



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:03 pm BST

PDB ID : 6JUW  
Title : BOVINE HEART CYTOCHROME C OXIDASE IN CATALITIC INTER-MEDIATES AT 1.80 ANGSTROM RESOLUTION  
Authors : Shimada, A.; Muramoto, K.; Shinzawa-Itoh, K.; Yoshikawa, S.; Tsukihara, T.  
Deposited on : 2019-04-15  
Resolution : 1.80 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](mailto: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.

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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	:	2.11
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)	:	2.11

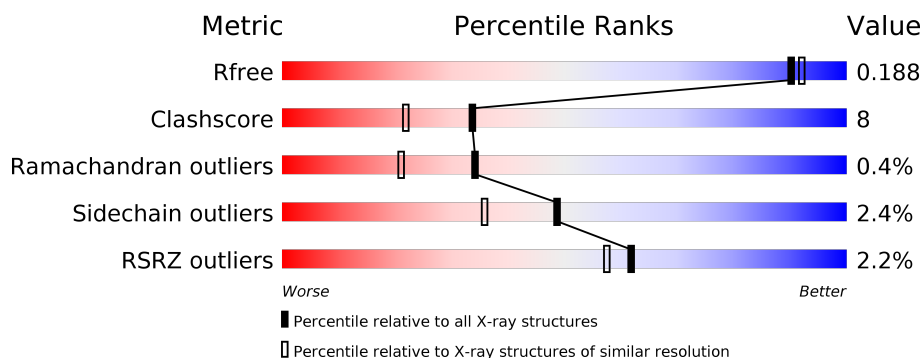
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
1	N	514	<div> <div>87%</div> <div>12%</div> <div>.</div> </div>
2	B	227	<div> <div>2%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
3	C	259	<div> <div>88%</div> <div>11%</div> </div>
3	P	259	<div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
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	602	X	-	-	-
14	HEA	N	602	X	-	-	-
18	DMU	K	103	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	EDO	N	612	-	-	X	-
22	EDO	N	617	-	-	X	-
22	EDO	U	102	-	-	X	-
25	CDL	G	102	-	-	X	-
25	CDL	T	102	-	-	X	-
7	TPO	G	11	-	-	-	X
9	SAC	V	1	-	-	-	X



## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 34360 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	37	0
			4192	2794	643	710	45			
1	N	514	Total	C	N	O	S	0	21	0
			4152	2770	639	703	40			

- 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	4	0
			1839	1196	281	343	19			
2	O	227	Total	C	N	O	S	0	7	0
			1857	1208	287	343	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	5	0
			2122	1417	336	355	14			
3	P	259	Total	C	N	O	S	0	2	0
			2114	1413	336	353	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1198	780	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	1	0
			751	465	135	146	5			
6	S	98	Total	C	N	O	S	0	1	0
			751	465	134	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			676	431	129	114	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			685	439	130	114	1	1		

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

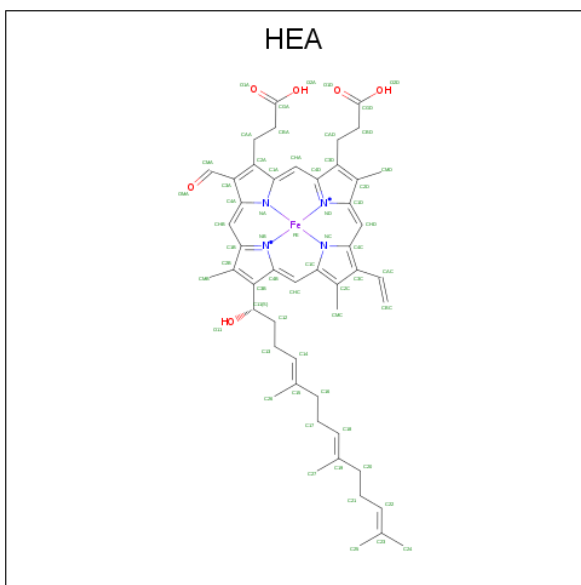
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			336	223	53	60			
13	Z	43	Total	C	N	O	0	0	0
			336	223	53	60			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 72	C 60	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 72	C 60	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		

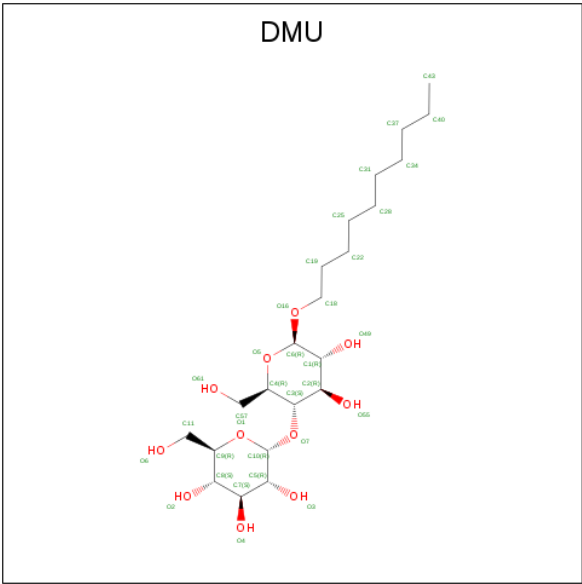
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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	P	1	Total	Na	0	0
			1	1		
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



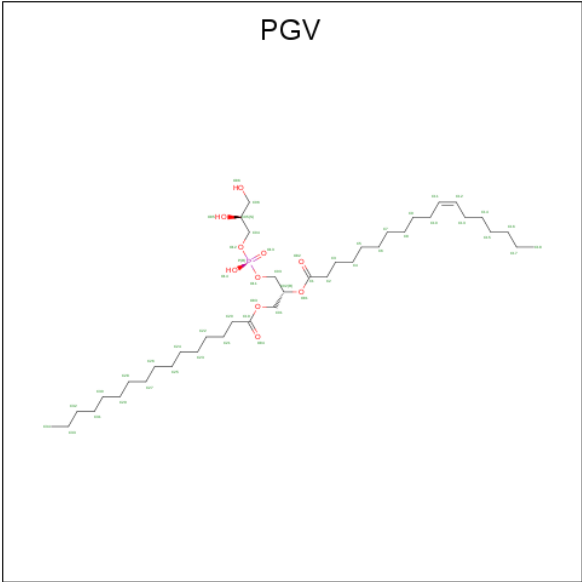
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			13	11	2		
18	B	1	Total	C	O	0	0
			11	10	1		
18	C	1	Total	C	O	0	0
			33	22	11		
18	C	1	Total	C	O	0	0
			22	16	6		
18	C	1	Total	C	O	0	0
			11	10	1		
18	D	1	Total	C	O	0	0
			21	16	5		
18	J	1	Total	C	O	0	0
			21	16	5		

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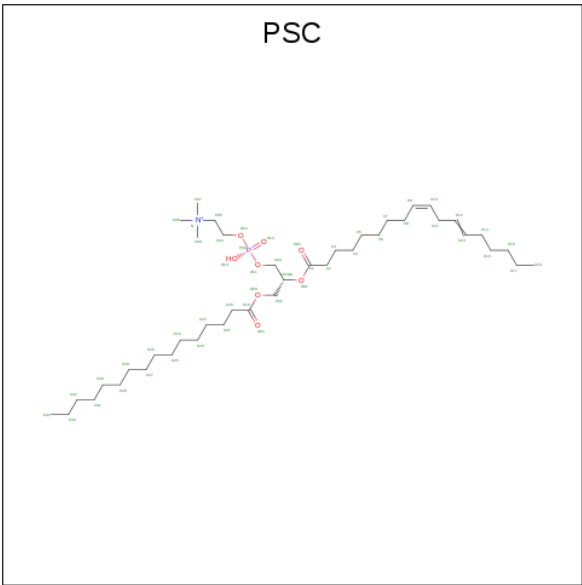
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	K	1	Total	C	O	0	0
			11	10	1		
18	K	1	Total	C	O	0	0
			14	11	3		
18	K	1	Total	C	O	0	0
			22	16	6		
18	K	1	Total	C	O	0	0
			11	10	1		
18	L	1	Total	C	O	0	0
			33	22	11		
18	M	1	Total	C	O	0	0
			33	22	11		
18	O	1	Total	C	O	0	0
			11	10	1		
18	P	1	Total	C	O	0	0
			11	10	1		
18	P	1	Total	C	O	0	0
			33	22	11		
18	Q	1	Total	C	O	0	0
			23	17	6		
18	W	1	Total	C	O	0	0
			21	16	5		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			21	16	5		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			11	10	1		
18	X	1	Total	C	O	0	0
			11	10	1		
18	Y	1	Total	C	O	0	0
			33	22	11		
18	Z	1	Total	C	O	0	0
			33	22	11		

- 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: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



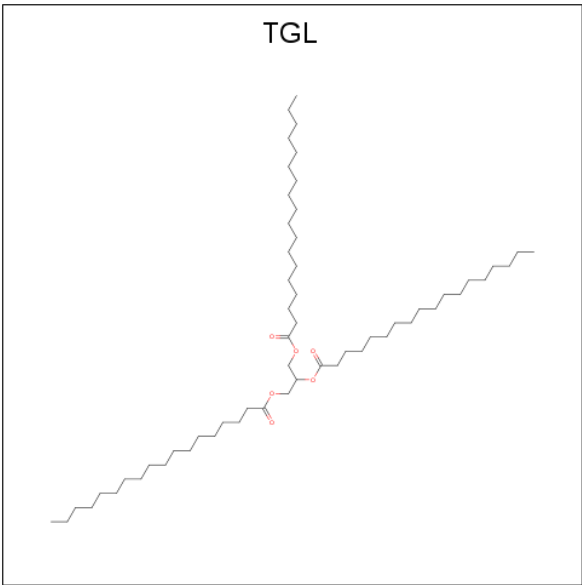
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
20	V	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	A	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

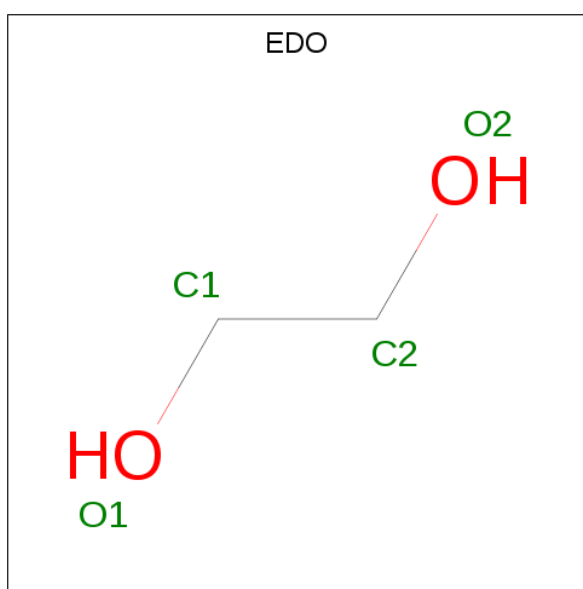
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

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

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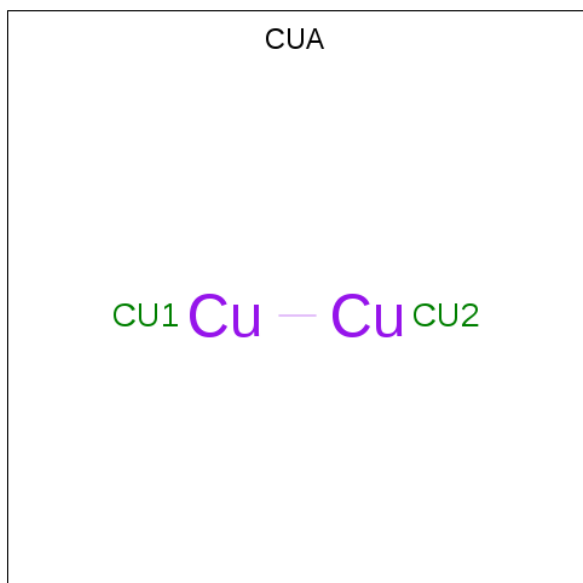
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	O	1	Total 4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

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

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



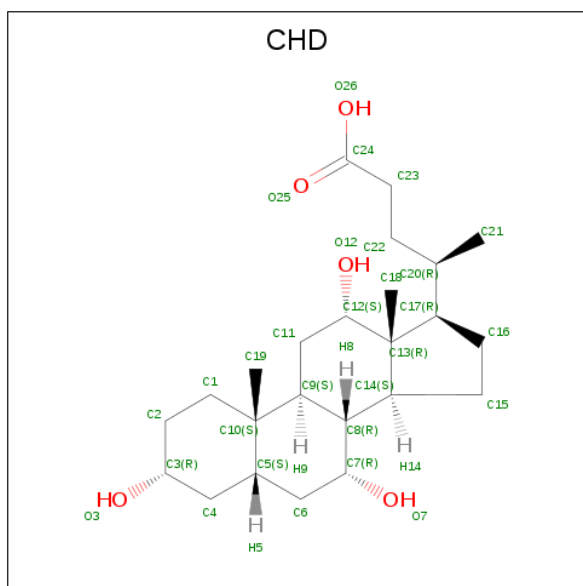
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total Cu 2 2	0	0

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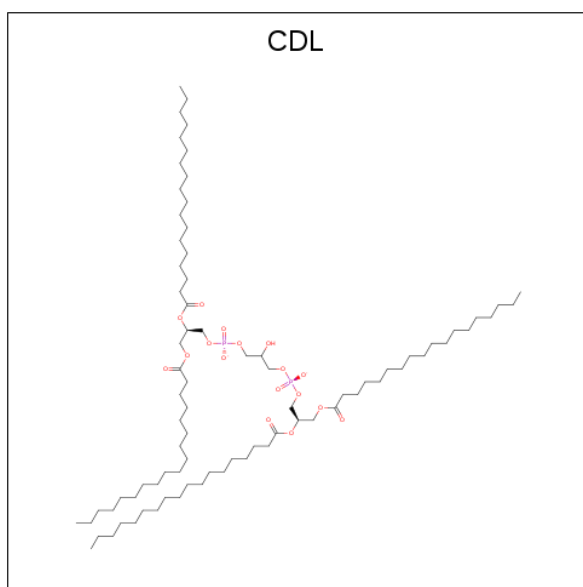
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	O	1	Total	Cu	0	0
			2	2		

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



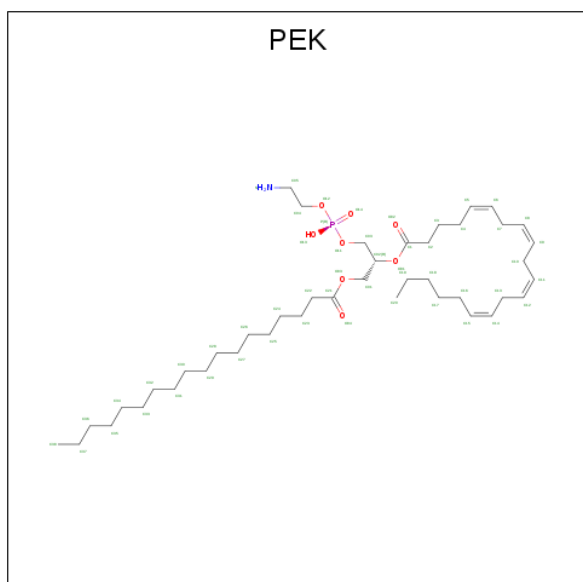
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	L	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	T	1	Total	C	O	0	0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

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



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

- Molecule 26 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).

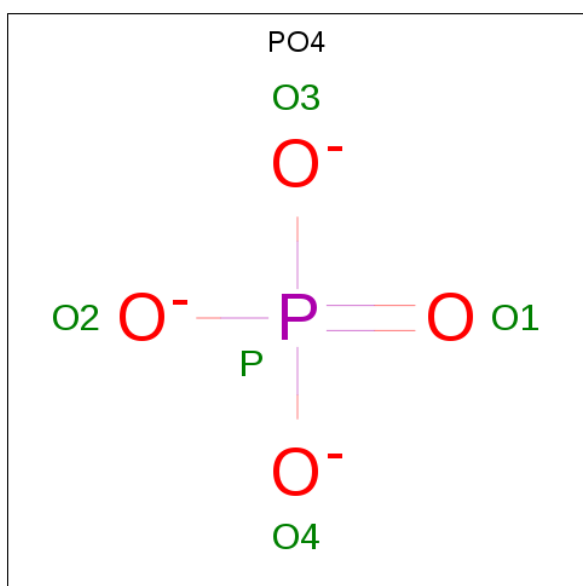


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	F	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
26	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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

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

- Molecule 28 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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



- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	247	Total O 250 250	0	4
29	B	200	Total O 200 200	0	0
29	C	136	Total O 136 136	0	0
29	D	174	Total O 174 174	0	0
29	E	133	Total O 133 133	0	0
29	F	117	Total O 117 117	0	0
29	G	72	Total O 72 72	0	0
29	H	79	Total O 79 79	0	0
29	I	56	Total O 56 56	0	0
29	J	44	Total O 44 44	0	0
29	K	36	Total O 36 36	0	0
29	L	42	Total O 42 42	0	0
29	M	34	Total O 34 34	0	0
29	N	245	Total O 247 247	0	3
29	O	166	Total O 166 166	0	0
29	P	132	Total O 132 132	0	0
29	Q	99	Total O 99 99	0	0
29	R	98	Total O 98 98	0	0
29	S	105	Total O 105 105	0	0
29	T	75	Total O 75 75	0	0
29	U	65	Total O 65 65	0	0

*Continued on next page...*

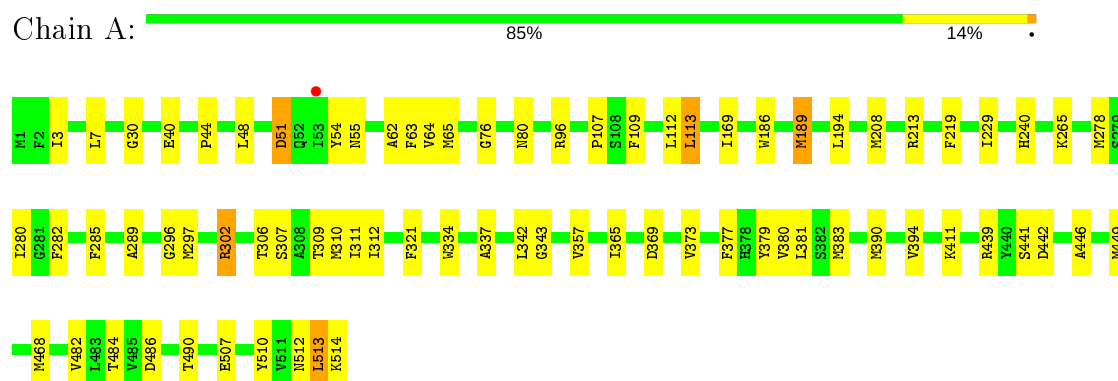
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	V	48	Total 48	O 48	0	0
29	W	27	Total 27	O 27	0	0
29	X	28	Total 28	O 28	0	0
29	Y	31	Total 31	O 31	0	0
29	Z	20	Total 20	O 20	0	0

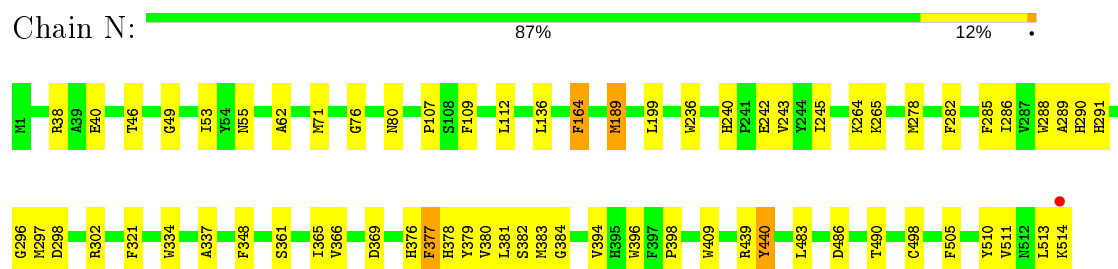
### 3 Residue-property plots

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

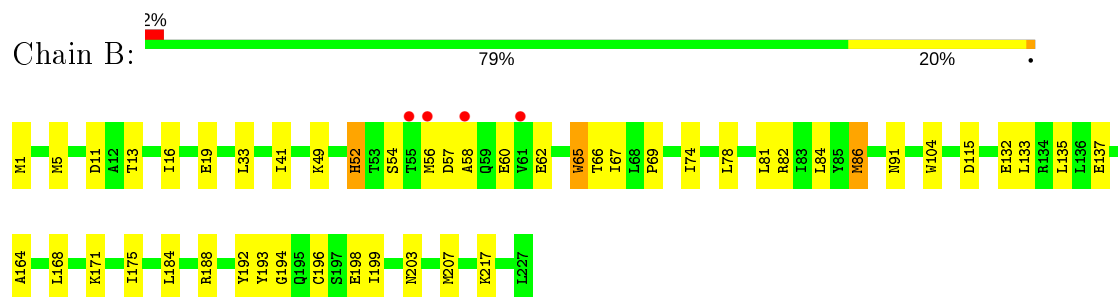
#### • Molecule 1: Cytochrome c oxidase subunit 1



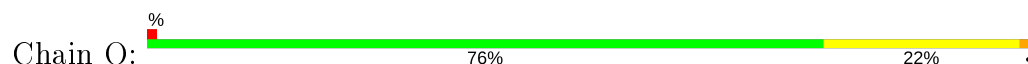
#### • Molecule 1: Cytochrome c oxidase subunit 1

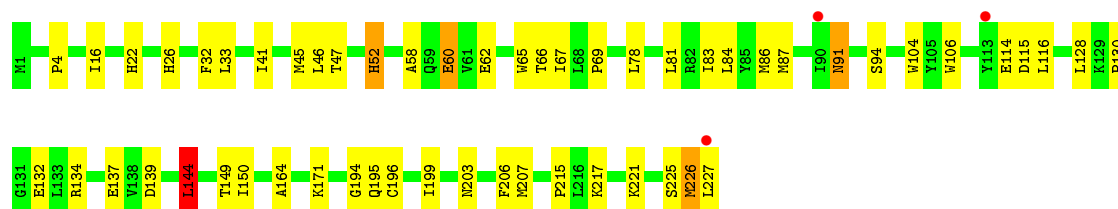


#### • Molecule 2: Cytochrome c oxidase subunit 2



#### • Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 88% 11%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 11%



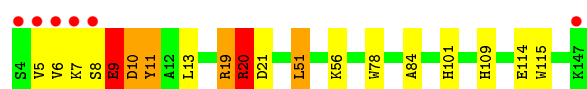
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 90% 10%



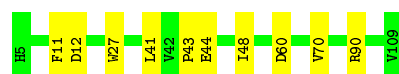
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 4% 87% 9%



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

Chain E: 90% 10%

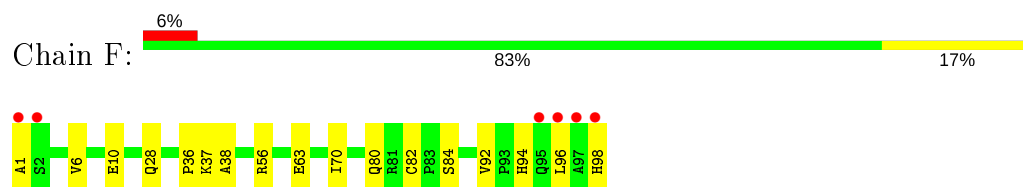


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

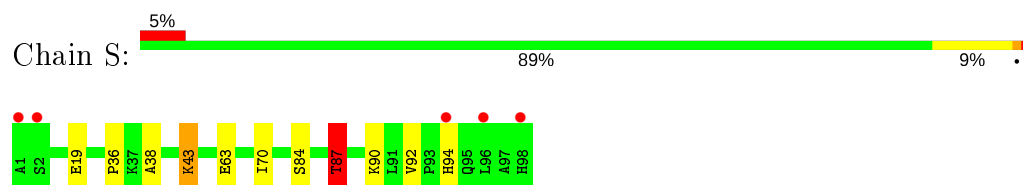
Chain R: 2% 88% 11%



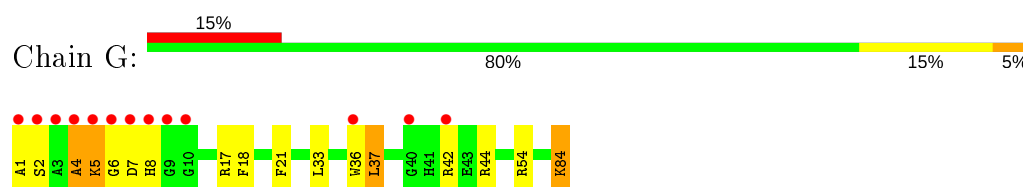
- Molecule 6: Cytochrome c oxidase subunit 5B



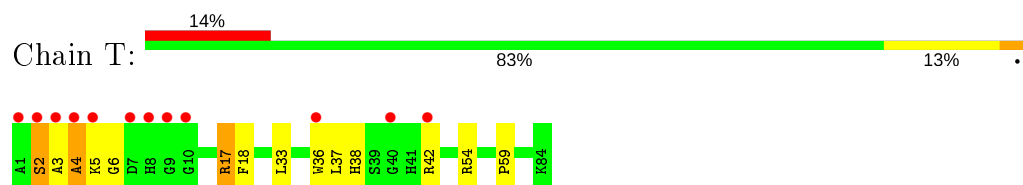
- Molecule 6: Cytochrome c oxidase subunit 5B



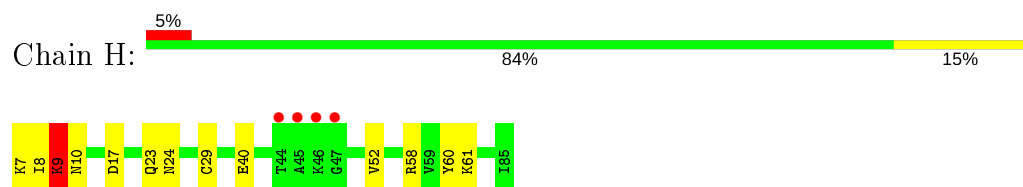
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



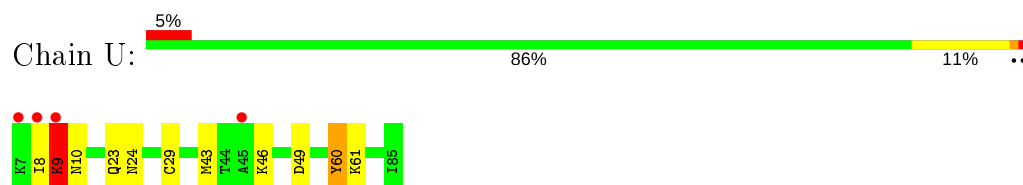
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



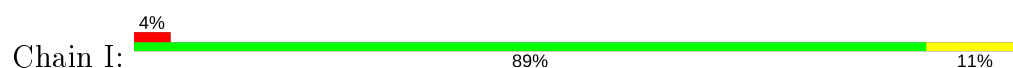
- Molecule 8: Cytochrome c oxidase subunit 6B1

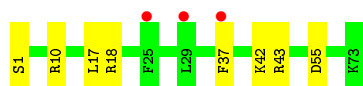


- Molecule 8: Cytochrome c oxidase subunit 6B1

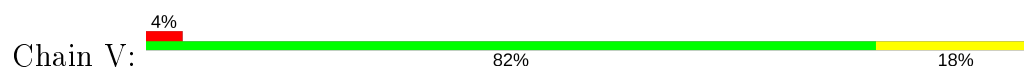


- Molecule 9: Cytochrome c oxidase subunit 6C

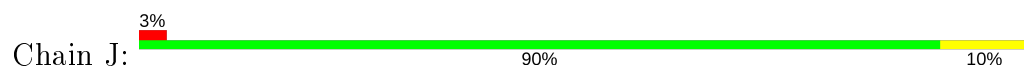




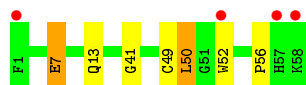
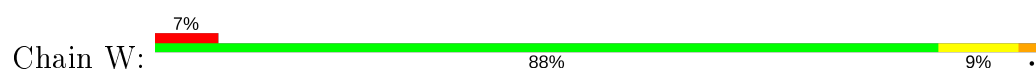
- Molecule 9: Cytochrome c oxidase subunit 6C



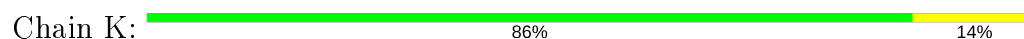
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



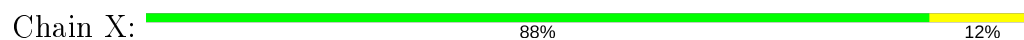
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



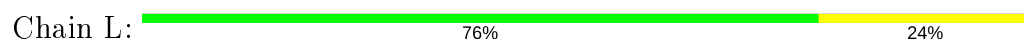
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



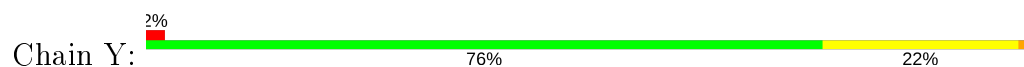
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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



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

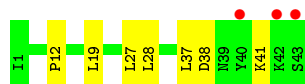
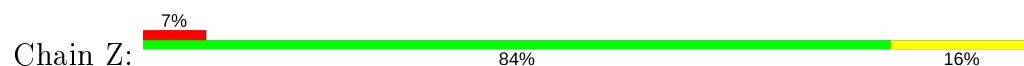




- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



- 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, $\alpha$ , $\beta$ , $\gamma$	182.22Å 204.65Å 177.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.88 – 1.80 136.09 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.88-1.80) 99.8 (136.09-1.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 1.80Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, $R_{free}$	0.157 , 0.188 0.157 , 0.188	Depositor DCC
$R_{free}$ test set	30366 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 83.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, TPO, CHD, TGL, CDL, PSC, PO4, PEK, MG, EDO, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.11	7/4445 (0.2%)	1.00	12/6063 (0.2%)
1	N	1.01	7/4321 (0.2%)	0.94	9/5899 (0.2%)
2	B	0.97	2/1896 (0.1%)	0.97	4/2582 (0.2%)
2	O	0.83	1/1934 (0.1%)	0.89	2/2634 (0.1%)
3	C	0.96	2/2236 (0.1%)	0.83	1/3056 (0.0%)
3	P	0.94	2/2211 (0.1%)	0.80	2/3024 (0.1%)
4	D	0.99	1/1234 (0.1%)	0.87	1/1665 (0.1%)
4	Q	0.69	0/1229	0.72	2/1658 (0.1%)
5	E	0.92	2/871 (0.2%)	0.80	1/1182 (0.1%)
5	R	0.75	0/871	0.82	4/1182 (0.3%)
6	F	0.90	3/774 (0.4%)	0.84	0/1050
6	S	0.81	1/774 (0.1%)	0.80	0/1050
7	G	0.82	0/691	0.87	1/937 (0.1%)
7	T	0.73	0/707	0.81	1/960 (0.1%)
8	H	0.88	0/682	0.90	3/921 (0.3%)
8	U	0.75	0/682	0.74	0/921
9	I	0.74	0/605	0.78	2/802 (0.2%)
9	V	0.59	0/605	0.71	1/802 (0.1%)
10	J	0.65	0/471	0.73	0/636
10	W	0.65	0/471	0.75	0/636
11	K	0.86	0/398	0.77	0/544
11	X	0.61	0/399	0.65	0/546
12	L	1.00	0/393	0.85	0/526
12	Y	0.84	1/393 (0.3%)	0.68	0/526
13	M	0.94	1/346 (0.3%)	0.81	0/470
13	Z	0.71	0/346	0.63	0/470
All	All	0.92	30/29985 (0.1%)	0.87	46/40742 (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
8	H	0	1
All	All	0	3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	27	TRP	CE3-CZ3	7.79	1.51	1.38
6	F	82	CYS	CB-SG	7.26	1.94	1.82
2	O	106	TRP	CE3-CZ3	6.62	1.49	1.38
2	B	198	GLU	CD-OE2	-6.60	1.18	1.25
2	B	193	TYR	CD1-CE1	6.54	1.49	1.39
6	F	10	GLU	CB-CG	6.24	1.64	1.52
1	N	396	TRP	CG-CD1	6.13	1.45	1.36
5	E	70	VAL	CB-CG1	-6.09	1.40	1.52
1	A	357	VAL	CB-CG1	5.58	1.64	1.52
3	C	193	TYR	CD2-CE2	5.55	1.47	1.39
1	N	440	TYR	CD2-CE2	5.51	1.47	1.39
1	A	411	LYS	CD-CE	5.47	1.65	1.51
1	A	507	GLU	CD-OE1	-5.45	1.19	1.25
13	M	21	VAL	CB-CG2	5.44	1.64	1.52
6	F	56	ARG	CG-CD	5.38	1.65	1.51
1	A	63	PHE	CE1-CZ	5.38	1.47	1.37
1	A	64	VAL	CB-CG1	5.30	1.64	1.52
1	N	264	LYS	CD-CE	5.30	1.64	1.51
12	Y	15	VAL	CB-CG1	5.25	1.63	1.52
4	D	55	GLU	CB-CG	5.25	1.62	1.52
3	P	94	PHE	CE2-CZ	5.22	1.47	1.37
1	A	186	TRP	CE3-CZ3	5.21	1.47	1.38
3	P	217	VAL	CB-CG1	5.18	1.63	1.52
1	A	373	VAL	CB-CG1	5.16	1.63	1.52
1	N	40	GLU	CB-CG	5.16	1.61	1.52
1	N	288	TRP	CE3-CZ3	5.14	1.47	1.38
6	S	87	THR	CB-CG2	-5.11	1.35	1.52
3	C	16	TRP	CE3-CZ3	5.04	1.47	1.38
1	N	377	PHE	CE1-CZ	5.03	1.47	1.37
1	N	164	PHE	CE2-CZ	5.00	1.46	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	71	MET	CG-SD-CE	-15.75	75.00	100.20
8	H	58	ARG	NE-CZ-NH2	-8.40	116.10	120.30
4	Q	20	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	213	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	51[A]	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	51[B]	ASP	CB-CG-OD1	6.79	124.41	118.30
5	R	53	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	N	366	VAL	CG1-CB-CG2	-6.17	101.03	110.90
8	H	17	ASP	CB-CG-OD1	6.17	123.85	118.30
1	N	38	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	96	ARG	NE-CZ-NH2	-5.93	117.34	120.30
5	R	66	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	B	188	ARG	NE-CZ-NH1	-5.83	117.39	120.30
9	V	59	ASP	CB-CG-OD1	5.82	123.54	118.30
2	O	144	LEU	CA-CB-CG	5.81	128.66	115.30
8	H	58	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	N	38	ARG	NE-CZ-NH1	5.76	123.18	120.30
5	R	25	ASP	CB-CG-OD2	-5.75	113.12	118.30
7	G	44	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	A	513	LEU	CA-CB-CG	-5.66	102.28	115.30
3	C	80	ARG	CG-CD-NE	-5.65	99.94	111.80
1	A	113	LEU	CB-CG-CD2	5.64	120.58	111.00
1	N	199	LEU	CB-CG-CD1	-5.60	101.48	111.00
7	T	17	ARG	NE-CZ-NH1	-5.52	117.54	120.30
9	I	43	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	N	189[A]	MET	CB-CG-SD	-5.37	96.29	112.40
1	N	189[B]	MET	CB-CG-SD	-5.37	96.29	112.40
4	D	21	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	442	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	N	189[A]	MET	CG-SD-CE	-5.23	91.83	100.20
1	N	189[B]	MET	CG-SD-CE	-5.23	91.83	100.20
5	E	60	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	O	139	ASP	CB-CG-OD1	5.19	122.97	118.30
5	R	25	ASP	CB-CG-OD1	5.17	122.96	118.30
2	B	184	LEU	CA-CB-CG	5.17	127.19	115.30
3	P	112	LEU	CB-CG-CD2	-5.15	102.25	111.00
9	I	55	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	189[A]	MET	CB-CG-SD	-5.14	96.98	112.40
1	A	189[B]	MET	CB-CG-SD	-5.14	96.98	112.40
2	B	11	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	302[A]	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	302[B]	ARG	NE-CZ-NH2	-5.11	117.75	120.30
4	Q	51	LEU	CA-CB-CG	5.11	127.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	233	PHE	CB-CG-CD1	-5.10	117.23	120.80
2	B	192	TYR	CA-CB-CG	-5.06	103.78	113.40
1	A	213	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4192	0	4181	73	0
1	N	4152	0	4129	61	0
2	B	1839	0	1848	34	0
2	O	1857	0	1858	45	0
3	C	2122	0	2032	33	0
3	P	2114	0	2028	24	0
4	D	1198	0	1189	15	0
4	Q	1195	0	1183	21	0
5	E	852	0	845	5	0
5	R	852	0	845	8	0
6	F	751	0	726	14	0
6	S	751	0	726	11	0
7	G	676	0	644	16	0
7	T	685	0	648	15	0
8	H	662	0	623	7	0
8	U	662	0	623	9	0
9	I	601	0	613	7	0
9	V	601	0	613	10	0
10	J	460	0	459	8	0
10	W	460	0	459	8	0
11	K	384	0	366	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	385	0	366	4	0
12	L	380	0	380	13	0
12	Y	380	0	380	11	0
13	M	336	0	352	2	0
13	Z	336	0	352	7	0
14	A	132	0	93	7	0
14	N	132	0	93	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	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	1	0
18	A	13	0	21	2	0
18	B	11	0	21	0	0
18	C	66	0	94	2	0
18	D	21	0	30	0	0
18	J	21	0	30	4	0
18	K	58	0	94	5	0
18	L	33	0	40	2	0
18	M	33	0	42	1	0
18	O	11	0	21	2	0
18	P	44	0	63	3	0
18	Q	23	0	31	2	0
18	W	21	0	30	4	0
18	X	65	0	114	1	0
18	Y	33	0	42	3	0
18	Z	33	0	42	2	0
19	A	102	0	152	6	0
19	C	51	0	76	4	0
19	N	102	0	152	9	0
19	P	102	0	152	12	0
19	T	51	0	74	1	0
20	A	52	0	79	17	0
20	V	52	0	78	7	0
21	A	63	0	110	2	0
21	D	63	0	110	15	0
21	L	63	0	110	16	0
21	N	63	0	110	4	0
21	Q	63	0	110	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	Y	63	0	110	3	0
22	A	36	0	54	10	0
22	B	20	0	30	3	0
22	C	28	0	42	3	0
22	D	20	0	30	3	0
22	E	12	0	18	2	0
22	F	32	0	48	3	0
22	G	4	0	6	0	0
22	H	4	0	6	2	0
22	J	4	0	6	0	0
22	L	8	0	11	1	0
22	M	4	0	6	0	0
22	N	60	0	90	14	0
22	O	8	0	12	1	0
22	P	28	0	42	3	0
22	Q	12	0	18	4	0
22	S	20	0	30	2	0
22	T	8	0	12	1	0
22	U	4	0	6	4	0
22	W	4	0	6	0	0
22	Y	4	0	6	0	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	C	58	0	78	3	0
24	G	29	0	39	1	0
24	J	29	0	39	1	0
24	L	29	0	39	0	0
24	P	58	0	78	3	0
24	T	29	0	39	1	0
24	Y	29	0	39	1	0
25	C	100	0	156	17	0
25	G	100	0	154	22	0
25	P	100	0	156	11	0
25	T	100	0	154	29	0
26	C	106	0	154	11	0
26	F	53	0	74	6	0
26	P	106	0	154	3	0
26	T	53	0	77	9	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	H	5	0	0	0	0
28	U	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	250	0	0	11	0
29	B	200	0	0	4	2
29	C	136	0	0	8	0
29	D	174	0	0	3	2
29	E	133	0	0	0	0
29	F	117	0	0	2	0
29	G	72	0	0	0	0
29	H	79	0	0	3	0
29	I	56	0	0	5	2
29	J	44	0	0	1	0
29	K	36	0	0	2	0
29	L	42	0	0	2	0
29	M	34	0	0	1	1
29	N	247	0	0	12	0
29	O	166	0	0	4	0
29	P	132	0	0	4	0
29	Q	99	0	0	2	0
29	R	98	0	0	2	0
29	S	105	0	0	4	0
29	T	75	0	0	4	0
29	U	65	0	0	2	0
29	V	48	0	0	1	1
29	W	27	0	0	1	0
29	X	28	0	0	0	0
29	Y	31	0	0	1	0
29	Z	20	0	0	0	0
All	All	34360	0	32701	548	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (548) 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)
25:G:102:CDL:H181	25:G:102:CDL:H512	1.32	1.09
1:A:55[B]:ASN:ND2	29:A:701:HOH:O	1.87	1.05
25:G:102:CDL:H551	25:G:102:CDL:H221	1.37	1.05
12:L:20:ARG:HH21	21:L:103:TGL:HC51	1.23	1.04
1:A:302[B]:ARG:HH12	1:A:365:ILE:HD11	1.25	1.01
8:U:24:ASN:HD21	22:U:102:EDO:H21	1.24	1.00
1:N:55[B]:ASN:ND2	29:N:701:HOH:O	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:NZ	29:T:201:HOH:O	1.96	0.97
26:F:102:PEK:N	29:F:201:HOH:O	1.99	0.93
2:O:221:LYS:O	29:O:401:HOH:O	1.88	0.91
7:T:17:ARG:HH12	26:T:103:PEK:H041	1.37	0.90
12:L:14:SER:H	21:L:103:TGL:HC31	1.38	0.87
25:P:306:CDL:H651	19:P:309:PGV:H172	1.56	0.87
4:Q:10:ASP:O	29:Q:301:HOH:O	1.93	0.86
1:A:486[B]:ASP:OD2	4:D:19:ARG:NH1	2.10	0.85
26:T:103:PEK:H31	26:T:103:PEK:H011	1.57	0.84
26:C:308:PEK:H361	25:T:102:CDL:H871	1.57	0.84
21:N:608:TGL:HA61	2:O:32[B]:PHE:HE1	1.42	0.83
1:A:514:LYS:OXT	6:F:37:LYS:NZ	2.13	0.82
10:J:50:LEU:HB2	18:J:101:DMU:H20	1.63	0.81
1:N:510:TYR:HA	22:N:617:EDO:H21	1.63	0.80
4:D:78:TRP:HB3	21:D:202:TGL:HB22	1.64	0.80
11:K:20:SER:HG	18:K:103:DMU:H27	1.17	0.79
1:A:446:ALA:HB2	22:A:615:EDO:H12	1.66	0.78
10:W:49:CYS:HB3	18:W:101:DMU:H11	1.65	0.78
3:C:67:PHE:CE2	25:C:307:CDL:HB22	2.18	0.78
25:C:307:CDL:H642	19:C:310:PGV:H161	1.66	0.78
2:O:22[B]:HIS:CE1	9:V:44:LYS:HE2	2.18	0.78
12:L:20:ARG:NH2	21:L:103:TGL:HC51	1.99	0.78
3:C:213:THR:HG23	25:C:307:CDL:H771	1.66	0.77
1:A:486[B]:ASP:OD1	22:A:618:EDO:O1	2.01	0.77
11:K:6:ALA:N	29:K:201:HOH:O	2.18	0.76
26:F:102:PEK:H312	2:O:66[A]:THR:HG21	1.67	0.76
22:N:615:EDO:H22	12:Y:10:ASN:HD22	1.52	0.75
11:X:7:PRO:O	11:X:12:LYS:NZ	2.21	0.74
26:F:102:PEK:H041	7:G:17:ARG:HH12	1.53	0.73
1:A:302[B]:ARG:NH1	1:A:365:ILE:HD11	2.02	0.73
1:A:112:LEU:HG	29:A:892:HOH:O	1.87	0.72
25:G:102:CDL:H762	25:G:102:CDL:H562	1.70	0.72
25:G:102:CDL:H381	25:G:102:CDL:H111	1.70	0.72
21:Q:202:TGL:H352	9:V:16:ARG:HE	1.53	0.72
12:Y:20:ARG:NH2	21:Y:103:TGL:HC32	2.04	0.72
21:Q:202:TGL:HG12	21:Q:202:TGL:HC32	1.71	0.71
1:A:302[B]:ARG:HE	2:B:84:LEU:HD11	1.56	0.71
21:L:103:TGL:OC1	21:L:103:TGL:HC41	1.89	0.70
1:A:390:MET:O	1:A:394[A]:VAL:HG12	1.92	0.69
1:A:468:MET:HG3	22:A:617:EDO:H22	1.74	0.69
12:Y:20:ARG:HH21	21:Y:103:TGL:HC32	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:236:GLU:HG3	22:P:316:EDO:H22	1.73	0.69
25:T:102:CDL:H273	26:T:103:PEK:H382	1.74	0.68
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.08	0.68
3:P:3:HIS:ND1	29:P:401:HOH:O	2.26	0.68
4:D:87:PHE:CZ	4:D:87:PHE:CD1	2.79	0.68
1:A:297[B]:MET:HG2	1:A:302[B]:ARG:HG2	1.75	0.68
2:O:47:THR:HB	21:Q:202:TGL:H181	1.74	0.68
3:C:67:PHE:HE2	25:C:307:CDL:HB22	1.58	0.67
4:D:4:SER:N	29:D:302:HOH:O	2.26	0.67
5:R:31:LYS:HE3	6:S:84:SER:O	1.94	0.67
18:L:101:DMU:H20	21:L:103:TGL:H301	1.75	0.67
1:A:482:VAL:O	29:A:702:HOH:O	2.13	0.66
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.77	0.66
22:Q:204:EDO:H12	29:S:231:HOH:O	1.97	0.66
12:Y:42:HIS:ND1	18:Y:101:DMU:O49	2.19	0.66
21:D:202:TGL:HC42	21:D:202:TGL:HG12	1.79	0.65
7:G:1:ALA:HB1	1:N:286:ILE:HG22	1.77	0.65
3:P:103:HIS:HA	19:P:310:PGV:H012	1.79	0.65
18:C:303:DMU:O61	29:C:401:HOH:O	2.13	0.64
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.32	0.64
1:A:510:TYR:OH	1:A:512[B]:ASN:ND2	2.26	0.64
10:W:7:GLU:HG2	29:W:221:HOH:O	1.97	0.64
7:G:37:LEU:HD23	25:G:102:CDL:H391	1.78	0.64
26:F:102:PEK:H312	2:O:66[A]:THR:CG2	2.27	0.64
6:S:19[B]:GLU:OE2	29:S:201:HOH:O	2.15	0.64
19:N:606:PGV:H302	13:Z:19:LEU:HD23	1.79	0.64
2:O:67:ILE:HD11	29:O:557:HOH:O	1.97	0.63
29:N:860:HOH:O	6:S:87:THR:HG21	1.98	0.63
22:B:305:EDO:H12	29:B:467:HOH:O	1.99	0.63
2:O:58:ALA:O	2:O:62:GLU:HG3	1.99	0.63
4:D:78:TRP:CB	21:D:202:TGL:HB22	2.28	0.62
1:A:379:TYR:O	1:A:383[B]:MET:HB2	1.99	0.62
19:N:606:PGV:H342	19:N:606:PGV:H162	1.80	0.62
7:T:38:HIS:CE1	25:T:102:CDL:H122	2.34	0.62
21:N:608:TGL:HA61	2:O:32[B]:PHE:CE1	2.29	0.62
1:A:307:SER:CB	25:T:102:CDL:H182	2.30	0.62
10:J:49:CYS:HB3	18:J:101:DMU:H11	1.80	0.62
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.82	0.61
2:O:225:SER:N	29:O:401:HOH:O	2.32	0.61
12:Y:35:ALA:HA	18:Y:101:DMU:H20	1.82	0.61
8:H:7:LYS:N	29:H:201:HOH:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:306:CDL:H332	25:P:306:CDL:H472	1.81	0.61
1:A:48[B]:LEU:HB2	29:A:708:HOH:O	2.00	0.61
25:C:307:CDL:H651	19:C:310:PGV:H182	1.83	0.61
19:N:606:PGV:H92	4:Q:84:ALA:HB2	1.81	0.61
3:C:224:LYS:CD	25:C:307:CDL:HB31	2.31	0.60
22:C:313:EDO:O2	6:F:1:ALA:O	2.17	0.60
13:Z:27:LEU:HD22	18:Z:101:DMU:H14	1.82	0.60
1:A:334:TRP:CZ3	21:D:202:TGL:HA52	2.36	0.60
20:A:609:PSC:H212	2:B:57:ASP:H	1.67	0.60
20:V:101:PSC:H42	20:V:101:PSC:H241	1.83	0.60
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.83	0.60
1:N:511:VAL:H	22:N:617:EDO:H21	1.66	0.60
19:N:606:PGV:H231	13:Z:12:PRO:HG3	1.82	0.60
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.37	0.60
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.83	0.60
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.83	0.60
1:A:297[B]:MET:CG	1:A:302[B]:ARG:HG2	2.32	0.59
20:A:609:PSC:C08	9:I:10:ARG:HH21	2.14	0.59
4:Q:20:ARG:HG2	29:Q:359:HOH:O	2.01	0.59
9:I:18:ARG:HG3	29:I:128:HOH:O	2.02	0.59
17:P:301:NA:NA	29:P:403:HOH:O	1.75	0.59
25:C:307:CDL:H131	25:C:307:CDL:HA61	1.84	0.59
1:N:365:ILE:HD11	29:N:891:HOH:O	2.01	0.59
21:N:608:TGL:HA71	21:N:608:TGL:H121	1.85	0.59
6:S:43:LYS:H	6:S:43:LYS:HD2	1.68	0.59
9:V:45:LYS:NZ	29:V:202:HOH:O	2.35	0.59
22:H:102:EDO:H11	29:H:262:HOH:O	2.03	0.59
4:Q:78:TRP:CA	21:Q:202:TGL:HB22	2.33	0.59
1:A:3:ILE:HG23	1:A:7[B]:LEU:HD12	1.85	0.58
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.84	0.58
19:A:607:PGV:H062	19:A:607:PGV:O13	2.03	0.58
1:A:311:ILE:HD11	25:T:102:CDL:H421	1.85	0.58
21:Q:202:TGL:H362	9:V:20:HIS:HE1	1.69	0.58
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.38	0.58
9:I:1:SAC:O	29:I:101:HOH:O	2.17	0.58
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.33	0.58
1:A:337:ALA:HB2	1:A:394[B]:VAL:HG23	1.85	0.58
25:T:102:CDL:H382	25:T:102:CDL:H161	1.85	0.57
1:A:334:TRP:CD1	21:D:202:TGL:HC41	2.38	0.57
3:C:156:ARG:HE	24:C:306:CHD:C24	2.17	0.57
11:X:24:PHE:O	11:X:28:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:177:GLN:HB3	26:C:309:PEK:H201	1.85	0.57
20:A:609:PSC:O02	29:A:703:HOH:O	2.17	0.56
25:T:102:CDL:H751	25:T:102:CDL:C25	2.36	0.56
25:T:102:CDL:H751	25:T:102:CDL:H252	1.86	0.56
4:D:78:TRP:CA	21:D:202:TGL:HB22	2.36	0.56
1:N:80:ASN:HD21	22:N:622:EDO:H12	1.70	0.56
22:S:105:EDO:H21	29:S:211:HOH:O	2.04	0.56
21:D:202:TGL:HC42	21:D:202:TGL:OG3	2.06	0.55
2:O:144:LEU:HG	2:O:150:ILE:HD13	1.87	0.55
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.55
20:A:609:PSC:H251	2:B:56:MET:HB3	1.87	0.55
25:G:102:CDL:HA61	25:G:102:CDL:H362	1.87	0.55
2:O:60:GLU:CD	2:O:60:GLU:H	2.10	0.55
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.36	0.55
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.89	0.55
9:V:1:SAC:OG	9:V:2:THR:N	2.37	0.55
1:N:381[B]:LEU:HB2	14:N:602:HEA:CAC	2.37	0.54
6:S:19[B]:GLU:OE2	22:S:105:EDO:O1	2.26	0.54
21:L:103:TGL:H362	21:L:103:TGL:H322	1.88	0.54
1:N:321:PHE:HB3	2:O:65[A]:TRP:CE3	2.42	0.54
7:T:38:HIS:CD2	25:T:102:CDL:H1	2.42	0.54
1:N:361:SER:OG	2:O:84:LEU:HD13	2.07	0.54
1:N:505:PHE:HA	22:N:612:EDO:H22	1.90	0.54
2:B:81:LEU:HD13	25:T:102:CDL:H131	1.89	0.54
1:N:49[B]:GLY:HA3	13:Z:41:LYS:HE3	1.89	0.54
1:A:311:ILE:CD1	25:T:102:CDL:H421	2.37	0.54
1:A:468:MET:CG	22:A:617:EDO:H22	2.36	0.54
2:B:74:ILE:HG13	25:T:102:CDL:H431	1.90	0.54
1:N:511:VAL:H	22:N:617:EDO:C2	2.21	0.54
19:A:607:PGV:H151	19:A:607:PGV:H321	1.90	0.54
20:A:609:PSC:C21	2:B:57:ASP:H	2.20	0.54
3:C:125:ASN:HB2	7:G:42:ARG:HH22	1.73	0.54
22:A:615:EDO:H11	2:B:1:FME:HE3	1.89	0.54
25:T:102:CDL:H581	25:T:102:CDL:C78	2.38	0.54
18:Y:101:DMU:H26	29:Y:229:HOH:O	2.08	0.54
20:A:609:PSC:H082	9:I:10:ARG:HH21	1.71	0.53
1:A:169[A]:ILE:HD11	1:A:189[A]:MET:HE3	1.90	0.53
1:A:51[B]:ASP:OD2	1:A:441:SER:OG	2.23	0.53
3:P:161:GLN:NE2	26:T:103:PEK:H22	2.23	0.53
21:D:202:TGL:HG32	29:D:336:HOH:O	2.08	0.53
13:M:43:SER:O	29:M:201:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3:HIS:N	29:C:409:HOH:O	2.41	0.53
1:N:53[B]:ILE:HG12	29:N:882:HOH:O	2.09	0.53
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.90	0.53
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.09	0.53
3:C:70:HIS:HE1	22:C:316:EDO:H22	1.74	0.53
8:U:43:MET:HE3	8:U:49:ASP:N	2.24	0.53
1:A:484:THR:HG22	29:A:921:HOH:O	2.09	0.52
20:A:609:PSC:H231	20:A:609:PSC:H22	1.89	0.52
25:G:102:CDL:H382	2:O:81:LEU:HD12	1.90	0.52
2:O:83:ILE:HA	2:O:86:MET:HG2	1.91	0.52
26:P:308:PEK:H42	26:P:308:PEK:H101	1.90	0.52
1:A:302[B]:ARG:HH12	1:A:365:ILE:CD1	2.11	0.52
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.92	0.52
2:B:135:LEU:HD21	22:B:307:EDO:H11	1.91	0.52
10:J:50:LEU:HB2	18:J:101:DMU:C37	2.37	0.52
19:P:310:PGV:O04	19:P:310:PGV:H71	2.08	0.52
3:C:80:ARG:NH1	29:C:403:HOH:O	2.23	0.52
3:C:127:LEU:HD22	25:G:102:CDL:HB61	1.91	0.52
21:D:202:TGL:HB31	21:D:202:TGL:HA21	1.92	0.52
11:K:20:SER:HA	18:K:103:DMU:H5	1.91	0.52
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.92	0.52
4:Q:101:HIS:ND1	18:Q:201:DMU:H5	2.25	0.52
10:W:50:LEU:HG	18:W:101:DMU:H23	1.91	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.52
4:Q:19:ARG:NH2	4:Q:21:ASP:OD2	2.42	0.52
7:T:36[B]:TRP:HZ2	26:T:103:PEK:H201	1.74	0.52
10:W:56:PRO:HD3	12:Y:46:LYS:HD2	1.92	0.52
3:C:80:ARG:HD3	29:C:403:HOH:O	2.11	0.51
2:B:49:LYS:HD3	21:D:202:TGL:HC72	1.91	0.51
25:G:102:CDL:H531	25:G:102:CDL:H202	1.92	0.51
3:P:224:LYS:CD	25:P:306:CDL:HB31	2.40	0.51
8:U:43:MET:HE3	8:U:49:ASP:H	1.75	0.51
21:L:103:TGL:HG31	29:L:228:HOH:O	2.10	0.51
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.51
22:A:614:EDO:H12	2:B:58:ALA:HB3	1.93	0.51
7:G:5:LYS:HB3	1:N:278[B]:MET:SD	2.51	0.51
1:A:381[B]:LEU:HB2	14:A:602:HEA:HAC	1.93	0.51
4:Q:101:HIS:HB2	18:Q:201:DMU:O49	2.10	0.51
13:Z:28:LEU:HD23	18:Z:101:DMU:H7	1.93	0.51
3:P:224:LYS:HD3	25:P:306:CDL:HB31	1.92	0.51
1:A:112:LEU:C	1:A:112:LEU:HD23	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486[B]:ASP:OD1	4:D:19:ARG:HD2	2.11	0.51
3:P:3:HIS:HA	29:P:502:HOH:O	2.11	0.51
3:C:224:LYS:HD2	25:C:307:CDL:HB31	1.93	0.50
21:A:610:TGL:H101	21:A:610:TGL:H283	1.93	0.50
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.91	0.50
8:H:61:LYS:NZ	29:H:202:HOH:O	2.43	0.50
9:I:42:LYS:NZ	29:I:104:HOH:O	2.44	0.50
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.92	0.50
1:N:505:PHE:H	22:N:612:EDO:C2	2.24	0.50
1:N:514:LYS:NZ	29:N:707:HOH:O	2.38	0.50
19:C:310:PGV:H12	19:C:310:PGV:H161	1.93	0.50
14:N:601[B]:HEA:H122	29:N:854:HOH:O	2.10	0.50
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.93	0.50
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.51	0.50
3:C:226:HIS:CE1	25:C:307:CDL:HB32	2.46	0.50
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.93	0.50
1:N:164:PHE:HE2	22:N:622:EDO:H22	1.77	0.50
3:P:135:SER:HB3	25:T:102:CDL:H562	1.94	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.93	0.50
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.11	0.50
2:O:66[A]:THR:HG22	2:O:67:ILE:HD13	1.93	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.50
7:G:84:LYS:HE2	7:G:84:LYS:H	1.77	0.49
3:C:224:LYS:NZ	25:C:307:CDL:H112	2.27	0.49
25:T:102:CDL:H581	25:T:102:CDL:H772	1.92	0.49
11:K:20:SER:HA	18:K:103:DMU:H7	1.93	0.49
1:A:113:LEU:HD12	21:L:103:TGL:H141	1.94	0.49
1:A:208[B]:MET:HG2	1:A:219:PHE:CE2	2.48	0.49
3:C:84:ILE:HG21	26:C:308:PEK:H222	1.94	0.49
2:O:41:ILE:O	2:O:45:MET:HG2	2.13	0.49
25:G:102:CDL:C79	25:G:102:CDL:H571	2.42	0.49
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.95	0.49
3:P:80:ARG:HH21	22:P:316:EDO:H21	1.78	0.49
2:O:22[B]:HIS:HE1	9:V:44:LYS:HE2	1.75	0.49
1:A:278[B]:MET:CE	7:T:5:LYS:HB3	2.43	0.49
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.95	0.49
7:G:7:ASP:OD1	7:G:8:HIS:N	2.45	0.49
3:P:62:ILE:HD12	25:P:306:CDL:H511	1.94	0.49
4:Q:56:LYS:NZ	22:Q:203:EDO:O1	2.46	0.49
6:F:94:HIS:HB2	6:F:98:HIS:CD2	2.48	0.48
3:C:240:TRP:CE2	26:C:308:PEK:H31	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.48	0.48
20:A:609:PSC:H252	2:B:56:MET:SD	2.54	0.48
6:F:92:VAL:O	6:F:92:VAL:HG23	2.14	0.48
1:N:334:TRP:CZ3	21:Q:202:TGL:HA51	2.49	0.48
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.95	0.48
1:A:289:ALA:HB1	1:A:297[B]:MET:HE1	1.95	0.48
20:A:609:PSC:H42	29:I:128:HOH:O	2.14	0.48
3:C:180[B]:GLU:HG3	29:C:467:HOH:O	2.13	0.48
3:C:3:HIS:HB2	29:C:520:HOH:O	2.13	0.48
20:A:609:PSC:H052	5:E:41:LEU:CD2	2.44	0.48
25:G:102:CDL:H512	25:G:102:CDL:C18	2.24	0.48
26:P:307:PEK:H383	19:P:310:PGV:H332	1.95	0.48
22:Q:205:EDO:H21	29:R:242:HOH:O	2.12	0.48
7:T:59:PRO:O	22:T:105:EDO:H22	2.13	0.48
19:A:607:PGV:H321	19:A:607:PGV:C15	2.44	0.48
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.12	0.48
5:R:11:PHE:CD1	20:V:101:PSC:H081	2.49	0.48
20:A:609:PSC:O02	29:A:704:HOH:O	2.20	0.48
22:A:611:EDO:C2	12:L:10:ASN:HB2	2.44	0.48
3:C:226:HIS:HE1	25:C:307:CDL:HB32	1.79	0.48
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.95	0.48
1:N:334:TRP:CE3	21:Q:202:TGL:HA51	2.49	0.48
1:N:381[B]:LEU:HB2	14:N:602:HEA:HAC	1.96	0.47
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.14	0.47
25:T:102:CDL:H341	25:T:102:CDL:H121	1.96	0.47
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.97	0.47
22:N:617:EDO:H12	6:S:36:PRO:HD3	1.96	0.47
1:N:483:LEU:HD11	4:Q:5:VAL:O	2.14	0.47
1:A:285:PHE:CE2	7:T:4:ALA:HB2	2.50	0.47
6:F:94:HIS:CD2	6:F:98:HIS:HB2	2.50	0.47
19:N:606:PGV:H142	19:N:606:PGV:H312	1.97	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.47
14:N:602:HEA:H243	2:O:69:PRO:HB3	1.94	0.47
12:Y:20:ARG:HH21	12:Y:24:MET:HG3	1.78	0.47
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.30	0.47
18:C:302:DMU:O6	29:C:402:HOH:O	2.20	0.47
26:C:309:PEK:H101	26:C:309:PEK:H71	1.42	0.47
18:P:303:DMU:H23	10:W:41:GLY:HA3	1.96	0.47
3:P:99:TRP:CD1	19:P:310:PGV:H211	2.50	0.47
9:V:61:GLU:OE1	9:V:64:ARG:NE	2.34	0.47
24:Y:102:CHD:H112	24:Y:102:CHD:H12A	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:TYR:O	22:D:203:EDO:H21	2.15	0.47
2:O:65[B]:TRP:HE1	20:V:101:PSC:H112	1.79	0.47
4:Q:78:TRP:HA	21:Q:202:TGL:HB22	1.96	0.47
3:C:257:TYR:O	3:C:261:SER:HB3	2.14	0.47
20:A:609:PSC:H052	5:E:41:LEU:HD23	1.96	0.47
21:L:103:TGL:H231	21:L:103:TGL:H262	1.74	0.47
25:T:102:CDL:H581	25:T:102:CDL:C77	2.44	0.47
22:P:313:EDO:H12	10:W:13:GLN:HG2	1.96	0.47
1:A:30:GLY:HA3	1:A:65[B]:MET:SD	2.55	0.46
25:T:102:CDL:H142	25:T:102:CDL:OB3	2.14	0.46
1:A:342:LEU:HB2	21:D:202:TGL:HA92	1.97	0.46
11:K:20:SER:OG	18:K:103:DMU:O49	2.02	0.46
1:A:307:SER:HB3	25:T:102:CDL:H182	1.97	0.46
3:C:99:TRP:CD1	19:T:104:PGV:H221	2.50	0.46
24:G:101:CHD:H12	24:G:101:CHD:H212	1.97	0.46
21:N:608:TGL:H121	21:N:608:TGL:CA7	2.44	0.46
29:N:801:HOH:O	22:U:102:EDO:H11	2.14	0.46
20:A:609:PSC:H083	5:E:11:PHE:CG	2.51	0.46
6:F:70:ILE:HG13	6:F:84:SER:HB3	1.97	0.46
22:N:618:EDO:H21	29:N:810:HOH:O	2.15	0.46
21:Y:103:TGL:HA91	21:Y:103:TGL:H222	1.52	0.46
11:K:7:PRO:HD2	29:K:210:HOH:O	2.16	0.46
20:A:609:PSC:C23	20:A:609:PSC:H22	2.45	0.46
21:L:103:TGL:H362	21:L:103:TGL:C32	2.45	0.46
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	2.15	0.46
21:L:103:TGL:H221	21:L:103:TGL:HA92	1.30	0.46
1:A:513:LEU:O	1:A:514:LYS:HB2	2.16	0.46
22:F:109:EDO:H22	29:F:279:HOH:O	2.16	0.46
8:H:24:ASN:HD21	22:H:102:EDO:C2	2.29	0.46
12:L:45:LEU:HA	12:L:45:LEU:HD23	1.82	0.46
1:N:112:LEU:HD23	1:N:112:LEU:C	2.37	0.46
1:N:298[B]:ASP:OD1	29:N:702:HOH:O	2.21	0.46
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.51	0.46
1:A:302[B]:ARG:HH21	2:B:84:LEU:CD1	2.29	0.46
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.51	0.46
12:L:20:ARG:HH22	21:L:103:TGL:HC72	1.80	0.45
21:Q:202:TGL:H362	9:V:20:HIS:CE1	2.51	0.45
8:U:61:LYS:NZ	29:U:201:HOH:O	2.37	0.45
6:F:96:LEU:C	6:F:98:HIS:H	2.20	0.45
12:L:41:ARG:HH22	18:L:101:DMU:H30	1.81	0.45
1:N:348:PHE:CE1	1:N:380[B]:VAL:HG22	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:308:PEK:C36	25:T:102:CDL:H871	2.38	0.45
21:A:610:TGL:H251	21:A:610:TGL:H282	1.62	0.45
18:P:303:DMU:H25	18:P:303:DMU:H19	1.69	0.45
25:P:306:CDL:H612	19:P:309:PGV:H131	1.99	0.45
4:Q:9:GLU:O	4:Q:11:TYR:N	2.49	0.45
1:N:112:LEU:HG	29:N:919:HOH:O	2.16	0.45
1:A:468:MET:HG3	22:A:617:EDO:C2	2.44	0.45
18:A:606:DMU:H6	11:K:30:VAL:HG21	1.98	0.45
5:E:12:ASP:OD2	5:E:44:GLU:HG3	2.16	0.45
7:G:1:ALA:N	19:P:310:PGV:H262	2.32	0.45
26:F:102:PEK:H372	25:G:102:CDL:H262	1.57	0.45
1:N:505:PHE:H	22:N:612:EDO:H22	1.81	0.45
29:O:482:HOH:O	21:Q:202:TGL:H331	2.16	0.45
10:W:52:TRP:CZ2	18:W:101:DMU:H4	2.51	0.45
26:C:309:PEK:H71	26:C:309:PEK:H42	1.74	0.45
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.53	0.45
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.51	0.45
1:N:486:ASP:OD2	4:Q:19:ARG:HD2	2.16	0.45
4:Q:78:TRP:HB3	21:Q:202:TGL:HB22	1.99	0.45
5:R:95:GLU:HG2	5:R:96:LEU:HD23	1.99	0.45
22:A:615:EDO:H22	2:B:133:LEU:HD22	1.98	0.45
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.98	0.45
24:P:304:CHD:C24	19:P:310:PGV:H011	2.47	0.45
24:T:101:CHD:H212	24:T:101:CHD:H12	1.99	0.45
3:P:127:LEU:HD22	25:T:102:CDL:HB61	1.99	0.44
4:Q:114:GLU:HG3	11:X:51:LYS:HE2	1.98	0.44
13:Z:37:LEU:HA	13:Z:37:LEU:HD23	1.83	0.44
1:A:512[B]:ASN:ND2	6:F:36:PRO:HB2	2.32	0.44
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.44
29:A:703:HOH:O	2:B:52:HIS:HD2	2.00	0.44
25:G:102:CDL:H801	25:G:102:CDL:H832	1.64	0.44
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.98	0.44
4:Q:13:LEU:C	22:Q:204:EDO:H21	2.38	0.44
10:W:52:TRP:CE2	18:W:101:DMU:H4	2.53	0.44
2:B:54:SER:CB	22:E:203:EDO:H11	2.47	0.44
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.16	0.44
2:O:52:HIS:HD2	29:R:247:HOH:O	2.00	0.44
22:U:102:EDO:H22	29:U:227:HOH:O	2.15	0.44
7:G:84:LYS:H	7:G:84:LYS:CE	2.30	0.44
26:T:103:PEK:H221	26:T:103:PEK:H5	1.98	0.44
6:F:28:GLN:O	22:F:108:EDO:O1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:616:EDO:H12	6:F:70:ILE:HD12	1.99	0.44
10:J:4:ARG:HD3	29:J:222:HOH:O	2.16	0.44
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.53	0.44
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.98	0.44
20:V:101:PSC:H343	20:V:101:PSC:C12	2.47	0.44
1:A:76:GLY:O	1:A:80:ASN:HB2	2.18	0.44
25:C:307:CDL:H251	25:C:307:CDL:H222	1.53	0.44
1:N:409:TRP:CZ2	19:N:606:PGV:H61	2.53	0.44
2:O:26:HIS:HE1	18:O:302:DMU:H9	1.82	0.44
2:B:67:ILE:HD11	29:T:268:HOH:O	2.17	0.44
12:L:24:MET:HG3	29:L:225:HOH:O	2.17	0.44
25:T:102:CDL:H321	29:T:257:HOH:O	2.18	0.44
3:C:180[B]:GLU:HG2	29:C:422:HOH:O	2.18	0.44
3:C:224:LYS:HD3	25:C:307:CDL:HB31	1.99	0.44
25:G:102:CDL:H122	25:G:102:CDL:H392	1.99	0.44
25:G:102:CDL:H422	25:G:102:CDL:H451	1.66	0.44
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.99	0.44
1:A:306:THR:O	1:A:310[B]:MET:HG2	2.18	0.44
21:L:103:TGL:HC52	21:L:103:TGL:HC22	1.68	0.44
3:C:210:ILE:HD13	19:C:310:PGV:H302	2.00	0.43
3:P:107:ALA:HB2	19:P:310:PGV:H031	1.99	0.43
3:P:99:TRP:CE2	19:P:310:PGV:H231	2.53	0.43
1:A:439:ARG:HD3	2:B:199:ILE:HB	1.99	0.43
1:A:510:TYR:CZ	1:A:512[B]:ASN:ND2	2.87	0.43
4:D:125:ASP:OD1	22:D:205:EDO:O2	2.36	0.43
1:N:378:HIS:O	1:N:382[B]:SER:HB2	2.17	0.43
3:P:47:LEU:O	3:P:51:MET:HG2	2.17	0.43
18:X:102:DMU:H11	18:X:102:DMU:H16	1.78	0.43
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.18	0.43
9:I:18:ARG:HD3	29:I:148:HOH:O	2.18	0.43
1:N:46:THR:HG22	1:N:49[B]:GLY:H	1.82	0.43
19:N:607:PGV:H343	26:P:308:PEK:H381	2.00	0.43
5:R:105:GLY:O	5:R:108:LYS:HG2	2.18	0.43
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.00	0.43
24:C:306:CHD:H12A	24:C:306:CHD:H112	1.70	0.43
1:A:343:GLY:HA2	21:D:202:TGL:H201	2.01	0.43
3:C:12:ASN:HD21	22:C:311:EDO:H12	1.83	0.43
29:A:868:HOH:O	21:D:202:TGL:HC32	2.18	0.43
8:H:9:LYS:O	8:H:10:ASN:HB2	2.19	0.43
18:A:606:DMU:H11	11:K:26:VAL:HG13	2.01	0.43
25:P:306:CDL:H121	29:P:519:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:O	8:U:10:ASN:HB2	2.18	0.43
2:O:4:PRO:HB2	11:X:43:SER:HA	2.01	0.43
1:N:243:VAL:HB	14:N:602:HEA:CAC	2.49	0.43
22:N:623:EDO:H11	29:N:876:HOH:O	2.18	0.43
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.43
6:S:92:VAL:HG23	6:S:92:VAL:O	2.18	0.43
25:T:102:CDL:H572	25:T:102:CDL:H752	2.01	0.43
25:T:102:CDL:H832	25:T:102:CDL:H801	1.36	0.43
22:B:305:EDO:H11	29:B:406:HOH:O	2.17	0.43
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.54	0.43
2:O:26:HIS:CE1	18:O:302:DMU:H9	2.54	0.43
2:O:206:PHE:CE1	22:O:304:EDO:H21	2.53	0.43
8:H:52:VAL:O	8:U:46:LYS:HD3	2.18	0.43
1:A:40:GLU:HG2	1:A:54[B]:TYR:CD1	2.54	0.43
25:G:102:CDL:H542	25:G:102:CDL:H511	1.73	0.43
7:G:1:ALA:H2	19:P:310:PGV:H262	1.84	0.43
12:L:20:ARG:HH21	21:L:103:TGL:CC5	2.11	0.43
5:R:80:GLU:CD	5:R:80:GLU:H	2.21	0.43
9:V:10:ARG:HH21	20:V:101:PSC:H081	1.84	0.43
25:P:306:CDL:H822	25:P:306:CDL:H852	1.87	0.42
7:T:42:ARG:NH2	29:T:208:HOH:O	2.52	0.42
3:C:51[A]:MET:SD	25:C:307:CDL:H622	2.59	0.42
25:C:307:CDL:HB21	10:J:8:LYS:CE	2.49	0.42
4:D:118:LYS:NZ	22:D:206:EDO:O2	2.49	0.42
5:R:11:PHE:CG	20:V:101:PSC:H081	2.54	0.42
10:J:52:TRP:CE2	18:J:101:DMU:H4	2.54	0.42
3:P:220:PHE:HB2	25:P:306:CDL:H712	2.01	0.42
14:A:601[B]:HEA:H122	29:A:819:HOH:O	2.18	0.42
12:L:2:HIS:CG	12:L:3:TYR:H	2.37	0.42
3:C:125:ASN:HB2	7:G:42:ARG:NH2	2.33	0.42
3:C:47:LEU:O	3:C:51[B]:MET:HG3	2.18	0.42
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.85	0.42
2:B:54:SER:HB2	22:E:203:EDO:H11	2.02	0.42
12:L:13:PHE:C	22:L:104:EDO:H22	2.40	0.42
19:A:607:PGV:H311	13:M:19:LEU:HD23	2.00	0.42
1:N:236:TRP:CH2	14:N:602:HEA:HBD1	2.54	0.42
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.01	0.42
25:T:102:CDL:H622	25:T:102:CDL:H651	1.73	0.42
20:A:609:PSC:H342	2:B:41:ILE:HD13	2.01	0.42
4:Q:78:TRP:CB	21:Q:202:TGL:HB22	2.50	0.42
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:16:ILE:HG23	2:O:16:ILE:HD12	1.83	0.42
2:B:69:PRO:HG2	29:B:429:HOH:O	2.19	0.42
5:E:43:PRO:HB2	5:E:48:ILE:HD11	2.02	0.42
11:K:23:THR:HB	18:K:103:DMU:H6	2.02	0.42
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.55	0.42
2:O:114:GLU:HG3	2:O:227:LEU:CD2	2.50	0.42
4:Q:109:HIS:HE1	4:Q:115:TRP:CZ3	2.37	0.42
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.01	0.41
25:G:102:CDL:H761	1:N:282:PHE:HZ	1.85	0.41
19:N:607:PGV:H262	19:P:309:PGV:H292	2.01	0.41
3:P:38:ASN:O	18:P:303:DMU:H35	2.20	0.41
3:P:161:GLN:HE22	26:T:103:PEK:H22	1.85	0.41
1:A:280:ILE:HG23	1:A:312[B]:ILE:HD11	2.01	0.41
1:A:486[B]:ASP:CG	4:D:19:ARG:HD2	2.40	0.41
26:C:309:PEK:H132	26:C:309:PEK:H161	1.79	0.41
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.20	0.41
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.08	0.41
26:C:308:PEK:H321	7:T:5:LYS:HB2	2.02	0.41
26:F:102:PEK:H222	7:G:21:PHE:CD1	2.55	0.41
2:O:41:ILE:HD13	20:V:101:PSC:H342	2.03	0.41
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.03	0.41
6:S:94:HIS:HB2	29:S:214:HOH:O	2.19	0.41
7:T:38:HIS:ND1	7:T:38:HIS:N	2.67	0.41
4:D:31:LYS:NZ	29:D:303:HOH:O	2.37	0.41
25:G:102:CDL:C55	25:G:102:CDL:H221	2.27	0.41
22:N:613:EDO:H12	6:S:70:ILE:HD12	2.02	0.41
1:A:334:TRP:CE3	21:D:202:TGL:HA32	2.56	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.50	0.41
21:L:103:TGL:H291	21:L:103:TGL:H122	1.81	0.41
24:P:305:CHD:H183	24:P:305:CHD:H212	2.03	0.41
1:A:512[B]:ASN:HD22	6:F:36:PRO:HB2	1.85	0.41
2:B:19:GLU:OE1	2:B:82:ARG:NH2	2.54	0.41
25:C:307:CDL:HB21	10:J:8:LYS:HE3	2.02	0.41
1:N:513:LEU:O	1:N:514:LYS:HB2	2.20	0.41
7:G:84:LYS:H	7:G:84:LYS:CD	2.32	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.20	0.41
19:N:606:PGV:H251	13:Z:12:PRO:HB3	2.03	0.41
19:A:607:PGV:C3	19:A:607:PGV:H011	2.51	0.41
3:P:59:ARG:HA	25:P:306:CDL:H512	2.02	0.41
1:A:54[B]:TYR:HB2	29:A:708:HOH:O	2.21	0.41
5:R:31:LYS:HE2	5:R:35:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:GLY:O	1:N:80:ASN:HB2	2.20	0.41
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.51	0.41
6:S:70:ILE:HG13	6:S:84:SER:HB2	2.03	0.41
7:T:36[B]:TRP:CZ2	26:T:103:PEK:H201	2.55	0.41
25:G:102:CDL:H311	25:G:102:CDL:H341	1.87	0.41
12:L:14:SER:N	21:L:103:TGL:HC31	2.20	0.41
3:P:80:ARG:HG2	3:P:233:PHE:CE1	2.56	0.41
8:U:24:ASN:ND2	22:U:102:EDO:H21	2.10	0.41
1:A:194:LEU:HD11	7:T:4:ALA:HB1	2.02	0.40
20:A:609:PSC:H042	20:A:609:PSC:H072	1.62	0.40
2:B:13:THR:HB	2:B:168:LEU:HD23	2.03	0.40
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.40
24:C:306:CHD:H193	24:C:306:CHD:H111	1.76	0.40
19:A:608:PGV:H322	26:C:309:PEK:H382	2.02	0.40
4:D:98:TRP:CE2	18:M:101:DMU:H10	2.56	0.40
10:J:36:MET:HG2	24:J:102:CHD:H221	2.04	0.40
25:T:102:CDL:H581	25:T:102:CDL:H781	2.03	0.40
2:B:66[A]:THR:CG2	26:T:103:PEK:H312	2.52	0.40
11:K:54:ARG:HB3	11:K:54:ARG:HE	1.63	0.40
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.03	0.40
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.22	0.40
1:N:53[B]:ILE:HD12	12:Y:44:LEU:CD2	2.51	0.40
4:Q:7:LYS:HB3	4:Q:8:SER:H	1.63	0.40
25:T:102:CDL:H151	25:T:102:CDL:H181	1.23	0.40
12:Y:14:SER:O	12:Y:20:ARG:NH1	2.53	0.40
20:A:609:PSC:H61	9:I:17:LEU:HD23	2.04	0.40
1:N:136:LEU:HB2	29:N:909:HOH:O	2.21	0.40
25:T:102:CDL:H751	25:T:102:CDL:H251	2.03	0.40
8:U:60:TYR:C	8:U:60:TYR:CD1	2.95	0.40
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.04	0.40
3:C:55:TYR:OH	25:C:307:CDL:HA62	2.20	0.40
6:F:96:LEU:HG	6:F:96:LEU:O	2.21	0.40
24:P:305:CHD:H182	24:P:305:CHD:H111	1.86	0.40
3:P:67:PHE:HE2	25:P:306:CDL:H1	1.86	0.40
1:A:44:PRO:HG3	4:D:111:PHE:CZ	2.56	0.40
26:C:309:PEK:H182	26:C:309:PEK:H15	1.91	0.40
29:B:552:HOH:O	21:D:202:TGL:HC81	2.22	0.40
25:G:102:CDL:H131	25:G:102:CDL:OB3	2.21	0.40
1:N:398:PRO:O	1:N:498:CYS:HB3	2.22	0.40
1:N:505:PHE:CA	22:N:612:EDO:H22	2.50	0.40
25:T:102:CDL:H401	25:T:102:CDL:H432	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:B:454:HOH:O	29:D:303:HOH:O[2_584]	2.03	0.17
29:I:129:HOH:O	29:V:201:HOH:O[3_647]	2.03	0.17
29:I:132:HOH:O	29:M:226:HOH:O[2_584]	2.09	0.11
29:B:500:HOH:O	29:D:437:HOH:O[2_584]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/514 (107%)	537 (98%)	13 (2%)	0	100	100
1	N	534/514 (104%)	517 (97%)	15 (3%)	2 (0%)	34	21
2	B	229/227 (101%)	220 (96%)	9 (4%)	0	100	100
2	O	232/227 (102%)	226 (97%)	6 (3%)	0	100	100
3	C	262/259 (101%)	256 (98%)	6 (2%)	0	100	100
3	P	259/259 (100%)	253 (98%)	6 (2%)	0	100	100
4	D	143/144 (99%)	139 (97%)	4 (3%)	0	100	100
4	Q	142/144 (99%)	135 (95%)	4 (3%)	3 (2%)	7	1
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	97/98 (99%)	95 (98%)	2 (2%)	0	100	100
6	S	97/98 (99%)	93 (96%)	4 (4%)	0	100	100
7	G	81/84 (96%)	71 (88%)	7 (9%)	3 (4%)	3	0
7	T	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	2	0
8	H	77/79 (98%)	74 (96%)	2 (3%)	1 (1%)	12	3
8	U	77/79 (98%)	73 (95%)	2 (3%)	2 (3%)	5	1
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
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%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
All	All	3586/3558 (101%)	3474 (97%)	97 (3%)	15 (0%)	34	21

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	6	GLY
4	Q	9	GLU
4	Q	10	ASP
4	Q	11	TYR
7	T	6	GLY
7	G	5	LYS
7	T	2	SER
7	T	3	ALA
7	T	4	ALA
8	U	9	LYS
1	N	384[A]	GLY
1	N	384[B]	GLY
8	H	8	ILE
8	U	8	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	461/426 (108%)	459 (100%)	2 (0%)	91	89
1	N	445/426 (104%)	441 (99%)	4 (1%)	78	75
2	B	214/210 (102%)	204 (95%)	10 (5%)	26	12
2	O	217/210 (103%)	206 (95%)	11 (5%)	24	10
3	C	229/224 (102%)	225 (98%)	4 (2%)	60	51
3	P	226/224 (101%)	223 (99%)	3 (1%)	69	62
4	D	129/128 (101%)	128 (99%)	1 (1%)	81	78
4	Q	128/128 (100%)	123 (96%)	5 (4%)	32	17
5	E	92/92 (100%)	91 (99%)	1 (1%)	73	68
5	R	92/92 (100%)	91 (99%)	1 (1%)	73	68
6	F	82/81 (101%)	79 (96%)	3 (4%)	34	19
6	S	82/81 (101%)	78 (95%)	4 (5%)	25	11
7	G	67/67 (100%)	60 (90%)	7 (10%)	7	1
7	T	68/67 (102%)	63 (93%)	5 (7%)	13	4
8	H	71/71 (100%)	67 (94%)	4 (6%)	21	8
8	U	71/71 (100%)	68 (96%)	3 (4%)	30	15
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	48
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	21
10	J	49/49 (100%)	49 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	16
11	K	39/39 (100%)	39 (100%)	0	100	100
11	X	39/39 (100%)	39 (100%)	0	100	100
12	L	39/39 (100%)	39 (100%)	0	100	100
12	Y	39/39 (100%)	37 (95%)	2 (5%)	24	10
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	36 (97%)	1 (3%)	44	31
All	All	3116/3040 (102%)	3040 (98%)	76 (2%)	49	36

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	369	ASP
2	B	33	LEU

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Mol	Chain	Res	Type
2	B	52	HIS
2	B	60	GLU
2	B	65	TRP
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	115	ASP
2	B	171	LYS
2	B	217	LYS
3	C	17	PRO
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	147	LYS
5	E	90	ARG
6	F	63	GLU
6	F	80[A]	GLN
6	F	80[B]	GLN
7	G	2	SER
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	29	CYS
8	H	40	GLU
8	H	60	TYR
9	I	37	PHE
1	N	109	PHE
1	N	189[A]	MET
1	N	189[B]	MET
1	N	369	ASP
2	O	33	LEU
2	O	52	HIS
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	144	LEU

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Mol	Chain	Res	Type
2	O	171	LYS
2	O	217	LYS
2	O	226	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	6	VAL
4	Q	9	GLU
4	Q	19	ARG
4	Q	20	ARG
4	Q	51	LEU
5	R	80	GLU
6	S	43	LYS
6	S	63	GLU
6	S	87	THR
6	S	90	LYS
7	T	2	SER
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	54	ARG
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	36	LYS
10	W	7	GLU
10	W	50	LEU
12	Y	20	ARG
12	Y	26	THR
13	Z	38	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	181	GLN
3	C	149	HIS
4	D	109	HIS
6	F	98	HIS
4	Q	101	HIS
4	Q	109	HIS
9	V	20	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.65	0	7,9,11	1.62	1 (14%)
9	SAC	I	1	9	7,8,9	0.64	0	8,9,11	0.96	0
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	0.61	0
7	TPO	G	11	7	8,10,11	1.33	1 (12%)	10,14,16	1.35	1 (10%)
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.70	2 (28%)
2	FME	B	1	2	8,9,10	0.96	0	7,9,11	2.08	3 (42%)
1	FME	N	1	1	8,9,10	0.51	0	7,9,11	1.62	1 (14%)
7	TPO	T	11	7	8,10,11	1.34	1 (12%)	10,14,16	1.23	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	4/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-
9	SAC	V	1	9	-	4/7/8/10	-
7	TPO	G	11	7	-	5/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	2.94	1.60	1.50
7	T	11	TPO	P-O1P	2.73	1.59	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.56	103.07	112.95
2	O	1	FME	CG-CB-CA	-3.51	103.19	112.95
1	N	1	FME	CE-SD-CG	3.25	111.55	100.40
7	G	11	TPO	CG2-CB-CA	3.09	119.27	113.16
1	A	1	FME	CE-SD-CG	2.87	110.25	100.40
7	T	11	TPO	CG2-CB-CA	2.47	118.04	113.16
2	B	1	FME	O-C-CA	-2.41	118.46	124.78
2	O	1	FME	O-C-CA	-2.30	118.76	124.78
2	B	1	FME	CB-CG-SD	-2.04	102.53	113.48

There are no chirality outliers.

All (27) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	T	11	TPO	CB-OG1-P-O2P
1	A	1	FME	C-CA-CB-CG
9	I	1	SAC	C-CA-CB-OG
7	G	11	TPO	CB-OG1-P-O3P
7	T	11	TPO	CB-OG1-P-O3P
1	A	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	SAC	1	0
9	V	1	SAC	1	0
2	B	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 160 ligands modelled in this entry, 10 are monoatomic - leaving 150 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
22	EDO	A	619	-	3,3,3	0.43	0	2,2,2	0.65	0
22	EDO	Y	104	-	3,3,3	0.56	0	2,2,2	0.12	0
22	EDO	G	103	-	3,3,3	0.88	0	2,2,2	0.54	0
26	PEK	C	308	-	52,52,52	1.17	2 (3%)	55,57,57	1.40	6 (10%)
22	EDO	C	311	-	3,3,3	0.90	0	2,2,2	0.45	0
22	EDO	T	105	-	3,3,3	0.57	0	2,2,2	0.31	0
19	PGV	T	104	-	50,50,50	1.07	2 (4%)	53,56,56	1.50	7 (13%)
22	EDO	C	312	-	3,3,3	0.93	0	2,2,2	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	CHD	P	305	-	29,32,32	0.66	0	48,51,51	1.79	10 (20%)
22	EDO	F	104	-	3,3,3	0.39	0	2,2,2	0.29	0
22	EDO	C	317	-	3,3,3	0.72	0	2,2,2	0.24	0
22	EDO	N	618	-	3,3,3	0.83	0	2,2,2	0.36	0
22	EDO	B	305	-	3,3,3	0.37	0	2,2,2	0.24	0
25	CDL	C	307	-	99,99,99	1.40	14 (14%)	105,111,111	1.66	17 (16%)
14	HEA	A	601[B]	-	44,67,67	1.55	6 (13%)	37,103,103	2.62	16 (43%)
22	EDO	C	315	-	3,3,3	0.50	0	2,2,2	0.57	0
18	DMU	Z	101	-	34,34,34	0.63	1 (2%)	45,45,45	1.06	3 (6%)
22	EDO	F	108	-	3,3,3	0.47	0	2,2,2	0.24	0
19	PGV	A	607	-	50,50,50	1.10	3 (6%)	53,56,56	1.31	7 (13%)
22	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.25	0
23	CUA	O	301	2	0,1,1	0.00	-	-	-	-
24	CHD	C	306	-	29,32,32	0.80	1 (3%)	48,51,51	2.20	16 (33%)
14	HEA	N	601[B]	-	44,67,67	1.16	3 (6%)	37,103,103	2.66	19 (51%)
22	EDO	N	611	-	3,3,3	1.12	0	2,2,2	0.36	0
24	CHD	T	101	-	29,32,32	1.06	2 (6%)	48,51,51	1.59	9 (18%)
18	DMU	P	302	-	10,10,34	0.44	0	9,9,45	0.38	0
20	PSC	V	101	-	51,51,51	1.19	4 (7%)	57,59,59	1.56	11 (19%)
22	EDO	W	102	-	3,3,3	0.47	0	2,2,2	0.41	0
20	PSC	A	609	-	51,51,51	1.13	3 (5%)	57,59,59	1.53	6 (10%)
22	EDO	E	202	-	3,3,3	0.45	0	2,2,2	0.40	0
22	EDO	D	205	-	3,3,3	0.55	0	2,2,2	0.37	0
18	DMU	M	101	-	34,34,34	0.46	0	45,45,45	1.12	4 (8%)
22	EDO	N	620	-	3,3,3	0.64	0	2,2,2	0.19	0
24	CHD	C	305	-	29,32,32	1.03	1 (3%)	48,51,51	1.56	6 (12%)
22	EDO	O	304	-	3,3,3	0.60	0	2,2,2	0.24	0
26	PEK	C	309	-	52,52,52	0.88	2 (3%)	55,57,57	1.23	6 (10%)
22	EDO	N	609	-	3,3,3	0.58	0	2,2,2	0.87	0
22	EDO	N	617	-	3,3,3	0.29	0	2,2,2	0.75	0
22	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.19	0
22	EDO	P	316	-	3,3,3	0.64	0	2,2,2	0.45	0
24	CHD	P	304	-	29,32,32	0.82	0	48,51,51	1.61	8 (16%)
25	CDL	T	102	-	99,99,99	1.36	12 (12%)	105,111,111	1.42	14 (13%)
22	EDO	A	615	-	3,3,3	0.34	0	2,2,2	0.92	0
22	EDO	F	107	-	3,3,3	0.73	0	2,2,2	0.31	0
23	CUA	B	301	2	0,1,1	0.00	-	-	-	-
22	EDO	N	622	-	3,3,3	1.10	0	2,2,2	1.30	0
19	PGV	P	310	-	50,50,50	1.04	2 (4%)	53,56,56	1.30	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	PGV	N	607	-	50,50,50	1.01	2 (4%)	53,56,56	1.37	7 (13%)
22	EDO	P	311	-	3,3,3	0.60	0	2,2,2	0.28	0
22	EDO	J	103	-	3,3,3	0.63	0	2,2,2	0.24	0
22	EDO	N	619	-	3,3,3	0.54	0	2,2,2	0.41	0
25	CDL	P	306	-	99,99,99	1.33	12 (12%)	105,111,111	1.58	18 (17%)
22	EDO	D	206	-	3,3,3	0.46	0	2,2,2	0.60	0
18	DMU	X	102	-	21,21,34	0.57	0	24,25,45	1.40	2 (8%)
22	EDO	S	106	-	3,3,3	0.73	0	2,2,2	0.32	0
22	EDO	A	612	-	3,3,3	0.72	0	2,2,2	1.12	0
24	CHD	J	102	-	29,32,32	0.73	0	48,51,51	1.65	13 (27%)
18	DMU	A	606	-	11,11,34	0.36	0	9,9,45	0.71	0
18	DMU	D	201	-	21,21,34	0.89	1 (4%)	24,25,45	1.55	5 (20%)
18	DMU	X	104	-	10,10,34	0.31	0	9,9,45	0.44	0
22	EDO	S	104	-	3,3,3	0.76	0	2,2,2	0.34	0
22	EDO	A	613	-	3,3,3	0.92	0	2,2,2	0.62	0
18	DMU	C	302	-	34,34,34	0.51	0	45,45,45	2.14	15 (33%)
22	EDO	A	617	-	3,3,3	0.39	0	2,2,2	0.65	0
22	EDO	A	618	-	3,3,3	0.66	0	2,2,2	0.24	0
18	DMU	L	101	-	34,34,34	0.68	0	45,45,45	1.64	9 (20%)
22	EDO	N	610	-	3,3,3	0.61	0	2,2,2	0.39	0
22	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.24	0
26	PEK	P	308	-	52,52,52	0.77	2 (3%)	55,57,57	1.30	5 (9%)
22	EDO	B	306	-	3,3,3	0.76	0	2,2,2	0.39	0
21	TGL	N	608	-	62,62,62	1.15	3 (4%)	65,65,65	1.32	6 (9%)
18	DMU	K	103	-	22,22,34	1.01	1 (4%)	27,27,45	1.33	4 (14%)
22	EDO	N	623	-	3,3,3	0.61	0	2,2,2	0.55	0
26	PEK	F	102	-	52,52,52	1.06	2 (3%)	55,57,57	1.50	5 (9%)
22	EDO	S	102	-	3,3,3	0.74	0	2,2,2	0.65	0
22	EDO	E	201	-	3,3,3	0.49	0	2,2,2	0.26	0
28	PO4	H	101	-	4,4,4	0.99	0	6,6,6	0.39	0
21	TGL	L	103	-	62,62,62	1.32	4 (6%)	65,65,65	2.12	16 (24%)
21	TGL	D	202	-	62,62,62	1.33	5 (8%)	65,65,65	1.16	6 (9%)
18	DMU	Q	201	-	22,22,34	0.86	1 (4%)	27,27,45	1.74	7 (25%)
18	DMU	X	101	-	10,10,34	0.44	0	9,9,45	0.45	0
22	EDO	B	304	-	3,3,3	0.41	0	2,2,2	0.49	0
22	EDO	N	614	-	3,3,3	0.54	0	2,2,2	0.22	0
22	EDO	M	102	-	3,3,3	0.40	0	2,2,2	0.19	0
26	PEK	P	307	-	52,52,52	1.09	2 (3%)	55,57,57	1.38	7 (12%)
14	HEA	A	601[A]	-	44,67,67	1.41	6 (13%)	37,103,103	2.50	13 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	F	105	-	3,3,3	0.65	0	2,2,2	0.64	0
22	EDO	L	104	-	3,3,3	0.68	0	2,2,2	0.54	0
22	EDO	B	303	-	3,3,3	0.67	0	2,2,2	0.65	0
22	EDO	Q	204	-	3,3,3	0.40	0	2,2,2	0.54	0
22	EDO	A	616	-	3,3,3	0.61	0	2,2,2	0.27	0
18	DMU	B	302	-	10,10,34	0.42	0	9,9,45	0.44	0
18	DMU	J	101	-	21,21,34	0.93	1 (4%)	24,25,45	1.36	4 (16%)
22	EDO	Q	205	-	3,3,3	0.75	0	2,2,2	0.28	0
22	EDO	N	616	-	3,3,3	0.68	0	2,2,2	0.26	0
19	PGV	N	606	-	50,50,50	1.02	2 (4%)	53,56,56	1.28	6 (11%)
21	TGL	Y	103	-	62,62,62	1.33	3 (4%)	65,65,65	1.57	9 (13%)
22	EDO	F	110	-	3,3,3	0.70	0	2,2,2	0.18	0
14	HEA	N	601[A]	-	44,67,67	1.10	2 (4%)	37,103,103	2.30	13 (35%)
18	DMU	O	302	-	10,10,34	0.40	0	9,9,45	0.40	0
22	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.55	0
22	EDO	A	611	-	3,3,3	0.69	0	2,2,2	0.50	0
22	EDO	S	105	-	3,3,3	0.36	0	2,2,2	0.28	0
22	EDO	P	314	-	3,3,3	0.92	0	2,2,2	0.07	0
22	EDO	F	109	-	3,3,3	0.59	0	2,2,2	0.30	0
18	DMU	Y	101	-	34,34,34	0.73	0	45,45,45	1.13	3 (6%)
19	PGV	C	310	-	50,50,50	0.76	1 (2%)	53,56,56	1.16	5 (9%)
28	PO4	U	101	-	4,4,4	0.91	0	6,6,6	0.58	0
21	TGL	A	610	-	62,62,62	1.18	3 (4%)	65,65,65	1.34	6 (9%)
22	EDO	H	102	-	3,3,3	0.27	0	2,2,2	0.79	0
19	PGV	A	608	-	50,50,50	0.89	4 (8%)	53,56,56	1.28	2 (3%)
18	DMU	P	303	-	34,34,34	0.64	0	45,45,45	2.08	15 (33%)
22	EDO	P	313	-	3,3,3	0.95	0	2,2,2	0.34	0
22	EDO	N	615	-	3,3,3	0.68	0	2,2,2	0.39	0
22	EDO	Q	203	-	3,3,3	0.48	0	2,2,2	0.27	0
22	EDO	T	106	-	3,3,3	0.86	0	2,2,2	1.06	0
22	EDO	O	303	-	3,3,3	0.71	0	2,2,2	0.62	0
19	PGV	P	309	-	50,50,50	0.82	4 (8%)	53,56,56	1.08	4 (7%)
18	DMU	K	102	-	12,12,34	0.49	0	10,11,45	0.47	0
18	DMU	W	101	-	21,21,34	0.92	1 (4%)	24,25,45	1.54	5 (20%)
22	EDO	F	106	-	3,3,3	0.96	0	2,2,2	0.29	0
22	EDO	D	207	-	3,3,3	0.58	0	2,2,2	0.31	0
22	EDO	P	317	-	3,3,3	0.69	0	2,2,2	0.60	0
18	DMU	K	104	-	10,10,34	0.31	0	9,9,45	0.50	0
18	DMU	X	105	-	10,10,34	0.38	0	9,9,45	0.32	0
22	EDO	S	103	-	3,3,3	0.65	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	EDO	D	203	-	3,3,3	0.75	0	2,2,2	0.28	0
22	EDO	B	307	-	3,3,3	0.77	0	2,2,2	0.69	0
14	HEA	N	602	1,29	44,67,67	1.20	5 (11%)	37,103,103	2.38	20 (54%)
18	DMU	C	304	-	10,10,34	0.40	0	9,9,45	0.29	0
18	DMU	X	103	-	10,10,34	0.38	0	9,9,45	0.27	0
22	EDO	C	314	-	3,3,3	0.75	0	2,2,2	1.02	0
22	EDO	P	312	-	3,3,3	0.39	0	2,2,2	0.78	0
18	DMU	C	303	-	22,22,34	0.80	1 (4%)	27,27,45	1.56	3 (11%)
24	CHD	Y	102	-	29,32,32	0.58	0	48,51,51	2.22	15 (31%)
22	EDO	L	105	-	3,3,3	0.49	0	2,2,2	0.27	0
21	TGL	Q	202	-	62,62,62	1.12	3 (4%)	65,65,65	0.95	5 (7%)
22	EDO	C	313	-	3,3,3	0.38	0	2,2,2	0.68	0
22	EDO	C	316	-	3,3,3	0.89	0	2,2,2	0.53	0
22	EDO	N	621	-	3,3,3	0.53	0	2,2,2	0.81	0
24	CHD	G	101	-	29,32,32	0.86	0	48,51,51	1.41	8 (16%)
22	EDO	P	315	-	3,3,3	1.08	0	2,2,2	0.66	0
22	EDO	U	102	-	3,3,3	0.53	0	2,2,2	0.13	0
18	DMU	K	101	-	10,10,34	0.27	0	9,9,45	0.78	0
25	CDL	G	102	-	99,99,99	1.41	12 (12%)	105,111,111	1.25	9 (8%)
24	CHD	L	102	-	29,32,32	0.57	0	48,51,51	2.52	18 (37%)
22	EDO	D	204	-	3,3,3	0.41	0	2,2,2	0.50	0
26	PEK	T	103	-	52,52,52	1.09	2 (3%)	55,57,57	1.48	6 (10%)
22	EDO	F	103	-	3,3,3	0.72	0	2,2,2	0.55	0
14	HEA	A	602	1,29	44,67,67	1.27	5 (11%)	37,103,103	2.28	13 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	Y	104	-	-	1/1/1/1	-
22	EDO	G	103	-	-	0/1/1/1	-
26	PEK	C	308	-	-	17/56/56/56	-
22	EDO	C	311	-	-	1/1/1/1	-
22	EDO	T	105	-	-	1/1/1/1	-
19	PGV	T	104	-	-	19/55/55/55	-
22	EDO	C	312	-	-	0/1/1/1	-
24	CHD	P	305	-	-	3/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	F	104	-	-	0/1/1/1	-
22	EDO	C	317	-	-	1/1/1/1	-
22	EDO	N	618	-	-	1/1/1/1	-
22	EDO	B	305	-	-	1/1/1/1	-
25	CDL	C	307	-	-	43/110/110/110	-
14	HEA	A	601[B]	-	-	0/24/76/76	-
22	EDO	C	315	-	-	0/1/1/1	-
18	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
22	EDO	F	108	-	-	0/1/1/1	-
19	PGV	A	607	-	-	18/55/55/55	-
22	EDO	N	613	-	-	0/1/1/1	-
24	CHD	C	306	-	-	7/7/74/74	0/4/4/4
14	HEA	N	601[B]	-	-	0/24/76/76	-
22	EDO	N	611	-	-	0/1/1/1	-
24	CHD	T	101	-	-	0/7/74/74	0/4/4/4
18	DMU	P	302	-	-	0/8/8/59	-
20	PSC	V	101	-	-	20/55/55/55	-
22	EDO	W	102	-	-	1/1/1/1	-
20	PSC	A	609	-	-	15/55/55/55	-
22	EDO	E	202	-	-	1/1/1/1	-
22	EDO	D	205	-	-	0/1/1/1	-
22	EDO	A	615	-	-	1/1/1/1	-
22	EDO	N	620	-	-	0/1/1/1	-
24	CHD	C	305	-	-	0/7/74/74	0/4/4/4
22	EDO	O	304	-	-	0/1/1/1	-
26	PEK	C	309	-	-	16/56/56/56	-
22	EDO	N	609	-	-	0/1/1/1	-
22	EDO	N	617	-	-	1/1/1/1	-
22	EDO	N	612	-	-	1/1/1/1	-
22	EDO	P	316	-	-	0/1/1/1	-
24	CHD	P	304	-	-	0/7/74/74	0/4/4/4
25	CDL	T	102	-	-	43/110/110/110	-
22	EDO	F	105	-	-	0/1/1/1	-
22	EDO	F	107	-	-	0/1/1/1	-
22	EDO	N	622	-	-	1/1/1/1	-
19	PGV	P	310	-	-	16/55/55/55	-
19	PGV	N	607	-	-	7/55/55/55	-
22	EDO	P	311	-	-	0/1/1/1	-
22	EDO	J	103	-	-	1/1/1/1	-
22	EDO	N	619	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CDL	P	306	-	-	42/110/110/110	-
22	EDO	D	206	-	-	0/1/1/1	-
18	DMU	X	102	-	-	8/13/29/59	0/1/1/2
22	EDO	S	106	-	-	0/1/1/1	-
22	EDO	A	612	-	-	0/1/1/1	-
24	CHD	J	102	-	-	3/7/74/74	0/4/4/4
18	DMU	A	606	-	-	2/8/8/59	-
18	DMU	D	201	-	-	4/13/29/59	0/1/1/2
18	DMU	X	104	-	-	3/8/8/59	-
22	EDO	S	104	-	-	0/1/1/1	-
22	EDO	A	613	-	-	0/1/1/1	-
18	DMU	C	302	-	-	10/19/59/59	0/2/2/2
22	EDO	A	617	-	-	0/1/1/1	-
22	EDO	A	618	-	-	1/1/1/1	-
18	DMU	L	101	-	-	8/19/59/59	0/2/2/2
22	EDO	N	610	-	-	0/1/1/1	-
18	DMU	M	101	-	-	7/19/59/59	0/2/2/2
22	EDO	A	614	-	-	0/1/1/1	-
26	PEK	P	308	-	-	11/56/56/56	-
22	EDO	B	306	-	-	1/1/1/1	-
21	TGL	N	608	-	-	33/65/65/65	-
18	DMU	K	103	-	-	6/13/33/59	0/1/1/2
22	EDO	N	623	-	-	1/1/1/1	-
26	PEK	F	102	-	-	24/56/56/56	-
22	EDO	S	102	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
21	TGL	L	103	-	-	32/65/65/65	-
21	TGL	D	202	-	-	21/65/65/65	-
18	DMU	Q	201	-	-	5/13/33/59	0/1/1/2
18	DMU	X	101	-	-	1/8/8/59	-
22	EDO	B	304	-	-	1/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
22	EDO	M	102	-	-	0/1/1/1	-
26	PEK	P	307	-	-	22/56/56/56	-
14	HEA	A	601[A]	-	-	2/24/76/76	-
22	EDO	L	104	-	-	0/1/1/1	-
22	EDO	B	303	-	-	0/1/1/1	-
22	EDO	Q	204	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	A	616	-	-	0/1/1/1	-
18	DMU	B	302	-	-	3/8/8/59	-
18	DMU	J	101	-	-	4/13/29/59	0/1/1/2
22	EDO	Q	205	-	-	1/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
19	PGV	N	606	-	-	15/55/55/55	-
21	TGL	Y	103	-	-	32/65/65/65	-
22	EDO	F	110	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	5/24/76/76	-
18	DMU	O	302	-	-	0/8/8/59	-
22	EDO	E	203	-	-	0/1/1/1	-
22	EDO	A	611	-	-	1/1/1/1	-
22	EDO	S	105	-	-	0/1/1/1	-
22	EDO	P	314	-	-	1/1/1/1	-
22	EDO	F	109	-	-	1/1/1/1	-
18	DMU	Y	101	-	-	5/19/59/59	0/2/2/2
19	PGV	C	310	-	-	8/55/55/55	-
21	TGL	A	610	-	-	36/65/65/65	-
22	EDO	H	102	-	-	0/1/1/1	-
19	PGV	A	608	-	-	4/55/55/55	-
18	DMU	P	303	-	-	6/19/59/59	0/2/2/2
22	EDO	P	313	-	-	1/1/1/1	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	Q	203	-	-	1/1/1/1	-
22	EDO	T	106	-	-	0/1/1/1	-
22	EDO	O	303	-	-	0/1/1/1	-
19	PGV	P	309	-	-	10/55/55/55	-
18	DMU	K	102	-	-	4/9/10/59	-
18	DMU	W	101	-	-	4/13/29/59	0/1/1/2
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	D	207	-	-	0/1/1/1	-
22	EDO	P	317	-	-	1/1/1/1	-
18	DMU	K	104	-	-	4/8/8/59	-
18	DMU	X	105	-	-	4/8/8/59	-
22	EDO	S	103	-	-	1/1/1/1	-
22	EDO	D	203	-	-	1/1/1/1	-
22	EDO	B	307	-	-	1/1/1/1	-
14	HEA	N	602	1,29	3/3/7/16	0/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	DMU	C	304	-	-	5/8/8/59	-
18	DMU	X	103	-	-	4/8/8/59	-
22	EDO	C	314	-	-	0/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
18	DMU	C	303	-	-	7/13/33/59	0/1/1/2
24	CHD	Y	102	-	-	1/7/74/74	0/4/4/4
22	EDO	L	105	-	-	0/1/1/1	-
21	TGL	Q	202	-	-	28/65/65/65	-
22	EDO	C	313	-	-	0/1/1/1	-
22	EDO	C	316	-	-	1/1/1/1	-
22	EDO	N	621	-	-	0/1/1/1	-
24	CHD	G	101	-	-	0/7/74/74	0/4/4/4
22	EDO	P	315	-	-	1/1/1/1	-
22	EDO	U	102	-	-	1/1/1/1	-
18	DMU	K	101	-	-	3/8/8/59	-
25	CDL	G	102	-	-	40/110/110/110	-
24	CHD	L	102	-	-	5/7/74/74	0/4/4/4
22	EDO	D	204	-	-	0/1/1/1	-
26	PEK	T	103	-	-	24/56/56/56	-
22	EDO	F	103	-	-	0/1/1/1	-
14	HEA	A	602	1,29	3/3/7/16	1/24/76/76	-

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	103	TGL	OG2-CB1	6.24	1.51	1.34
21	Y	103	TGL	OG2-CB1	6.12	1.51	1.34
21	Y	103	TGL	OG3-CC1	5.88	1.50	1.33
25	G	102	CDL	OA6-CA5	5.48	1.49	1.34
21	N	608	TGL	OG2-CB1	5.38	1.49	1.34
26	C	308	PEK	O03-C21	5.35	1.49	1.33
21	A	610	TGL	OG2-CB1	5.23	1.49	1.34
21	A	610	TGL	OG1-CA1	5.09	1.48	1.33
21	D	202	TGL	OG2-CB1	5.07	1.48	1.34
21	L	103	TGL	OG3-CC1	5.04	1.48	1.33
19	N	606	PGV	O03-C19	5.03	1.48	1.33
26	C	308	PEK	O01-C1	4.98	1.48	1.34
21	D	202	TGL	OG3-CC1	4.94	1.47	1.33
19	A	607	PGV	O03-C19	4.93	1.47	1.33
21	Y	103	TGL	OG1-CA1	4.92	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	102	CDL	OA8-CA7	4.92	1.47	1.33
26	P	307	PEK	O01-C1	4.87	1.48	1.34
25	G	102	CDL	OB8-CB7	4.86	1.47	1.33
25	T	102	CDL	OA6-CA5	4.85	1.48	1.34
26	T	103	PEK	O03-C21	4.84	1.47	1.33
26	F	102	PEK	O03-C21	4.82	1.47	1.33
19	T	104	PGV	O01-C1	4.79	1.47	1.34
26	P	307	PEK	O03-C21	4.79	1.47	1.33
19	P	310	PGV	O03-C19	4.77	1.47	1.33
20	A	609	PSC	O01-C1	4.77	1.47	1.34
21	Q	202	TGL	OG2-CB1	4.76	1.47	1.34
25	T	102	CDL	OB8-CB7	4.75	1.47	1.33
14	A	601[B]	HEA	C3B-C11	-4.75	1.49	1.52
26	F	102	PEK	O01-C1	4.75	1.47	1.34
25	P	306	CDL	OA8-CA7	4.75	1.47	1.33
25	C	307	CDL	OB8-CB7	4.69	1.47	1.33
21	L	103	TGL	OG1-CA1	4.69	1.47	1.33
20	V	101	PSC	O01-C1	4.64	1.47	1.34
26	T	103	PEK	O01-C1	4.62	1.47	1.34
19	T	104	PGV	O03-C19	4.57	1.46	1.33
21	A	610	TGL	OG3-CC1	4.57	1.46	1.33
21	N	608	TGL	OG1-CA1	4.57	1.46	1.33
25	P	306	CDL	OA6-CA5	4.47	1.46	1.34
21	D	202	TGL	OG1-CA1	4.47	1.46	1.33
21	N	608	TGL	OG3-CC1	4.39	1.46	1.33
21	Q	202	TGL	OG1-CA1	4.38	1.46	1.33
19	P	310	PGV	O01-C1	4.37	1.46	1.34
19	A	607	PGV	O01-C1	4.36	1.46	1.34
20	V	101	PSC	O03-C19	4.32	1.46	1.33
25	C	307	CDL	OA8-CA7	4.28	1.45	1.33
25	T	102	CDL	OB6-CB5	4.23	1.46	1.34
25	G	102	CDL	OB6-CB5	4.19	1.46	1.34
19	N	606	PGV	O01-C1	4.16	1.46	1.34
25	C	307	CDL	OA6-CA5	4.09	1.45	1.34
14	A	601[B]	HEA	CAD-C3D	3.97	1.57	1.52
14	A	601[A]	HEA	CAD-C3D	3.97	1.57	1.52
26	C	309	PEK	O03-C21	3.97	1.44	1.33
20	V	101	PSC	C13-C12	3.91	1.54	1.31
25	T	102	CDL	OA8-CA7	3.91	1.44	1.33
25	P	306	CDL	OB8-CB7	3.90	1.44	1.33
21	Q	202	TGL	OG3-CC1	3.89	1.44	1.33
21	D	202	TGL	OB1-CB1	3.75	1.33	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	609	PSC	C13-C12	3.73	1.53	1.31
25	C	307	CDL	C59-C58	-3.70	1.30	1.51
20	A	609	PSC	O03-C19	3.67	1.44	1.33
18	K	103	DMU	O16-C6	3.61	1.46	1.40
25	C	307	CDL	OB6-CB5	3.61	1.44	1.34
14	A	602	HEA	C3A-C2A	-3.58	1.35	1.40
25	P	306	CDL	OB6-CB5	3.49	1.44	1.34
18	W	101	DMU	O16-C6	3.49	1.46	1.40
25	C	307	CDL	C79-C78	-3.48	1.32	1.51
25	T	102	CDL	C59-C58	-3.45	1.32	1.51
25	T	102	CDL	C19-C18	-3.45	1.32	1.51
18	J	101	DMU	O16-C6	3.44	1.46	1.40
19	N	607	PGV	O01-C1	3.40	1.43	1.34
26	P	308	PEK	O03-C21	3.35	1.43	1.33
25	T	102	CDL	C82-C81	-3.35	1.32	1.51
14	N	601[B]	HEA	CAD-C3D	3.33	1.56	1.52
14	N	601[A]	HEA	CAD-C3D	3.33	1.56	1.52
25	G	102	CDL	C59-C58	-3.32	1.32	1.51
14	A	601[B]	HEA	CMC-C2C	3.30	1.58	1.51
14	A	601[A]	HEA	CMC-C2C	3.30	1.58	1.51
25	P	306	CDL	C79-C78	-3.30	1.33	1.51
19	N	607	PGV	O03-C19	3.29	1.43	1.33
25	C	307	CDL	C39-C38	-3.26	1.33	1.51
25	T	102	CDL	C22-C21	-3.23	1.33	1.51
25	C	307	CDL	C82-C81	-3.22	1.33	1.51
25	P	306	CDL	C22-C21	-3.21	1.33	1.51
25	T	102	CDL	C79-C78	-3.21	1.33	1.51
25	P	306	CDL	C19-C18	-3.21	1.33	1.51
25	G	102	CDL	C62-C61	-3.21	1.33	1.51
25	T	102	CDL	C62-C61	-3.20	1.33	1.51
25	G	102	CDL	C82-C81	-3.20	1.33	1.51
25	T	102	CDL	C42-C41	-3.20	1.33	1.51
25	C	307	CDL	C42-C41	-3.19	1.33	1.51
25	G	102	CDL	C79-C78	-3.19	1.33	1.51
25	C	307	CDL	C22-C21	-3.15	1.33	1.51
25	C	307	CDL	C62-C61	-3.15	1.33	1.51
25	C	307	CDL	C19-C18	-3.15	1.33	1.51
25	T	102	CDL	C39-C38	-3.09	1.34	1.51
14	A	601[B]	HEA	CAA-C2A	3.08	1.57	1.52
14	A	601[A]	HEA	CAA-C2A	3.08	1.57	1.52
25	P	306	CDL	C59-C58	-3.04	1.34	1.51
25	P	306	CDL	C82-C81	-3.04	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	306	CDL	C39-C38	-3.03	1.34	1.51
14	N	601[B]	HEA	C3B-C11	-3.03	1.50	1.52
18	D	201	DMU	O16-C6	3.02	1.45	1.40
25	G	102	CDL	C42-C41	-3.02	1.34	1.51
25	P	306	CDL	C62-C61	-3.01	1.34	1.51
25	G	102	CDL	C39-C38	-2.99	1.34	1.51
25	C	307	CDL	O1-C1	2.96	1.52	1.43
25	P	306	CDL	C42-C41	-2.95	1.35	1.51
24	C	305	CHD	O12-C12	2.91	1.48	1.43
18	C	303	DMU	O16-C6	2.89	1.45	1.40
19	P	309	PGV	O01-C1	2.87	1.42	1.34
19	P	309	PGV	O01-C02	-2.85	1.39	1.46
25	G	102	CDL	C19-C18	-2.85	1.35	1.51
26	C	309	PEK	O01-C1	2.83	1.42	1.34
14	A	601[B]	HEA	C3A-C2A	-2.81	1.36	1.40
14	A	601[A]	HEA	C3A-C2A	-2.81	1.36	1.40
19	A	608	PGV	O01-C1	2.80	1.42	1.34
25	G	102	CDL	C22-C21	-2.75	1.36	1.51
18	Q	201	DMU	O16-C6	2.72	1.44	1.40
24	T	101	CHD	O7-C7	2.68	1.49	1.43
14	A	602	HEA	C18-C19	2.62	1.39	1.33
18	Z	101	DMU	O16-C6	2.58	1.44	1.40
14	N	602	HEA	CAD-C3D	2.58	1.55	1.52
21	D	202	TGL	CB2-CB1	2.54	1.58	1.50
19	A	608	PGV	O03-C19	2.53	1.40	1.33
24	C	306	CHD	C10-C9	-2.51	1.51	1.56
14	N	601[B]	HEA	C3C-C2C	-2.50	1.36	1.40
14	N	601[A]	HEA	C3C-C2C	-2.50	1.36	1.40
26	P	308	PEK	C05-C04	2.46	1.60	1.50
21	L	103	TGL	CC2-CC1	2.33	1.57	1.50
24	T	101	CHD	C13-C17	-2.29	1.51	1.55
14	A	602	HEA	C14-C15	2.29	1.38	1.33
14	N	602	HEA	C1B-CHB	2.27	1.47	1.41
14	N	602	HEA	C18-C19	2.27	1.38	1.33
19	A	608	PGV	C20-C19	2.24	1.57	1.50
19	A	607	PGV	O02-C1	2.22	1.29	1.22
14	A	601[A]	HEA	C12-C13	2.21	1.60	1.53
25	C	307	CDL	PB2-OB3	2.17	1.58	1.50
19	P	309	PGV	P-O14	-2.17	1.45	1.55
14	N	602	HEA	C14-C15	2.15	1.38	1.33
14	A	602	HEA	C1B-CHB	2.15	1.47	1.41
19	P	309	PGV	O03-C19	2.11	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	310	PGV	O01-C1	2.11	1.40	1.34
19	A	608	PGV	O03-C01	2.09	1.49	1.45
14	A	602	HEA	CMC-C2C	2.09	1.56	1.51
20	V	101	PSC	C08-N	-2.08	1.43	1.50
14	A	601[B]	HEA	C1B-CHB	2.05	1.46	1.41
14	A	601[A]	HEA	C1B-CHB	2.05	1.46	1.41
14	N	602	HEA	CAA-C2A	2.04	1.55	1.52

All (477) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	102	CHD	C10-C9-C8	7.39	119.75	111.82
21	L	103	TGL	OG2-CB1-CB2	7.35	127.34	111.50
20	A	609	PSC	C03-C02-C01	-7.04	95.14	111.79
14	N	601[B]	HEA	C1B-C2B-C3B	-6.78	102.28	107.00
14	N	601[A]	HEA	C1B-C2B-C3B	-6.78	102.28	107.00
21	Y	103	TGL	OG2-CB1-CB2	6.56	125.64	111.50
14	N	601[B]	HEA	C13-C12-C11	-6.35	104.81	114.35
21	A	610	TGL	OG2-CB1-CB2	6.30	125.08	111.50
18	C	302	DMU	C10-O1-C9	6.26	125.97	113.69
25	P	306	CDL	CB4-OB6-CB5	-6.25	102.41	117.79
24	C	306	CHD	C23-C22-C20	-6.17	106.41	114.72
24	Y	102	CHD	C6-C5-C4	-6.14	104.12	111.19
14	A	602	HEA	C26-C15-C16	5.94	125.26	115.27
21	L	103	TGL	OG3-CC1-OC1	-5.85	108.83	123.59
14	A	601[B]	HEA	CAA-CBA-CGA	-5.59	103.29	112.67
14	A	601[A]	HEA	CAA-CBA-CGA	-5.59	103.29	112.67
21	N	608	TGL	OG2-CB1-CB2	5.56	123.47	111.50
19	T	104	PGV	O03-C19-C20	5.54	129.29	111.91
21	L	103	TGL	CG2-OG2-CB1	5.49	131.30	117.79
14	N	601[A]	HEA	C13-C12-C11	-5.34	106.33	114.35
18	X	102	DMU	C6-O5-C4	5.29	119.00	113.13
18	C	303	DMU	O16-C6-C1	5.22	116.46	108.30
25	P	306	CDL	C52-C51-CB5	-5.19	94.74	113.62
26	T	103	PEK	O01-C1-C2	5.18	122.66	111.50
26	F	102	PEK	O03-C21-C22	5.16	128.09	111.91
14	A	601[A]	HEA	C13-C12-C11	-5.08	106.72	114.35
14	A	601[A]	HEA	C26-C15-C16	5.05	123.77	115.27
24	L	102	CHD	C6-C5-C4	-5.04	105.39	111.19
14	N	602	HEA	C13-C12-C11	-5.04	106.78	114.35
24	Y	102	CHD	C1-C10-C5	5.03	115.21	107.77
26	T	103	PEK	O03-C21-C22	5.03	127.68	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	101	PSC	O01-C1-C2	4.99	122.25	111.50
26	C	308	PEK	O01-C1-C2	4.97	122.22	111.50
24	Y	102	CHD	C14-C8-C7	4.97	118.40	111.81
18	L	101	DMU	C10-O1-C9	4.94	123.38	113.69
25	C	307	CDL	O1-C1-CB2	4.94	126.87	109.56
14	A	601[B]	HEA	C13-C12-C11	-4.94	106.93	114.35
14	N	601[B]	HEA	C4B-C3B-C2B	4.93	110.31	106.87
14	N	601[A]	HEA	C4B-C3B-C2B	4.93	110.31	106.87
14	A	601[B]	HEA	C1B-C2B-C3B	-4.87	103.61	107.00
14	A	601[A]	HEA	C1B-C2B-C3B	-4.87	103.61	107.00
24	L	102	CHD	C11-C12-C13	4.85	116.23	111.24
24	L	102	CHD	C13-C17-C20	4.83	125.26	119.50
25	C	307	CDL	CB4-OB6-CB5	-4.82	105.92	117.79
14	A	602	HEA	C27-C19-C20	4.81	123.36	115.27
19	P	310	PGV	O03-C19-C20	4.80	126.97	111.91
21	D	202	TGL	OG3-CC1-CC2	4.79	126.95	111.91
18	P	303	DMU	O1-C10-C5	4.79	120.48	110.35
25	G	102	CDL	OA6-CA5-C11	4.77	121.77	111.50
24	C	305	CHD	C18-C13-C12	4.76	113.91	109.07
25	C	307	CDL	CB2-C1-CA2	-4.72	98.91	112.79
24	Y	102	CHD	C19-C10-C1	-4.71	100.67	108.26
24	L	102	CHD	C11-C9-C10	-4.69	108.89	113.73
14	A	602	HEA	CAD-CBD-CGD	-4.69	104.80	112.67
25	C	307	CDL	OB8-CB7-C71	4.68	126.60	111.91
19	T	104	PGV	C01-O03-C19	4.63	134.28	117.12
18	L	101	DMU	O7-C3-C2	4.62	119.57	107.28
19	P	310	PGV	O01-C1-C2	4.59	121.40	111.50
24	C	306	CHD	C14-C8-C9	-4.59	103.41	109.71
18	P	303	DMU	C10-O1-C9	4.57	122.67	113.69
21	L	103	TGL	OG3-CC1-CC2	4.56	126.23	111.91
18	C	302	DMU	C8-C7-C5	4.52	118.71	110.82
21	L	103	TGL	CG3-CG2-CG1	-4.50	101.13	111.79
14	A	601[B]	HEA	CBD-CAD-C3D	-4.47	104.24	112.49
14	A	601[A]	HEA	CBD-CAD-C3D	-4.47	104.24	112.49
14	A	601[B]	HEA	C17-C18-C19	-4.44	116.97	127.66
26	C	308	PEK	O03-C01-C02	4.42	121.29	108.43
24	P	304	CHD	C22-C20-C17	-4.41	101.17	110.28
14	N	602	HEA	CAA-CBA-CGA	-4.40	105.28	112.67
18	Q	201	DMU	O5-C4-C3	4.38	117.64	109.69
24	J	102	CHD	C13-C17-C20	4.38	124.72	119.50
20	A	609	PSC	O01-C1-C2	4.37	120.92	111.50
25	P	306	CDL	OB8-CB7-C71	4.36	125.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	307	PEK	O03-C21-C22	4.33	125.50	111.91
26	C	308	PEK	O03-C21-C22	4.33	125.49	111.91
25	T	102	CDL	OB6-CB5-C51	4.29	120.75	111.50
24	C	306	CHD	C11-C9-C10	-4.29	109.31	113.73
24	P	305	CHD	C15-C14-C13	4.24	107.71	103.55
26	F	102	PEK	C01-O03-C21	4.23	132.77	117.12
25	C	307	CDL	OB2-PB2-OB3	4.21	125.53	109.07
24	P	305	CHD	C1-C2-C3	4.20	115.86	110.47
14	A	601[B]	HEA	CAD-CBD-CGD	-4.20	105.63	112.67
14	A	601[A]	HEA	CAD-CBD-CGD	-4.20	105.63	112.67
24	P	304	CHD	C16-C17-C13	4.18	107.66	103.55
14	N	601[B]	HEA	C12-C11-C3B	4.17	123.50	112.56
21	Y	103	TGL	CG2-OG2-CB1	4.15	128.02	117.79
26	F	102	PEK	O01-C1-C2	4.14	120.43	111.50
14	A	601[B]	HEA	C12-C11-C3B	4.14	123.42	112.56
19	N	606	PGV	C03-C02-C01	-4.12	102.04	111.79
25	P	306	CDL	OB6-CB5-C51	4.11	120.37	111.50
19	A	607	PGV	C4-C3-C2	-4.08	98.51	113.19
19	A	608	PGV	O03-C19-O04	-4.06	113.33	123.59
14	N	601[B]	HEA	CMB-C2B-C3B	4.06	132.65	124.69
14	N	601[A]	HEA	CMB-C2B-C3B	4.06	132.65	124.69
21	N	608	TGL	CG3-CG2-CG1	-4.05	102.21	111.79
24	C	305	CHD	C22-C20-C17	-4.03	101.96	110.28
24	P	305	CHD	C18-C13-C12	-4.03	104.96	109.07
19	A	608	PGV	O03-C19-C20	4.02	124.54	111.91
25	T	102	CDL	OA8-CA7-C31	4.01	124.48	111.91
18	P	303	DMU	O1-C9-C11	3.94	116.22	106.44
26	F	102	PEK	O03-C21-O04	-3.89	113.78	123.59
24	P	304	CHD	C15-C14-C13	3.89	107.36	103.55
25	P	306	CDL	OB8-CB7-OB9	-3.89	113.78	123.59
18	C	302	DMU	O1-C10-C5	3.89	118.57	110.35
14	A	602	HEA	C16-C15-C14	-3.88	113.26	121.12
14	N	602	HEA	C16-C15-C14	-3.87	113.29	121.12
24	C	306	CHD	C18-C13-C12	-3.85	105.14	109.07
14	N	602	HEA	CMC-C2C-C3C	3.84	131.87	124.68
14	A	601[A]	HEA	C16-C15-C14	-3.81	113.41	121.12
25	T	102	CDL	OA6-CA5-C11	3.80	119.68	111.50
24	L	102	CHD	C14-C13-C12	3.78	110.92	107.40
14	A	602	HEA	C20-C19-C18	-3.77	113.48	121.12
24	C	306	CHD	C19-C10-C9	-3.77	105.99	111.18
24	L	102	CHD	C15-C14-C8	3.77	123.60	118.33
26	P	308	PEK	O03-C21-C22	3.72	123.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	307	CDL	OB6-CB5-C51	3.72	119.51	111.50
24	C	306	CHD	C14-C13-C12	3.71	110.86	107.40
24	C	305	CHD	C22-C23-C24	-3.71	105.62	113.59
24	L	102	CHD	C21-C20-C17	3.71	118.59	112.92
24	G	101	CHD	C13-C17-C20	-3.70	115.07	119.50
18	C	302	DMU	O5-C6-O16	-3.70	101.21	109.97
24	L	102	CHD	C5-C6-C7	3.69	118.54	114.46
19	T	104	PGV	O03-C19-O04	-3.69	114.27	123.59
18	D	201	DMU	O5-C4-C57	3.68	112.73	106.83
25	C	307	CDL	OB8-CB7-OB9	-3.67	114.34	123.59
19	N	606	PGV	O03-C19-C20	3.66	123.40	111.91
25	G	102	CDL	CB6-OB8-CB7	3.65	130.66	117.12
26	P	307	PEK	O03-C21-O04	-3.65	114.38	123.59
24	T	101	CHD	C13-C14-C8	-3.64	110.08	114.74
21	Y	103	TGL	OG3-CG3-CG2	3.64	119.04	108.43
24	Y	102	CHD	C21-C20-C17	3.62	118.46	112.92
18	P	303	DMU	O1-C9-C8	3.60	116.22	109.69
18	L	101	DMU	O1-C10-C5	3.58	117.94	110.35
19	N	607	PGV	O03-C19-C20	3.58	123.15	111.91
21	L	103	TGL	CC5-CC4-CC3	-3.57	96.31	114.42
19	N	606	PGV	O01-C1-C2	3.52	119.09	111.50
24	C	306	CHD	C15-C14-C13	3.52	107.01	103.55
19	N	607	PGV	O01-C1-O02	-3.51	115.22	123.70
24	C	305	CHD	C23-C22-C20	-3.50	110.00	114.72
14	N	602	HEA	C27-C19-C20	3.49	121.15	115.27
19	T	104	PGV	O01-C1-C2	3.49	119.02	111.50
14	A	601[B]	HEA	C20-C19-C18	3.45	128.11	121.12
24	Y	102	CHD	C13-C17-C20	3.44	123.61	119.50
20	V	101	PSC	C21-C20-C19	-3.43	101.13	113.62
21	A	610	TGL	OG1-CA1-CA2	3.43	122.68	111.91
14	A	601[B]	HEA	CMC-C2C-C3C	3.43	131.09	124.68
14	A	601[A]	HEA	CMC-C2C-C3C	3.43	131.09	124.68
14	A	602	HEA	CMC-C2C-C3C	3.43	131.09	124.68
18	Q	201	DMU	C3-C2-C1	-3.41	104.86	110.82
24	P	305	CHD	C19-C10-C9	-3.40	106.50	111.18
24	Y	102	CHD	C10-C9-C8	3.40	115.47	111.82
24	L	102	CHD	C23-C22-C20	-3.40	110.14	114.72
26	T	103	PEK	O03-C21-O04	-3.40	115.02	123.59
24	C	306	CHD	C22-C23-C24	-3.39	106.31	113.59
14	A	601[B]	HEA	C27-C19-C18	-3.39	114.99	123.68
14	N	601[B]	HEA	CAA-CBA-CGA	-3.39	106.99	112.67
14	N	601[A]	HEA	CAA-CBA-CGA	-3.39	106.99	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	102	CDL	OB6-CB5-C51	3.38	118.80	111.50
24	P	305	CHD	C11-C12-C13	-3.37	107.78	111.24
26	P	308	PEK	O03-C21-O04	-3.34	115.15	123.59
20	A	609	PSC	C04-C05-N	-3.33	104.64	115.78
21	Y	103	TGL	OG3-CC1-CC2	3.33	122.37	111.91
24	T	101	CHD	C6-C5-C4	-3.33	107.35	111.19
24	T	101	CHD	C11-C9-C10	-3.33	110.30	113.73
26	P	307	PEK	C03-C02-C01	-3.30	103.98	111.79
24	P	305	CHD	C16-C17-C13	3.30	106.79	103.55
18	P	303	DMU	C10-O7-C3	-3.29	109.83	117.96
19	N	607	PGV	O03-C19-O04	-3.28	115.30	123.59
18	C	302	DMU	O5-C4-C3	3.28	116.67	109.75
24	C	306	CHD	C6-C5-C4	-3.28	107.41	111.19
18	K	103	DMU	C3-C2-C1	-3.28	105.09	110.82
18	P	303	DMU	C7-C8-C9	3.26	116.06	110.24
14	A	602	HEA	CAA-CBA-CGA	-3.25	107.21	112.67
24	L	102	CHD	C14-C8-C7	3.25	116.12	111.81
14	A	601[B]	HEA	C20-C21-C22	-3.24	101.22	111.88
14	A	601[A]	HEA	C20-C21-C22	-3.24	101.22	111.88
18	C	302	DMU	C10-O7-C3	-3.23	109.97	117.96
24	L	102	CHD	C1-C10-C9	-3.22	106.28	111.35
14	N	602	HEA	CMB-C2B-C3B	3.22	131.00	124.69
14	N	601[B]	HEA	O11-C11-C3B	-3.22	102.72	112.00
18	Y	101	DMU	O1-C9-C11	3.22	114.44	106.44
21	L	103	TGL	C20-CA9-CA8	-3.22	98.10	114.42
18	C	302	DMU	O5-C6-C1	3.20	117.12	110.35
24	T	101	CHD	C19-C10-C1	-3.20	103.11	108.26
18	C	302	DMU	C7-C8-C9	3.19	115.93	110.24
14	A	601[B]	HEA	CMC-C2C-C1C	-3.18	123.58	128.46
14	A	601[A]	HEA	CMC-C2C-C1C	-3.18	123.58	128.46
18	P	303	DMU	O6-C11-C9	3.17	122.17	111.29
18	P	303	DMU	C8-C7-C5	3.17	116.35	110.82
24	Y	102	CHD	C2-C1-C10	3.16	118.21	112.78
18	L	101	DMU	C10-O7-C3	3.16	125.79	117.96
21	N	608	TGL	OG3-CC1-CC2	3.16	121.82	111.91
26	P	307	PEK	O01-C1-C2	3.15	118.29	111.50
24	P	305	CHD	C14-C8-C9	-3.13	105.42	109.71
21	D	202	TGL	OG3-CC1-OC1	-3.13	115.70	123.59
25	P	306	CDL	OA8-CA7-C31	3.12	121.69	111.91
18	P	303	DMU	O16-C6-C1	3.12	113.17	108.30
24	Y	102	CHD	C11-C12-C13	3.11	114.44	111.24
18	D	201	DMU	O16-C6-C1	3.09	113.13	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	C20-C19-C18	-3.09	114.87	121.12
25	C	307	CDL	OA8-CA7-C31	3.08	121.56	111.91
24	T	101	CHD	C5-C4-C3	-3.07	108.25	112.76
25	T	102	CDL	OA8-CA7-OA9	-3.07	115.86	123.59
21	L	103	TGL	CC4-CC3-CC2	-3.06	102.19	113.19
18	Q	201	DMU	O16-C6-C1	3.05	113.06	108.30
21	D	202	TGL	CG3-CG2-CG1	-3.04	104.59	111.79
18	P	303	DMU	C6-O5-C4	-3.04	107.72	113.69
19	A	607	PGV	O01-C1-C2	3.04	118.06	111.50
14	N	602	HEA	C26-C15-C16	3.04	120.38	115.27
14	N	602	HEA	CAD-CBD-CGD	-3.02	107.61	112.67
24	G	101	CHD	C11-C12-C13	3.00	114.33	111.24
24	L	102	CHD	C22-C23-C24	-3.00	107.14	113.59
18	P	303	DMU	C10-C5-C7	3.00	116.24	110.00
19	A	607	PGV	O03-C19-C20	2.99	121.30	111.91
18	Y	101	DMU	O7-C10-C5	2.99	115.85	108.10
19	N	606	PGV	C4-C3-C2	-2.99	102.44	113.19
14	N	602	HEA	CMB-C2B-C1B	-2.98	123.88	128.46
26	P	308	PEK	C11-C10-C9	-2.98	97.35	112.02
19	C	310	PGV	O03-C19-O04	-2.98	116.07	123.59
14	N	601[B]	HEA	CBD-CAD-C3D	-2.98	107.00	112.49
14	N	601[A]	HEA	CBD-CAD-C3D	-2.98	107.00	112.49
26	P	307	PEK	O03-C01-C02	2.97	117.08	108.43
24	J	102	CHD	C5-C6-C7	2.97	117.74	114.46
25	C	307	CDL	C61-C60-C59	-2.97	99.36	114.42
24	G	101	CHD	C15-C14-C13	2.97	106.46	103.55
24	J	102	CHD	C6-C5-C4	-2.96	107.78	111.19
24	C	306	CHD	C13-C17-C20	-2.95	115.98	119.50
18	C	302	DMU	O4-C7-C5	-2.94	103.56	110.35
24	C	306	CHD	C1-C10-C5	2.94	112.11	107.77
24	T	101	CHD	C15-C14-C13	2.92	106.42	103.55
21	L	103	TGL	OB1-CB1-CB2	-2.92	112.33	123.73
24	J	102	CHD	C22-C20-C17	2.92	116.32	110.28
18	W	101	DMU	O16-C18-C19	2.91	119.78	109.56
19	P	310	PGV	O03-C19-O04	-2.91	116.25	123.59
24	Y	102	CHD	C4-C5-C10	2.91	115.75	112.66
18	K	103	DMU	C18-O16-C6	2.90	118.66	113.84
21	L	103	TGL	C26-C25-C24	-2.90	99.69	114.42
26	T	103	PEK	C01-O03-C21	2.90	127.84	117.12
14	A	601[B]	HEA	C16-C17-C18	2.89	121.39	111.88
14	N	601[B]	HEA	C17-C18-C19	-2.89	120.69	127.66
14	A	601[B]	HEA	O11-C11-C3B	-2.89	103.66	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	N	608	TGL	OG1-CA1-CA2	2.89	120.98	111.91
24	T	101	CHD	C6-C7-C8	-2.89	108.40	111.48
25	P	306	CDL	OB2-PB2-OB3	2.89	120.34	109.07
26	C	309	PEK	O03-C21-C22	2.88	120.95	111.91
19	N	607	PGV	O01-C1-C2	2.88	117.71	111.50
20	V	101	PSC	O01-C02-C03	2.87	118.81	108.40
14	N	602	HEA	CBD-CAD-C3D	2.87	117.78	112.49
18	Q	201	DMU	O55-C2-C3	2.87	116.99	110.35
26	C	308	PEK	O01-C1-O02	-2.86	116.79	123.70
21	A	610	TGL	CG3-OG3-CC1	2.86	127.71	117.12
24	P	304	CHD	C1-C2-C3	-2.85	106.81	110.47
25	P	306	CDL	OA6-CA5-C11	2.84	117.62	111.50
14	N	602	HEA	C1B-C2B-C3B	-2.83	105.03	107.00
20	V	101	PSC	C07-N-C06	2.83	116.24	108.97
18	C	302	DMU	C6-O5-C4	2.82	119.22	113.69
21	D	202	TGL	CB3-CB2-CB1	2.82	123.87	113.62
18	Q	201	DMU	C6-O5-C4	2.82	119.21	113.69
18	W	101	DMU	O16-C6-C1	2.81	112.69	108.30
14	A	602	HEA	C21-C20-C19	2.81	122.22	112.98
24	J	102	CHD	C11-C9-C10	-2.81	110.83	113.73
24	P	305	CHD	C22-C23-C24	-2.81	107.56	113.59
19	P	310	PGV	C01-O03-C19	2.80	127.50	117.12
21	Q	202	TGL	OG2-CB1-CB2	2.80	117.53	111.50
24	L	102	CHD	C21-C20-C22	-2.78	106.00	110.36
20	V	101	PSC	C08-N-C07	-2.77	101.84	108.97
21	Y	103	TGL	OB1-CB1-CB2	-2.76	112.96	123.73
21	L	103	TGL	OG1-CA1-CA2	2.76	120.56	111.91
21	L	103	TGL	CC3-CC2-CC1	2.75	123.63	113.62
20	V	101	PSC	C01-O03-C19	2.75	127.31	117.12
18	J	101	DMU	C6-O5-C4	2.75	116.17	113.13
18	Z	101	DMU	O16-C6-C1	2.75	112.59	108.30
21	L	103	TGL	CB9-CB8-CB7	-2.73	100.56	114.42
24	C	306	CHD	C4-C5-C10	2.73	115.56	112.66
21	L	103	TGL	OG3-CG3-CG2	2.73	116.37	108.43
14	N	601[B]	HEA	CAD-CBD-CGD	-2.71	108.12	112.67
14	N	601[A]	HEA	CAD-CBD-CGD	-2.71	108.12	112.67
21	N	608	TGL	OG3-CC1-OC1	-2.70	116.78	123.59
26	P	308	PEK	C2-C3-C4	-2.70	108.42	113.23
25	T	102	CDL	OA6-CA4-CA3	2.69	118.15	108.40
24	Y	102	CHD	C15-C14-C8	2.68	122.08	118.33
19	P	309	PGV	O01-C1-O02	-2.68	117.23	123.70
25	C	307	CDL	C53-C52-C51	-2.67	103.58	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	PGV	C3-C2-C1	2.67	123.34	113.62
14	A	602	HEA	C4B-C3B-C2B	-2.67	105.00	106.87
24	L	102	CHD	C1-C10-C5	2.67	111.71	107.77
21	Q	202	TGL	OG3-CC1-OC1	-2.66	116.87	123.59
26	C	309	PEK	O11-P-O14	-2.66	98.69	109.07
18	C	302	DMU	O49-C1-C2	-2.65	104.22	110.35
20	V	101	PSC	C02-O01-C1	2.65	124.31	117.79
25	T	102	CDL	CA6-OA8-CA7	2.65	126.92	117.12
20	V	101	PSC	C3-C2-C1	-2.64	104.01	113.62
19	A	607	PGV	C04-C05-C06	-2.64	102.28	111.67
18	W	101	DMU	C6-O5-C4	2.64	116.05	113.13
14	N	602	HEA	C20-C19-C18	-2.63	115.78	121.12
14	A	602	HEA	C25-C23-C24	2.63	120.41	114.60
18	J	101	DMU	O5-C4-C57	2.61	111.02	106.83
26	C	309	PEK	C11-C10-C9	-2.61	99.17	112.02
24	Y	102	CHD	O7-C7-C8	2.61	115.25	109.43
21	L	103	TGL	C25-C24-C23	-2.60	101.21	114.42
14	N	602	HEA	CMD-C2D-C3D	2.60	129.85	124.94
25	P	306	CDL	C82-C81-C80	2.60	127.63	114.42
21	Q	202	TGL	OG3-CC1-CC2	2.60	120.06	111.91
25	C	307	CDL	CA6-CA4-CA3	-2.60	105.64	111.79
24	P	304	CHD	C22-C23-C24	-2.58	108.04	113.59
19	A	607	PGV	O02-C1-C2	-2.58	113.65	123.73
14	N	602	HEA	O11-C11-C3B	-2.58	104.57	112.00
26	P	307	PEK	C3-C4-C5	-2.58	97.66	112.43
19	T	104	PGV	C21-C20-C19	-2.57	104.28	113.62
25	T	102	CDL	OA8-CA6-CA4	-2.57	100.96	108.43
24	G	101	CHD	C19-C10-C5	-2.56	106.02	110.36
24	J	102	CHD	C18-C13-C17	2.56	115.21	111.21
21	Y	103	TGL	OG1-CA1-CA2	2.55	119.91	111.91
19	P	309	PGV	C27-C26-C25	-2.55	101.49	114.42
14	A	601[A]	HEA	O11-C11-C3B	-2.54	104.67	112.00
21	A	610	TGL	OB1-CB1-CB2	-2.53	113.87	123.73
14	N	602	HEA	C13-C14-C15	-2.53	121.58	127.66
18	C	302	DMU	O55-C2-C1	-2.53	104.51	110.35
25	G	102	CDL	OA8-CA7-C31	2.52	119.82	111.91
18	D	201	DMU	O5-C6-O16	2.52	115.94	109.97
14	N	601[B]	HEA	OMA-CMA-C3A	-2.51	119.44	124.91
14	N	601[A]	HEA	OMA-CMA-C3A	-2.51	119.44	124.91
18	Z	101	DMU	O2-C8-C7	-2.51	104.54	110.35
19	C	310	PGV	C22-C21-C20	-2.51	104.17	113.19
25	G	102	CDL	OA8-CA6-CA4	2.50	115.72	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	K	103	DMU	C6-O5-C4	2.50	118.60	113.69
18	D	201	DMU	C3-C4-C57	-2.50	108.21	112.60
18	C	302	DMU	O1-C9-C8	2.49	114.22	109.69
14	N	601[B]	HEA	C16-C17-C18	2.49	120.05	111.88
24	P	304	CHD	C19-C10-C1	-2.49	104.26	108.26
18	J	101	DMU	O16-C18-C19	2.48	118.26	109.56
14	N	601[B]	HEA	C13-C14-C15	-2.48	121.69	127.66
19	C	310	PGV	C26-C25-C24	-2.47	101.87	114.42
24	L	102	CHD	C9-C10-C5	2.47	112.05	108.58
14	N	602	HEA	OMA-CMA-C3A	-2.46	119.56	124.91
18	J	101	DMU	O16-C6-C1	2.45	112.14	108.30
14	N	601[A]	HEA	C16-C17-C18	-2.45	103.82	111.88
21	Y	103	TGL	CG3-CG2-CG1	-2.45	105.99	111.79
19	P	309	PGV	O03-C01-C02	-2.45	101.30	108.43
19	N	606	PGV	O14-P-O13	2.45	124.34	112.24
25	P	306	CDL	C59-C58-C57	2.45	126.84	114.42
24	Y	102	CHD	C5-C6-C7	2.44	117.16	114.46
18	X	102	DMU	O5-C4-C3	2.44	113.93	110.04
26	T	103	PEK	C2-C3-C4	2.44	117.58	113.23
25	P	306	CDL	C83-C82-C81	2.44	126.80	114.42
21	A	610	TGL	OG2-CG2-CG3	2.43	117.19	108.40
19	N	607	PGV	C9-C10-C11	-2.43	98.53	112.43
18	Q	201	DMU	O49-C1-C6	2.43	115.94	110.05
25	T	102	CDL	C19-C18-C17	2.42	126.70	114.42
25	P	306	CDL	OA8-CA6-CA4	2.42	115.47	108.43
25	G	102	CDL	OA6-CA4-CA3	2.42	117.15	108.40
20	V	101	PSC	C04-C05-N	2.41	123.83	115.78
19	C	310	PGV	O03-C19-C20	2.40	119.44	111.91
24	J	102	CHD	C9-C8-C7	-2.40	109.01	111.88
25	P	306	CDL	CB2-C1-CA2	-2.39	105.75	112.79
24	T	101	CHD	C5-C6-C7	2.39	117.10	114.46
14	N	601[B]	HEA	CMD-C2D-C3D	2.39	129.45	124.94
14	N	601[A]	HEA	CMD-C2D-C3D	2.39	129.45	124.94
26	C	309	PEK	O01-C1-O02	-2.39	117.93	123.70
24	C	306	CHD	C1-C10-C9	-2.39	107.60	111.35
21	N	608	TGL	OG2-CG2-CG3	2.37	116.99	108.40
14	N	601[B]	HEA	CMC-C2C-C3C	2.37	129.12	124.68
14	N	601[A]	HEA	CMC-C2C-C3C	2.37	129.12	124.68
14	N	601[B]	HEA	C26-C15-C14	-2.37	117.60	123.68
24	T	101	CHD	C16-C17-C13	2.36	105.86	103.55
25	T	102	CDL	C61-C60-C59	-2.35	102.47	114.42
14	A	602	HEA	C13-C14-C15	-2.35	122.01	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	607	PGV	C22-C21-C20	-2.35	104.75	113.19
24	L	102	CHD	C6-C7-C8	2.34	113.98	111.48
24	P	304	CHD	C6-C5-C4	-2.33	108.51	111.19
25	T	102	CDL	OB8-CB7-C71	2.33	119.21	111.91
26	T	103	PEK	O01-C1-O02	-2.32	118.10	123.70
18	L	101	DMU	O1-C9-C11	2.32	112.20	106.44
26	C	308	PEK	O03-C21-O04	-2.32	117.74	123.59
18	C	302	DMU	C10-C5-C7	2.31	114.81	110.00
25	T	102	CDL	C60-C59-C58	2.31	126.16	114.42
19	P	309	PGV	C03-C02-C01	-2.31	106.33	111.79
19	N	607	PGV	O12-P-O13	2.31	118.09	109.07
14	A	601[B]	HEA	CBA-CAA-C2A	-2.31	108.23	112.48
14	A	601[A]	HEA	CBA-CAA-C2A	-2.31	108.23	112.48
14	N	601[B]	HEA	C26-C15-C16	2.29	119.13	115.27
14	A	602	HEA	CBA-CAA-C2A	-2.29	108.25	112.48
24	J	102	CHD	C1-C10-C5	2.29	111.16	107.77
25	C	307	CDL	PB2-OB2-CB2	2.29	135.09	121.68
21	Y	103	TGL	C26-C25-C24	-2.28	102.83	114.42
25	P	306	CDL	OA8-CA7-OA9	-2.28	117.83	123.59
18	P	303	DMU	C6-C1-C2	2.28	114.74	110.00
24	P	304	CHD	C11-C12-C13	-2.28	108.91	111.24
25	C	307	CDL	OA6-CA5-C11	2.27	116.40	111.50
18	K	103	DMU	O7-C3-C4	2.27	114.93	109.30
26	C	308	PEK	C03-C02-C01	2.27	117.15	111.79
24	L	102	CHD	C6-C5-C10	2.26	115.06	112.66
25	G	102	CDL	C19-C18-C17	2.26	125.89	114.42
24	G	101	CHD	C11-C9-C10	-2.26	111.40	113.73
20	V	101	PSC	C08-N-C05	-2.26	100.69	109.92
24	J	102	CHD	C6-C5-C10	2.25	115.05	112.66
18	L	101	DMU	O5-C4-C3	2.25	114.50	109.75
19	T	104	PGV	C22-C21-C20	2.25	121.28	113.19
24	G	101	CHD	O3-C3-C4	-2.24	105.39	109.85
25	C	307	CDL	C62-C61-C60	2.24	125.80	114.42
18	P	303	DMU	O5-C6-O16	-2.24	104.67	109.97
25	G	102	CDL	CA6-CA4-CA3	-2.24	106.50	111.79
24	J	102	CHD	C17-C13-C14	-2.24	97.84	100.09
21	Q	202	TGL	CG2-OG2-CB1	-2.24	112.29	117.79
18	M	101	DMU	O1-C9-C8	2.23	113.75	109.69
21	Q	202	TGL	OG1-CA1-CA2	2.22	118.86	111.91
14	N	601[B]	HEA	CMB-C2B-C1B	-2.21	125.06	128.46
14	N	601[A]	HEA	CMB-C2B-C1B	-2.21	125.06	128.46
14	N	602	HEA	C3C-C4C-NC	2.21	112.06	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	102	CHD	C19-C10-C9	-2.21	108.14	111.18
25	P	306	CDL	OA4-PA1-OA3	2.20	123.13	112.24
26	C	309	PEK	C03-C02-C01	-2.20	106.58	111.79
21	D	202	TGL	OG1-CA1-OA1	-2.20	118.05	123.59
18	M	101	DMU	C22-C19-C18	-2.19	103.79	113.49
18	M	101	DMU	C31-C28-C25	-2.19	103.31	114.42
24	P	305	CHD	C6-C5-C4	-2.19	108.67	111.19
24	J	102	CHD	C9-C10-C5	2.19	111.65	108.58
24	C	306	CHD	O7-C7-C8	2.18	114.31	109.43
18	L	101	DMU	O55-C2-C1	-2.18	105.30	110.35
18	Q	201	DMU	C6-C1-C2	-2.18	105.46	110.00
25	C	307	CDL	OA8-CA7-OA9	-2.18	118.09	123.59
18	Z	101	DMU	O7-C10-C5	2.18	113.74	108.10
19	N	606	PGV	O03-C19-O04	-2.17	118.11	123.59
25	T	102	CDL	C62-C61-C60	2.17	125.44	114.42
24	C	305	CHD	C6-C5-C10	-2.16	110.36	112.66
18	W	101	DMU	O5-C6-C1	-2.16	105.78	110.35
18	Y	101	DMU	O6-C11-C9	2.16	118.69	111.29
26	F	102	PEK	O11-P-O14	-2.16	100.64	109.07
20	A	609	PSC	C29-C28-C27	-2.16	103.48	114.42
21	A	610	TGL	CB3-CB2-CB1	-2.15	105.80	113.62
14	N	602	HEA	C3A-C4A-NA	-2.14	106.90	110.94
20	A	609	PSC	C27-C26-C25	-2.14	103.57	114.42
24	C	305	CHD	C5-C6-C7	2.13	116.81	114.46
26	P	308	PEK	O01-C1-C2	2.12	116.08	111.50
25	P	306	CDL	O1-C1-CA2	-2.12	102.11	109.56
19	T	104	PGV	C02-O01-C1	2.12	123.01	117.79
25	T	102	CDL	OB6-CB5-OB7	-2.11	118.59	123.70
19	P	310	PGV	O01-C1-O02	-2.11	118.60	123.70
18	P	303	DMU	C37-C34-C31	-2.11	103.72	114.42
19	C	310	PGV	O01-C1-C2	2.11	116.05	111.50
14	N	602	HEA	C12-C13-C14	-2.11	106.67	112.23
21	Y	103	TGL	CG1-OG1-CA1	2.11	124.92	117.12
24	Y	102	CHD	C14-C13-C12	2.10	109.36	107.40
18	D	201	DMU	O49-C1-C6	2.10	115.15	110.05
26	P	307	PEK	C8-C7-C6	-2.09	101.72	112.02
18	C	303	DMU	C3-C2-C1	2.09	114.48	110.82
19	N	607	PGV	O11-P-O13	-2.09	100.89	109.07
14	N	601[B]	HEA	C3C-C4C-NC	2.09	111.91	109.21
14	N	601[A]	HEA	C3C-C4C-NC	2.09	111.91	109.21
24	G	101	CHD	C6-C5-C4	-2.08	108.79	111.19
25	G	102	CDL	C39-C38-C37	2.08	125.00	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	306	CHD	C16-C15-C14	-2.08	101.01	105.13
25	P	306	CDL	O1-C1-CB2	2.08	116.84	109.56
26	C	309	PEK	C3-C2-C1	-2.07	106.08	113.62
20	V	101	PSC	O03-C01-C02	-2.07	102.40	108.43
25	C	307	CDL	OA6-CA4-CA3	2.06	115.87	108.40
18	L	101	DMU	O7-C3-C4	-2.06	103.80	109.45
18	M	101	DMU	O7-C10-C5	2.06	113.43	108.10
24	J	102	CHD	C6-C7-C8	2.05	113.67	111.48
18	W	101	DMU	O5-C4-C57	2.05	110.12	106.83
14	A	602	HEA	O11-C11-C3B	-2.05	106.09	112.00
24	P	305	CHD	C22-C20-C17	-2.05	106.06	110.28
24	G	101	CHD	C4-C5-C10	-2.04	110.49	112.66
21	L	103	TGL	C21-C20-CA9	-2.04	104.08	114.42
25	C	307	CDL	OA4-PA1-OA3	2.04	122.30	112.24
18	P	303	DMU	O4-C7-C5	-2.04	105.64	110.35
18	C	303	DMU	O55-C2-C3	-2.04	105.64	110.35
18	C	302	DMU	O5-C4-C57	2.03	111.49	106.44
18	L	101	DMU	O55-C2-C3	2.03	115.33	109.94
25	T	102	CDL	OB8-CB6-CB4	2.02	114.32	108.43
14	A	601[B]	HEA	C26-C15-C16	2.02	118.67	115.27
24	C	306	CHD	C9-C10-C5	2.01	111.40	108.58
24	Y	102	CHD	C21-C20-C22	-2.01	107.22	110.36
25	P	306	CDL	C39-C38-C37	2.01	124.61	114.42
20	A	609	PSC	O01-C1-O02	-2.00	118.86	123.70
14	N	602	HEA	CBA-CAA-C2A	-2.00	108.79	112.48
21	D	202	TGL	OG1-CA1-CA2	2.00	118.18	111.91

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NA
14	A	602	HEA	NB

All (769) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	C	308	PEK	C03-O11-P-O12
26	C	308	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
26	C	308	PEK	C03-O11-P-O14
26	C	308	PEK	O04-C21-O03-C01
26	C	308	PEK	C22-C21-O03-C01
26	C	308	PEK	C6-C7-C8-C9
26	C	308	PEK	C9-C10-C11-C12
19	T	104	PGV	C03-O11-P-O13
19	T	104	PGV	C03-O11-P-O14
19	T	104	PGV	O04-C19-O03-C01
19	T	104	PGV	C20-C19-O03-C01
25	C	307	CDL	OA9-CA7-OA8-CA6
25	C	307	CDL	C31-CA7-OA8-CA6
25	C	307	CDL	CB2-OB2-PB2-OB4
25	C	307	CDL	CB3-OB5-PB2-OB3
25	C	307	CDL	C51-CB5-OB6-CB4
19	A	607	PGV	C2-C1-O01-C02
19	A	607	PGV	O04-C19-O03-C01
19	A	607	PGV	C20-C19-O03-C01
24	C	306	CHD	C20-C22-C23-C24
20	V	101	PSC	C2-C1-O01-C02
20	A	609	PSC	O12-C04-C05-N
20	A	609	PSC	O02-C1-O01-C02
20	A	609	PSC	C2-C1-O01-C02
25	T	102	CDL	CA3-OA5-PA1-OA4
19	P	310	PGV	O04-C19-O03-C01
19	P	310	PGV	C20-C19-O03-C01
22	N	619	EDO	O1-C1-C2-O2
25	P	306	CDL	CA2-OA2-PA1-OA3
25	P	306	CDL	CA2-OA2-PA1-OA5
25	P	306	CDL	CA3-OA5-PA1-OA2
25	P	306	CDL	OA9-CA7-OA8-CA6
25	P	306	CDL	C31-CA7-OA8-CA6
25	P	306	CDL	CB2-OB2-PB2-OB4
25	P	306	CDL	CB3-OB5-PB2-OB4
18	X	102	DMU	C3-C4-C57-O61
18	X	102	DMU	O5-C4-C57-O61
18	C	302	DMU	C1-C6-O16-C18
18	C	302	DMU	O5-C6-O16-C18
26	F	102	PEK	C04-O12-P-O13
21	L	103	TGL	OB1-CB1-OG2-CG2
26	P	307	PEK	O04-C21-O03-C01
26	P	307	PEK	C22-C21-O03-C01
26	P	307	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	N	606	PGV	O02-C1-O01-C02
19	N	606	PGV	C2-C1-O01-C02
19	N	606	PGV	O04-C19-O03-C01
19	N	606	PGV	C20-C19-O03-C01
21	Y	103	TGL	CB2-CB1-OG2-CG2
14	N	601[A]	HEA	C18-C19-C20-C21
14	N	601[A]	HEA	C27-C19-C20-C21
19	P	309	PGV	C10-C11-C12-C13
18	W	101	DMU	O5-C6-O16-C18
25	G	102	CDL	OA9-CA7-OA8-CA6
25	G	102	CDL	C31-CA7-OA8-CA6
25	G	102	CDL	CB2-OB2-PB2-OB3
26	T	103	PEK	O04-C21-O03-C01
26	T	103	PEK	C22-C21-O03-C01
26	T	103	PEK	C5-C6-C7-C8
14	A	602	HEA	O11-C11-C12-C13
25	T	102	CDL	OA9-CA7-OA8-CA6
26	F	102	PEK	O04-C21-O03-C01
18	L	101	DMU	O1-C10-O7-C3
26	F	102	PEK	C22-C21-O03-C01
20	A	609	PSC	O04-C19-O03-C01
21	Y	103	TGL	OA1-CA1-OG1-CG1
24	L	102	CHD	C13-C17-C20-C21
25	C	307	CDL	OA7-CA5-OA6-CA4
25	C	307	CDL	OB7-CB5-OB6-CB4
19	A	607	PGV	O02-C1-O01-C02
20	V	101	PSC	O02-C1-O01-C02
21	Y	103	TGL	OB1-CB1-OG2-CG2
26	T	103	PEK	O02-C1-O01-C02
25	T	102	CDL	C31-CA7-OA8-CA6
21	L	103	TGL	CA2-CA1-OG1-CG1
21	L	103	TGL	CB2-CB1-OG2-CG2
26	T	103	PEK	C2-C1-O01-C02
20	A	609	PSC	C20-C19-O03-C01
21	Y	103	TGL	CA2-CA1-OG1-CG1
26	C	308	PEK	C4-C5-C6-C7
26	C	308	PEK	C7-C8-C9-C10
20	V	101	PSC	C11-C10-C9-C8
19	P	310	PGV	C10-C11-C12-C13
26	P	307	PEK	C4-C5-C6-C7
26	T	103	PEK	C13-C14-C15-C16
21	L	103	TGL	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
18	C	302	DMU	O6-C11-C9-O1
19	A	607	PGV	O12-C04-C05-O05
18	K	103	DMU	C3-C4-C57-O61
25	C	307	CDL	C11-CA5-OA6-CA4
21	L	103	TGL	CC1-CC2-CC3-CC4
18	K	103	DMU	O5-C4-C57-O61
25	P	306	CDL	C80-C81-C82-C83
24	L	102	CHD	C16-C17-C20-C22
18	C	302	DMU	O5-C4-C57-O61
18	Y	101	DMU	O5-C4-C57-O61
18	C	303	DMU	O5-C4-C57-O61
25	T	102	CDL	C15-C16-C17-C18
24	P	305	CHD	C21-C20-C22-C23
24	P	305	CHD	C17-C20-C22-C23
24	C	306	CHD	C17-C20-C22-C23
19	N	606	PGV	C19-C20-C21-C22
21	N	608	TGL	CC2-CC1-OG3-CG3
18	C	302	DMU	C3-C4-C57-O61
18	Y	101	DMU	C3-C4-C57-O61
18	C	303	DMU	C3-C4-C57-O61
24	C	306	CHD	C21-C20-C22-C23
21	A	610	TGL	C22-C23-C24-C25
21	N	608	TGL	CA1-CA2-CA3-CA4
25	G	102	CDL	CA5-C11-C12-C13
21	N	608	TGL	OC1-CC1-OG3-CG3
21	N	608	TGL	CC1-CC2-CC3-CC4
26	F	102	PEK	C10-C11-C12-C13
18	L	101	DMU	C4-C3-O7-C10
25	G	102	CDL	C80-C81-C82-C83
21	D	202	TGL	OB1-CB1-OG2-CG2
21	A	610	TGL	CA9-C20-C21-C22
22	W	102	EDO	O1-C1-C2-O2
18	C	302	DMU	O16-C18-C19-C22
24	J	102	CHD	C13-C17-C20-C21
24	J	102	CHD	C13-C17-C20-C22
14	A	601[A]	HEA	C15-C16-C17-C18
14	N	601[A]	HEA	C15-C16-C17-C18
18	M	101	DMU	O16-C18-C19-C22
25	T	102	CDL	C80-C81-C82-C83
21	N	608	TGL	CC6-CC7-CC8-CC9
21	L	103	TGL	C21-C22-C23-C24
24	J	102	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
18	L	101	DMU	C2-C3-O7-C10
18	K	102	DMU	O16-C18-C19-C22
19	A	607	PGV	C10-C11-C12-C13
19	A	608	PGV	C10-C11-C12-C13
25	P	306	CDL	C11-CA5-OA6-CA4
25	P	306	CDL	C51-CB5-OB6-CB4
21	D	202	TGL	CB2-CB1-OG2-CG2
19	T	104	PGV	C03-O11-P-O12
25	C	307	CDL	CA3-OA5-PA1-OA2
25	C	307	CDL	CB2-OB2-PB2-OB5
25	C	307	CDL	CB3-OB5-PB2-OB2
25	T	102	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CB2-OB2-PB2-OB5
25	T	102	CDL	CB3-OB5-PB2-OB2
25	P	306	CDL	CB2-OB2-PB2-OB5
25	P	306	CDL	CB3-OB5-PB2-OB2
26	F	102	PEK	C04-O12-P-O11
25	G	102	CDL	CA3-OA5-PA1-OA2
21	L	103	TGL	CB1-CB2-CB3-CB4
25	C	307	CDL	C63-C64-C65-C66
18	X	102	DMU	O16-C18-C19-C22
18	J	101	DMU	O16-C18-C19-C22
25	P	306	CDL	OA7-CA5-OA6-CA4
20	V	101	PSC	C04-C05-N-C06
20	V	101	PSC	C04-C05-N-C08
21	Q	202	TGL	CC2-CC1-OG3-CG3
24	P	305	CHD	C20-C22-C23-C24
21	Y	103	TGL	CA9-C20-C21-C22
21	Q	202	TGL	CC1-CC2-CC3-CC4
21	A	610	TGL	C16-C17-C18-C19
26	P	307	PEK	C2-C1-O01-C02
20	V	101	PSC	C21-C22-C23-C24
26	C	309	PEK	C31-C32-C33-C34
25	T	102	CDL	C57-C58-C59-C60
25	T	102	CDL	C77-C78-C79-C80
21	N	608	TGL	C21-C20-CA9-CA8
21	D	202	TGL	C21-C20-CA9-CA8
18	X	105	DMU	C31-C34-C37-C40
25	C	307	CDL	C40-C41-C42-C43
18	X	103	DMU	C19-C22-C25-C28
25	G	102	CDL	C54-C55-C56-C57
25	P	306	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
26	P	307	PEK	O02-C1-O01-C02
21	A	610	TGL	OB1-CB1-OG2-CG2
19	N	607	PGV	C26-C27-C28-C29
26	P	308	PEK	C4-C5-C6-C7
18	Z	101	DMU	C22-C25-C28-C31
21	N	608	TGL	CB1-CB2-CB3-CB4
21	Q	202	TGL	CB1-CB2-CB3-CB4
18	P	303	DMU	C1-C6-O16-C18
18	W	101	DMU	C1-C6-O16-C18
21	A	610	TGL	CC2-CC1-OG3-CG3
21	Y	103	TGL	CA4-CA5-CA6-CA7
18	X	105	DMU	C25-C28-C31-C34
25	C	307	CDL	C17-C18-C19-C20
21	N	608	TGL	CB4-CB5-CB6-CB7
19	N	606	PGV	C20-C21-C22-C23
19	P	309	PGV	C7-C8-C9-C10
25	G	102	CDL	C57-C58-C59-C60
18	Q	201	DMU	C28-C31-C34-C37
21	Q	202	TGL	C15-C16-C17-C18
21	N	608	TGL	CA7-CA8-CA9-C20
21	L	103	TGL	CB5-CB6-CB7-CB8
21	D	202	TGL	C16-C17-C18-C19
21	A	610	TGL	CB2-CB1-OG2-CG2
25	C	307	CDL	C80-C81-C82-C83
21	L	103	TGL	C10-C11-C12-C13
26	C	308	PEK	C30-C31-C32-C33
25	P	306	CDL	C60-C61-C62-C63
18	L	101	DMU	C31-C34-C37-C40
26	F	102	PEK	C29-C30-C31-C32
21	D	202	TGL	C20-C21-C22-C23
19	N	606	PGV	C3-C4-C5-C6
21	Y	103	TGL	CA6-CA7-CA8-CA9
21	Y	103	TGL	CB5-CB6-CB7-CB8
21	Y	103	TGL	CC3-CC4-CC5-CC6
21	Y	103	TGL	C21-C22-C23-C24
19	C	310	PGV	C7-C8-C9-C10
25	G	102	CDL	C40-C41-C42-C43
18	P	303	DMU	O5-C6-O16-C18
21	N	608	TGL	CC5-CC6-CC7-CC8
19	C	310	PGV	C27-C28-C29-C30
26	C	309	PEK	O12-C04-C05-N
21	Y	103	TGL	CA2-CA3-CA4-CA5

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Mol	Chain	Res	Type	Atoms
25	C	307	CDL	C51-C52-C53-C54
21	N	608	TGL	CA6-CA7-CA8-CA9
21	D	202	TGL	C19-C33-C34-C35
21	A	610	TGL	CC4-CC5-CC6-CC7
20	A	609	PSC	C24-C25-C26-C27
21	N	608	TGL	CA4-CA5-CA6-CA7
18	Q	201	DMU	C22-C25-C28-C31
21	Q	202	TGL	C11-C10-CB9-CB8
18	P	303	DMU	C19-C18-O16-C6
18	M	101	DMU	C25-C28-C31-C34
21	L	103	TGL	CA3-CA4-CA5-CA6
18	C	303	DMU	C22-C25-C28-C31
21	Q	202	TGL	C19-C33-C34-C35
25	G	102	CDL	C55-C56-C57-C58
19	P	310	PGV	C1-C2-C3-C4
26	F	102	PEK	C26-C27-C28-C29
21	L	103	TGL	C18-C19-C33-C34
19	T	104	PGV	C3-C4-C5-C6
25	C	307	CDL	C59-C60-C61-C62
21	D	202	TGL	CB5-CB6-CB7-CB8
18	K	102	DMU	C25-C28-C31-C34
18	X	103	DMU	C25-C28-C31-C34
25	G	102	CDL	C77-C78-C79-C80
18	C	302	DMU	O6-C11-C9-C8
18	C	302	DMU	O1-C10-O7-C3
25	P	306	CDL	C36-C37-C38-C39
21	Q	202	TGL	CA6-CA7-CA8-CA9
25	C	307	CDL	O1-C1-CA2-OA2
19	P	310	PGV	C20-C21-C22-C23
21	N	608	TGL	CB6-CB7-CB8-CB9
21	D	202	TGL	CC7-CC8-CC9-C15
21	Y	103	TGL	C22-C23-C24-C25
21	A	610	TGL	CC9-C15-C16-C17
21	A	610	TGL	C10-C11-C12-C13
21	Q	202	TGL	C13-C14-C29-C30
21	D	202	TGL	C11-C10-CB9-CB8
21	Y	103	TGL	CB9-C10-C11-C12
21	Q	202	TGL	OC1-CC1-OG3-CG3
26	C	309	PEK	C32-C33-C34-C35
21	N	608	TGL	C20-C21-C22-C23
19	P	309	PGV	C30-C31-C32-C33
18	C	303	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
20	V	101	PSC	C04-C05-N-C07
22	C	311	EDO	O1-C1-C2-O2
22	T	105	EDO	O1-C1-C2-O2
22	A	615	EDO	O1-C1-C2-O2
22	Q	205	EDO	O1-C1-C2-O2
22	A	611	EDO	O1-C1-C2-O2
22	P	312	EDO	O1-C1-C2-O2
22	P	315	EDO	O1-C1-C2-O2
18	D	201	DMU	O16-C18-C19-C22
21	L	103	TGL	CA2-CA3-CA4-CA5
21	A	610	TGL	C16-C15-CC9-CC8
25	C	307	CDL	C31-C32-C33-C34
25	G	102	CDL	C56-C57-C58-C59
18	K	104	DMU	C18-C19-C22-C25
24	L	102	CHD	C16-C17-C20-C21
25	C	307	CDL	C20-C21-C22-C23
18	J	101	DMU	C31-C34-C37-C40
21	A	610	TGL	CA5-CA6-CA7-CA8
24	L	102	CHD	C13-C17-C20-C22
21	N	608	TGL	OB1-CB1-OG2-CG2
21	Q	202	TGL	OB1-CB1-OG2-CG2
21	L	103	TGL	C11-C12-C13-C14
21	D	202	TGL	CC9-C15-C16-C17
19	T	104	PGV	C24-C25-C26-C27
25	T	102	CDL	C20-C21-C22-C23
21	N	608	TGL	C11-C10-CB9-CB8
21	Q	202	TGL	CC2-CC3-CC4-CC5
26	C	309	PEK	C26-C27-C28-C29
25	P	306	CDL	C58-C59-C60-C61
18	Y	101	DMU	C28-C31-C34-C37
20	V	101	PSC	C20-C19-O03-C01
18	X	102	DMU	C18-C19-C22-C25
25	T	102	CDL	C14-C15-C16-C17
18	K	103	DMU	C19-C22-C25-C28
21	D	202	TGL	C16-C15-CC9-CC8
21	A	610	TGL	C24-C25-C26-C27
25	G	102	CDL	C37-C38-C39-C40
25	G	102	CDL	C60-C61-C62-C63
25	T	102	CDL	C11-CA5-OA6-CA4
21	N	608	TGL	CB2-CB1-OG2-CG2
21	Q	202	TGL	CB2-CB1-OG2-CG2
25	G	102	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	P	310	PGV	O01-C02-C03-O11
21	A	610	TGL	CB4-CB5-CB6-CB7
20	A	609	PSC	C3-C4-C5-C6
25	G	102	CDL	OB7-CB5-OB6-CB4
18	X	102	DMU	C28-C31-C34-C37
21	N	608	TGL	C16-C15-CC9-CC8
21	Y	103	TGL	C19-C33-C34-C35
18	L	101	DMU	O5-C4-C57-O61
19	P	310	PGV	C28-C29-C30-C31
21	Q	202	TGL	C22-C23-C24-C25
25	T	102	CDL	OA7-CA5-OA6-CA4
18	X	104	DMU	C22-C25-C28-C31
18	M	101	DMU	C19-C22-C25-C28
21	N	608	TGL	CA2-CA1-OG1-CG1
25	C	307	CDL	OA5-CA3-CA4-CA6
25	G	102	CDL	OB5-CB3-CB4-CB6
26	T	103	PEK	C01-C02-C03-O11
26	C	308	PEK	C21-C22-C23-C24
26	P	308	PEK	C26-C27-C28-C29
21	N	608	TGL	CC9-C15-C16-C17
18	Y	101	DMU	C25-C28-C31-C34
26	F	102	PEK	C27-C28-C29-C30
25	T	102	CDL	CB3-CB4-CB6-OB8
18	X	102	DMU	C34-C37-C40-C43
26	P	308	PEK	C10-C11-C12-C13
20	V	101	PSC	O04-C19-O03-C01
21	A	610	TGL	OC1-CC1-OG3-CG3
25	G	102	CDL	C24-C25-C26-C27
20	A	609	PSC	C2-C3-C4-C5
25	T	102	CDL	C79-C80-C81-C82
18	L	101	DMU	C25-C28-C31-C34
18	X	101	DMU	C18-C19-C22-C25
19	A	607	PGV	C2-C3-C4-C5
25	P	306	CDL	C77-C78-C79-C80
18	K	102	DMU	C18-C19-C22-C25
20	V	101	PSC	C03-C02-O01-C1
25	C	307	CDL	C58-C59-C60-C61
25	C	307	CDL	C83-C84-C85-C86
18	A	606	DMU	C22-C25-C28-C31
21	Y	103	TGL	C13-C14-C29-C30
18	Q	201	DMU	O5-C4-C57-O61
18	Z	101	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
21	Q	202	TGL	C21-C20-CA9-CA8
21	Q	202	TGL	CC9-C15-C16-C17
19	N	607	PGV	C29-C30-C31-C32
25	C	307	CDL	OA5-CA3-CA4-OA6
25	T	102	CDL	OA5-CA3-CA4-OA6
26	C	309	PEK	C13-C14-C15-C16
26	P	308	PEK	C7-C8-C9-C10
26	P	308	PEK	C13-C14-C15-C16
26	T	103	PEK	C4-C5-C6-C7
20	V	101	PSC	C23-C24-C25-C26
18	K	104	DMU	C22-C25-C28-C31
18	K	101	DMU	C18-C19-C22-C25
22	F	110	EDO	O1-C1-C2-O2
22	C	316	EDO	O1-C1-C2-O2
21	L	103	TGL	C11-C10-CB9-CB8
18	P	303	DMU	O6-C11-C9-C8
21	Y	103	TGL	CB1-CB2-CB3-CB4
18	K	103	DMU	C1-C6-O16-C18
20	V	101	PSC	O03-C01-C02-O01
25	T	102	CDL	OB6-CB4-CB6-OB8
21	Y	103	TGL	OG2-CG2-CG3-OG3
21	Y	103	TGL	CB4-CB5-CB6-CB7
25	C	307	CDL	C37-C38-C39-C40
21	N	608	TGL	OA1-CA1-OG1-CG1
19	N	606	PGV	C4-C5-C6-C7
26	C	309	PEK	C30-C31-C32-C33
24	C	306	CHD	C16-C17-C20-C21
19	A	607	PGV	O12-C04-C05-C06
25	T	102	CDL	C39-C40-C41-C42
21	L	103	TGL	CC2-CC1-OG3-CG3
19	T	104	PGV	C31-C32-C33-C34
18	M	101	DMU	C34-C37-C40-C43
21	A	610	TGL	C12-C13-C14-C29
26	F	102	PEK	C13-C14-C15-C16
19	P	310	PGV	C01-C02-C03-O11
25	P	306	CDL	OA5-CA3-CA4-CA6
18	X	104	DMU	O16-C18-C19-C22
26	C	308	PEK	C27-C28-C29-C30
21	A	610	TGL	C15-C16-C17-C18
19	A	607	PGV	C20-C21-C22-C23
25	T	102	CDL	CA7-C31-C32-C33
25	G	102	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
21	A	610	TGL	C14-C29-C30-C31
18	M	101	DMU	C22-C25-C28-C31
21	D	202	TGL	CC5-CC6-CC7-CC8
20	V	101	PSC	C3-C4-C5-C6
25	C	307	CDL	CB3-CB4-CB6-OB8
25	P	306	CDL	CB3-CB4-CB6-OB8
26	F	102	PEK	O03-C01-C02-C03
21	L	103	TGL	OG1-CG1-CG2-CG3
19	N	606	PGV	O03-C01-C02-C03
25	G	102	CDL	CB3-CB4-CB6-OB8
18	B	302	DMU	C31-C34-C37-C40
26	C	309	PEK	C4-C5-C6-C7
19	N	607	PGV	C10-C11-C12-C13
26	F	102	PEK	C4-C5-C6-C7
19	N	606	PGV	C10-C11-C12-C13
21	Q	202	TGL	C17-C18-C19-C33
25	C	307	CDL	C55-C56-C57-C58
25	C	307	CDL	C82-C83-C84-C85
18	X	103	DMU	C22-C25-C28-C31
25	P	306	CDL	C17-C18-C19-C20
25	C	307	CDL	C78-C79-C80-C81
25	P	306	CDL	C59-C60-C61-C62
26	C	308	PEK	C5-C6-C7-C8
26	C	308	PEK	C11-C10-C9-C8
26	C	308	PEK	C11-C12-C13-C14
26	C	308	PEK	C12-C13-C14-C15
20	V	101	PSC	C10-C11-C12-C13
20	A	609	PSC	C03-O11-P-O12
20	A	609	PSC	C9-C10-C11-C12
20	A	609	PSC	C10-C11-C12-C13
26	C	309	PEK	C5-C6-C7-C8
26	C	309	PEK	C9-C10-C11-C12
26	C	309	PEK	C11-C12-C13-C14
26	P	308	PEK	C11-C12-C13-C14
26	P	308	PEK	C12-C13-C14-C15
26	F	102	PEK	C5-C6-C7-C8
26	F	102	PEK	C6-C7-C8-C9
26	F	102	PEK	C11-C10-C9-C8
26	F	102	PEK	C9-C10-C11-C12
26	F	102	PEK	C11-C12-C13-C14
26	F	102	PEK	C12-C13-C14-C15
26	P	307	PEK	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	P	307	PEK	C6-C7-C8-C9
26	P	307	PEK	C11-C10-C9-C8
26	P	307	PEK	C12-C13-C14-C15
26	T	103	PEK	C6-C7-C8-C9
26	T	103	PEK	C11-C10-C9-C8
26	T	103	PEK	C9-C10-C11-C12
26	T	103	PEK	C11-C12-C13-C14
26	T	103	PEK	C12-C13-C14-C15
21	A	610	TGL	CB1-CB2-CB3-CB4
25	G	102	CDL	OB9-CB7-OB8-CB6
21	D	202	TGL	CB4-CB5-CB6-CB7
21	Y	103	TGL	C11-C10-CB9-CB8
18	C	304	DMU	C34-C37-C40-C43
25	G	102	CDL	C33-C34-C35-C36
25	P	306	CDL	OA5-CA3-CA4-OA6
25	G	102	CDL	OB5-CB3-CB4-OB6
21	L	103	TGL	C15-C16-C17-C18
18	X	105	DMU	C22-C25-C28-C31
24	C	306	CHD	C13-C17-C20-C21
19	N	606	PGV	O03-C01-C02-O01
25	G	102	CDL	OB6-CB4-CB6-OB8
21	N	608	TGL	C13-C14-C29-C30
18	W	101	DMU	C18-C19-C22-C25
25	T	102	CDL	C56-C57-C58-C59
25	G	102	CDL	C81-C82-C83-C84
19	T	104	PGV	O02-C1-O01-C02
18	B	302	DMU	C19-C22-C25-C28
25	T	102	CDL	C82-C83-C84-C85
19	C	310	PGV	C24-C25-C26-C27
18	C	304	DMU	C31-C34-C37-C40
18	C	304	DMU	C18-C19-C22-C25
20	V	101	PSC	C24-C25-C26-C27
19	P	309	PGV	C02-C03-O11-P
21	L	103	TGL	C14-C29-C30-C31
25	T	102	CDL	C71-C72-C73-C74
22	N	623	EDO	O1-C1-C2-O2
22	P	313	EDO	O1-C1-C2-O2
18	X	102	DMU	C22-C25-C28-C31
21	L	103	TGL	C12-C13-C14-C29
25	G	102	CDL	C14-C15-C16-C17
25	T	102	CDL	OB7-CB5-OB6-CB4
19	T	104	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	T	102	CDL	C51-CB5-OB6-CB4
25	T	102	CDL	C40-C41-C42-C43
18	Z	101	DMU	O6-C11-C9-C8
24	C	306	CHD	C16-C17-C20-C22
25	T	102	CDL	C33-C34-C35-C36
25	C	307	CDL	CA7-C31-C32-C33
20	A	609	PSC	C15-C16-C17-C18
21	N	608	TGL	CB7-CB8-CB9-C10
26	P	307	PEK	C29-C30-C31-C32
21	Y	103	TGL	C20-C21-C22-C23
21	Q	202	TGL	CC5-CC6-CC7-CC8
18	Q	201	DMU	C25-C28-C31-C34
21	Y	103	TGL	C12-C13-C14-C29
24	C	306	CHD	C13-C17-C20-C22
21	L	103	TGL	C17-C18-C19-C33
21	D	202	TGL	CA1-CA2-CA3-CA4
21	Q	202	TGL	CA9-C20-C21-C22
25	T	102	CDL	C71-CB7-OB8-CB6
21	A	610	TGL	C29-C30-C31-C32
18	Z	101	DMU	C28-C31-C34-C37
26	P	308	PEK	C22-C23-C24-C25
19	C	310	PGV	C13-C14-C15-C16
19	T	104	PGV	C1-C2-C3-C4
25	T	102	CDL	CA3-CA4-CA6-OA8
21	Y	103	TGL	CG1-CG2-CG3-OG3
21	A	610	TGL	CG1-CG2-CG3-OG3
25	G	102	CDL	CA3-CA4-CA6-OA8
21	L	103	TGL	OG1-CA1-CA2-CA3
21	Q	202	TGL	CB9-C10-C11-C12
25	T	102	CDL	O1-C1-CA2-OA2
25	P	306	CDL	C72-C73-C74-C75
25	C	307	CDL	OB6-CB4-CB6-OB8
25	P	306	CDL	OB6-CB4-CB6-OB8
21	L	103	TGL	OG1-CG1-CG2-OG2
21	A	610	TGL	OG2-CG2-CG3-OG3
18	C	304	DMU	C19-C22-C25-C28
21	L	103	TGL	OC1-CC1-OG3-CG3
21	N	608	TGL	CC7-CC8-CC9-C15
25	T	102	CDL	OB9-CB7-OB8-CB6
19	N	607	PGV	C14-C15-C16-C17
21	Y	103	TGL	CB7-CB8-CB9-C10
21	Y	103	TGL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	P	309	PGV	C24-C25-C26-C27
18	D	201	DMU	C3-C4-C57-O61
19	C	310	PGV	C1-C2-C3-C4
18	C	302	DMU	C34-C37-C40-C43
26	T	103	PEK	C04-O12-P-O11
21	Y	103	TGL	C25-C26-C27-C28
19	T	104	PGV	C02-C03-O11-P
19	P	310	PGV	C02-C03-O11-P
19	C	310	PGV	C02-C03-O11-P
25	C	307	CDL	CA3-OA5-PA1-OA3
25	C	307	CDL	CB3-OB5-PB2-OB4
25	T	102	CDL	CB2-OB2-PB2-OB3
25	T	102	CDL	CB3-OB5-PB2-OB3
25	P	306	CDL	CA3-OA5-PA1-OA3
25	P	306	CDL	CB2-OB2-PB2-OB3
26	F	102	PEK	C04-O12-P-O14
25	G	102	CDL	CA3-OA5-PA1-OA3
25	T	102	CDL	OA5-CA3-CA4-CA6
22	A	619	EDO	O1-C1-C2-O2
22	N	618	EDO	O1-C1-C2-O2
22	E	202	EDO	O1-C1-C2-O2
22	P	317	EDO	O1-C1-C2-O2
19	P	310	PGV	C25-C26-C27-C28
26	C	309	PEK	C7-C8-C9-C10
18	C	303	DMU	O16-C18-C19-C22
25	G	102	CDL	CA7-C31-C32-C33
19	A	607	PGV	C14-C15-C16-C17
19	P	309	PGV	C12-C13-C14-C15
19	T	104	PGV	C29-C30-C31-C32
25	C	307	CDL	CB7-C71-C72-C73
18	M	101	DMU	O6-C11-C9-C8
26	T	103	PEK	O01-C02-C03-O11
20	V	101	PSC	C20-C21-C22-C23
18	K	101	DMU	C25-C28-C31-C34
21	N	608	TGL	CB3-CB4-CB5-CB6
21	L	103	TGL	C24-C25-C26-C27
26	T	103	PEK	C28-C29-C30-C31
26	F	102	PEK	O03-C01-C02-O01
26	F	102	PEK	C33-C34-C35-C36
21	L	103	TGL	C25-C26-C27-C28
18	K	104	DMU	C25-C28-C31-C34
25	P	306	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
25	P	306	CDL	C55-C56-C57-C58
24	L	102	CHD	C20-C22-C23-C24
18	Z	101	DMU	C34-C37-C40-C43
18	J	101	DMU	C25-C28-C31-C34
25	T	102	CDL	C32-C31-CA7-OA8
21	Q	202	TGL	OG3-CC1-CC2-CC3
25	C	307	CDL	C61-C62-C63-C64
21	L	103	TGL	C16-C15-CC9-CC8
19	A	607	PGV	C11-C10-C9-C8
21	Y	103	TGL	CB6-CB7-CB8-CB9
18	K	104	DMU	C31-C34-C37-C40
21	A	610	TGL	CB9-C10-C11-C12
21	Q	202	TGL	C12-C13-C14-C29
21	Y	103	TGL	CC2-CC3-CC4-CC5
21	A	610	TGL	CB6-CB7-CB8-CB9
18	Q	201	DMU	C31-C34-C37-C40
25	P	306	CDL	C42-C43-C44-C45
25	T	102	CDL	CA3-CA4-OA6-CA5
26	F	102	PEK	C16-C17-C18-C19
18	D	201	DMU	C18-C19-C22-C25
18	C	303	DMU	C28-C31-C34-C37
21	A	610	TGL	C17-C18-C19-C33
25	C	307	CDL	CA4-CA3-OA5-PA1
26	P	307	PEK	C10-C11-C12-C13
21	Y	103	TGL	C24-C25-C26-C27
22	N	612	EDO	O1-C1-C2-O2
22	P	314	EDO	O1-C1-C2-O2
22	S	103	EDO	O1-C1-C2-O2
18	X	104	DMU	C31-C34-C37-C40
18	K	103	DMU	O5-C6-O16-C18
19	N	606	PGV	C11-C12-C13-C14
21	A	610	TGL	OG1-CG1-CG2-OG2
25	T	102	CDL	CA2-OA2-PA1-OA5
19	P	310	PGV	C03-O11-P-O12
25	G	102	CDL	CA2-OA2-PA1-OA5
25	G	102	CDL	CB2-OB2-PB2-OB5
25	G	102	CDL	CB3-OB5-PB2-OB2
19	P	309	PGV	C1-C2-C3-C4
21	A	610	TGL	CC7-CC8-CC9-C15
21	L	103	TGL	C21-C20-CA9-CA8
18	J	101	DMU	C18-C19-C22-C25
21	A	610	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	C	309	PEK	C25-C26-C27-C28
21	D	202	TGL	CA3-CA4-CA5-CA6
18	P	303	DMU	C34-C37-C40-C43
19	P	309	PGV	C20-C21-C22-C23
21	A	610	TGL	CA4-CA5-CA6-CA7
25	C	307	CDL	C1-CA2-OA2-PA1
19	A	607	PGV	C05-C04-O12-P
20	V	101	PSC	C7-C8-C9-C10
19	A	608	PGV	C11-C12-C13-C14
19	P	309	PGV	C28-C29-C30-C31
25	P	306	CDL	CB7-C71-C72-C73
21	A	610	TGL	CA2-CA1-OG1-CG1
25	P	306	CDL	C41-C42-C43-C44
19	T	104	PGV	C19-C20-C21-C22
21	Q	202	TGL	CC6-CC7-CC8-CC9
14	N	601[A]	HEA	C19-C20-C21-C22
21	Q	202	TGL	CA4-CA5-CA6-CA7
26	P	308	PEK	O12-C04-C05-N
24	Y	102	CHD	C13-C17-C20-C21
21	N	608	TGL	CC2-CC3-CC4-CC5
25	G	102	CDL	C72-C73-C74-C75
21	Y	103	TGL	CB3-CB4-CB5-CB6
21	Y	103	TGL	C17-C18-C19-C33
25	P	306	CDL	C73-C74-C75-C76
22	D	203	EDO	O1-C1-C2-O2
25	P	306	CDL	C20-C21-C22-C23
18	X	105	DMU	C19-C22-C25-C28
26	P	307	PEK	C7-C8-C9-C10
21	N	608	TGL	CA2-CA3-CA4-CA5
19	T	104	PGV	C14-C15-C16-C17
21	Q	202	TGL	C11-C12-C13-C14
26	P	307	PEK	C03-C02-O01-C1
20	V	101	PSC	C9-C10-C11-C12
26	C	309	PEK	C12-C13-C14-C15
26	P	308	PEK	C6-C7-C8-C9
26	P	307	PEK	C9-C10-C11-C12
18	C	303	DMU	C18-C19-C22-C25
19	A	607	PGV	C4-C5-C6-C7
18	L	101	DMU	C5-C10-O7-C3
19	A	607	PGV	C19-C20-C21-C22
18	M	101	DMU	C28-C31-C34-C37
18	X	102	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
21	Q	202	TGL	CB3-CB4-CB5-CB6
25	P	306	CDL	OA6-CA4-CA6-OA8
19	P	310	PGV	C5-C6-C7-C8
21	D	202	TGL	OC1-CC1-OG3-CG3
18	X	103	DMU	O16-C18-C19-C22
18	A	606	DMU	C28-C31-C34-C37
18	K	103	DMU	O16-C18-C19-C22
21	L	103	TGL	CC3-CC4-CC5-CC6
14	A	601[A]	HEA	C19-C20-C21-C22
19	N	606	PGV	C31-C32-C33-C34
25	P	306	CDL	C51-C52-C53-C54
18	P	303	DMU	C31-C34-C37-C40
26	P	307	PEK	C27-C28-C29-C30
21	L	103	TGL	CA9-C20-C21-C22
26	T	103	PEK	C34-C35-C36-C37
19	A	608	PGV	O03-C19-C20-C21
25	P	306	CDL	C38-C39-C40-C41
22	J	103	EDO	O1-C1-C2-O2
22	Q	203	EDO	O1-C1-C2-O2
26	T	103	PEK	C33-C34-C35-C36
25	G	102	CDL	C11-C12-C13-C14
25	P	306	CDL	C34-C35-C36-C37
21	L	103	TGL	C33-C34-C35-C36
26	C	308	PEK	C3-C4-C5-C6
19	P	310	PGV	C11-C12-C13-C14
26	T	103	PEK	C14-C15-C16-C17
18	C	302	DMU	C5-C10-O7-C3
19	A	607	PGV	O01-C1-C2-C3
21	D	202	TGL	CC2-CC1-OG3-CG3
25	C	307	CDL	C72-C73-C74-C75
25	P	306	CDL	C24-C25-C26-C27
25	G	102	CDL	OA6-CA4-CA6-OA8
20	V	101	PSC	C5-C6-C7-C8
18	B	302	DMU	C22-C25-C28-C31
21	N	608	TGL	CA9-C20-C21-C22
19	A	607	PGV	C23-C24-C25-C26
26	C	309	PEK	C14-C15-C16-C17
26	F	102	PEK	C3-C4-C5-C6
26	P	307	PEK	C3-C4-C5-C6
25	G	102	CDL	C59-C60-C61-C62
26	P	307	PEK	O03-C21-C22-C23
26	C	309	PEK	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	T	103	PEK	C35-C36-C37-C38
19	T	104	PGV	C9-C10-C11-C12
20	V	101	PSC	C12-C13-C14-C15
20	A	609	PSC	C7-C8-C9-C10
19	N	607	PGV	C11-C12-C13-C14
26	P	308	PEK	C14-C15-C16-C17
19	N	606	PGV	C9-C10-C11-C12
19	C	310	PGV	C9-C10-C11-C12
25	P	306	CDL	C82-C83-C84-C85
25	T	102	CDL	C32-C31-CA7-OA9
21	A	610	TGL	OA1-CA1-OG1-CG1
25	C	307	CDL	C21-C22-C23-C24
19	P	310	PGV	C15-C16-C17-C18
21	A	610	TGL	OG1-CA1-CA2-CA3
26	P	307	PEK	C24-C25-C26-C27
18	Y	101	DMU	C19-C22-C25-C28
19	T	104	PGV	C11-C12-C13-C14
26	T	103	PEK	C3-C4-C5-C6
21	A	610	TGL	CA3-CA4-CA5-CA6
21	A	610	TGL	CC5-CC6-CC7-CC8
18	C	304	DMU	C25-C28-C31-C34
19	N	607	PGV	O03-C19-C20-C21
25	P	306	CDL	C72-C71-CB7-OB8
21	Q	202	TGL	CA2-CA3-CA4-CA5
22	Y	104	EDO	O1-C1-C2-O2
22	B	305	EDO	O1-C1-C2-O2
22	N	622	EDO	O1-C1-C2-O2
22	A	618	EDO	O1-C1-C2-O2
22	B	306	EDO	O1-C1-C2-O2
22	B	304	EDO	O1-C1-C2-O2
22	N	617	EDO	O1-C1-C2-O2
22	F	109	EDO	O1-C1-C2-O2
22	B	307	EDO	O1-C1-C2-O2
22	U	102	EDO	O1-C1-C2-O2
21	Q	202	TGL	OG1-CA1-CA2-CA3
21	D	202	TGL	CC1-CC2-CC3-CC4
21	N	608	TGL	OG3-CC1-CC2-CC3
21	N	608	TGL	OG2-CG2-CG3-OG3
18	W	101	DMU	C22-C25-C28-C31
21	Y	103	TGL	C29-C30-C31-C32
18	K	101	DMU	C34-C37-C40-C43
18	D	201	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
19	A	607	PGV	C31-C32-C33-C34
19	P	310	PGV	C24-C25-C26-C27
26	F	102	PEK	C14-C15-C16-C17
19	C	310	PGV	C11-C12-C13-C14
21	D	202	TGL	OG1-CA1-CA2-CA3
25	C	307	CDL	C22-C23-C24-C25
21	A	610	TGL	OA1-CA1-CA2-CA3
19	A	608	PGV	C26-C27-C28-C29
21	L	103	TGL	OA1-CA1-CA2-CA3
26	P	307	PEK	O04-C21-C22-C23
25	T	102	CDL	C24-C25-C26-C27
14	N	601[A]	HEA	C12-C13-C14-C15
25	G	102	CDL	C32-C31-CA7-OA8
25	P	306	CDL	C72-C71-CB7-OB9
20	A	609	PSC	C23-C24-C25-C26
21	A	610	TGL	CA1-CA2-CA3-CA4
26	C	309	PEK	C17-C18-C19-C20
21	N	608	TGL	CC3-CC4-CC5-CC6
19	T	104	PGV	C21-C22-C23-C24
21	Y	103	TGL	C16-C17-C18-C19
21	A	610	TGL	CA6-CA7-CA8-CA9
26	F	102	PEK	C30-C31-C32-C33
25	C	307	CDL	CA2-OA2-PA1-OA3
25	T	102	CDL	CA2-OA2-PA1-OA3
19	N	606	PGV	C04-O12-P-O13
25	G	102	CDL	CB3-OB5-PB2-OB3
26	T	103	PEK	C04-O12-P-O13
26	T	103	PEK	C04-O12-P-O14
26	T	103	PEK	C30-C31-C32-C33
21	N	608	TGL	OC1-CC1-CC2-CC3
21	D	202	TGL	OA1-CA1-CA2-CA3
26	P	307	PEK	O12-C04-C05-N
19	T	104	PGV	C5-C6-C7-C8
22	C	317	EDO	O1-C1-C2-O2
19	A	607	PGV	O03-C19-C20-C21
26	P	307	PEK	C01-C02-O01-C1
20	A	609	PSC	C12-C13-C14-C15
19	P	310	PGV	C26-C27-C28-C29
19	N	607	PGV	C30-C31-C32-C33
25	T	102	CDL	C31-C32-C33-C34
25	G	102	CDL	C32-C31-CA7-OA9
18	L	101	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
25	C	307	CDL	C42-C43-C44-C45
21	D	202	TGL	OG2-CB1-CB2-CB3
19	P	309	PGV	C9-C10-C11-C12
25	G	102	CDL	C17-C18-C19-C20
21	L	103	TGL	CB2-CB3-CB4-CB5
21	N	608	TGL	OG1-CA1-CA2-CA3
25	T	102	CDL	C37-C38-C39-C40
25	T	102	CDL	C43-C44-C45-C46
25	C	307	CDL	C32-C31-CA7-OA8
21	Q	202	TGL	OG2-CB1-CB2-CB3
18	K	102	DMU	C28-C31-C34-C37

There are no ring outliers.

89 monomers are involved in 316 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	C	308	PEK	5	0
22	C	311	EDO	1	0
22	T	105	EDO	1	0
19	T	104	PGV	1	0
24	P	305	CHD	2	0
22	N	618	EDO	1	0
22	B	305	EDO	2	0
25	C	307	CDL	17	0
14	A	601[B]	HEA	1	0
18	Z	101	DMU	2	0
22	F	108	EDO	1	0
19	A	607	PGV	5	0
22	N	613	EDO	1	0
24	C	306	CHD	3	0
14	N	601[B]	HEA	1	0
24	T	101	CHD	1	0
20	V	101	PSC	7	0
20	A	609	PSC	17	0
22	D	205	EDO	1	0
18	M	101	DMU	1	0
22	O	304	EDO	1	0
26	C	309	PEK	6	0
22	N	617	EDO	4	0
22	N	612	EDO	4	0
22	P	316	EDO	2	0
24	P	304	CHD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	T	102	CDL	29	0
22	A	615	EDO	3	0
22	N	622	EDO	2	0
19	P	310	PGV	9	0
19	N	607	PGV	2	0
25	P	306	CDL	11	0
22	D	206	EDO	1	0
18	X	102	DMU	1	0
24	J	102	CHD	1	0
18	A	606	DMU	2	0
18	C	302	DMU	1	0
22	A	617	EDO	3	0
22	A	618	EDO	1	0
18	L	101	DMU	2	0
22	A	614	EDO	1	0
26	P	308	PEK	2	0
21	N	608	TGL	4	0
18	K	103	DMU	5	0
22	N	623	EDO	1	0
26	F	102	PEK	6	0
21	L	103	TGL	16	0
21	D	202	TGL	15	0
18	Q	201	DMU	2	0
26	P	307	PEK	1	0
14	A	601[A]	HEA	1	0
22	L	104	EDO	1	0
22	Q	204	EDO	2	0
22	A	616	EDO	1	0
18	J	101	DMU	4	0
22	Q	205	EDO	1	0
19	N	606	PGV	7	0
21	Y	103	TGL	3	0
22	F	110	EDO	1	0
14	N	601[A]	HEA	1	0
18	O	302	DMU	2	0
22	E	203	EDO	2	0
22	A	611	EDO	1	0
22	S	105	EDO	2	0
22	F	109	EDO	1	0
18	Y	101	DMU	3	0
19	C	310	PGV	4	0
21	A	610	TGL	2	0

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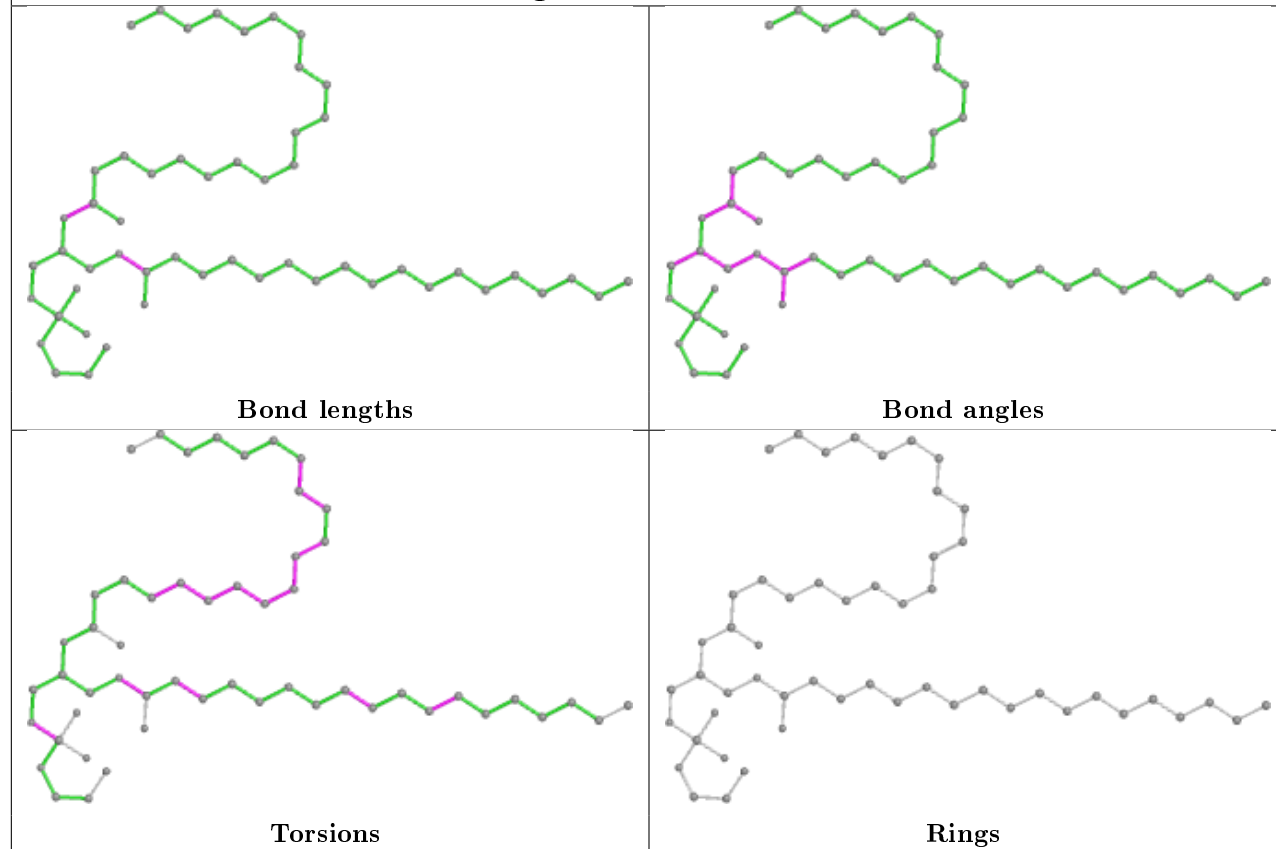
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	H	102	EDO	2	0
19	A	608	PGV	1	0
18	P	303	DMU	3	0
22	P	313	EDO	1	0
22	N	615	EDO	1	0
22	Q	203	EDO	1	0
19	P	309	PGV	3	0
18	W	101	DMU	4	0
22	D	203	EDO	1	0
22	B	307	EDO	1	0
14	N	602	HEA	6	0
18	C	303	DMU	1	0
24	Y	102	CHD	1	0
21	Q	202	TGL	12	0
22	C	313	EDO	1	0
22	C	316	EDO	1	0
24	G	101	CHD	1	0
22	U	102	EDO	4	0
25	G	102	CDL	22	0
26	T	103	PEK	9	0
14	A	602	HEA	5	0

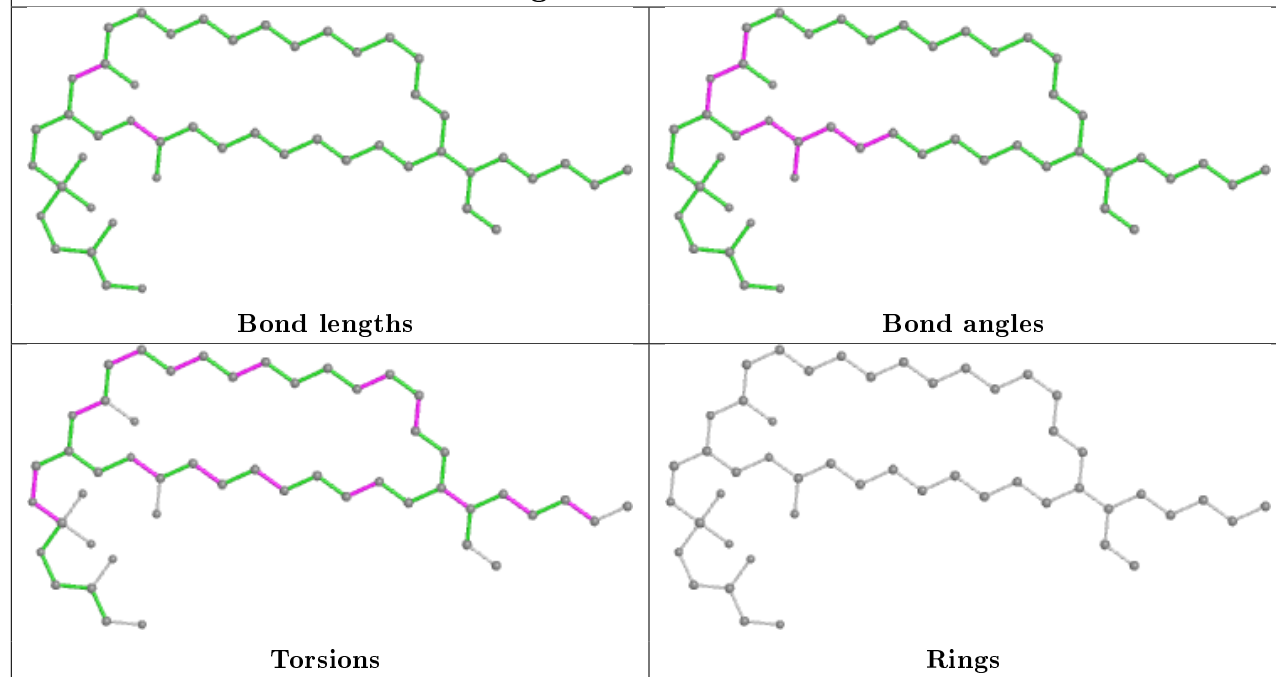
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

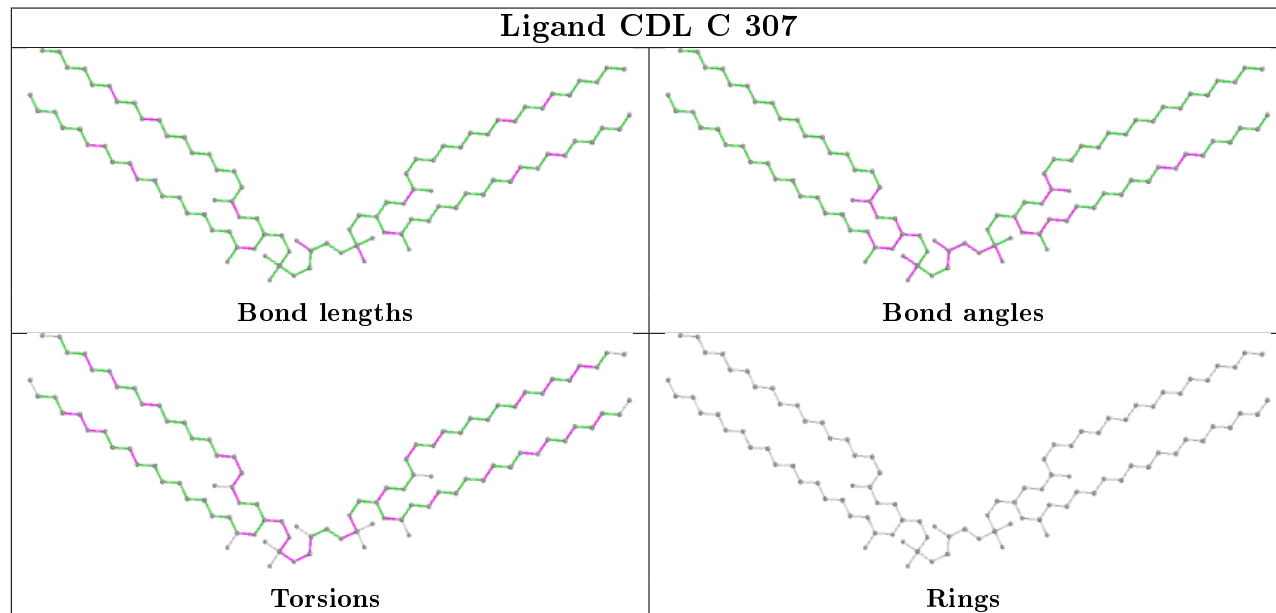
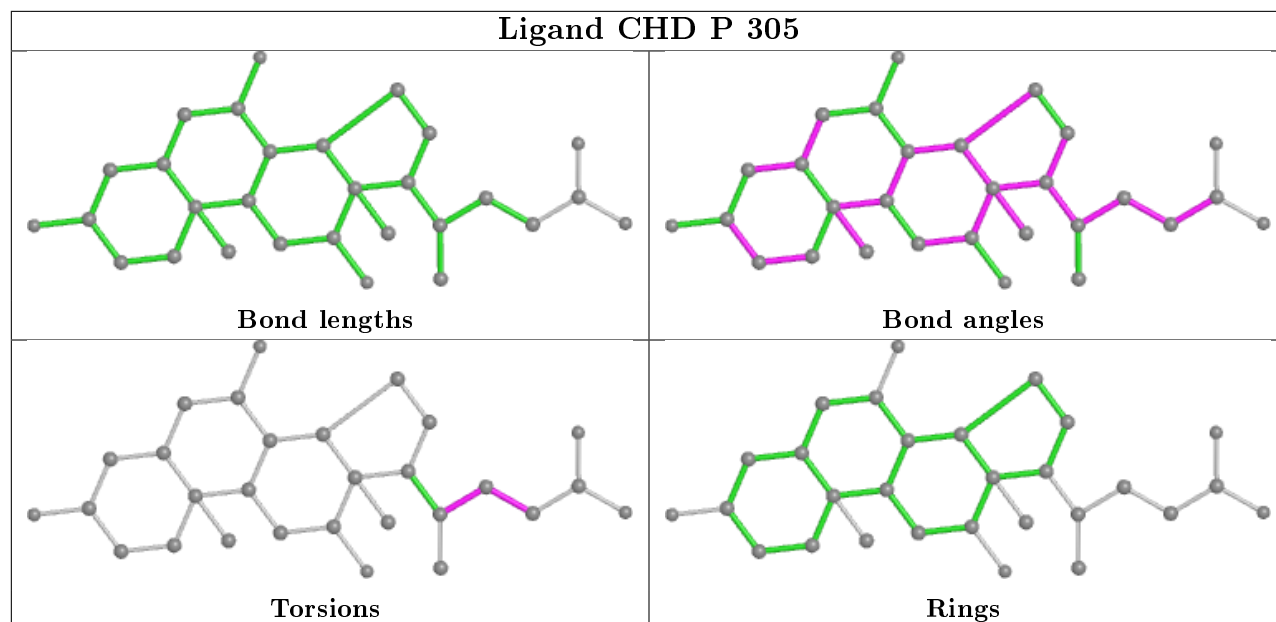


## Ligand PEK C 308

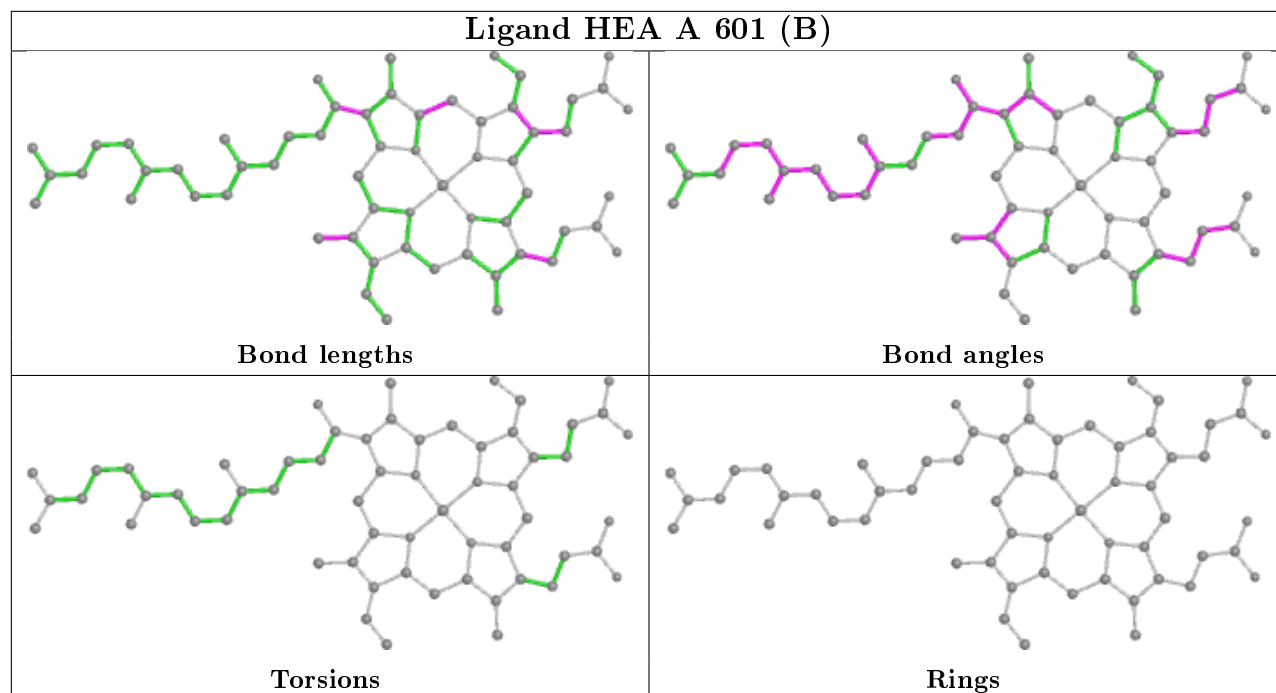


## Ligand PGV T 104

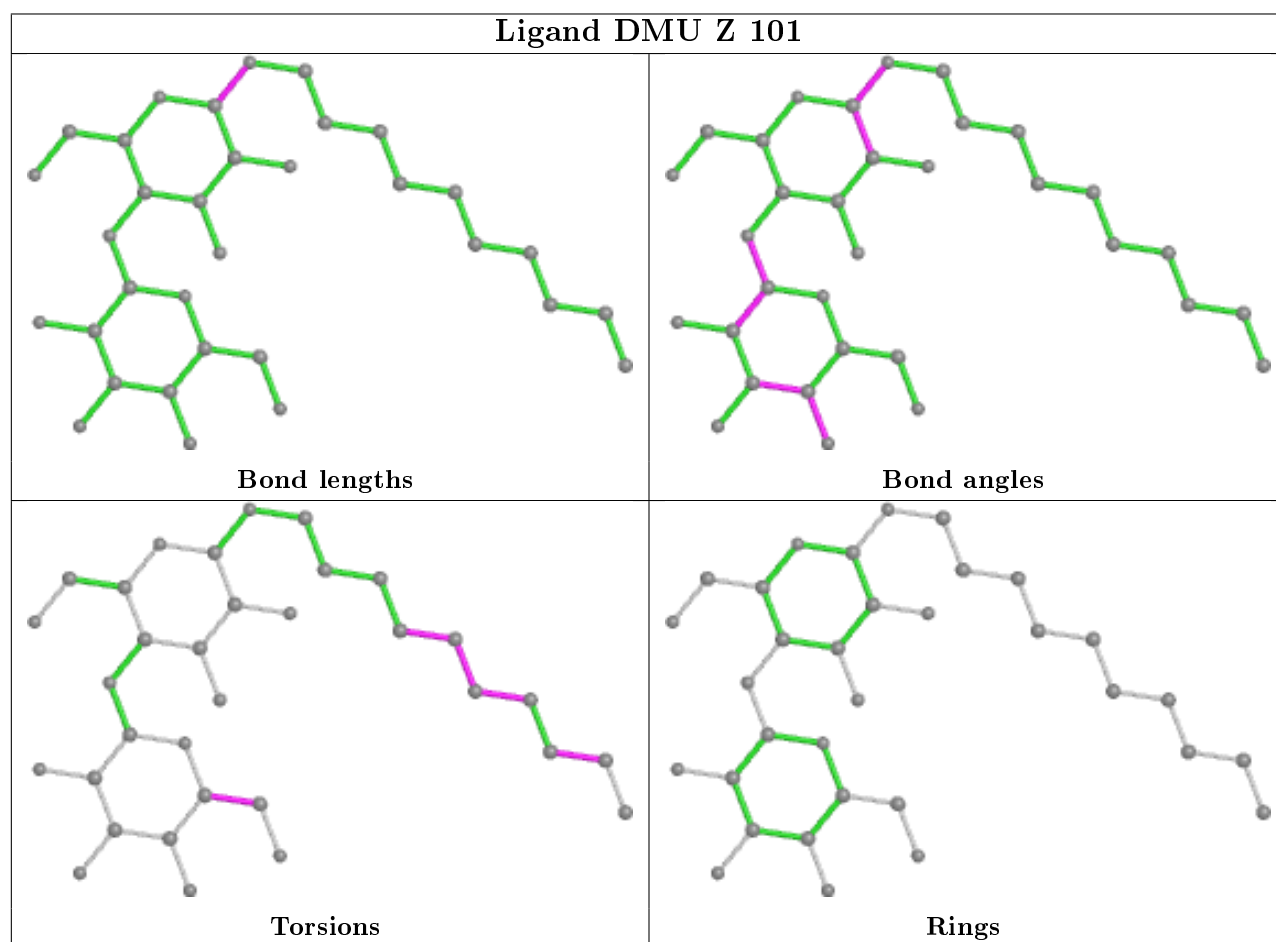


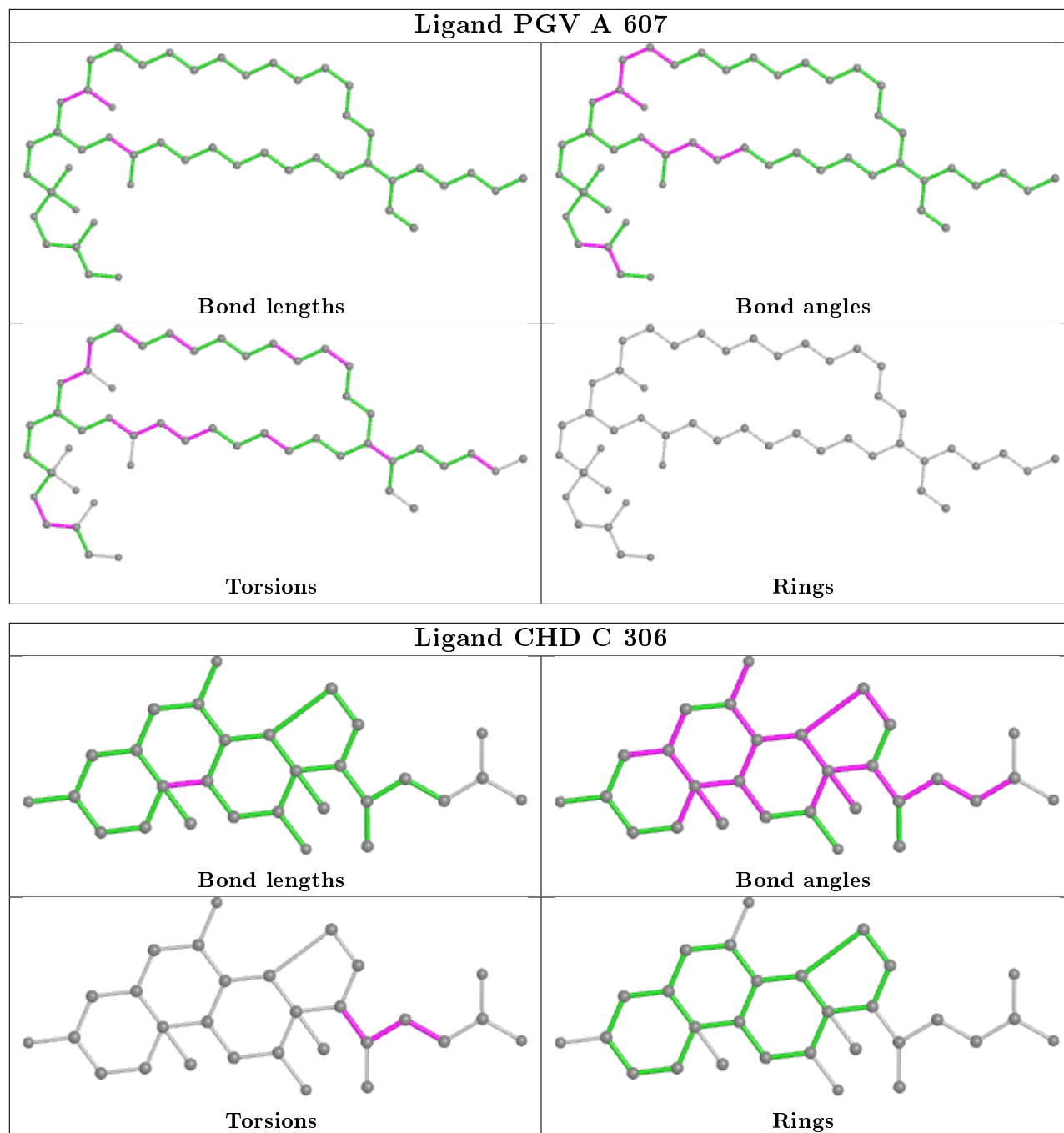


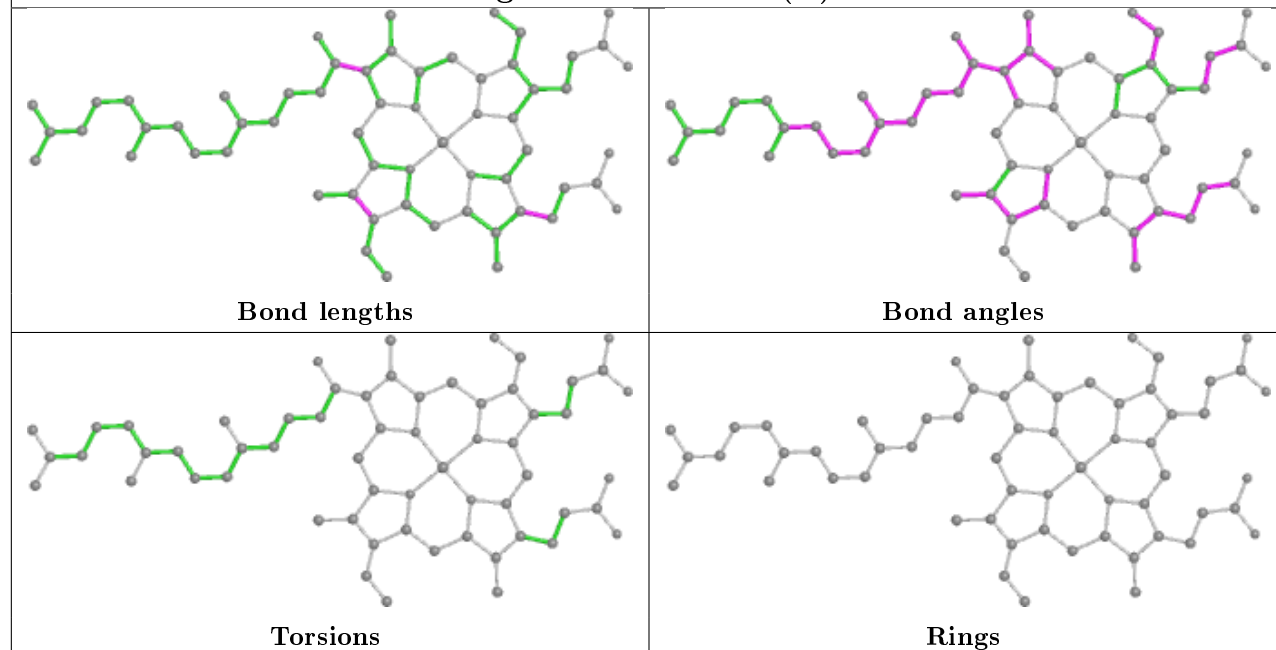
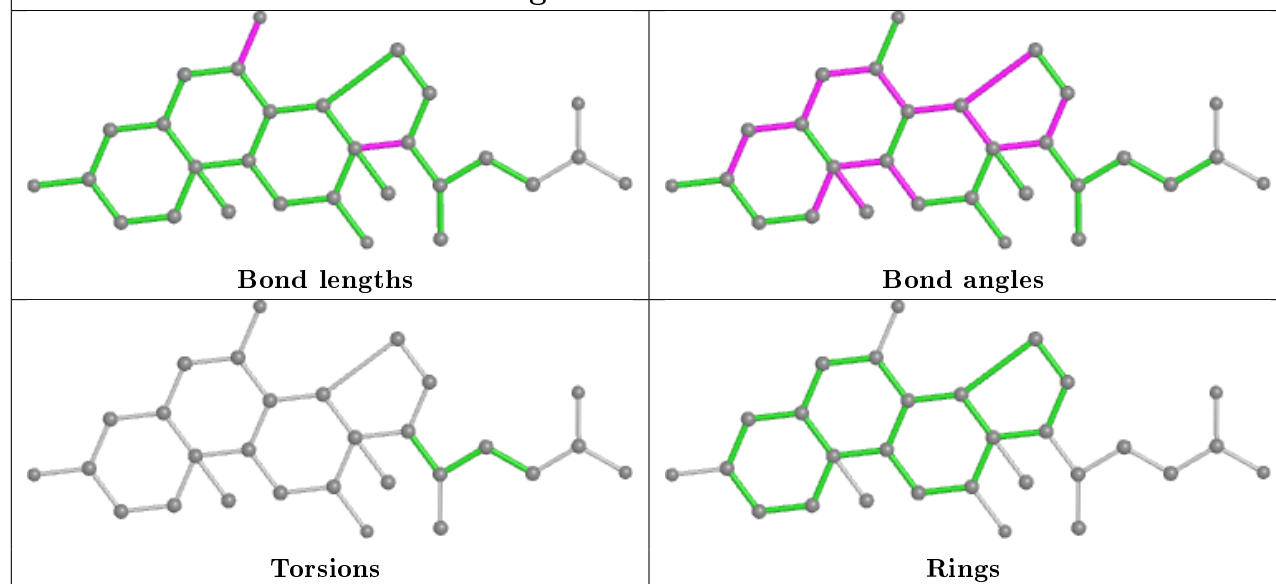
## Ligand HEA A 601 (B)

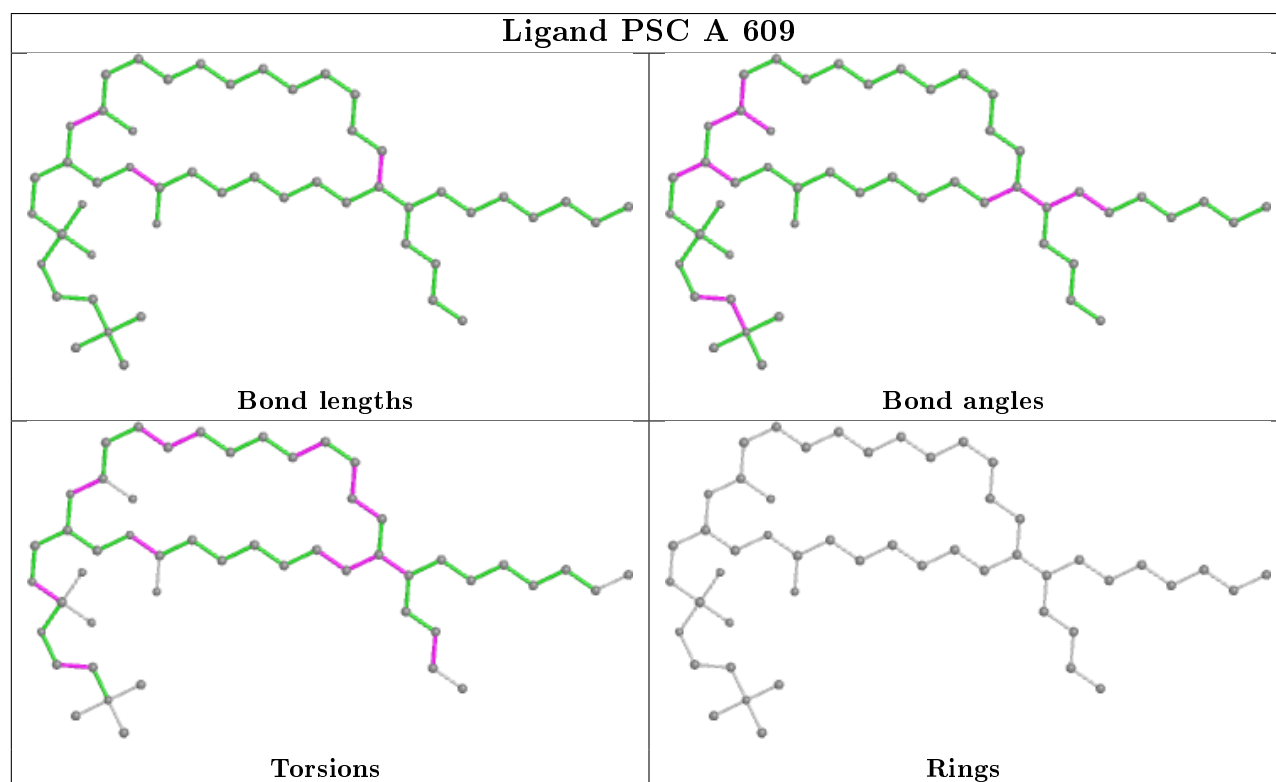
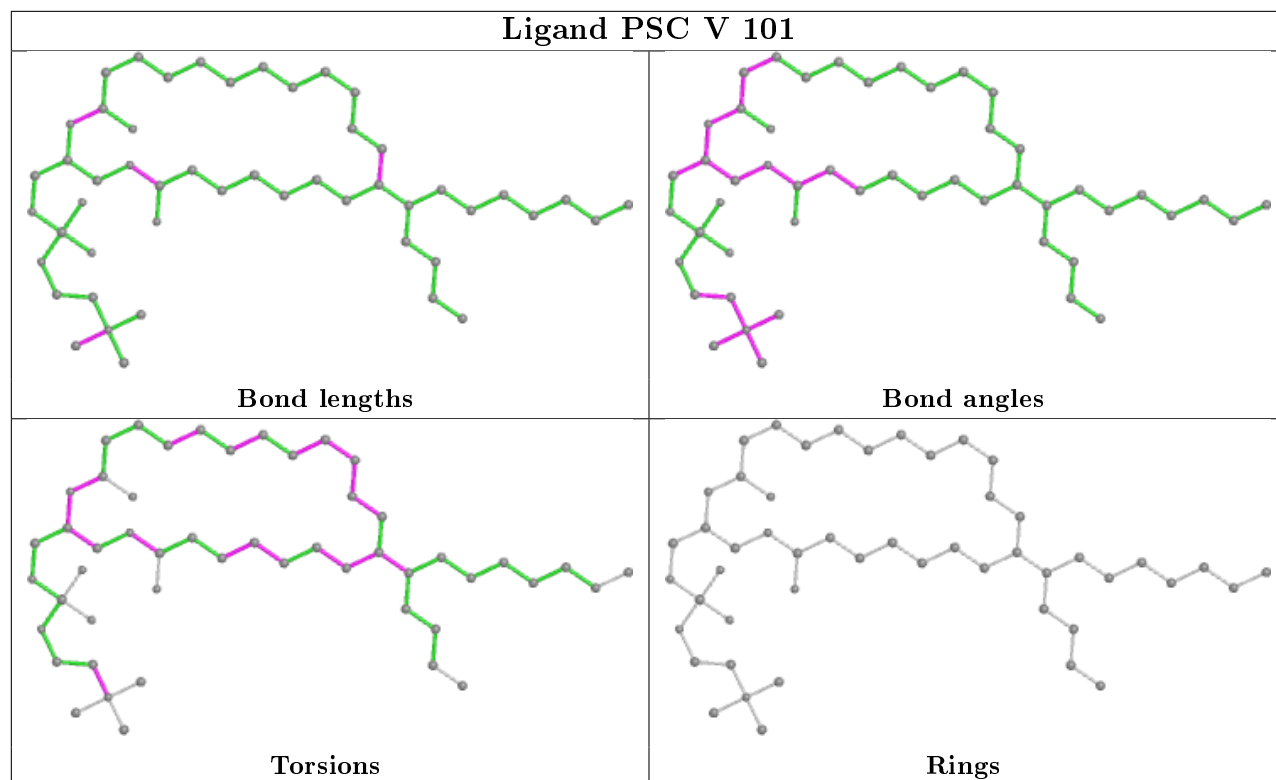


## Ligand DMU Z 101

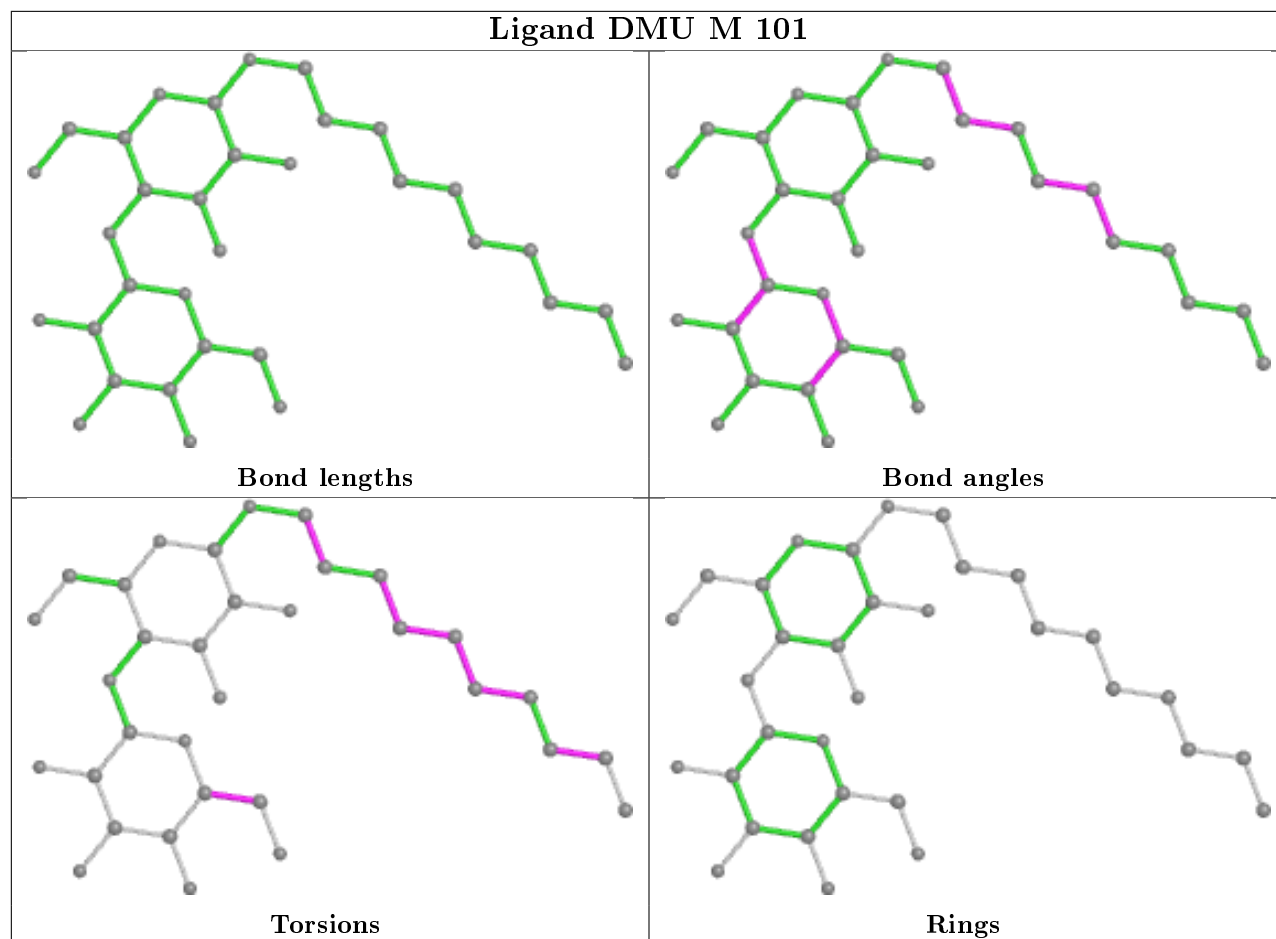




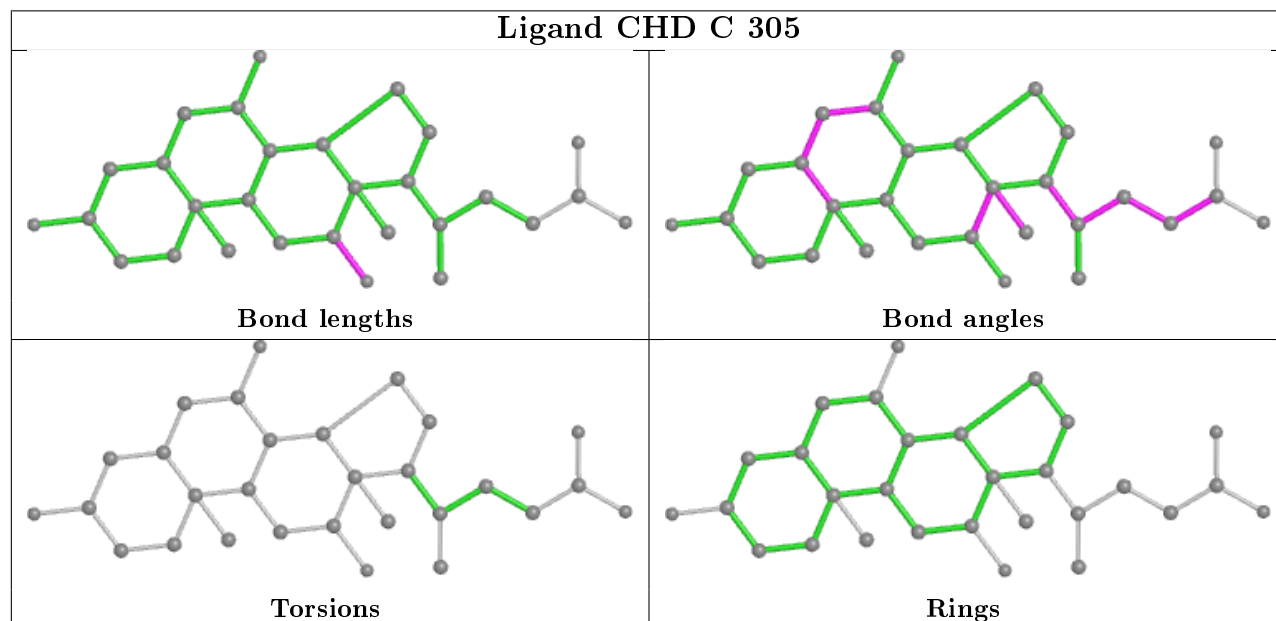
**Ligand HEA N 601 (B)****Ligand CHD T 101**



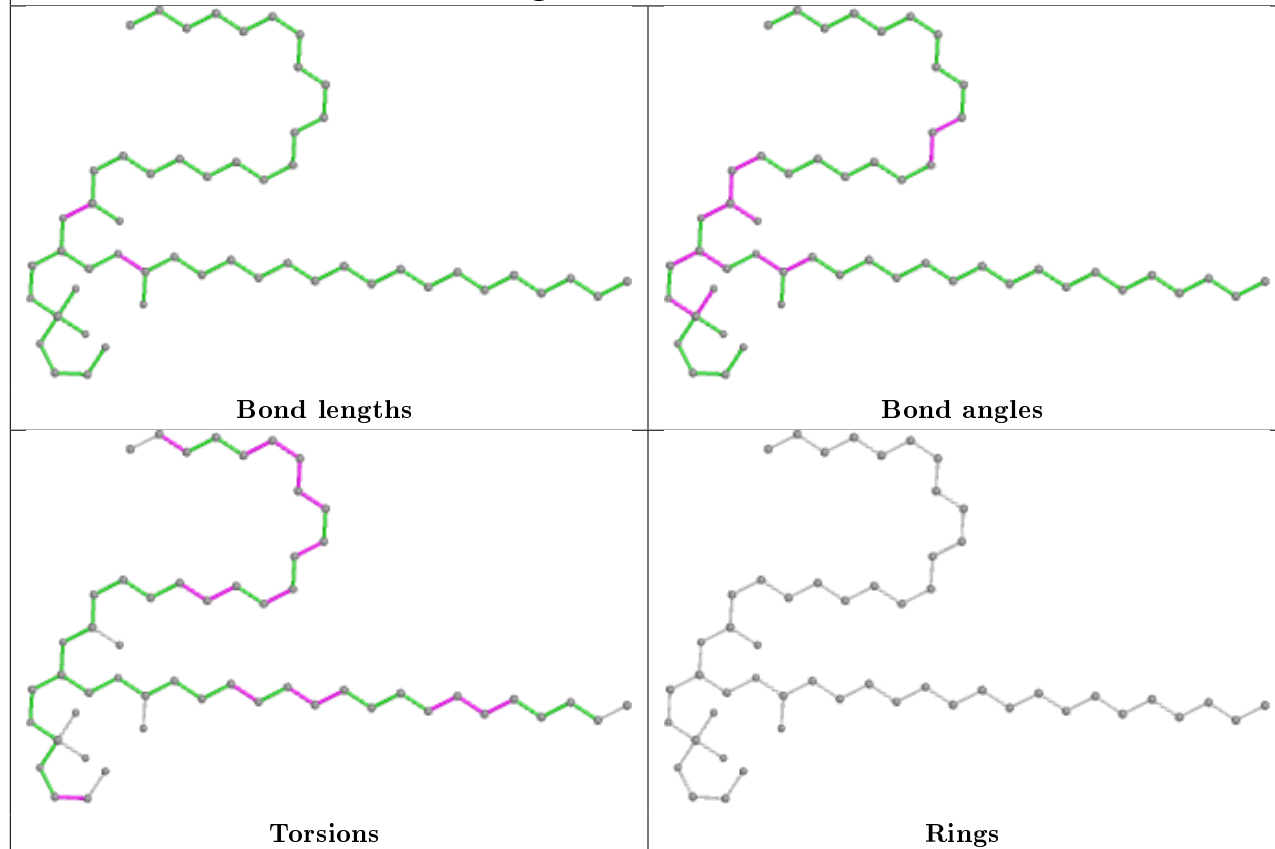
## Ligand DMU M 101



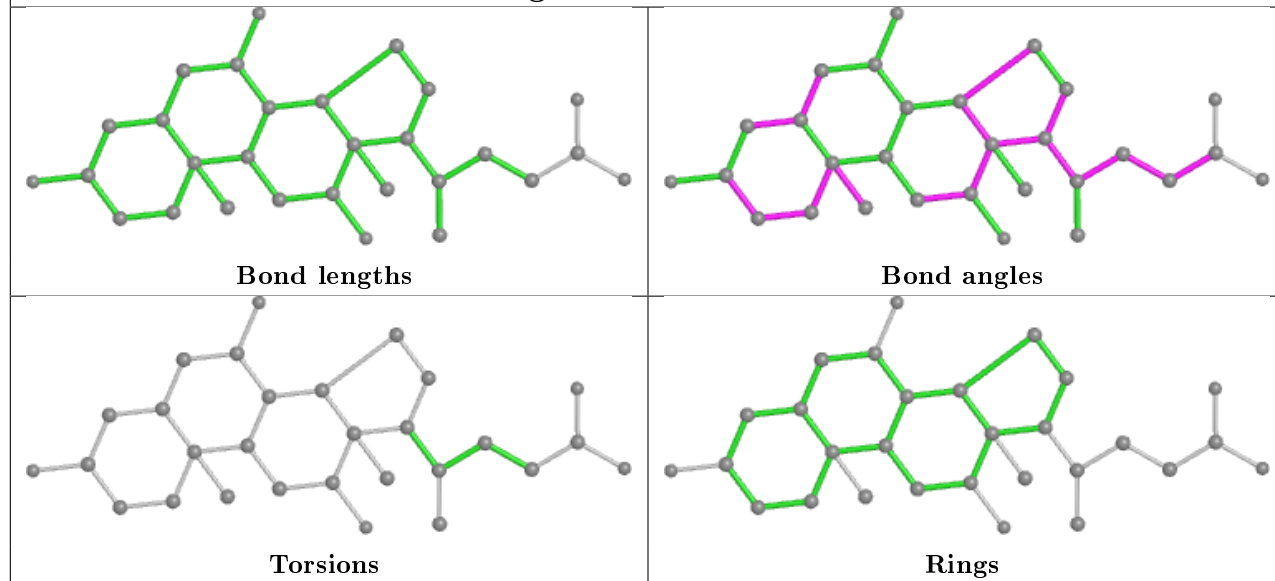
## Ligand CHD C 305



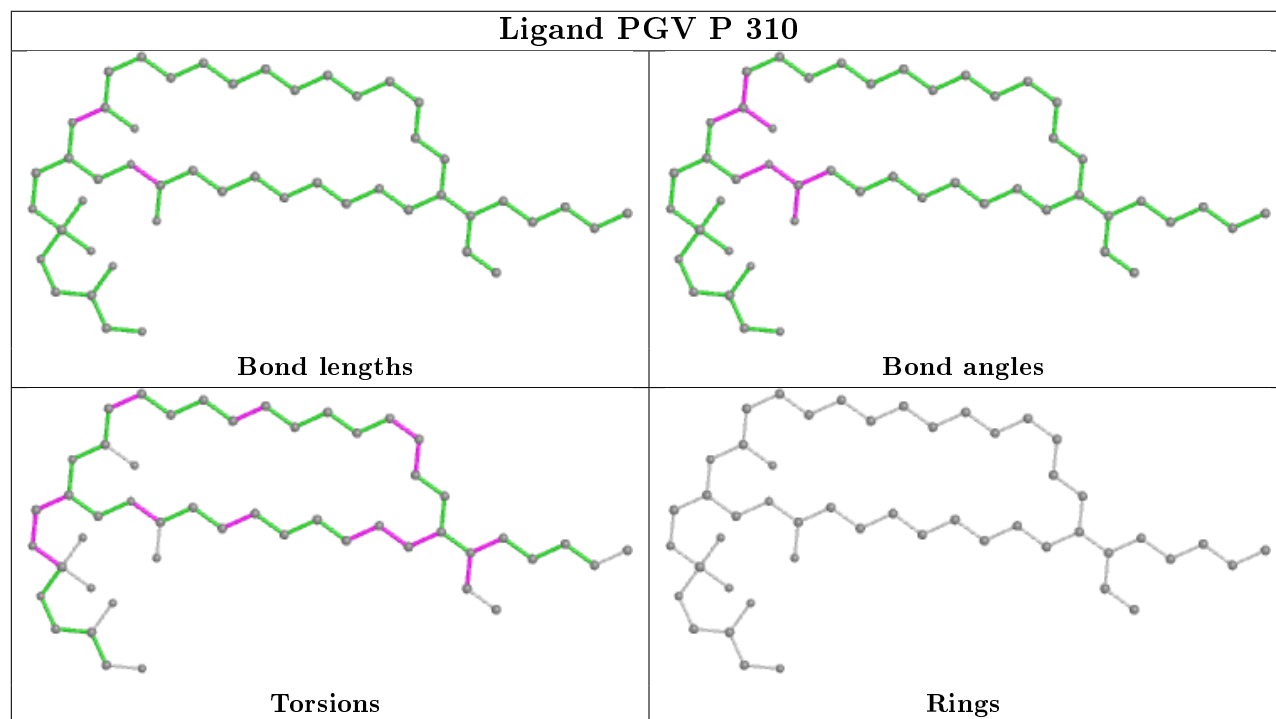
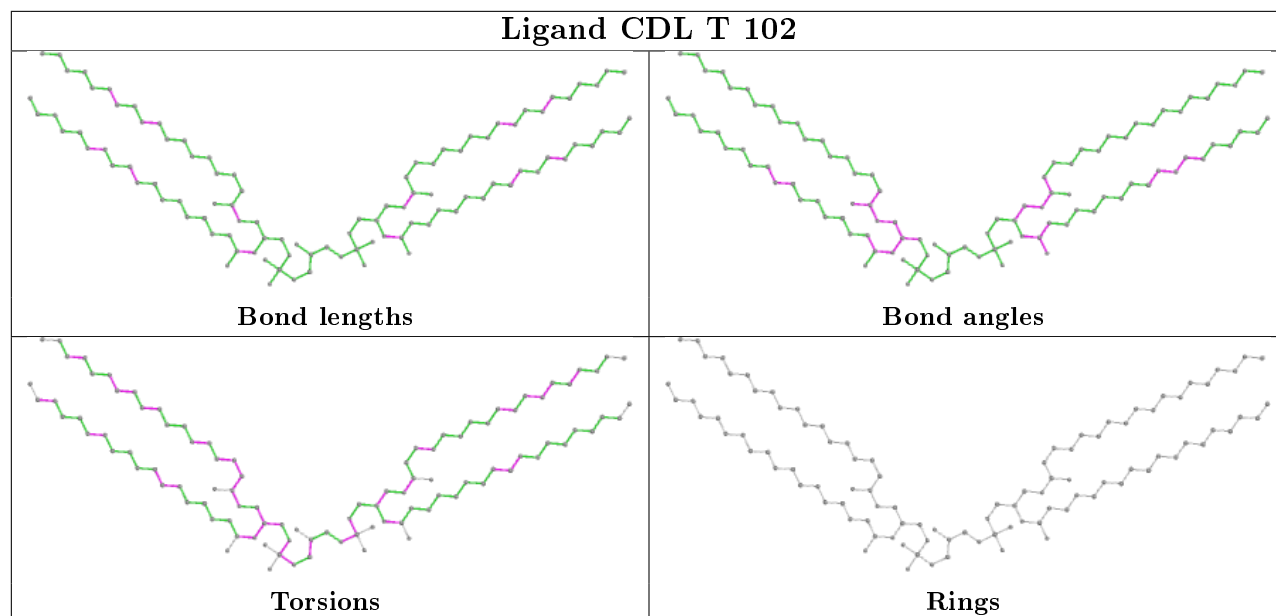
## Ligand PEK C 309

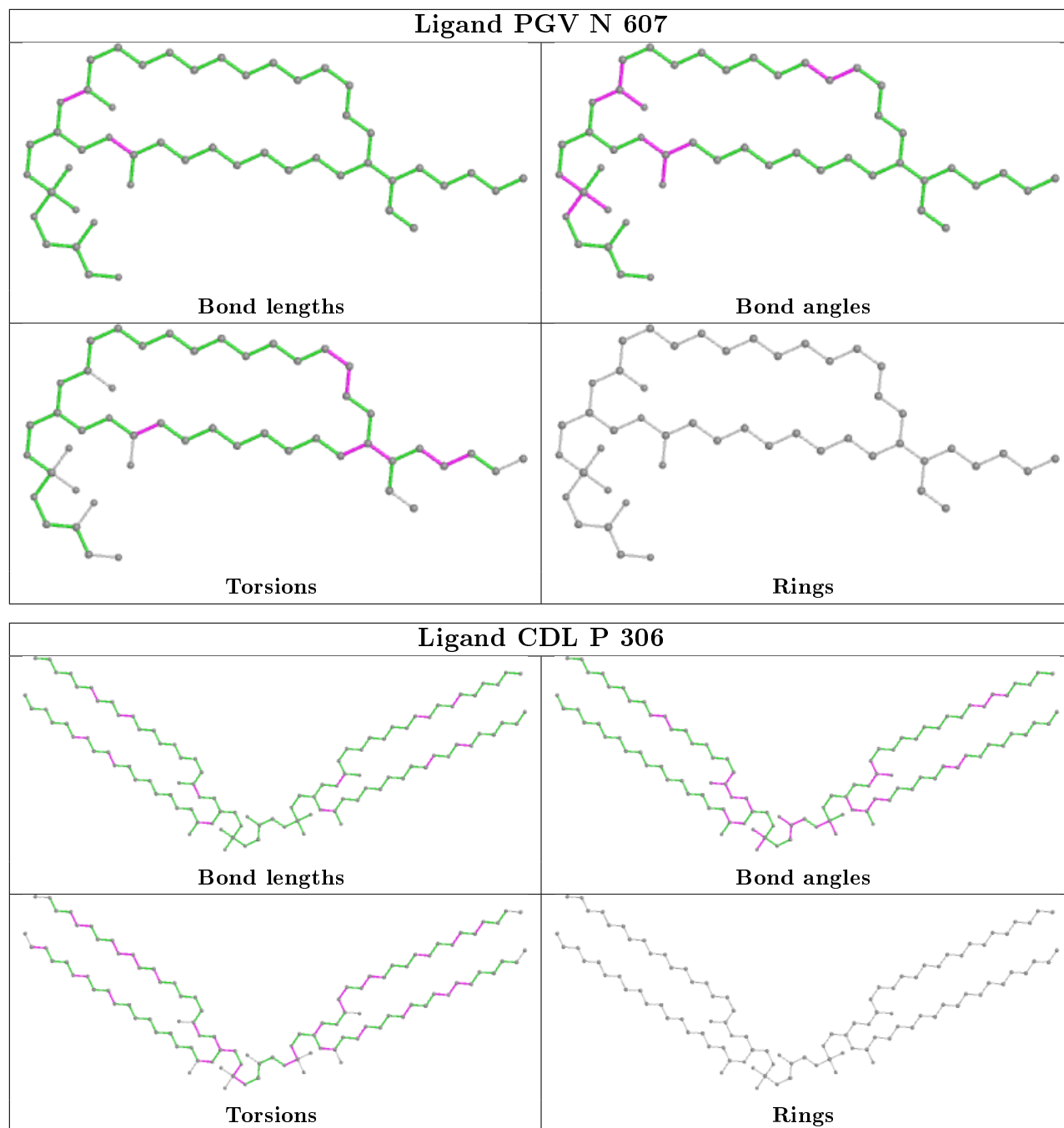


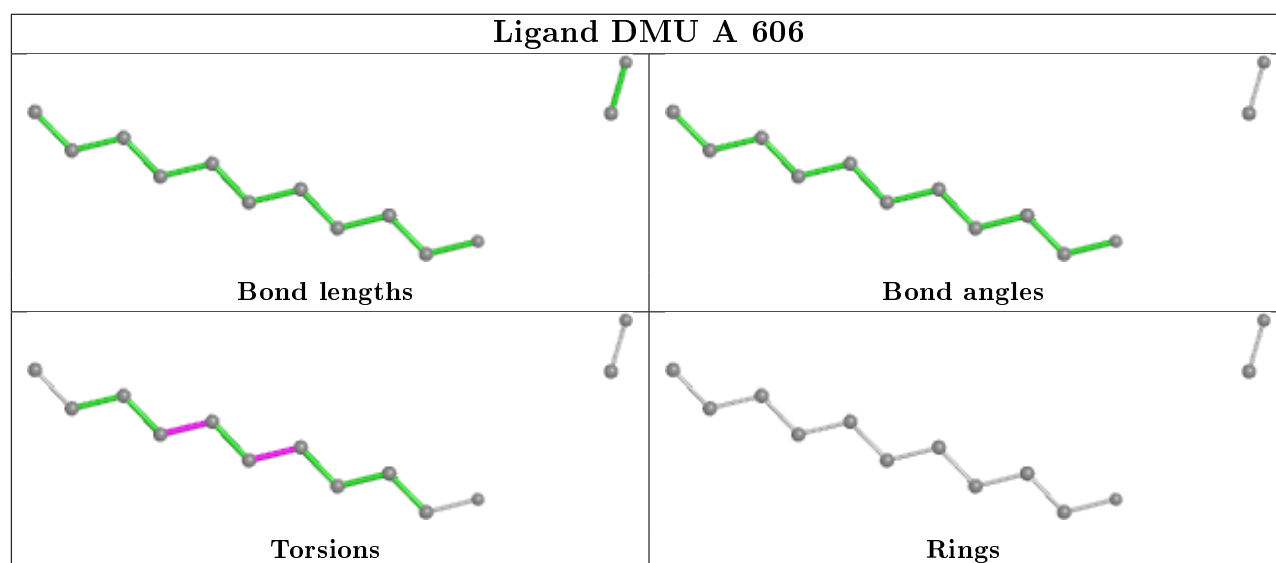
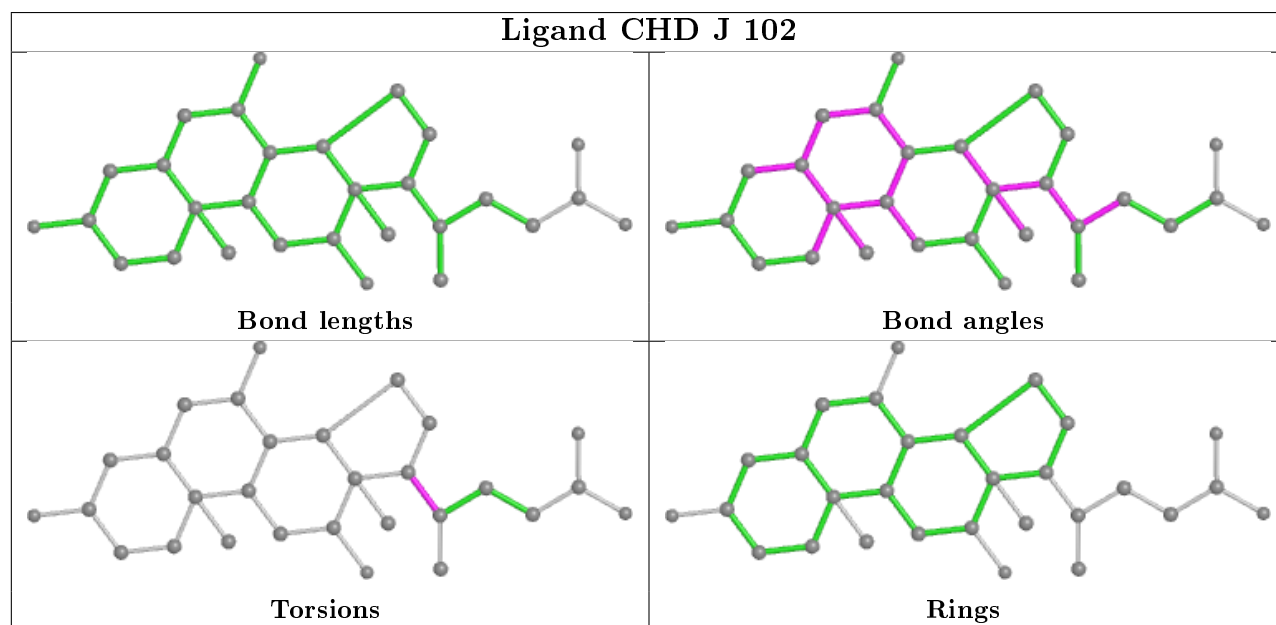
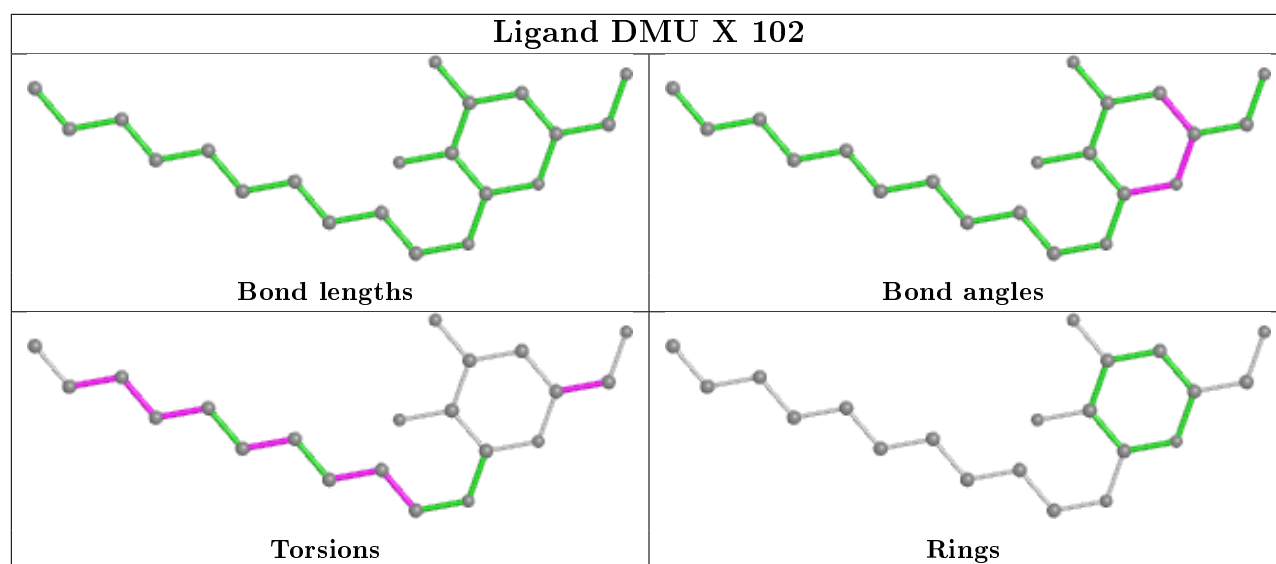
## Ligand CHD P 304

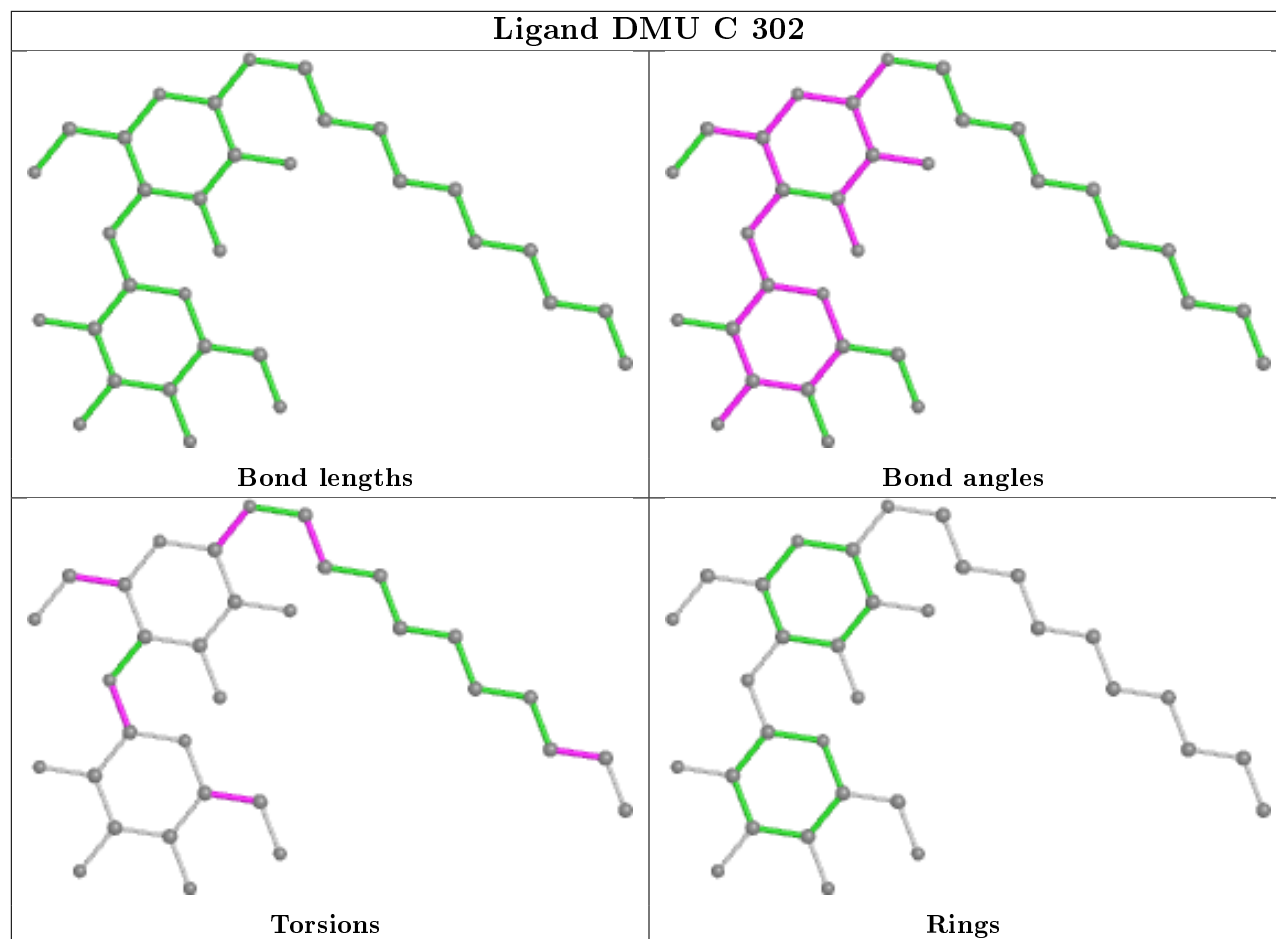
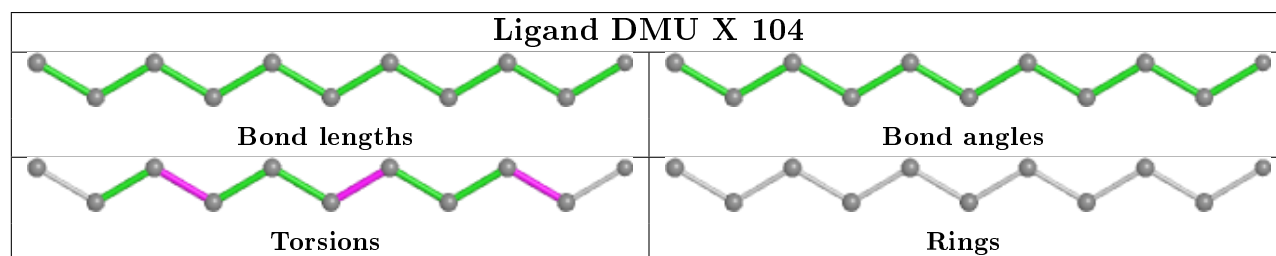
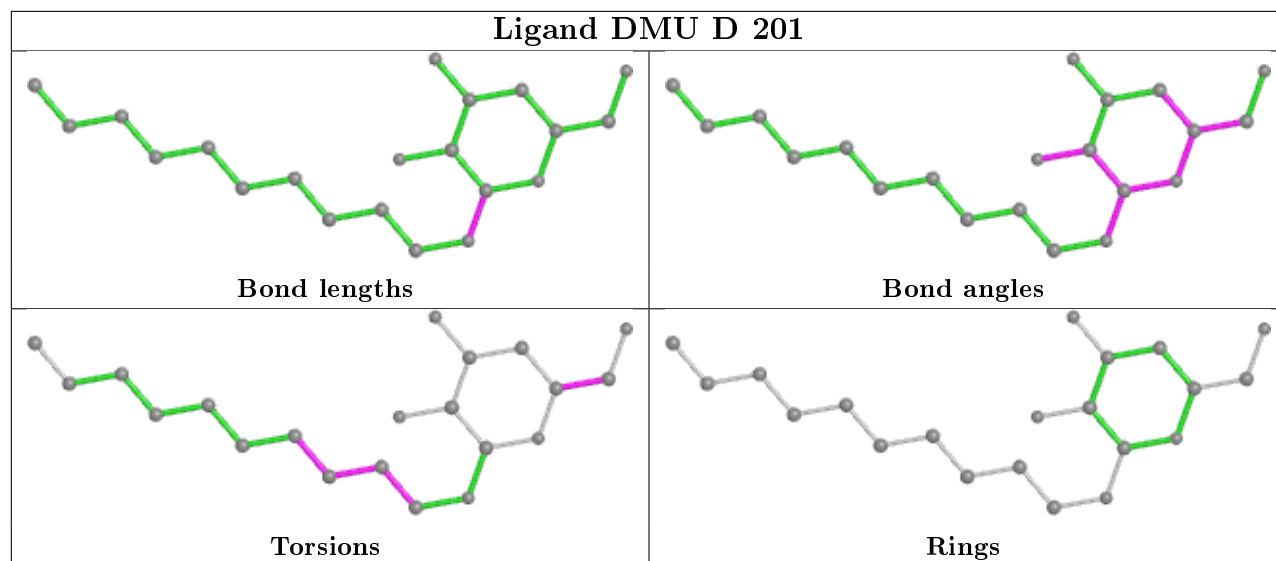


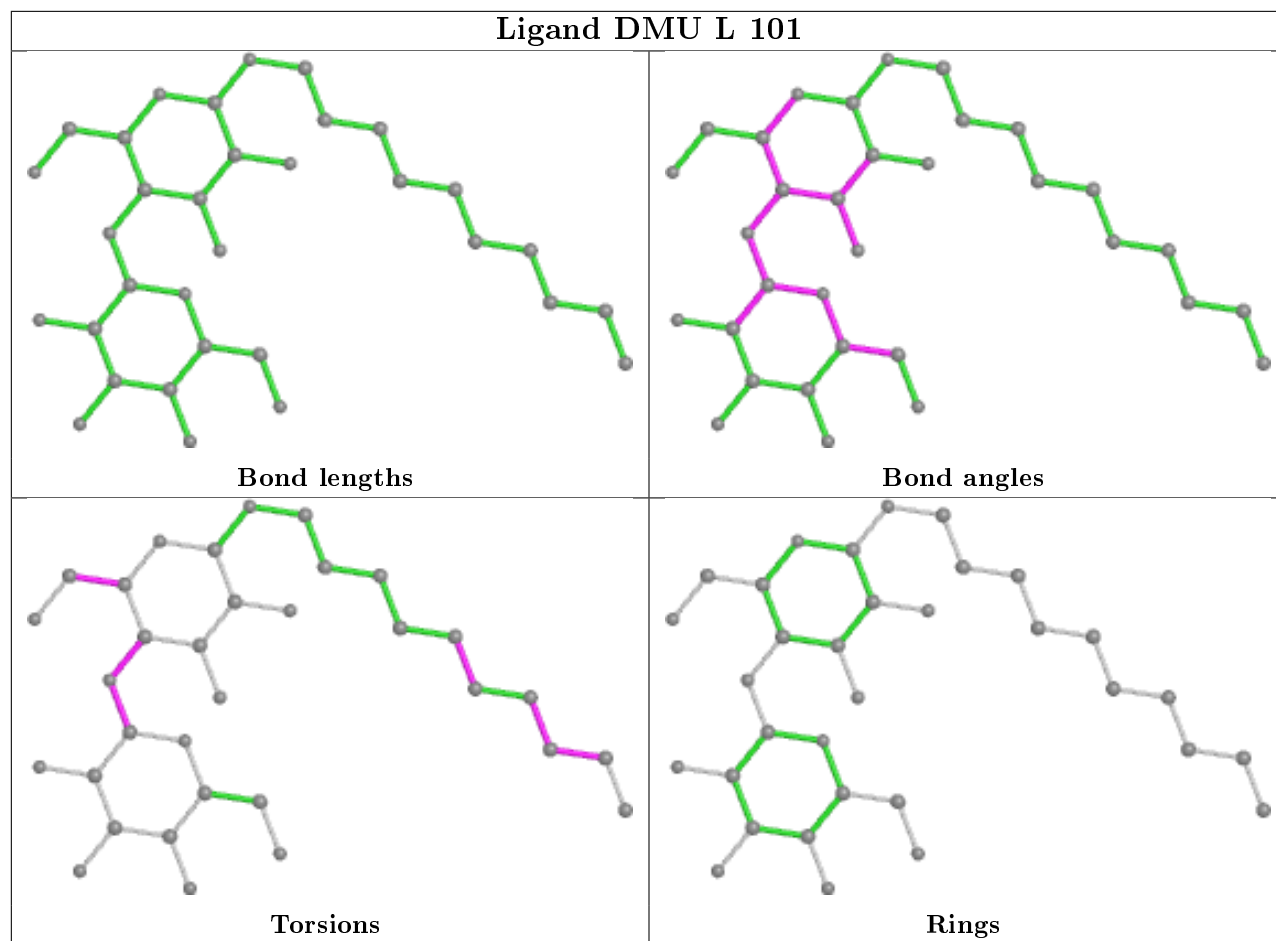


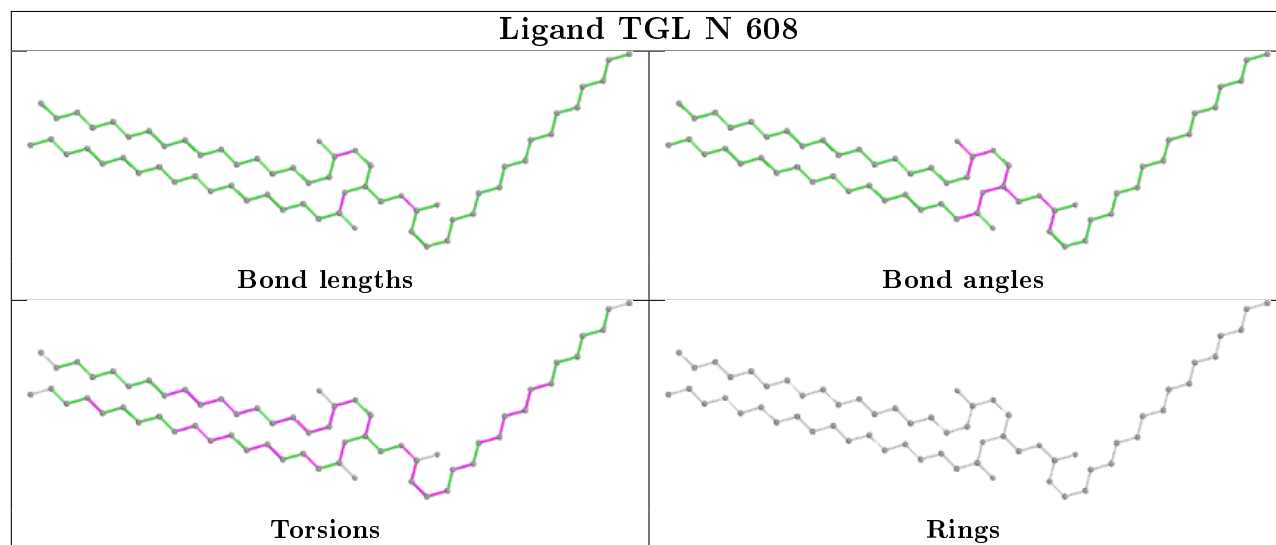
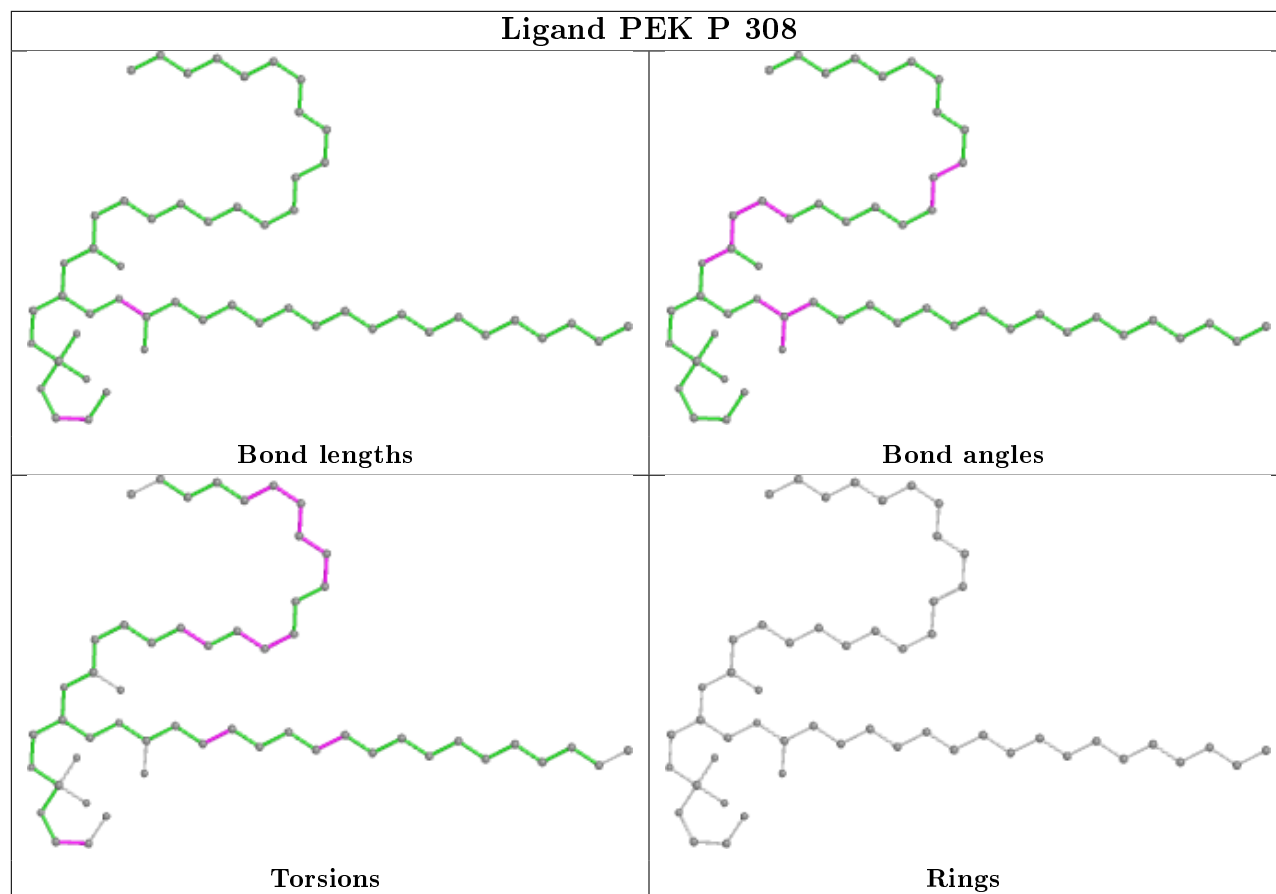


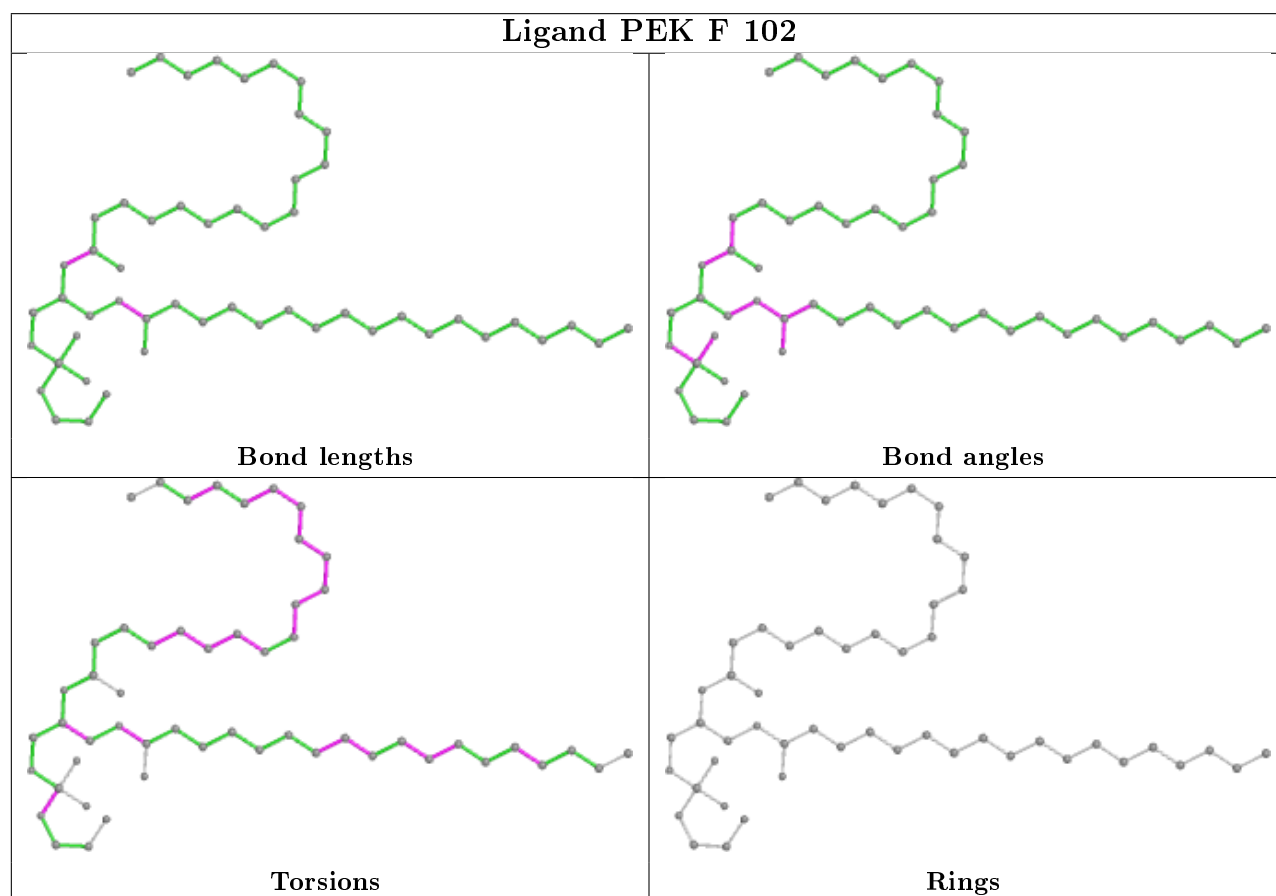
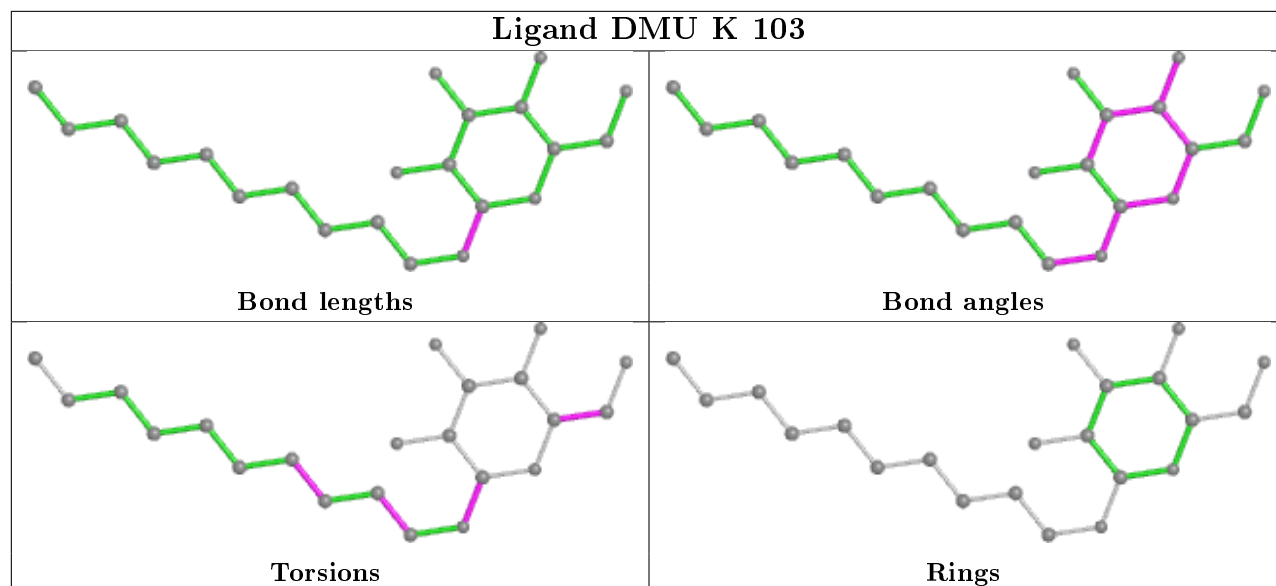


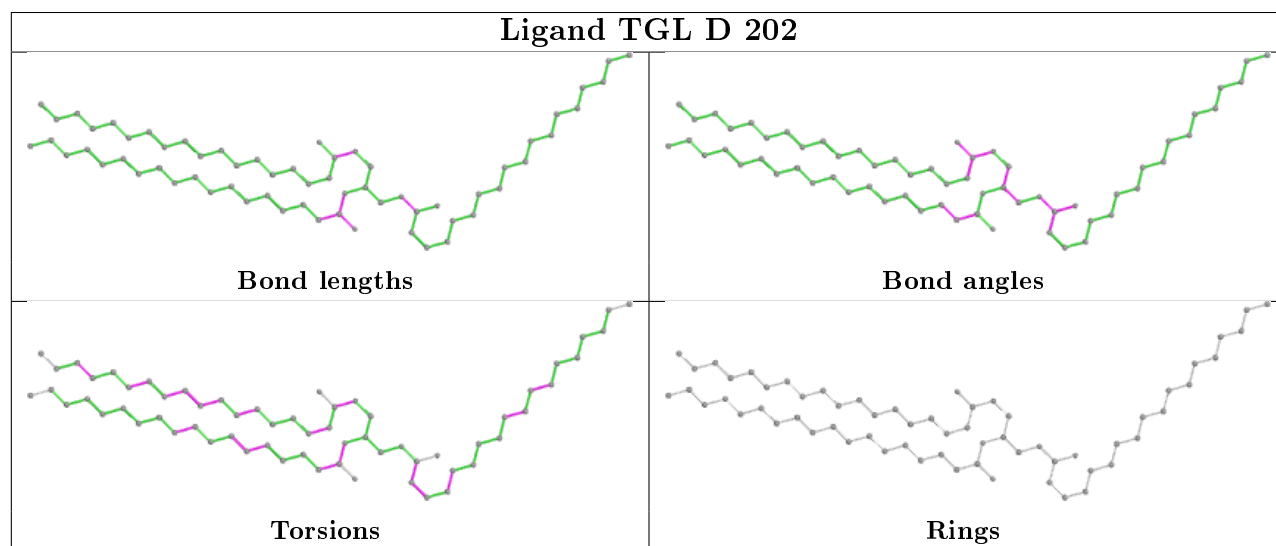
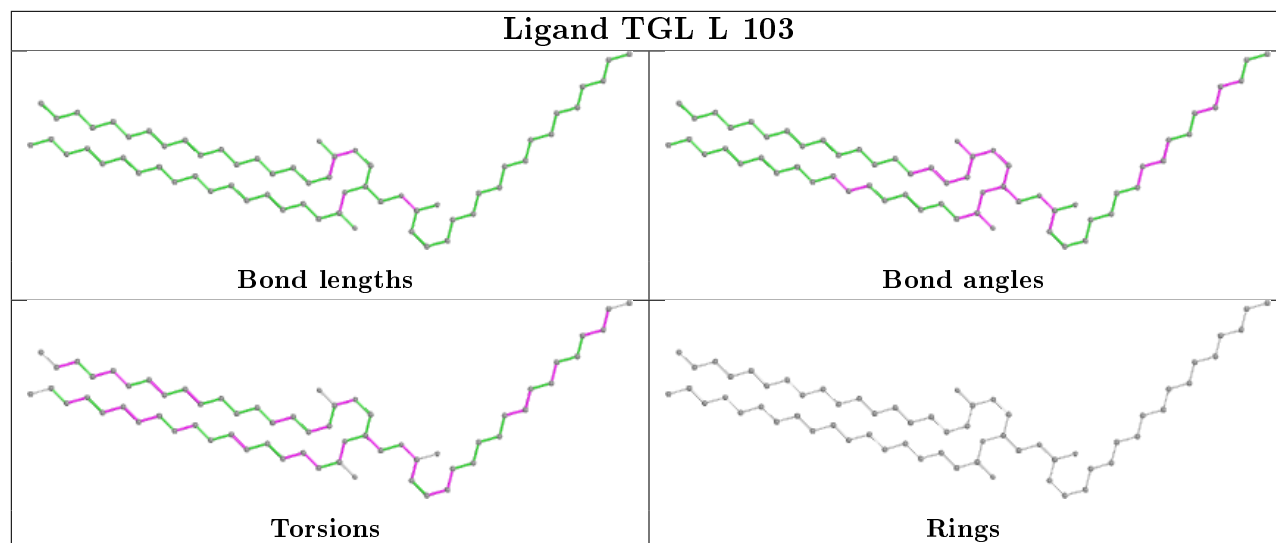




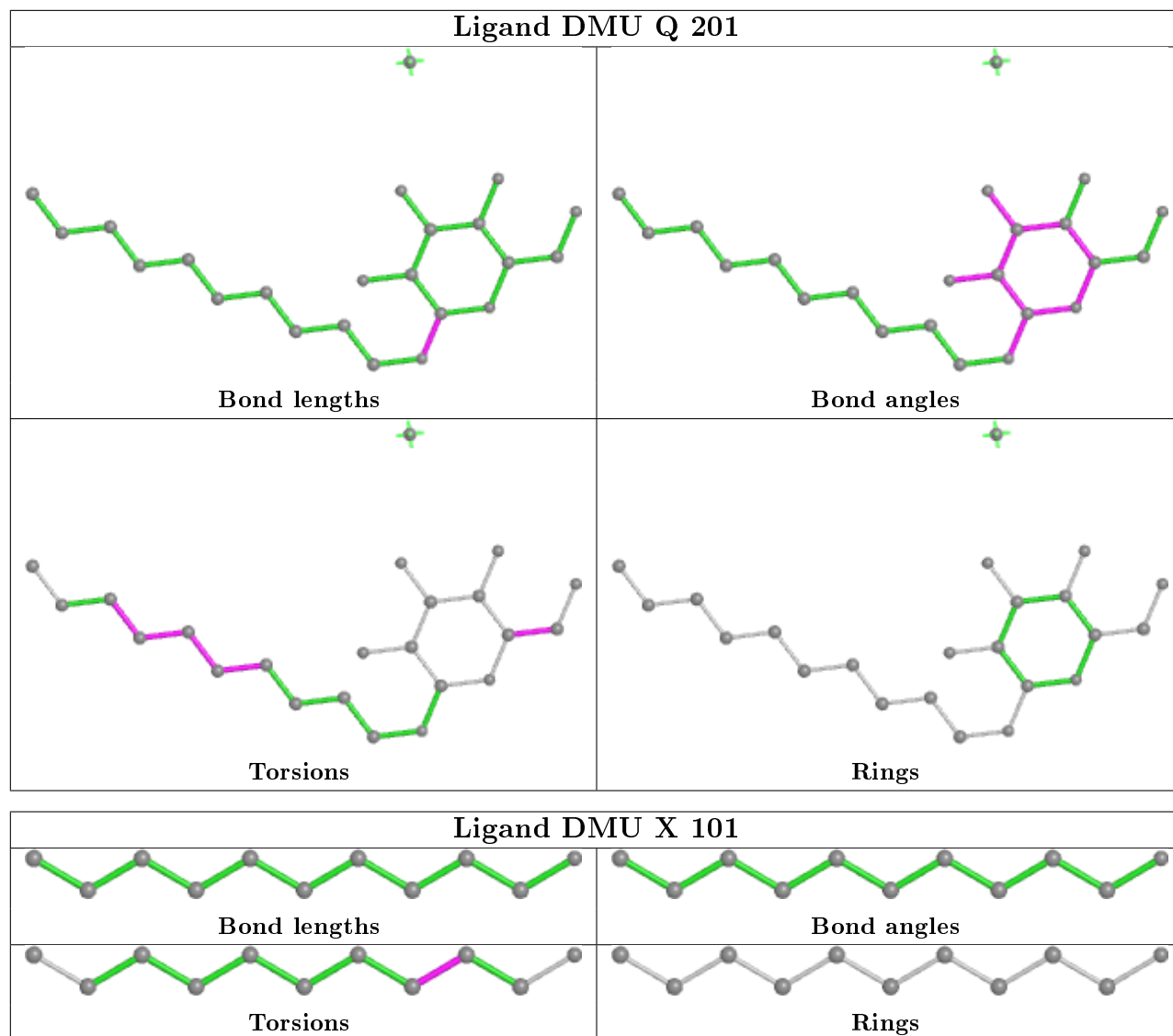




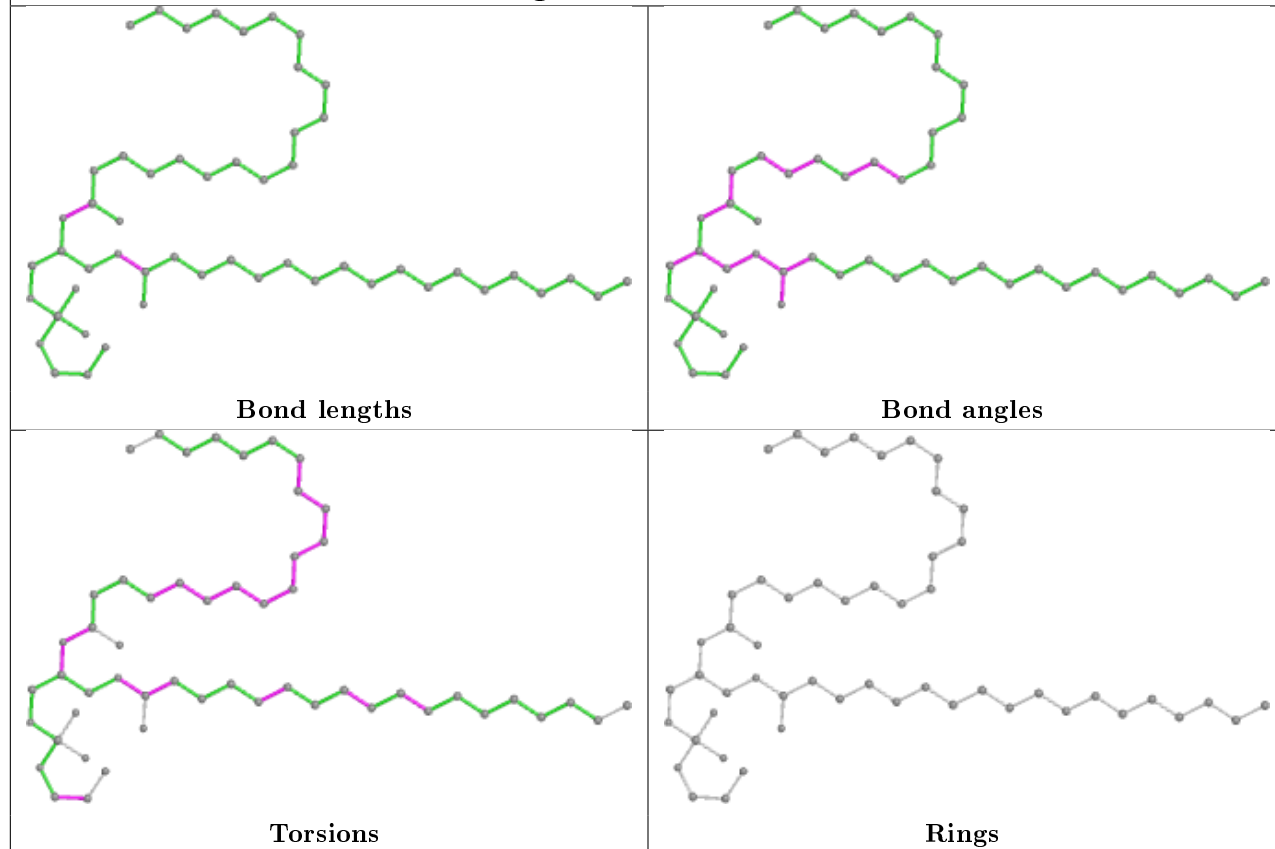




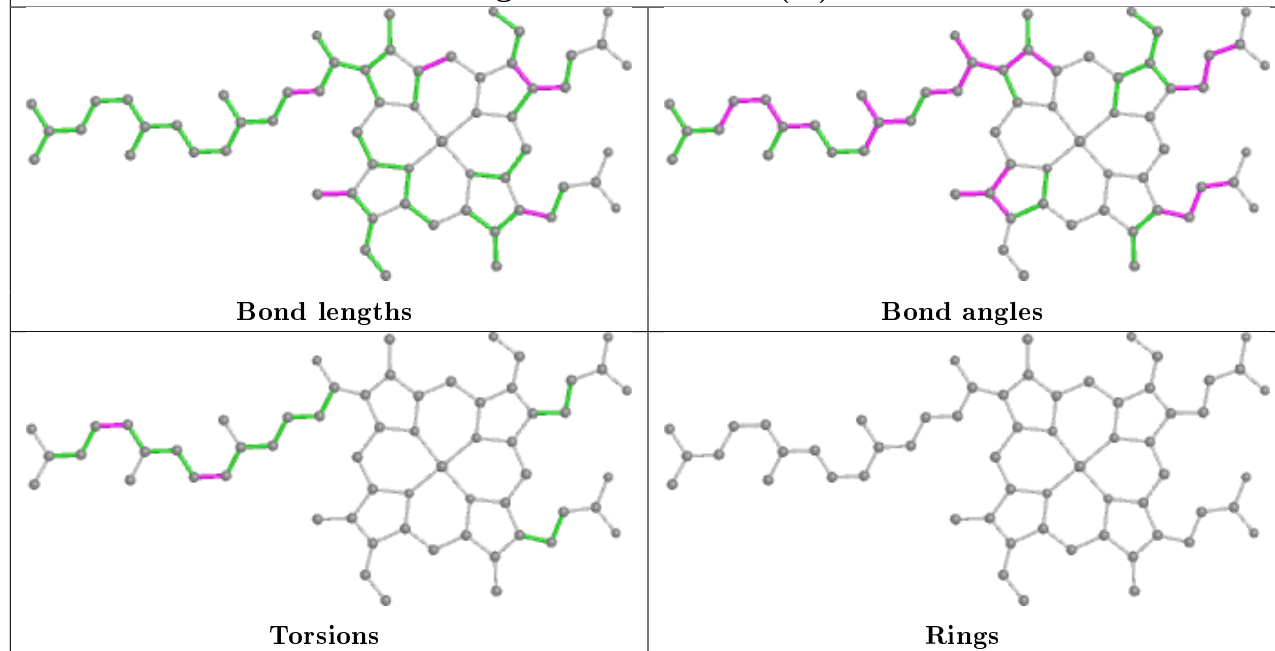


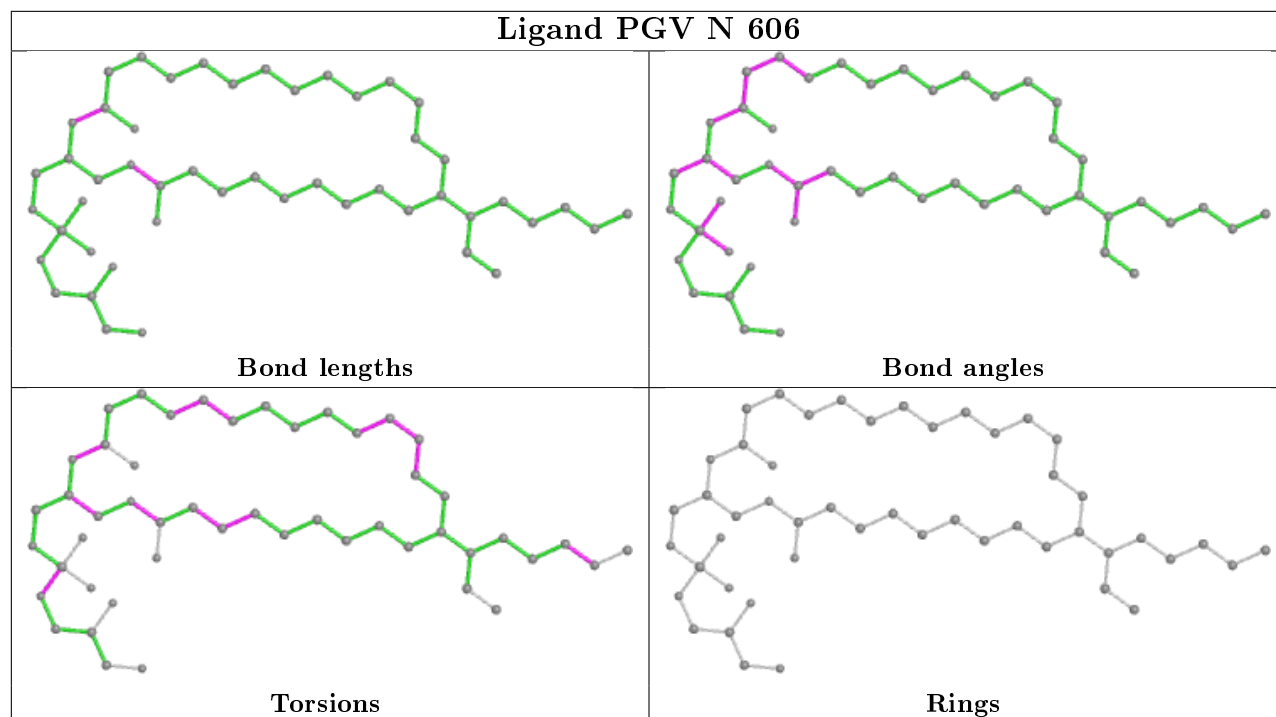
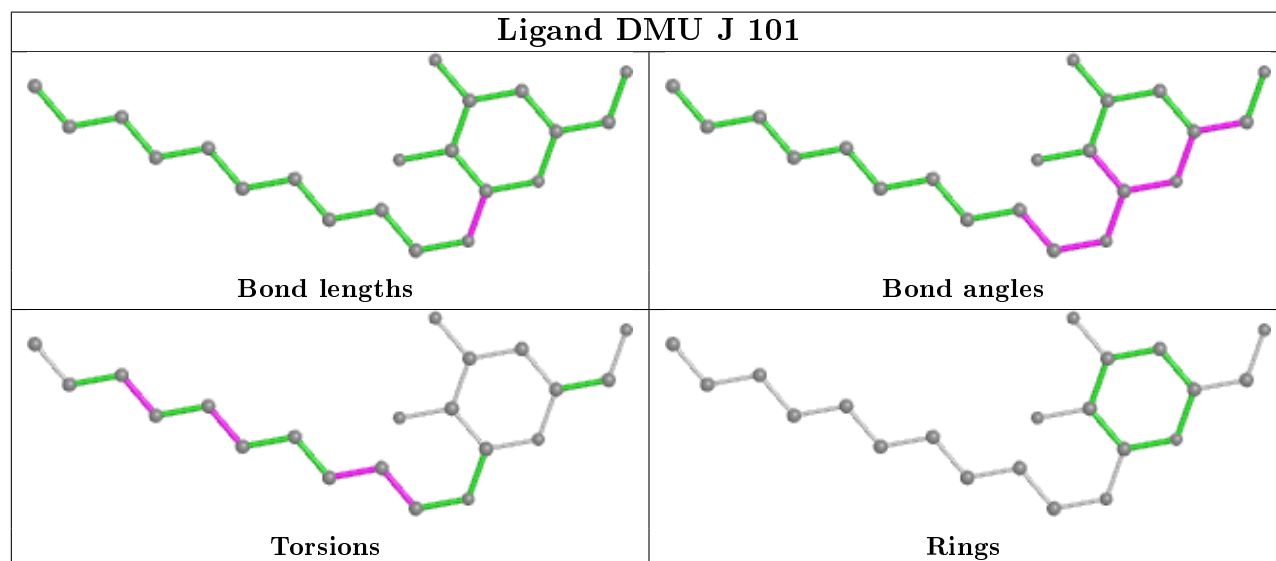
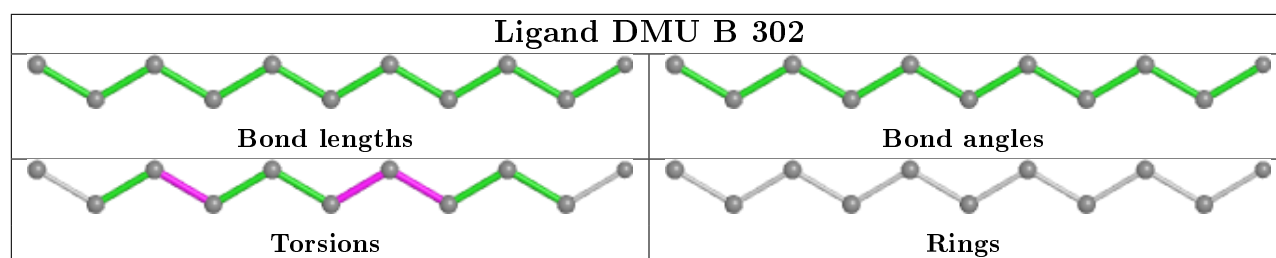


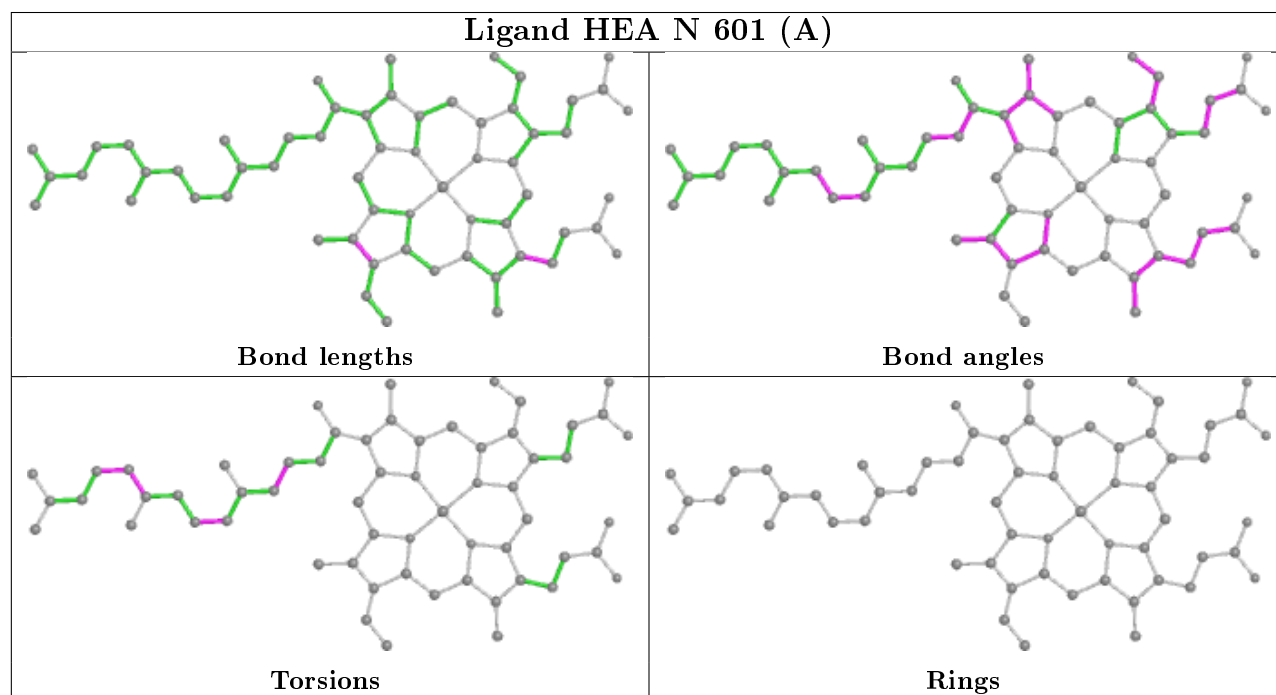
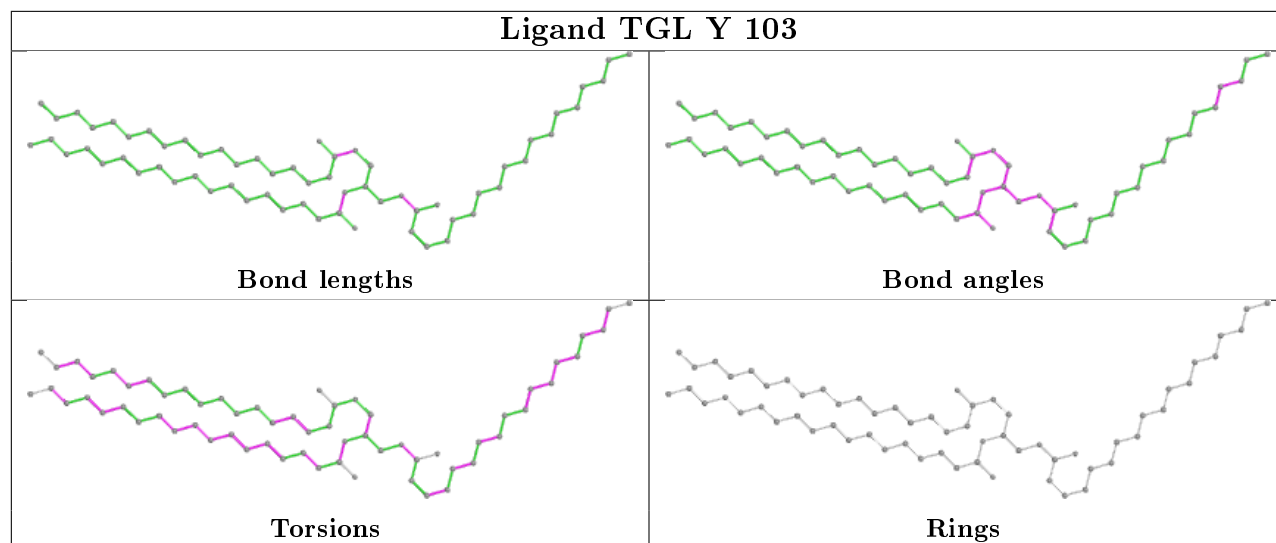
## Ligand PEK P 307



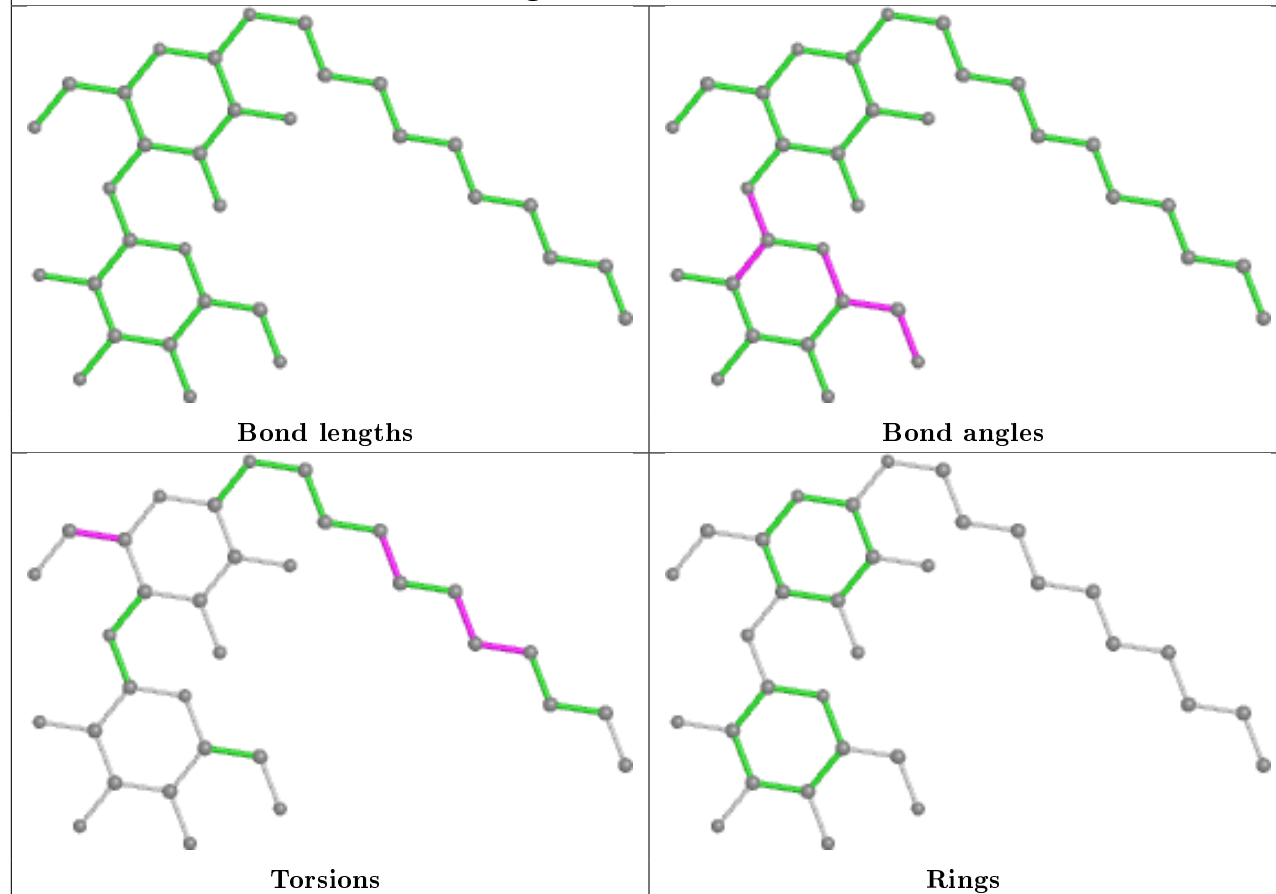
## Ligand HEA A 601 (A)



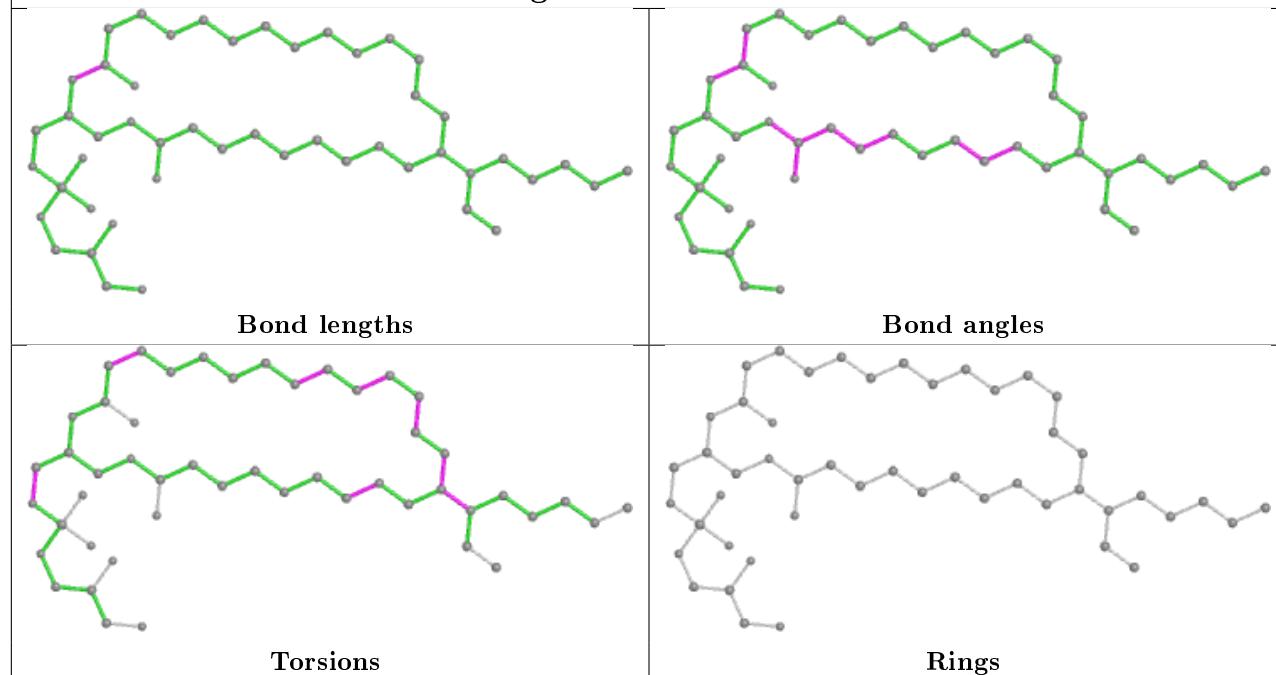


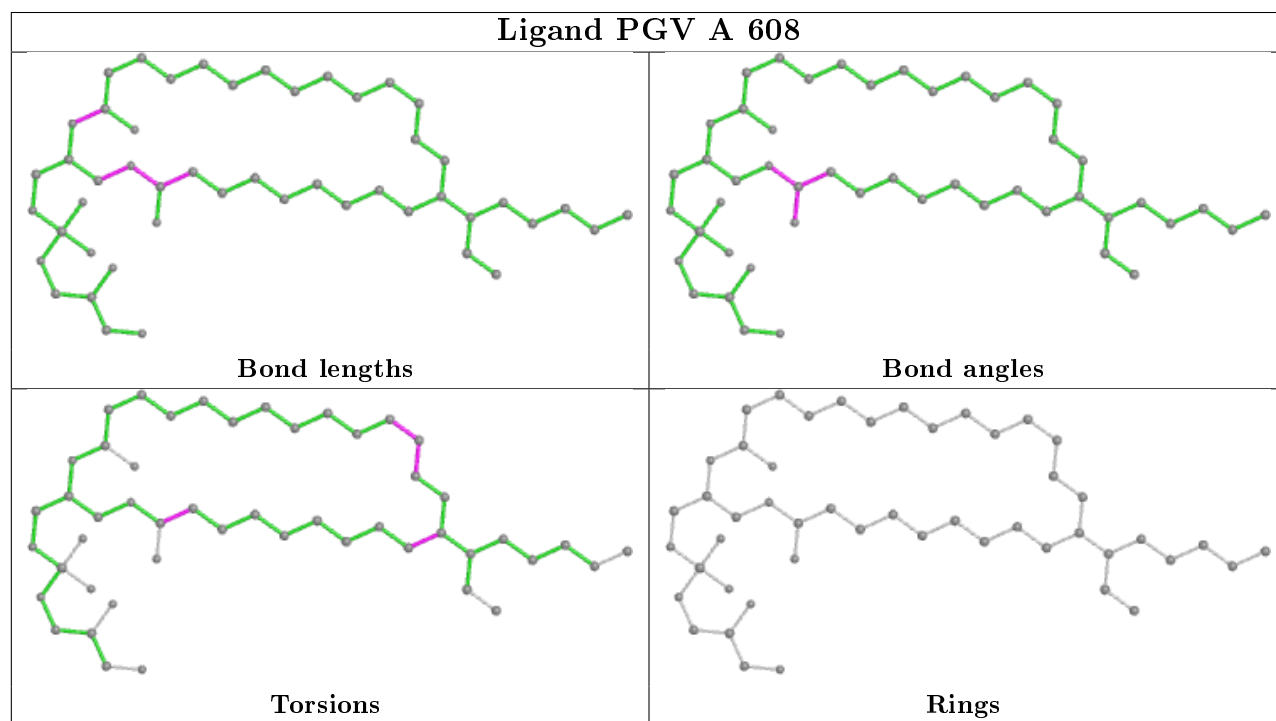
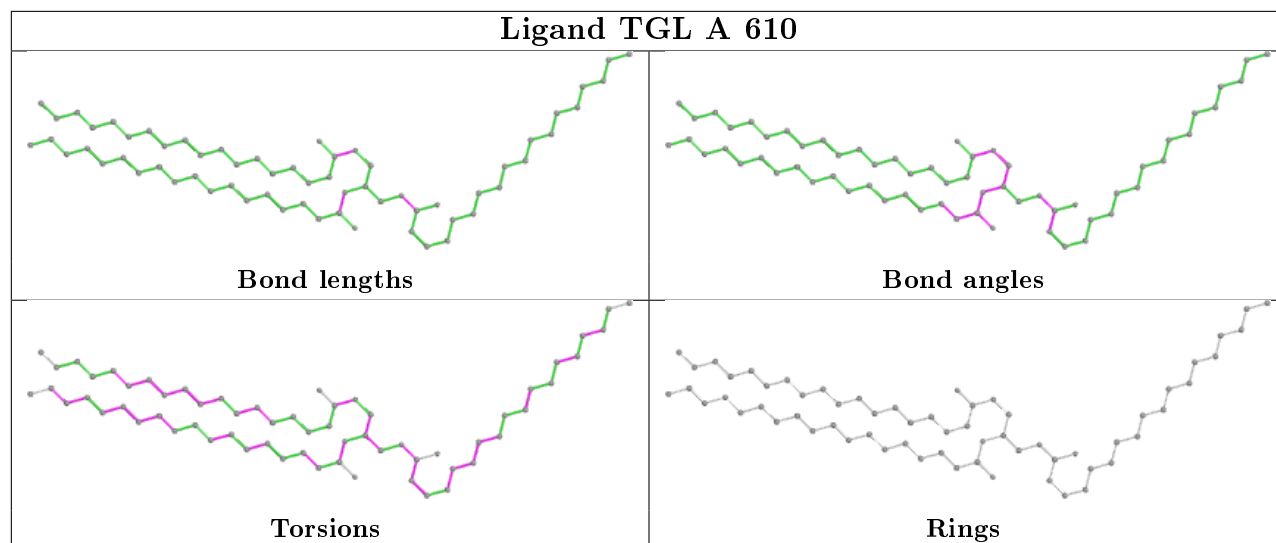


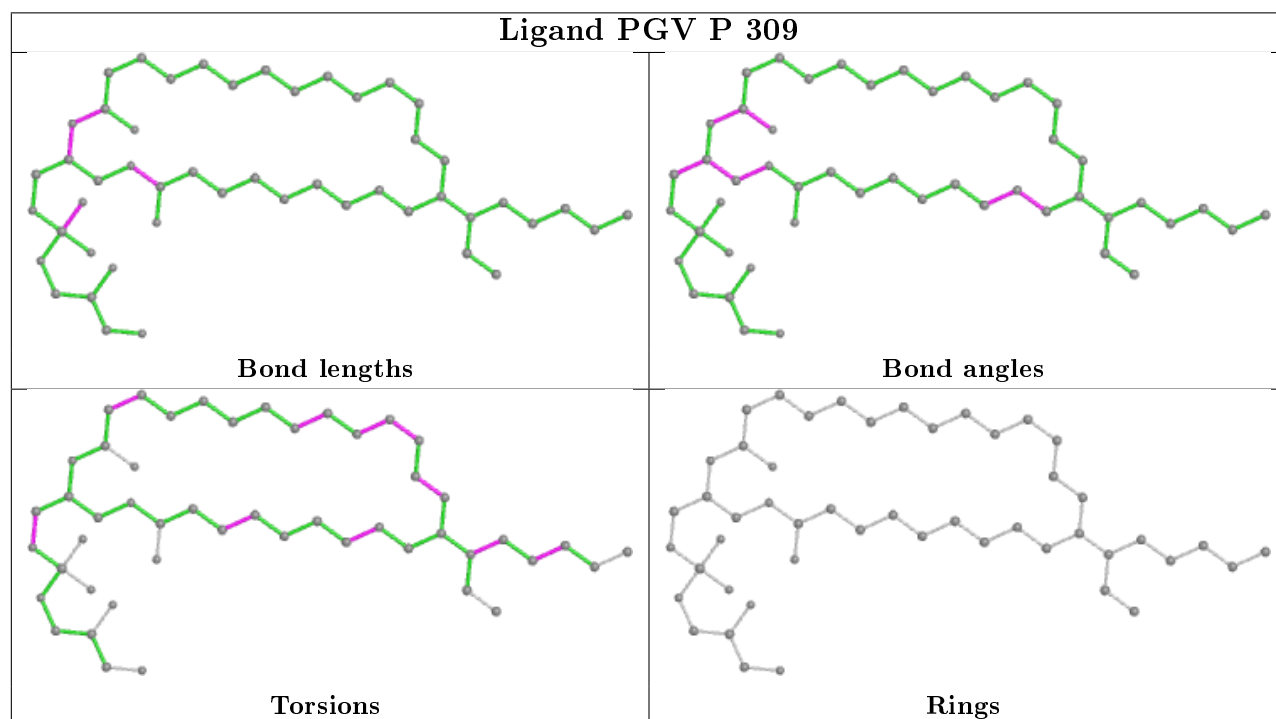
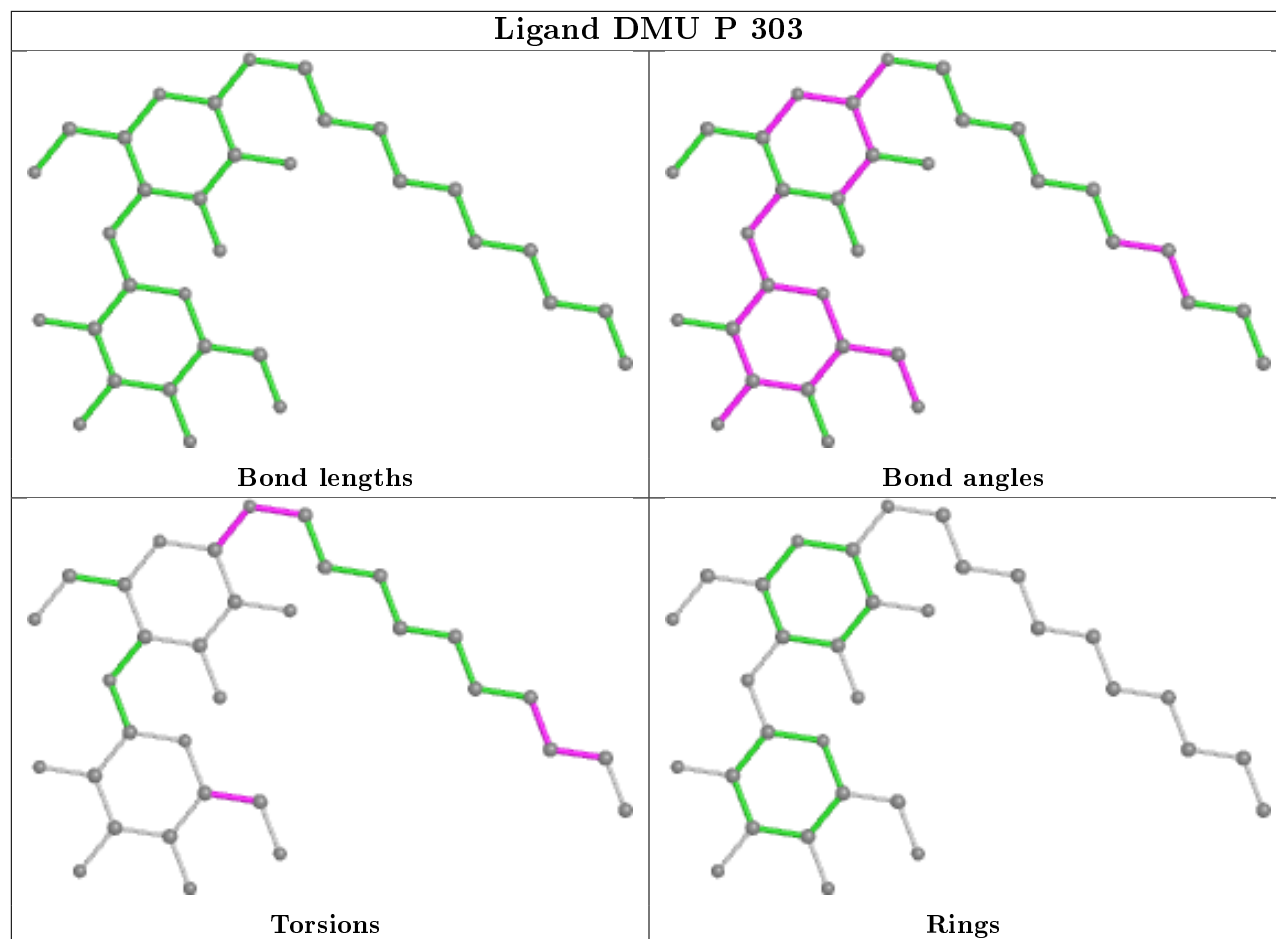
## Ligand DMU Y 101

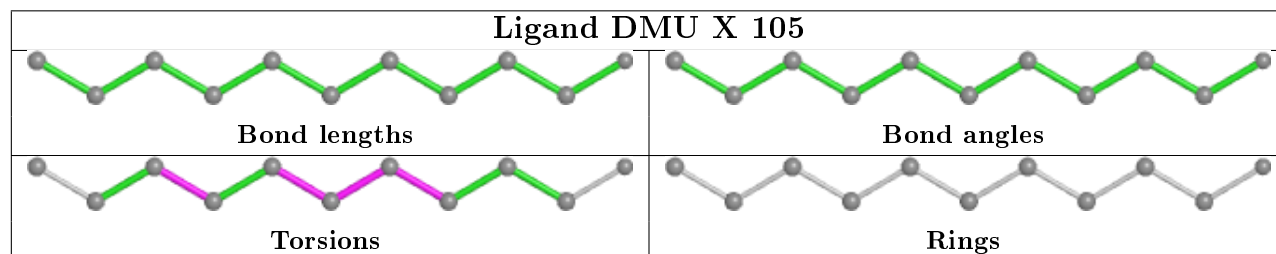
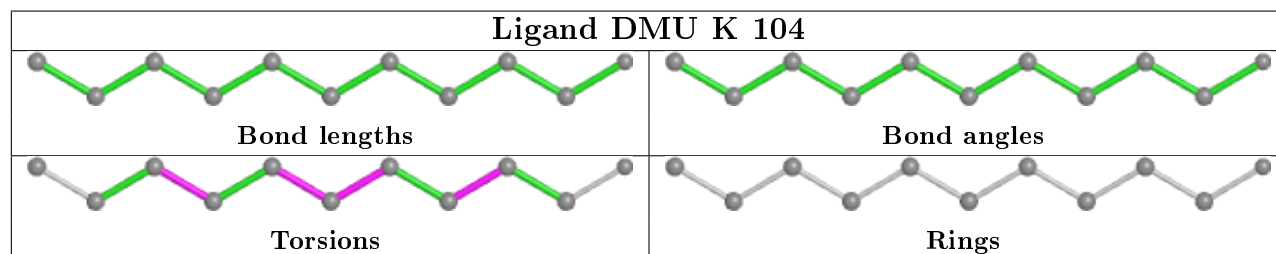
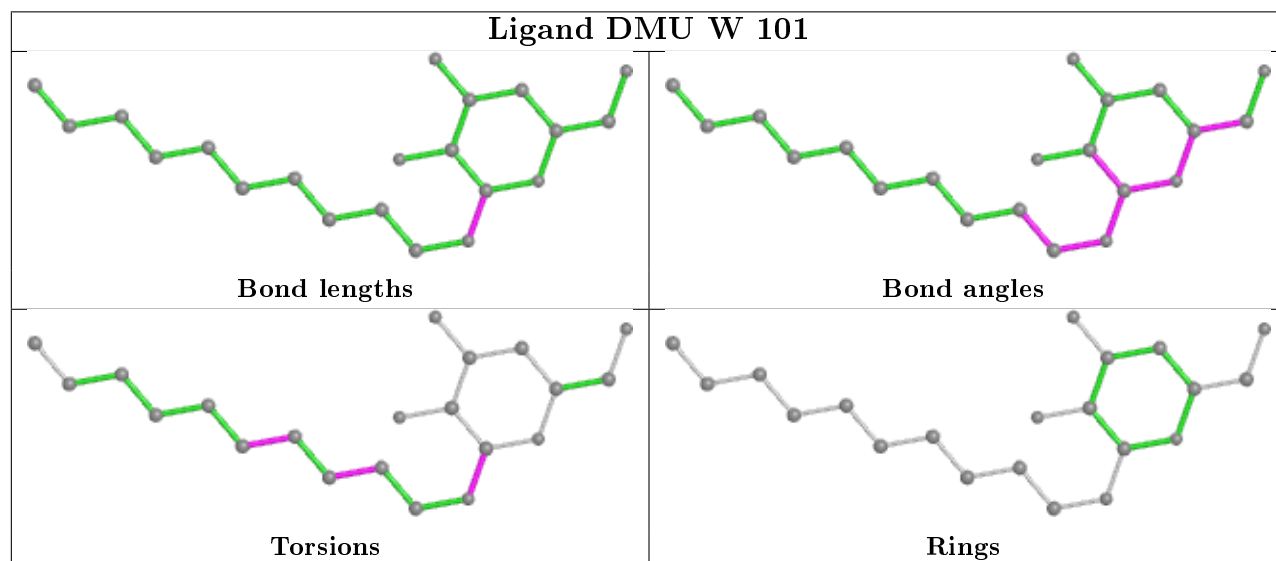
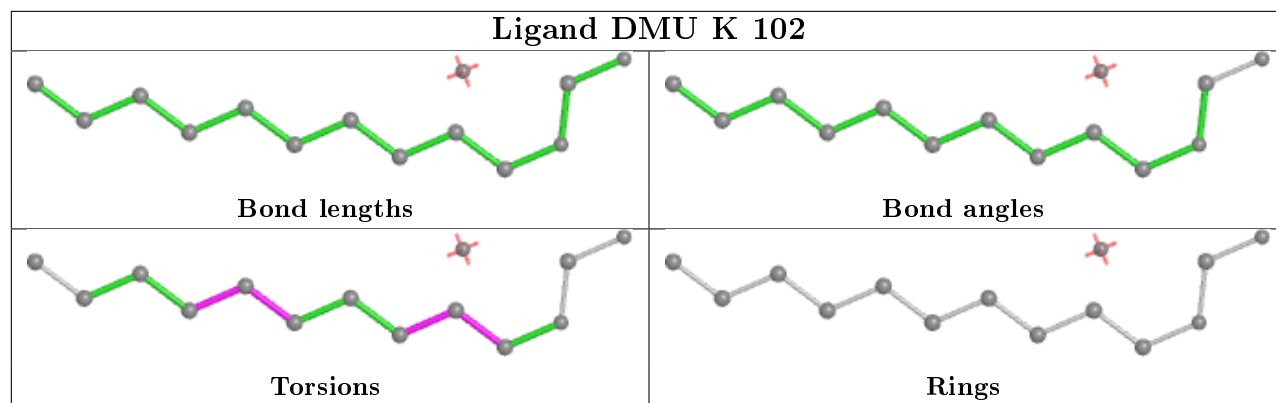


## Ligand PGV C 310

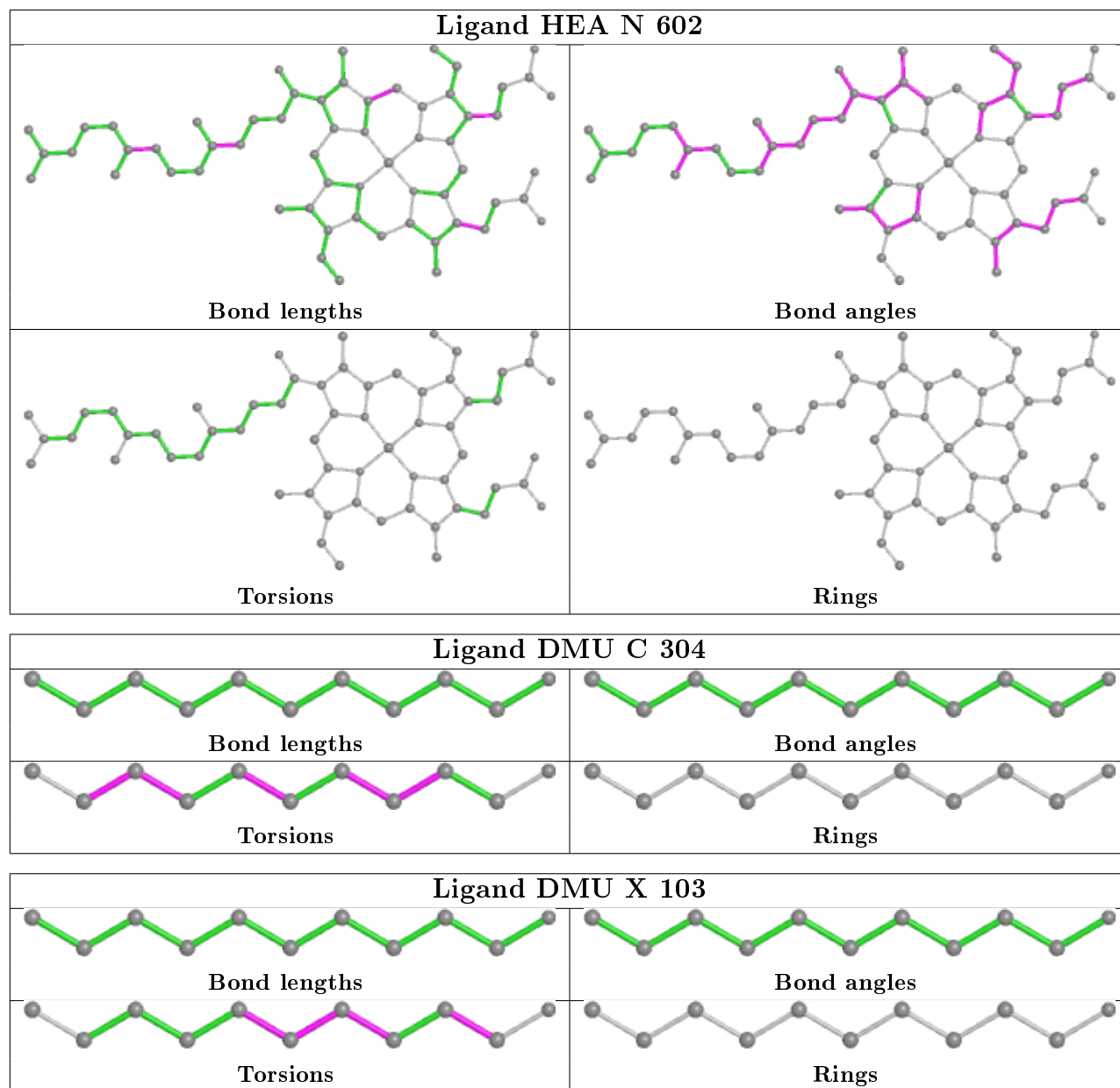


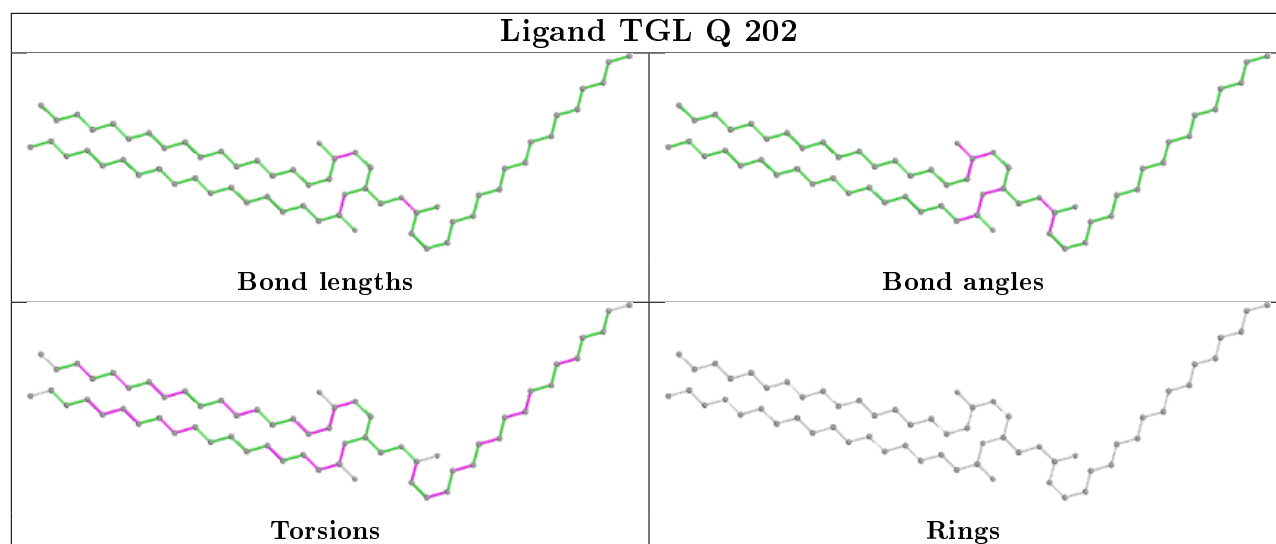
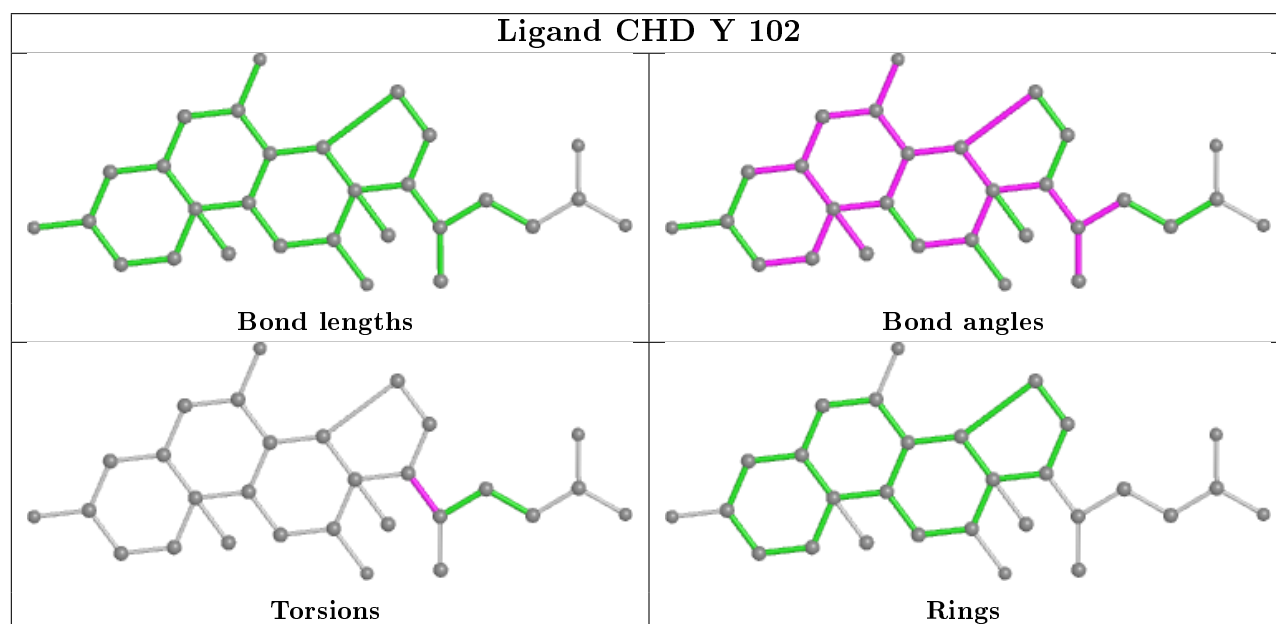
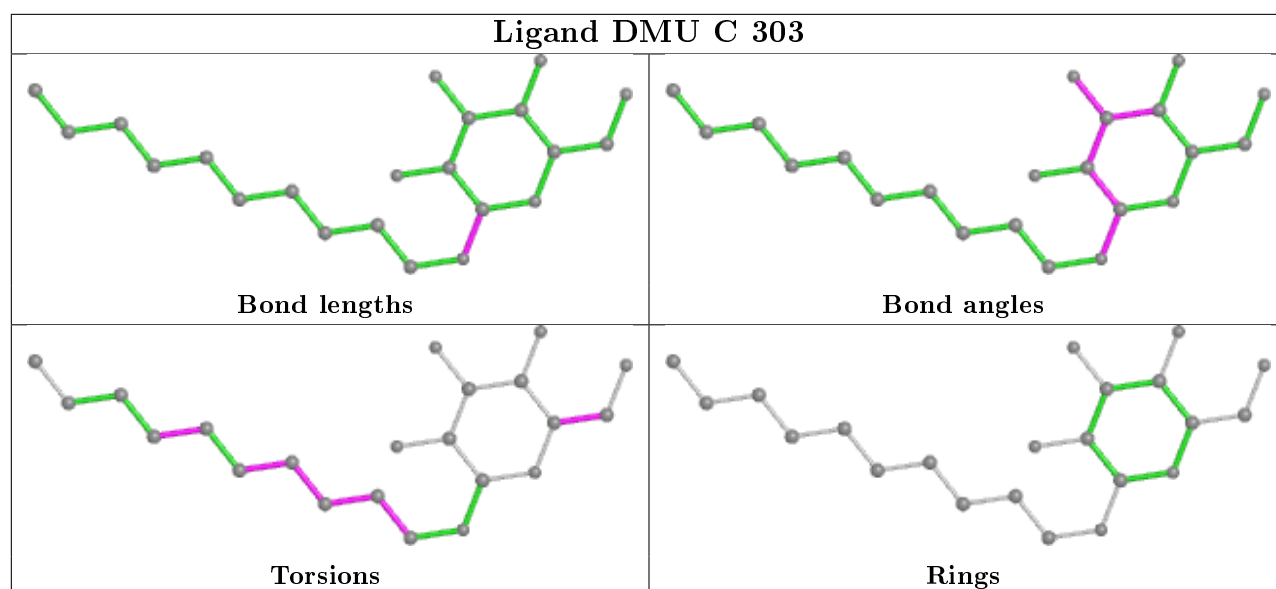


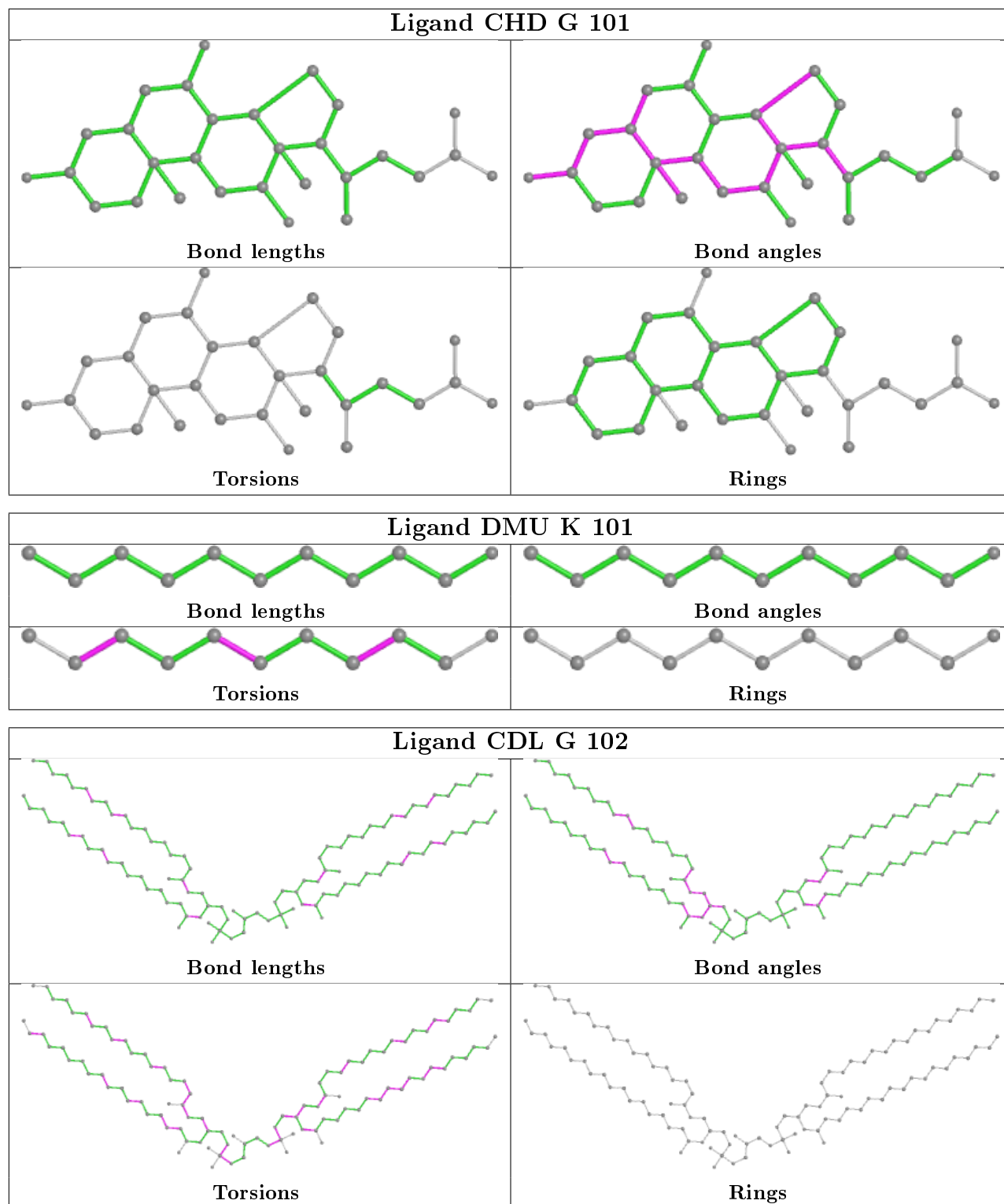


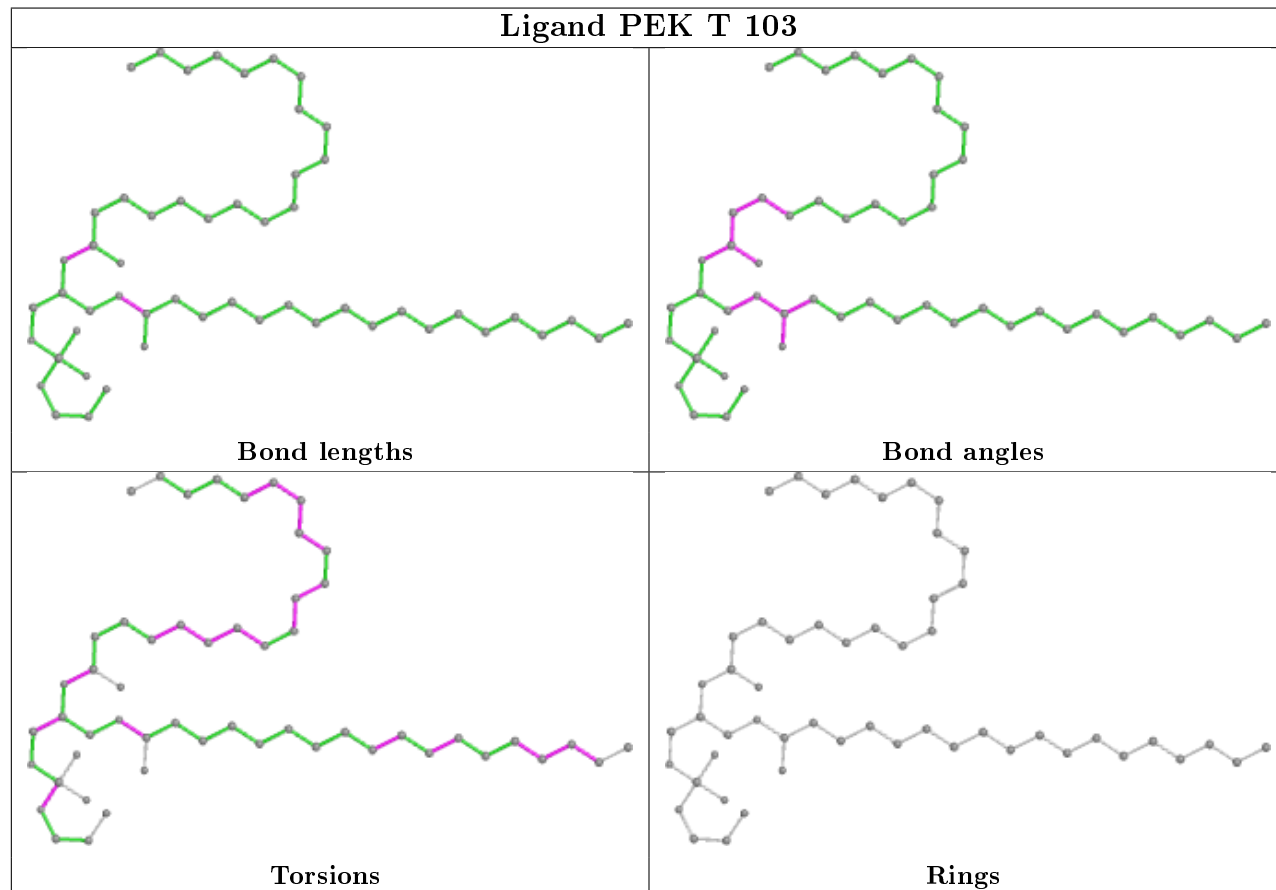
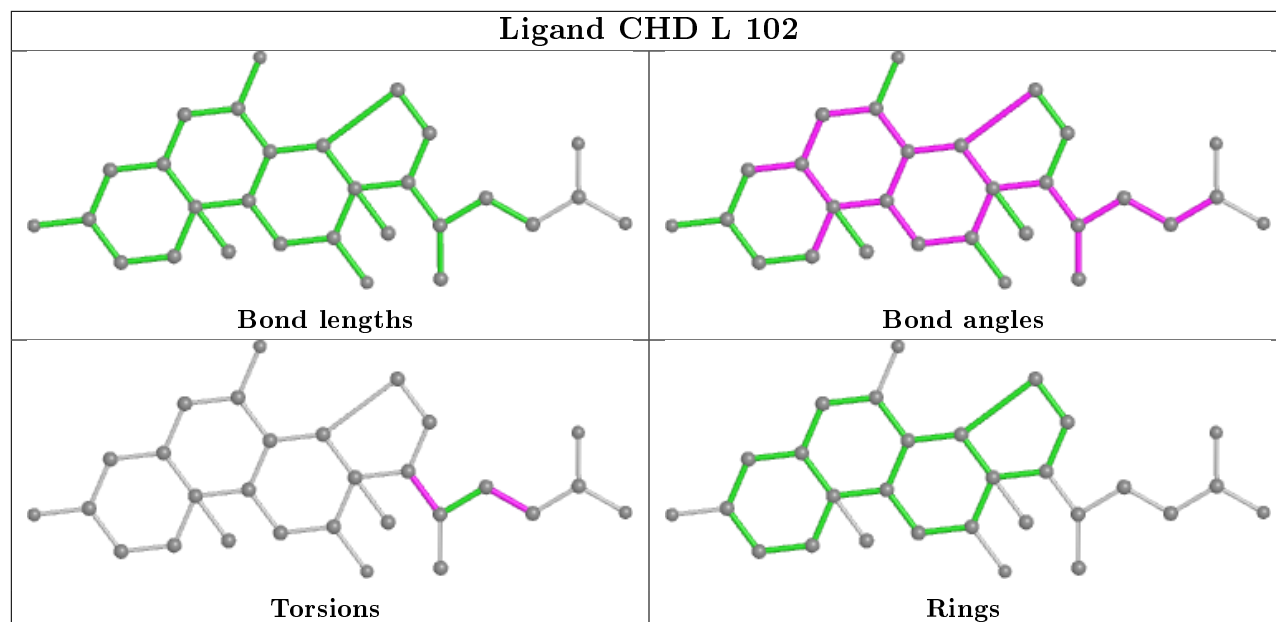


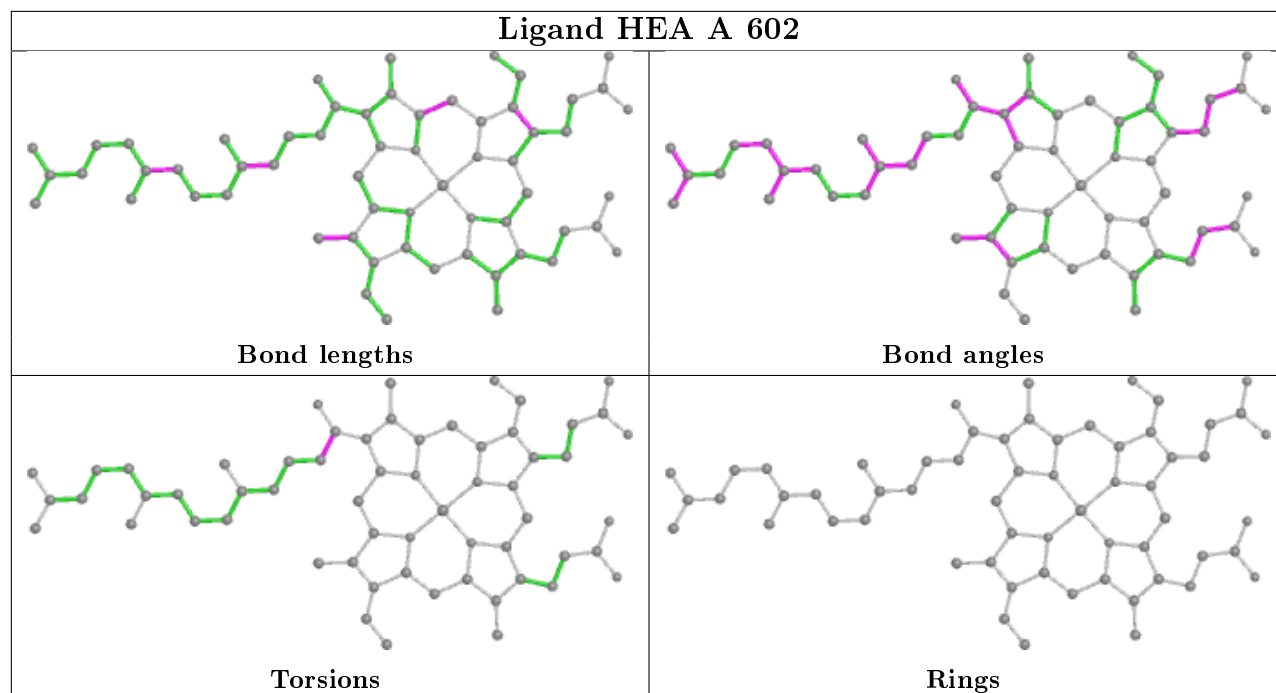












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	-0.04	1 (0%) 95 93	22, 28, 38, 103	0
1	N	513/514 (99%)	-0.16	1 (0%) 95 93	23, 31, 43, 111	0
2	B	226/227 (99%)	-0.13	4 (1%) 68 64	26, 37, 73, 143	0
2	O	226/227 (99%)	-0.15	3 (1%) 77 74	30, 42, 81, 124	0
3	C	259/259 (100%)	-0.09	0 100 100	25, 32, 50, 99	0
3	P	259/259 (100%)	-0.13	0 100 100	26, 33, 55, 94	0
4	D	144/144 (100%)	-0.25	0 100 100	28, 39, 64, 120	0
4	Q	144/144 (100%)	0.47	6 (4%) 36 30	36, 52, 106, 286	0
5	E	105/105 (100%)	-0.27	0 100 100	29, 37, 72, 132	0
5	R	105/105 (100%)	-0.20	2 (1%) 66 63	33, 47, 83, 161	0
6	F	98/98 (100%)	0.28	6 (6%) 21 16	28, 41, 147, 232	0
6	S	98/98 (100%)	0.15	5 (5%) 28 22	29, 42, 130, 198	0
7	G	83/84 (98%)	0.63	13 (15%) 2 1	29, 41, 129, 212	0
7	T	83/84 (98%)	0.72	12 (14%) 2 1	28, 45, 138, 226	0
8	H	79/79 (100%)	0.18	4 (5%) 28 22	33, 45, 118, 155	0
8	U	79/79 (100%)	0.26	4 (5%) 28 22	36, 48, 144, 220	0
9	I	72/73 (98%)	0.07	3 (4%) 36 30	34, 54, 87, 116	0
9	V	72/73 (98%)	0.14	3 (4%) 36 30	34, 61, 104, 191	0
10	J	58/58 (100%)	0.03	2 (3%) 45 39	31, 43, 94, 131	0
10	W	58/58 (100%)	0.09	4 (6%) 16 13	33, 47, 94, 161	0
11	K	49/49 (100%)	-0.18	0 100 100	35, 43, 67, 78	0
11	X	49/49 (100%)	-0.12	0 100 100	43, 54, 93, 113	0
12	L	46/46 (100%)	-0.09	0 100 100	29, 33, 62, 118	0
12	Y	46/46 (100%)	-0.16	1 (2%) 62 57	34, 42, 87, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/43 (100%)	0.05	2 (4%) 31 25	29, 34, 83, 143	0
13	Z	43/43 (100%)	0.11	3 (6%) 16 13	40, 46, 123, 185	0
All	All	3550/3558 (99%)	-0.01	79 (2%) 62 57	22, 37, 85, 286	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	21.7
4	Q	6	VAL	19.2
4	Q	4	SER	16.8
4	Q	8	SER	15.6
7	T	8	HIS	14.2
6	S	1	ALA	13.2
7	T	3	ALA	12.0
6	F	97	ALA	11.8
6	F	1	ALA	10.6
4	Q	7	LYS	9.9
7	G	8	HIS	9.3
6	F	2	SER	6.9
8	U	7	LYS	6.6
10	W	58	LYS	6.3
10	J	58	LYS	6.0
8	U	8	ILE	5.7
10	W	57	HIS	5.7
8	H	46	LYS	5.7
5	R	5	HIS	5.5
7	T	10	GLY	5.2
7	G	3	ALA	5.2
6	F	96	LEU	5.1
8	H	45	ALA	4.8
7	G	6	GLY	4.6
9	V	37	PHE	4.6
7	G	2	SER	4.5
13	Z	43	SER	4.4
7	T	4	ALA	4.4
7	G	40	GLY	4.1
6	S	2	SER	4.1
7	T	2	SER	4.1
7	G	42	ARG	4.0
6	F	95	GLN	4.0
6	F	98	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
6	S	96	LEU	3.9
8	U	9	LYS	3.8
7	G	1	ALA	3.6
10	J	1	PHE	3.6
8	U	45	ALA	3.4
7	T	7	ASP	3.2
9	I	37	PHE	3.2
2	O	90	ILE	3.2
13	Z	40	TYR	3.1
7	T	9	GLY	3.1
7	G	4	ALA	3.1
13	M	42	LYS	3.0
2	B	58	ALA	3.0
7	G	5	LYS	3.0
7	G	36	TRP	3.0
7	T	36[A]	TRP	3.0
13	Z	42	LYS	2.9
6	S	94	HIS	2.9
4	Q	147	LYS	2.9
9	I	25	PHE	2.9
7	T	42	ARG	2.8
9	V	2	THR	2.8
8	H	47	GLY	2.7
2	O	113	TYR	2.7
2	B	61	VAL	2.7
1	N	514	LYS	2.6
9	V	34	PHE	2.6
7	G	9	GLY	2.6
7	G	10	GLY	2.6
12	Y	47	LYS	2.5
5	R	109	VAL	2.5
2	O	227	LEU	2.5
7	G	7	ASP	2.5
10	W	52	TRP	2.4
10	W	1	PHE	2.4
2	B	55	THR	2.4
8	H	44	THR	2.4
7	T	40	GLY	2.3
9	I	29	LEU	2.3
13	M	43	SER	2.3
7	T	1	ALA	2.1
7	T	5	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	56	MET	2.1
1	A	53[A]	ILE	2.1
6	S	98	HIS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.45	0.62	210,249,270,285	0
7	TPO	G	11	11/12	0.63	0.41	137,171,213,223	0
7	TPO	T	11	11/12	0.81	0.31	124,161,188,220	0
9	SAC	I	1	9/10	0.82	0.20	131,136,147,157	0
1	FME	N	1	10/11	0.96	0.11	38,54,95,119	0
1	FME	A	1	10/11	0.96	0.13	39,52,94,106	0
2	FME	O	1	10/11	0.98	0.10	35,40,46,125	0
2	FME	B	1	10/11	0.98	0.10	32,35,43,114	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
22	EDO	Q	205	4/4	0.48	0.27	67,78,84,107	0
18	DMU	X	105	11/33	0.58	0.38	80,95,123,124	0
18	DMU	K	104	11/33	0.62	0.39	73,94,107,107	0
18	DMU	Q	201	23/33	0.67	0.35	52,92,138,154	0
22	EDO	C	316	4/4	0.67	0.22	52,60,77,128	0
18	DMU	K	103	22/33	0.68	0.54	66,110,139,152	0
22	EDO	S	103	4/4	0.71	0.19	61,71,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	P	313	4/4	0.71	0.21	50,57,70,84	0
24	CHD	J	102	29/29	0.73	0.32	61,109,143,153	0
18	DMU	X	103	11/33	0.73	0.25	67,83,110,113	0
22	EDO	P	317	4/4	0.73	0.10	61,66,67,80	0
18	DMU	C	303	22/33	0.74	0.26	53,89,148,160	0
22	EDO	F	110	4/4	0.75	0.22	66,70,80,81	0
25	CDL	T	102	100/100	0.76	0.30	42,103,168,206	0
22	EDO	P	315	4/4	0.76	0.33	41,52,78,113	0
26	PEK	C	308	53/53	0.77	0.31	48,101,182,205	0
24	CHD	Y	102	29/29	0.77	0.35	68,98,143,174	0
18	DMU	C	304	11/33	0.77	0.15	56,65,86,100	0
18	DMU	P	303	33/33	0.77	0.23	49,107,135,152	0
18	DMU	O	302	11/33	0.79	0.15	57,67,89,89	0
18	DMU	Y	101	33/33	0.79	0.26	52,105,145,149	0
22	EDO	D	203	4/4	0.79	0.17	45,66,83,84	0
26	PEK	T	103	53/53	0.79	0.31	49,78,169,233	0
18	DMU	C	302	33/33	0.80	0.25	53,103,152,162	0
20	PSC	A	609	52/52	0.80	0.35	42,101,181,243	0
25	CDL	G	102	100/100	0.80	0.28	51,99,177,197	0
18	DMU	D	201	21/33	0.80	0.21	51,85,132,140	0
26	PEK	P	307	53/53	0.81	0.22	50,74,159,190	0
18	DMU	X	102	21/33	0.81	0.21	68,102,136,151	0
19	PGV	T	104	51/51	0.81	0.26	50,97,182,229	0
19	PGV	P	310	51/51	0.81	0.28	51,97,153,200	0
18	DMU	X	101	11/33	0.81	0.16	48,75,115,125	0
22	EDO	L	104	4/4	0.82	0.34	41,94,96,97	0
24	CHD	L	102	29/29	0.82	0.27	51,91,123,145	0
21	TGL	Q	202	63/63	0.82	0.21	37,73,125,139	0
22	EDO	S	105	4/4	0.83	0.49	73,85,94,103	0
18	DMU	P	302	11/33	0.83	0.14	52,60,93,94	0
26	PEK	F	102	53/53	0.83	0.27	46,79,162,232	0
22	EDO	N	618	4/4	0.83	0.24	41,54,66,72	0
18	DMU	W	101	21/33	0.83	0.33	42,75,111,128	0
25	CDL	P	306	100/100	0.84	0.25	40,100,173,211	0
18	DMU	J	101	21/33	0.84	0.27	32,68,123,131	0
22	EDO	M	102	4/4	0.84	0.14	71,76,76,93	0
22	EDO	C	314	4/4	0.84	0.16	41,45,49,59	0
21	TGL	Y	103	63/63	0.84	0.23	39,73,128,179	0
22	EDO	C	311	4/4	0.84	0.35	35,61,78,103	0
20	PSC	V	101	52/52	0.85	0.29	43,92,191,241	0
21	TGL	D	202	63/63	0.85	0.18	34,68,120,140	0
24	CHD	P	305	29/29	0.85	0.17	59,75,113,132	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	T	105	4/4	0.86	0.23	58,81,89,108	0
22	EDO	E	203	4/4	0.86	0.47	67,79,81,82	0
22	EDO	A	613	4/4	0.86	0.19	39,40,46,80	0
18	DMU	K	101	11/33	0.86	0.15	47,70,93,99	0
22	EDO	P	314	4/4	0.86	0.21	46,48,65,82	0
25	CDL	C	307	100/100	0.86	0.20	39,85,148,175	0
21	TGL	N	608	63/63	0.86	0.15	48,70,116,129	0
18	DMU	X	104	11/33	0.87	0.30	56,71,105,109	0
22	EDO	N	616	4/4	0.87	0.11	49,54,55,66	0
22	EDO	Q	203	4/4	0.87	0.27	78,86,87,105	0
18	DMU	K	102	14/33	0.87	0.19	60,80,119,123	0
22	EDO	N	611	4/4	0.87	0.17	37,37,43,56	0
22	EDO	A	619	4/4	0.87	0.25	59,67,69,89	0
18	DMU	L	101	33/33	0.87	0.22	49,102,136,160	0
22	EDO	C	317	4/4	0.87	0.28	45,73,80,84	0
18	DMU	Z	101	33/33	0.87	0.12	44,58,89,96	0
18	DMU	B	302	11/33	0.87	0.24	61,78,97,105	0
19	PGV	A	607	51/51	0.87	0.22	31,70,159,167	0
24	CHD	C	306	29/29	0.88	0.16	51,80,118,135	0
21	TGL	A	610	63/63	0.88	0.14	36,73,112,133	0
19	PGV	N	606	51/51	0.88	0.27	41,94,148,194	0
22	EDO	N	623	4/4	0.88	0.19	67,76,79,96	0
22	EDO	D	206	4/4	0.88	0.41	46,59,99,113	0
22	EDO	F	109	4/4	0.88	0.18	53,57,67,98	0
24	CHD	C	305	29/29	0.89	0.12	35,42,60,67	0
21	TGL	L	103	63/63	0.89	0.18	29,63,125,169	0
22	EDO	A	618	4/4	0.89	0.13	38,57,68,73	0
22	EDO	N	620	4/4	0.89	0.21	45,56,92,96	0
22	EDO	N	615	4/4	0.90	0.26	40,56,59,88	0
18	DMU	A	606	13/33	0.90	0.19	43,67,113,117	0
22	EDO	U	102	4/4	0.90	0.25	42,53,67,72	0
22	EDO	L	105	4/4	0.90	0.11	56,59,64,85	0
22	EDO	C	312	4/4	0.90	0.09	38,46,49,49	0
22	EDO	F	107	4/4	0.90	0.25	54,60,63,83	0
22	EDO	O	304	4/4	0.90	0.18	56,64,81,84	0
22	EDO	B	307	4/4	0.91	0.14	36,57,74,101	0
22	EDO	D	204	4/4	0.91	0.13	54,55,56,95	0
22	EDO	B	306	4/4	0.91	0.12	35,46,51,94	0
22	EDO	W	102	4/4	0.92	0.20	53,80,80,128	0
24	CHD	P	304	29/29	0.92	0.11	34,44,64,70	0
22	EDO	F	106	4/4	0.92	0.10	43,43,53,54	0
22	EDO	T	106	4/4	0.92	0.16	38,40,45,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	DMU	M	101	33/33	0.93	0.12	36,46,68,80	0
22	EDO	F	108	4/4	0.93	0.31	74,76,86,88	0
22	EDO	A	611	4/4	0.93	0.18	37,41,41,94	0
22	EDO	N	619	4/4	0.93	0.30	49,65,71,83	0
22	EDO	N	612	4/4	0.93	0.21	40,55,59,61	0
22	EDO	B	304	4/4	0.93	0.15	59,73,85,88	0
22	EDO	Y	104	4/4	0.93	0.29	56,71,73,83	0
22	EDO	N	613	4/4	0.93	0.24	52,55,73,74	0
22	EDO	N	617	4/4	0.93	0.19	48,48,58,79	0
22	EDO	P	316	4/4	0.94	0.17	32,52,92,94	0
22	EDO	A	617	4/4	0.94	0.66	49,69,96,141	0
22	EDO	N	622	4/4	0.94	0.24	29,50,67,70	0
22	EDO	D	207	4/4	0.94	0.20	42,70,72,108	0
28	PO4	U	101	5/5	0.94	0.16	59,65,141,151	0
22	EDO	J	103	4/4	0.94	0.19	44,70,75,83	0
22	EDO	H	102	4/4	0.94	0.23	41,41,57,84	0
22	EDO	A	615	4/4	0.95	0.23	30,61,69,139	0
22	EDO	S	106	4/4	0.95	0.16	38,45,59,63	0
22	EDO	Q	204	4/4	0.95	0.20	35,64,73,77	0
22	EDO	A	612	4/4	0.95	0.12	24,28,31,31	0
22	EDO	F	104	4/4	0.95	0.28	60,66,79,83	0
22	EDO	G	103	4/4	0.95	0.08	31,37,40,44	0
22	EDO	D	205	4/4	0.95	0.18	53,58,60,87	0
28	PO4	H	101	5/5	0.95	0.19	63,70,118,149	0
22	EDO	P	312	4/4	0.96	0.13	37,43,47,68	0
22	EDO	S	102	4/4	0.96	0.11	33,33,35,39	0
22	EDO	B	305	4/4	0.96	0.16	44,56,58,76	0
26	PEK	P	308	53/53	0.96	0.12	31,50,93,125	0
22	EDO	F	105	4/4	0.96	0.20	36,39,40,42	0
22	EDO	N	621	4/4	0.96	0.17	37,47,53,79	0
24	CHD	G	101	29/29	0.96	0.09	27,32,38,49	0
22	EDO	P	311	4/4	0.96	0.22	40,46,48,56	0
22	EDO	S	104	4/4	0.96	0.10	32,35,38,42	0
22	EDO	A	616	4/4	0.96	0.17	48,53,72,112	0
22	EDO	C	315	4/4	0.96	0.25	51,65,79,108	0
22	EDO	O	303	4/4	0.96	0.10	33,35,37,38	0
24	CHD	T	101	29/29	0.96	0.09	28,33,41,65	0
26	PEK	C	309	53/53	0.96	0.13	31,48,111,119	0
19	PGV	P	309	51/51	0.97	0.12	26,37,83,126	0
19	PGV	N	607	51/51	0.97	0.12	26,38,64,78	0
27	ZN	S	101	1/1	0.97	0.19	55,55,55,55	0
19	PGV	A	608	51/51	0.97	0.12	26,33,69,92	0

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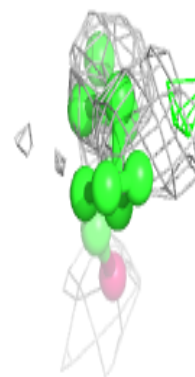
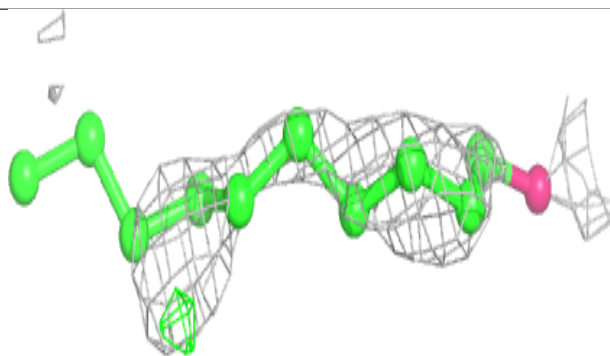
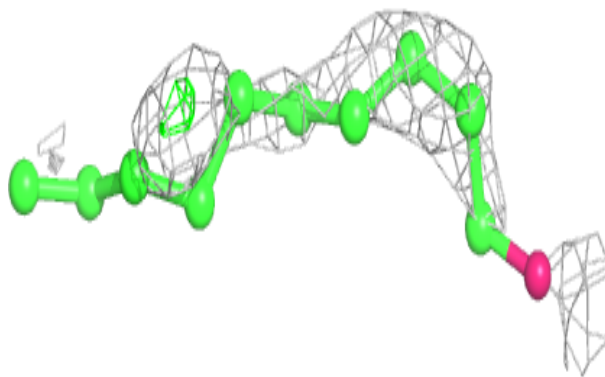
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
22	EDO	N	610	4/4	0.97	0.25	33,57,77,86	0
22	EDO	E	202	4/4	0.97	0.08	37,40,47,53	0
27	ZN	F	101	1/1	0.97	0.17	55,55,55,55	0
19	PGV	C	310	51/51	0.97	0.12	26,33,93,120	0
22	EDO	N	609	4/4	0.97	0.15	29,32,35,37	0
22	EDO	C	313	4/4	0.97	0.17	34,41,56,57	0
14	HEA	A	602	60/60	0.97	0.11	22,27,38,47	0
14	HEA	N	601[B]	60/60	0.98	0.12	24,30,48,56	12
16	MG	A	604	1/1	0.98	0.07	29,29,29,29	0
17	NA	N	605	1/1	0.98	0.07	34,34,34,34	0
14	HEA	A	601[A]	60/60	0.98	0.11	20,24,41,51	12
22	EDO	E	201	4/4	0.98	0.10	44,47,50,56	0
17	NA	P	301	1/1	0.98	0.26	22,22,22,22	0
14	HEA	N	602	60/60	0.98	0.10	24,28,33,47	0
22	EDO	B	303	4/4	0.98	0.11	30,31,32,40	0
15	CU	N	603	1/1	0.98	0.15	30,30,30,30	0
14	HEA	A	601[B]	60/60	0.98	0.11	20,24,41,51	12
14	HEA	N	601[A]	60/60	0.98	0.12	23,30,48,53	12
22	EDO	N	614	4/4	0.98	0.23	38,45,67,71	0
22	EDO	F	103	4/4	0.98	0.12	31,35,37,40	0
22	EDO	A	614	4/4	0.98	0.12	36,57,62,82	0
17	NA	A	605	1/1	0.99	0.08	29,29,29,29	0
17	NA	C	301	1/1	0.99	0.24	22,22,22,22	0
16	MG	N	604	1/1	0.99	0.05	31,31,31,31	0
23	CUA	O	301	2/2	0.99	0.14	32,32,32,33	0
15	CU	A	603	1/1	1.00	0.13	29,29,29,29	0
23	CUA	B	301	2/2	1.00	0.16	28,28,28,29	0

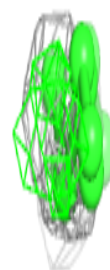
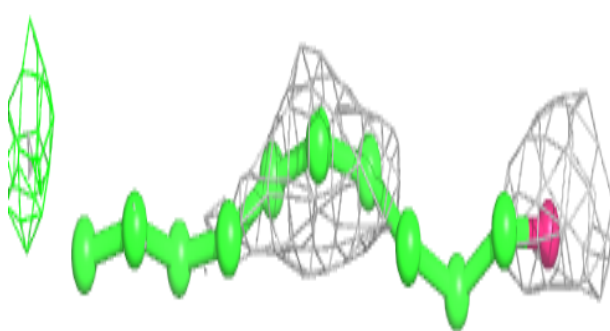
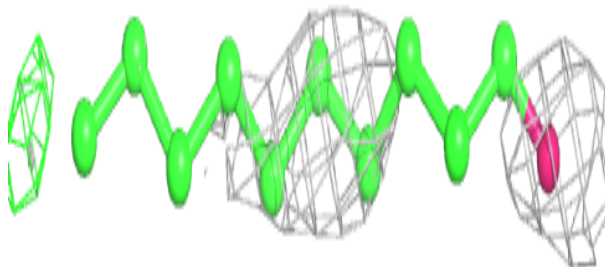
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DMU X 105:**

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

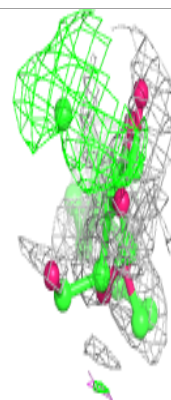
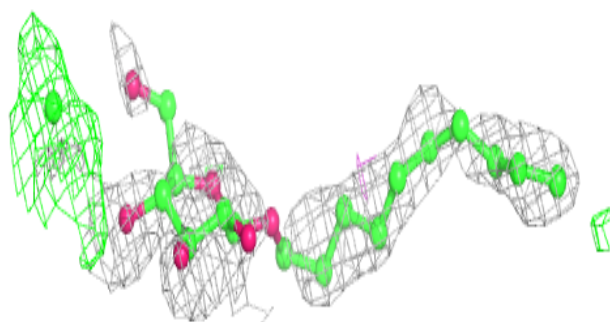
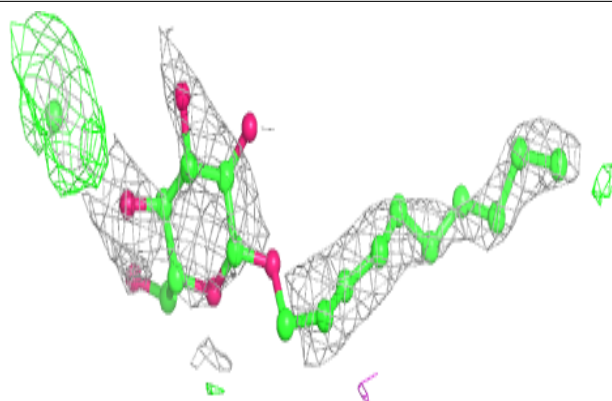
**Electron density around DMU K 104:**

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

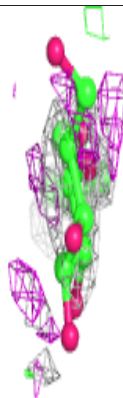
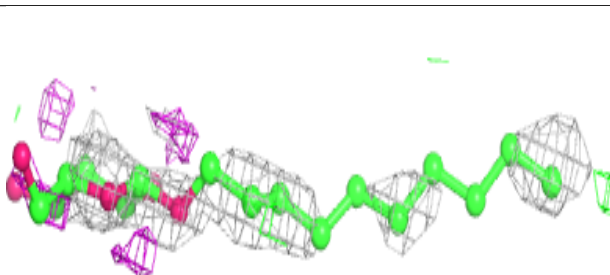
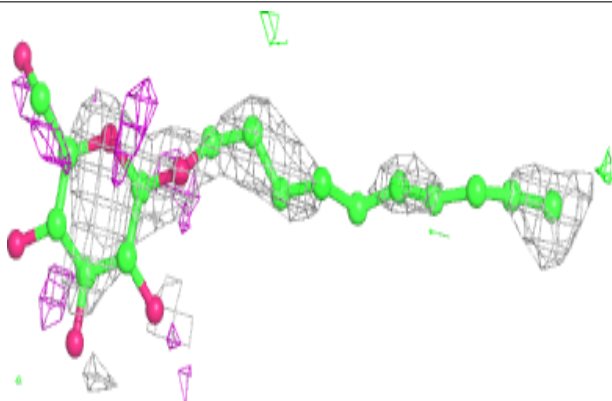


**Electron density around DMU Q 201:**

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

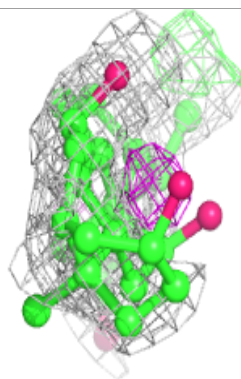
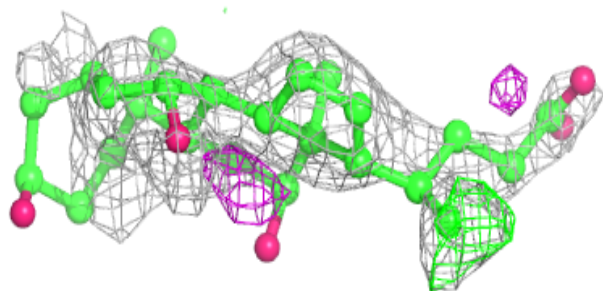
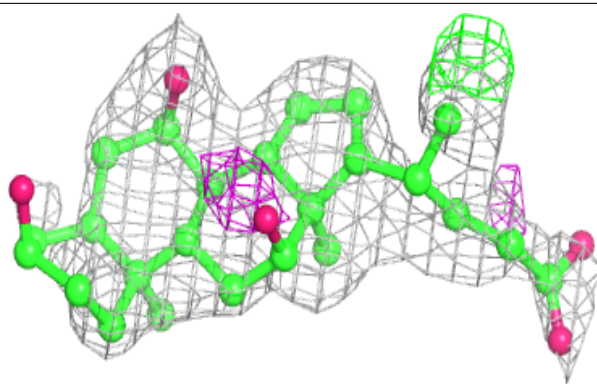
**Electron density around DMU K 103:**

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

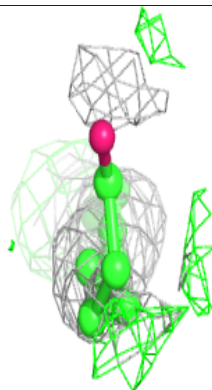
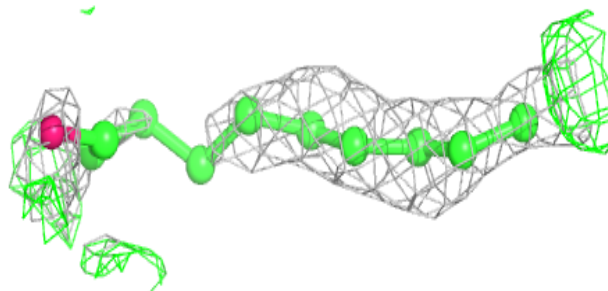
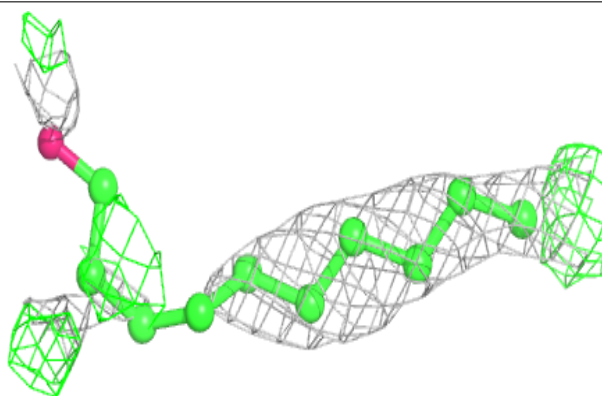


**Electron density around CHD J 102:**

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

**Electron density around DMU X 103:**

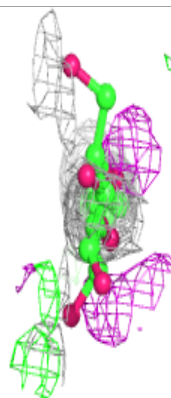
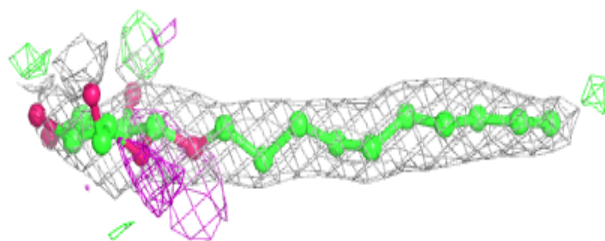
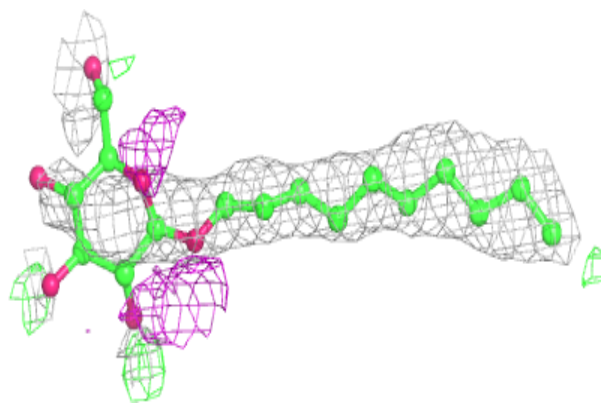
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



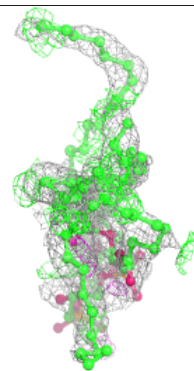
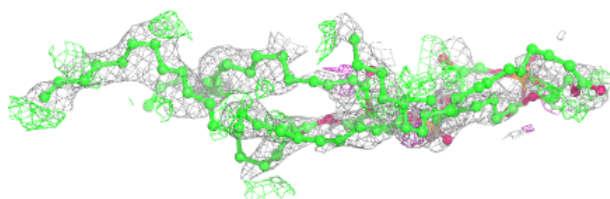
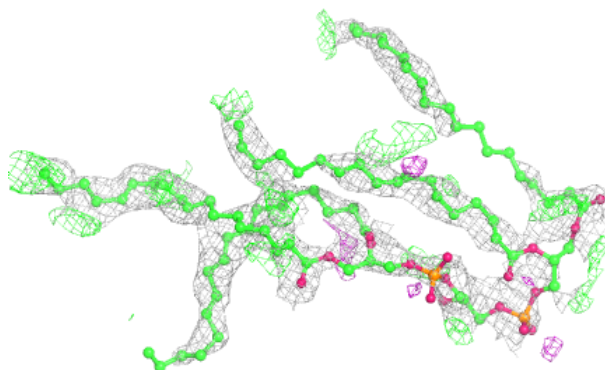


**Electron density around DMU C 303:**

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

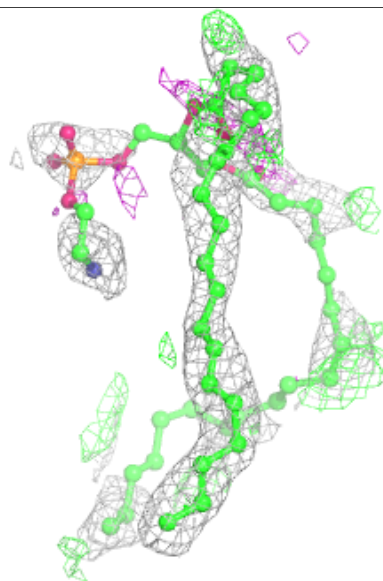
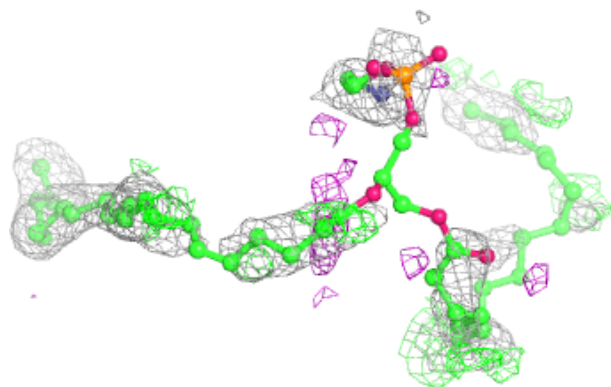
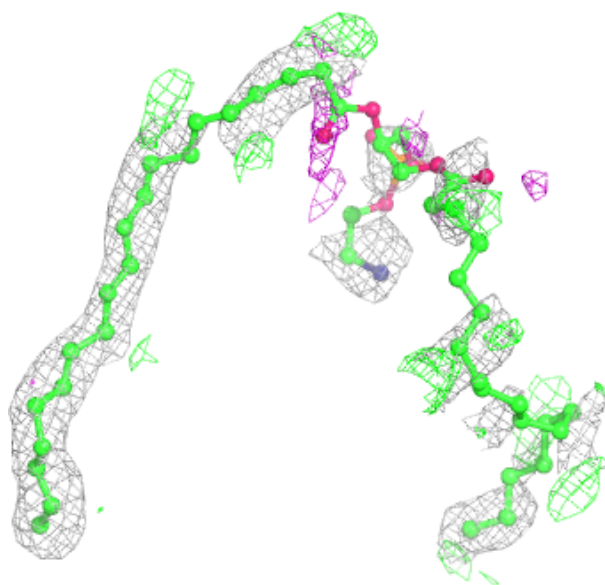
**Electron density around CDL T 102:**

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



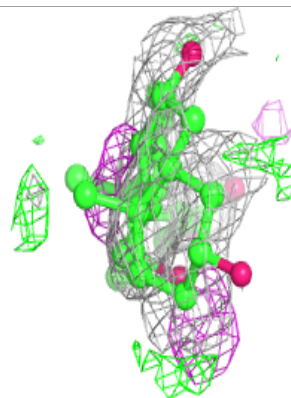
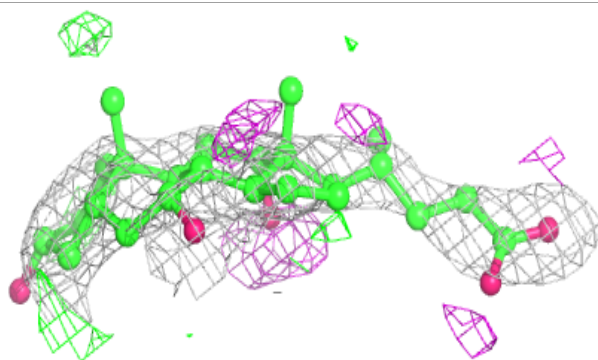
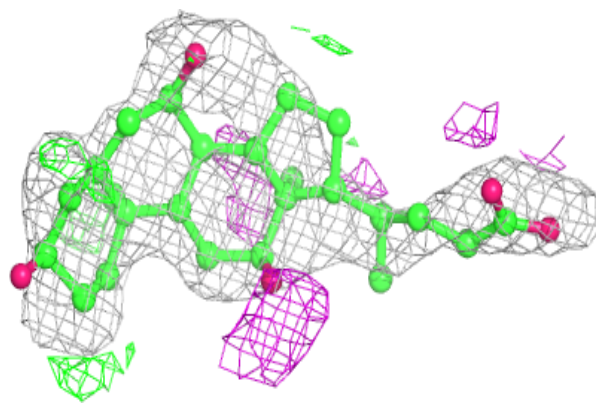
**Electron density around PEK C 308:**

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

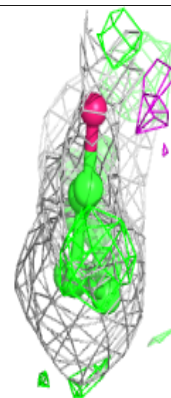
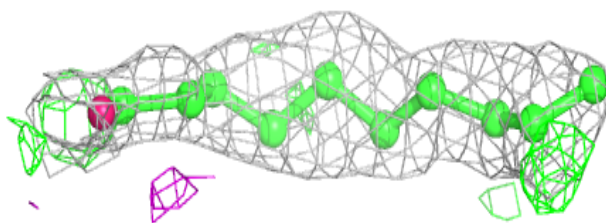
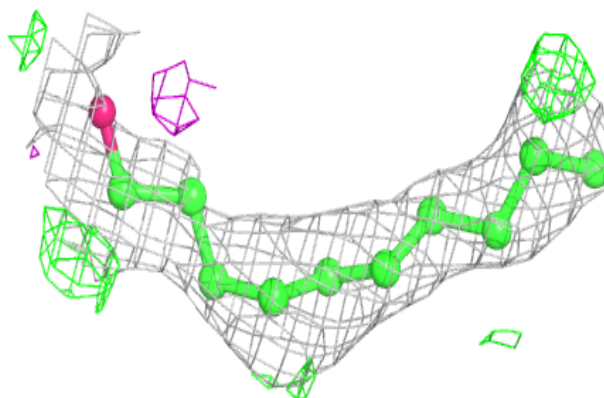


**Electron density around CHD Y 102:**

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

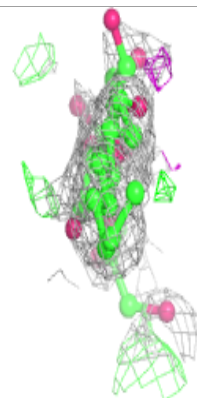
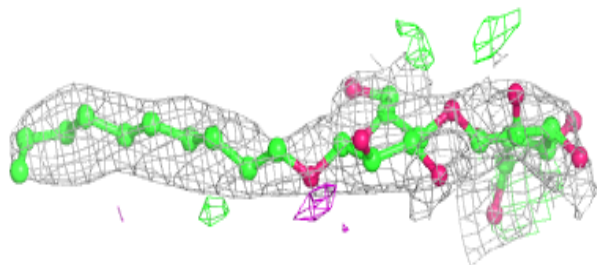
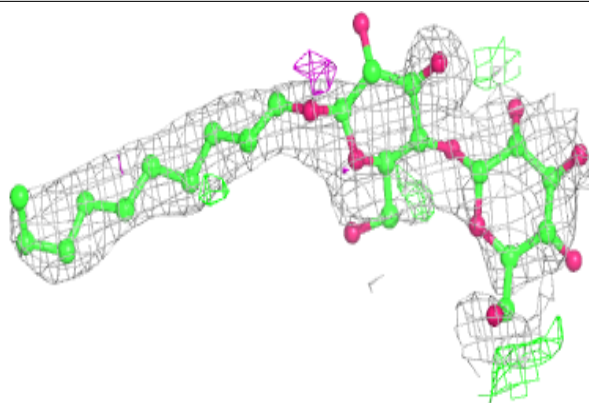
**Electron density around DMU C 304:**

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

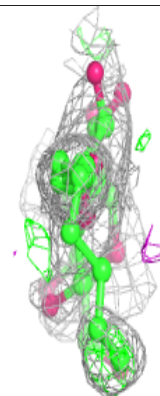
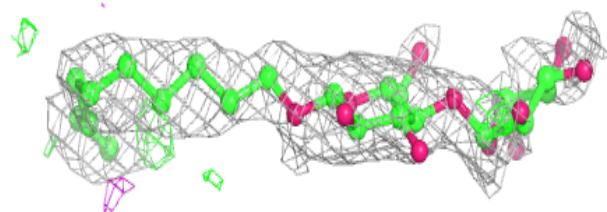
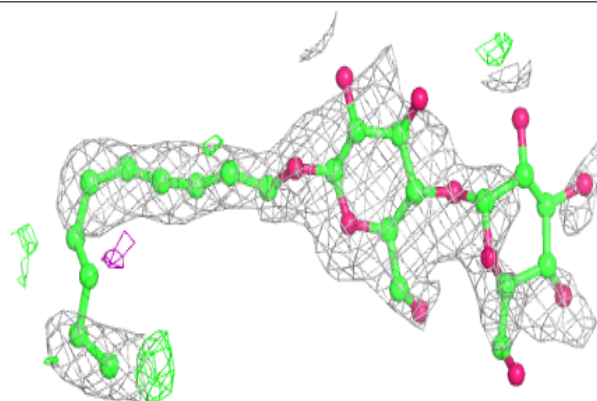


**Electron density around DMU P 303:**

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

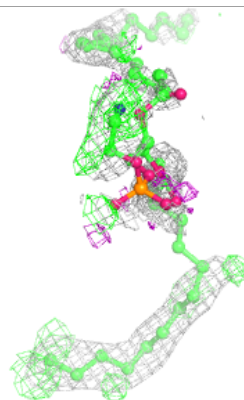
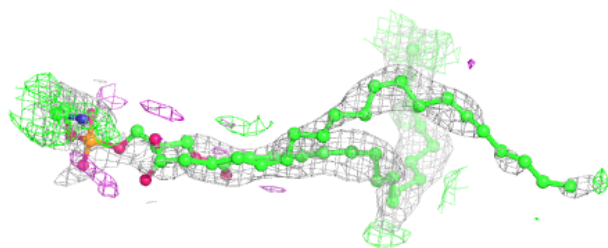
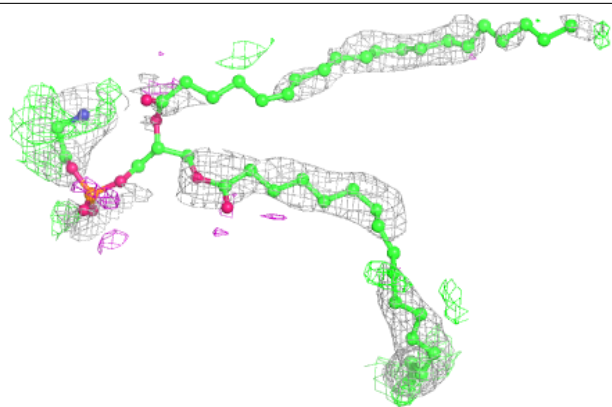
**Electron density around DMU Y 101:**

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

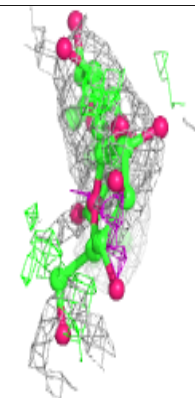
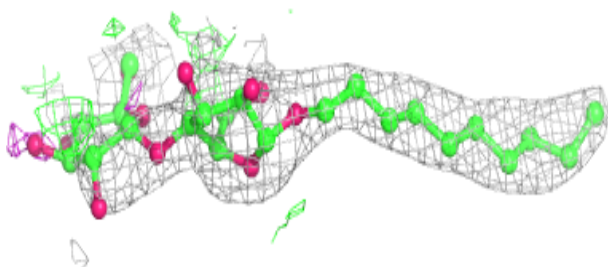
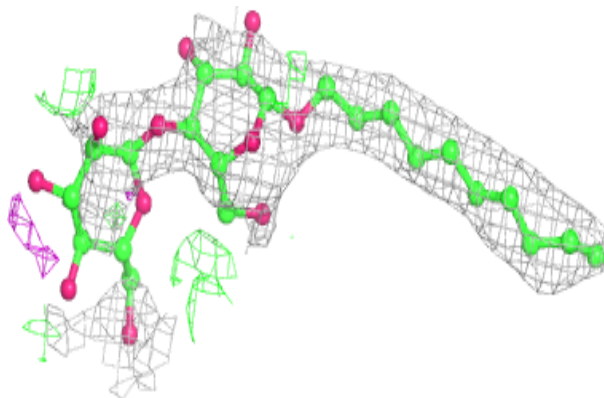


**Electron density around PEK T 103:**

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

**Electron density around DMU C 302:**

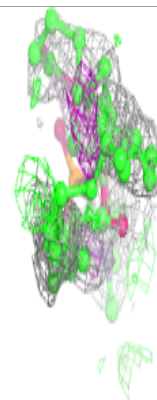
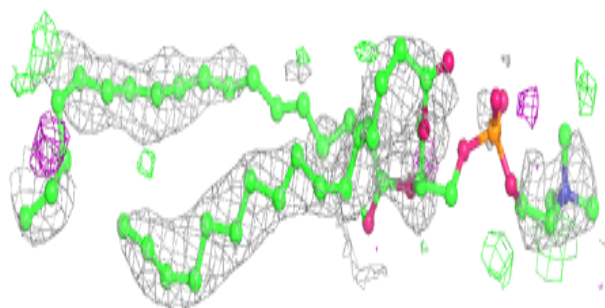
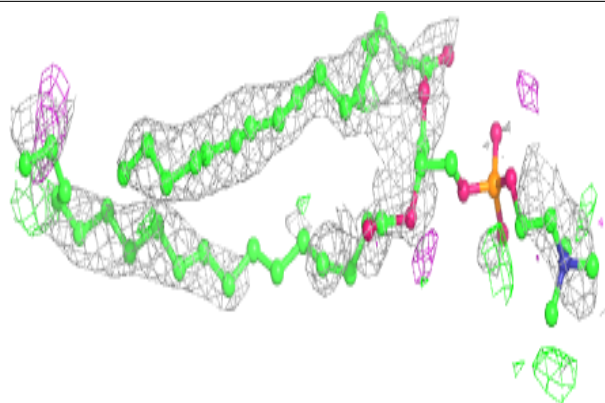
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



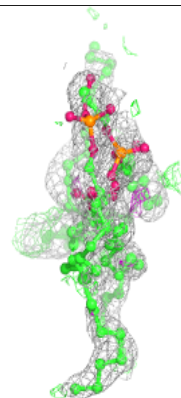
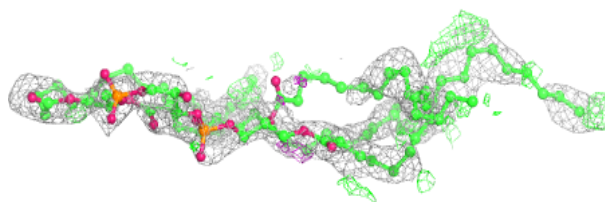
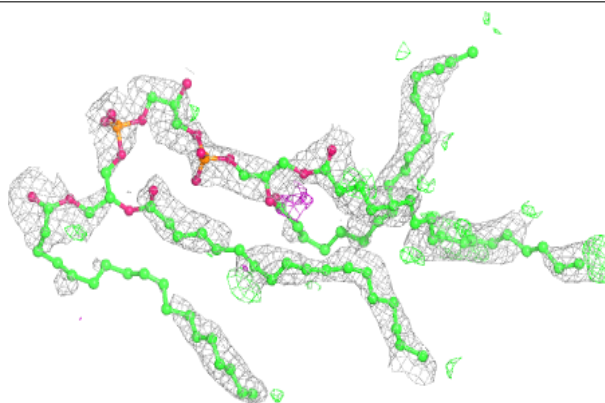


**Electron density around PSC A 609:**

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

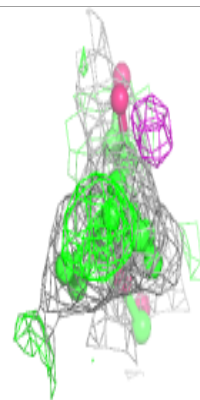
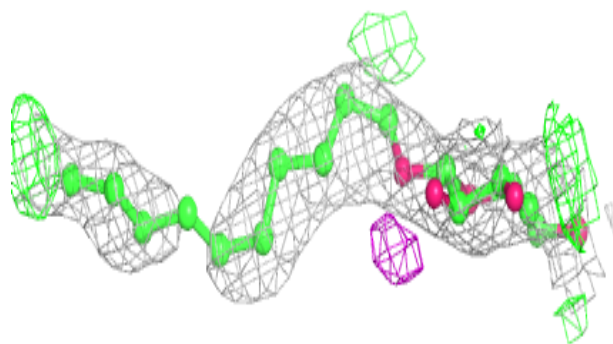
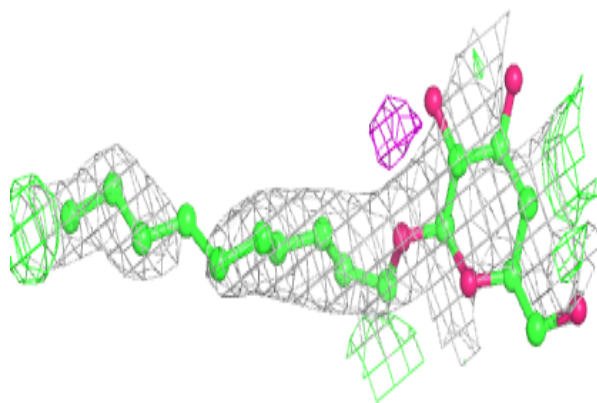
**Electron density around CDL G 102:**

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

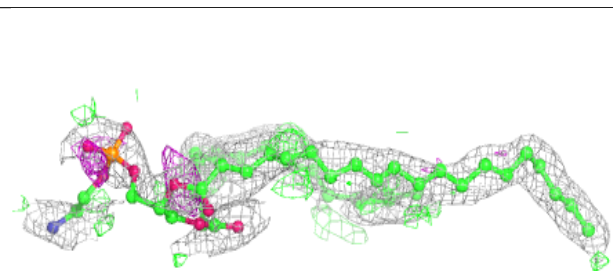
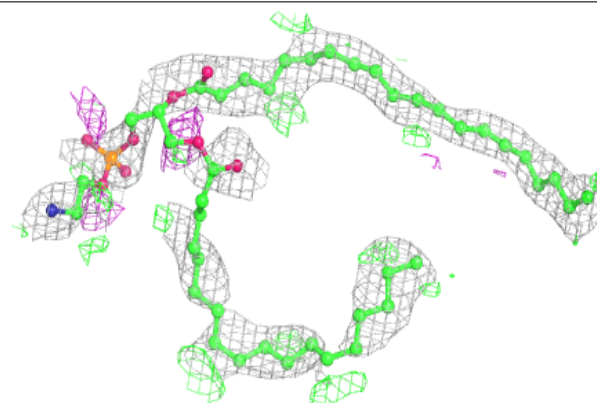


**Electron density around DMU D 201:**

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

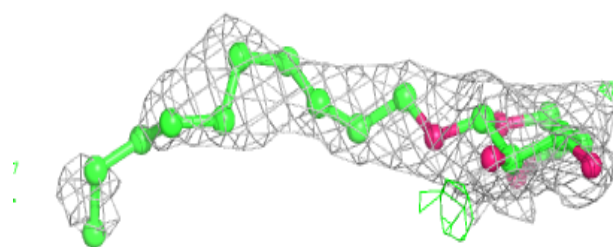
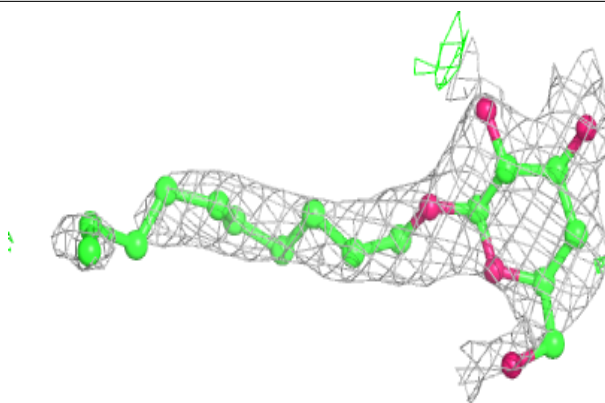
**Electron density around PEK P 307:**

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

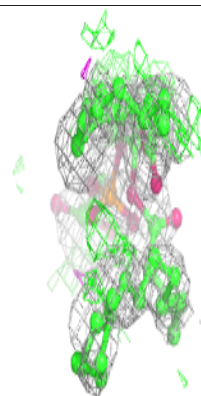
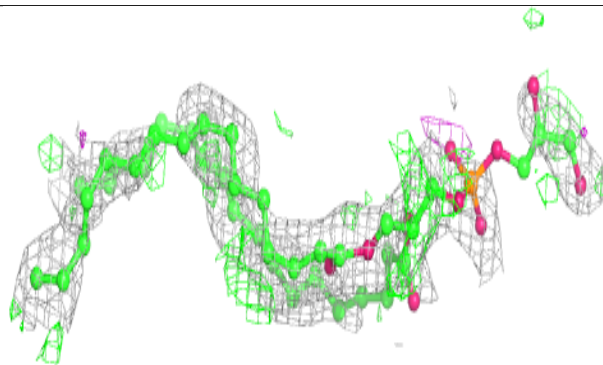
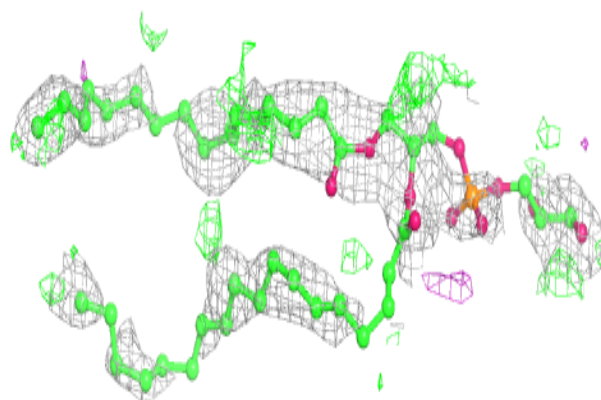


**Electron density around DMU X 102:**

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

**Electron density around PGV T 104:**

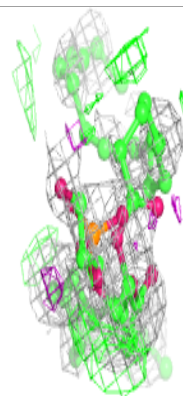
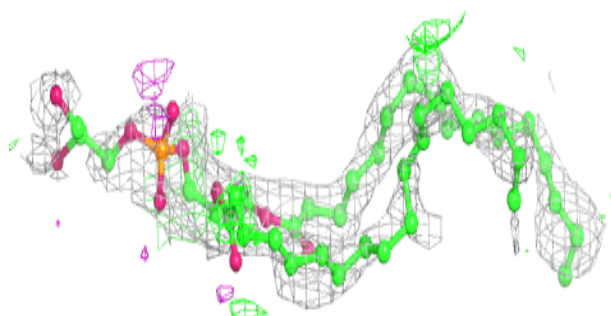
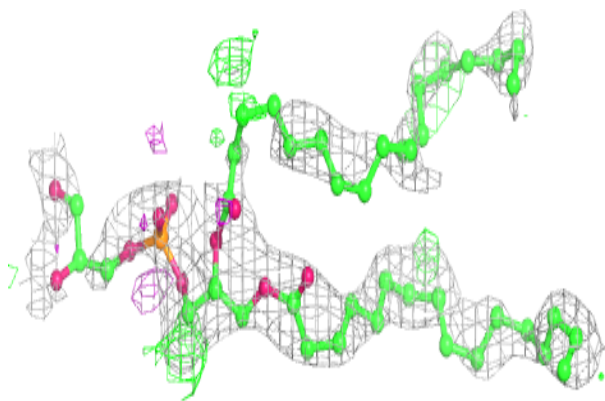
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



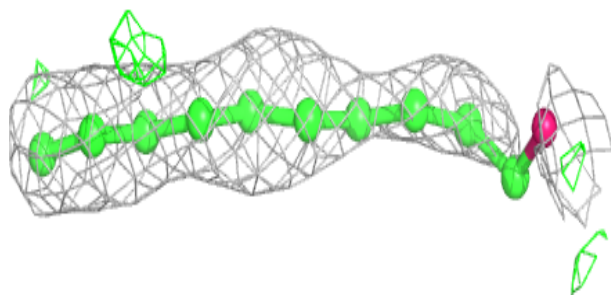
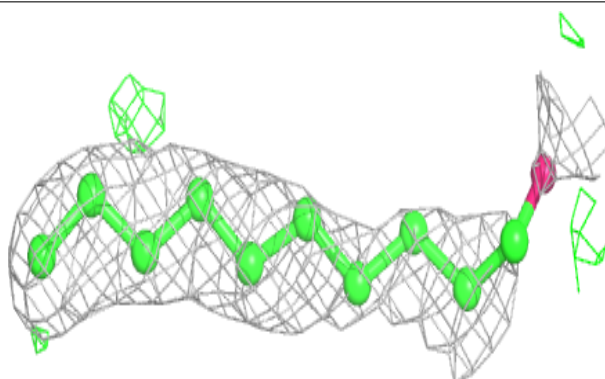


**Electron density around PGV P 310:**

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

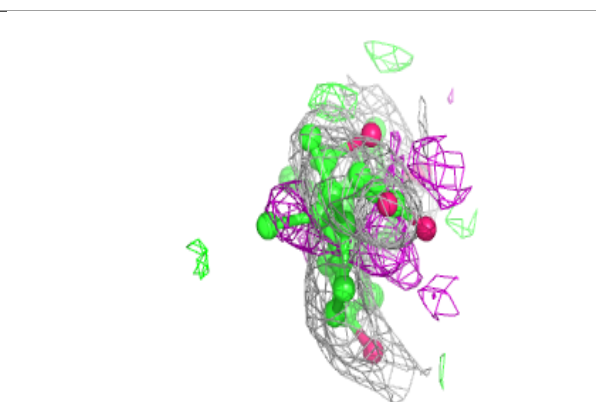
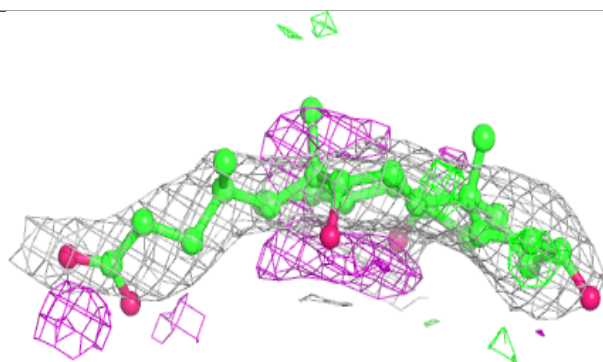
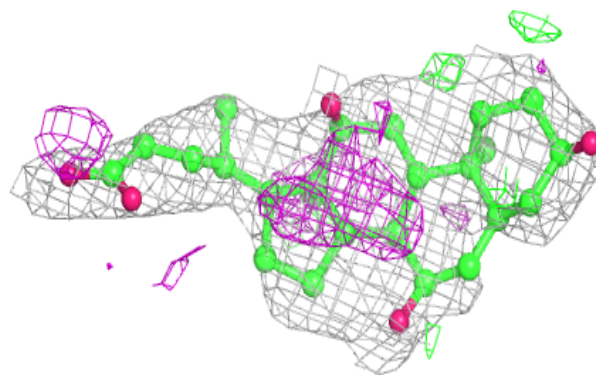
**Electron density around DMU X 101:**

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

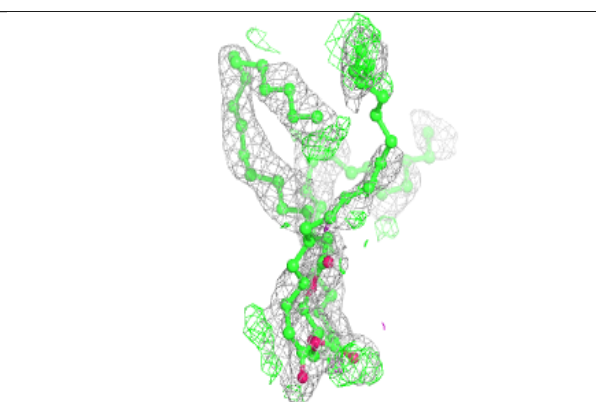
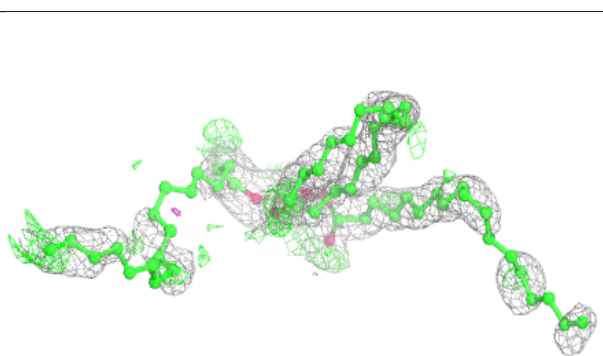
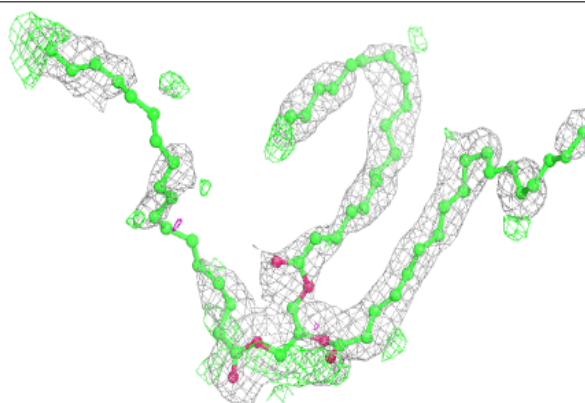


**Electron density around CHD L 102:**

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

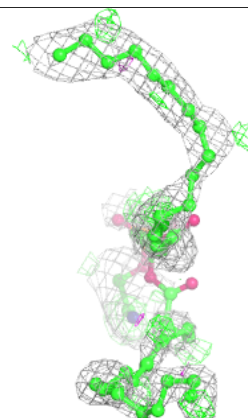
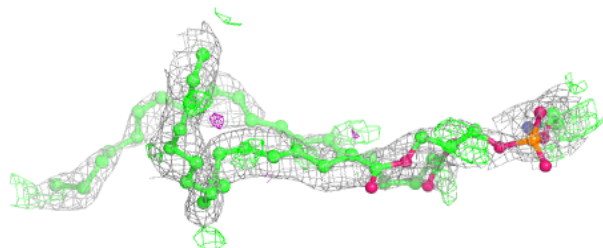
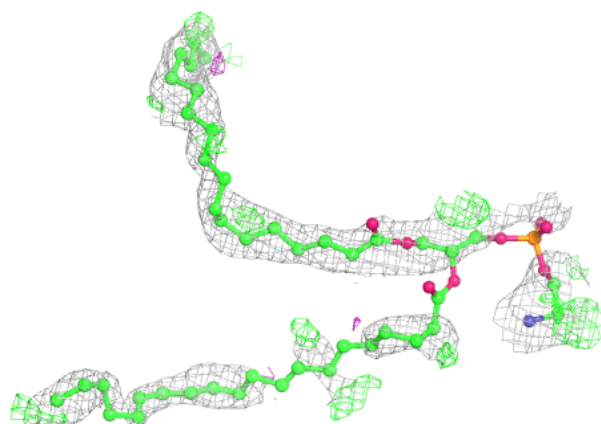
**Electron density around TGL Q 202:**

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

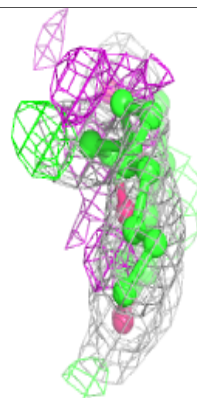
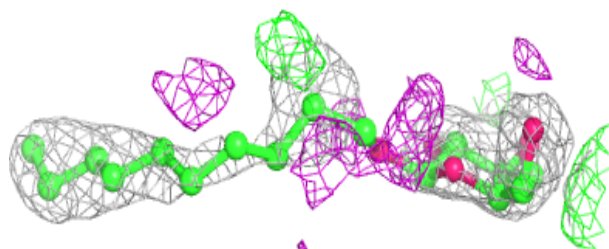
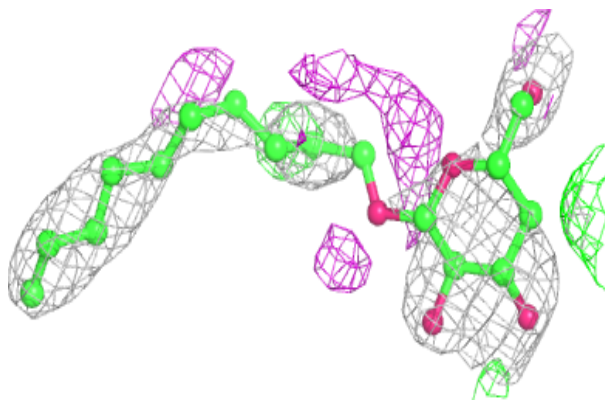


**Electron density around PEK F 102:**

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

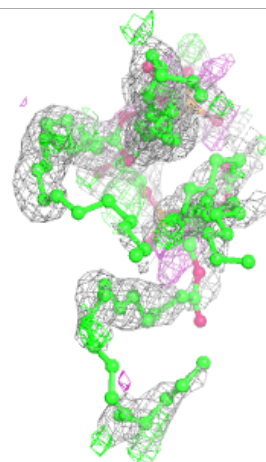
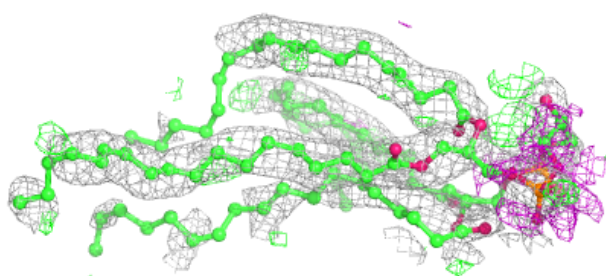
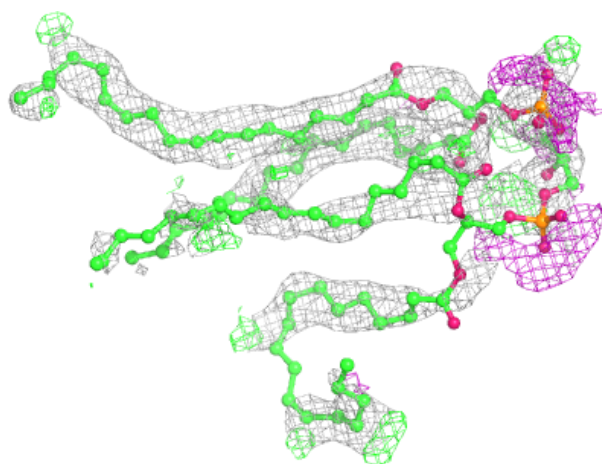
**Electron density around DMU W 101:**

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



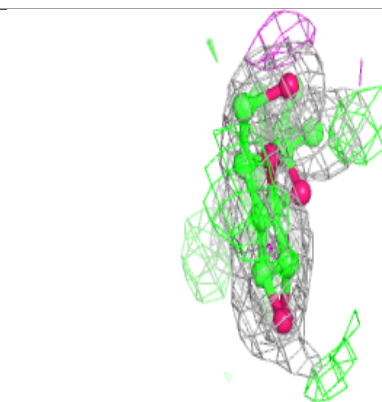
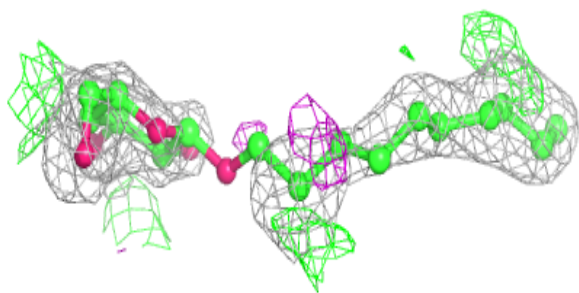
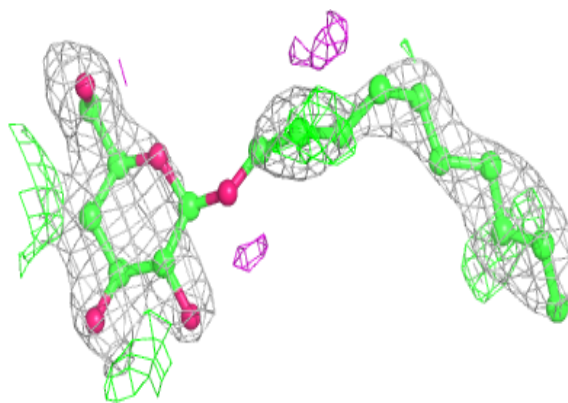
**Electron density around CDL P 306:**

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

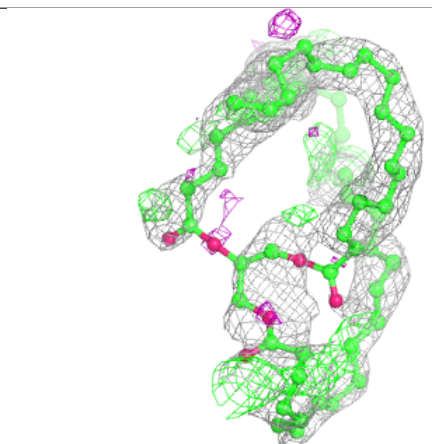
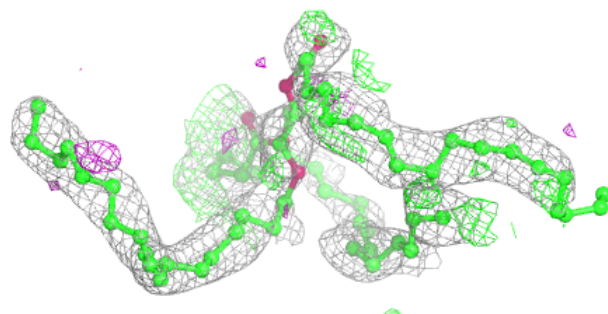
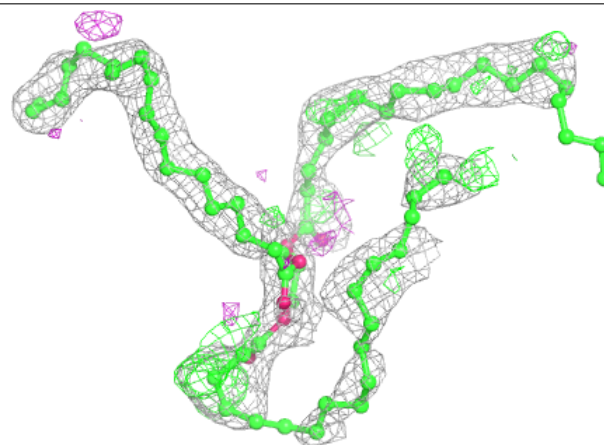


**Electron density around DMU J 101:**

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

**Electron density around TGL Y 103:**

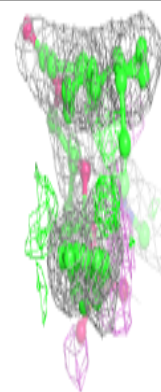
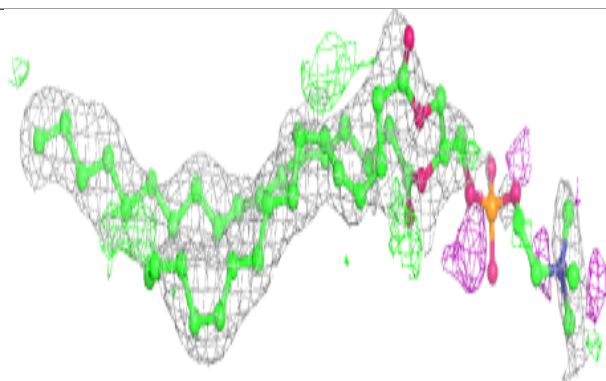
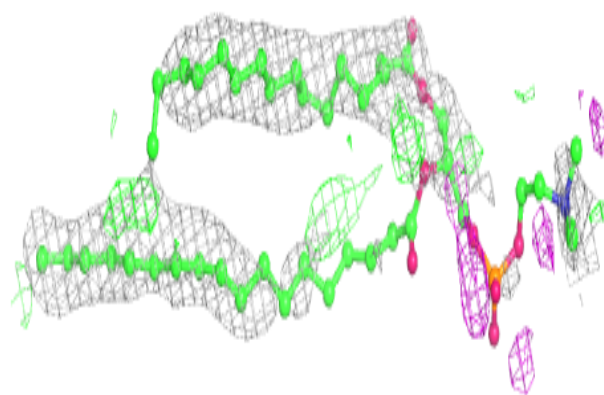
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



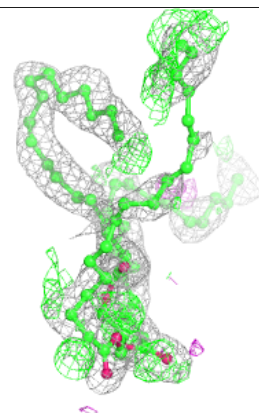
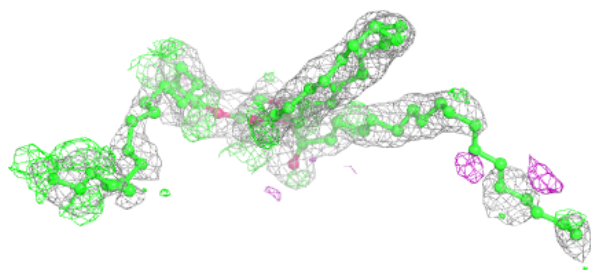
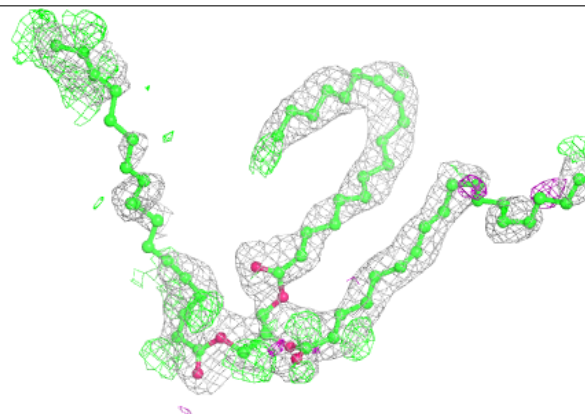


**Electron density around PSC V 101:**

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

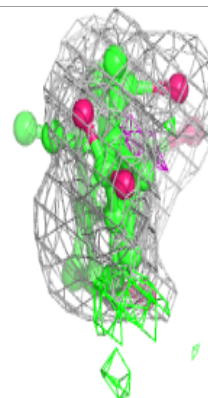
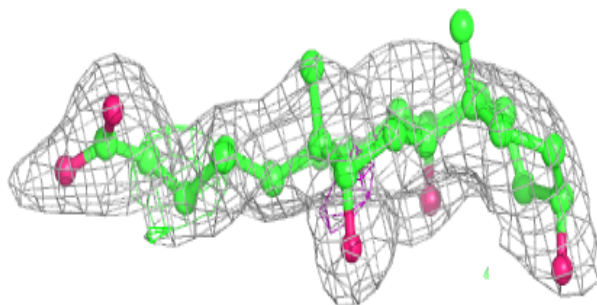
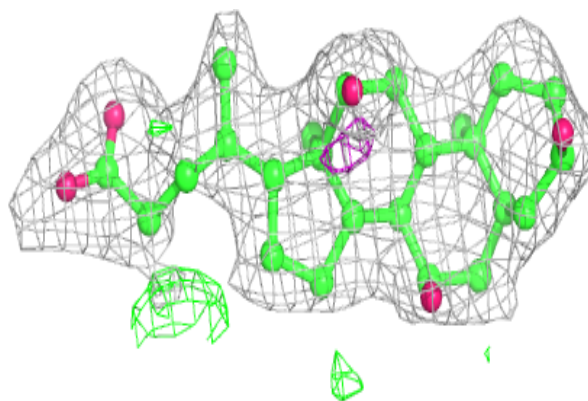
**Electron density around TGL D 202:**

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

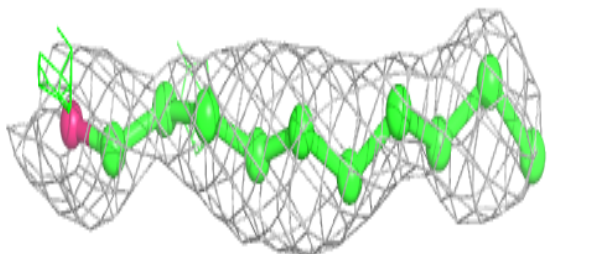
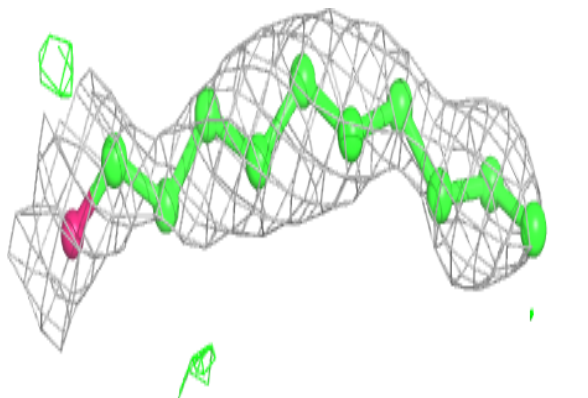


**Electron density around CHD P 305:**

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

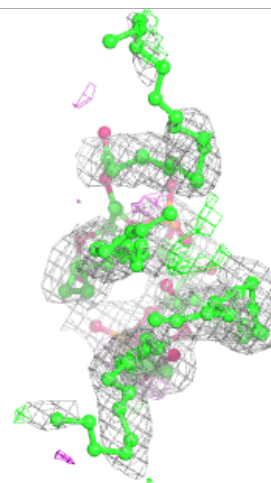
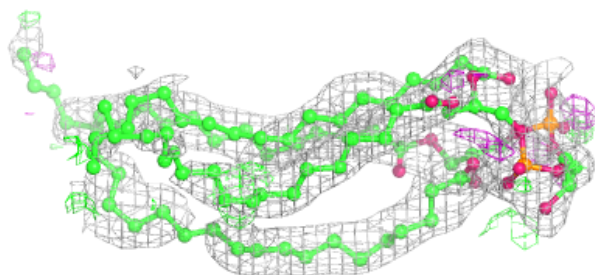
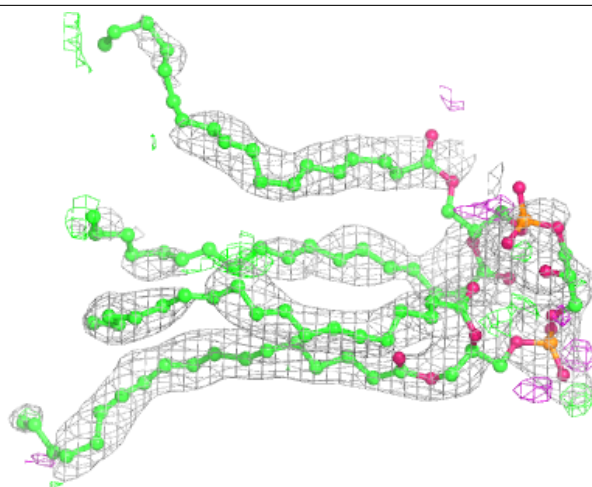
**Electron density around DMU K 101:**

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



**Electron density around CDL C 307:**

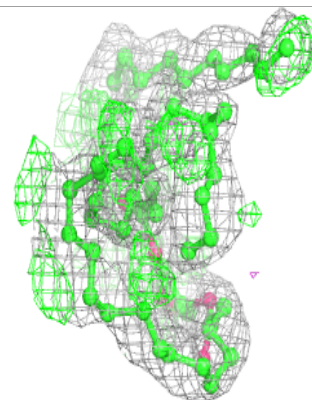
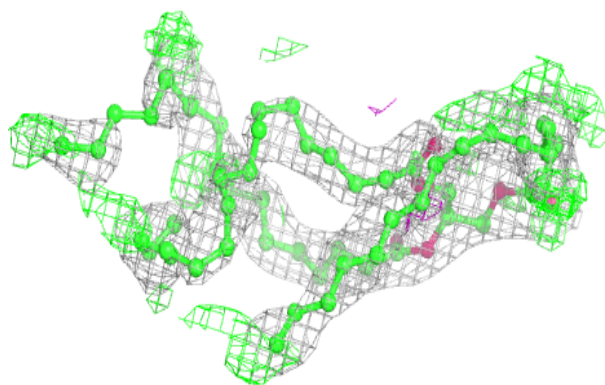
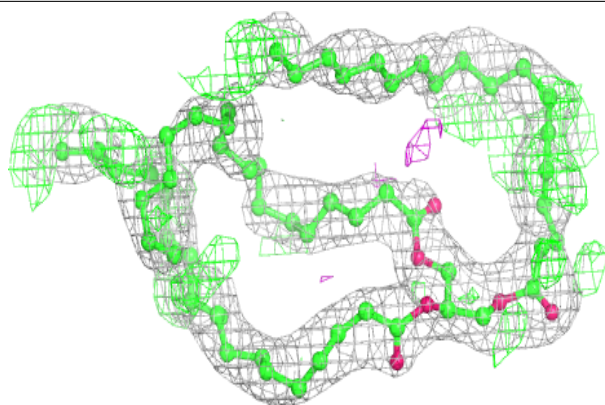
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



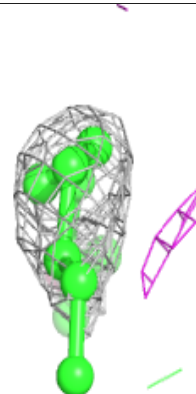
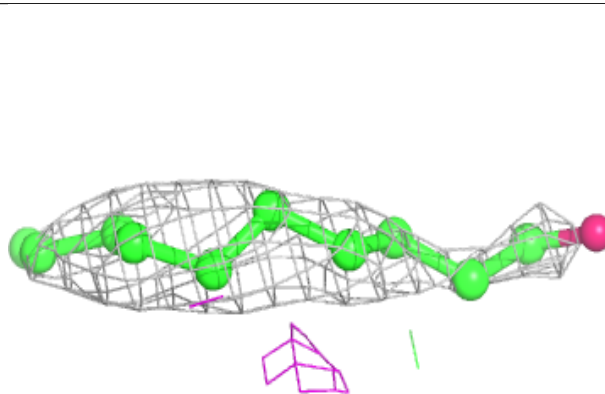
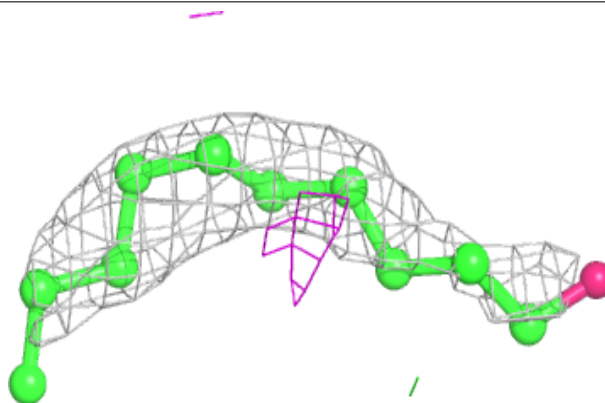


**Electron density around TGL N 608:**

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

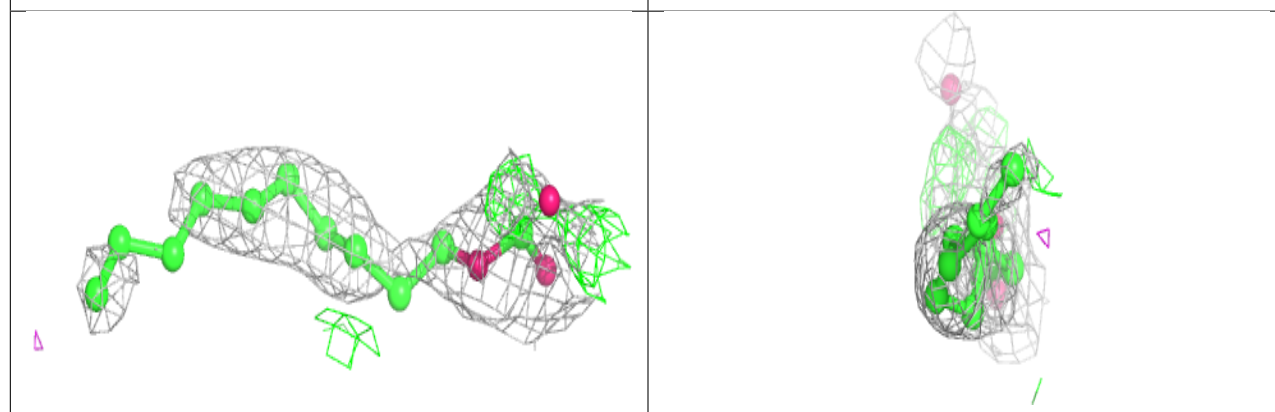
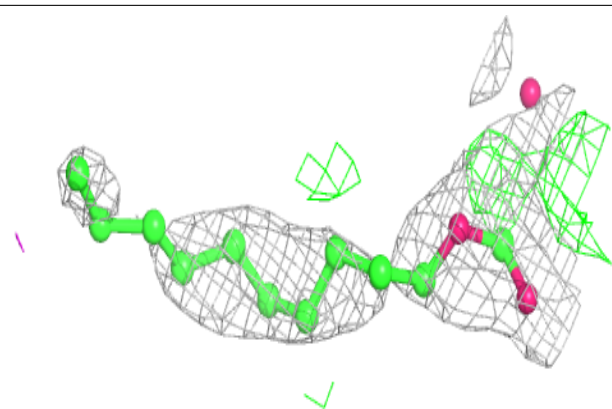
**Electron density around DMU X 104:**

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

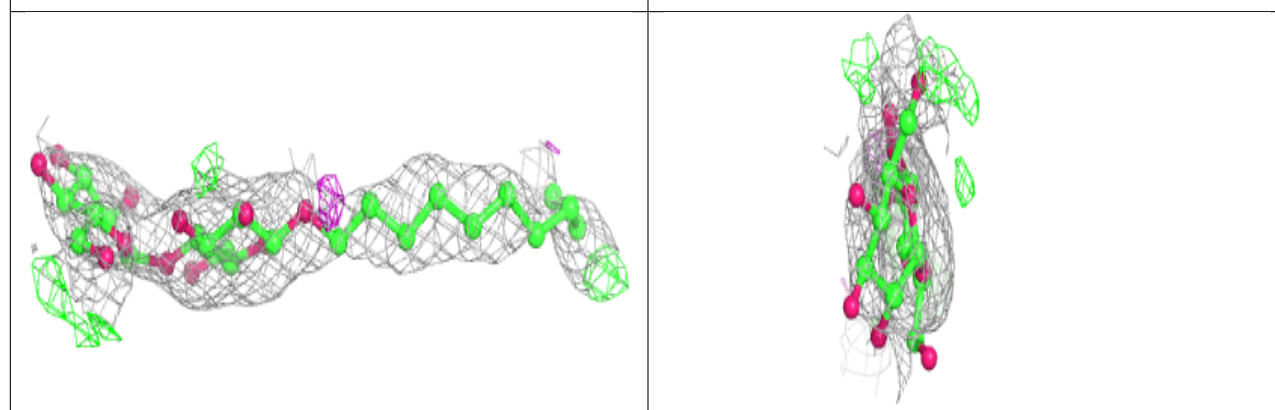
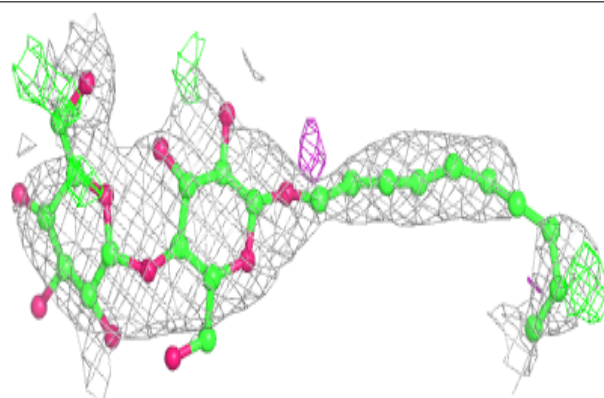


**Electron density around DMU K 102:**

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

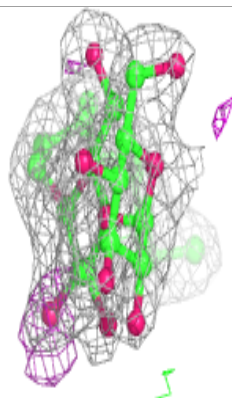
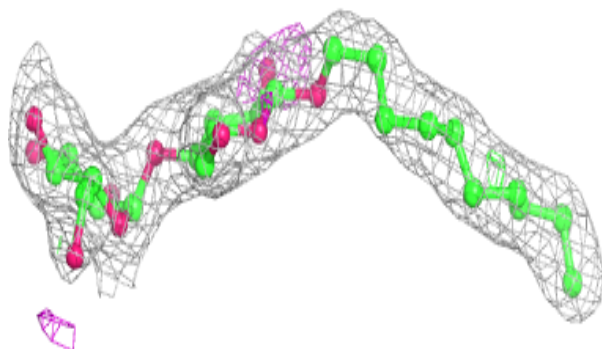
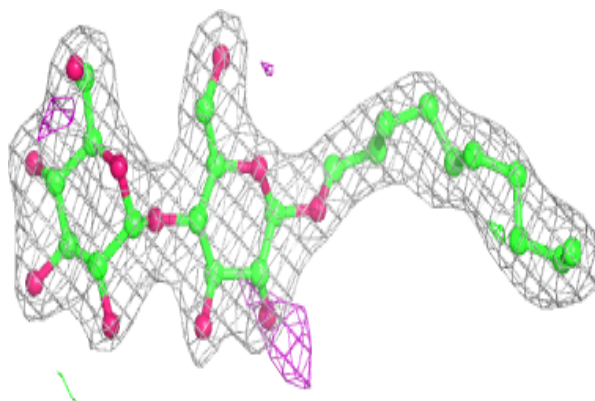
**Electron density around DMU L 101:**

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

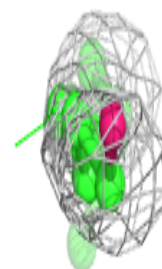
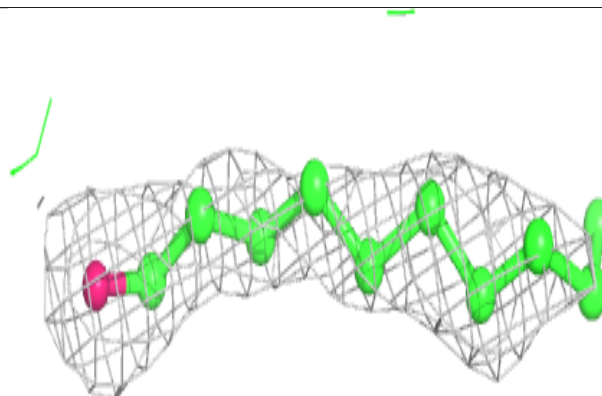
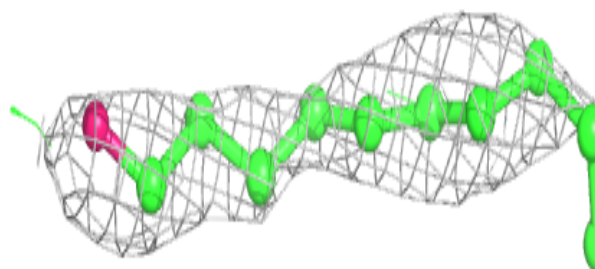


**Electron density around DMU Z 101:**

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

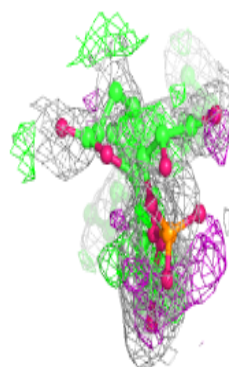
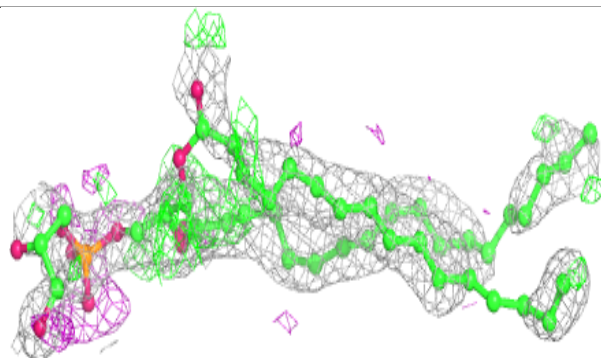
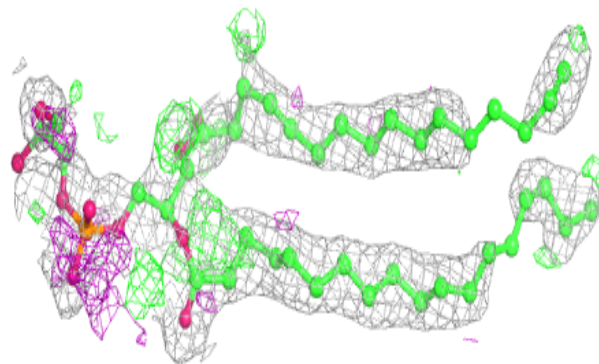
**Electron density around DMU B 302:**

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

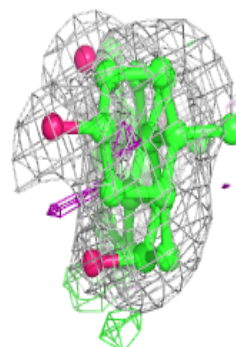
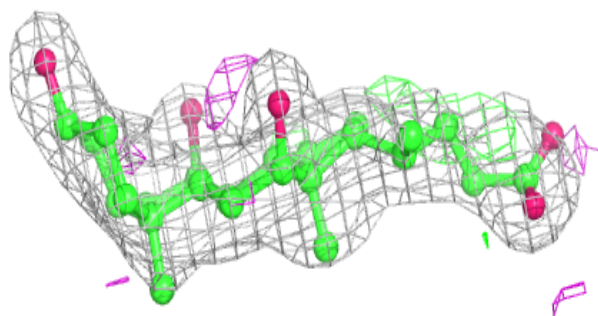
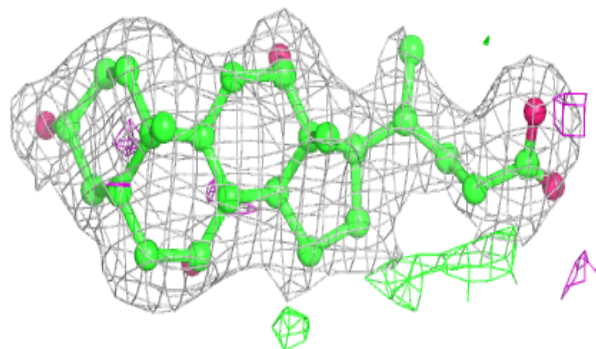


**Electron density around PGV A 607:**

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

**Electron density around CHD C 306:**

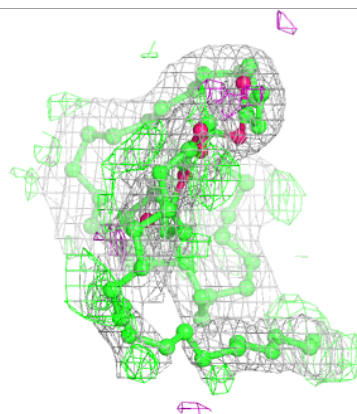
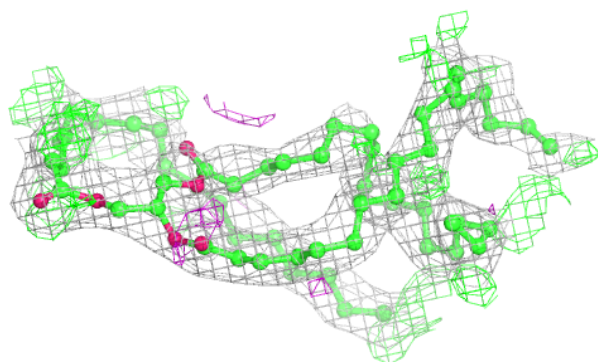
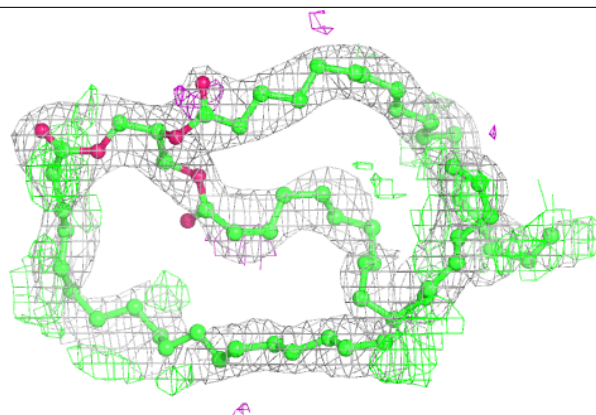
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



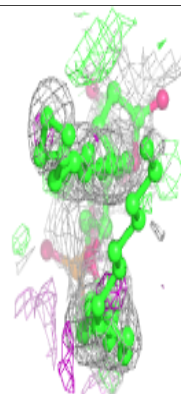
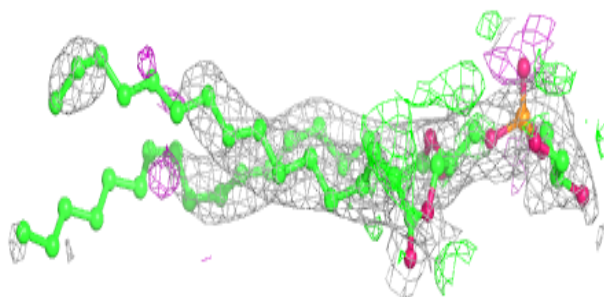
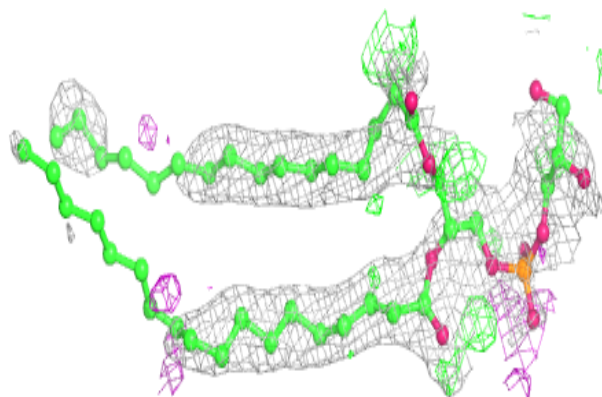


**Electron density around TGL A 610:**

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

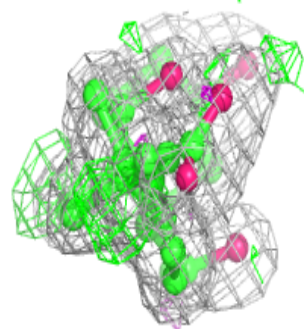
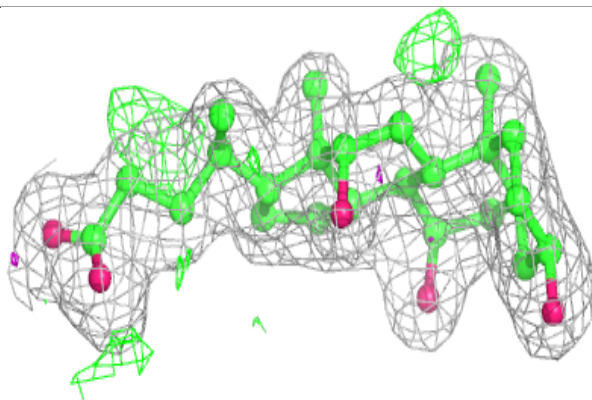
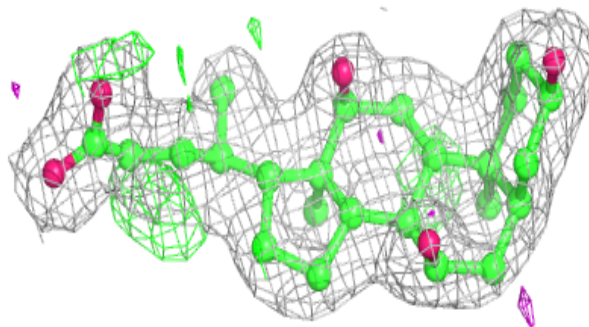
**Electron density around PGV N 606:**

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



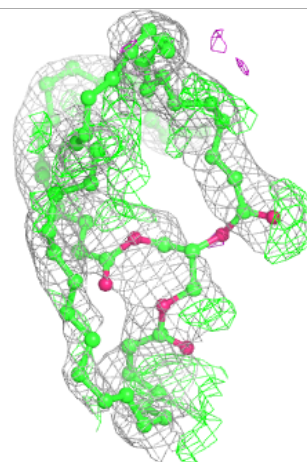
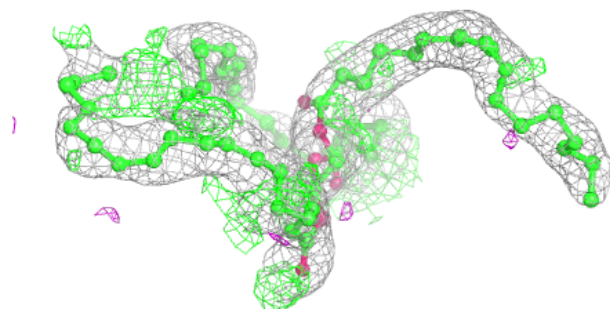
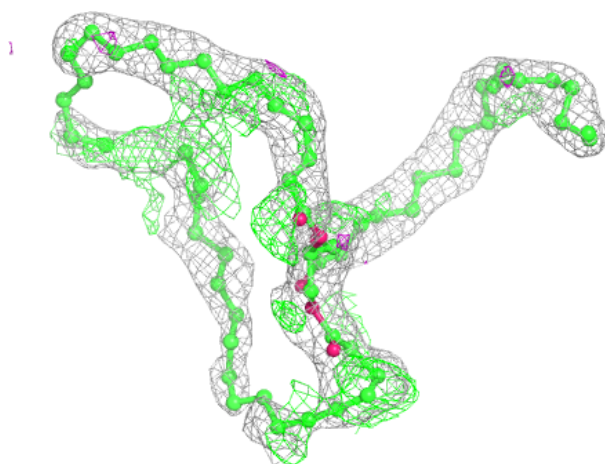
**Electron density around CHD C 305:**

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



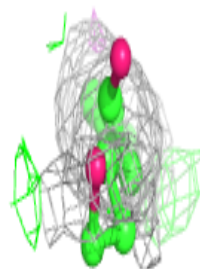
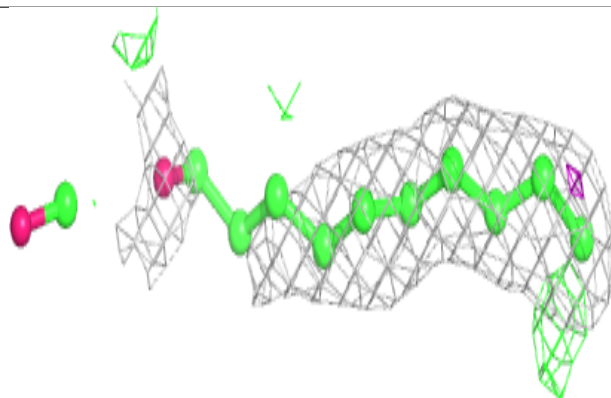
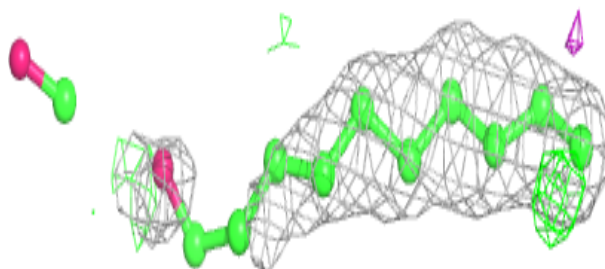
**Electron density around TGL L 103:**

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

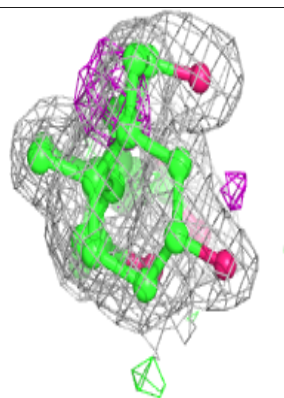
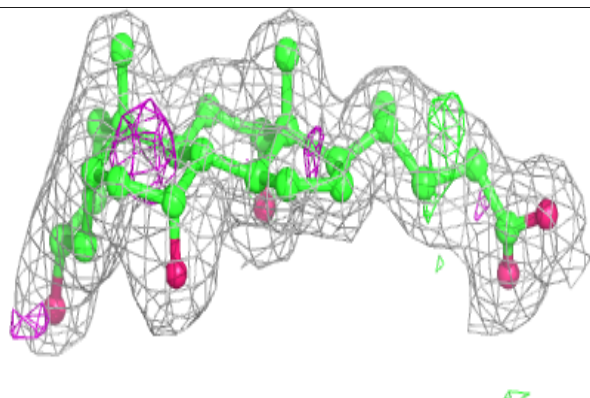
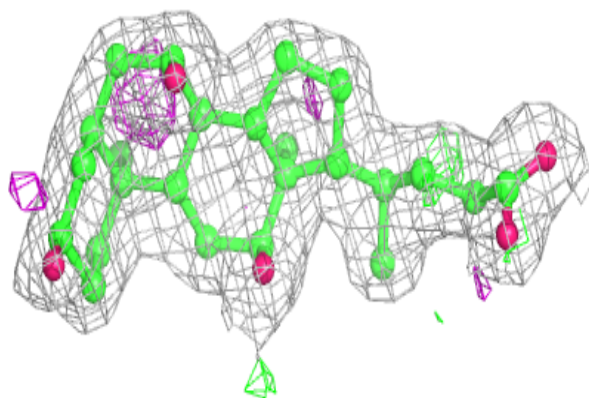


**Electron density around DMU A 606:**

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

**Electron density around CHD P 304:**

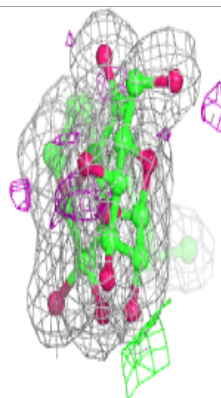
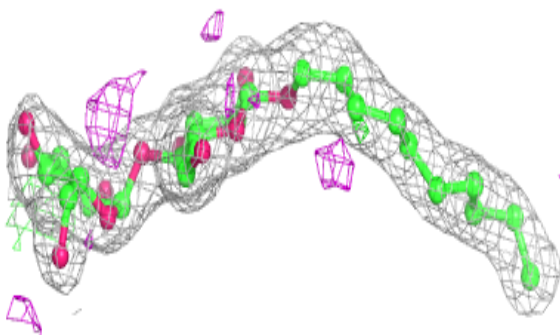
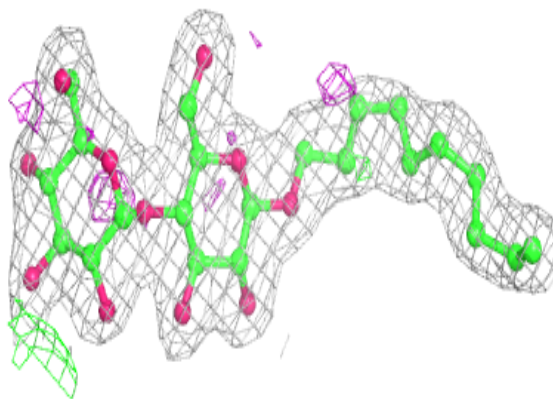
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



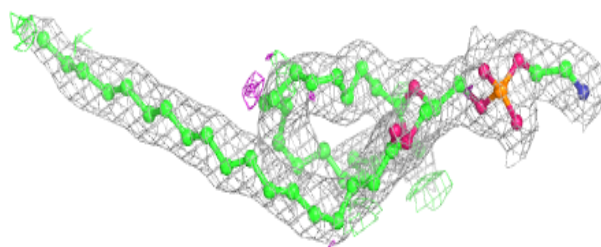
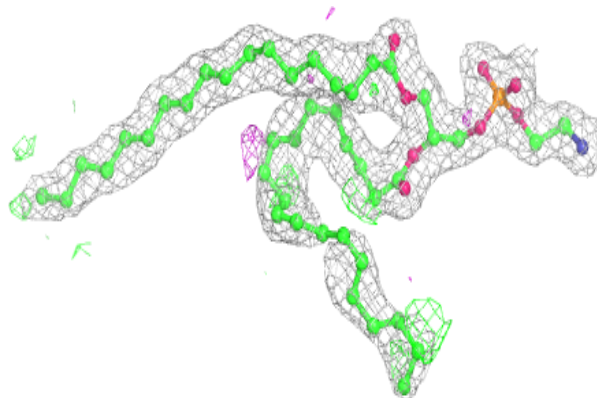


**Electron density around DMU M 101:**

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

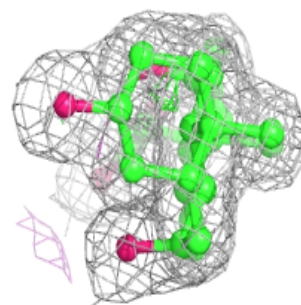
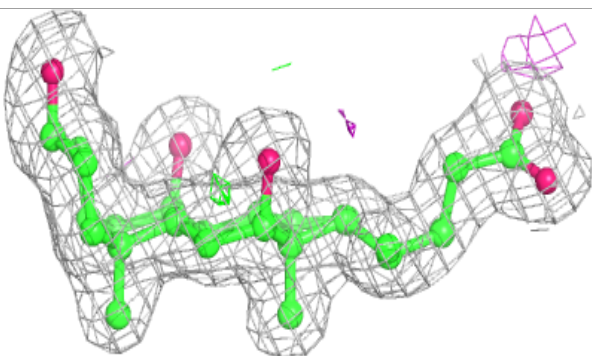
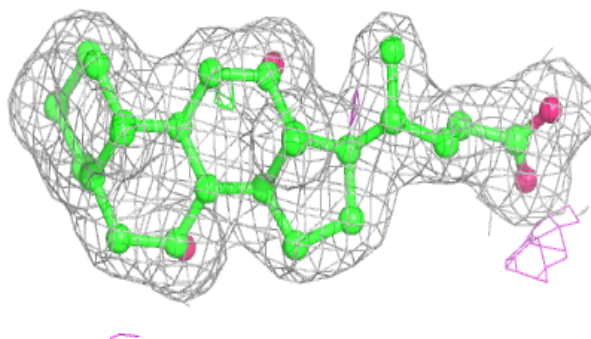
**Electron density around PEK P 308:**

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

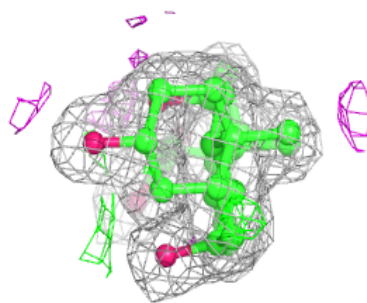
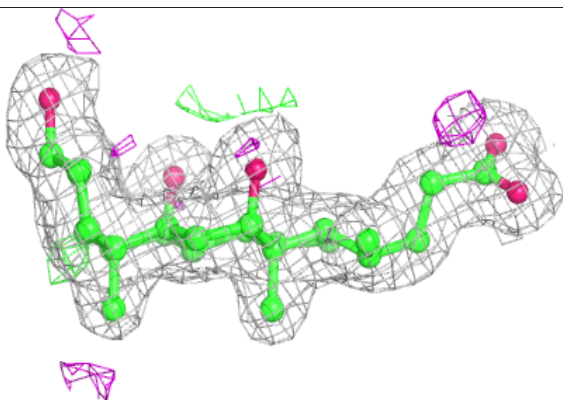
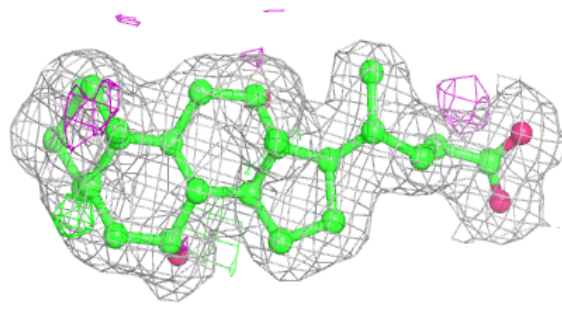


**Electron density around CHD G 101:**

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

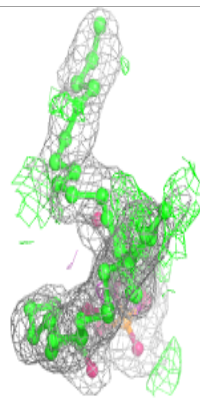
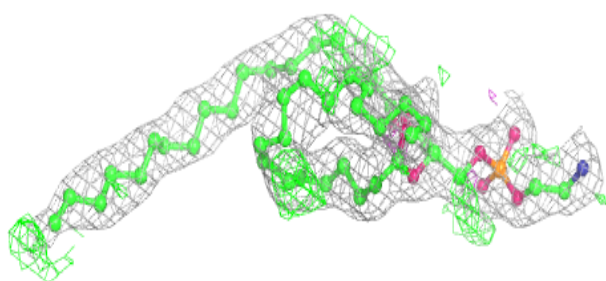
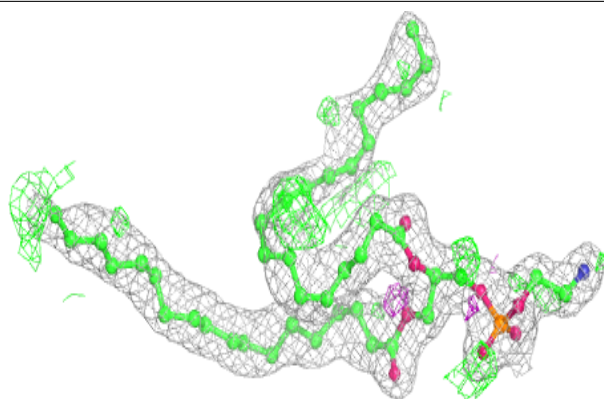
**Electron density around CHD T 101:**

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

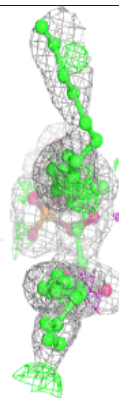
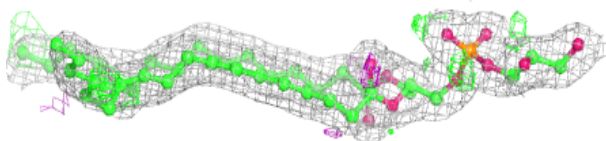
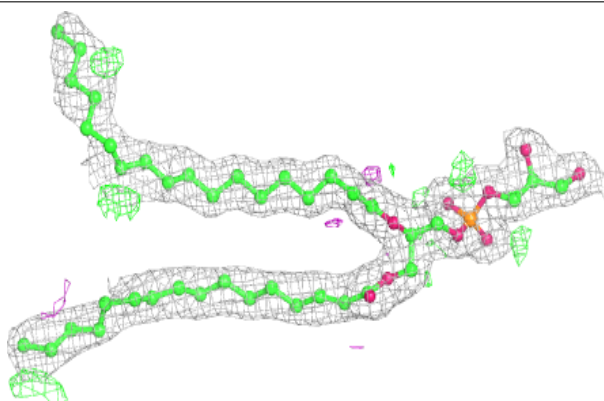


**Electron density around PEK C 309:**

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

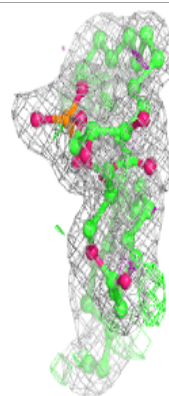
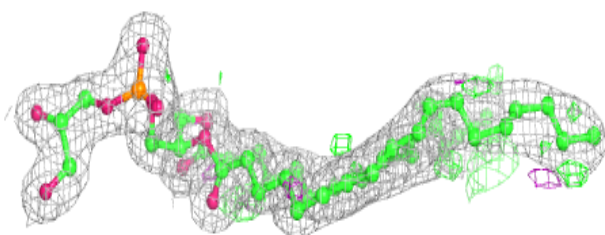
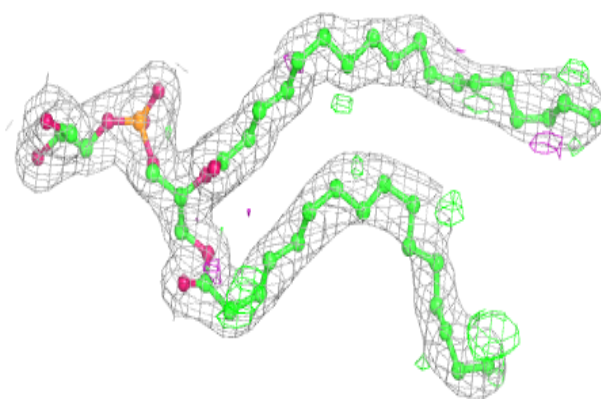
**Electron density around PGV P 309:**

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

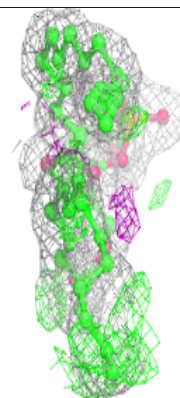
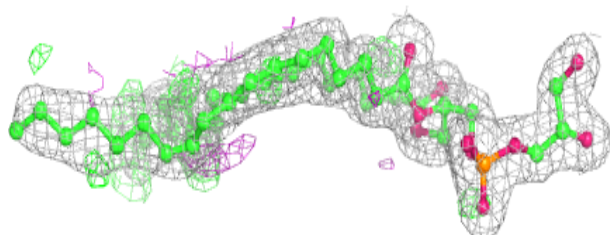
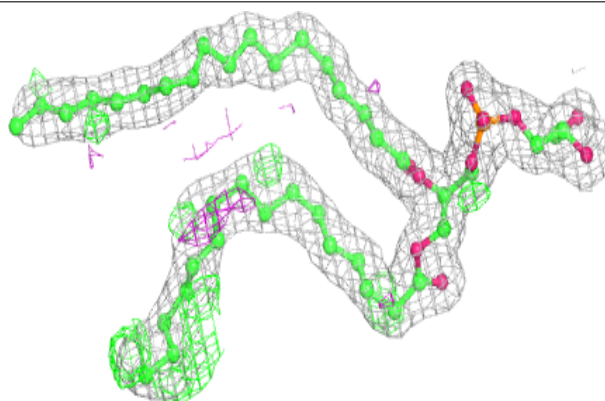


**Electron density around PGV N 607:**

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

**Electron density around PGV A 608:**

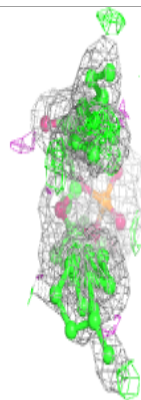
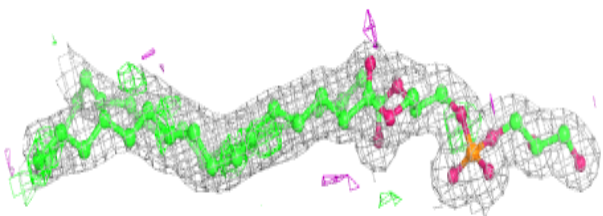
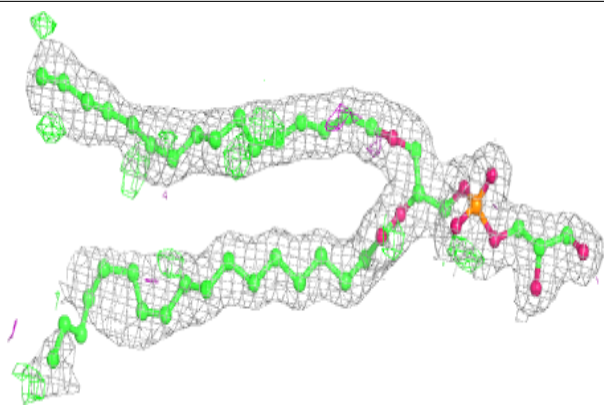
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



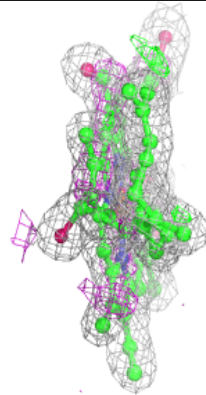
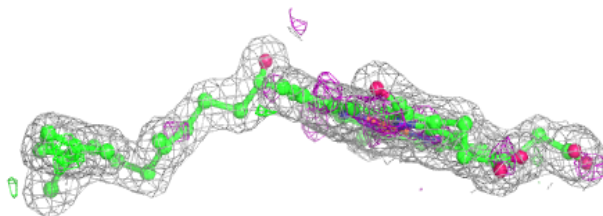
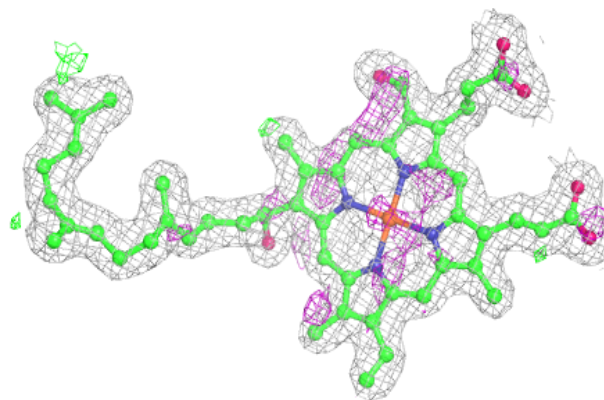


**Electron density around PGV C 310:**

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

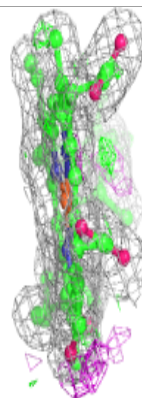
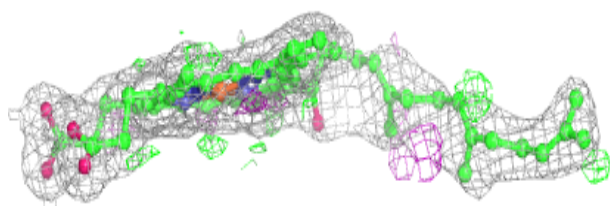
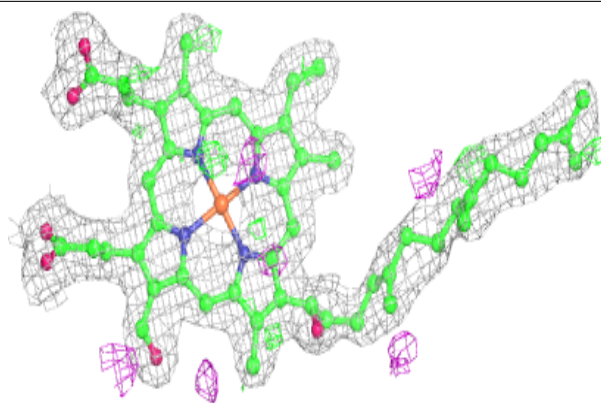
**Electron density around HEA A 602:**

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

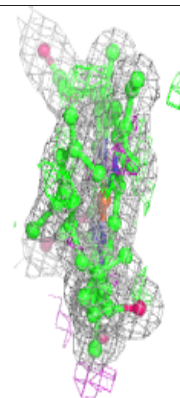
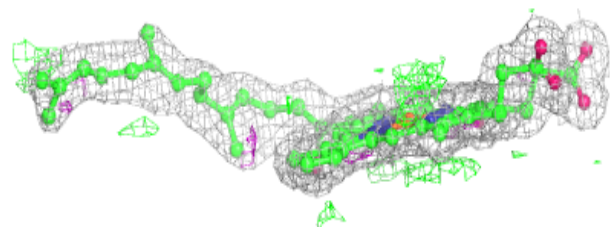
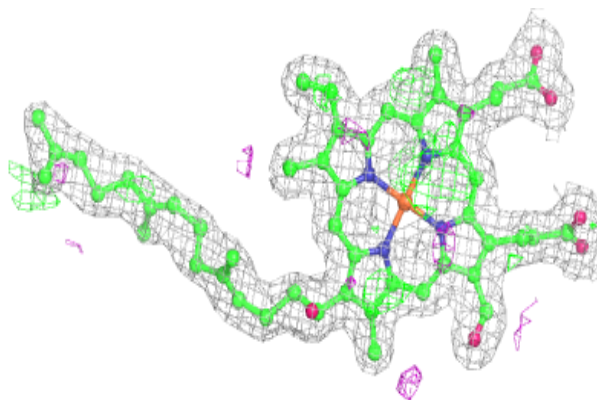


**Electron density around HEA N 601 (B):**

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

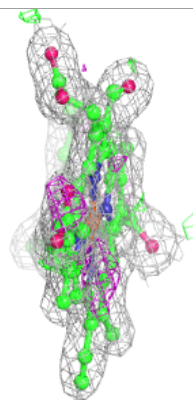
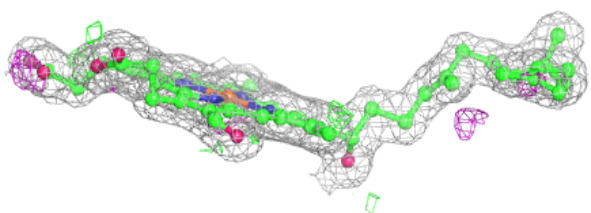
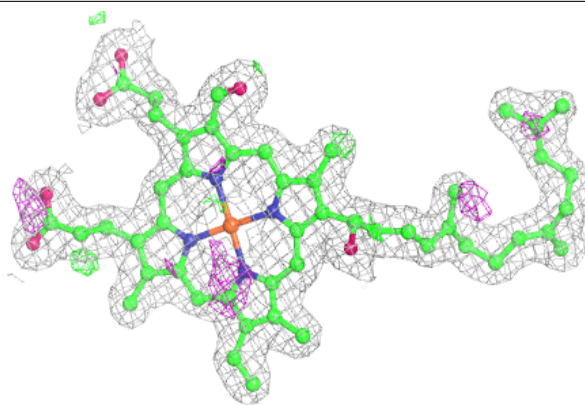
**Electron density around HEA A 601 (A):**

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

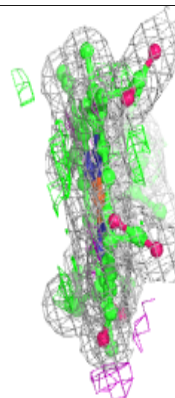
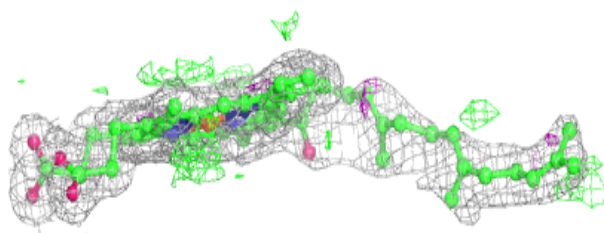
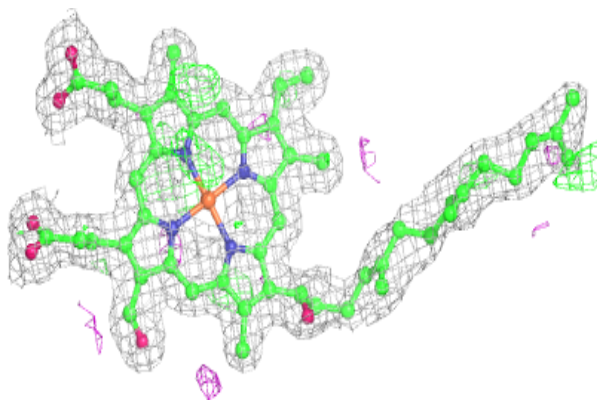


**Electron density around HEA N 602:**

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

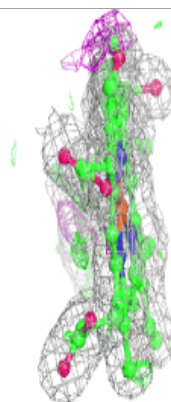
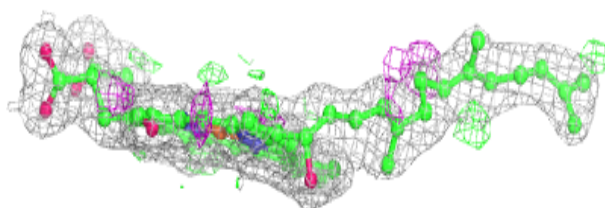
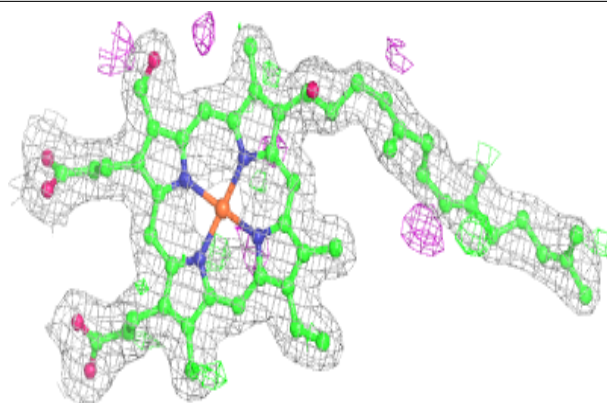
**Electron density around HEA A 601 (B):**

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



**Electron density around HEA N 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.