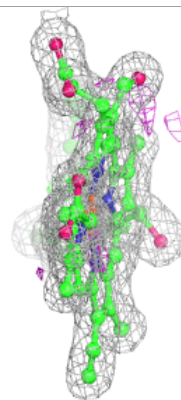
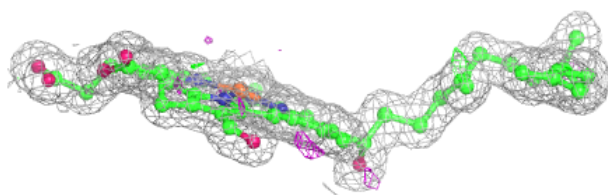
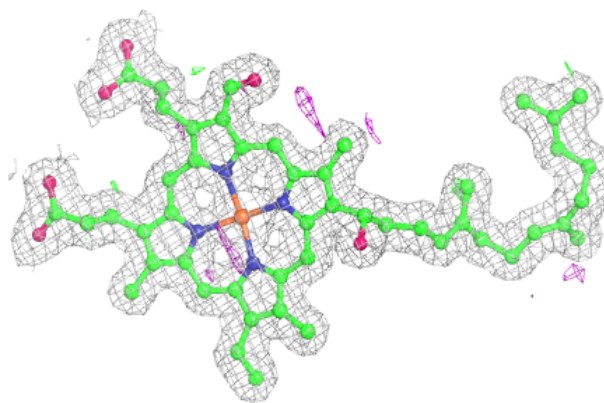
**Electron density around HEA A 601 (C):**

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

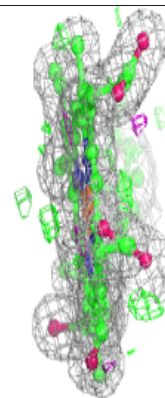
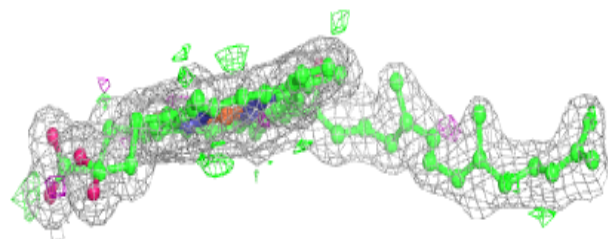
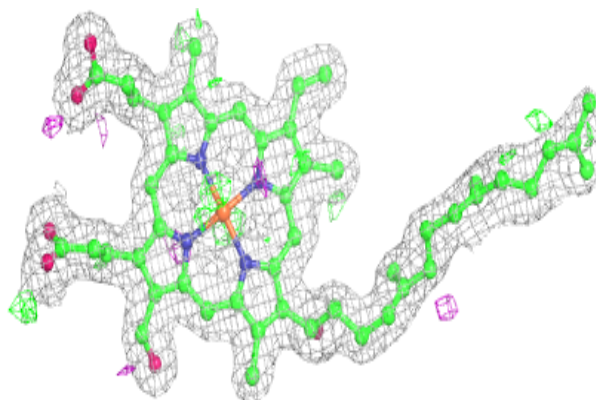


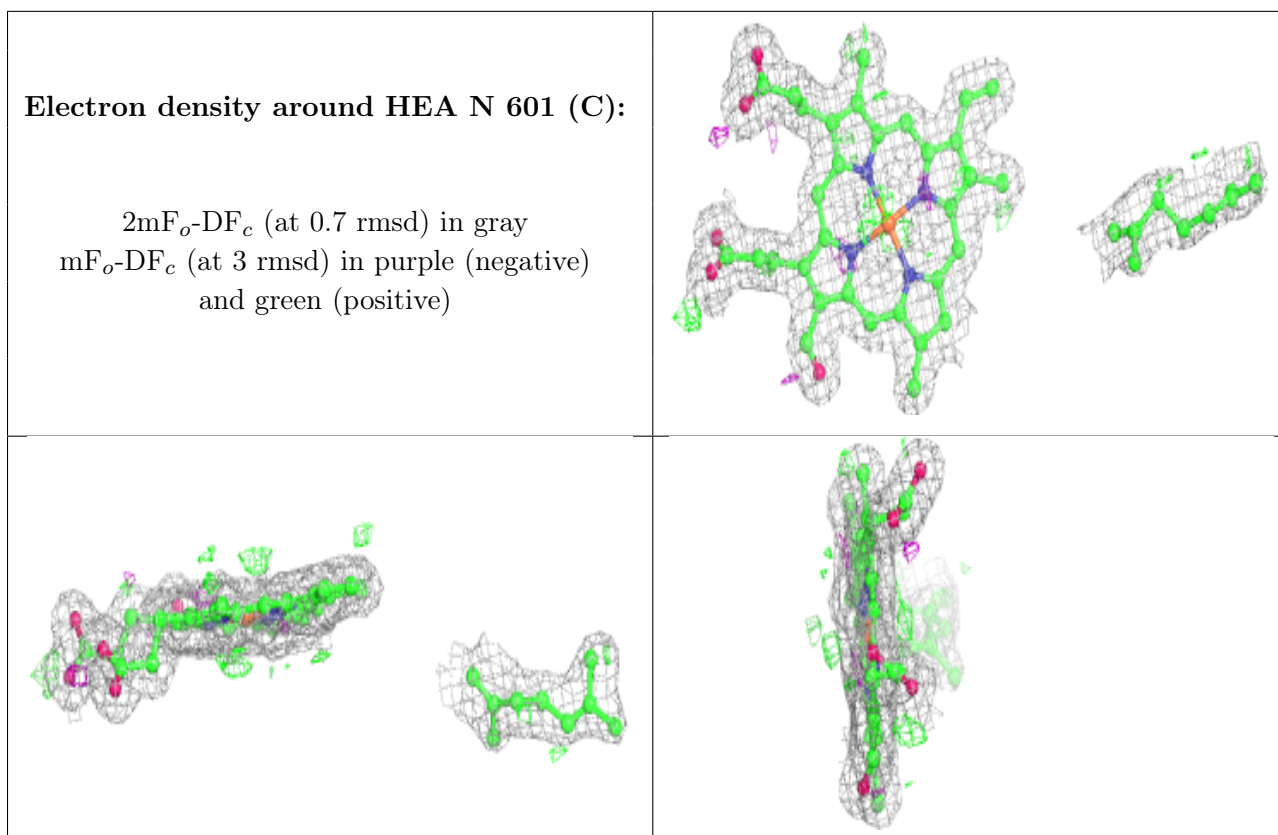
Electron density around HEA A 602:

$2mF_o-DF_c$ (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 (A):**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.