



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 04:38 AM JST

PDB ID : 7VUW  
Title : Bovine heart cytochrome c oxidase in the cyanide-bound fully oxidized state at 50 K  
Authors : Shimada, A.; Tsukihara, T.  
Deposited on : 2021-11-04  
Resolution : 1.60 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.31.2
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)	:	2.31.2

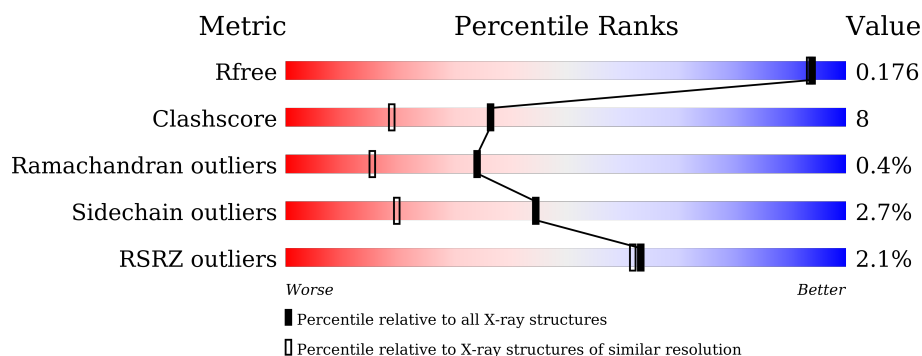
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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.






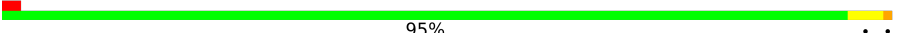











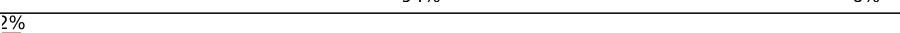

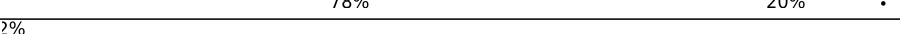


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>87%</div> <div>12%</div> <div>.</div> </div>
1	N	514	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	B	227	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
2	O	227	<div> <div>%</div> <div>81%</div> <div>19%</div> </div>
3	C	259	<div> <div>94%</div> <div>6%</div> </div>
3	P	259	<div> <div>86%</div> <div>13%</div> <div>.</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	94	
6	S	94	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	601[A]	X	-	-	-
14	HEA	A	601[B]	X	-	-	-
14	HEA	A	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601[A]	X	-	-	-
14	HEA	N	601[B]	X	-	-	-
14	HEA	N	602	X	-	-	-
20	EDO	A	609	-	-	X	-
20	EDO	A	623	-	-	X	-
20	EDO	A	626	-	-	X	-
20	EDO	A	627	-	-	X	-
20	EDO	A	633	-	-	X	-
20	EDO	B	312	-	-	X	-
20	EDO	B	321	-	-	X	-
20	EDO	C	325	-	-	X	-
20	EDO	D	202	-	-	X	-
20	EDO	D	209	-	-	X	-
20	EDO	D	214	-	-	-	X
20	EDO	L	110	-	-	X	-
20	EDO	O	314	-	-	X	-
20	EDO	Q	207	-	-	-	X



## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34951 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	35	0
			4152	2768	638	705	41			
1	N	513	Total	C	N	O	S	0	30	0
			4123	2751	632	701	39			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	11	0
			1854	1202	283	349	20			
2	O	227	Total	C	N	O	S	0	12	0
			1857	1204	286	349	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	9	0
			2138	1428	341	355	14			
3	P	259	Total	C	N	O	S	0	9	0
			2138	1428	341	355	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	3	0
			1207	786	199	218	4			
4	Q	138	Total	C	N	O	S	0	2	0
			1159	758	189	208	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	1	0
			854	546	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	1	0
			718	445	127	140	6			
6	S	94	Total	C	N	O	S	0	1	0
			718	445	127	140	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	1	0
			663	417	121	120	5			
8	U	79	Total	C	N	O	S	0	1	0
			663	417	121	120	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	2	0
			613	398	109	102	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			387	252	65	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			387	252	65	68	2			

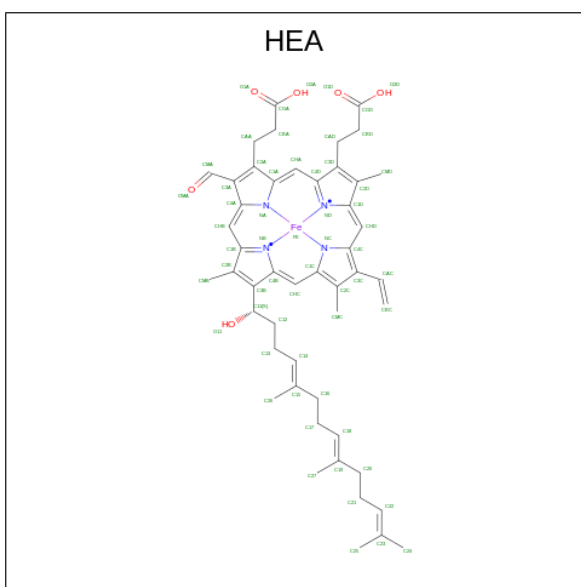
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			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 69	C 58	Fe 1	N 4	O 6	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

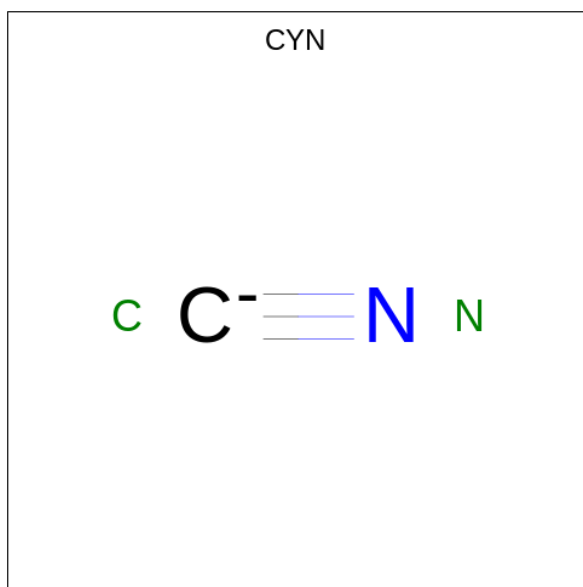
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

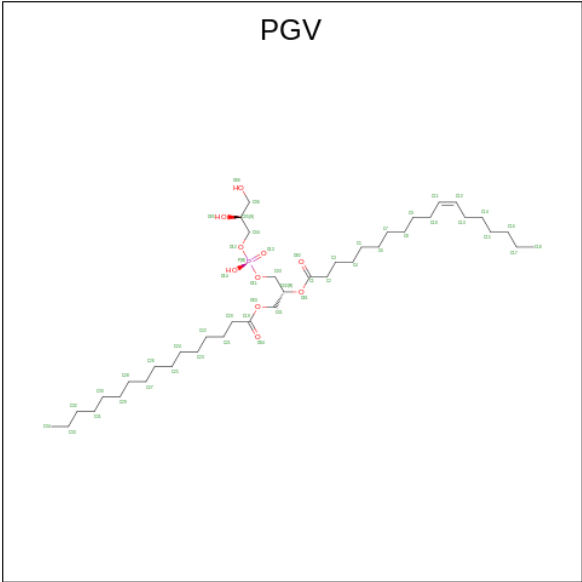
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

- Molecule 18 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- 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
			47	36	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			50	39	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			42	31	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		

- Molecule 20 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
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		
20	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 4	C 2	O 2	0	0
20	A	1	Total 3	C 1	O 2	0	1
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0
20	B	1	Total 4	C 2	O 2	0	0

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

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

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

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

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

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

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

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

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

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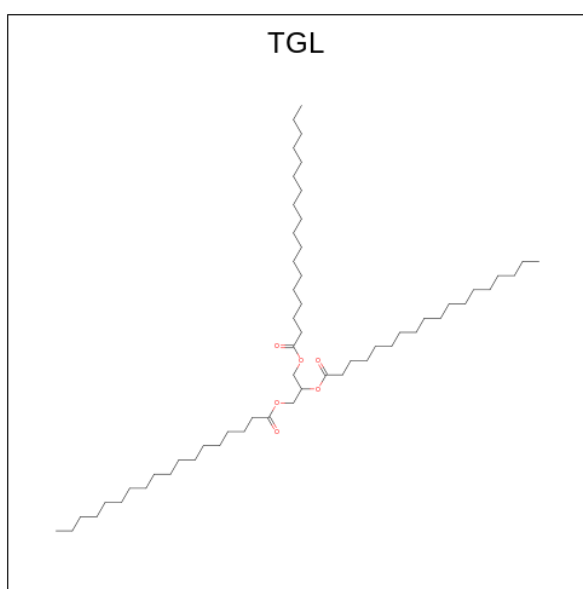
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20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	U	1	Total 4	C 2	O 2	0	0
20	U	1	Total 4	C 2	O 2	0	0
20	U	1	Total 4	C 2	O 2	0	0
20	V	1	Total 4	C 2	O 2	0	0
20	V	1	Total 4	C 2	O 2	0	0
20	V	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	Y	1	Total 4	C 2	O 2	0	0
20	Y	1	Total 4	C 2	O 2	0	0
20	Y	1	Total 4	C 2	O 2	0	0

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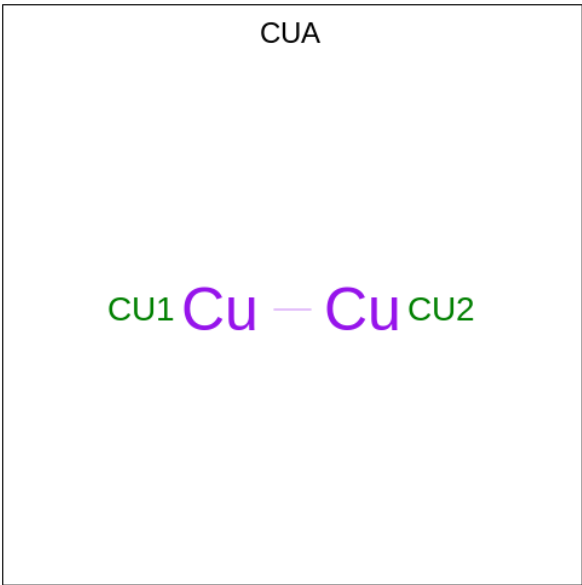
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Y	1	Total	C	O	0	0
			4	2	2		
20	Z	1	Total	C	O	0	0
			4	2	2		

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



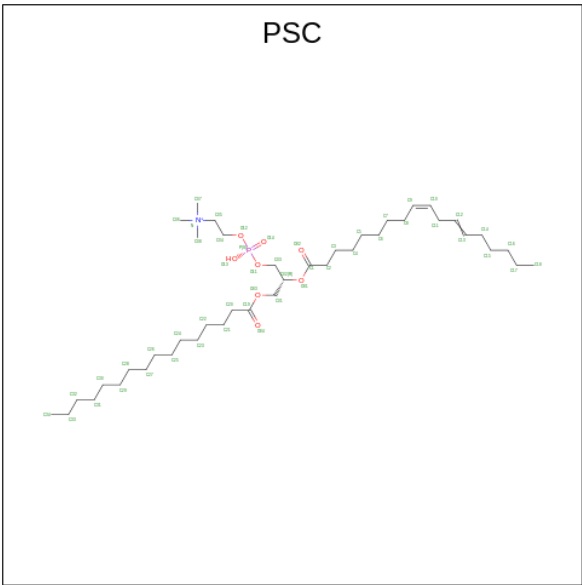
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	B	1	Total	C	O	0	0
			62	56	6		
21	L	1	Total	C	O	0	0
			60	54	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			60	54	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula:  $Cu_2$ ).



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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



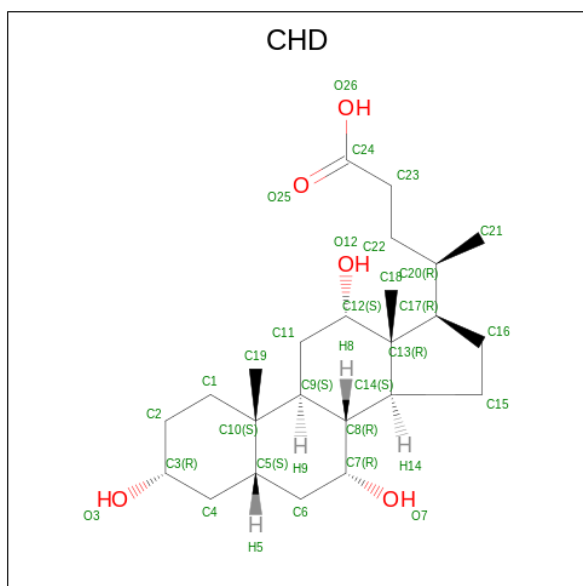
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

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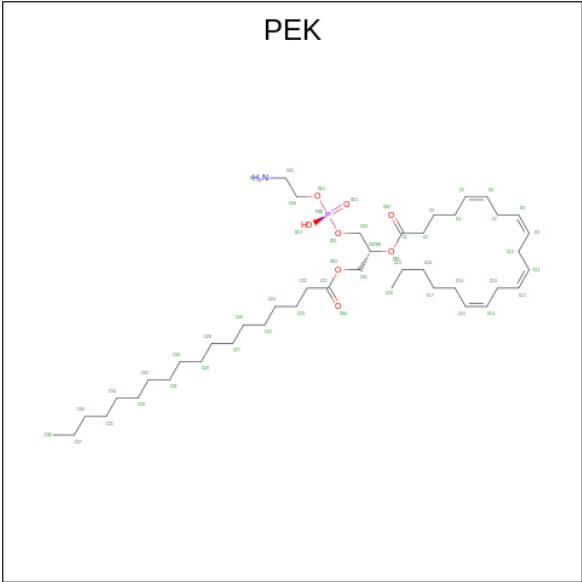
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	O	1	Total	C	O	P	0	0
			43	34	8	1		

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



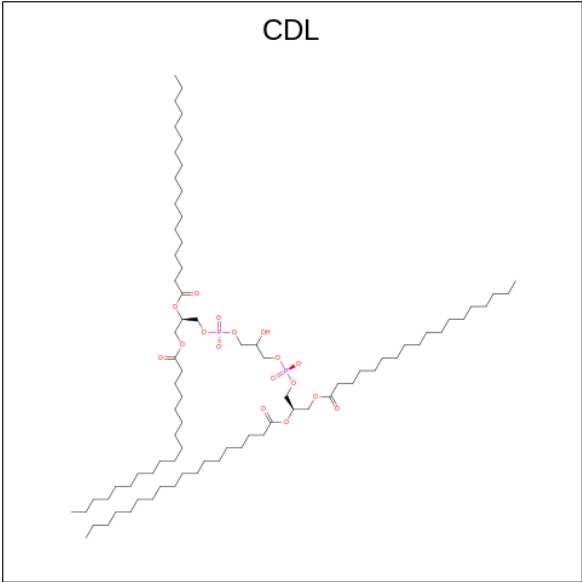
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	Y	1	Total	C	O	0	0
			29	24	5		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula:  $C_{43}H_{78}NO_8P$ ).



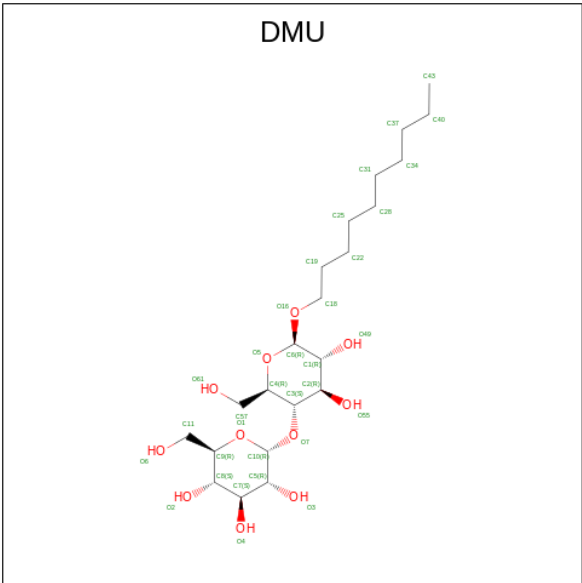
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			33	25	1	6	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			96	78	16	2		
26	G	1	Total	C	O	P	0	0
			90	74	14	2		
26	P	1	Total	C	O	P	0	0
			85	67	16	2		
26	T	1	Total	C	O	P	0	0
			92	75	15	2		

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



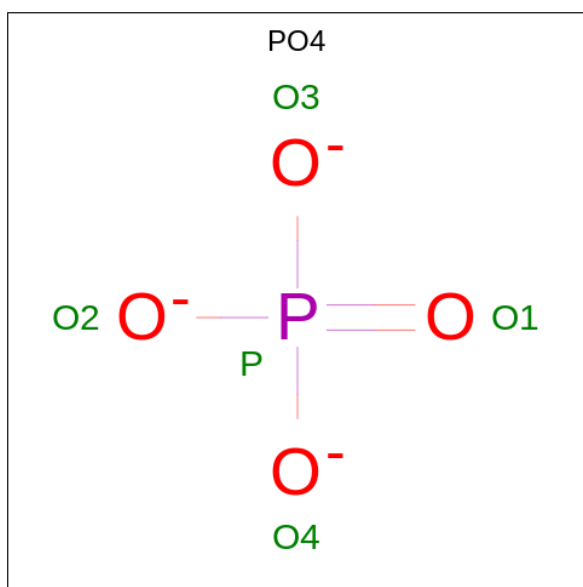
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 22 16 6	0	0
27	C	1	Total C O 33 22 11	0	0
27	J	1	Total C O 23 12 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	N	1	Total C O 17 15 2	0	0
27	O	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 21 16 5	0	0
27	X	1	Total C 10 10	0	0
27	X	1	Total C O 22 16 6	0	0
27	X	1	Total C O 33 22 11	0	0
27	X	1	Total C O 12 11 1	0	0
27	Z	1	Total C O 33 22 11	0	0

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

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

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).





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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	239	Total	O	0	3
			239	239		
30	B	211	Total	O	0	2
			212	212		
30	C	132	Total	O	0	1
			132	132		
30	D	195	Total	O	0	0
			195	195		
30	E	143	Total	O	0	0
			143	143		
30	F	148	Total	O	0	0
			148	148		
30	G	84	Total	O	0	0
			84	84		
30	H	92	Total	O	0	0
			92	92		
30	I	76	Total	O	0	0
			76	76		
30	J	51	Total	O	0	0
			51	51		

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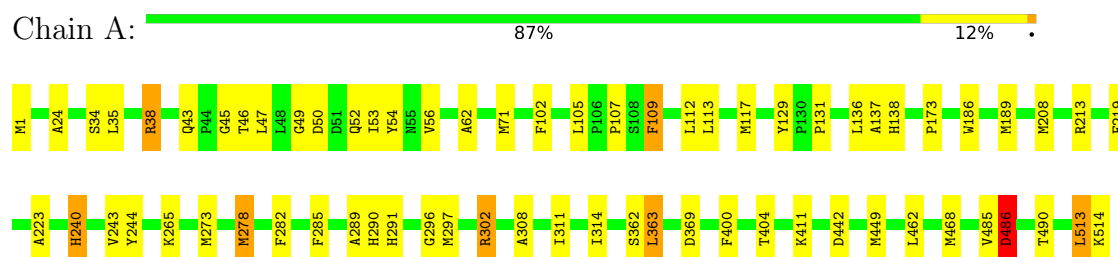
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	49	Total 49	O 49	0	0
30	L	39	Total 39	O 39	0	1
30	M	34	Total 34	O 34	0	0
30	N	248	Total 248	O 248	0	2
30	O	187	Total 188	O 188	0	2
30	P	160	Total 160	O 160	0	0
30	Q	118	Total 118	O 118	0	0
30	R	105	Total 105	O 105	0	0
30	S	136	Total 136	O 136	0	0
30	T	68	Total 68	O 68	0	0
30	U	82	Total 82	O 82	0	0
30	V	64	Total 64	O 64	0	0
30	W	43	Total 43	O 43	0	0
30	X	41	Total 41	O 41	0	0
30	Y	35	Total 35	O 35	0	0
30	Z	23	Total 23	O 23	0	0

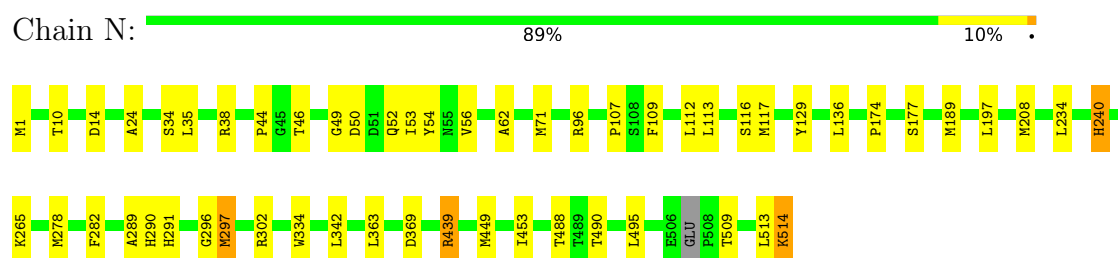
### 3 Residue-property plots

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

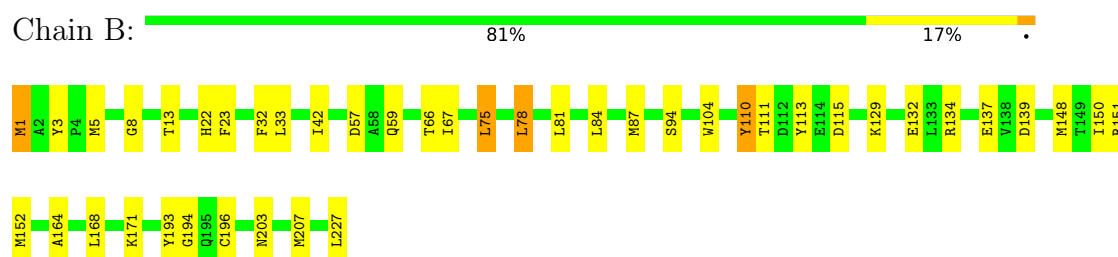
#### • Molecule 1: Cytochrome c oxidase subunit 1



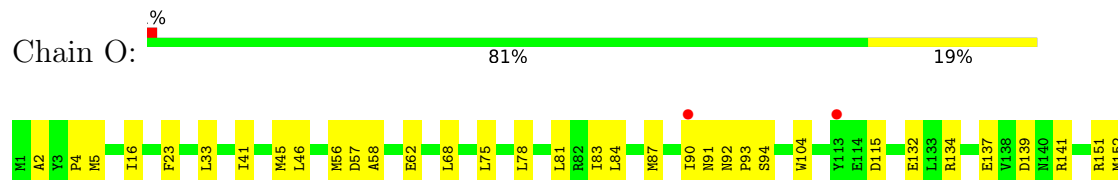
#### • Molecule 1: Cytochrome c oxidase subunit 1



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



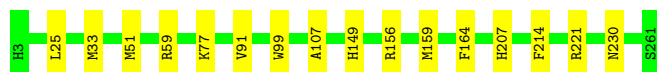
#### • Molecule 2: Cytochrome c oxidase subunit 2





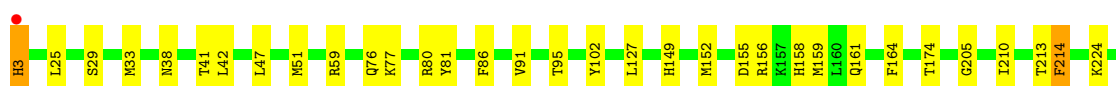
- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 94% 6%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 86% 13%



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

Chain D: 90% 9%



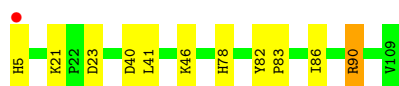
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 88% 8%



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

Chain E: 90% 10%

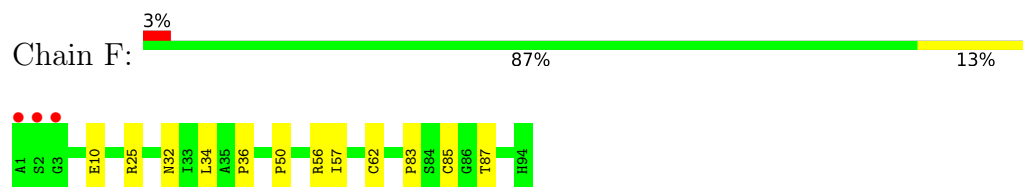


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

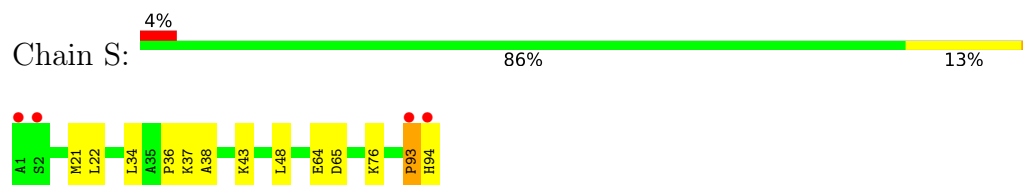
Chain R: 95%



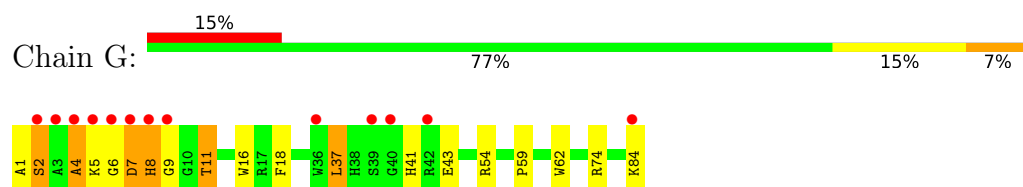
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



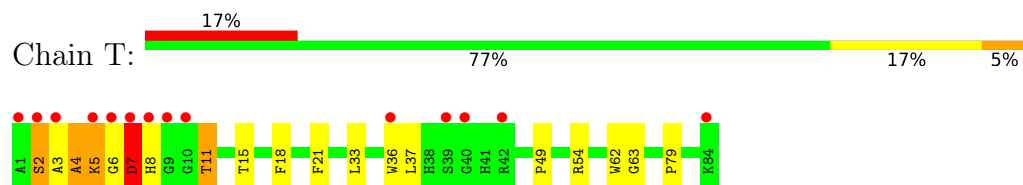
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



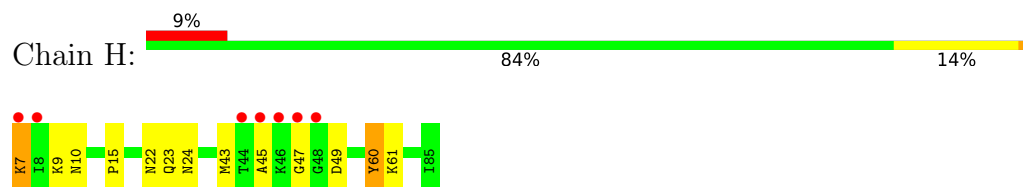
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



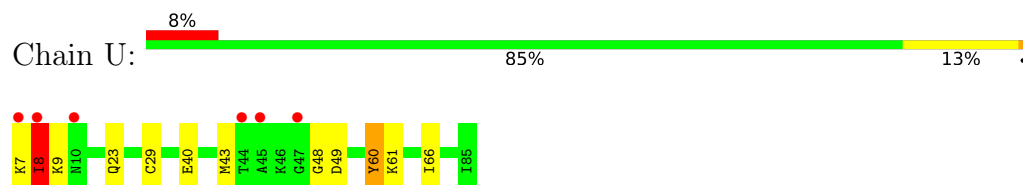
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



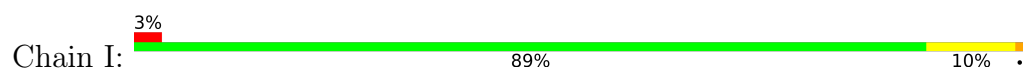
- Molecule 8: Cytochrome c oxidase subunit 6B1

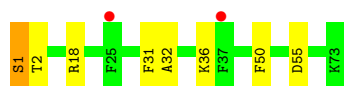


- Molecule 8: Cytochrome c oxidase subunit 6B1

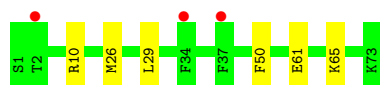
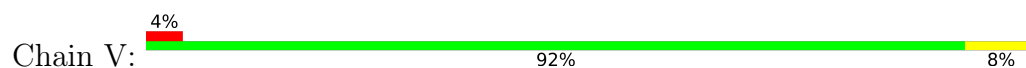


- Molecule 9: Cytochrome c oxidase subunit 6C

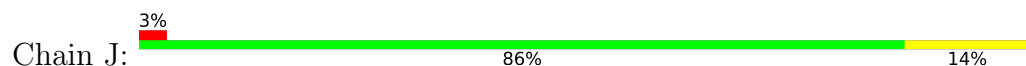




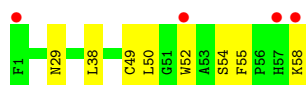
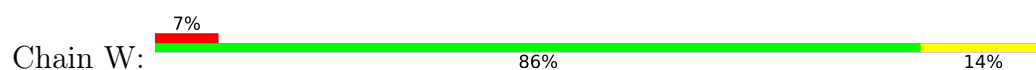
- Molecule 9: Cytochrome c oxidase subunit 6C



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



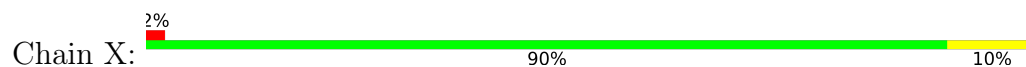
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



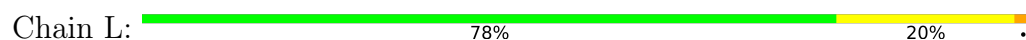
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



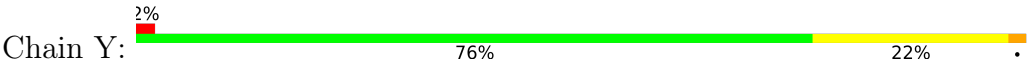
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



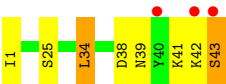
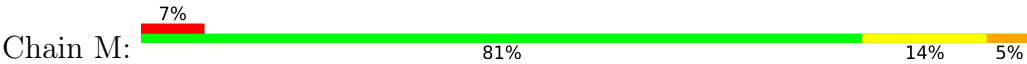
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



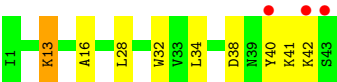
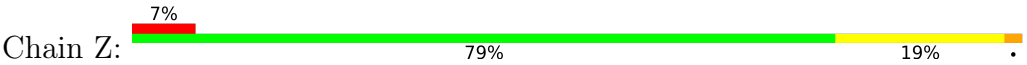
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.08Å 204.48Å 177.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.92 – 1.60 135.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.92-1.60) 99.7 (135.98-1.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.12 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.153 , 0.175 0.154 , 0.176	Depositor DCC
$R_{free}$ test set	43213 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 71.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34951	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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: CUA, NA, TGL, FME, TPO, SAC, CHD, CYN, DMU, ZN, CDL, PEK, PO4, CU, PSC, EDO, MG, HEA, PGV

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.96	4/4426 (0.1%)	1.04	20/6039 (0.3%)
1	N	0.87	0/4373	0.92	7/5966 (0.1%)
2	B	0.85	1/1947 (0.1%)	1.03	5/2650 (0.2%)
2	O	0.76	0/1958	0.91	4/2665 (0.2%)
3	C	0.85	0/2278	0.83	1/3111 (0.0%)
3	P	0.82	0/2278	0.80	3/3111 (0.1%)
4	D	0.84	0/1259	0.88	3/1698 (0.2%)
4	Q	0.67	0/1204	0.75	2/1625 (0.1%)
5	E	0.79	0/878	0.87	1/1192 (0.1%)
5	R	0.64	0/871	0.73	1/1182 (0.1%)
6	F	0.83	0/740	0.84	0/1003
6	S	0.75	0/740	0.83	0/1003
7	G	0.80	0/691	0.86	0/937
7	T	0.69	0/691	0.86	1/937 (0.1%)
8	H	0.82	0/688	0.81	0/929
8	U	0.67	0/688	0.78	0/929
9	I	0.76	0/605	0.80	1/802 (0.1%)
9	V	0.62	0/622	0.79	1/825 (0.1%)
10	J	0.59	0/472	0.83	1/636 (0.2%)
10	W	0.54	0/472	0.71	0/636
11	K	0.74	0/406	0.76	0/556
11	X	0.57	0/406	0.66	0/556
12	L	0.94	0/401	0.80	0/536
12	Y	0.66	0/401	0.68	0/536
13	M	0.80	0/346	0.83	1/470 (0.2%)
13	Z	0.66	0/346	0.72	0/470
All	All	0.82	5/30187 (0.0%)	0.88	52/41000 (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
7	T	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362[A]	SER	CB-OG	-5.77	1.34	1.42
1	A	362[B]	SER	CB-OG	-5.77	1.34	1.42
1	A	34[A]	SER	CB-OG	-5.57	1.35	1.42
1	A	34[B]	SER	CB-OG	-5.57	1.35	1.42
2	B	110	TYR	CD2-CE2	5.03	1.46	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278[A]	MET	CG-SD-CE	-15.51	75.39	100.20
1	A	278[B]	MET	CG-SD-CE	-15.51	75.39	100.20
2	B	152[A]	MET	CG-SD-CE	-11.45	81.88	100.20
2	B	152[B]	MET	CG-SD-CE	-11.45	81.88	100.20
1	A	189[A]	MET	CG-SD-CE	-9.80	84.51	100.20
1	A	189[B]	MET	CG-SD-CE	-9.80	84.51	100.20
1	N	71	MET	CG-SD-CE	-9.20	85.49	100.20
1	N	189[A]	MET	CG-SD-CE	-8.67	86.33	100.20
1	N	189[B]	MET	CG-SD-CE	-8.67	86.33	100.20
1	A	38	ARG	NE-CZ-NH2	-8.32	116.14	120.30
5	E	40	ASP	CB-CG-OD2	8.12	125.61	118.30
9	V	10	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	A	486[A]	ASP	CB-CG-OD1	7.98	125.49	118.30
1	A	486[B]	ASP	CB-CG-OD1	7.98	125.49	118.30
1	N	278	MET	CG-SD-CE	-7.59	88.06	100.20
4	Q	20	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	A	302[A]	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	A	213	ARG	NE-CZ-NH2	-7.49	116.56	120.30
4	Q	20	ARG	NE-CZ-NH1	7.42	124.01	120.30
4	D	20	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	A	513	LEU	CA-CB-CG	-6.83	99.60	115.30
3	P	155	ASP	CB-CG-OD1	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	233	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	A	38	ARG	NE-CZ-NH1	6.36	123.48	120.30
4	D	21	ASP	CB-CG-OD2	6.18	123.86	118.30
1	N	96	ARG	NE-CZ-NH2	-6.17	117.22	120.30
4	D	20	ARG	NE-CZ-NH2	6.04	123.32	120.30
7	T	33	LEU	CA-CB-CG	5.91	128.88	115.30
1	A	71	MET	CG-SD-CE	-5.89	90.78	100.20
2	B	134	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	363[A]	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	363[B]	LEU	CA-CB-CG	5.73	128.48	115.30
1	A	129	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	A	400	PHE	CB-CG-CD2	-5.60	116.88	120.80
9	I	55	ASP	CB-CG-OD1	5.60	123.34	118.30
5	R	36	LEU	CB-CG-CD2	-5.49	101.66	111.00
2	O	152	MET	CG-SD-CE	-5.40	91.56	100.20
2	O	139	ASP	CB-CG-OD2	5.28	123.06	118.30
2	B	139	ASP	CB-CG-OD2	5.27	123.04	118.30
3	C	221	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	442	ASP	CB-CG-OD2	5.20	122.98	118.30
2	O	134	ARG	NE-CZ-NH2	-5.17	117.72	120.30
13	M	34	LEU	CB-CG-CD1	5.13	119.72	111.00
2	B	151	ARG	NE-CZ-NH1	5.12	122.86	120.30
3	P	214	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	A	102	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	N	129	TYR	CB-CG-CD1	-5.10	117.94	121.00
10	J	36	MET	CG-SD-CE	-5.09	92.06	100.20
1	N	439	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	244	TYR	CB-CG-CD1	-5.05	117.97	121.00
2	O	68	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
7	T	7	ASP	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4152	0	4121	67	0
1	N	4123	0	4090	46	0
2	B	1854	0	1860	35	0
2	O	1857	0	1855	29	0
3	C	2138	0	2046	17	0
3	P	2138	0	2046	38	0
4	D	1207	0	1194	12	0
4	Q	1159	0	1146	9	0
5	E	854	0	850	8	0
5	R	852	0	845	3	0
6	F	718	0	698	11	0
6	S	718	0	698	14	0
7	G	676	0	644	10	0
7	T	676	0	643	12	0
8	H	663	0	624	9	0
8	U	663	0	624	10	0
9	I	601	0	613	7	0
9	V	613	0	627	3	0
10	J	461	0	459	6	0
10	W	461	0	459	7	0
11	K	387	0	371	2	0
11	X	387	0	371	5	0
12	L	382	0	381	14	0
12	Y	382	0	381	15	0
13	M	336	0	352	7	0
13	Z	336	0	352	4	0
14	A	129	0	88	3	0
14	N	129	0	88	3	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	98	0	141	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	C	101	0	147	9	0
19	N	93	0	128	4	0
19	P	102	0	152	11	0
20	A	115	0	168	44	0
20	B	76	0	114	16	0
20	C	64	0	96	9	0
20	D	84	0	126	18	0
20	E	52	0	78	5	0
20	F	32	0	48	5	0
20	G	12	0	18	3	0
20	H	16	0	24	6	0
20	I	24	0	36	4	0
20	J	12	0	18	1	0
20	K	20	0	30	0	0
20	L	40	0	60	7	0
20	M	20	0	30	3	0
20	N	100	0	150	16	0
20	O	64	0	96	16	0
20	P	68	0	102	8	0
20	Q	32	0	48	5	0
20	R	24	0	36	4	0
20	S	52	0	78	5	0
20	T	20	0	30	5	0
20	U	12	0	18	3	0
20	V	12	0	18	0	0
20	W	16	0	24	3	0
20	Y	24	0	36	0	0
20	Z	4	0	6	0	0
21	B	125	0	215	15	0
21	L	60	0	97	7	0
21	N	63	0	110	4	0
21	Q	63	0	110	9	0
21	Y	60	0	101	11	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	48	0	66	8	0
23	O	43	0	58	1	0
24	B	29	0	39	0	0
24	C	58	0	78	4	0
24	G	29	0	39	0	0
24	P	58	0	78	2	0
24	Y	29	0	39	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	155	0	220	11	0
25	P	138	0	189	9	0
26	C	96	0	150	6	0
26	G	90	0	138	8	0
26	P	85	0	122	11	0
26	T	92	0	141	11	0
27	C	55	0	73	5	0
27	J	23	0	21	2	0
27	M	33	0	42	0	0
27	N	17	0	22	0	0
27	O	33	0	42	0	0
27	P	66	0	84	9	0
27	T	21	0	27	3	0
27	X	77	0	113	4	0
27	Z	33	0	42	2	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	239	0	0	19	0
30	B	212	0	0	9	0
30	C	132	0	0	5	0
30	D	195	0	0	2	0
30	E	143	0	0	3	0
30	F	148	0	0	2	0
30	G	84	0	0	0	0
30	H	92	0	0	0	0
30	I	76	0	0	2	0
30	J	51	0	0	2	0
30	K	49	0	0	2	0
30	L	39	0	0	2	0
30	M	34	0	0	0	0
30	N	248	0	0	10	0
30	O	188	0	0	3	0
30	P	160	0	0	4	0
30	Q	118	0	0	4	0
30	R	105	0	0	0	0
30	S	136	0	0	10	0
30	T	68	0	0	3	0
30	U	82	0	0	4	0
30	V	64	0	0	3	0
30	W	43	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	41	0	0	0	0
30	Y	35	0	0	1	0
30	Z	23	0	0	1	0
All	All	34951	0	33038	511	0

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

All (511) 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)
20:A:609:EDO:H22	20:A:633:EDO:H22	1.41	1.01
12:L:6:GLY:H	20:L:110:EDO:H21	1.25	1.01
20:N:631:EDO:H11	20:S:105:EDO:H11	1.47	0.95
8:H:24:ASN:HD21	20:H:104:EDO:H12	1.40	0.87
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.57	0.86
2:B:8:GLY:H	20:B:312:EDO:H21	1.41	0.85
20:A:629:EDO:H12	30:A:789:HOH:O	1.80	0.81
20:B:313:EDO:H11	8:H:15:PRO:HA	1.62	0.81
5:E:78:HIS:NE2	20:I:104:EDO:H12	1.96	0.80
12:Y:20:ARG:HH22	21:Y:101:TGL:HC62	1.47	0.80
20:N:618:EDO:H12	30:N:780:HOH:O	1.81	0.80
13:M:1:ILE:HG22	20:M:106:EDO:H21	1.63	0.79
20:A:630:EDO:H21	30:A:808:HOH:O	1.83	0.79
7:T:79:PRO:HG2	20:T:107:EDO:H11	1.67	0.77
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.65	0.77
7:G:7:ASP:O	7:G:9:GLY:N	2.18	0.76
26:C:307:CDL:H391	30:C:529:HOH:O	1.86	0.75
27:P:309:DMU:H24	10:W:38:LEU:HA	1.69	0.73
20:A:635:EDO:H11	13:M:1:ILE:HG23	1.70	0.73
1:N:50[B]:ASP:HA	30:N:712:HOH:O	1.88	0.72
6:S:94:HIS:HE1	30:S:215:HOH:O	1.72	0.72
30:N:943:HOH:O	25:P:303:PEK:H381	1.90	0.72
20:N:632:EDO:H22	12:Y:10:ASN:HD22	1.55	0.71
3:P:80[A]:ARG:NE	20:P:318:EDO:O2	2.21	0.71
8:U:66:ILE:HG23	20:U:102:EDO:H11	1.73	0.71
12:L:6:GLY:N	20:L:110:EDO:H21	2.04	0.71
1:A:105:LEU:HD11	20:A:629:EDO:H11	1.72	0.70
20:A:626:EDO:H11	23:B:304:PSC:H21	1.74	0.70
6:F:25:ARG:HH21	20:F:106:EDO:H11	1.56	0.69
20:A:609:EDO:H11	30:A:779:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:310:DMU:H23	10:J:41:GLY:HA3	1.75	0.69
4:D:20:ARG:O	20:E:210:EDO:H12	1.93	0.68
20:D:212:EDO:H22	20:D:213:EDO:H22	1.75	0.68
20:A:635:EDO:H21	30:A:792:HOH:O	1.92	0.68
20:T:107:EDO:H12	30:T:256:HOH:O	1.92	0.68
20:A:623:EDO:H12	20:B:321:EDO:H22	1.76	0.68
19:C:306:PGV:H221	20:C:319:EDO:H12	1.75	0.67
2:O:141:ARG:HH22	20:O:318:EDO:H22	1.60	0.67
21:B:302:TGL:HC31	20:D:202:EDO:C2	2.24	0.67
23:B:304:PSC:H212	23:B:304:PSC:O01	1.95	0.67
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.76	0.66
2:O:90:ILE:HG13	20:O:311:EDO:H21	1.76	0.66
27:P:309:DMU:H24	10:W:38:LEU:HD23	1.78	0.66
20:D:219:EDO:H11	30:D:313:HOH:O	1.97	0.65
1:A:223:ALA:HB2	20:A:609:EDO:H12	1.77	0.65
27:C:309:DMU:H29	7:G:62:TRP:HB3	1.77	0.65
7:T:11:TPO:O2P	7:T:15:THR:HG21	1.98	0.64
12:L:24[B]:MET:SD	21:L:101:TGL:HC21	2.37	0.63
3:P:229:SER:O	20:P:321:EDO:H12	1.98	0.63
27:C:310:DMU:H29	27:C:310:DMU:O1	1.99	0.63
1:A:308:ALA:O	1:A:311[B]:ILE:HG12	1.98	0.63
21:Y:101:TGL:HC51	21:Y:101:TGL:OC1	1.99	0.63
20:B:321:EDO:O2	20:D:209:EDO:H11	1.99	0.62
1:A:43:GLN:HG3	20:A:627:EDO:H22	1.81	0.62
2:O:16[B]:ILE:HG22	20:O:314:EDO:H11	1.80	0.62
1:N:54[B]:TYR:HB2	30:N:826:HOH:O	1.99	0.62
23:O:302:PSC:H61	30:O:580:HOH:O	1.99	0.62
30:A:707:HOH:O	21:B:302:TGL:HG11	1.99	0.62
1:A:54[B]:TYR:HB2	30:A:826:HOH:O	2.00	0.62
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.82	0.62
7:G:59:PRO:O	20:G:104:EDO:H22	2.00	0.62
20:E:208:EDO:H22	30:E:411:HOH:O	1.98	0.61
6:F:10:GLU:HB2	20:F:106:EDO:H22	1.83	0.61
9:I:1:SAC:HB3	9:I:1:SAC:H2A1	1.80	0.61
19:C:306:PGV:O06	20:H:102:EDO:H12	1.99	0.61
21:Q:201:TGL:H361	30:V:255:HOH:O	2.00	0.61
1:N:174:PRO:HD2	20:N:618:EDO:H22	1.82	0.61
3:P:156:ARG:HE	24:P:308:CHD:C24	2.14	0.61
20:U:101:EDO:H11	30:U:224:HOH:O	2.00	0.61
27:P:310:DMU:H10	10:W:49:CYS:HB3	1.82	0.61
12:Y:20:ARG:HH12	21:Y:101:TGL:HC32	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:301:TGL:HC22	30:I:261:HOH:O	2.01	0.61
20:A:623:EDO:H12	20:B:321:EDO:H11	1.83	0.60
20:G:105:EDO:H21	19:P:306:PGV:H301	1.81	0.60
2:B:57:ASP:H	23:B:304:PSC:H202	1.66	0.60
4:D:94:LEU:HB3	20:D:207:EDO:H21	1.84	0.60
1:A:50[B]:ASP:HA	30:A:704:HOH:O	2.01	0.60
20:A:618:EDO:H11	6:F:32:ASN:HD21	1.67	0.60
21:L:101:TGL:H321	20:L:104:EDO:O1	2.02	0.60
21:B:302:TGL:HC31	20:D:202:EDO:O2	2.01	0.60
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.83	0.59
2:B:111:THR:O	20:B:315:EDO:H12	2.02	0.59
30:D:334:HOH:O	20:E:209:EDO:H21	2.01	0.59
1:A:43:GLN:HE21	20:A:627:EDO:H11	1.66	0.59
1:N:53[B]:ILE:HG12	30:N:865:HOH:O	2.03	0.59
7:T:49:PRO:O	20:T:106:EDO:H22	2.03	0.59
1:A:49[B]:GLY:HA3	13:M:41:LYS:HE3	1.83	0.59
5:E:23:ASP:O	20:E:205:EDO:H11	2.02	0.59
1:N:514:LYS:HD3	30:S:263:HOH:O	2.03	0.59
24:Y:102:CHD:H22	13:Z:13:LYS:HE3	1.83	0.59
20:A:616:EDO:H11	19:C:306:PGV:H142	1.84	0.59
19:C:306:PGV:H282	20:C:319:EDO:O1	2.02	0.59
30:N:900:HOH:O	4:Q:20:ARG:HG2	2.03	0.58
4:D:36:SER:OG	20:D:218:EDO:H11	2.03	0.58
1:N:136[B]:LEU:HD11	20:N:627:EDO:O1	2.03	0.58
1:N:297[A]:MET:CG	1:N:302:ARG:HG3	2.33	0.58
20:N:623:EDO:O2	19:P:306:PGV:H51	2.02	0.58
26:T:101:CDL:H712	26:T:101:CDL:H552	1.86	0.58
25:C:304:PEK:H031	20:O:305:EDO:O1	2.04	0.58
2:B:3:TYR:OH	20:B:312:EDO:H22	2.03	0.57
26:G:101:CDL:H162	26:G:101:CDL:H511	1.86	0.57
19:N:608:PGV:H011	19:N:608:PGV:H22	1.84	0.57
2:O:2:ALA:O	20:O:319:EDO:O2	2.22	0.57
25:C:304:PEK:O13	20:O:305:EDO:H11	2.04	0.57
1:A:485:VAL:HB	20:A:636:EDO:H22	1.87	0.57
26:P:307:CDL:H112	30:P:538:HOH:O	2.04	0.57
1:A:468:MET:HG3	30:A:926:HOH:O	2.03	0.57
1:N:509:THR:O	20:N:618:EDO:H11	2.05	0.57
2:B:22[A]:HIS:HE1	30:B:573:HOH:O	1.86	0.57
3:P:80[A]:ARG:HE	20:P:318:EDO:HO2	1.51	0.56
8:H:9:LYS:O	8:H:10:ASN:HB2	2.05	0.56
2:B:8:GLY:N	20:B:312:EDO:H21	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:131:ILE:O	20:Q:206:EDO:H21	2.06	0.56
1:A:43:GLN:NE2	20:A:627:EDO:H11	2.21	0.56
3:P:247:VAL:HG11	25:P:302:PEK:H11	1.87	0.56
25:P:303:PEK:H261	27:T:102:DMU:H17	1.87	0.56
21:B:302:TGL:H241	21:B:302:TGL:HA91	1.88	0.56
7:T:62:TRP:HB2	27:T:102:DMU:H3	1.88	0.56
1:A:302[B]:ARG:HH21	2:B:84:LEU:CD1	2.18	0.56
1:A:136[B]:LEU:HD11	30:A:930:HOH:O	2.05	0.55
5:E:21:LYS:HD3	20:E:201:EDO:H21	1.88	0.55
30:B:574:HOH:O	8:H:61:LYS:HE3	2.06	0.55
3:P:38:ASN:ND2	27:P:309:DMU:O2	2.39	0.55
7:G:9:GLY:HA3	30:N:702:HOH:O	2.06	0.55
2:O:141:ARG:NH2	20:O:318:EDO:H22	2.21	0.55
26:T:101:CDL:H322	26:T:101:CDL:HA62	1.88	0.55
1:N:297[A]:MET:HG2	1:N:302:ARG:HG3	1.88	0.55
20:O:314:EDO:H21	30:O:573:HOH:O	2.07	0.55
30:Q:329:HOH:O	20:R:204:EDO:H21	2.07	0.55
6:S:94:HIS:CE1	30:S:215:HOH:O	2.53	0.55
30:A:748:HOH:O	20:H:104:EDO:H22	2.06	0.54
2:O:84:LEU:HD12	2:O:87[A]:MET:CE	2.38	0.54
20:A:622:EDO:H11	30:L:220:HOH:O	2.07	0.54
4:Q:145:TRP:HD1	20:Q:203:EDO:H12	1.73	0.54
2:O:56:MET:O	20:O:315:EDO:H22	2.07	0.54
20:G:105:EDO:C2	19:P:306:PGV:H301	2.38	0.54
20:C:326:EDO:O2	20:H:103:EDO:H22	2.08	0.54
20:A:626:EDO:H21	23:B:304:PSC:H222	1.90	0.53
19:N:609:PGV:H183	25:P:303:PEK:H352	1.90	0.53
6:S:93:PRO:HB3	30:S:247:HOH:O	2.07	0.53
21:N:607:TGL:HC22	30:V:253:HOH:O	2.07	0.53
6:S:36:PRO:HG3	20:S:109:EDO:H12	1.91	0.53
23:B:304:PSC:H42	23:B:304:PSC:H231	1.90	0.53
2:O:57:ASP:HA	20:O:315:EDO:H22	1.90	0.53
1:A:50[B]:ASP:HB2	30:A:824:HOH:O	2.08	0.53
3:P:152:MET:HB3	20:P:321:EDO:H11	1.91	0.53
20:N:630:EDO:H21	12:Y:2:HIS:CD2	2.44	0.53
3:C:77[B]:LYS:HD2	20:C:325:EDO:H22	1.90	0.53
5:E:90:ARG:HD2	30:E:399:HOH:O	2.08	0.53
26:G:101:CDL:H782	26:G:101:CDL:H562	1.89	0.52
20:N:628:EDO:H11	30:S:262:HOH:O	2.08	0.52
5:R:14:ARG:NH1	20:R:201:EDO:O2	2.34	0.52
25:C:302:PEK:H252	7:T:8:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:297[A]:MET:SD	1:N:302:ARG:HG2	2.49	0.52
1:A:486[A]:ASP:OD2	4:D:19[A]:ARG:HD3	2.10	0.52
30:A:939:HOH:O	21:B:301:TGL:H222	2.10	0.52
1:N:53[A]:ILE:HD11	12:Y:40:VAL:HG13	1.92	0.52
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.91	0.52
2:B:113:TYR:CE2	20:B:317:EDO:H12	2.44	0.52
1:N:14:ASP:OD2	20:N:632:EDO:H11	2.10	0.52
1:N:449[A]:MET:SD	2:O:5:MET:HG2	2.49	0.52
20:A:609:EDO:H22	20:A:633:EDO:C2	2.27	0.52
12:Y:2:HIS:N	30:Y:202:HOH:O	2.43	0.52
10:J:7:GLU:HG3	30:J:232:HOH:O	2.09	0.52
26:P:307:CDL:H151	26:P:307:CDL:H332	1.92	0.52
2:B:94:SER:HB2	2:B:148[B]:MET:SD	2.50	0.51
20:T:106:EDO:H12	30:T:205:HOH:O	2.08	0.51
3:C:91:VAL:HG22	25:C:302:PEK:H12	1.93	0.51
1:A:513:LEU:O	1:A:514:LYS:HB2	2.10	0.51
3:P:33:MET:SD	27:P:310:DMU:H8	2.51	0.51
11:X:34:THR:HG22	27:X:102:DMU:H6	1.93	0.51
1:N:113:LEU:HD11	1:N:117[A]:MET:SD	2.51	0.51
1:A:273:MET:HE2	30:A:769:HOH:O	2.11	0.51
20:A:609:EDO:C1	30:A:779:HOH:O	2.54	0.51
4:D:97:ILE:HG22	20:D:201:EDO:H21	1.93	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
4:D:131:ILE:O	20:I:103:EDO:H12	2.11	0.51
8:U:43:MET:HE3	8:U:49:ASP:H	1.74	0.51
12:Y:20:ARG:NH2	21:Y:101:TGL:HC62	2.23	0.51
1:A:24:ALA:HB2	14:A:601[B]:HEA:H253	1.93	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.93	0.51
21:B:302:TGL:HC61	30:B:554:HOH:O	2.10	0.51
7:G:1:ALA:HB2	19:P:306:PGV:H321	1.93	0.50
7:G:1:ALA:N	19:P:306:PGV:H342	2.25	0.50
1:A:514:LYS:HD2	30:F:224:HOH:O	2.11	0.50
20:A:637[A]:EDO:O2	20:A:637[A]:EDO:O1	2.30	0.50
3:P:29:SER:HB2	27:P:310:DMU:H21	1.92	0.50
13:M:43:SER:O	13:M:43:SER:OG	2.29	0.50
20:N:614:EDO:HO2	20:N:625:EDO:HO1	1.56	0.50
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.12	0.50
20:A:609:EDO:C2	20:A:633:EDO:H22	2.28	0.50
3:P:33:MET:HE1	3:P:42:LEU:H	1.76	0.50
12:Y:24[B]:MET:HE1	21:Y:101:TGL:H161	1.93	0.50
8:H:7:LYS:HE2	30:U:269:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:634:EDO:C1	19:P:306:PGV:H12	2.41	0.50
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.50
20:A:620:EDO:C2	6:F:57:ILE:H	2.25	0.49
21:B:302:TGL:HC52	20:D:202:EDO:O2	2.11	0.49
12:L:5:GLU:HA	20:L:110:EDO:C1	2.42	0.49
1:N:116[A]:SER:HB3	30:N:701:HOH:O	2.11	0.49
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.52	0.49
3:P:149:HIS:NE2	20:P:316:EDO:H21	2.27	0.49
7:T:63:GLY:H	27:T:102:DMU:C10	2.25	0.49
12:Y:14:SER:H	21:Y:101:TGL:HC31	1.77	0.49
21:B:302:TGL:HC31	20:D:202:EDO:H22	1.94	0.49
1:A:223:ALA:CB	20:A:609:EDO:H12	2.43	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.93	0.49
20:B:317:EDO:H22	30:B:577:HOH:O	2.13	0.49
3:P:213:THR:HG23	26:P:307:CDL:H771	1.94	0.49
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.95	0.49
6:F:83:PRO:HD3	20:F:105:EDO:H21	1.93	0.49
1:N:513:LEU:O	1:N:514:LYS:HB2	2.12	0.49
11:K:39:GLU:HB3	30:K:206:HOH:O	2.13	0.49
6:F:50:PRO:HG2	30:F:275:HOH:O	2.12	0.49
8:U:43:MET:HE3	8:U:49:ASP:N	2.27	0.49
21:B:301:TGL:HA92	21:B:301:TGL:HA42	1.94	0.49
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.95	0.49
30:N:847:HOH:O	20:O:319:EDO:H21	2.12	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
30:B:522:HOH:O	26:T:101:CDL:H312	2.12	0.48
9:I:50:PHE:HB2	20:I:103:EDO:H21	1.94	0.48
19:A:607:PGV:H162	30:K:249:HOH:O	2.13	0.48
3:C:99:TRP:HB2	20:C:319:EDO:H11	1.96	0.48
21:L:101:TGL:H311	30:L:239:HOH:O	2.13	0.48
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.94	0.48
12:L:24[A]:MET:SD	21:L:101:TGL:HC82	2.53	0.48
1:N:513:LEU:O	1:N:514:LYS:CB	2.60	0.48
12:Y:12:PRO:HB2	21:Y:101:TGL:HG11	1.96	0.48
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.49	0.48
12:L:26:THR:HG23	13:M:25:SER:CB	2.44	0.48
2:O:16[B]:ILE:CG2	20:O:314:EDO:H11	2.43	0.48
6:S:64:GLU:O	6:S:65:ASP:HB2	2.14	0.48
1:A:302[B]:ARG:HE	2:B:84:LEU:HD11	1.78	0.48
21:B:302:TGL:HC32	21:B:302:TGL:OG1	2.13	0.48
21:Q:201:TGL:HG12	30:Q:310:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:623:EDO:H12	20:B:321:EDO:C2	2.40	0.48
2:B:227:LEU:HD21	30:B:544:HOH:O	2.12	0.48
21:Y:101:TGL:H222	21:Y:101:TGL:HA91	1.44	0.48
4:D:58:GLU:HG2	20:D:215:EDO:O1	2.14	0.48
1:N:24:ALA:HB2	14:N:601[B]:HEA:H253	1.96	0.48
6:S:43:LYS:HE3	30:S:320:HOH:O	2.13	0.48
26:C:307:CDL:H522	26:C:307:CDL:OB9	2.13	0.47
3:P:102[B]:TYR:CE2	20:P:324:EDO:H22	2.49	0.47
8:H:43:MET:HE3	8:H:49:ASP:N	2.29	0.47
1:N:35[A]:LEU:HB3	27:Z:101:DMU:H24	1.97	0.47
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.95	0.47
1:A:289:ALA:HB1	1:A:297[B]:MET:HE1	1.95	0.47
2:B:78:LEU:HD12	26:T:101:CDL:H352	1.95	0.47
3:C:156:ARG:HE	24:C:308:CHD:C24	2.26	0.47
26:G:101:CDL:H142	26:G:101:CDL:H171	1.53	0.47
5:R:18:TYR:CE1	20:R:202:EDO:H21	2.49	0.47
3:C:149:HIS:NE2	20:C:320:EDO:H12	2.29	0.47
2:O:58:ALA:O	2:O:62:GLU:HG3	2.15	0.47
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.14	0.47
1:A:302[B]:ARG:HH21	2:B:84:LEU:HD12	1.77	0.47
2:B:8:GLY:H	20:B:312:EDO:C2	2.21	0.47
25:C:302:PEK:H252	7:T:8:HIS:NE2	2.30	0.47
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.47
3:P:205:GLY:HA3	25:P:303:PEK:H181	1.97	0.47
3:P:127:LEU:HD22	26:T:101:CDL:HB32	1.96	0.47
1:A:113[B]:LEU:HD11	1:A:117[B]:MET:SD	2.54	0.47
21:B:302:TGL:HA42	21:B:302:TGL:HB51	1.97	0.47
20:O:317:EDO:O1	8:U:61:LYS:HD2	2.14	0.47
3:P:224:LYS:HE3	26:P:307:CDL:HB32	1.96	0.47
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.15	0.46
20:A:618:EDO:H21	6:F:50:PRO:HB2	1.97	0.46
20:A:626:EDO:H22	23:B:304:PSC:H21	1.96	0.46
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.14	0.46
20:Q:206:EDO:H12	9:V:50:PHE:HB2	1.95	0.46
13:M:39:ASN:O	13:M:43:SER:HB3	2.16	0.46
12:L:24[B]:MET:SD	21:L:101:TGL:CC2	3.02	0.46
3:P:77[A]:LYS:HE2	30:P:546:HOH:O	2.15	0.46
2:B:42:ILE:HG21	21:B:302:TGL:H242	1.97	0.46
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.81	0.46
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.72	0.46
26:T:101:CDL:H561	26:T:101:CDL:H592	1.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:MET:SD	27:J:101:DMU:O16	2.73	0.46
3:P:33:MET:HB2	27:P:310:DMU:C19	2.46	0.46
4:D:108:PRO:HA	20:D:209:EDO:H22	1.97	0.46
1:N:342:LEU:HB2	21:Q:201:TGL:HA92	1.98	0.46
3:P:164:PHE:CD1	24:P:308:CHD:H192	2.51	0.46
26:P:307:CDL:H321	20:W:104:EDO:H12	1.98	0.46
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.45	0.46
8:H:22:ASN:ND2	20:H:102:EDO:O1	2.36	0.46
1:N:10:THR:O	20:N:635:EDO:H22	2.16	0.46
12:Y:26:THR:HA	30:Z:211:HOH:O	2.14	0.46
20:A:627:EDO:O1	20:D:209:EDO:O1	2.29	0.46
3:C:77[B]:LYS:NZ	20:C:325:EDO:H12	2.31	0.46
24:C:308:CHD:H183	24:C:308:CHD:H20	1.77	0.46
24:Y:102:CHD:H112	24:Y:102:CHD:H12A	1.66	0.46
3:P:224:LYS:CD	26:P:307:CDL:HB32	2.46	0.45
9:I:1:SAC:H2A1	9:I:1:SAC:CB	2.46	0.45
25:P:303:PEK:H203	25:P:303:PEK:H171	1.69	0.45
1:A:173:PRO:O	20:A:630:EDO:H22	2.16	0.45
2:B:13:THR:HB	2:B:168:LEU:HD23	1.97	0.45
3:P:77[A]:LYS:NZ	3:P:81:TYR:OH	2.46	0.45
3:P:210:ILE:HG23	19:P:305:PGV:H91	1.98	0.45
20:A:623:EDO:H12	20:B:321:EDO:C1	2.45	0.45
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.97	0.45
5:R:79:LYS:HD2	5:R:79:LYS:HA	1.71	0.45
2:B:22[A]:HIS:HD2	30:B:583:HOH:O	2.00	0.45
1:N:439:ARG:HD3	2:O:199:ILE:HB	1.98	0.45
2:B:1:FME:O1	2:B:193:TYR:N	2.35	0.45
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.97	0.45
26:G:101:CDL:H362	2:O:81:LEU:HD12	1.97	0.45
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.98	0.45
20:N:623:EDO:H21	19:P:306:PGV:H32	1.99	0.45
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.82	0.45
1:A:186:TRP:CZ3	1:A:278[B]:MET:HE3	2.52	0.45
1:A:411:LYS:HZ1	20:A:631:EDO:H12	1.82	0.45
19:C:306:PGV:H312	20:T:103:EDO:C2	2.47	0.45
26:P:307:CDL:H522	26:P:307:CDL:OB9	2.15	0.45
6:S:76:LYS:CE	6:S:93:PRO:HG2	2.47	0.45
8:U:7:LYS:O	8:U:8:ILE:HB	2.16	0.45
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.57	0.45
1:A:112:LEU:HG	30:A:915:HOH:O	2.16	0.44
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:101:EDO:O1	30:U:201:HOH:O	2.21	0.44
20:S:112:EDO:H21	30:S:254:HOH:O	2.17	0.44
3:C:77[B]:LYS:CD	20:C:325:EDO:H22	2.48	0.44
25:C:304:PEK:H032	30:C:415:HOH:O	2.17	0.44
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.05	0.44
3:P:3:HIS:ND1	3:P:3:HIS:N	2.65	0.44
1:A:46:THR:HG22	1:A:49[B]:GLY:H	1.82	0.44
5:E:46:LYS:NZ	30:E:303:HOH:O	2.51	0.44
5:E:86:ILE:O	5:E:90:ARG:HG2	2.17	0.44
1:N:52[B]:GLN:O	1:N:56:VAL:HG23	2.17	0.44
20:N:621:EDO:H11	30:N:719:HOH:O	2.17	0.44
20:P:316:EDO:O1	20:P:326:EDO:O1	2.29	0.44
1:A:404:THR:HG21	20:A:635:EDO:H12	2.00	0.44
21:B:301:TGL:HC31	20:B:312:EDO:H11	1.99	0.44
3:C:51[A]:MET:SD	26:C:307:CDL:H621	2.58	0.44
25:C:302:PEK:H322	7:T:2:SER:O	2.17	0.44
11:K:24:PHE:CE1	11:K:28[B]:VAL:HG21	2.52	0.44
1:N:334:TRP:CZ3	21:Q:201:TGL:HA51	2.52	0.44
21:N:607:TGL:H211	21:N:607:TGL:H241	1.46	0.44
2:B:129:LYS:HE3	30:B:585:HOH:O	2.17	0.44
27:C:310:DMU:H5	30:J:202:HOH:O	2.17	0.44
20:O:314:EDO:H12	20:O:316:EDO:H22	1.99	0.44
26:T:101:CDL:H181	26:T:101:CDL:OB6	2.18	0.44
26:G:101:CDL:H521	26:G:101:CDL:H551	1.68	0.44
3:P:174:THR:HG21	26:P:307:CDL:H851	2.00	0.44
20:Q:205:EDO:H12	30:Q:317:HOH:O	2.16	0.44
2:O:4:PRO:HD3	20:O:319:EDO:H12	1.99	0.44
3:P:38:ASN:O	27:P:309:DMU:H35	2.18	0.44
1:A:363[A]:LEU:HG	2:B:23:PHE:HD1	1.82	0.43
26:G:101:CDL:H522	26:G:101:CDL:H201	1.98	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.43
26:P:307:CDL:H532	26:P:307:CDL:H561	1.73	0.43
1:A:43:GLN:HE21	20:A:627:EDO:C1	2.30	0.43
1:A:131:PRO:HB3	20:A:633:EDO:H12	2.00	0.43
2:B:81:LEU:HD12	26:T:101:CDL:H371	2.00	0.43
25:C:303:PEK:H102	25:C:303:PEK:H72	1.70	0.43
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.17	0.43
26:T:101:CDL:H1	30:T:246:HOH:O	2.18	0.43
19:A:608:PGV:H322	25:C:303:PEK:H383	2.00	0.43
3:P:91:VAL:HG22	25:P:302:PEK:H12	2.00	0.43
4:Q:81:VAL:HG11	21:Q:201:TGL:HB52	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:HD12	2:B:75:LEU:HA	1.80	0.43
4:D:37:GLN:HG3	20:D:218:EDO:H22	2.00	0.43
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.06	0.43
19:C:306:PGV:C06	20:H:102:EDO:H12	2.47	0.43
3:P:3:HIS:N	3:P:3:HIS:HD1	2.16	0.43
30:S:219:HOH:O	20:W:102:EDO:H11	2.18	0.43
12:Y:24[B]:MET:SD	21:Y:101:TGL:CC2	3.07	0.43
1:A:43:GLN:HE21	20:A:627:EDO:C2	2.31	0.43
4:Q:146:LYS:NZ	30:Q:304:HOH:O	2.51	0.43
10:W:54:SER:O	12:Y:46:LYS:HD3	2.19	0.43
19:N:608:PGV:H12	4:Q:87[B]:PHE:CD2	2.53	0.43
11:X:24:PHE:O	11:X:28[B]:VAL:HG23	2.18	0.43
1:A:411:LYS:NZ	20:A:631:EDO:H12	2.33	0.43
19:C:306:PGV:H52	19:C:306:PGV:H21	1.57	0.43
21:L:101:TGL:CA9	21:L:101:TGL:H231	2.49	0.43
1:N:453:ILE:HD11	27:X:102:DMU:H19	2.01	0.43
21:N:607:TGL:H101	21:N:607:TGL:C28	2.49	0.43
12:Y:25:MET:HG2	21:Y:101:TGL:HA51	2.00	0.43
1:A:314:ILE:CG2	2:B:66[A]:THR:HG23	2.49	0.43
24:C:308:CHD:H112	24:C:308:CHD:H12A	1.79	0.43
26:T:101:CDL:HA62	26:T:101:CDL:C32	2.47	0.43
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.72	0.43
1:A:45:GLY:HA3	20:A:627:EDO:O1	2.20	0.42
1:N:46:THR:HG22	1:N:49[B]:GLY:H	1.84	0.42
20:O:314:EDO:H12	20:O:316:EDO:C2	2.49	0.42
10:J:27:THR:HG22	20:J:104:EDO:H11	2.00	0.42
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.42
6:S:22:LEU:HD12	30:S:308:HOH:O	2.18	0.42
13:Z:28:LEU:HD23	27:Z:101:DMU:H7	2.00	0.42
1:A:363[A]:LEU:HG	2:B:23:PHE:CD1	2.54	0.42
20:A:626:EDO:C1	23:B:304:PSC:H21	2.45	0.42
23:B:304:PSC:H041	5:E:41:LEU:HD23	2.01	0.42
20:B:321:EDO:C2	20:D:209:EDO:H11	2.49	0.42
3:P:33:MET:HE1	3:P:41:THR:HB	2.00	0.42
10:W:55:PHE:C	20:W:103:EDO:H22	2.40	0.42
1:A:208[B]:MET:HG2	1:A:219:PHE:CE1	2.54	0.42
1:A:411:LYS:CE	20:A:631:EDO:H22	2.49	0.42
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.33	0.42
6:S:37:LYS:HE2	30:S:220:HOH:O	2.20	0.42
9:V:26:MET:HE1	30:V:264:HOH:O	2.20	0.42
2:B:87:MET:HE2	30:B:491:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:51[B]:MET:HE2	30:C:529:HOH:O	2.20	0.42
3:C:59:ARG:HG3	26:C:307:CDL:H512	2.01	0.42
9:I:50:PHE:HB2	20:I:103:EDO:C2	2.50	0.42
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.55	0.42
1:N:363[A]:LEU:HG	2:O:23:PHE:HD1	1.84	0.42
27:P:310:DMU:H41	10:W:52:TRP:HZ2	1.84	0.42
20:P:316:EDO:HO1	20:P:326:EDO:C1	2.32	0.42
1:A:35[B]:LEU:HD11	1:A:462:LEU:HD13	2.01	0.42
1:A:137:ALA:O	20:A:617:EDO:H21	2.18	0.42
3:C:164:PHE:CD1	24:C:308:CHD:H192	2.54	0.42
25:P:304:PEK:H222	7:T:21:PHE:CG	2.55	0.42
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.08	0.42
6:F:36:PRO:HD3	20:F:109:EDO:H22	2.02	0.42
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.02	0.42
1:N:297[A]:MET:SD	1:N:302:ARG:CG	3.08	0.42
21:N:607:TGL:HB32	21:N:607:TGL:HB61	1.91	0.42
1:A:109:PHE:HB3	21:L:101:TGL:H122	2.02	0.42
26:C:307:CDL:H561	26:C:307:CDL:H532	1.90	0.42
26:G:101:CDL:H562	26:G:101:CDL:H762	2.02	0.42
12:L:5:GLU:HA	20:L:110:EDO:C2	2.50	0.42
12:L:47:LYS:HD2	12:L:47:LYS:HA	1.46	0.42
1:A:468:MET:SD	20:A:637[A]:EDO:O2	2.78	0.42
21:B:301:TGL:HC31	20:B:312:EDO:C1	2.49	0.42
2:O:16[B]:ILE:HD11	2:O:83:ILE:HG23	2.01	0.42
10:W:29:ASN:HD22	10:W:29:ASN:H	1.67	0.42
1:A:47:LEU:HD12	20:M:104:EDO:H22	2.01	0.41
1:A:50[B]:ASP:HB3	1:A:53[B]:ILE:HB	2.02	0.41
12:L:5:GLU:HA	20:L:110:EDO:H21	2.01	0.41
1:N:289:ALA:HB1	1:N:297[A]:MET:HE1	2.01	0.41
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.55	0.41
20:R:201:EDO:O1	20:R:202:EDO:H22	2.20	0.41
10:J:29:ASN:HD22	10:J:29:ASN:H	1.67	0.41
27:C:310:DMU:H22	10:J:38:LEU:HA	2.03	0.41
13:M:1:ILE:CG2	20:M:106:EDO:H21	2.42	0.41
25:P:304:PEK:H22	30:P:452:HOH:O	2.19	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.94	0.41
25:C:303:PEK:H302	25:C:303:PEK:H271	1.71	0.41
4:D:114:GLU:HG2	20:D:203:EDO:H12	2.03	0.41
9:V:65:LYS:HB2	9:V:65:LYS:HE3	1.52	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.46	0.41
8:H:60:TYR:CD1	8:H:60:TYR:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[B]:ILE:HG12	30:A:877:HOH:O	2.21	0.41
1:A:243:VAL:HB	14:A:602:HEA:C3C	2.50	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.82	0.41
21:Q:201:TGL:HC21	21:Q:201:TGL:HG31	1.72	0.41
8:U:43:MET:CE	8:U:49:ASP:H	2.33	0.41
12:Y:24[B]:MET:CE	21:Y:101:TGL:H161	2.51	0.41
1:A:53[B]:ILE:HG12	30:A:927:HOH:O	2.20	0.41
1:A:113[B]:LEU:HD13	12:L:39:ILE:HD11	2.03	0.41
21:Q:201:TGL:H321	27:X:101:DMU:H22	2.03	0.41
21:Q:201:TGL:HB31	21:Q:201:TGL:HG11	2.02	0.41
20:A:620:EDO:H22	6:F:56:ARG:HA	2.02	0.41
2:B:81:LEU:HD13	26:T:101:CDL:H121	2.03	0.41
3:C:107:ALA:HB2	19:C:306:PGV:H031	2.01	0.41
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.41
8:U:60:TYR:OH	8:U:61:LYS:NZ	2.49	0.41
26:C:307:CDL:H252	30:C:531:HOH:O	2.20	0.41
4:D:58:GLU:OE2	20:D:218:EDO:H21	2.21	0.41
7:G:2:SER:HB2	1:N:197:LEU:HD21	2.02	0.41
1:N:112:LEU:HD23	1:N:112:LEU:C	2.41	0.41
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.21	0.41
3:P:95:THR:HG21	19:P:306:PGV:H302	2.03	0.41
8:U:48:GLY:HA2	30:U:202:HOH:O	2.19	0.41
11:X:24:PHE:O	11:X:28[A]:VAL:HG12	2.21	0.41
9:I:32:ALA:O	9:I:36:LYS:HE3	2.20	0.41
19:N:608:PGV:H291	13:Z:16:ALA:HA	2.03	0.41
3:P:76:GLN:HE21	3:P:233:PHE:HB2	1.86	0.41
3:C:207:HIS:CE1	19:C:305:PGV:H343	2.57	0.40
20:C:325:EDO:H11	30:C:525:HOH:O	2.21	0.40
26:G:101:CDL:H332	30:O:416:HOH:O	2.20	0.40
10:J:52:TRP:CH2	27:J:101:DMU:H4	2.56	0.40
20:L:102:EDO:H21	20:L:109:EDO:H11	2.02	0.40
1:N:240:HIS:CD2	1:N:240:HIS:C	2.94	0.40
2:O:224:ALA:O	2:O:227:LEU:HG	2.21	0.40
4:Q:34:SER:O	4:Q:38:LYS:HG3	2.20	0.40
20:A:636:EDO:H12	30:A:848:HOH:O	2.20	0.40
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.02	0.40
9:I:1:SAC:H2A3	30:I:255:HOH:O	2.21	0.40
1:N:177:SER:HB3	20:N:615:EDO:H21	2.03	0.40
1:N:208[B]:MET:HE1	1:N:234:LEU:CD1	2.50	0.40
3:P:3:HIS:HB2	30:P:508:HOH:O	2.21	0.40
3:P:158:HIS:HD2	3:P:161[B]:GLN:OE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:201:TGL:HA91	21:Q:201:TGL:C24	2.51	0.40
11:X:26:VAL:HG13	27:X:101:DMU:H10	2.03	0.40
30:A:757:HOH:O	12:L:7:PRO:HG3	2.21	0.40
14:N:601[A]:HEA:H212	14:N:601[A]:HEA:H271	1.74	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.04	0.40
3:P:59:ARG:HA	26:P:307:CDL:H512	2.03	0.40
6:S:36:PRO:CG	20:S:109:EDO:H12	2.51	0.40
2:B:67:ILE:HD13	2:B:67:ILE:HA	1.88	0.40
2:B:148[B]:MET:HG2	2:B:150:ILE:HG13	2.03	0.40
4:D:125:ASP:OD2	20:D:206:EDO:O1	2.40	0.40
6:F:34:LEU:O	20:F:109:EDO:H11	2.20	0.40
3:P:210:ILE:HG23	19:P:305:PGV:H11	2.04	0.40
3:C:91:VAL:CG2	25:C:302:PEK:H12	2.51	0.40
3:P:86:PHE:CZ	19:P:305:PGV:H281	2.57	0.40
6:S:34:LEU:HD11	20:S:107:EDO:H11	2.03	0.40

There are no symmetry-related clashes.

## 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	547/514 (106%)	534 (98%)	13 (2%)	0	100	100
1	N	539/514 (105%)	523 (97%)	16 (3%)	0	100	100
2	B	236/227 (104%)	229 (97%)	7 (3%)	0	100	100
2	O	237/227 (104%)	230 (97%)	6 (2%)	1 (0%)	34	15
3	C	266/259 (103%)	260 (98%)	6 (2%)	0	100	100
3	P	266/259 (103%)	261 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	138/144 (96%)	135 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	104/105 (99%)	104 (100%)	0	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	93/94 (99%)	92 (99%)	1 (1%)	0	100	100
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	81/84 (96%)	71 (88%)	5 (6%)	5 (6%)	1	0
7	T	81/84 (96%)	72 (89%)	4 (5%)	5 (6%)	1	0
8	H	78/79 (99%)	71 (91%)	5 (6%)	2 (3%)	5	0
8	U	78/79 (99%)	71 (91%)	6 (8%)	1 (1%)	12	2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	73/73 (100%)	72 (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	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
11	X	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	42 (93%)	3 (7%)	0	100	100
12	Y	45/46 (98%)	43 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3609/3550 (102%)	3500 (97%)	95 (3%)	14 (0%)	34	15

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	T	3	ALA
7	T	4	ALA
7	T	7	ASP
8	U	8	ILE
7	G	37	LEU
8	H	45	ALA
7	T	5	LYS
2	O	92	ASN
7	T	6	GLY
7	G	6	GLY

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Mol	Chain	Res	Type
8	H	47	GLY

### 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	460/426 (108%)	454 (99%)	6 (1%)	69	50
1	N	454/426 (107%)	448 (99%)	6 (1%)	69	50
2	B	221/210 (105%)	213 (96%)	8 (4%)	35	12
2	O	222/210 (106%)	213 (96%)	9 (4%)	30	9
3	C	233/224 (104%)	230 (99%)	3 (1%)	69	50
3	P	233/224 (104%)	229 (98%)	4 (2%)	60	38
4	D	131/128 (102%)	129 (98%)	2 (2%)	65	44
4	Q	124/128 (97%)	122 (98%)	2 (2%)	62	41
5	E	93/92 (101%)	91 (98%)	2 (2%)	52	27
5	R	92/92 (100%)	90 (98%)	2 (2%)	52	27
6	F	79/78 (101%)	78 (99%)	1 (1%)	69	50
6	S	79/78 (101%)	77 (98%)	2 (2%)	47	22
7	G	67/67 (100%)	59 (88%)	8 (12%)	5	0
7	T	67/67 (100%)	61 (91%)	6 (9%)	9	1
8	H	72/71 (101%)	70 (97%)	2 (3%)	43	18
8	U	72/71 (101%)	68 (94%)	4 (6%)	21	5
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	13
9	V	59/57 (104%)	57 (97%)	2 (3%)	37	13
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	31
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	9
11	K	40/39 (103%)	40 (100%)	0	100	100
11	X	40/39 (103%)	40 (100%)	0	100	100
12	L	40/39 (103%)	39 (98%)	1 (2%)	47	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
12	Y	40/39 (103%)	38 (95%)	2 (5%)	24 6
13	M	37/37 (100%)	33 (89%)	4 (11%)	6 1
13	Z	37/37 (100%)	32 (86%)	5 (14%)	4 0
All	All	3147/3034 (104%)	3061 (97%)	86 (3%)	44 20

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	369	ASP
1	A	486[A]	ASP
1	A	486[B]	ASP
2	B	33	LEU
2	B	59	GLN
2	B	75	LEU
2	B	78	LEU
2	B	110	TYR
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	33	LEU
4	D	147	LYS
5	E	5	HIS
5	E	90	ARG
6	F	87	THR
7	G	2	SER
7	G	5	LYS
7	G	8	HIS
7	G	18	PHE
7	G	37	LEU
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	60	TYR
9	I	2	THR

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Mol	Chain	Res	Type
9	I	18	ARG
10	J	50	LEU
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
13	M	43	SER
1	N	38	ARG
1	N	109	PHE
1	N	297[A]	MET
1	N	297[B]	MET
1	N	369	ASP
1	N	514	LYS
2	O	33	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115[A]	ASP
2	O	115[B]	ASP
2	O	171	LYS
2	O	217	LYS
3	P	3	HIS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	20	ARG
4	Q	31	LYS
5	R	79	LYS
5	R	80	GLU
6	S	48	LEU
6	S	93	PRO
7	T	2	SER
7	T	7	ASP
7	T	18	PHE
7	T	36	TRP
7	T	37	LEU
7	T	54	ARG
8	U	8	ILE
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR

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Mol	Chain	Res	Type
9	V	29	LEU
9	V	61	GLU
10	W	50	LEU
10	W	58	LYS
12	Y	2	HIS
12	Y	47	LYS
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	41	LYS
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
2	B	10	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	29	HIS
4	D	109	HIS
5	E	94	ASN
6	F	94	HIS
10	J	29	ASN
11	K	35	GLN
2	O	59	GLN
2	O	181	GLN
2	O	195	GLN
3	P	38	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	109	HIS
5	R	94	ASN
6	S	94	HIS
9	V	53	ASN
10	W	29	ASN



### 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	N	1	1	8,9,10	0.48	0	7,9,11	1.65	2 (28%)
7	TPO	T	11	7	8,10,11	1.33	1 (12%)	10,14,16	1.11	1 (10%)
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	1.35	0
7	TPO	G	11	7	8,10,11	1.53	1 (12%)	10,14,16	1.05	1 (10%)
1	FME	A	1	1	8,9,10	0.69	0	7,9,11	2.16	3 (42%)
2	FME	O	1	2	8,9,10	0.84	0	7,9,11	1.27	0
9	SAC	I	1	9	7,8,9	0.54	0	8,9,11	1.76	2 (25%)
2	FME	B	1	2	8,9,10	2.49	4 (50%)	7,9,11	2.06	3 (42%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CN-N	5.46	1.51	1.33
7	T	11	TPO	P-O1P	3.03	1.60	1.50
7	G	11	TPO	P-O1P	3.01	1.60	1.50
2	B	1	FME	CG-SD	-2.35	1.68	1.81
2	B	1	FME	O1-CN	-2.30	1.15	1.22
2	B	1	FME	CA-N	2.25	1.49	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	CA-N-CN	-4.04	116.60	122.82
7	T	11	TPO	CG2-CB-CA	3.04	119.16	113.16
9	I	1	SAC	CA-N-C1A	2.88	128.47	123.15
2	B	1	FME	CA-N-CN	-2.81	118.50	122.82
1	A	1	FME	O1-CN-N	-2.69	118.19	125.27
1	N	1	FME	CE-SD-CG	2.65	109.51	100.40
1	A	1	FME	O-C-CA	-2.58	118.01	124.78
1	N	1	FME	O-C-CA	-2.58	118.01	124.78
2	B	1	FME	O1-CN-N	2.50	131.84	125.27
2	B	1	FME	C-CA-N	2.44	114.13	109.73
9	I	1	SAC	C2A-C1A-N	2.18	119.79	116.10
7	G	11	TPO	CG2-CB-CA	2.16	117.42	113.16

There are no chirality outliers.

All (31) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CB-OG1-P-O1P
9	V	1	SAC	C-CA-CB-OG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	N-CA-CB-OG
9	V	1	SAC	N-CA-CB-OG
2	B	1	FME	O1-CN-N-CA
7	T	11	TPO	CB-OG1-P-O2P
1	A	1	FME	CA-CB-CG-SD
2	O	1	FME	CB-CG-SD-CE
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	G	11	TPO	O-C-CA-CB
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0
7	G	11	TPO	1	0
9	I	1	SAC	3	0
2	B	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 8 are monoatomic - leaving 308 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	EDO	D	216	-	3,3,3	0.67	0	2,2,2	0.51	0
20	EDO	M	102	-	3,3,3	0.59	0	2,2,2	0.25	0
20	EDO	O	313	-	3,3,3	0.55	0	2,2,2	0.33	0
20	EDO	A	637[A]	-	1,1,3	0.38	0	-		
20	EDO	C	311	-	3,3,3	1.00	0	2,2,2	0.13	0
20	EDO	A	622	-	3,3,3	0.76	0	2,2,2	0.43	0
20	EDO	O	309	-	3,3,3	0.66	0	2,2,2	0.25	0
20	EDO	N	621	-	3,3,3	0.31	0	2,2,2	0.37	0
20	EDO	A	620	-	3,3,3	0.51	0	2,2,2	0.31	0
25	PEK	P	304	-	51,51,52	1.15	2 (3%)	54,56,57	1.57	6 (11%)
20	EDO	K	102	-	3,3,3	0.80	0	2,2,2	0.42	0
20	EDO	A	609	-	3,3,3	0.21	0	2,2,2	0.18	0
20	EDO	C	325	-	3,3,3	0.68	0	2,2,2	0.28	0
20	EDO	B	308	-	3,3,3	0.79	0	2,2,2	0.20	0
20	EDO	E	209	-	3,3,3	0.78	0	2,2,2	0.16	0
20	EDO	R	201	-	3,3,3	0.23	0	2,2,2	1.03	0
14	HEA	A	601[B]	-	57,67,67	1.56	12 (21%)	61,103,103	1.86	21 (34%)
20	EDO	V	103	-	3,3,3	0.54	0	2,2,2	0.13	0
20	EDO	H	102	-	3,3,3	0.44	0	2,2,2	0.04	0
20	EDO	P	317	-	3,3,3	0.52	0	2,2,2	0.24	0
21	TGL	B	301	-	62,62,62	1.15	3 (4%)	65,65,65	1.57	7 (10%)
20	EDO	F	102	-	3,3,3	0.65	0	2,2,2	0.50	0
20	EDO	T	107	-	3,3,3	0.67	0	2,2,2	0.31	0
20	EDO	Y	105	-	3,3,3	0.75	0	2,2,2	0.41	0
20	EDO	J	104	-	3,3,3	0.32	0	2,2,2	0.75	0
20	EDO	E	206	-	3,3,3	0.34	0	2,2,2	0.92	0
20	EDO	L	102	-	3,3,3	0.65	0	2,2,2	0.76	0
20	EDO	L	108	-	3,3,3	0.55	0	2,2,2	0.15	0
20	EDO	P	316	-	3,3,3	0.58	0	2,2,2	0.16	0
20	EDO	A	626	-	3,3,3	0.55	0	2,2,2	0.40	0
20	EDO	N	625	-	3,3,3	0.43	0	2,2,2	0.64	0
20	EDO	Q	205	-	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	N	626	-	3,3,3	0.61	0	2,2,2	0.56	0
20	EDO	D	215	-	3,3,3	0.42	0	2,2,2	0.54	0
20	EDO	Y	103	-	3,3,3	0.66	0	2,2,2	0.40	0
20	EDO	F	103	-	3,3,3	0.91	0	2,2,2	0.32	0
25	PEK	C	303	-	52,52,52	0.67	1 (1%)	55,57,57	1.23	5 (9%)
19	PGV	A	607	-	46,46,50	1.26	5 (10%)	49,52,56	2.11	13 (26%)
20	EDO	S	109	-	3,3,3	0.54	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	Q	203	-	3,3,3	0.55	0	2,2,2	0.33	0
20	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.37	0
20	EDO	B	306	-	3,3,3	0.59	0	2,2,2	0.20	0
24	CHD	C	308	-	32,32,32	0.92	1 (3%)	51,51,51	2.53	22 (43%)
20	EDO	C	318	-	3,3,3	0.44	0	2,2,2	0.12	0
19	PGV	N	608	-	41,41,50	1.09	2 (4%)	44,47,56	1.35	6 (13%)
20	EDO	B	312	-	3,3,3	0.63	0	2,2,2	0.18	0
20	EDO	A	628	-	3,3,3	0.45	0	2,2,2	0.24	0
20	EDO	P	324	-	3,3,3	0.37	0	2,2,2	0.79	0
19	PGV	A	608	-	50,50,50	0.89	2 (4%)	53,56,56	1.12	3 (5%)
20	EDO	C	316	-	3,3,3	0.50	0	2,2,2	0.21	0
26	CDL	C	307	-	94,94,99	1.42	14 (14%)	102,104,111	1.68	22 (21%)
27	DMU	M	101	-	34,34,34	0.67	1 (2%)	45,45,45	1.11	3 (6%)
20	EDO	N	630	-	3,3,3	0.32	0	2,2,2	1.26	0
20	EDO	E	212	-	3,3,3	0.52	0	2,2,2	0.54	0
20	EDO	N	615	-	3,3,3	0.60	0	2,2,2	0.81	0
20	EDO	N	619	-	3,3,3	0.43	0	2,2,2	0.75	0
20	EDO	R	202	-	3,3,3	0.47	0	2,2,2	0.52	0
20	EDO	E	202	-	3,3,3	0.57	0	2,2,2	0.34	0
21	TGL	B	302	-	61,61,62	1.16	3 (4%)	64,64,65	1.59	7 (10%)
20	EDO	C	317	-	3,3,3	0.77	0	2,2,2	0.20	0
20	EDO	A	619	-	3,3,3	0.71	0	2,2,2	0.72	0
20	EDO	C	313	-	3,3,3	0.54	0	2,2,2	0.17	0
20	EDO	A	633	-	3,3,3	0.51	0	2,2,2	0.46	0
20	EDO	D	204	-	3,3,3	0.74	0	2,2,2	0.09	0
14	HEA	N	601[B]	-	57,67,67	1.33	10 (17%)	61,103,103	1.74	18 (29%)
20	EDO	D	214	-	3,3,3	0.70	0	2,2,2	0.12	0
20	EDO	E	211	-	3,3,3	0.99	0	2,2,2	1.11	0
18	CYN	N	606	15	0,1,1	-	-	-	-	-
20	EDO	S	107	-	3,3,3	0.54	0	2,2,2	0.13	0
20	EDO	C	320	-	3,3,3	0.62	0	2,2,2	0.08	0
20	EDO	A	631	-	3,3,3	0.64	0	2,2,2	0.30	0
20	EDO	E	208	-	3,3,3	0.64	0	2,2,2	0.47	0
20	EDO	Y	107	-	3,3,3	0.65	0	2,2,2	0.18	0
23	PSC	B	304	-	47,47,51	1.20	4 (8%)	50,52,59	1.55	6 (12%)
20	EDO	B	315	-	3,3,3	0.50	0	2,2,2	0.29	0
21	TGL	Q	201	-	62,62,62	1.07	3 (4%)	65,65,65	1.73	11 (16%)
20	EDO	P	322	-	3,3,3	0.46	0	2,2,2	0.69	0
20	EDO	B	310	-	3,3,3	0.38	0	2,2,2	1.00	0
20	EDO	N	627	-	3,3,3	0.79	0	2,2,2	0.36	0
20	EDO	L	109	-	3,3,3	0.39	0	2,2,2	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	S	104	-	3,3,3	0.68	0	2,2,2	0.36	0
20	EDO	M	105	-	3,3,3	0.45	0	2,2,2	0.36	0
20	EDO	D	206	-	3,3,3	0.49	0	2,2,2	0.76	0
20	EDO	E	210	-	3,3,3	0.58	0	2,2,2	1.60	1 (50%)
20	EDO	E	204	-	3,3,3	0.30	0	2,2,2	0.92	0
27	DMU	P	309	-	34,34,34	0.73	0	45,45,45	2.19	16 (35%)
20	EDO	M	103	-	3,3,3	0.92	0	2,2,2	0.50	0
20	EDO	C	315	-	3,3,3	0.76	0	2,2,2	0.58	0
20	EDO	N	632	-	3,3,3	0.59	0	2,2,2	0.77	0
20	EDO	N	635	-	3,3,3	0.49	0	2,2,2	0.30	0
20	EDO	N	613	-	3,3,3	0.70	0	2,2,2	0.17	0
20	EDO	E	207	-	3,3,3	0.48	0	2,2,2	0.52	0
20	EDO	N	629	-	3,3,3	0.41	0	2,2,2	0.93	0
20	EDO	A	617	-	3,3,3	0.76	0	2,2,2	0.30	0
20	EDO	A	634	-	3,3,3	0.49	0	2,2,2	0.50	0
20	EDO	E	205	-	3,3,3	0.67	0	2,2,2	0.25	0
20	EDO	N	634	-	3,3,3	0.34	0	2,2,2	1.13	0
24	CHD	B	305	-	32,32,32	1.01	0	51,51,51	1.67	13 (25%)
20	EDO	O	311	-	3,3,3	0.41	0	2,2,2	0.26	0
20	EDO	W	104	-	3,3,3	0.41	0	2,2,2	0.39	0
26	CDL	T	101	-	89,91,99	1.46	11 (12%)	94,100,111	1.92	23 (24%)
20	EDO	D	217	-	3,3,3	0.50	0	2,2,2	0.35	0
20	EDO	G	105	-	3,3,3	0.36	0	2,2,2	0.49	0
20	EDO	Y	106	-	3,3,3	0.68	0	2,2,2	0.47	0
20	EDO	A	629	-	3,3,3	0.23	0	2,2,2	1.22	0
20	EDO	C	319	-	3,3,3	0.42	0	2,2,2	0.43	0
20	EDO	B	317	-	3,3,3	0.60	0	2,2,2	0.26	0
20	EDO	B	313	-	3,3,3	0.55	0	2,2,2	0.26	0
20	EDO	N	622	-	3,3,3	0.47	0	2,2,2	0.55	0
20	EDO	P	323	-	3,3,3	0.84	0	2,2,2	0.32	0
20	EDO	A	615	-	3,3,3	0.88	0	2,2,2	0.46	0
20	EDO	O	305	-	3,3,3	0.52	0	2,2,2	0.23	0
20	EDO	B	309	-	3,3,3	0.94	0	2,2,2	0.85	0
20	EDO	L	106	-	3,3,3	0.71	0	2,2,2	0.61	0
20	EDO	D	211	-	3,3,3	0.66	0	2,2,2	0.18	0
27	DMU	C	309	-	22,22,34	0.90	1 (4%)	27,27,45	1.66	6 (22%)
20	EDO	A	618	-	3,3,3	0.38	0	2,2,2	0.87	0
20	EDO	N	611	-	3,3,3	1.06	0	2,2,2	0.14	0
20	EDO	K	104	-	3,3,3	0.42	0	2,2,2	0.60	0
27	DMU	O	303	-	34,34,34	1.07	2 (5%)	45,45,45	1.57	10 (22%)
20	EDO	A	627	-	3,3,3	0.40	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	PGV	N	609	-	50,50,50	1.04	4 (8%)	53,56,56	1.40	8 (15%)
27	DMU	N	610	-	17,17,34	0.77	0	17,18,45	1.26	3 (17%)
20	EDO	Y	108	-	3,3,3	0.38	0	2,2,2	0.34	0
27	DMU	C	310	-	34,34,34	0.88	1 (2%)	45,45,45	1.92	12 (26%)
20	EDO	O	314	-	3,3,3	0.78	0	2,2,2	0.77	0
20	EDO	L	111	-	3,3,3	0.62	0	2,2,2	0.18	0
20	EDO	K	103	-	3,3,3	0.60	0	2,2,2	0.14	0
20	EDO	S	112	-	3,3,3	0.53	0	2,2,2	0.60	0
27	DMU	X	104	-	11,11,34	0.48	0	10,10,45	0.43	0
20	EDO	J	103	-	3,3,3	0.88	0	2,2,2	0.21	0
27	DMU	P	310	-	34,34,34	0.93	1 (2%)	45,45,45	1.33	5 (11%)
20	EDO	O	316	-	3,3,3	0.47	0	2,2,2	0.20	0
20	EDO	M	106	-	3,3,3	0.91	0	2,2,2	0.92	0
20	EDO	I	103	-	3,3,3	0.67	0	2,2,2	0.63	0
20	EDO	D	208	-	3,3,3	0.48	0	2,2,2	0.44	0
20	EDO	C	312	-	3,3,3	0.78	0	2,2,2	0.50	0
20	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.77	0
20	EDO	L	103	-	3,3,3	0.71	0	2,2,2	0.47	0
20	EDO	D	213	-	3,3,3	0.57	0	2,2,2	0.21	0
20	EDO	D	201	-	3,3,3	0.49	0	2,2,2	0.41	0
25	PEK	P	303	-	52,52,52	0.75	2 (3%)	55,57,57	2.27	12 (21%)
20	EDO	J	102	-	3,3,3	0.55	0	2,2,2	0.34	0
20	EDO	D	212	-	3,3,3	0.68	0	2,2,2	0.97	0
20	EDO	L	107	-	3,3,3	0.39	0	2,2,2	0.66	0
20	EDO	A	624	-	3,3,3	0.55	0	2,2,2	0.39	0
14	HEA	A	601[A]	-	57,67,67	1.55	12 (21%)	61,103,103	1.82	19 (31%)
20	EDO	F	105	-	3,3,3	0.57	0	2,2,2	0.31	0
20	EDO	N	624	-	3,3,3	0.46	0	2,2,2	0.21	0
20	EDO	A	635	-	3,3,3	0.37	0	2,2,2	0.52	0
20	EDO	R	204	-	3,3,3	0.69	0	2,2,2	0.72	0
20	EDO	B	319	-	3,3,3	0.54	0	2,2,2	0.08	0
20	EDO	U	103	-	3,3,3	0.66	0	2,2,2	0.42	0
20	EDO	D	220	-	3,3,3	0.51	0	2,2,2	0.18	0
20	EDO	S	102	-	3,3,3	0.97	0	2,2,2	0.66	0
14	HEA	A	602	1	57,67,67	1.35	6 (10%)	61,103,103	1.90	14 (22%)
19	PGV	P	305	-	50,50,50	0.73	3 (6%)	53,56,56	1.10	5 (9%)
20	EDO	B	307	-	3,3,3	1.11	0	2,2,2	0.16	0
20	EDO	P	318	-	3,3,3	0.45	0	2,2,2	0.39	0
20	EDO	F	104	-	3,3,3	0.95	0	2,2,2	0.13	0
20	EDO	N	631	-	3,3,3	0.50	0	2,2,2	0.74	0
20	EDO	A	625	-	3,3,3	0.68	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	A	610	-	3,3,3	0.26	0	2,2,2	1.18	0
20	EDO	I	105	-	3,3,3	0.41	0	2,2,2	0.65	0
22	CUA	B	303	2	0,1,1	-	-	-		
19	PGV	C	305	-	49,49,50	0.75	1 (2%)	52,55,56	0.87	1 (1%)
20	EDO	B	316	-	3,3,3	0.63	0	2,2,2	0.25	0
27	DMU	T	102	-	21,21,34	0.85	2 (9%)	25,25,45	1.08	0
20	EDO	O	318	-	3,3,3	0.83	0	2,2,2	0.37	0
20	EDO	C	314	-	3,3,3	0.52	0	2,2,2	0.11	0
20	EDO	D	205	-	3,3,3	0.46	0	2,2,2	1.11	0
20	EDO	C	322	-	3,3,3	0.72	0	2,2,2	0.15	0
20	EDO	D	219	-	3,3,3	0.67	0	2,2,2	0.34	0
20	EDO	Q	202	-	3,3,3	0.57	0	2,2,2	0.26	0
27	DMU	J	101	-	24,24,34	0.55	0	35,35,45	1.55	10 (28%)
20	EDO	I	101	-	3,3,3	0.56	0	2,2,2	0.83	0
20	EDO	N	628	-	3,3,3	0.49	0	2,2,2	0.56	0
24	CHD	C	301	-	32,32,32	1.03	3 (9%)	51,51,51	1.46	9 (17%)
20	EDO	R	206	-	3,3,3	0.61	0	2,2,2	0.64	0
20	EDO	A	623	-	3,3,3	0.64	0	2,2,2	0.35	0
21	TGL	Y	101	-	59,59,62	1.29	3 (5%)	62,62,65	1.77	14 (22%)
20	EDO	P	327	-	3,3,3	0.68	0	2,2,2	0.42	0
25	PEK	C	302	-	48,48,52	1.23	2 (4%)	51,53,57	1.37	7 (13%)
20	EDO	E	201	-	3,3,3	0.87	0	2,2,2	2.08	1 (50%)
20	EDO	H	103	-	3,3,3	0.59	0	2,2,2	0.40	0
20	EDO	O	307	-	3,3,3	0.55	0	2,2,2	0.29	0
20	EDO	O	315	-	3,3,3	0.56	0	2,2,2	0.40	0
20	EDO	A	636	-	3,3,3	0.42	0	2,2,2	0.49	0
26	CDL	G	101	-	87,87,99	1.32	12 (13%)	89,94,111	1.47	14 (15%)
19	PGV	C	306	-	50,50,50	1.23	3 (6%)	53,56,56	1.44	7 (13%)
20	EDO	S	110	-	3,3,3	0.43	0	2,2,2	0.74	0
20	EDO	S	114	-	3,3,3	0.41	0	2,2,2	0.58	0
20	EDO	P	311	-	3,3,3	0.26	0	2,2,2	1.42	0
20	EDO	N	623	-	3,3,3	0.53	0	2,2,2	0.20	0
24	CHD	G	102	-	32,32,32	0.95	1 (3%)	51,51,51	1.38	8 (15%)
20	EDO	S	108	-	3,3,3	0.56	0	2,2,2	0.24	0
20	EDO	W	103	-	3,3,3	0.53	0	2,2,2	0.41	0
27	DMU	X	102	-	22,22,34	0.74	1 (4%)	27,27,45	1.01	1 (3%)
20	EDO	P	313	-	3,3,3	0.63	0	2,2,2	0.32	0
20	EDO	Y	104	-	3,3,3	0.49	0	2,2,2	0.28	0
24	CHD	Y	102	-	32,32,32	0.85	2 (6%)	51,51,51	2.80	22 (43%)
20	EDO	D	221	-	3,3,3	0.75	0	2,2,2	0.48	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	F	106	-	3,3,3	0.58	0	2,2,2	0.21	0
20	EDO	Q	207	-	3,3,3	0.63	0	2,2,2	0.25	0
20	EDO	N	620	-	3,3,3	0.65	0	2,2,2	0.41	0
20	EDO	U	101	-	3,3,3	0.64	0	2,2,2	0.51	0
20	EDO	A	630	-	3,3,3	0.68	0	2,2,2	0.41	0
29	PO4	U	104	-	4,4,4	0.74	0	6,6,6	0.72	0
20	EDO	G	104	-	3,3,3	0.59	0	2,2,2	0.14	0
25	PEK	C	304	-	52,52,52	1.16	3 (5%)	55,57,57	1.43	7 (12%)
20	EDO	O	317	-	3,3,3	0.42	0	2,2,2	0.74	0
20	EDO	Z	102	-	3,3,3	0.38	0	2,2,2	0.79	0
20	EDO	W	102	-	3,3,3	0.33	0	2,2,2	0.36	0
20	EDO	S	113	-	3,3,3	0.38	0	2,2,2	1.01	0
20	EDO	A	621	-	3,3,3	0.51	0	2,2,2	0.69	0
20	EDO	R	203	-	3,3,3	0.66	0	2,2,2	0.22	0
20	EDO	B	311	-	3,3,3	0.50	0	2,2,2	0.80	0
20	EDO	P	325	-	3,3,3	0.68	0	2,2,2	0.27	0
20	EDO	T	106	-	3,3,3	0.63	0	2,2,2	0.40	0
20	EDO	D	209	-	3,3,3	0.38	0	2,2,2	0.59	0
20	EDO	D	203	-	3,3,3	0.62	0	2,2,2	1.06	0
24	CHD	P	308	-	32,32,32	0.78	0	51,51,51	2.04	16 (31%)
20	EDO	C	323	-	3,3,3	0.57	0	2,2,2	0.27	0
20	EDO	O	308	-	3,3,3	0.75	0	2,2,2	0.34	0
18	CYN	A	606	15	0,1,1	-	-	-	-	-
20	EDO	O	310	-	3,3,3	0.80	0	2,2,2	0.45	0
20	EDO	B	314	-	3,3,3	0.47	0	2,2,2	1.11	0
20	EDO	H	104	-	3,3,3	0.43	0	2,2,2	0.55	0
20	EDO	A	632	-	3,3,3	1.00	0	2,2,2	0.29	0
20	EDO	H	101	-	3,3,3	0.49	0	2,2,2	0.70	0
20	EDO	S	111	-	3,3,3	0.62	0	2,2,2	0.28	0
27	DMU	Z	101	-	34,34,34	0.62	1 (2%)	45,45,45	1.06	2 (4%)
20	EDO	A	613	-	3,3,3	1.32	0	2,2,2	0.97	0
20	EDO	L	105	-	3,3,3	0.57	0	2,2,2	0.11	0
20	EDO	N	633	-	3,3,3	1.07	0	2,2,2	0.20	0
20	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.82	0
20	EDO	F	107	-	3,3,3	0.51	0	2,2,2	0.40	0
27	DMU	X	101	-	9,9,34	0.33	0	8,8,45	0.54	0
20	EDO	K	101	-	3,3,3	0.76	0	2,2,2	0.16	0
26	CDL	P	307	-	83,83,99	1.41	11 (13%)	91,93,111	1.79	22 (24%)
20	EDO	K	105	-	3,3,3	0.46	0	2,2,2	0.76	0
20	EDO	A	612	-	3,3,3	0.64	0	2,2,2	0.34	0
20	EDO	E	203	-	3,3,3	0.56	0	2,2,2	0.38	0
20	EDO	O	306	-	3,3,3	0.57	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	C	324	-	3,3,3	0.94	0	2,2,2	0.31	0
20	EDO	T	105	-	3,3,3	0.55	0	2,2,2	0.06	0
24	CHD	P	301	-	32,32,32	0.94	1 (3%)	51,51,51	1.41	10 (19%)
20	EDO	N	614	-	3,3,3	0.58	0	2,2,2	0.19	0
20	EDO	P	326	-	3,3,3	0.83	0	2,2,2	0.28	0
20	EDO	P	312	-	3,3,3	0.48	0	2,2,2	0.22	0
20	EDO	G	103	-	3,3,3	0.66	0	2,2,2	0.69	0
20	EDO	T	103	-	3,3,3	0.43	0	2,2,2	0.46	0
20	EDO	A	614	-	3,3,3	0.39	0	2,2,2	0.49	0
20	EDO	L	110	-	3,3,3	0.74	0	2,2,2	0.82	0
20	EDO	I	104	-	3,3,3	0.82	0	2,2,2	0.39	0
20	EDO	F	109	-	3,3,3	0.70	0	2,2,2	0.76	0
20	EDO	L	104	-	3,3,3	0.43	0	2,2,2	0.16	0
29	PO4	H	105	-	4,4,4	0.83	0	6,6,6	1.17	0
23	PSC	O	302	-	42,42,51	1.25	4 (9%)	46,47,59	2.03	11 (23%)
20	EDO	W	101	-	3,3,3	0.38	0	2,2,2	0.78	0
20	EDO	A	611	-	3,3,3	0.52	0	2,2,2	0.65	0
20	EDO	P	320	-	3,3,3	0.35	0	2,2,2	0.66	0
20	EDO	P	321	-	3,3,3	0.59	0	2,2,2	0.62	0
20	EDO	B	320	-	3,3,3	0.56	0	2,2,2	0.29	0
20	EDO	P	314	-	3,3,3	0.54	0	2,2,2	0.30	0
20	EDO	S	106	-	3,3,3	0.69	0	2,2,2	0.82	0
20	EDO	D	218	-	3,3,3	0.87	0	2,2,2	0.36	0
20	EDO	C	326	-	3,3,3	1.04	0	2,2,2	0.92	0
20	EDO	Q	209	-	3,3,3	0.48	0	2,2,2	0.08	0
20	EDO	I	102	-	3,3,3	0.66	0	2,2,2	0.52	0
20	EDO	B	322	-	3,3,3	0.85	0	2,2,2	0.66	0
20	EDO	Q	206	-	3,3,3	0.55	0	2,2,2	0.40	0
20	EDO	U	102	-	3,3,3	0.85	0	2,2,2	0.35	0
20	EDO	B	323	-	3,3,3	0.50	0	2,2,2	0.65	0
20	EDO	Q	208	-	3,3,3	0.58	0	2,2,2	0.31	0
20	EDO	B	318	-	3,3,3	0.51	0	2,2,2	0.05	0
20	EDO	Q	204	-	3,3,3	0.43	0	2,2,2	0.49	0
20	EDO	D	207	-	3,3,3	0.68	0	2,2,2	0.37	0
19	PGV	P	306	-	50,50,50	1.12	2 (4%)	53,56,56	1.45	10 (18%)
14	HEA	N	601[A]	-	57,67,67	1.31	10 (17%)	61,103,103	1.82	21 (34%)
20	EDO	V	102	-	3,3,3	0.50	0	2,2,2	0.32	0
21	TGL	L	101	-	58,58,62	1.30	3 (5%)	60,60,65	1.87	15 (25%)
27	DMU	X	103	-	34,34,34	0.98	1 (2%)	45,45,45	1.93	16 (35%)
20	EDO	N	618	-	3,3,3	0.86	0	2,2,2	1.00	0
20	EDO	V	101	-	3,3,3	0.59	0	2,2,2	0.09	0
22	CUA	O	301	2	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	S	105	-	3,3,3	0.34	0	2,2,2	0.65	0
20	EDO	O	304	-	3,3,3	0.44	0	2,2,2	0.59	0
20	EDO	N	617	-	3,3,3	0.80	0	2,2,2	0.68	0
20	EDO	T	104	-	3,3,3	0.75	0	2,2,2	0.70	0
20	EDO	S	103	-	3,3,3	0.73	0	2,2,2	0.68	0
20	EDO	O	312	-	3,3,3	0.66	0	2,2,2	0.55	0
20	EDO	D	202	-	3,3,3	0.22	0	2,2,2	0.93	0
20	EDO	B	324	-	3,3,3	0.54	0	2,2,2	0.81	0
20	EDO	F	108	-	3,3,3	0.39	0	2,2,2	1.29	0
20	EDO	D	210	-	3,3,3	0.39	0	2,2,2	0.50	0
20	EDO	C	321	-	3,3,3	0.65	0	2,2,2	0.07	0
20	EDO	P	319	-	3,3,3	0.70	0	2,2,2	0.35	0
20	EDO	P	315	-	3,3,3	0.57	0	2,2,2	0.50	0
20	EDO	M	104	-	3,3,3	0.45	0	2,2,2	0.24	0
25	PEK	P	302	-	32,32,52	1.03	1 (3%)	34,36,57	1.38	4 (11%)
20	EDO	E	213	-	3,3,3	0.35	0	2,2,2	0.65	0
20	EDO	O	319	-	3,3,3	0.40	0	2,2,2	0.37	0
20	EDO	B	321	-	3,3,3	0.31	0	2,2,2	1.01	0
21	TGL	N	607	-	62,62,62	1.13	3 (4%)	65,65,65	1.30	8 (12%)
14	HEA	N	602	1	57,67,67	1.35	8 (14%)	61,103,103	1.80	18 (29%)
20	EDO	R	205	-	3,3,3	0.64	0	2,2,2	0.33	0
20	EDO	I	106	-	3,3,3	0.42	0	2,2,2	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	C	315	-	-	1/1/1/1	-
20	EDO	U	103	-	-	0/1/1/1	-
20	EDO	N	633	-	-	1/1/1/1	-
20	EDO	D	216	-	-	0/1/1/1	-
20	EDO	N	632	-	-	0/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
20	EDO	O	313	-	-	0/1/1/1	-
20	EDO	D	220	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
20	EDO	F	107	-	-	1/1/1/1	-
27	DMU	X	101	-	-	2/7/7/59	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	K	101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	635	-	-	1/1/1/1	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	A	622	-	-	0/1/1/1	-
20	EDO	E	207	-	-	0/1/1/1	-
20	EDO	S	102	-	-	0/1/1/1	-
26	CDL	P	307	-	-	39/87/87/110	-
20	EDO	N	629	-	-	1/1/1/1	-
20	EDO	K	105	-	-	1/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
14	HEA	A	602	1	3/3/7/16	4/32/76/76	-
19	PGV	P	305	-	-	7/55/55/55	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
20	EDO	O	306	-	-	0/1/1/1	-
20	EDO	N	621	-	-	1/1/1/1	-
20	EDO	O	309	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
20	EDO	C	324	-	-	1/1/1/1	-
20	EDO	A	634	-	-	0/1/1/1	-
20	EDO	P	318	-	-	1/1/1/1	-
20	EDO	A	620	-	-	0/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	E	205	-	-	0/1/1/1	-
20	EDO	N	631	-	-	0/1/1/1	-
20	EDO	T	105	-	-	0/1/1/1	-
20	EDO	A	625	-	-	0/1/1/1	-
20	EDO	N	634	-	-	1/1/1/1	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
25	PEK	P	304	-	-	24/55/55/56	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	K	102	-	-	1/1/1/1	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	P	326	-	-	1/1/1/1	-
20	EDO	P	312	-	-	1/1/1/1	-
20	EDO	A	610	-	-	1/1/1/1	-
24	CHD	B	305	-	-	2/9/74/74	0/4/4/4
20	EDO	I	105	-	-	0/1/1/1	-
20	EDO	G	103	-	-	0/1/1/1	-
20	EDO	C	325	-	-	1/1/1/1	-
19	PGV	C	305	-	-	13/54/54/55	-
20	EDO	O	311	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	T	103	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
20	EDO	B	316	-	-	1/1/1/1	-
20	EDO	L	110	-	-	0/1/1/1	-
20	EDO	E	209	-	-	1/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	3/3/7/16	5/32/76/76	-
20	EDO	I	104	-	-	0/1/1/1	-
20	EDO	O	318	-	-	1/1/1/1	-
20	EDO	H	102	-	-	1/1/1/1	-
20	EDO	V	103	-	-	0/1/1/1	-
20	EDO	W	104	-	-	1/1/1/1	-
26	CDL	T	101	-	-	35/96/100/110	-
20	EDO	P	317	-	-	1/1/1/1	-
27	DMU	T	102	-	-	6/13/30/59	0/1/1/2
21	TGL	B	301	-	-	27/65/65/65	-
20	EDO	C	314	-	-	1/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	T	107	-	-	1/1/1/1	-
20	EDO	C	322	-	-	1/1/1/1	-
20	EDO	Y	105	-	-	1/1/1/1	-
20	EDO	D	219	-	-	1/1/1/1	-
20	EDO	F	109	-	-	0/1/1/1	-
20	EDO	J	104	-	-	0/1/1/1	-
20	EDO	L	104	-	-	1/1/1/1	-
20	EDO	D	217	-	-	0/1/1/1	-
20	EDO	E	206	-	-	0/1/1/1	-
20	EDO	L	102	-	-	0/1/1/1	-
20	EDO	L	108	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	0/1/1/1	-
20	EDO	G	105	-	-	0/1/1/1	-
20	EDO	P	316	-	-	1/1/1/1	-
23	PSC	O	302	-	-	21/44/44/55	-
20	EDO	A	626	-	-	1/1/1/1	-
20	EDO	W	101	-	-	1/1/1/1	-
20	EDO	A	611	-	-	0/1/1/1	-
20	EDO	N	625	-	-	0/1/1/1	-
20	EDO	Y	106	-	-	0/1/1/1	-
20	EDO	A	629	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	Q	205	-	-	1/1/1/1	-
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	P	320	-	-	1/1/1/1	-
20	EDO	D	215	-	-	1/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-
20	EDO	C	319	-	-	1/1/1/1	-
27	DMU	J	101	-	-	1/8/48/59	0/2/2/2
20	EDO	B	317	-	-	1/1/1/1	-
20	EDO	P	321	-	-	1/1/1/1	-
20	EDO	B	320	-	-	1/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	I	101	-	-	1/1/1/1	-
20	EDO	N	628	-	-	0/1/1/1	-
20	EDO	B	313	-	-	0/1/1/1	-
20	EDO	N	622	-	-	0/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
20	EDO	P	323	-	-	0/1/1/1	-
20	EDO	D	218	-	-	0/1/1/1	-
19	PGV	A	607	-	-	27/51/51/55	-
20	EDO	S	109	-	-	1/1/1/1	-
25	PEK	C	303	-	-	9/56/56/56	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	C	326	-	-	0/1/1/1	-
20	EDO	R	206	-	-	0/1/1/1	-
20	EDO	O	305	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	0/1/1/1	-
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	Q	209	-	-	1/1/1/1	-
20	EDO	A	623	-	-	0/1/1/1	-
20	EDO	B	309	-	-	1/1/1/1	-
20	EDO	L	106	-	-	1/1/1/1	-
21	TGL	Y	101	-	-	35/62/62/65	-
20	EDO	P	327	-	-	0/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
25	PEK	C	302	-	-	21/52/52/56	-
20	EDO	E	201	-	-	0/1/1/1	-
24	CHD	C	308	-	-	9/9/74/74	0/4/4/4
20	EDO	D	211	-	-	1/1/1/1	-
20	EDO	H	103	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	C	309	-	-	11/13/33/59	0/1/1/2
20	EDO	C	318	-	-	1/1/1/1	-
20	EDO	I	102	-	-	1/1/1/1	-
19	PGV	N	608	-	-	19/46/46/55	-
20	EDO	B	312	-	-	1/1/1/1	-
20	EDO	O	307	-	-	0/1/1/1	-
20	EDO	A	618	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	B	322	-	-	1/1/1/1	-
20	EDO	Q	206	-	-	1/1/1/1	-
20	EDO	A	628	-	-	0/1/1/1	-
20	EDO	O	315	-	-	1/1/1/1	-
20	EDO	A	636	-	-	0/1/1/1	-
20	EDO	K	104	-	-	0/1/1/1	-
26	CDL	G	101	-	-	42/90/90/110	-
20	EDO	U	102	-	-	1/1/1/1	-
20	EDO	P	324	-	-	0/1/1/1	-
19	PGV	C	306	-	-	19/55/55/55	-
27	DMU	O	303	-	-	8/19/59/59	0/2/2/2
20	EDO	A	627	-	-	1/1/1/1	-
20	EDO	B	323	-	-	1/1/1/1	-
19	PGV	A	608	-	-	5/55/55/55	-
19	PGV	N	609	-	-	7/55/55/55	-
20	EDO	S	110	-	-	0/1/1/1	-
27	DMU	N	610	-	-	9/11/19/59	0/1/1/2
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	Q	208	-	-	1/1/1/1	-
20	EDO	Y	108	-	-	0/1/1/1	-
20	EDO	S	114	-	-	1/1/1/1	-
20	EDO	B	318	-	-	0/1/1/1	-
27	DMU	C	310	-	-	3/19/59/59	0/2/2/2
20	EDO	Q	204	-	-	1/1/1/1	-
20	EDO	P	311	-	-	1/1/1/1	-
20	EDO	O	314	-	-	1/1/1/1	-
26	CDL	C	307	-	-	55/98/98/110	-
20	EDO	D	207	-	-	1/1/1/1	-
20	EDO	N	623	-	-	1/1/1/1	-
20	EDO	L	111	-	-	1/1/1/1	-
27	DMU	M	101	-	-	5/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHD	G	102	-	-	2/9/74/74	0/4/4/4
19	PGV	P	306	-	-	26/55/55/55	-
20	EDO	N	630	-	-	0/1/1/1	-
20	EDO	K	103	-	-	1/1/1/1	-
20	EDO	S	108	-	-	0/1/1/1	-
20	EDO	W	103	-	-	0/1/1/1	-
14	HEA	N	601[A]	-	3/3/7/16	6/32/76/76	-
20	EDO	V	102	-	-	1/1/1/1	-
20	EDO	E	212	-	-	1/1/1/1	-
21	TGL	L	101	-	-	34/59/59/65	-
27	DMU	X	103	-	-	7/19/59/59	0/2/2/2
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	V	101	-	-	1/1/1/1	-
20	EDO	S	112	-	-	1/1/1/1	-
27	DMU	X	104	-	-	3/9/9/59	-
27	DMU	X	102	-	-	10/13/33/59	0/1/1/2
20	EDO	P	313	-	-	0/1/1/1	-
20	EDO	S	105	-	-	1/1/1/1	-
20	EDO	J	103	-	-	1/1/1/1	-
20	EDO	N	615	-	-	1/1/1/1	-
20	EDO	N	619	-	-	1/1/1/1	-
20	EDO	D	221	-	-	0/1/1/1	-
20	EDO	F	106	-	-	1/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-
20	EDO	Y	104	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	O	316	-	-	0/1/1/1	-
20	EDO	E	202	-	-	1/1/1/1	-
20	EDO	Q	207	-	-	0/1/1/1	-
20	EDO	M	106	-	-	1/1/1/1	-
20	EDO	I	103	-	-	1/1/1/1	-
20	EDO	N	620	-	-	1/1/1/1	-
20	EDO	R	202	-	-	1/1/1/1	-
20	EDO	U	101	-	-	1/1/1/1	-
20	EDO	T	104	-	-	0/1/1/1	-
21	TGL	B	302	-	-	37/64/64/65	-
20	EDO	D	208	-	-	1/1/1/1	-
20	EDO	C	312	-	-	1/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-
20	EDO	A	619	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	630	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	C	313	-	-	1/1/1/1	-
20	EDO	A	633	-	-	0/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
20	EDO	D	204	-	-	1/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	G	104	-	-	1/1/1/1	-
14	HEA	N	601[B]	-	3/3/7/16	4/32/76/76	-
20	EDO	D	213	-	-	0/1/1/1	-
20	EDO	D	201	-	-	0/1/1/1	-
20	EDO	O	312	-	-	1/1/1/1	-
20	EDO	D	202	-	-	0/1/1/1	-
20	EDO	B	324	-	-	0/1/1/1	-
20	EDO	D	214	-	-	1/1/1/1	-
20	EDO	O	317	-	-	1/1/1/1	-
25	PEK	C	304	-	-	22/56/56/56	-
20	EDO	Z	102	-	-	0/1/1/1	-
20	EDO	W	102	-	-	1/1/1/1	-
25	PEK	P	303	-	-	19/56/56/56	-
20	EDO	J	102	-	-	0/1/1/1	-
20	EDO	E	211	-	-	1/1/1/1	-
20	EDO	S	107	-	-	0/1/1/1	-
20	EDO	D	212	-	-	1/1/1/1	-
20	EDO	S	113	-	-	1/1/1/1	-
20	EDO	L	107	-	-	0/1/1/1	-
20	EDO	A	621	-	-	1/1/1/1	-
20	EDO	F	108	-	-	1/1/1/1	-
20	EDO	R	203	-	-	1/1/1/1	-
20	EDO	D	210	-	-	0/1/1/1	-
20	EDO	B	311	-	-	1/1/1/1	-
20	EDO	C	320	-	-	0/1/1/1	-
20	EDO	A	624	-	-	0/1/1/1	-
20	EDO	A	631	-	-	1/1/1/1	-
20	EDO	C	321	-	-	0/1/1/1	-
20	EDO	P	325	-	-	0/1/1/1	-
20	EDO	T	106	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	3/3/7/16	8/32/76/76	-
20	EDO	D	209	-	-	1/1/1/1	-
20	EDO	E	208	-	-	1/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	D	203	-	-	1/1/1/1	-
20	EDO	N	624	-	-	1/1/1/1	-
20	EDO	P	315	-	-	1/1/1/1	-
20	EDO	P	319	-	-	0/1/1/1	-
20	EDO	Y	107	-	-	1/1/1/1	-
24	CHD	P	308	-	-	5/9/74/74	0/4/4/4
23	PSC	B	304	-	-	24/51/51/55	-
20	EDO	B	315	-	-	0/1/1/1	-
20	EDO	C	323	-	-	1/1/1/1	-
20	EDO	M	104	-	-	0/1/1/1	-
20	EDO	O	308	-	-	0/1/1/1	-
25	PEK	P	302	-	-	16/34/34/56	-
24	CHD	Y	102	-	-	6/9/74/74	0/4/4/4
21	TGL	Q	201	-	-	36/65/65/65	-
20	EDO	O	310	-	-	0/1/1/1	-
20	EDO	E	213	-	-	0/1/1/1	-
20	EDO	B	314	-	-	1/1/1/1	-
20	EDO	P	322	-	-	0/1/1/1	-
20	EDO	B	310	-	-	1/1/1/1	-
20	EDO	N	627	-	-	1/1/1/1	-
20	EDO	A	635	-	-	1/1/1/1	-
20	EDO	L	109	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	M	105	-	-	0/1/1/1	-
20	EDO	H	104	-	-	1/1/1/1	-
20	EDO	D	206	-	-	0/1/1/1	-
20	EDO	A	632	-	-	0/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-
20	EDO	H	101	-	-	1/1/1/1	-
20	EDO	S	111	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	B	321	-	-	1/1/1/1	-
20	EDO	O	319	-	-	1/1/1/1	-
20	EDO	E	210	-	-	0/1/1/1	-
21	TGL	N	607	-	-	30/65/65/65	-
20	EDO	E	204	-	-	1/1/1/1	-
20	EDO	B	319	-	-	0/1/1/1	-
14	HEA	N	602	1	3/3/7/16	4/32/76/76	-
20	EDO	R	205	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	P	309	-	-	6/19/59/59	0/2/2/2
20	EDO	I	106	-	-	1/1/1/1	-
27	DMU	P	310	-	-	5/19/59/59	0/2/2/2
20	EDO	L	105	-	-	1/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-

All (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Y	101	TGL	OG2-CB1	6.39	1.52	1.34
21	L	101	TGL	OG2-CB1	6.13	1.51	1.34
19	C	306	PGV	O01-C1	5.33	1.49	1.34
26	T	101	CDL	OB8-CB7	5.25	1.48	1.33
21	B	301	TGL	OG1-CA1	5.20	1.48	1.33
25	C	302	PEK	O03-C21	5.20	1.48	1.33
19	C	306	PGV	O03-C19	5.08	1.48	1.33
21	L	101	TGL	OG3-CC1	5.08	1.48	1.33
21	Y	101	TGL	OG3-CC1	5.07	1.48	1.33
25	C	302	PEK	O01-C1	5.07	1.48	1.34
21	B	302	TGL	OG2-CB1	4.99	1.48	1.34
26	T	101	CDL	OA6-CA5	4.96	1.48	1.34
19	A	607	PGV	O03-C19	4.95	1.47	1.33
19	P	306	PGV	O01-C1	4.94	1.48	1.34
21	N	607	TGL	OG2-CB1	4.93	1.48	1.34
25	C	304	PEK	O01-C1	4.90	1.48	1.34
25	P	304	PEK	O01-C1	4.90	1.48	1.34
25	C	304	PEK	O03-C21	4.87	1.47	1.33
25	P	304	PEK	O03-C21	4.87	1.47	1.33
26	G	101	CDL	OB8-CB7	4.84	1.47	1.33
26	T	101	CDL	OA8-CA7	4.83	1.47	1.33
26	G	101	CDL	OB6-CB5	4.80	1.47	1.34
25	P	302	PEK	O01-C1	4.78	1.47	1.34
23	O	302	PSC	O01-C1	4.75	1.47	1.34
26	C	307	CDL	OA8-CA7	4.68	1.47	1.33
19	P	306	PGV	O03-C19	4.67	1.47	1.33
26	P	307	CDL	OB8-CB7	4.64	1.46	1.33
26	T	101	CDL	OB6-CB5	4.62	1.47	1.34
19	N	608	PGV	O03-C19	4.57	1.46	1.33
26	P	307	CDL	OA8-CA7	4.56	1.46	1.33
21	B	302	TGL	OG1-CA1	4.55	1.46	1.33
21	L	101	TGL	OG1-CA1	4.53	1.46	1.33
21	B	301	TGL	OG3-CC1	4.52	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	304	PSC	O01-C1	4.52	1.47	1.34
19	A	607	PGV	O01-C1	4.50	1.47	1.34
26	C	307	CDL	OB8-CB7	4.48	1.46	1.33
21	N	607	TGL	OG1-CA1	4.44	1.46	1.33
21	N	607	TGL	OG3-CC1	4.43	1.46	1.33
21	B	301	TGL	OG2-CB1	4.33	1.46	1.34
21	Q	201	TGL	OG3-CC1	4.31	1.45	1.33
21	Q	201	TGL	OG1-CA1	4.22	1.45	1.33
21	B	302	TGL	OG3-CC1	4.20	1.45	1.33
26	P	307	CDL	OA6-CA5	4.18	1.46	1.34
23	B	304	PSC	O03-C19	4.14	1.45	1.33
19	N	608	PGV	O01-C1	4.02	1.45	1.34
21	Y	101	TGL	OG1-CA1	3.99	1.45	1.33
21	Q	201	TGL	OG2-CB1	3.92	1.45	1.34
26	C	307	CDL	OA6-CA5	3.86	1.45	1.34
23	O	302	PSC	C13-C12	3.84	1.54	1.31
26	G	101	CDL	OA8-CA7	-3.78	1.22	1.42
14	N	602	HEA	C1D-ND	-3.75	1.33	1.40
23	B	304	PSC	C13-C12	3.73	1.53	1.31
14	A	601[A]	HEA	C3C-C2C	-3.67	1.35	1.40
14	A	601[B]	HEA	C3C-C2C	-3.67	1.35	1.40
27	P	310	DMU	O16-C6	3.67	1.46	1.40
26	C	307	CDL	C59-C58	-3.57	1.31	1.51
14	N	601[A]	HEA	CHC-C4B	3.52	1.44	1.35
14	N	601[B]	HEA	CHC-C4B	3.52	1.44	1.35
26	P	307	CDL	C79-C78	-3.52	1.31	1.51
26	T	101	CDL	C62-C61	-3.47	1.32	1.51
26	T	101	CDL	C59-C58	-3.46	1.32	1.51
26	G	101	CDL	C59-C58	-3.46	1.32	1.51
26	C	307	CDL	C79-C78	-3.45	1.32	1.51
26	G	101	CDL	C62-C61	-3.44	1.32	1.51
14	A	602	HEA	CHC-C4B	3.42	1.43	1.35
26	P	307	CDL	OB6-CB5	3.39	1.43	1.34
26	C	307	CDL	C19-C18	-3.38	1.32	1.51
26	C	307	CDL	C62-C61	-3.33	1.32	1.51
26	C	307	CDL	C22-C21	-3.30	1.33	1.51
26	P	307	CDL	C82-C81	-3.26	1.33	1.51
26	P	307	CDL	C19-C18	-3.25	1.33	1.51
26	P	307	CDL	C59-C58	-3.21	1.33	1.51
27	C	309	DMU	O16-C6	3.21	1.45	1.40
14	A	602	HEA	CHD-C1D	3.21	1.43	1.35
14	A	601[A]	HEA	CHD-C1D	3.20	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[B]	HEA	CHD-C1D	3.20	1.43	1.35
26	G	101	CDL	C42-C41	-3.18	1.33	1.51
26	C	307	CDL	C82-C81	-3.17	1.33	1.51
26	T	101	CDL	C82-C81	-3.16	1.33	1.51
23	O	302	PSC	O03-C19	3.13	1.42	1.33
19	N	609	PGV	O03-C19	3.10	1.42	1.33
26	T	101	CDL	C42-C41	-3.10	1.34	1.51
26	T	101	CDL	C79-C78	-3.07	1.34	1.51
19	N	609	PGV	O01-C1	3.05	1.42	1.34
14	N	602	HEA	CHD-C1D	3.03	1.42	1.35
26	C	307	CDL	C39-C38	-3.03	1.34	1.51
26	P	307	CDL	C22-C21	-3.03	1.34	1.51
26	G	101	CDL	C18-C17	-3.01	1.34	1.51
27	C	310	DMU	O16-C6	3.00	1.45	1.40
14	A	601[A]	HEA	CBD-CGD	2.99	1.57	1.50
14	A	601[B]	HEA	CBD-CGD	2.99	1.57	1.50
26	G	101	CDL	C39-C38	-2.94	1.35	1.51
26	C	307	CDL	OB6-CB5	2.92	1.42	1.34
14	A	602	HEA	C1D-C2D	-2.92	1.38	1.44
19	N	609	PGV	O01-C02	-2.89	1.39	1.46
27	X	103	DMU	O16-C6	2.86	1.45	1.40
26	C	307	CDL	C42-C41	-2.83	1.35	1.51
14	A	601[A]	HEA	C1D-ND	-2.83	1.35	1.40
14	A	601[B]	HEA	C1D-ND	-2.83	1.35	1.40
14	N	602	HEA	O11-C11	2.81	1.48	1.42
26	G	101	CDL	C82-C81	-2.79	1.35	1.51
14	N	601[A]	HEA	CHD-C1D	2.78	1.42	1.35
14	N	601[B]	HEA	CHD-C1D	2.78	1.42	1.35
26	T	101	CDL	C19-C18	-2.77	1.36	1.51
25	P	303	PEK	C2-C1	2.77	1.58	1.50
26	C	307	CDL	OB6-CB4	-2.76	1.39	1.46
14	A	601[A]	HEA	C4D-C3D	-2.75	1.40	1.45
14	A	601[B]	HEA	C4D-C3D	-2.75	1.40	1.45
26	T	101	CDL	C39-C38	-2.75	1.36	1.51
19	A	608	PGV	O01-C1	2.74	1.42	1.34
14	A	602	HEA	C18-C19	2.71	1.39	1.33
14	N	601[A]	HEA	C4B-NB	-2.71	1.35	1.40
14	N	601[B]	HEA	C4B-NB	-2.71	1.35	1.40
14	A	601[A]	HEA	C4B-NB	-2.70	1.35	1.40
14	A	601[B]	HEA	C4B-NB	-2.70	1.35	1.40
26	G	101	CDL	C79-C78	-2.67	1.36	1.51
26	P	307	CDL	C62-C61	-2.64	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	102	DMU	O16-C6	2.55	1.44	1.40
19	C	306	PGV	C01-C02	2.53	1.58	1.50
27	M	101	DMU	O16-C6	2.52	1.44	1.40
19	A	607	PGV	O02-C1	2.47	1.29	1.22
14	A	601[A]	HEA	CHC-C4B	2.43	1.41	1.35
14	A	601[B]	HEA	CHC-C4B	2.43	1.41	1.35
14	A	601[A]	HEA	O11-C11	2.43	1.48	1.42
14	A	601[B]	HEA	O11-C11	2.43	1.48	1.42
14	A	602	HEA	C3C-C2C	-2.41	1.37	1.40
19	P	305	PGV	O01-C1	2.41	1.41	1.34
14	A	601[A]	HEA	C4B-C3B	-2.41	1.40	1.44
14	A	601[B]	HEA	C4B-C3B	-2.41	1.40	1.44
14	A	601[A]	HEA	C3D-C2D	2.40	1.41	1.36
14	A	601[B]	HEA	C3D-C2D	2.40	1.41	1.36
26	P	307	CDL	C39-C38	-2.40	1.34	1.51
14	N	602	HEA	CHC-C4B	2.36	1.41	1.35
14	A	601[A]	HEA	CMB-C2B	2.35	1.55	1.50
14	A	601[B]	HEA	CMB-C2B	2.35	1.55	1.50
14	N	601[A]	HEA	O1D-CGD	2.34	1.29	1.22
14	N	601[B]	HEA	O1D-CGD	2.34	1.29	1.22
25	C	303	PEK	O01-C1	2.33	1.40	1.34
24	C	301	CHD	O25-C24	2.28	1.29	1.22
23	O	302	PSC	O03-C01	-2.28	1.40	1.45
26	G	101	CDL	C21-C20	-2.27	1.35	1.51
27	Z	101	DMU	O16-C6	2.23	1.44	1.40
14	N	602	HEA	CBA-CGA	2.22	1.55	1.50
19	C	305	PGV	O01-C1	2.21	1.40	1.34
27	O	303	DMU	O7-C10	2.20	1.47	1.41
14	N	602	HEA	C4B-NB	-2.19	1.36	1.40
27	T	102	DMU	O16-C6	2.18	1.43	1.40
24	Y	102	CHD	C20-C17	2.16	1.58	1.54
27	O	303	DMU	O16-C6	2.16	1.43	1.40
24	P	301	CHD	C13-C14	-2.15	1.51	1.55
19	A	608	PGV	C03-C02	2.15	1.57	1.50
14	N	601[A]	HEA	O1A-CGA	2.15	1.29	1.22
14	N	601[B]	HEA	O1A-CGA	2.15	1.29	1.22
14	N	601[A]	HEA	CMD-C2D	2.14	1.55	1.50
14	N	601[B]	HEA	CMD-C2D	2.14	1.55	1.50
19	A	607	PGV	P-O13	2.14	1.58	1.50
23	B	304	PSC	C2-C1	2.13	1.56	1.50
19	A	607	PGV	O01-C02	-2.13	1.41	1.46
14	N	602	HEA	C4D-C3D	-2.12	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	305	PGV	P-O14	-2.12	1.45	1.55
19	N	609	PGV	O03-C01	2.12	1.50	1.45
14	N	601[A]	HEA	O11-C11	2.10	1.47	1.42
14	N	601[B]	HEA	O11-C11	2.10	1.47	1.42
24	Y	102	CHD	C8-C7	2.10	1.57	1.53
14	N	601[A]	HEA	C1D-C2D	-2.09	1.40	1.44
14	N	601[B]	HEA	C1D-C2D	-2.09	1.40	1.44
26	C	307	CDL	PA1-OA2	2.09	1.62	1.54
14	N	601[A]	HEA	C1D-ND	-2.07	1.36	1.40
14	N	601[B]	HEA	C1D-ND	-2.07	1.36	1.40
24	C	301	CHD	O12-C12	2.06	1.47	1.43
27	T	102	DMU	C4-C3	2.05	1.55	1.51
14	N	602	HEA	C12-C11	2.05	1.56	1.52
25	C	304	PEK	C01-C02	2.04	1.57	1.50
14	A	602	HEA	O2D-CGD	-2.03	1.23	1.30
24	C	301	CHD	O26-C24	-2.03	1.23	1.30
24	G	102	CHD	O25-C24	2.03	1.28	1.22
19	P	305	PGV	O01-C02	-2.02	1.41	1.46
24	C	308	CHD	C10-C9	-2.02	1.52	1.56
14	N	601[A]	HEA	O2D-CGD	-2.01	1.24	1.30
14	N	601[B]	HEA	O2D-CGD	-2.01	1.24	1.30
14	A	601[A]	HEA	C12-C13	2.01	1.60	1.53
14	A	601[B]	HEA	C12-C13	2.01	1.60	1.53
26	G	101	CDL	CB6-CB4	2.01	1.56	1.50
25	P	303	PEK	C3-C2	2.00	1.59	1.52

All (551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	303	PEK	C2-C3-C4	11.82	134.29	113.23
24	C	308	CHD	C23-C22-C20	-8.32	99.32	114.52
19	A	607	PGV	O01-C1-O02	8.26	143.67	123.70
26	T	101	CDL	OA6-CA5-C11	7.58	127.84	111.50
21	B	301	TGL	OG2-CB1-CB2	7.36	127.37	111.50
21	B	302	TGL	OG2-CB1-CB2	7.22	127.06	111.50
23	O	302	PSC	O01-C1-C2	7.14	126.90	111.50
21	Q	201	TGL	CG2-OG2-CB1	-6.93	100.72	117.79
24	Y	102	CHD	C6-C5-C4	-6.75	103.41	111.19
26	T	101	CDL	OB5-CB3-CB4	6.66	128.37	108.31
26	G	101	CDL	OB6-CB5-C51	6.65	125.84	111.50
21	Y	101	TGL	OG2-CB1-CB2	6.59	125.71	111.50
23	B	304	PSC	O01-C1-C2	6.51	125.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	303	PEK	O01-C1-O02	-6.26	108.57	123.70
24	Y	102	CHD	C14-C8-C7	6.26	120.11	111.81
24	P	308	CHD	C15-C14-C13	6.23	109.66	103.55
25	P	304	PEK	O01-C1-C2	6.03	124.50	111.50
26	P	307	CDL	CB4-OB6-CB5	-6.00	103.01	117.79
24	Y	102	CHD	C21-C20-C17	5.93	122.00	112.92
21	Q	201	TGL	OG2-CB1-CB2	5.84	124.09	111.50
26	P	307	CDL	C52-C51-CB5	-5.78	92.61	113.62
26	C	307	CDL	C52-C51-CB5	-5.70	92.88	113.62
21	L	101	TGL	CG2-OG2-CB1	5.63	131.66	117.79
21	L	101	TGL	OG2-CB1-CB2	5.63	123.63	111.50
23	O	302	PSC	C03-C02-C01	-5.59	98.56	111.79
24	C	308	CHD	C13-C17-C20	-5.58	112.83	119.50
24	Y	102	CHD	C14-C13-C12	5.43	112.46	107.40
21	L	101	TGL	OG3-CC1-CC2	5.38	125.50	111.38
26	T	101	CDL	OA8-CA7-C31	5.27	128.44	111.91
24	Y	102	CHD	C11-C9-C10	-5.26	108.30	113.73
26	T	101	CDL	OB6-CB5-C51	5.26	122.84	111.50
14	A	602	HEA	CHA-C4D-ND	5.22	130.10	124.43
19	A	607	PGV	O01-C1-C2	-5.17	100.35	111.50
14	N	602	HEA	CHA-C4D-ND	5.15	130.03	124.43
26	P	307	CDL	OB2-PB2-OB5	-5.11	93.14	106.73
24	Y	102	CHD	C1-C10-C5	5.07	115.27	107.77
24	Y	102	CHD	C11-C12-C13	5.02	116.40	111.24
21	N	607	TGL	OG2-CB1-CB2	4.95	122.17	111.50
19	P	306	PGV	O03-C19-C20	4.86	127.17	111.91
19	A	607	PGV	C02-O01-C1	4.85	129.74	117.79
24	C	308	CHD	C21-C20-C17	4.77	120.23	112.92
27	C	310	DMU	O4-C7-C5	-4.72	99.43	110.35
27	P	310	DMU	O1-C9-C11	4.72	118.16	106.44
24	C	308	CHD	C17-C13-C12	-4.71	113.37	117.67
24	C	308	CHD	C6-C5-C4	-4.62	105.87	111.19
24	P	308	CHD	C19-C10-C9	-4.59	104.85	111.18
26	P	307	CDL	OB8-CB7-C71	4.59	126.30	111.91
23	O	302	PSC	O03-C01-C02	-4.56	95.17	108.43
27	C	310	DMU	O16-C6-C1	4.55	115.41	108.30
21	B	301	TGL	OG1-CA1-CA2	4.50	126.02	111.91
27	P	309	DMU	O16-C6-C1	4.48	115.30	108.30
19	C	306	PGV	O03-C19-C20	4.48	125.95	111.91
19	N	609	PGV	O01-C1-O02	-4.44	112.98	123.70
21	B	302	TGL	OB1-CB1-CB2	-4.43	106.47	123.73
14	A	602	HEA	C27-C19-C20	4.38	122.64	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	304	PEK	O03-C21-C22	4.37	125.64	111.91
19	P	306	PGV	O01-C1-C2	4.37	120.91	111.50
25	C	302	PEK	O03-C21-C22	4.37	125.61	111.91
27	P	309	DMU	C10-O1-C9	4.36	122.25	113.69
25	C	304	PEK	O01-C1-C2	4.33	120.82	111.50
14	A	602	HEA	CMC-C2C-C1C	-4.30	121.85	128.46
24	P	308	CHD	C18-C13-C12	-4.30	104.69	109.07
25	C	304	PEK	O03-C21-O04	-4.28	112.80	123.59
21	B	301	TGL	CB3-CB2-CB1	-4.26	98.12	113.62
26	T	101	CDL	OA6-CA5-OA7	-4.26	113.41	123.70
14	N	601[A]	HEA	C3C-C4C-NC	4.21	114.65	109.21
14	N	601[B]	HEA	C3C-C4C-NC	4.21	114.65	109.21
27	X	103	DMU	C10-O7-C3	-4.21	107.56	117.96
27	P	309	DMU	O1-C10-C5	4.18	119.21	110.35
25	C	304	PEK	O03-C21-C22	4.18	125.02	111.91
26	C	307	CDL	OB8-CB7-C71	4.15	124.94	111.91
26	C	307	CDL	OA8-CA7-C31	4.13	124.88	111.91
19	C	306	PGV	O01-C1-C2	4.12	120.38	111.50
24	Y	102	CHD	C21-C20-C22	-4.11	103.92	110.36
27	X	103	DMU	O1-C10-C5	4.09	119.00	110.35
24	Y	102	CHD	C19-C10-C1	-4.08	101.69	108.26
27	P	309	DMU	O1-C9-C11	4.07	116.56	106.44
26	C	307	CDL	OB2-PB2-OB5	-4.05	95.97	106.73
26	C	307	CDL	OB4-PB2-OB3	4.04	126.49	110.68
21	Q	201	TGL	OG2-CB1-OB1	-4.02	113.98	123.70
14	A	602	HEA	C20-C19-C18	-3.98	113.07	121.12
14	A	601[A]	HEA	C3D-C4D-ND	3.95	114.18	110.36
14	A	601[B]	HEA	C3D-C4D-ND	3.95	114.18	110.36
27	P	309	DMU	O4-C7-C5	-3.92	101.30	110.35
21	Q	201	TGL	OG1-CA1-OA1	-3.91	113.73	123.59
27	C	309	DMU	C2-C3-C4	-3.90	103.29	110.24
26	C	307	CDL	OB6-CB4-CB3	-3.89	94.31	108.40
24	Y	102	CHD	C16-C17-C20	3.88	118.16	112.15
23	O	302	PSC	O01-C1-O02	-3.87	114.35	123.70
24	C	301	CHD	C18-C13-C12	3.84	112.98	109.07
24	Y	102	CHD	C15-C14-C8	3.83	123.69	118.33
25	P	302	PEK	C01-C02-C03	-3.83	101.63	112.63
25	P	303	PEK	C24-C23-C22	-3.81	99.48	113.19
14	A	602	HEA	C13-C12-C11	-3.79	108.65	114.35
27	C	310	DMU	O1-C10-C5	3.76	118.31	110.35
14	N	602	HEA	C3C-C4C-NC	3.73	114.03	109.21
21	Q	201	TGL	OG1-CA1-CA2	3.72	123.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	304	PSC	O01-C1-O02	-3.72	114.71	123.70
25	P	304	PEK	O03-C21-O04	-3.70	114.26	123.59
24	P	301	CHD	C22-C20-C17	-3.69	102.66	110.28
27	J	101	DMU	C7-C8-C9	3.68	116.80	110.24
14	A	602	HEA	C3C-C4C-NC	3.68	113.96	109.21
21	L	101	TGL	OG1-CA1-CA2	3.67	123.42	111.91
27	C	310	DMU	C6-C1-C2	3.67	117.63	110.00
23	O	302	PSC	C21-C20-C19	-3.65	100.34	113.62
25	C	303	PEK	C24-C23-C22	-3.65	100.07	113.19
21	Y	101	TGL	CG2-OG2-CB1	3.63	126.72	117.79
24	B	305	CHD	C11-C9-C10	-3.62	109.99	113.73
26	C	307	CDL	OB8-CB7-OB9	-3.60	114.51	123.59
24	C	308	CHD	C11-C9-C10	-3.60	110.02	113.73
19	N	608	PGV	O03-C19-C20	3.59	123.17	111.91
14	A	601[A]	HEA	C13-C12-C11	-3.58	108.97	114.35
14	A	601[B]	HEA	C13-C12-C11	-3.58	108.97	114.35
25	P	303	PEK	O02-C1-C2	3.58	137.71	123.73
27	C	310	DMU	C10-O1-C9	3.57	120.70	113.69
24	C	308	CHD	C22-C23-C24	-3.57	103.04	112.51
24	C	308	CHD	C15-C14-C13	3.55	107.03	103.55
25	P	304	PEK	O11-P-O14	-3.53	95.28	109.07
24	B	305	CHD	C4-C5-C10	-3.52	108.92	112.66
19	A	607	PGV	O12-P-O13	3.50	122.73	109.07
21	Y	101	TGL	CG3-CG2-CG1	-3.48	103.56	111.79
21	Q	201	TGL	CG3-CG2-CG1	3.48	120.01	111.79
27	P	309	DMU	C6-O5-C4	-3.48	106.87	113.69
27	X	103	DMU	C10-O1-C9	3.46	120.49	113.69
25	C	302	PEK	O03-C01-C02	3.45	118.49	108.43
24	C	308	CHD	C19-C10-C9	-3.43	106.46	111.18
14	N	602	HEA	O1A-CGA-CBA	-3.41	112.14	123.08
26	G	101	CDL	CB6-OB8-CB7	3.34	129.49	117.12
26	P	307	CDL	OB8-CB7-OB9	-3.33	115.18	123.59
27	P	310	DMU	C10-O1-C9	-3.33	107.16	113.69
14	A	602	HEA	CAD-CBD-CGD	-3.32	106.46	113.60
27	O	303	DMU	O5-C4-C3	3.31	116.74	109.75
21	B	302	TGL	OG1-CA1-CA2	3.31	122.28	111.91
25	P	302	PEK	O01-C1-C2	3.29	118.60	111.50
27	X	103	DMU	O55-C2-C3	3.29	118.66	109.94
26	T	101	CDL	CB4-OB6-CB5	-3.29	109.69	117.79
26	P	307	CDL	OA6-CA5-C11	3.28	118.57	111.50
14	A	601[A]	HEA	C3C-C4C-NC	3.27	113.43	109.21
14	A	601[B]	HEA	C3C-C4C-NC	3.27	113.43	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	305	CHD	C6-C5-C4	-3.27	107.43	111.19
14	N	601[A]	HEA	C27-C19-C18	-3.26	115.32	123.68
27	P	309	DMU	C7-C8-C9	3.25	116.05	110.24
26	C	307	CDL	OA8-CA7-OA9	-3.25	115.38	123.59
14	A	601[A]	HEA	C2B-C1B-NB	3.24	113.77	109.88
14	A	601[B]	HEA	C2B-C1B-NB	3.24	113.77	109.88
14	N	601[B]	HEA	C17-C18-C19	3.24	135.46	127.66
14	N	602	HEA	O2D-CGD-O1D	3.23	131.35	123.30
27	O	303	DMU	C10-O7-C3	3.23	125.95	117.96
25	C	302	PEK	O01-C1-C2	3.22	118.43	111.50
24	Y	102	CHD	C5-C6-C7	3.20	118.00	114.46
24	P	308	CHD	C5-C4-C3	-3.20	108.06	112.76
27	P	310	DMU	C6-O5-C4	3.19	119.94	113.69
24	B	305	CHD	C13-C14-C8	-3.15	110.72	114.74
26	G	101	CDL	C58-C57-C56	-3.14	98.47	114.42
24	Y	102	CHD	C16-C17-C13	-3.13	100.48	103.55
24	G	102	CHD	C16-C17-C20	-3.13	107.31	112.15
21	B	301	TGL	OB1-CB1-CB2	-3.12	111.54	123.73
26	G	101	CDL	OB6-CB5-OB7	-3.12	116.16	123.70
14	A	601[A]	HEA	CMC-C2C-C1C	-3.11	123.68	128.46
14	A	601[B]	HEA	CMC-C2C-C1C	-3.11	123.68	128.46
24	P	308	CHD	C13-C17-C20	-3.11	115.78	119.50
24	P	308	CHD	C14-C8-C9	-3.10	105.46	109.71
21	Y	101	TGL	OG1-CA1-CA2	3.10	121.63	111.91
24	C	301	CHD	C22-C20-C17	-3.10	103.89	110.28
27	P	309	DMU	C2-C3-C4	-3.10	103.82	110.93
14	A	601[A]	HEA	C2D-C1D-ND	3.09	113.51	109.84
14	A	601[B]	HEA	C2D-C1D-ND	3.09	113.51	109.84
19	A	607	PGV	C4-C3-C2	-3.09	102.07	113.19
14	A	601[A]	HEA	C25-C23-C24	3.09	121.43	114.60
21	L	101	TGL	CG3-CG2-CG1	-3.09	104.48	111.79
27	X	103	DMU	O7-C10-C5	3.08	116.08	108.10
27	C	310	DMU	O2-C8-C9	-3.07	101.68	109.30
24	P	308	CHD	C21-C20-C17	3.06	117.60	112.92
23	O	302	PSC	O12-P-O11	-3.04	98.63	106.73
27	P	309	DMU	C8-C7-C5	3.04	116.14	110.82
27	M	101	DMU	C18-O16-C6	-3.04	108.81	113.84
21	Y	101	TGL	OG3-CC1-CC2	3.03	121.43	111.91
24	C	301	CHD	C1-C2-C3	-3.02	106.59	110.47
23	B	304	PSC	C3-C2-C1	3.02	124.61	113.62
21	Y	101	TGL	CC3-CC2-CC1	3.02	124.61	113.62
27	O	303	DMU	C7-C8-C9	-3.02	104.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	608	PGV	O03-C19-C20	3.01	121.34	111.91
19	N	609	PGV	C22-C21-C20	3.00	123.98	113.19
21	L	101	TGL	C26-C25-C24	-3.00	99.19	114.42
14	A	602	HEA	C4A-CHB-C1B	-3.00	118.60	122.56
25	P	303	PEK	C3-C2-C1	-2.99	102.73	113.62
24	Y	102	CHD	C6-C7-C8	2.99	114.67	111.48
27	P	309	DMU	O1-C9-C8	2.98	115.10	109.69
24	P	301	CHD	C14-C13-C12	2.97	110.17	107.40
14	N	601[A]	HEA	O2A-CGA-CBA	2.97	123.58	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	2.97	123.58	114.03
19	N	609	PGV	C9-C10-C11	-2.97	95.43	112.43
24	P	308	CHD	C11-C12-C13	-2.96	108.20	111.24
27	C	310	DMU	O1-C9-C11	2.96	113.81	106.44
20	E	201	EDO	O2-C2-C1	-2.95	90.70	111.91
27	P	309	DMU	C6-C1-C2	2.95	116.13	110.00
24	C	308	CHD	C1-C10-C5	2.95	112.12	107.77
21	Q	201	TGL	OG1-CG1-CG2	2.94	117.00	108.43
25	C	304	PEK	O03-C01-C02	2.94	116.98	108.43
14	A	601[B]	HEA	C27-C19-C20	2.93	120.20	115.27
24	P	308	CHD	C16-C17-C13	2.93	106.42	103.55
14	N	602	HEA	CHD-C1D-ND	2.92	127.99	124.38
21	B	302	TGL	OG1-CA1-OA1	-2.92	116.22	123.59
14	N	601[A]	HEA	OMA-CMA-C3A	-2.92	118.56	124.91
14	N	601[B]	HEA	OMA-CMA-C3A	-2.92	118.56	124.91
27	O	303	DMU	C10-C5-C7	2.92	116.07	110.00
21	N	607	TGL	CG3-CG2-CG1	-2.92	104.89	111.79
21	Q	201	TGL	OG3-CG3-CG2	2.91	116.92	108.43
27	C	309	DMU	C18-O16-C6	2.91	118.67	113.84
27	J	101	DMU	C10-O7-C3	-2.90	110.80	117.96
14	N	602	HEA	C27-C19-C20	2.90	120.14	115.27
24	B	305	CHD	C5-C4-C3	-2.89	108.51	112.76
14	N	601[A]	HEA	C13-C14-C15	-2.89	120.71	127.66
14	N	601[B]	HEA	C13-C14-C15	-2.89	120.71	127.66
24	C	308	CHD	C16-C17-C20	2.88	116.61	112.15
24	G	102	CHD	C13-C14-C8	-2.88	111.06	114.74
19	N	608	PGV	O03-C19-O04	-2.88	116.33	123.59
14	A	601[A]	HEA	O2A-CGA-CBA	2.88	123.27	114.03
14	A	601[B]	HEA	O2A-CGA-CBA	2.88	123.27	114.03
26	C	307	CDL	OA6-CA4-CA6	-2.87	98.00	108.40
26	G	101	CDL	C39-C38-C37	2.87	129.00	114.42
25	P	303	PEK	C31-C30-C29	-2.87	99.85	114.42
14	A	602	HEA	CHA-C4D-C3D	-2.87	120.63	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	103	DMU	O3-C5-C10	2.87	117.01	110.05
19	A	608	PGV	O03-C19-O04	-2.87	116.36	123.59
21	B	302	TGL	OG1-CG1-CG2	2.86	116.77	108.43
26	T	101	CDL	OB8-CB6-CB4	2.86	116.75	108.43
19	N	609	PGV	O03-C19-O04	-2.85	116.39	123.59
14	A	602	HEA	CMC-C2C-C3C	2.83	129.97	124.68
25	C	302	PEK	O03-C21-O04	-2.82	116.46	123.59
24	B	305	CHD	C19-C10-C1	-2.82	103.72	108.26
27	O	303	DMU	C10-O1-C9	2.82	119.22	113.69
19	A	607	PGV	O14-P-O11	-2.82	94.66	107.75
14	N	601[A]	HEA	O2D-CGD-CBD	2.81	123.07	114.03
14	N	601[B]	HEA	O2D-CGD-CBD	2.81	123.07	114.03
27	X	103	DMU	C6-C1-C2	-2.81	104.14	110.00
21	B	301	TGL	CG2-OG2-CB1	-2.81	110.87	117.79
27	C	309	DMU	O5-C4-C57	2.81	113.42	106.44
19	N	609	PGV	C01-O03-C19	-2.80	106.74	117.12
26	C	307	CDL	OA6-CA4-CA3	2.80	118.53	108.40
24	C	308	CHD	C14-C13-C12	2.80	110.00	107.40
24	G	102	CHD	C11-C9-C10	-2.77	110.87	113.73
27	X	103	DMU	C10-C5-C7	2.77	115.77	110.00
26	P	307	CDL	OA8-CA7-C31	2.75	120.55	111.91
19	P	305	PGV	O01-C1-O02	-2.74	117.07	123.70
27	P	309	DMU	O61-C57-C4	-2.74	101.88	111.29
24	Y	102	CHD	C4-C5-C10	2.74	115.57	112.66
14	N	602	HEA	C4A-CHB-C1B	-2.74	118.95	122.56
25	C	302	PEK	O12-C04-C05	2.72	119.27	109.10
14	A	601[A]	HEA	O1A-CGA-CBA	-2.72	114.35	123.08
14	A	601[B]	HEA	O1A-CGA-CBA	-2.72	114.35	123.08
26	C	307	CDL	C61-C60-C59	-2.71	100.65	114.42
14	N	602	HEA	CHB-C1B-NB	2.71	127.38	124.43
21	N	607	TGL	CA8-CA7-CA6	-2.71	100.66	114.42
14	N	602	HEA	C13-C12-C11	-2.71	110.28	114.35
26	C	307	CDL	C39-C38-C37	2.71	128.18	114.42
21	N	607	TGL	OG1-CA1-CA2	2.71	120.40	111.91
26	P	307	CDL	OA6-CA4-CA3	2.71	118.20	108.40
14	A	601[B]	HEA	C17-C18-C19	2.71	134.17	127.66
14	A	602	HEA	O1A-CGA-CBA	-2.70	114.39	123.08
24	B	305	CHD	O3-C3-C4	-2.69	104.48	109.85
25	P	304	PEK	O01-C1-O02	-2.68	117.22	123.70
27	O	303	DMU	O1-C10-C5	2.68	116.02	110.35
19	N	608	PGV	C03-C02-C01	-2.67	105.47	111.79
27	P	310	DMU	C18-O16-C6	2.66	118.26	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	X	103	DMU	O4-C7-C8	2.66	116.50	110.35
19	P	305	PGV	C30-C29-C28	-2.66	100.94	114.42
21	L	101	TGL	OG1-CG1-CG2	2.65	116.15	108.43
14	A	601[B]	HEA	C21-C22-C23	-2.65	118.70	127.75
24	Y	102	CHD	C1-C2-C3	-2.64	107.08	110.47
21	Y	101	TGL	OG3-CC1-OC1	-2.63	116.95	123.59
14	N	602	HEA	C1D-C2D-C3D	2.63	109.72	106.96
26	P	307	CDL	OB5-PB2-OB3	2.63	113.84	106.47
14	N	601[A]	HEA	C13-C12-C11	-2.63	110.40	114.35
14	N	601[B]	HEA	C13-C12-C11	-2.63	110.40	114.35
19	C	305	PGV	C22-C21-C20	-2.62	103.76	113.19
26	G	101	CDL	C79-C78-C77	2.62	127.74	114.42
27	C	310	DMU	C10-C5-C7	2.62	115.46	110.00
24	B	305	CHD	C19-C10-C5	-2.62	105.92	110.36
27	P	309	DMU	C10-C5-C7	2.61	115.44	110.00
14	N	602	HEA	CHA-C4D-C3D	-2.61	121.00	124.84
26	T	101	CDL	C81-C80-C79	-2.60	101.22	114.42
14	A	602	HEA	O1D-CGD-CBD	-2.60	114.73	123.08
25	C	304	PEK	C36-C35-C34	-2.60	101.24	114.42
26	T	101	CDL	C80-C79-C78	2.60	127.61	114.42
24	C	308	CHD	C16-C17-C13	2.59	106.10	103.55
14	N	601[A]	HEA	CMC-C2C-C1C	-2.59	124.48	128.46
14	N	601[B]	HEA	CMC-C2C-C1C	-2.59	124.48	128.46
23	O	302	PSC	O01-C02-C03	2.59	117.80	108.40
19	P	306	PGV	O14-P-O13	2.59	125.06	112.24
24	Y	102	CHD	C4-C3-C2	-2.59	107.46	110.55
23	O	302	PSC	O13-P-O14	2.59	120.82	110.68
14	N	601[A]	HEA	C17-C18-C19	-2.58	121.45	127.66
24	Y	102	CHD	C18-C13-C17	-2.57	107.18	111.21
26	G	101	CDL	C61-C60-C59	-2.57	101.38	114.42
21	B	302	TGL	CG1-OG1-CA1	2.57	126.63	117.12
27	X	103	DMU	C18-O16-C6	2.56	118.09	113.84
26	T	101	CDL	OA8-CA7-OA9	-2.56	117.14	123.59
14	N	601[A]	HEA	O1A-CGA-CBA	-2.56	114.87	123.08
14	N	601[B]	HEA	O1A-CGA-CBA	-2.56	114.87	123.08
19	A	607	PGV	C8-C9-C10	-2.55	102.67	113.79
14	N	602	HEA	CAD-CBD-CGD	-2.55	108.11	113.60
24	C	301	CHD	C22-C23-C24	-2.54	105.76	112.51
25	C	303	PEK	C02-O01-C1	-2.54	111.54	117.79
24	P	301	CHD	C11-C9-C10	-2.52	111.13	113.73
27	N	610	DMU	O5-C4-C3	2.52	115.84	110.73
24	Y	102	CHD	O7-C7-C8	2.52	115.05	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	C4B-NB-C1B	-2.51	102.48	105.07
14	A	601[B]	HEA	C4B-NB-C1B	-2.51	102.48	105.07
24	P	308	CHD	C16-C17-C20	2.51	116.03	112.15
27	X	103	DMU	O5-C6-O16	2.51	115.91	109.97
21	N	607	TGL	OG3-CC1-OC1	-2.50	117.27	123.59
19	C	306	PGV	O03-C01-C02	2.50	115.72	108.43
14	A	601[A]	HEA	C26-C15-C16	2.50	119.48	115.27
14	A	601[B]	HEA	C26-C15-C16	2.50	119.48	115.27
14	N	601[A]	HEA	C4A-CHB-C1B	2.50	125.86	122.56
14	N	601[B]	HEA	C4A-CHB-C1B	2.50	125.86	122.56
21	Y	101	TGL	OG1-CA1-OA1	-2.50	117.29	123.59
21	Y	101	TGL	OB1-CB1-CB2	-2.50	113.99	123.73
14	A	601[A]	HEA	C16-C15-C14	-2.50	116.07	121.12
14	A	601[B]	HEA	C16-C15-C14	-2.50	116.07	121.12
27	C	310	DMU	O7-C3-C4	-2.49	102.62	109.45
26	T	101	CDL	C61-C60-C59	-2.49	101.78	114.42
24	P	301	CHD	C19-C10-C1	-2.49	104.25	108.26
26	T	101	CDL	C40-C39-C38	2.49	127.07	114.42
21	B	301	TGL	OG1-CA1-OA1	-2.49	117.31	123.59
14	A	602	HEA	C4D-CHA-C1A	-2.49	119.28	122.56
27	P	309	DMU	O5-C6-O16	-2.48	104.09	109.97
19	P	306	PGV	C4-C3-C2	-2.48	104.27	113.19
27	C	310	DMU	O6-C11-C9	2.48	119.81	111.29
21	L	101	TGL	C20-CA9-CA8	-2.48	101.86	114.42
14	A	601[A]	HEA	CAA-CBA-CGA	-2.47	106.83	113.76
14	A	601[B]	HEA	CAA-CBA-CGA	-2.47	106.83	113.76
19	N	609	PGV	O03-C19-C20	2.47	119.65	111.91
27	Z	101	DMU	C1-C2-C3	2.47	115.31	109.68
27	J	101	DMU	C10-C5-C7	2.46	115.13	110.00
26	G	101	CDL	C40-C39-C38	2.46	126.93	114.42
24	Y	102	CHD	C13-C17-C20	2.46	122.43	119.50
26	T	101	CDL	C32-C31-CA7	2.46	122.56	113.62
24	G	102	CHD	C2-C1-C10	-2.46	108.56	112.78
24	B	305	CHD	C1-C10-C5	2.46	111.40	107.77
27	X	103	DMU	O7-C3-C2	2.46	113.82	107.28
26	G	101	CDL	C18-C17-C16	2.45	126.89	114.42
24	C	308	CHD	C14-C8-C9	-2.45	106.36	109.71
26	G	101	CDL	CB4-OB6-CB5	-2.44	111.77	117.79
26	T	101	CDL	OA9-CA7-C31	-2.44	114.20	123.73
19	A	607	PGV	O02-C1-C2	-2.44	114.21	123.73
14	A	601[A]	HEA	C3B-C4B-NB	2.44	112.73	109.84
14	A	601[B]	HEA	C3B-C4B-NB	2.44	112.73	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	O	303	DMU	O1-C9-C11	2.44	112.50	106.44
25	C	303	PEK	C26-C25-C24	-2.44	102.04	114.42
27	C	309	DMU	O61-C57-C4	2.44	119.66	111.29
19	P	306	PGV	O04-C19-C20	-2.44	114.23	123.73
23	O	302	PSC	C26-C25-C24	-2.43	102.06	114.42
26	P	307	CDL	OB4-PB2-OB3	2.43	120.19	110.68
26	P	307	CDL	PB2-OB5-CB3	2.43	124.98	118.30
24	G	102	CHD	C21-C20-C17	-2.42	109.22	112.92
19	N	608	PGV	O14-P-O13	2.42	124.19	112.24
27	X	103	DMU	O49-C1-C6	2.42	115.91	110.05
26	P	307	CDL	OB6-CB5-C51	2.42	116.71	111.50
19	N	609	PGV	O01-C1-C2	2.41	116.70	111.50
21	Y	101	TGL	OG2-CG2-CG3	2.41	117.13	108.40
24	P	301	CHD	C21-C20-C22	-2.41	106.58	110.36
19	N	608	PGV	C01-O03-C19	2.41	126.04	117.12
26	P	307	CDL	C55-C54-C53	-2.40	102.22	114.42
19	A	608	PGV	C22-C21-C20	2.40	121.83	113.19
27	O	303	DMU	O5-C4-C57	2.40	112.41	106.44
21	L	101	TGL	C24-C23-C22	-2.40	102.24	114.42
27	O	303	DMU	O2-C8-C9	2.40	115.26	109.30
26	P	307	CDL	OA8-CA6-CA4	2.40	115.42	108.43
27	C	309	DMU	C6-O5-C4	2.39	118.39	113.69
27	X	102	DMU	C2-C3-C4	2.39	114.50	110.24
19	A	607	PGV	C3-C2-C1	2.39	122.31	113.62
24	C	308	CHD	C9-C11-C12	-2.39	111.15	114.30
24	P	308	CHD	C23-C22-C20	-2.39	110.16	114.52
24	P	301	CHD	O12-C12-C13	-2.38	107.00	111.03
19	C	306	PGV	O04-C19-C20	-2.38	114.44	123.73
26	P	307	CDL	C83-C82-C81	2.38	126.50	114.42
26	T	101	CDL	OB8-CB7-C71	2.37	119.35	111.91
14	A	601[A]	HEA	C16-C17-C18	2.37	119.66	111.88
21	Y	101	TGL	C26-C25-C24	-2.37	102.41	114.42
14	A	601[B]	HEA	C21-C20-C19	-2.36	105.20	112.98
21	L	101	TGL	OG1-CA1-OA1	-2.36	117.65	123.59
26	G	101	CDL	C19-C18-C17	2.35	126.35	114.42
24	C	301	CHD	C23-C22-C20	-2.35	110.23	114.52
14	A	601[A]	HEA	CHB-C1B-C2B	-2.35	121.31	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-2.35	121.31	124.98
26	P	307	CDL	C82-C81-C80	2.34	126.33	114.42
26	G	101	CDL	C80-C79-C78	2.34	126.32	114.42
27	X	103	DMU	O5-C4-C3	2.34	114.69	109.75
24	C	301	CHD	C4-C5-C10	-2.34	110.17	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	610	DMU	C2-C3-C4	2.34	115.85	110.40
19	A	607	PGV	C03-C02-C01	-2.33	106.27	111.79
25	C	304	PEK	O11-P-O14	-2.33	99.95	109.07
21	L	101	TGL	OG3-CG3-CG2	2.33	115.22	108.43
14	N	601[A]	HEA	CHD-C1D-ND	2.33	127.26	124.38
14	N	601[B]	HEA	CHD-C1D-ND	2.33	127.26	124.38
19	C	306	PGV	C01-O03-C19	2.32	125.71	117.12
26	T	101	CDL	CA6-OA8-CA7	2.32	125.71	117.12
26	P	307	CDL	OA2-PA1-OA3	-2.32	101.60	110.68
14	N	601[A]	HEA	CAA-CBA-CGA	-2.32	107.27	113.76
14	N	601[B]	HEA	CAA-CBA-CGA	-2.32	107.27	113.76
26	P	307	CDL	CB6-CB4-CB3	2.30	117.23	111.79
27	J	101	DMU	C6-C1-C2	-2.30	105.54	110.31
25	P	303	PEK	C14-C13-C12	-2.30	100.69	112.02
14	N	601[A]	HEA	C2B-C1B-NB	2.30	112.64	109.88
14	N	601[B]	HEA	C2B-C1B-NB	2.30	112.64	109.88
27	C	310	DMU	O5-C6-O16	-2.30	104.53	109.97
19	P	305	PGV	O03-C19-O04	-2.30	117.80	123.59
21	L	101	TGL	CA4-CA3-CA2	-2.30	104.94	113.19
25	C	303	PEK	C25-C24-C23	-2.30	102.77	114.42
25	C	302	PEK	C8-C7-C6	-2.29	100.73	112.02
27	Z	101	DMU	C18-O16-C6	2.29	117.64	113.84
24	C	308	CHD	O25-C24-C23	-2.29	115.72	123.08
21	Y	101	TGL	C24-C23-C22	-2.29	102.80	114.42
21	N	607	TGL	OG2-CG2-CG3	2.29	116.68	108.40
26	C	307	CDL	C78-C77-C76	-2.29	102.82	114.42
14	N	601[A]	HEA	CHA-C4D-C3D	-2.29	121.48	124.84
14	N	601[B]	HEA	CHA-C4D-C3D	-2.29	121.48	124.84
26	C	307	CDL	OA6-CA5-C11	2.29	116.43	111.50
26	P	307	CDL	C81-C80-C79	-2.28	102.84	114.42
26	T	101	CDL	CB6-OB8-CB7	2.28	125.57	117.12
27	J	101	DMU	C8-C7-C5	2.28	114.81	110.82
27	N	610	DMU	O16-C6-C1	2.28	113.60	108.68
24	P	308	CHD	C22-C23-C24	-2.28	106.45	112.51
24	C	308	CHD	C6-C5-C10	2.28	115.08	112.66
26	T	101	CDL	C83-C82-C81	2.27	125.94	114.42
27	P	309	DMU	C1-C2-C3	2.27	114.86	109.68
14	N	602	HEA	C4D-CHA-C1A	-2.25	119.58	122.56
27	C	310	DMU	O61-C57-C4	-2.25	103.58	111.29
14	N	601[A]	HEA	CAD-C3D-C2D	2.24	132.06	127.88
14	N	601[B]	HEA	CAD-C3D-C2D	2.24	132.06	127.88
21	Y	101	TGL	CC6-CC5-CC4	2.24	125.81	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	302	PEK	O01-C02-C03	2.24	111.32	106.13
24	C	301	CHD	C5-C4-C3	-2.24	109.47	112.76
27	J	101	DMU	O1-C10-C5	2.24	115.09	110.35
14	N	601[A]	HEA	C20-C19-C18	2.24	125.65	121.12
26	C	307	CDL	PB2-OB5-CB3	-2.24	112.13	118.30
14	A	601[A]	HEA	C1B-C2B-C3B	-2.24	104.13	106.80
14	A	601[B]	HEA	C1B-C2B-C3B	-2.24	104.13	106.80
27	X	103	DMU	C1-C2-C3	-2.24	104.58	109.68
24	P	308	CHD	C14-C8-C7	-2.23	108.84	111.81
24	P	308	CHD	C14-C13-C12	2.23	109.48	107.40
14	A	602	HEA	C2B-C1B-NB	2.23	112.55	109.88
14	A	601[A]	HEA	C1D-ND-C4D	-2.22	102.78	105.07
14	A	601[B]	HEA	C1D-ND-C4D	-2.22	102.78	105.07
14	N	602	HEA	CAD-C3D-C4D	2.22	128.54	124.66
14	N	601[A]	HEA	C27-C19-C20	2.22	119.00	115.27
24	C	308	CHD	C11-C12-C13	-2.22	108.97	111.24
27	C	309	DMU	O7-C3-C4	2.22	114.80	109.30
27	P	309	DMU	O2-C8-C9	-2.22	103.79	109.30
14	N	601[A]	HEA	CHD-C1D-C2D	-2.22	120.59	126.72
14	N	601[B]	HEA	CHD-C1D-C2D	-2.22	120.59	126.72
19	P	306	PGV	C21-C20-C19	-2.21	105.57	113.62
27	J	101	DMU	O5-C4-C57	2.21	111.93	106.44
24	B	305	CHD	C18-C13-C12	-2.21	106.82	109.07
24	P	308	CHD	C1-C10-C9	2.21	114.82	111.35
26	G	101	CDL	OB6-CB4-CB3	2.20	116.38	108.40
24	C	301	CHD	C5-C6-C7	2.20	116.89	114.46
26	C	307	CDL	C21-C20-C19	-2.20	103.26	114.42
21	B	301	TGL	OG2-CG2-CG3	2.19	116.34	108.40
25	C	303	PEK	O04-C21-C22	2.18	132.24	123.73
20	E	210	EDO	O1-C1-C2	-2.18	96.23	111.91
19	P	306	PGV	O12-P-O13	-2.18	100.56	109.07
25	P	304	PEK	C01-O03-C21	2.18	125.18	117.12
24	Y	102	CHD	C10-C9-C8	2.17	114.15	111.82
25	P	303	PEK	C26-C25-C24	-2.17	103.41	114.42
26	P	307	CDL	OA6-CA4-CA6	-2.17	100.56	108.40
14	N	602	HEA	C16-C15-C14	-2.16	116.74	121.12
26	T	101	CDL	OB2-CB2-C1	2.16	114.39	108.93
26	C	307	CDL	OA2-PA1-OA5	2.16	112.48	106.73
21	N	607	TGL	OG3-CC1-CC2	2.16	118.68	111.91
25	C	302	PEK	C01-O03-C21	2.16	125.11	117.12
19	A	607	PGV	C22-C21-C20	-2.15	105.45	113.19
21	Q	201	TGL	OG3-CC1-CC2	2.15	118.66	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	CDL	C19-C18-C17	2.15	125.33	114.42
23	O	302	PSC	C23-C22-C21	-2.15	103.53	114.42
24	P	301	CHD	C11-C9-C8	2.15	114.02	110.88
26	C	307	CDL	OA8-CA6-CA4	2.15	114.68	108.43
24	B	305	CHD	O12-C12-C13	-2.14	107.41	111.03
26	P	307	CDL	OA4-PA1-OA3	2.14	119.06	110.68
25	C	304	PEK	C24-C23-C22	2.14	120.88	113.19
21	L	101	TGL	CA8-CA7-CA6	-2.14	103.57	114.42
26	C	307	CDL	OA4-PA1-OA3	2.14	119.05	110.68
23	B	304	PSC	C29-C28-C27	-2.13	103.60	114.42
14	N	602	HEA	C26-C15-C16	2.13	118.85	115.27
24	Y	102	CHD	O25-C24-C23	-2.13	116.25	123.08
24	G	102	CHD	C1-C10-C5	2.13	110.91	107.77
26	C	307	CDL	C81-C80-C79	-2.12	103.69	114.42
23	O	302	PSC	C3-C2-C1	2.11	121.31	113.62
19	N	608	PGV	C24-C23-C22	-2.11	103.69	114.42
25	P	303	PEK	O03-C01-C02	-2.11	102.29	108.43
27	M	101	DMU	C28-C25-C22	-2.10	103.74	114.42
19	A	607	PGV	C01-O03-C19	2.10	124.91	117.12
27	J	101	DMU	C6-O5-C4	-2.10	109.69	113.66
25	P	303	PEK	C34-C33-C32	-2.10	103.76	114.42
21	B	302	TGL	CB3-CB2-CB1	-2.10	105.98	113.62
19	P	305	PGV	C22-C21-C20	-2.10	105.65	113.19
23	B	304	PSC	C4-C3-C2	2.10	120.73	113.19
25	P	303	PEK	C29-C28-C27	-2.10	103.79	114.42
14	N	601[A]	HEA	C4D-C3D-C2D	-2.09	103.85	106.90
14	N	601[B]	HEA	C4D-C3D-C2D	-2.09	103.85	106.90
27	X	103	DMU	O1-C9-C8	2.09	113.49	109.69
27	O	303	DMU	O7-C10-O1	2.09	116.50	110.67
25	P	303	PEK	O11-P-O14	-2.08	100.92	109.07
26	G	101	CDL	CB2-C1-CA2	-2.08	106.66	112.79
23	B	304	PSC	O03-C01-C02	-2.08	102.37	108.43
24	C	308	CHD	C11-C9-C8	2.08	113.92	110.88
26	T	101	CDL	C52-C51-CB5	-2.08	106.06	113.62
19	C	306	PGV	C4-C3-C2	-2.08	105.72	113.19
26	C	307	CDL	C55-C54-C53	-2.08	103.89	114.42
27	J	101	DMU	O7-C10-C5	2.08	113.48	108.10
24	C	308	CHD	C22-C20-C17	-2.07	106.00	110.28
19	C	306	PGV	C3-C2-C1	2.07	121.16	113.62
24	B	305	CHD	C23-C22-C20	-2.07	110.74	114.52
27	M	101	DMU	C22-C19-C18	-2.07	104.33	113.49
24	C	301	CHD	C2-C1-C10	2.07	116.33	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	308	CHD	C15-C14-C8	2.06	121.22	118.33
14	N	602	HEA	C1D-ND-C4D	2.06	107.20	105.07
24	B	305	CHD	C4-C3-C2	2.06	113.01	110.55
26	T	101	CDL	OB6-CB5-OB7	-2.06	118.73	123.70
24	P	301	CHD	C22-C23-C24	-2.06	107.05	112.51
26	T	101	CDL	CA4-OA6-CA5	-2.05	112.75	117.79
24	C	308	CHD	C4-C5-C10	2.04	114.83	112.66
21	Q	201	TGL	CA3-CA2-CA1	2.04	121.05	113.62
21	N	607	TGL	OG1-CA1-OA1	-2.04	118.44	123.59
19	P	305	PGV	C27-C26-C25	-2.04	104.08	114.42
24	P	308	CHD	C11-C9-C8	2.04	113.86	110.88
19	P	306	PGV	O03-C01-C02	2.03	114.35	108.43
26	C	307	CDL	C82-C81-C80	2.03	124.74	114.42
14	N	602	HEA	CMC-C2C-C3C	2.03	128.47	124.68
21	L	101	TGL	OB1-CB1-CB2	-2.03	115.83	123.73
24	G	102	CHD	C22-C23-C24	-2.03	107.13	112.51
21	Y	101	TGL	CC9-CC8-CC7	-2.02	104.16	114.42
19	A	607	PGV	O14-P-O13	2.02	122.23	112.24
27	P	310	DMU	O16-C6-C1	2.02	111.46	108.30
21	Q	201	TGL	CB7-CB6-CB5	-2.02	104.17	114.42
19	N	609	PGV	O03-C01-C02	2.02	114.31	108.43
19	P	306	PGV	O03-C19-O04	-2.02	118.50	123.59
27	J	101	DMU	O1-C9-C8	2.02	113.36	109.69
24	G	102	CHD	C19-C10-C1	-2.02	105.02	108.26
26	P	307	CDL	OA8-CA7-OA9	-2.01	118.51	123.59
14	N	601[A]	HEA	C3D-C4D-ND	2.01	112.30	110.36
14	N	601[B]	HEA	C3D-C4D-ND	2.01	112.30	110.36
25	P	302	PEK	C8-C7-C6	-2.01	102.12	112.02
24	P	301	CHD	C5-C4-C3	-2.01	109.81	112.76
19	P	306	PGV	O14-P-O11	-2.01	98.43	107.75
24	P	301	CHD	C1-C2-C3	-2.01	107.89	110.47
21	L	101	TGL	OG2-CG2-CG1	2.01	115.66	108.40
14	A	601[A]	HEA	C4D-C3D-C2D	-2.00	103.98	106.90
14	A	601[B]	HEA	C4D-C3D-C2D	-2.00	103.98	106.90

All (18) chirality outliers are listed below:

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

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

All (909) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
14	A	601[A]	HEA	C27-C19-C20-C21
19	A	607	PGV	C03-O11-P-O13
19	A	607	PGV	C03-O11-P-O14
19	A	607	PGV	C04-C05-C06-O06
19	A	607	PGV	O04-C19-O03-C01
19	A	607	PGV	C20-C19-O03-C01
19	C	306	PGV	C04-O12-P-O13
19	C	306	PGV	C2-C1-O01-C02
19	N	608	PGV	C03-O11-P-O12
19	N	608	PGV	C04-O12-P-O11
19	N	608	PGV	C02-C03-O11-P
19	N	608	PGV	C2-C1-O01-C02
19	N	608	PGV	O04-C19-O03-C01
19	N	608	PGV	C20-C19-O03-C01
19	N	608	PGV	C10-C11-C12-C13
19	P	306	PGV	C03-O11-P-O13
19	P	306	PGV	C04-O12-P-O13
19	P	306	PGV	C04-O12-P-O14
19	P	306	PGV	C2-C1-O01-C02
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	Y	101	TGL	OB1-CB1-OG2-CG2
23	B	304	PSC	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
23	B	304	PSC	C03-C02-O01-C1
23	B	304	PSC	O12-C04-C05-N
23	O	302	PSC	C03-O11-P-O12
23	O	302	PSC	C03-O11-P-O13
23	O	302	PSC	C03-O11-P-O14
24	Y	102	CHD	C13-C17-C20-C21
25	C	302	PEK	C6-C7-C8-C9
25	C	302	PEK	C9-C10-C11-C12
25	C	304	PEK	C04-O12-P-O11
25	C	304	PEK	C04-O12-P-O13
25	C	304	PEK	O12-C04-C05-N
25	C	304	PEK	C2-C1-O01-C02
25	P	302	PEK	O01-C02-C03-O11
25	P	302	PEK	C01-C02-O01-C1
25	P	302	PEK	O12-C04-C05-N
25	P	303	PEK	C4-C5-C6-C7
26	G	101	CDL	CA2-C1-CB2-OB2
26	G	101	CDL	CA2-OA2-PA1-OA3
26	G	101	CDL	CA2-OA2-PA1-OA4
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CA3-OA5-PA1-OA2
26	G	101	CDL	CA3-OA5-PA1-OA3
26	G	101	CDL	CA3-OA5-PA1-OA4
26	G	101	CDL	CB2-OB2-PB2-OB5
26	G	101	CDL	CB3-OB5-PB2-OB3
26	G	101	CDL	CB3-OB5-PB2-OB4
26	G	101	CDL	OB6-CB4-CB6-OB8
26	P	307	CDL	CA3-OA5-PA1-OA3
26	P	307	CDL	OA7-CA5-OA6-CA4
26	P	307	CDL	C11-CA5-OA6-CA4
26	P	307	CDL	CB3-OB5-PB2-OB2
26	P	307	CDL	CB3-OB5-PB2-OB4
26	T	101	CDL	OA9-CA7-OA8-CA6
26	T	101	CDL	C31-CA7-OA8-CA6
27	C	309	DMU	C1-C6-O16-C18
27	C	309	DMU	O5-C6-O16-C18
27	N	610	DMU	C1-C6-O16-C18
27	N	610	DMU	O5-C6-O16-C18
27	N	610	DMU	C19-C18-O16-C6
27	X	102	DMU	C1-C6-O16-C18
27	X	102	DMU	O5-C6-O16-C18
21	Q	201	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
26	P	307	CDL	OA9-CA7-OA8-CA6
21	B	302	TGL	CG2-CG1-OG1-CA1
27	O	303	DMU	O1-C10-O7-C3
21	Q	201	TGL	CC2-CC1-OG3-CG3
26	P	307	CDL	C31-CA7-OA8-CA6
21	B	302	TGL	OA1-CA1-OG1-CG1
21	B	302	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	OA1-CA1-OG1-CG1
25	C	302	PEK	O04-C21-O03-C01
26	C	307	CDL	OA9-CA7-OA8-CA6
19	C	306	PGV	O02-C1-O01-C02
19	N	608	PGV	O02-C1-O01-C02
19	P	306	PGV	O02-C1-O01-C02
23	B	304	PSC	O02-C1-O01-C02
25	C	304	PEK	O02-C1-O01-C02
26	C	307	CDL	OA7-CA5-OA6-CA4
21	B	302	TGL	CA2-CA1-OG1-CG1
21	B	302	TGL	CC2-CC1-OG3-CG3
21	Q	201	TGL	CA2-CA1-OG1-CG1
25	C	302	PEK	C22-C21-O03-C01
26	C	307	CDL	C31-CA7-OA8-CA6
27	P	310	DMU	O6-C11-C9-O1
21	Y	101	TGL	CB2-CB1-OG2-CG2
26	P	307	CDL	C51-CB5-OB6-CB4
27	P	309	DMU	O6-C11-C9-O1
24	Y	102	CHD	C16-C17-C20-C22
24	Y	102	CHD	C13-C17-C20-C22
21	B	301	TGL	CC2-CC1-OG3-CG3
25	P	304	PEK	C22-C21-O03-C01
27	C	310	DMU	O5-C4-C57-O61
19	P	306	PGV	C10-C11-C12-C13
23	O	302	PSC	C11-C12-C13-C14
25	C	302	PEK	C13-C14-C15-C16
25	C	303	PEK	C10-C11-C12-C13
25	P	302	PEK	C13-C14-C15-C16
25	P	304	PEK	C7-C8-C9-C10
27	O	303	DMU	C4-C3-O7-C10
25	C	302	PEK	O02-C1-O01-C02
25	P	304	PEK	O04-C21-O03-C01
24	Y	102	CHD	C16-C17-C20-C21
19	N	608	PGV	O12-C04-C05-O05
27	P	310	DMU	O6-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	CB2-CB1-OG2-CG2
25	C	302	PEK	C2-C1-O01-C02
26	C	307	CDL	C11-CA5-OA6-CA4
26	P	307	CDL	C80-C81-C82-C83
26	T	101	CDL	C40-C41-C42-C43
26	T	101	CDL	C52-C53-C54-C55
27	X	102	DMU	O5-C4-C57-O61
21	Y	101	TGL	CC2-CC3-CC4-CC5
14	N	601[A]	HEA	C27-C19-C20-C21
14	N	601[A]	HEA	C18-C19-C20-C21
26	G	101	CDL	C52-C53-C54-C55
24	C	308	CHD	C21-C20-C22-C23
24	P	308	CHD	C17-C20-C22-C23
23	O	302	PSC	C11-C10-C9-C8
25	P	303	PEK	C13-C14-C15-C16
21	B	301	TGL	OC1-CC1-OG3-CG3
27	P	309	DMU	O6-C11-C9-C8
19	A	607	PGV	O12-C04-C05-C06
21	B	301	TGL	OB1-CB1-OG2-CG2
21	Q	201	TGL	OB1-CB1-OG2-CG2
26	P	307	CDL	OB7-CB5-OB6-CB4
19	P	306	PGV	C20-C19-O03-C01
21	N	607	TGL	CC2-CC1-OG3-CG3
23	O	302	PSC	C20-C19-O03-C01
23	B	304	PSC	C22-C23-C24-C25
26	G	101	CDL	C77-C78-C79-C80
24	C	308	CHD	C17-C20-C22-C23
27	C	310	DMU	C3-C4-C57-O61
19	P	306	PGV	C2-C3-C4-C5
19	C	306	PGV	O01-C02-C03-O11
26	G	101	CDL	O1-C1-CB2-OB2
23	O	302	PSC	C1-C2-C3-C4
27	M	101	DMU	C28-C31-C34-C37
23	B	304	PSC	C20-C21-C22-C23
27	P	310	DMU	C22-C25-C28-C31
24	P	308	CHD	C20-C22-C23-C24
21	B	301	TGL	CB2-CB1-OG2-CG2
23	B	304	PSC	C2-C1-O01-C02
24	P	308	CHD	C21-C20-C22-C23
19	A	608	PGV	C10-C11-C12-C13
25	C	304	PEK	C13-C14-C15-C16
26	C	307	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
19	A	607	PGV	C19-C20-C21-C22
19	C	306	PGV	C1-C2-C3-C4
21	Q	201	TGL	CB1-CB2-CB3-CB4
23	B	304	PSC	C19-C20-C21-C22
19	C	306	PGV	C20-C19-O03-C01
27	P	310	DMU	O16-C18-C19-C22
19	P	306	PGV	C19-C20-C21-C22
20	A	610	EDO	O1-C1-C2-O2
20	F	107	EDO	O1-C1-C2-O2
20	F	108	EDO	O1-C1-C2-O2
20	N	629	EDO	O1-C1-C2-O2
20	O	317	EDO	O1-C1-C2-O2
19	P	306	PGV	O04-C19-O03-C01
21	N	607	TGL	OC1-CC1-OG3-CG3
25	C	304	PEK	O04-C21-O03-C01
14	A	601[A]	HEA	C15-C16-C17-C18
14	N	601[A]	HEA	C15-C16-C17-C18
21	L	101	TGL	CB1-CB2-CB3-CB4
19	C	306	PGV	O04-C19-O03-C01
23	O	302	PSC	O04-C19-O03-C01
21	Y	101	TGL	CB1-CB2-CB3-CB4
27	O	303	DMU	C2-C3-O7-C10
25	P	304	PEK	C10-C11-C12-C13
21	Y	101	TGL	CA9-C20-C21-C22
19	A	607	PGV	C03-O11-P-O12
19	C	306	PGV	C04-O12-P-O11
19	P	306	PGV	C03-O11-P-O12
19	P	306	PGV	C04-O12-P-O11
23	B	304	PSC	C04-O12-P-O11
25	P	304	PEK	C04-O12-P-O11
26	G	101	CDL	CB3-OB5-PB2-OB2
26	T	101	CDL	CA3-OA5-PA1-OA2
21	Y	101	TGL	CC1-CC2-CC3-CC4
21	N	607	TGL	CA2-CA1-OG1-CG1
25	C	304	PEK	C22-C21-O03-C01
27	C	309	DMU	O16-C18-C19-C22
21	B	302	TGL	CB1-CB2-CB3-CB4
27	M	101	DMU	C19-C22-C25-C28
21	B	301	TGL	CA5-CA6-CA7-CA8
21	B	301	TGL	CB5-CB6-CB7-CB8
21	B	302	TGL	CB5-CB6-CB7-CB8
21	B	302	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	C10-C11-C12-C13
21	L	101	TGL	C16-C17-C18-C19
21	N	607	TGL	C16-C15-CC9-CC8
21	N	607	TGL	C23-C24-C25-C26
25	P	303	PEK	C24-C25-C26-C27
26	C	307	CDL	C74-C75-C76-C77
26	T	101	CDL	C32-C33-C34-C35
27	C	309	DMU	C28-C31-C34-C37
21	Q	201	TGL	CA4-CA5-CA6-CA7
21	Q	201	TGL	C20-C21-C22-C23
21	Y	101	TGL	CA3-CA4-CA5-CA6
21	Y	101	TGL	CB7-CB8-CB9-C10
23	B	304	PSC	C29-C30-C31-C32
26	P	307	CDL	C35-C36-C37-C38
27	X	103	DMU	C22-C25-C28-C31
23	O	302	PSC	O02-C1-O01-C02
21	B	302	TGL	CC4-CC5-CC6-CC7
21	B	302	TGL	CC6-CC7-CC8-CC9
21	L	101	TGL	C22-C23-C24-C25
21	Y	101	TGL	CB4-CB5-CB6-CB7
26	G	101	CDL	C16-C17-C18-C19
19	P	306	PGV	O01-C02-C03-O11
21	B	302	TGL	C16-C15-CC9-CC8
21	L	101	TGL	CA3-CA4-CA5-CA6
21	Q	201	TGL	CC4-CC5-CC6-CC7
21	N	607	TGL	C21-C22-C23-C24
21	Q	201	TGL	CA2-CA3-CA4-CA5
27	N	610	DMU	O16-C18-C19-C22
26	C	307	CDL	CB7-C71-C72-C73
19	A	607	PGV	C22-C23-C24-C25
21	B	302	TGL	C21-C20-CA9-CA8
21	B	302	TGL	C15-C16-C17-C18
21	L	101	TGL	CB6-CB7-CB8-CB9
21	Q	201	TGL	CC3-CC4-CC5-CC6
21	Y	101	TGL	C16-C15-CC9-CC8
21	B	302	TGL	CC2-CC3-CC4-CC5
26	P	307	CDL	C17-C18-C19-C20
26	P	307	CDL	C36-C37-C38-C39
26	T	101	CDL	C37-C38-C39-C40
26	T	101	CDL	C71-C72-C73-C74
27	X	103	DMU	C28-C31-C34-C37
19	C	305	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	C17-C18-C19-C33
21	N	607	TGL	C13-C14-C29-C30
21	Q	201	TGL	C11-C10-CB9-CB8
26	C	307	CDL	C61-C62-C63-C64
26	C	307	CDL	C82-C83-C84-C85
26	P	307	CDL	C16-C17-C18-C19
27	N	610	DMU	C22-C25-C28-C31
21	Y	101	TGL	CB9-C10-C11-C12
19	P	306	PGV	C04-C05-C06-O06
21	B	301	TGL	CB2-CB3-CB4-CB5
21	L	101	TGL	CB9-C10-C11-C12
27	T	102	DMU	C28-C31-C34-C37
24	Y	102	CHD	C21-C20-C22-C23
23	B	304	PSC	C1-C2-C3-C4
21	B	302	TGL	CC7-CC8-CC9-C15
21	N	607	TGL	CA5-CA6-CA7-CA8
21	N	607	TGL	C17-C18-C19-C33
21	Y	101	TGL	C17-C18-C19-C33
26	P	307	CDL	C11-C12-C13-C14
27	X	101	DMU	C28-C31-C34-C37
21	B	302	TGL	C11-C10-CB9-CB8
21	L	101	TGL	C21-C20-CA9-CA8
26	C	307	CDL	C17-C18-C19-C20
26	C	307	CDL	C72-C73-C74-C75
26	P	307	CDL	C57-C58-C59-C60
21	Q	201	TGL	CA7-CA8-CA9-C20
26	C	307	CDL	C12-C13-C14-C15
26	P	307	CDL	CA5-C11-C12-C13
19	C	305	PGV	C25-C26-C27-C28
21	B	302	TGL	CC5-CC6-CC7-CC8
25	P	304	PEK	C29-C30-C31-C32
27	X	102	DMU	C22-C25-C28-C31
19	C	306	PGV	C14-C15-C16-C17
21	B	301	TGL	C13-C14-C29-C30
27	X	102	DMU	C19-C18-O16-C6
27	X	103	DMU	C19-C18-O16-C6
21	B	301	TGL	CC7-CC8-CC9-C15
21	Y	101	TGL	C21-C22-C23-C24
25	C	302	PEK	C25-C26-C27-C28
26	C	307	CDL	C18-C19-C20-C21
26	C	307	CDL	C23-C24-C25-C26
21	Y	101	TGL	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
26	C	307	CDL	C59-C60-C61-C62
19	A	607	PGV	O03-C01-C02-C03
25	P	304	PEK	C4-C5-C6-C7
27	Z	101	DMU	C22-C25-C28-C31
21	L	101	TGL	CA2-CA1-OG1-CG1
21	Q	201	TGL	C21-C20-CA9-CA8
21	Y	101	TGL	C16-C17-C18-C19
19	A	607	PGV	O05-C05-C06-O06
21	B	301	TGL	C16-C17-C18-C19
21	B	302	TGL	C17-C18-C19-C33
21	N	607	TGL	C10-C11-C12-C13
26	P	307	CDL	C58-C59-C60-C61
19	A	607	PGV	C12-C13-C14-C15
19	P	305	PGV	C11-C10-C9-C8
27	X	103	DMU	O6-C11-C9-C8
26	C	307	CDL	C57-C58-C59-C60
27	X	104	DMU	C18-C19-C22-C25
19	A	607	PGV	C21-C22-C23-C24
19	C	305	PGV	C27-C28-C29-C30
27	Z	101	DMU	C25-C28-C31-C34
21	N	607	TGL	OA1-CA1-OG1-CG1
21	N	607	TGL	OB1-CB1-OG2-CG2
25	P	302	PEK	O02-C1-O01-C02
26	T	101	CDL	OA7-CA5-OA6-CA4
26	G	101	CDL	CA7-C31-C32-C33
19	P	306	PGV	C23-C24-C25-C26
25	C	303	PEK	C24-C25-C26-C27
25	C	304	PEK	C25-C26-C27-C28
19	N	608	PGV	C19-C20-C21-C22
21	B	301	TGL	CB1-CB2-CB3-CB4
25	P	303	PEK	C1-C2-C3-C4
20	A	619	EDO	O1-C1-C2-O2
20	A	626	EDO	O1-C1-C2-O2
20	A	627	EDO	O1-C1-C2-O2
20	B	320	EDO	O1-C1-C2-O2
20	B	321	EDO	O1-C1-C2-O2
20	C	322	EDO	O1-C1-C2-O2
20	C	323	EDO	O1-C1-C2-O2
20	D	212	EDO	O1-C1-C2-O2
20	E	208	EDO	O1-C1-C2-O2
20	E	212	EDO	O1-C1-C2-O2
20	G	104	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	H	101	EDO	O1-C1-C2-O2
20	I	103	EDO	O1-C1-C2-O2
20	I	106	EDO	O1-C1-C2-O2
20	J	103	EDO	O1-C1-C2-O2
20	L	104	EDO	O1-C1-C2-O2
20	N	627	EDO	O1-C1-C2-O2
20	N	633	EDO	O1-C1-C2-O2
20	N	635	EDO	O1-C1-C2-O2
20	O	314	EDO	O1-C1-C2-O2
20	O	319	EDO	O1-C1-C2-O2
20	P	316	EDO	O1-C1-C2-O2
20	P	318	EDO	O1-C1-C2-O2
20	S	114	EDO	O1-C1-C2-O2
20	T	107	EDO	O1-C1-C2-O2
20	U	101	EDO	O1-C1-C2-O2
20	V	101	EDO	O1-C1-C2-O2
20	V	102	EDO	O1-C1-C2-O2
20	Y	105	EDO	O1-C1-C2-O2
21	Q	201	TGL	CA5-CA6-CA7-CA8
26	C	307	CDL	C42-C43-C44-C45
21	N	607	TGL	CB2-CB1-OG2-CG2
25	P	302	PEK	C2-C1-O01-C02
26	C	307	CDL	C51-CB5-OB6-CB4
26	C	307	CDL	C38-C39-C40-C41
26	P	307	CDL	C77-C78-C79-C80
21	Q	201	TGL	CC5-CC6-CC7-CC8
26	C	307	CDL	C21-C22-C23-C24
26	T	101	CDL	C80-C81-C82-C83
25	P	302	PEK	C7-C8-C9-C10
21	L	101	TGL	OA1-CA1-OG1-CG1
25	P	302	PEK	C15-C16-C17-C18
21	B	302	TGL	OB1-CB1-OG2-CG2
21	B	301	TGL	CA1-CA2-CA3-CA4
26	C	307	CDL	C78-C79-C80-C81
21	B	301	TGL	C12-C13-C14-C29
21	Q	201	TGL	C24-C25-C26-C27
19	C	305	PGV	C24-C25-C26-C27
21	B	301	TGL	CA9-C20-C21-C22
21	Q	201	TGL	CB2-CB3-CB4-CB5
27	M	101	DMU	C34-C37-C40-C43
21	B	302	TGL	CB2-CB1-OG2-CG2
23	O	302	PSC	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
26	T	101	CDL	C11-CA5-OA6-CA4
26	T	101	CDL	C51-CB5-OB6-CB4
26	P	307	CDL	OB5-CB3-CB4-OB6
21	Y	101	TGL	CC4-CC5-CC6-CC7
21	Q	201	TGL	CC7-CC8-CC9-C15
21	Y	101	TGL	C18-C19-C33-C34
26	C	307	CDL	OB7-CB5-OB6-CB4
26	T	101	CDL	OB7-CB5-OB6-CB4
27	X	102	DMU	C3-C4-C57-O61
21	B	301	TGL	CA6-CA7-CA8-CA9
27	O	303	DMU	O5-C4-C57-O61
26	C	307	CDL	C71-C72-C73-C74
25	P	303	PEK	C10-C11-C12-C13
27	C	310	DMU	C18-C19-C22-C25
19	C	305	PGV	C28-C29-C30-C31
26	G	101	CDL	OB7-CB5-OB6-CB4
26	C	307	CDL	C73-C74-C75-C76
26	T	101	CDL	C54-C55-C56-C57
24	C	308	CHD	C13-C17-C20-C22
19	A	607	PGV	C7-C8-C9-C10
21	Y	101	TGL	CC5-CC6-CC7-CC8
19	C	306	PGV	C01-C02-C03-O11
26	C	307	CDL	OB5-CB3-CB4-CB6
26	P	307	CDL	OA5-CA3-CA4-CA6
21	L	101	TGL	CA9-C20-C21-C22
26	G	101	CDL	C32-C33-C34-C35
21	N	607	TGL	C20-C21-C22-C23
26	C	307	CDL	C51-C52-C53-C54
21	L	101	TGL	C15-C16-C17-C18
21	Q	201	TGL	CC2-CC3-CC4-CC5
27	P	309	DMU	C31-C34-C37-C40
27	C	309	DMU	C3-C4-C57-O61
21	N	607	TGL	C16-C17-C18-C19
26	C	307	CDL	C36-C37-C38-C39
21	N	607	TGL	CC4-CC5-CC6-CC7
19	N	608	PGV	O03-C01-C02-C03
21	B	302	TGL	OG1-CG1-CG2-CG3
21	L	101	TGL	OG1-CG1-CG2-CG3
21	Y	101	TGL	C22-C23-C24-C25
24	C	308	CHD	C16-C17-C20-C22
25	C	303	PEK	C7-C8-C9-C10
21	B	302	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	C29-C30-C31-C32
21	Y	101	TGL	C33-C34-C35-C36
23	B	304	PSC	C2-C3-C4-C5
25	C	302	PEK	C30-C31-C32-C33
27	C	309	DMU	C31-C34-C37-C40
21	B	302	TGL	C19-C33-C34-C35
27	X	102	DMU	O16-C18-C19-C22
19	C	306	PGV	C5-C6-C7-C8
27	X	102	DMU	C25-C28-C31-C34
19	A	607	PGV	C11-C10-C9-C8
19	C	305	PGV	C12-C13-C14-C15
21	N	607	TGL	CB4-CB5-CB6-CB7
26	G	101	CDL	C51-CB5-OB6-CB4
21	L	101	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	CB2-CB3-CB4-CB5
27	Z	101	DMU	C28-C31-C34-C37
27	Z	101	DMU	C34-C37-C40-C43
19	A	607	PGV	C20-C21-C22-C23
21	N	607	TGL	C29-C30-C31-C32
25	C	304	PEK	C35-C36-C37-C38
27	X	102	DMU	C34-C37-C40-C43
27	X	103	DMU	C25-C28-C31-C34
21	Q	201	TGL	CB3-CB4-CB5-CB6
26	T	101	CDL	C59-C60-C61-C62
27	X	102	DMU	C18-C19-C22-C25
26	P	307	CDL	CB3-OB5-PB2-OB3
26	P	307	CDL	OA5-CA3-CA4-OA6
19	C	305	PGV	C10-C11-C12-C13
21	B	302	TGL	CB4-CB5-CB6-CB7
24	C	308	CHD	C16-C17-C20-C21
20	C	317	EDO	O1-C1-C2-O2
20	D	214	EDO	O1-C1-C2-O2
20	R	204	EDO	O1-C1-C2-O2
20	S	112	EDO	O1-C1-C2-O2
19	A	608	PGV	C31-C32-C33-C34
27	T	102	DMU	C34-C37-C40-C43
26	C	307	CDL	C64-C65-C66-C67
21	L	101	TGL	OG1-CA1-CA2-CA3
21	N	607	TGL	CA9-C20-C21-C22
21	Q	201	TGL	C16-C15-CC9-CC8
21	L	101	TGL	CB3-CB4-CB5-CB6
21	L	101	TGL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C14-C15-C16-C17
23	B	304	PSC	C20-C19-O03-C01
21	B	302	TGL	C21-C22-C23-C24
26	T	101	CDL	OB9-CB7-OB8-CB6
26	C	307	CDL	C40-C41-C42-C43
26	T	101	CDL	C36-C37-C38-C39
26	G	101	CDL	C59-C60-C61-C62
26	T	101	CDL	C71-CB7-OB8-CB6
26	G	101	CDL	C57-C58-C59-C60
26	G	101	CDL	C62-C63-C64-C65
27	N	610	DMU	C25-C28-C31-C34
25	C	304	PEK	C4-C5-C6-C7
25	P	303	PEK	C26-C27-C28-C29
19	C	305	PGV	C14-C15-C16-C17
19	P	306	PGV	C27-C28-C29-C30
19	A	607	PGV	C01-C02-C03-O11
19	P	306	PGV	C01-C02-C03-O11
26	P	307	CDL	OB5-CB3-CB4-CB6
19	N	609	PGV	C31-C32-C33-C34
21	B	301	TGL	CB4-CB5-CB6-CB7
26	C	307	CDL	C43-C44-C45-C46
26	P	307	CDL	C15-C16-C17-C18
27	X	103	DMU	C34-C37-C40-C43
19	A	607	PGV	O12-C04-C05-O05
19	N	609	PGV	C29-C30-C31-C32
26	C	307	CDL	C83-C84-C85-C86
19	A	607	PGV	C02-C03-O11-P
19	P	306	PGV	C02-C03-O11-P
27	C	309	DMU	C19-C18-O16-C6
21	N	607	TGL	C15-C16-C17-C18
26	G	101	CDL	C38-C39-C40-C41
26	G	101	CDL	C32-C31-CA7-OA8
21	Y	101	TGL	OG1-CG1-CG2-CG3
25	P	302	PEK	C01-C02-C03-O11
26	T	101	CDL	CA3-CA4-CA6-OA8
19	A	607	PGV	C10-C11-C12-C13
19	N	609	PGV	C10-C11-C12-C13
25	C	303	PEK	C13-C14-C15-C16
25	P	303	PEK	C7-C8-C9-C10
26	C	307	CDL	C19-C20-C21-C22
26	G	101	CDL	C79-C80-C81-C82
19	C	306	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	C17-C18-C19-C33
27	T	102	DMU	C25-C28-C31-C34
23	B	304	PSC	C9-C10-C11-C12
23	B	304	PSC	C10-C11-C12-C13
23	O	302	PSC	C9-C10-C11-C12
25	C	302	PEK	C5-C6-C7-C8
25	C	302	PEK	C11-C10-C9-C8
25	C	302	PEK	C12-C13-C14-C15
25	C	304	PEK	C5-C6-C7-C8
25	C	304	PEK	C6-C7-C8-C9
25	C	304	PEK	C11-C10-C9-C8
25	C	304	PEK	C9-C10-C11-C12
25	C	304	PEK	C11-C12-C13-C14
25	C	304	PEK	C12-C13-C14-C15
25	P	302	PEK	C5-C6-C7-C8
25	P	302	PEK	C6-C7-C8-C9
25	P	302	PEK	C11-C10-C9-C8
25	P	302	PEK	C12-C13-C14-C15
25	P	303	PEK	C5-C6-C7-C8
25	P	303	PEK	C9-C10-C11-C12
25	P	304	PEK	C5-C6-C7-C8
25	P	304	PEK	C11-C10-C9-C8
25	P	304	PEK	C12-C13-C14-C15
21	Y	101	TGL	CA1-CA2-CA3-CA4
24	C	308	CHD	C13-C17-C20-C21
26	C	307	CDL	C16-C17-C18-C19
19	A	607	PGV	O01-C02-C03-O11
23	B	304	PSC	O01-C02-C03-O11
26	T	101	CDL	OA5-CA3-CA4-OA6
19	A	607	PGV	O03-C01-C02-O01
21	B	302	TGL	OG2-CG2-CG3-OG3
21	L	101	TGL	OG1-CG1-CG2-OG2
23	O	302	PSC	O03-C01-C02-O01
25	C	302	PEK	O03-C01-C02-O01
26	T	101	CDL	OA6-CA4-CA6-OA8
21	B	301	TGL	C29-C30-C31-C32
26	G	101	CDL	C40-C41-C42-C43
27	P	309	DMU	C28-C31-C34-C37
25	C	303	PEK	C23-C24-C25-C26
19	P	305	PGV	C02-C03-O11-P
27	O	303	DMU	O6-C11-C9-C8
26	C	307	CDL	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
20	A	609	EDO	O1-C1-C2-O2
20	A	629	EDO	O1-C1-C2-O2
20	A	635	EDO	O1-C1-C2-O2
20	B	309	EDO	O1-C1-C2-O2
20	B	310	EDO	O1-C1-C2-O2
20	B	314	EDO	O1-C1-C2-O2
20	C	312	EDO	O1-C1-C2-O2
20	C	319	EDO	O1-C1-C2-O2
20	D	204	EDO	O1-C1-C2-O2
20	D	208	EDO	O1-C1-C2-O2
20	L	105	EDO	O1-C1-C2-O2
20	M	106	EDO	O1-C1-C2-O2
20	N	620	EDO	O1-C1-C2-O2
20	O	315	EDO	O1-C1-C2-O2
20	U	102	EDO	O1-C1-C2-O2
21	N	607	TGL	CB1-CB2-CB3-CB4
27	C	309	DMU	C25-C28-C31-C34
23	B	304	PSC	C01-C02-C03-O11
23	O	302	PSC	C01-C02-C03-O11
25	C	304	PEK	C01-C02-C03-O11
21	N	607	TGL	CB9-C10-C11-C12
26	P	307	CDL	C59-C60-C61-C62
19	P	305	PGV	C24-C25-C26-C27
23	B	304	PSC	C5-C6-C7-C8
26	C	307	CDL	C35-C36-C37-C38
27	T	102	DMU	C31-C34-C37-C40
26	C	307	CDL	C44-C45-C46-C47
26	C	307	CDL	CB3-OB5-PB2-OB4
26	G	101	CDL	C43-C44-C45-C46
23	O	302	PSC	C3-C4-C5-C6
27	Z	101	DMU	O16-C18-C19-C22
23	O	302	PSC	C20-C21-C22-C23
21	L	101	TGL	CG1-CG2-CG3-OG3
21	Q	201	TGL	OG1-CG1-CG2-CG3
23	O	302	PSC	O03-C01-C02-C03
26	C	307	CDL	CB3-CB4-CB6-OB8
26	G	101	CDL	C1-CB2-OB2-PB2
26	G	101	CDL	CB3-CB4-CB6-OB8
26	P	307	CDL	CA3-CA4-CA6-OA8
23	O	302	PSC	O01-C02-C03-O11
21	B	302	TGL	C16-C17-C18-C19
26	T	101	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	CC4-CC5-CC6-CC7
21	L	101	TGL	CC6-CC7-CC8-CC9
19	N	608	PGV	O03-C01-C02-O01
21	Y	101	TGL	OG1-CG1-CG2-OG2
26	C	307	CDL	OB6-CB4-CB6-OB8
27	N	610	DMU	C31-C34-C37-C40
26	T	101	CDL	C33-C34-C35-C36
23	B	304	PSC	O04-C19-O03-C01
26	C	307	CDL	CA5-C11-C12-C13
19	A	607	PGV	O02-C1-O01-C02
27	P	310	DMU	C18-C19-C22-C25
21	Y	101	TGL	C20-C21-C22-C23
26	G	101	CDL	C80-C81-C82-C83
21	N	607	TGL	C18-C19-C33-C34
21	Q	201	TGL	C18-C19-C33-C34
19	C	306	PGV	C31-C32-C33-C34
27	O	303	DMU	O16-C18-C19-C22
21	B	301	TGL	C22-C23-C24-C25
19	C	305	PGV	C02-C03-O11-P
27	J	101	DMU	C5-C10-O7-C3
19	C	306	PGV	C04-O12-P-O14
19	N	608	PGV	C03-O11-P-O13
19	N	608	PGV	C04-O12-P-O14
19	P	306	PGV	C03-O11-P-O14
25	P	304	PEK	C04-O12-P-O13
26	G	101	CDL	CB2-OB2-PB2-OB4
26	T	101	CDL	CA3-OA5-PA1-OA3
21	B	302	TGL	CA4-CA5-CA6-CA7
20	B	317	EDO	O1-C1-C2-O2
20	D	209	EDO	O1-C1-C2-O2
20	H	102	EDO	O1-C1-C2-O2
20	L	106	EDO	O1-C1-C2-O2
20	P	320	EDO	O1-C1-C2-O2
20	Q	204	EDO	O1-C1-C2-O2
20	R	203	EDO	O1-C1-C2-O2
20	R	205	EDO	O1-C1-C2-O2
24	C	308	CHD	C20-C22-C23-C24
21	L	101	TGL	CC5-CC6-CC7-CC8
21	Q	201	TGL	C16-C17-C18-C19
26	C	307	CDL	C56-C57-C58-C59
26	P	307	CDL	CB7-C71-C72-C73
21	B	302	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C42-C43-C44-C45
26	C	307	CDL	C20-C21-C22-C23
26	G	101	CDL	C56-C57-C58-C59
19	N	608	PGV	O12-C04-C05-C06
25	C	304	PEK	O01-C02-C03-O11
26	C	307	CDL	OB5-CB3-CB4-OB6
27	T	102	DMU	C22-C25-C28-C31
21	L	101	TGL	CB2-CB3-CB4-CB5
21	B	302	TGL	CG1-CG2-CG3-OG3
25	C	302	PEK	O03-C01-C02-C03
27	X	101	DMU	C31-C34-C37-C40
26	P	307	CDL	OA6-CA4-CA6-OA8
19	A	608	PGV	C23-C24-C25-C26
21	B	302	TGL	CA3-CA4-CA5-CA6
21	Y	101	TGL	C24-C25-C26-C27
26	C	307	CDL	C58-C59-C60-C61
26	P	307	CDL	C19-C20-C21-C22
23	B	304	PSC	C30-C31-C32-C33
25	P	303	PEK	C23-C24-C25-C26
26	P	307	CDL	C82-C83-C84-C85
26	P	307	CDL	C32-C33-C34-C35
25	C	302	PEK	C4-C5-C6-C7
21	B	301	TGL	CB9-C10-C11-C12
27	C	309	DMU	C22-C25-C28-C31
27	M	101	DMU	C31-C34-C37-C40
19	P	305	PGV	C7-C8-C9-C10
19	C	306	PGV	C19-C20-C21-C22
19	C	305	PGV	C11-C12-C13-C14
26	C	307	CDL	C31-C32-C33-C34
27	O	303	DMU	C5-C10-O7-C3
25	P	304	PEK	O02-C1-O01-C02
20	A	631	EDO	O1-C1-C2-O2
20	B	312	EDO	O1-C1-C2-O2
20	B	322	EDO	O1-C1-C2-O2
20	C	324	EDO	O1-C1-C2-O2
20	C	325	EDO	O1-C1-C2-O2
20	D	207	EDO	O1-C1-C2-O2
20	D	219	EDO	O1-C1-C2-O2
20	E	202	EDO	O1-C1-C2-O2
20	E	211	EDO	O1-C1-C2-O2
20	F	106	EDO	O1-C1-C2-O2
20	N	623	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	N	634	EDO	O1-C1-C2-O2
20	P	317	EDO	O1-C1-C2-O2
20	P	326	EDO	O1-C1-C2-O2
20	Q	206	EDO	O1-C1-C2-O2
20	W	101	EDO	O1-C1-C2-O2
20	W	102	EDO	O1-C1-C2-O2
26	G	101	CDL	C37-C38-C39-C40
27	X	104	DMU	C22-C25-C28-C31
19	P	306	PGV	C9-C10-C11-C12
21	B	302	TGL	OG1-CG1-CG2-OG2
19	A	607	PGV	C04-O12-P-O11
26	T	101	CDL	C76-C77-C78-C79
19	P	306	PGV	C13-C14-C15-C16
25	P	303	PEK	C2-C1-O01-C02
21	Q	201	TGL	CA9-C20-C21-C22
19	A	607	PGV	C05-C04-O12-P
21	N	607	TGL	CA6-CA7-CA8-CA9
21	Q	201	TGL	C15-C16-C17-C18
25	P	302	PEK	C10-C11-C12-C13
21	B	301	TGL	C21-C22-C23-C24
26	T	101	CDL	C17-C18-C19-C20
21	Q	201	TGL	CC1-CC2-CC3-CC4
21	B	301	TGL	C18-C19-C33-C34
14	N	601[B]	HEA	C16-C17-C18-C19
21	B	302	TGL	CB3-CB4-CB5-CB6
26	C	307	CDL	C37-C38-C39-C40
25	C	303	PEK	C17-C18-C19-C20
21	L	101	TGL	OG2-CG2-CG3-OG3
26	C	307	CDL	CA4-CA3-OA5-PA1
21	Y	101	TGL	C10-C11-C12-C13
24	B	305	CHD	C22-C23-C24-O25
24	G	102	CHD	C22-C23-C24-O25
20	B	311	EDO	O1-C1-C2-O2
20	C	313	EDO	O1-C1-C2-O2
20	D	205	EDO	O1-C1-C2-O2
20	I	101	EDO	O1-C1-C2-O2
20	P	311	EDO	O1-C1-C2-O2
20	Q	205	EDO	O1-C1-C2-O2
24	B	305	CHD	C22-C23-C24-O26
19	C	306	PGV	C13-C14-C15-C16
19	P	305	PGV	C13-C14-C15-C16
26	C	307	CDL	C63-C64-C65-C66

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	CB5-CB6-CB7-CB8
14	A	602	HEA	CAA-CBA-CGA-O2A
25	C	303	PEK	C4-C5-C6-C7
25	C	302	PEK	C31-C32-C33-C34
26	P	307	CDL	C73-C74-C75-C76
27	O	303	DMU	O5-C6-O16-C18
27	X	103	DMU	C31-C34-C37-C40
19	N	608	PGV	C01-C02-O01-C1
26	T	101	CDL	C61-C62-C63-C64
19	N	609	PGV	C11-C12-C13-C14
27	N	610	DMU	C28-C31-C34-C37
25	P	302	PEK	C9-C10-C11-C12
25	P	303	PEK	C11-C10-C9-C8
25	P	304	PEK	C6-C7-C8-C9
25	P	304	PEK	C9-C10-C11-C12
25	P	304	PEK	C11-C12-C13-C14
21	N	607	TGL	CA2-CA3-CA4-CA5
23	B	304	PSC	O01-C1-C2-C3
24	G	102	CHD	C22-C23-C24-O26
26	G	101	CDL	C51-C52-C53-C54
25	C	304	PEK	C10-C11-C12-C13
21	L	101	TGL	CB4-CB5-CB6-CB7
25	P	304	PEK	C01-C02-C03-O11
26	T	101	CDL	OA5-CA3-CA4-CA6
25	P	304	PEK	C21-C22-C23-C24
21	L	101	TGL	CA2-CA3-CA4-CA5
27	C	309	DMU	O5-C4-C57-O61
25	P	303	PEK	C15-C16-C17-C18
14	A	601[A]	HEA	C16-C17-C18-C19
24	P	301	CHD	C22-C23-C24-O25
14	A	601[B]	HEA	C27-C19-C20-C21
24	C	308	CHD	C22-C23-C24-O25
25	P	303	PEK	C3-C4-C5-C6
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
24	C	308	CHD	C22-C23-C24-O26
26	G	101	CDL	C78-C79-C80-C81
21	L	101	TGL	OA1-CA1-CA2-CA3
21	Y	101	TGL	CG1-CG2-CG3-OG3
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
20	B	323	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	E	209	EDO	O1-C1-C2-O2
20	H	104	EDO	O1-C1-C2-O2
20	I	102	EDO	O1-C1-C2-O2
20	K	105	EDO	O1-C1-C2-O2
20	N	621	EDO	O1-C1-C2-O2
20	Q	209	EDO	O1-C1-C2-O2
20	R	202	EDO	O1-C1-C2-O2
20	S	109	EDO	O1-C1-C2-O2
20	S	113	EDO	O1-C1-C2-O2
26	T	101	CDL	C15-C16-C17-C18
27	X	104	DMU	C19-C18-O16-C6
21	B	301	TGL	C15-C16-C17-C18
27	P	309	DMU	C18-C19-C22-C25
19	C	306	PGV	C9-C10-C11-C12
21	N	607	TGL	C22-C23-C24-C25
14	N	602	HEA	CAD-CBD-CGD-O1D
24	C	301	CHD	C22-C23-C24-O25
23	B	304	PSC	C4-C5-C6-C7
24	P	308	CHD	C22-C23-C24-O26
26	G	101	CDL	C58-C59-C60-C61
21	Q	201	TGL	CB6-CB7-CB8-CB9
14	A	602	HEA	CAD-CBD-CGD-O1D
19	P	306	PGV	C30-C31-C32-C33
14	A	602	HEA	CAD-CBD-CGD-O2D
14	N	602	HEA	CAD-CBD-CGD-O2D
19	A	607	PGV	C9-C10-C11-C12
25	P	303	PEK	O01-C1-C2-C3
26	T	101	CDL	C43-C44-C45-C46
26	C	307	CDL	C79-C80-C81-C82
19	C	305	PGV	C9-C10-C11-C12
19	N	608	PGV	C9-C10-C11-C12
23	B	304	PSC	C12-C13-C14-C15
25	C	303	PEK	C14-C15-C16-C17
23	O	302	PSC	C03-C02-O01-C1
25	C	302	PEK	C01-C02-O01-C1
25	P	303	PEK	C16-C17-C18-C19
14	A	602	HEA	CAA-CBA-CGA-O1A
21	Y	101	TGL	OG1-CA1-CA2-CA3
25	C	302	PEK	C26-C27-C28-C29
24	C	301	CHD	C22-C23-C24-O26
27	N	610	DMU	C19-C22-C25-C28
27	T	102	DMU	O5-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
21	B	302	TGL	OG2-CB1-CB2-CB3
19	P	306	PGV	C11-C12-C13-C14
23	B	304	PSC	C7-C8-C9-C10
23	O	302	PSC	C7-C8-C9-C10
25	C	303	PEK	C15-C16-C17-C18
25	P	304	PEK	C2-C3-C4-C5
25	C	302	PEK	C7-C8-C9-C10
21	Q	201	TGL	OG3-CC1-CC2-CC3
25	P	304	PEK	C32-C33-C34-C35
20	A	621	EDO	O1-C1-C2-O2
20	C	314	EDO	O1-C1-C2-O2
20	C	318	EDO	O1-C1-C2-O2
20	E	204	EDO	O1-C1-C2-O2
20	K	102	EDO	O1-C1-C2-O2
20	K	103	EDO	O1-C1-C2-O2
20	N	615	EDO	O1-C1-C2-O2
20	N	618	EDO	O1-C1-C2-O2
20	N	624	EDO	O1-C1-C2-O2
20	O	304	EDO	O1-C1-C2-O2
20	O	312	EDO	O1-C1-C2-O2
20	O	318	EDO	O1-C1-C2-O2
20	P	312	EDO	O1-C1-C2-O2
20	P	315	EDO	O1-C1-C2-O2
20	P	321	EDO	O1-C1-C2-O2
20	W	104	EDO	O1-C1-C2-O2
20	Y	107	EDO	O1-C1-C2-O2
19	A	608	PGV	C11-C12-C13-C14
19	N	609	PGV	C26-C27-C28-C29
21	B	302	TGL	OG1-CA1-CA2-CA3
21	L	101	TGL	OG2-CB1-CB2-CB3
21	N	607	TGL	OG1-CA1-CA2-CA3
26	P	307	CDL	C21-C22-C23-C24
21	Y	101	TGL	OG2-CB1-CB2-CB3
21	Y	101	TGL	OG2-CG2-CG3-OG3
19	P	306	PGV	C1-C2-C3-C4
19	P	305	PGV	C9-C10-C11-C12
25	P	303	PEK	C14-C15-C16-C17
26	C	307	CDL	C32-C31-CA7-OA8
26	C	307	CDL	C52-C51-CB5-OB6
26	T	101	CDL	C14-C15-C16-C17
19	N	609	PGV	O03-C19-C20-C21
19	P	305	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
25	C	304	PEK	C14-C15-C16-C17
25	P	304	PEK	O01-C1-C2-C3
26	P	307	CDL	C12-C11-CA5-OA6
26	T	101	CDL	C52-C51-CB5-OB6
14	N	602	HEA	CAA-CBA-CGA-O1A
26	G	101	CDL	C33-C34-C35-C36
14	A	601[A]	HEA	CAA-CBA-CGA-O1A
14	A	601[B]	HEA	CAA-CBA-CGA-O1A
19	A	608	PGV	O03-C19-C20-C21
21	N	607	TGL	OA1-CA1-CA2-CA3
25	P	303	PEK	O02-C1-C2-C3
19	P	306	PGV	C22-C23-C24-C25
26	C	307	CDL	C12-C11-CA5-OA6
21	N	607	TGL	CC9-C15-C16-C17
25	P	304	PEK	C3-C4-C5-C6
27	C	309	DMU	C18-C19-C22-C25
23	O	302	PSC	C2-C3-C4-C5
14	N	602	HEA	CAA-CBA-CGA-O2A
21	B	302	TGL	OB1-CB1-CB2-CB3
21	L	101	TGL	OB1-CB1-CB2-CB3
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
24	P	308	CHD	C22-C23-C24-O25
21	L	101	TGL	C17-C18-C19-C33
21	Y	101	TGL	OA1-CA1-CA2-CA3
26	T	101	CDL	C52-C51-CB5-OB7
19	C	305	PGV	C22-C23-C24-C25
26	G	101	CDL	C72-C73-C74-C75
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
24	P	301	CHD	C22-C23-C24-O26
24	Y	102	CHD	C20-C22-C23-C24
19	C	306	PGV	C22-C23-C24-C25
21	B	302	TGL	OA1-CA1-CA2-CA3
25	C	304	PEK	C3-C4-C5-C6
21	B	301	TGL	CC2-CC3-CC4-CC5
19	A	607	PGV	C04-O12-P-O14
19	C	306	PGV	C03-O11-P-O13
26	P	307	CDL	C24-C25-C26-C27
21	Y	101	TGL	OB1-CB1-CB2-CB3
25	P	304	PEK	O02-C1-C2-C3
21	N	607	TGL	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	P	303	PEK	O12-C04-C05-N
21	B	301	TGL	CB3-CB4-CB5-CB6
27	M	101	DMU	C22-C25-C28-C31
20	B	316	EDO	O1-C1-C2-O2
20	C	315	EDO	O1-C1-C2-O2
20	D	203	EDO	O1-C1-C2-O2
20	D	211	EDO	O1-C1-C2-O2
20	D	215	EDO	O1-C1-C2-O2
20	L	111	EDO	O1-C1-C2-O2
20	N	619	EDO	O1-C1-C2-O2
20	Q	208	EDO	O1-C1-C2-O2
20	S	105	EDO	O1-C1-C2-O2
25	C	302	PEK	O03-C21-C22-C23
25	C	302	PEK	O04-C21-C22-C23
26	P	307	CDL	C78-C79-C80-C81
25	P	304	PEK	C14-C15-C16-C17
21	Q	201	TGL	OC1-CC1-CC2-CC3
19	P	306	PGV	C5-C6-C7-C8
26	G	101	CDL	C75-C76-C77-C78
25	P	302	PEK	C16-C17-C18-C19
21	L	101	TGL	CA5-CA6-CA7-CA8
21	Q	201	TGL	CB9-C10-C11-C12
21	Y	101	TGL	C25-C26-C27-C28
21	B	301	TGL	C11-C12-C13-C14
21	Q	201	TGL	CC6-CC7-CC8-CC9
26	T	101	CDL	C55-C56-C57-C58
21	Y	101	TGL	C23-C24-C25-C26
26	C	307	CDL	C52-C51-CB5-OB7
19	C	305	PGV	C05-C04-O12-P
26	C	307	CDL	C32-C31-CA7-OA9
21	L	101	TGL	C23-C24-C25-C26
19	N	608	PGV	O03-C19-C20-C21
26	P	307	CDL	C52-C51-CB5-OB6
23	O	302	PSC	C12-C13-C14-C15
19	N	608	PGV	C5-C6-C7-C8
26	C	307	CDL	C12-C11-CA5-OA7
14	N	601[A]	HEA	CAA-CBA-CGA-O1A
14	N	601[B]	HEA	CAA-CBA-CGA-O1A
27	P	309	DMU	C19-C18-O16-C6
26	T	101	CDL	C32-C31-CA7-OA8
26	P	307	CDL	C14-C15-C16-C17
25	P	304	PEK	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	N	609	PGV	C30-C31-C32-C33
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
14	A	601[B]	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

146 monomers are involved in 324 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	637[A]	EDO	2	0
20	A	622	EDO	1	0
20	N	621	EDO	1	0
20	A	620	EDO	2	0
25	P	304	PEK	2	0
20	A	609	EDO	7	0
20	C	325	EDO	4	0
20	E	209	EDO	1	0
20	R	201	EDO	2	0
14	A	601[B]	HEA	1	0
20	H	102	EDO	3	0
21	B	301	TGL	5	0
20	T	107	EDO	2	0
20	J	104	EDO	1	0
20	L	102	EDO	1	0
20	P	316	EDO	3	0
20	A	626	EDO	4	0
20	N	625	EDO	1	0
20	Q	205	EDO	1	0
20	D	215	EDO	1	0
25	C	303	PEK	3	0
19	A	607	PGV	1	0
20	S	109	EDO	2	0
20	Q	203	EDO	1	0
24	C	308	CHD	4	0
19	N	608	PGV	3	0
20	B	312	EDO	6	0
20	P	324	EDO	1	0
19	A	608	PGV	1	0
26	C	307	CDL	6	0
20	N	630	EDO	1	0
20	N	615	EDO	1	0
20	R	202	EDO	2	0
21	B	302	TGL	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	633	EDO	4	0
14	N	601[B]	HEA	1	0
20	S	107	EDO	1	0
20	C	320	EDO	1	0
20	A	631	EDO	3	0
20	E	208	EDO	1	0
23	B	304	PSC	8	0
20	B	315	EDO	1	0
21	Q	201	TGL	9	0
20	N	627	EDO	1	0
20	L	109	EDO	1	0
20	D	206	EDO	1	0
20	E	210	EDO	1	0
27	P	309	DMU	4	0
20	N	632	EDO	2	0
20	N	635	EDO	1	0
20	A	617	EDO	1	0
20	E	205	EDO	1	0
20	N	634	EDO	1	0
20	O	311	EDO	1	0
20	W	104	EDO	1	0
26	T	101	CDL	11	0
20	G	105	EDO	2	0
20	A	629	EDO	2	0
20	C	319	EDO	3	0
20	B	317	EDO	2	0
20	B	313	EDO	1	0
20	O	305	EDO	2	0
27	C	309	DMU	1	0
20	A	618	EDO	2	0
20	A	627	EDO	7	0
19	N	609	PGV	1	0
27	C	310	DMU	4	0
20	O	314	EDO	5	0
20	S	112	EDO	1	0
27	P	310	DMU	5	0
20	O	316	EDO	2	0
20	M	106	EDO	2	0
20	I	103	EDO	3	0
20	A	616	EDO	1	0
20	D	213	EDO	1	0
20	D	201	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	303	PEK	5	0
20	D	212	EDO	1	0
20	F	105	EDO	1	0
20	A	635	EDO	3	0
20	R	204	EDO	1	0
14	A	602	HEA	2	0
19	P	305	PGV	3	0
20	P	318	EDO	2	0
20	N	631	EDO	1	0
19	C	305	PGV	1	0
27	T	102	DMU	3	0
20	O	318	EDO	2	0
20	D	219	EDO	1	0
27	J	101	DMU	2	0
20	N	628	EDO	1	0
20	A	623	EDO	4	0
21	Y	101	TGL	11	0
25	C	302	PEK	5	0
20	E	201	EDO	1	0
20	H	103	EDO	1	0
20	O	315	EDO	2	0
20	A	636	EDO	2	0
26	G	101	CDL	8	0
19	C	306	PGV	8	0
20	N	623	EDO	2	0
20	W	103	EDO	1	0
27	X	102	DMU	2	0
24	Y	102	CHD	2	0
20	F	106	EDO	2	0
20	Q	207	EDO	1	0
20	U	101	EDO	2	0
20	A	630	EDO	2	0
20	G	104	EDO	1	0
25	C	304	PEK	3	0
20	O	317	EDO	1	0
20	W	102	EDO	1	0
20	T	106	EDO	2	0
20	D	209	EDO	4	0
20	D	203	EDO	1	0
24	P	308	CHD	2	0
20	H	104	EDO	2	0
27	Z	101	DMU	2	0

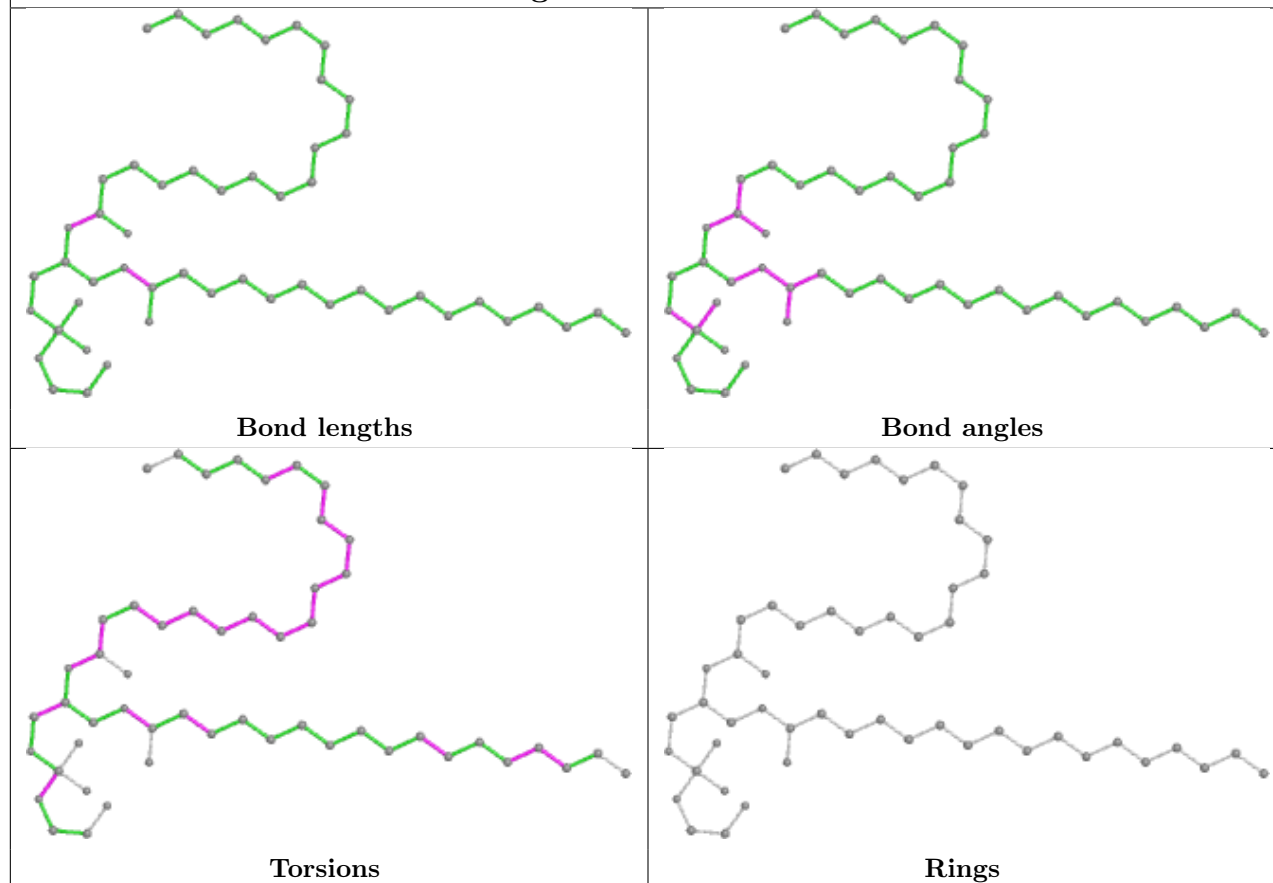
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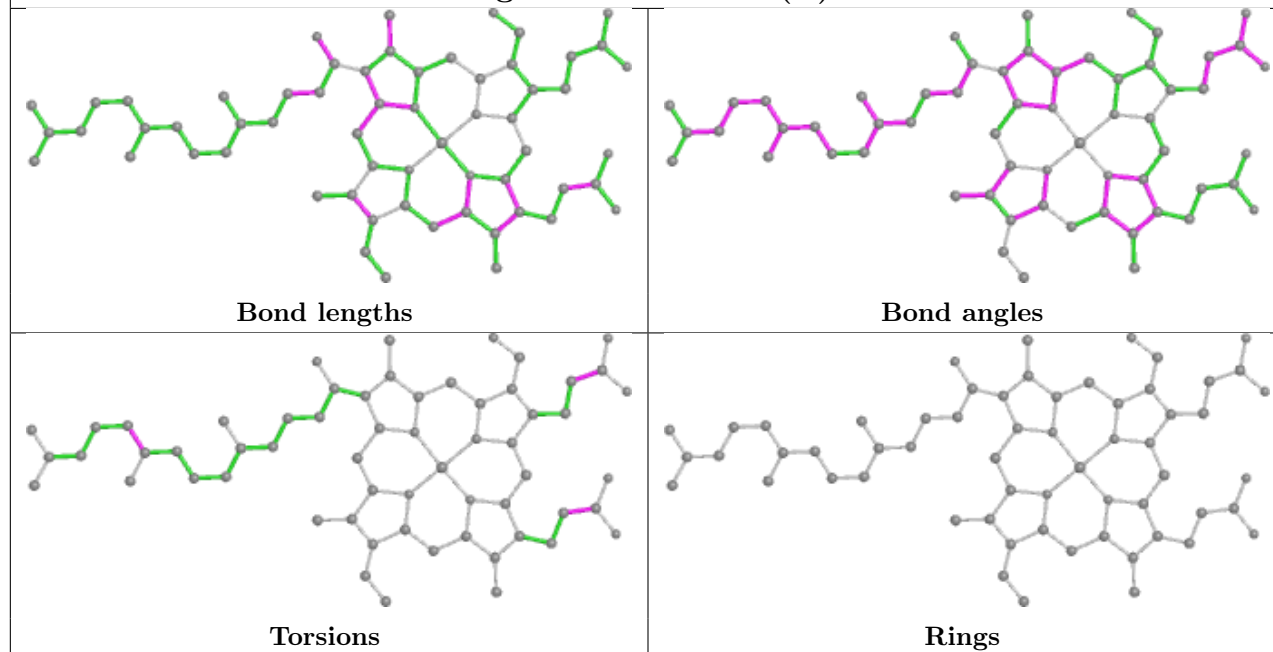
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	X	101	DMU	2	0
26	P	307	CDL	11	0
20	N	614	EDO	1	0
20	P	326	EDO	2	0
20	T	103	EDO	1	0
20	L	110	EDO	5	0
20	I	104	EDO	1	0
20	F	109	EDO	2	0
20	L	104	EDO	1	0
23	O	302	PSC	1	0
20	P	321	EDO	2	0
20	D	218	EDO	3	0
20	C	326	EDO	1	0
20	Q	206	EDO	2	0
20	U	102	EDO	1	0
20	D	207	EDO	1	0
19	P	306	PGV	8	0
14	N	601[A]	HEA	1	0
21	L	101	TGL	7	0
20	N	618	EDO	3	0
20	S	105	EDO	1	0
20	D	202	EDO	4	0
20	M	104	EDO	1	0
25	P	302	PEK	2	0
20	O	319	EDO	3	0
20	B	321	EDO	6	0
21	N	607	TGL	4	0
14	N	602	HEA	1	0

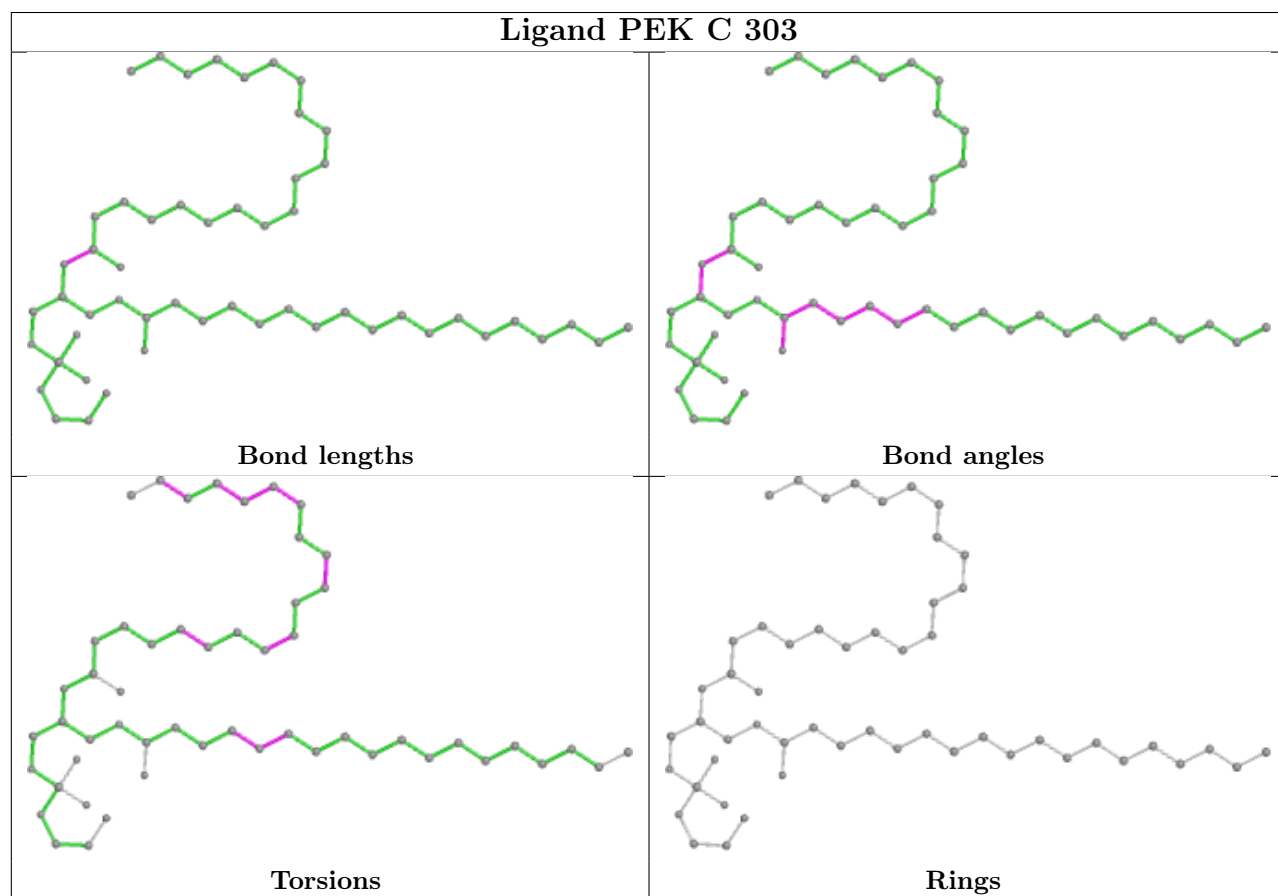
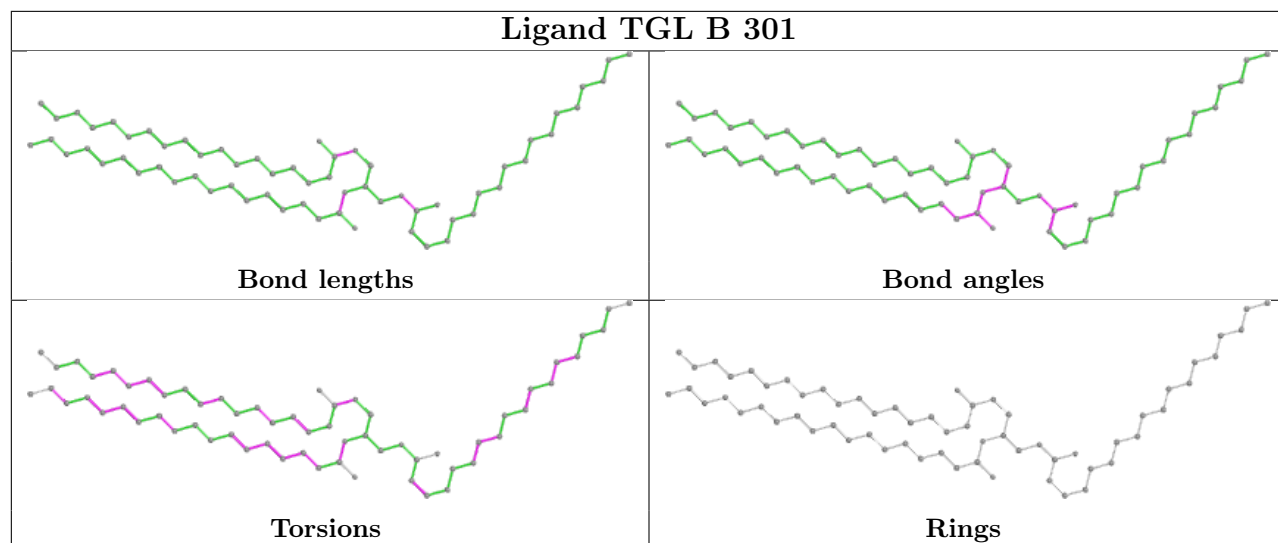
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

## Ligand PEK P 304

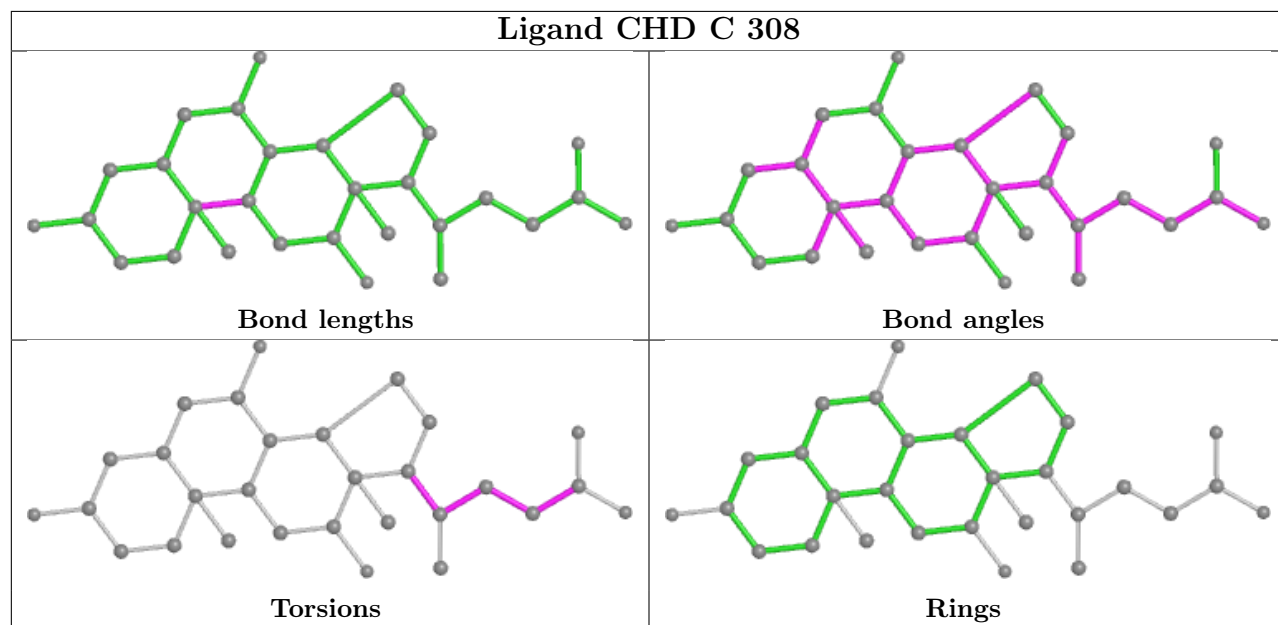
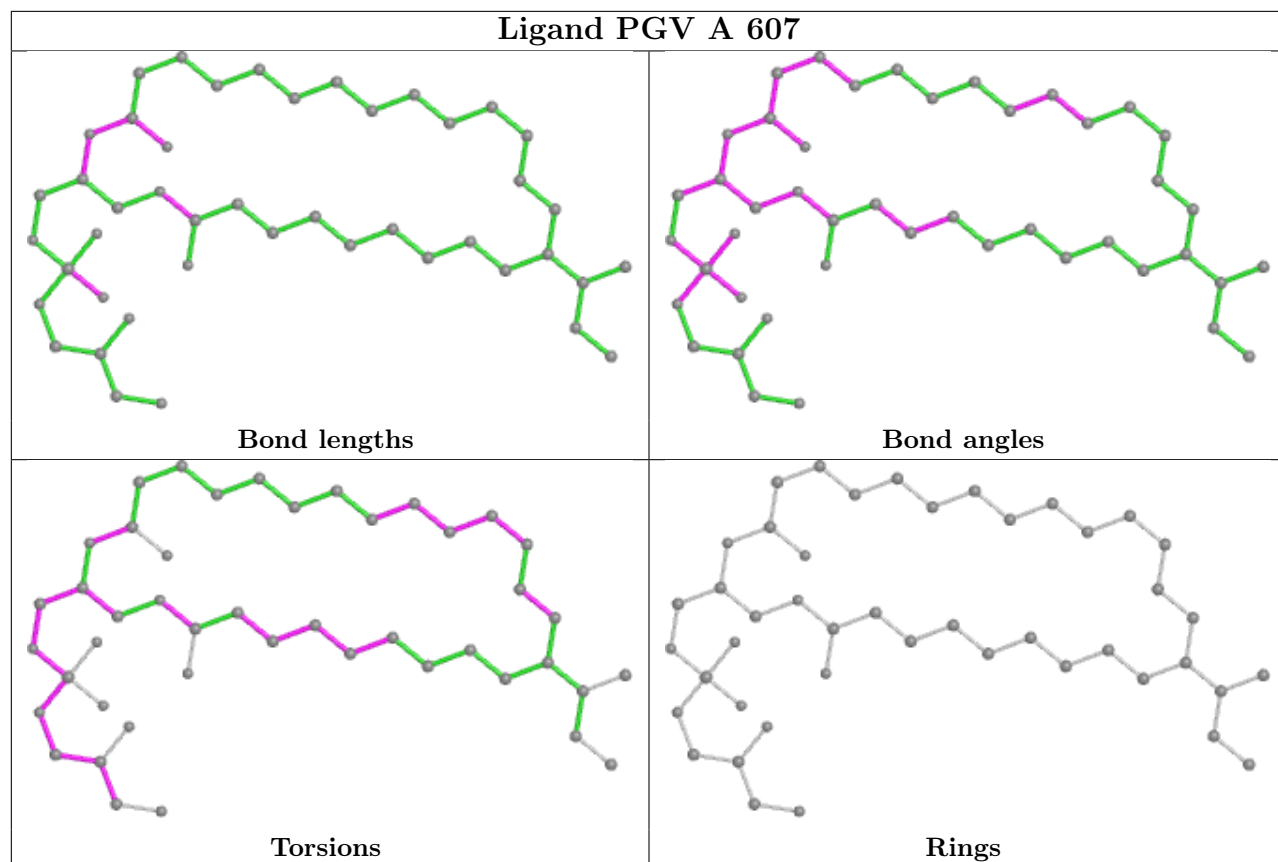


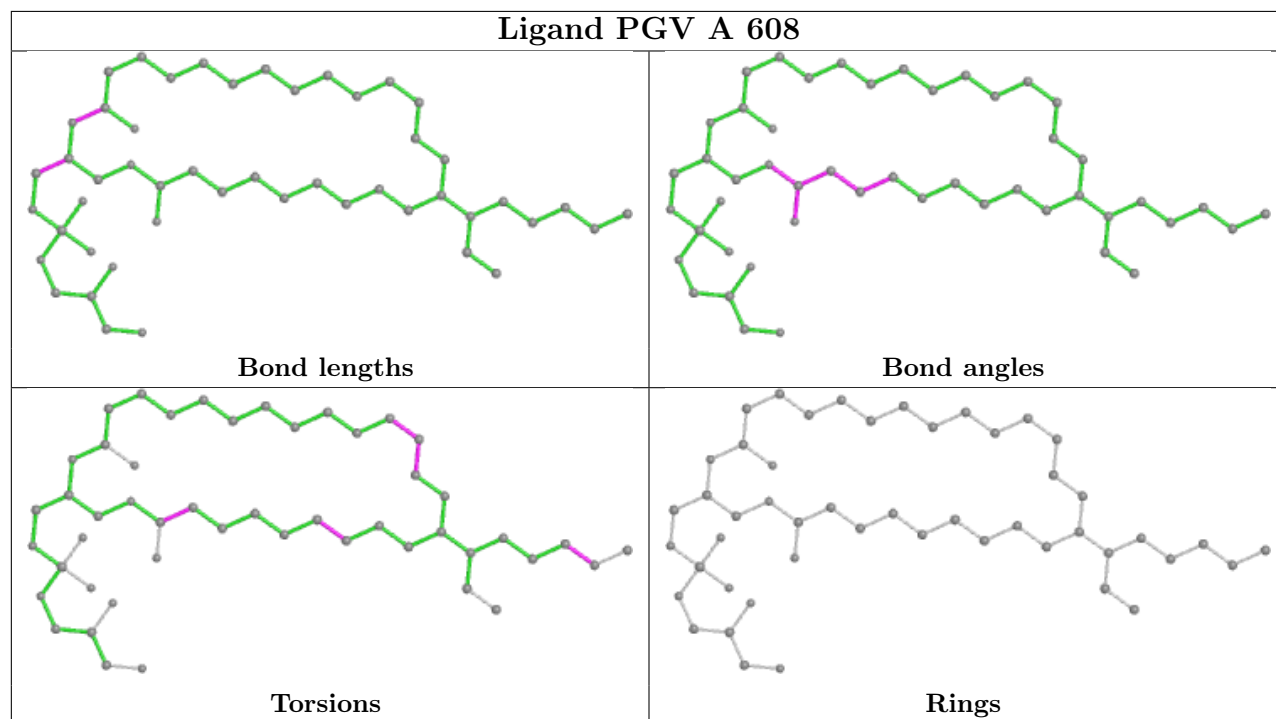
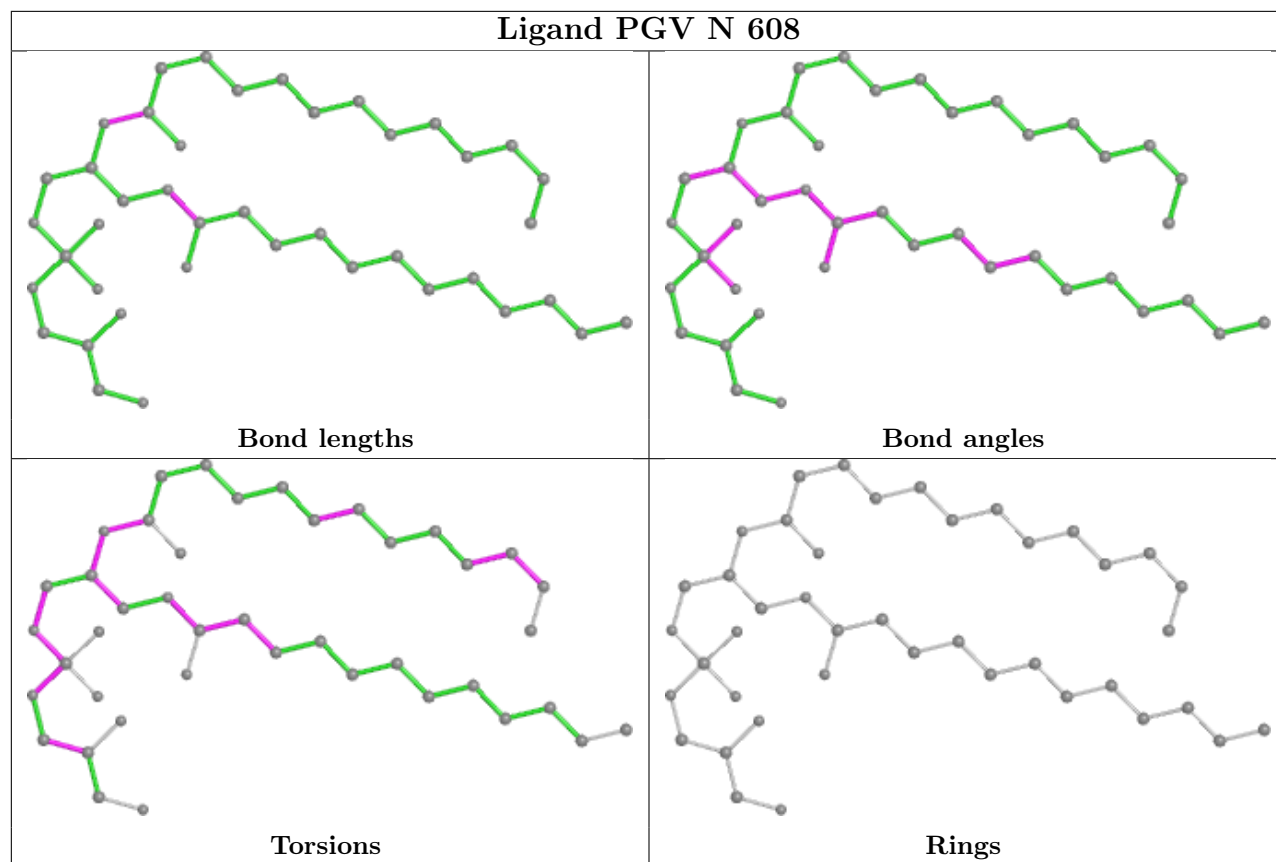
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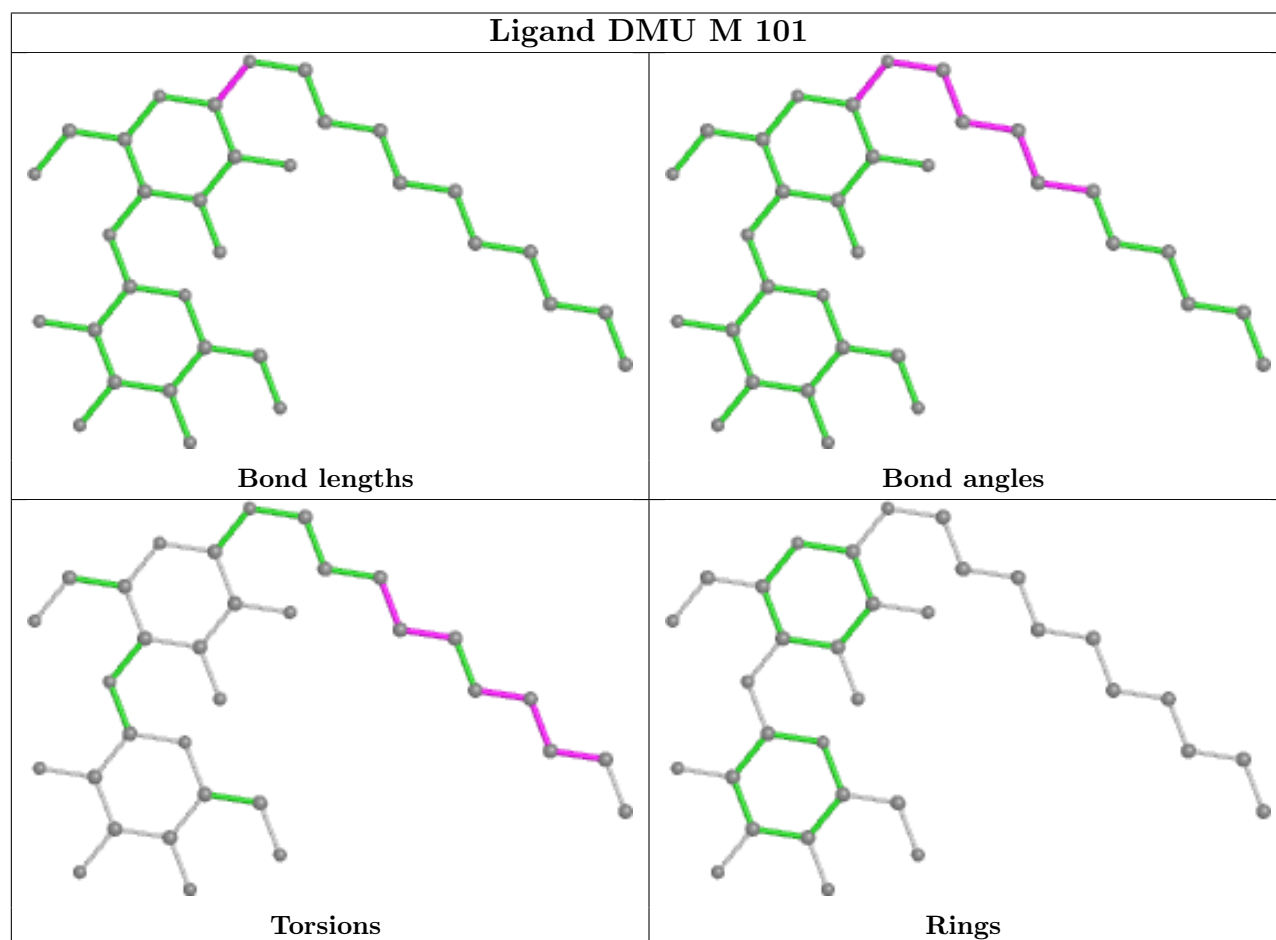
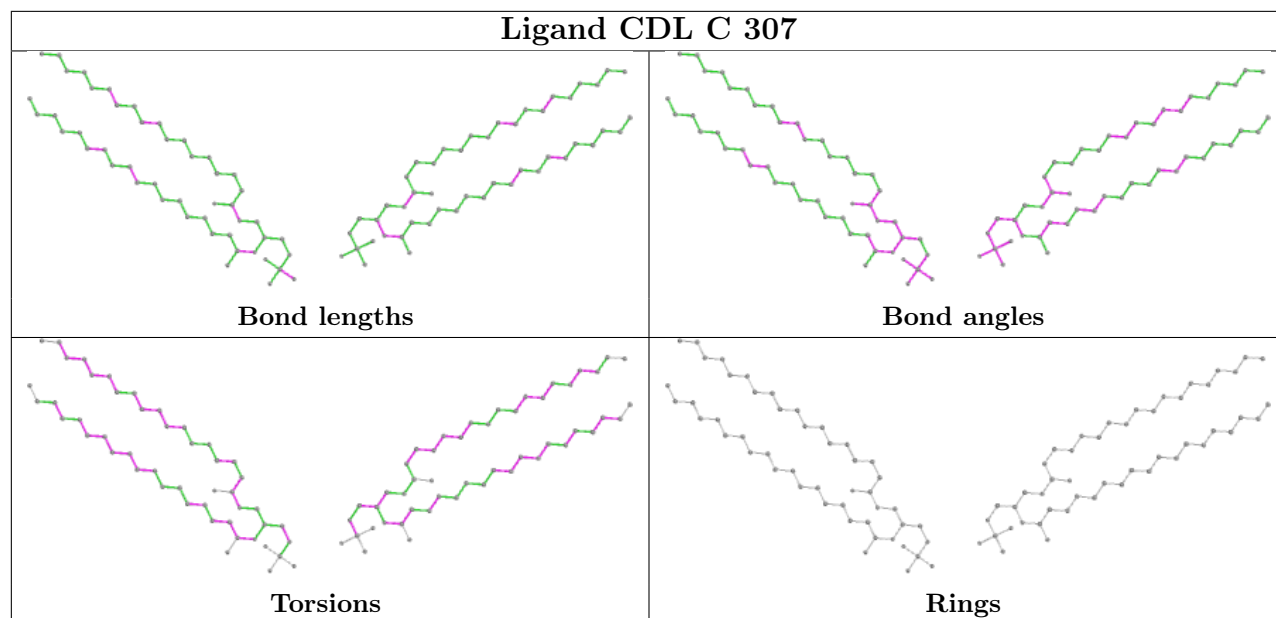


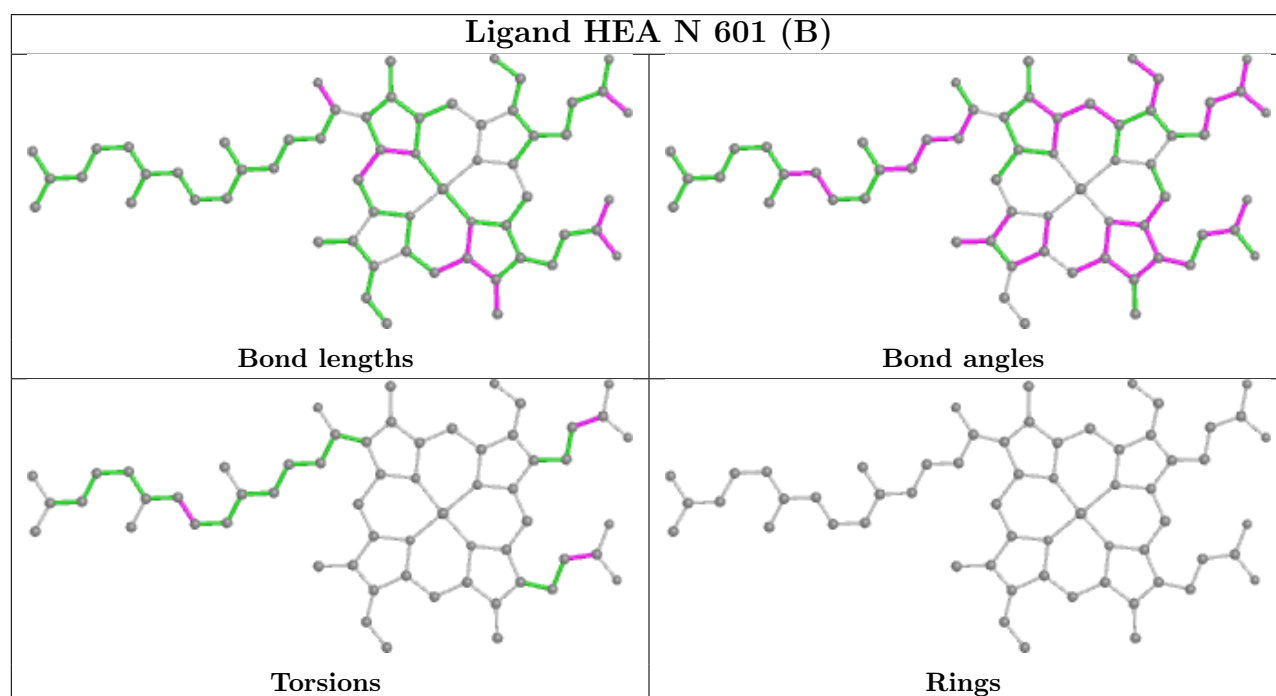
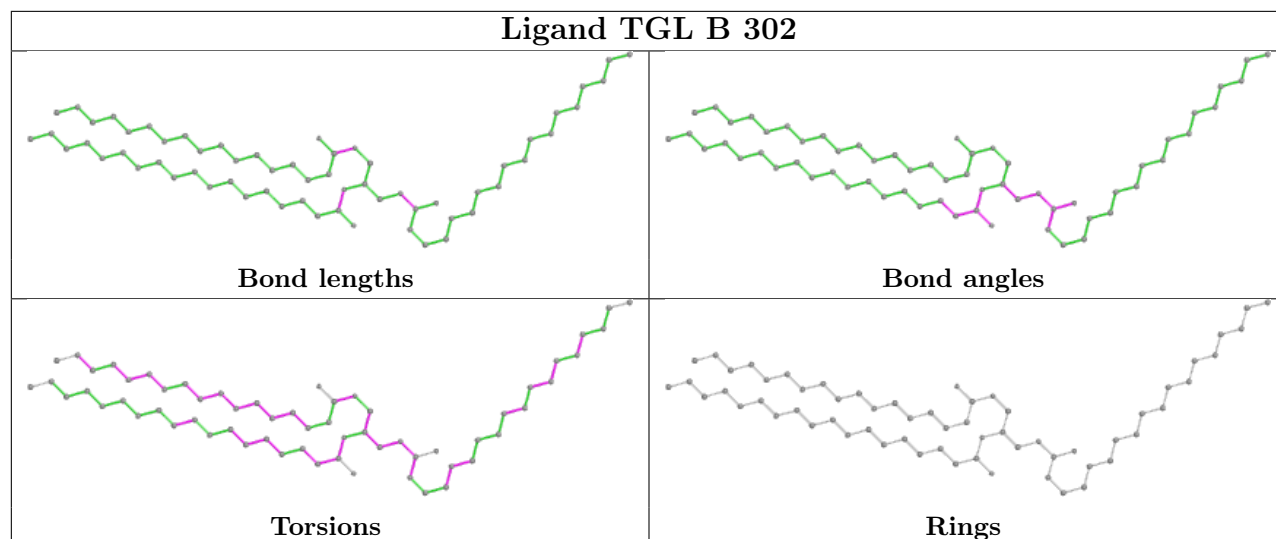




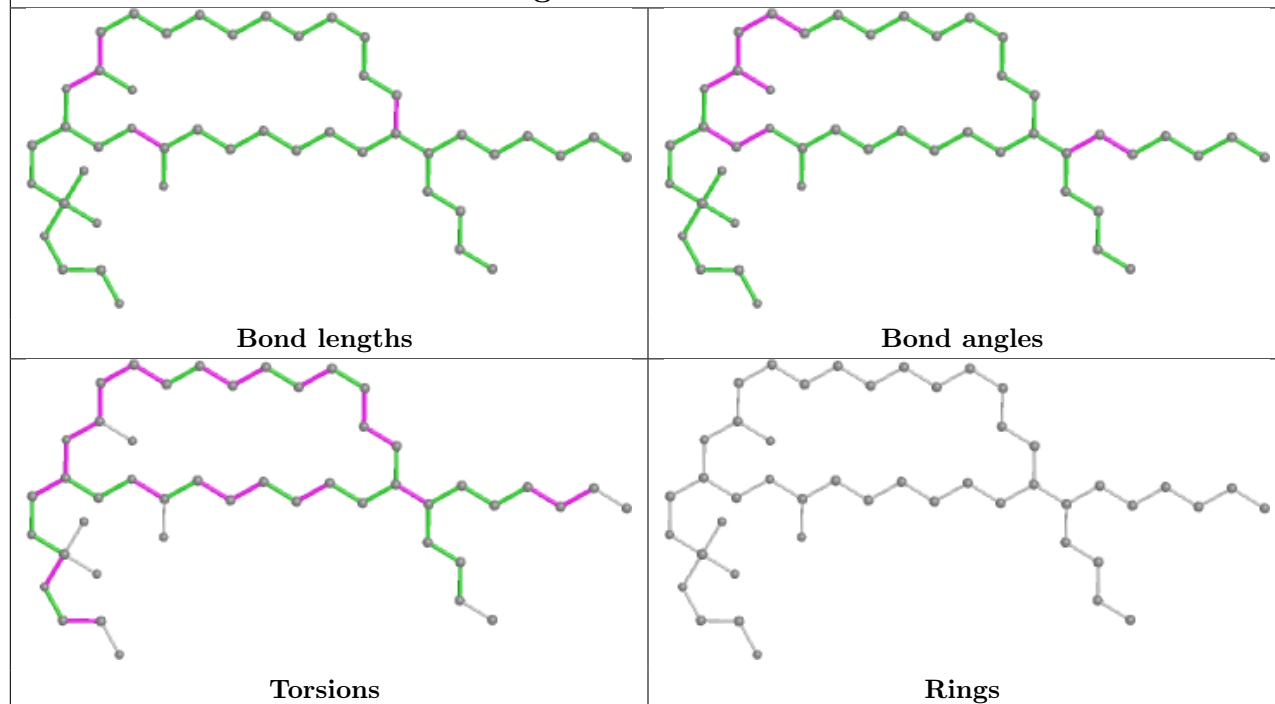




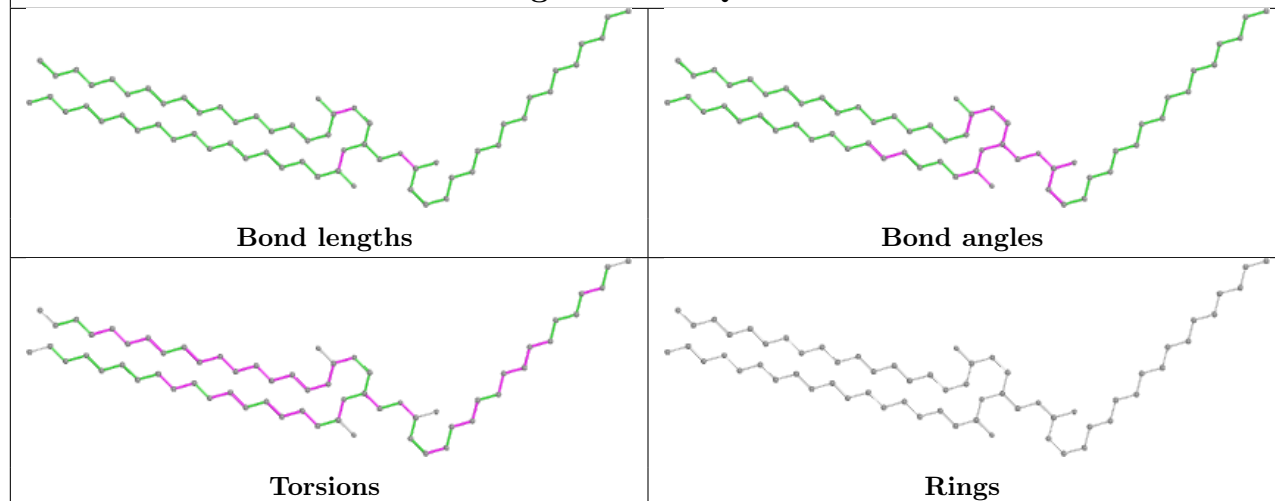


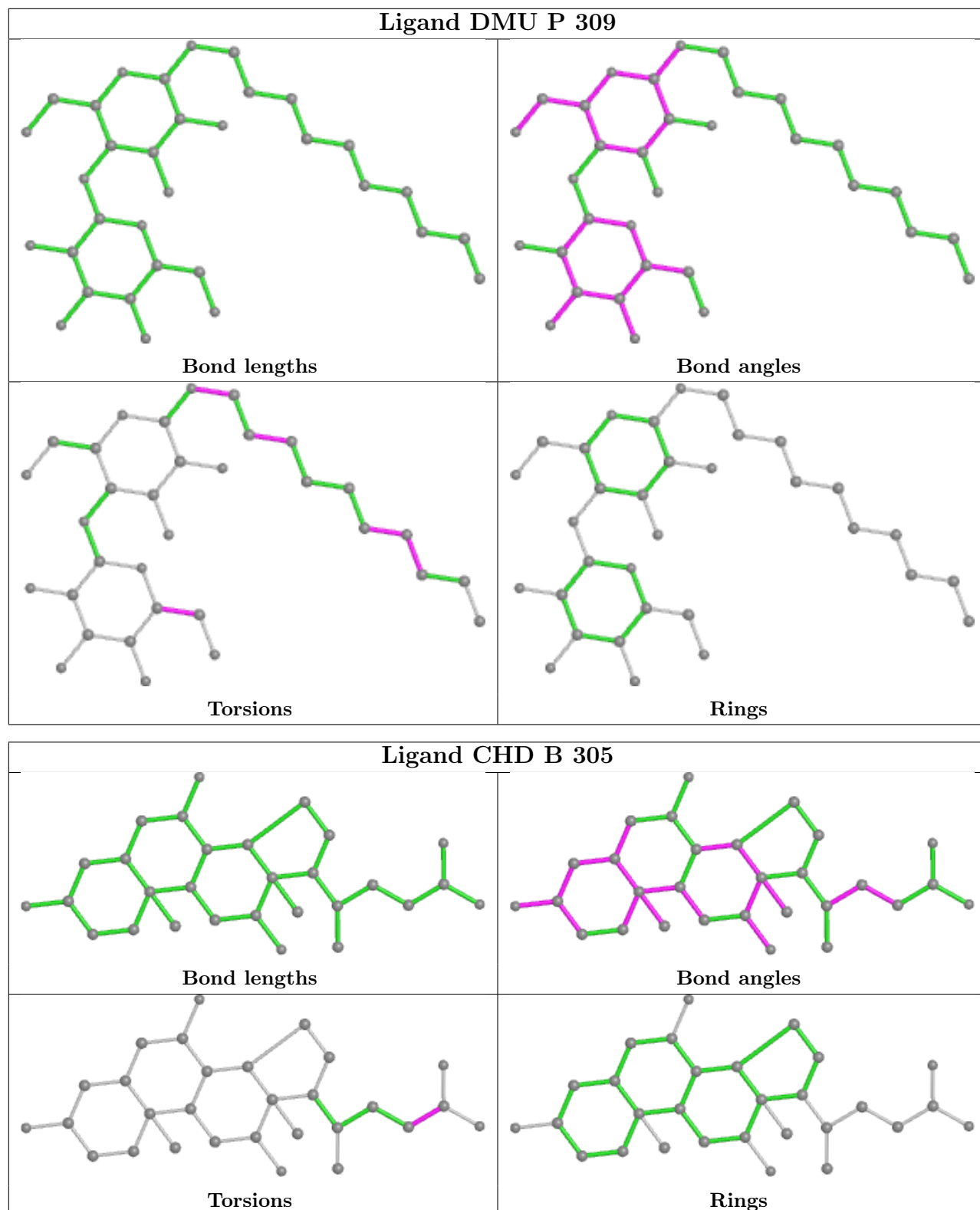


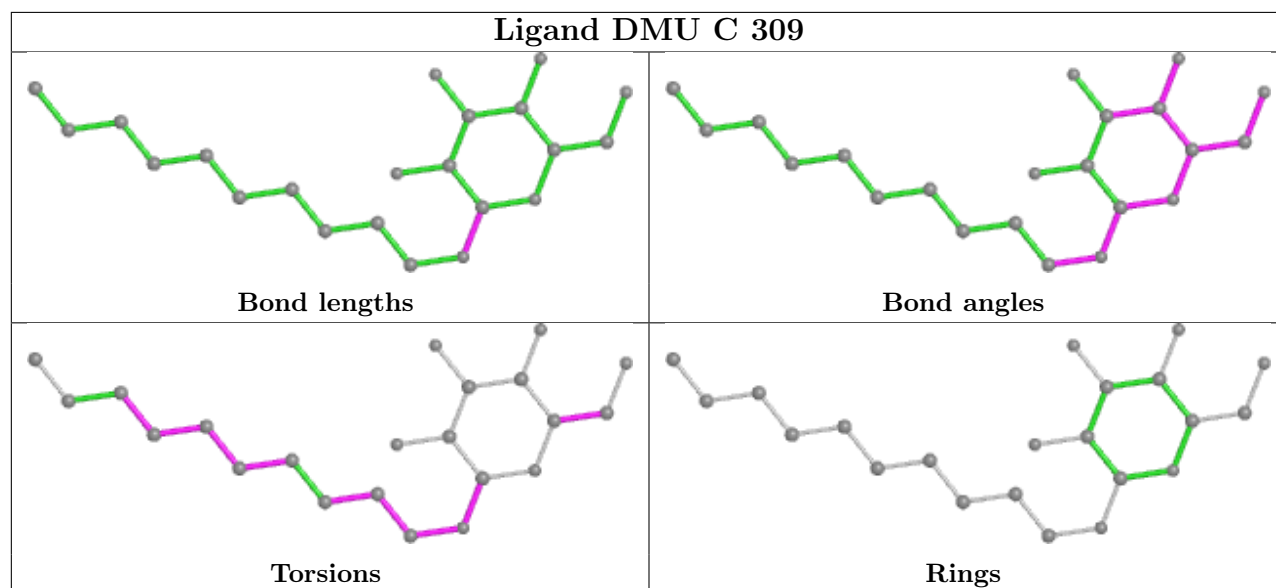
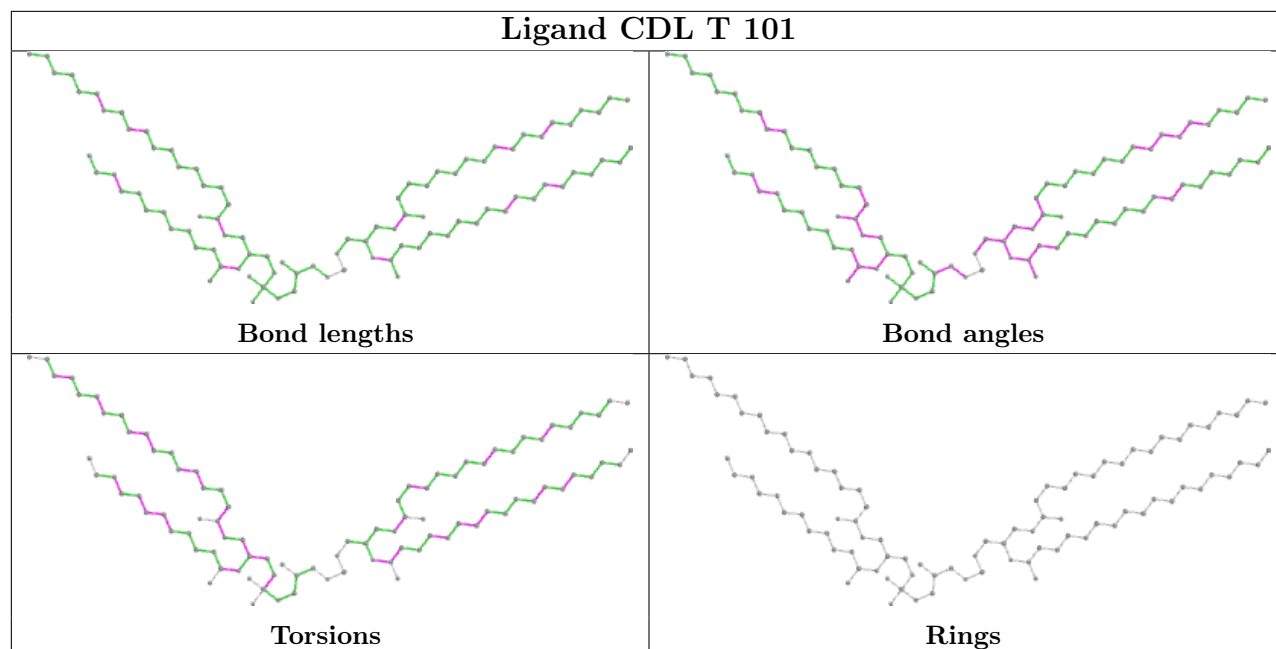
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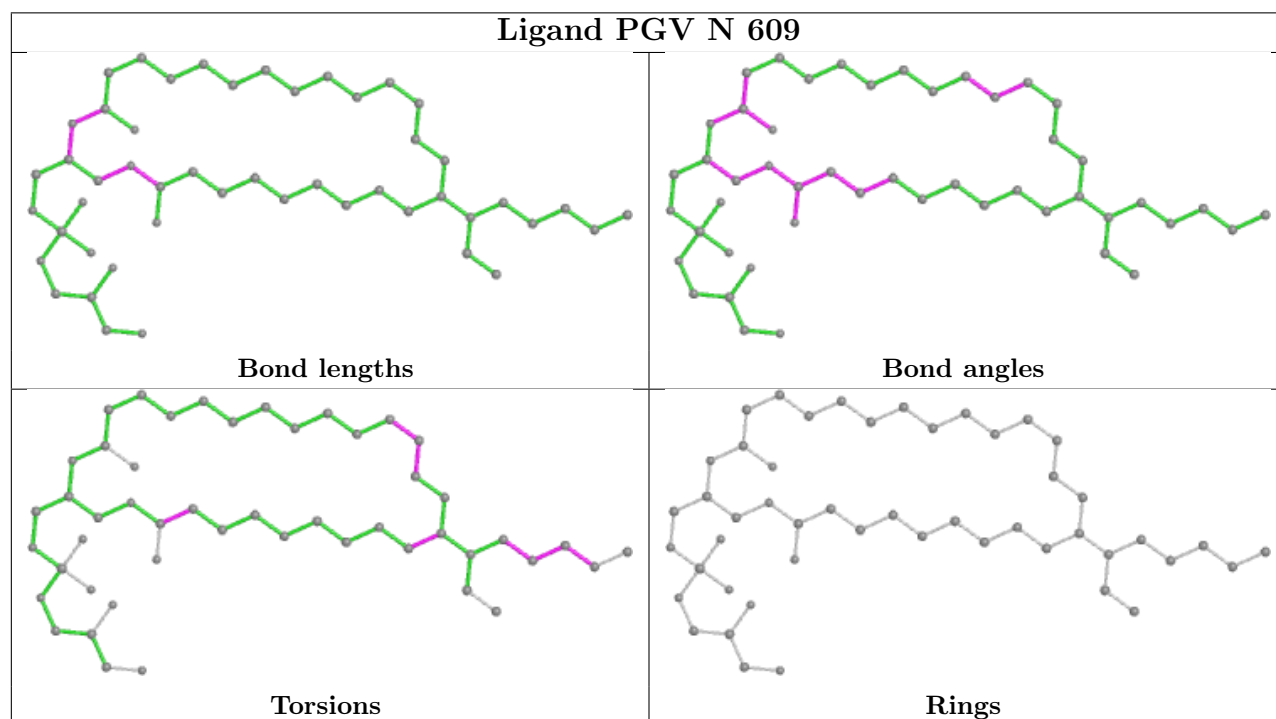
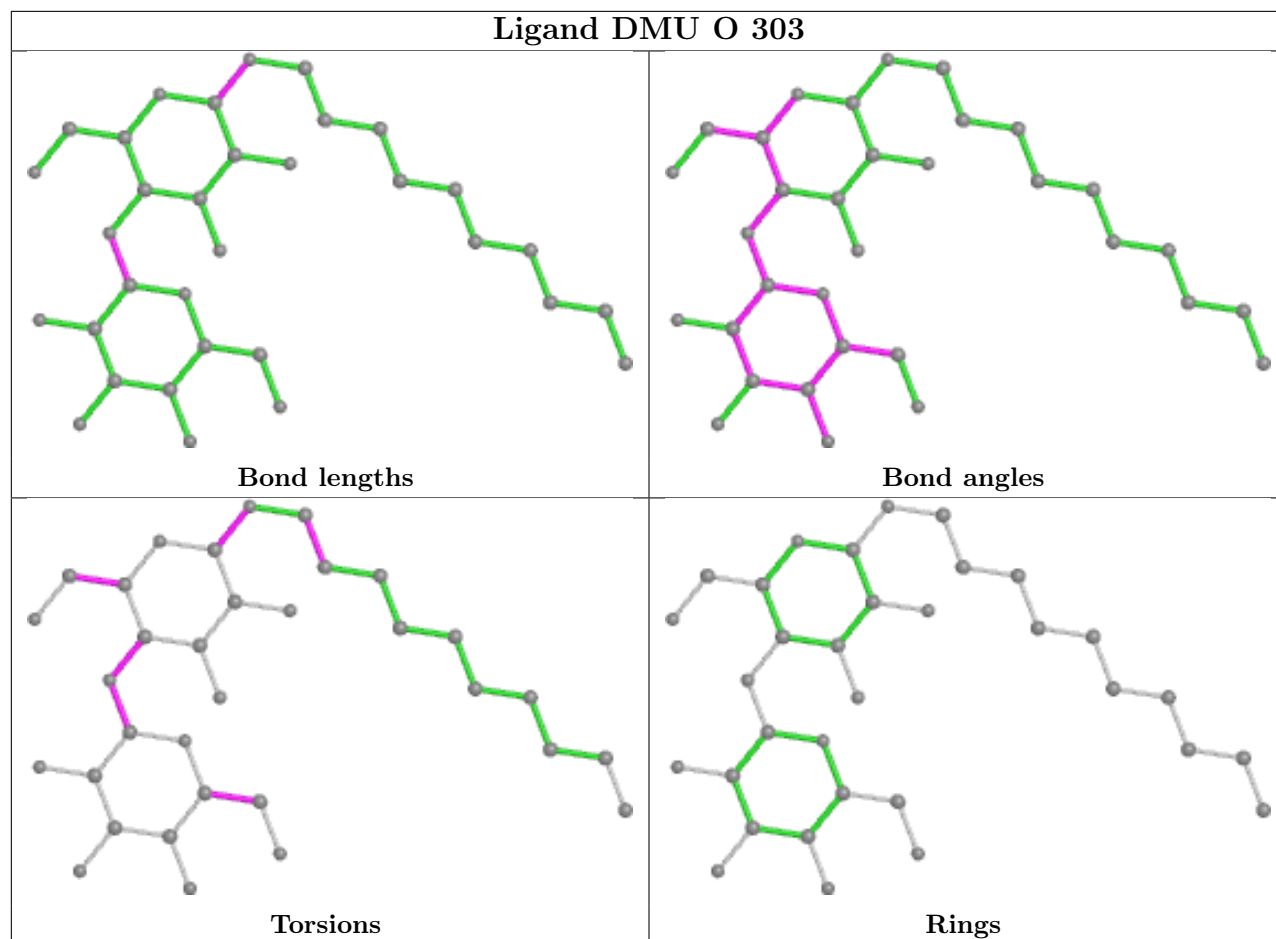


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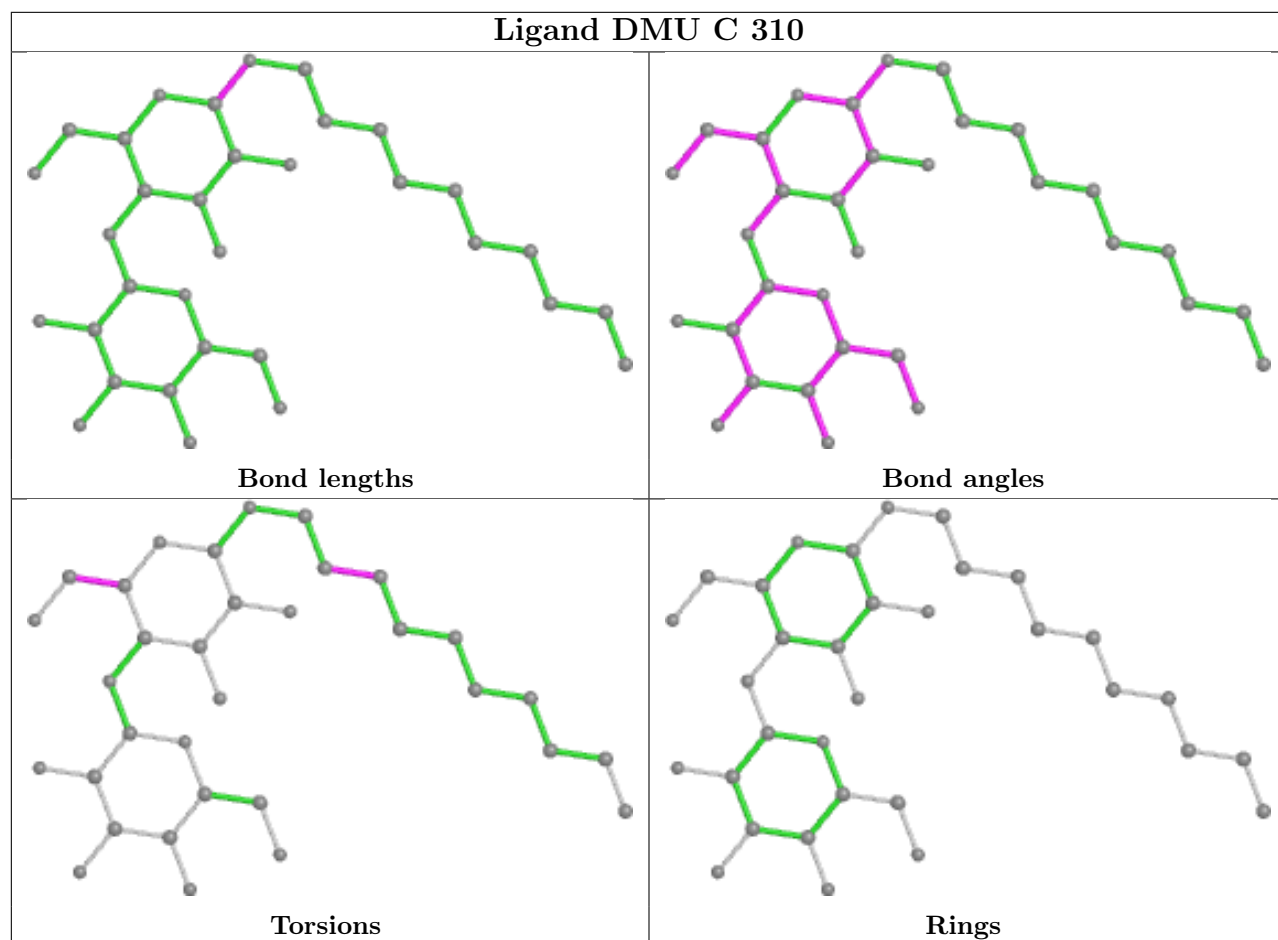
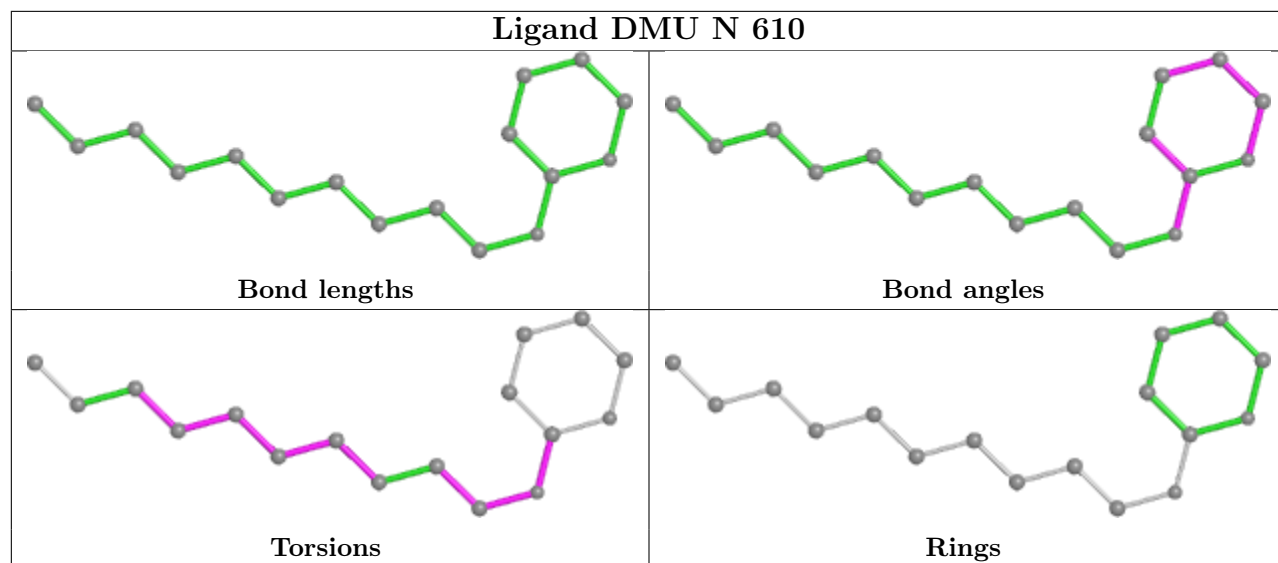


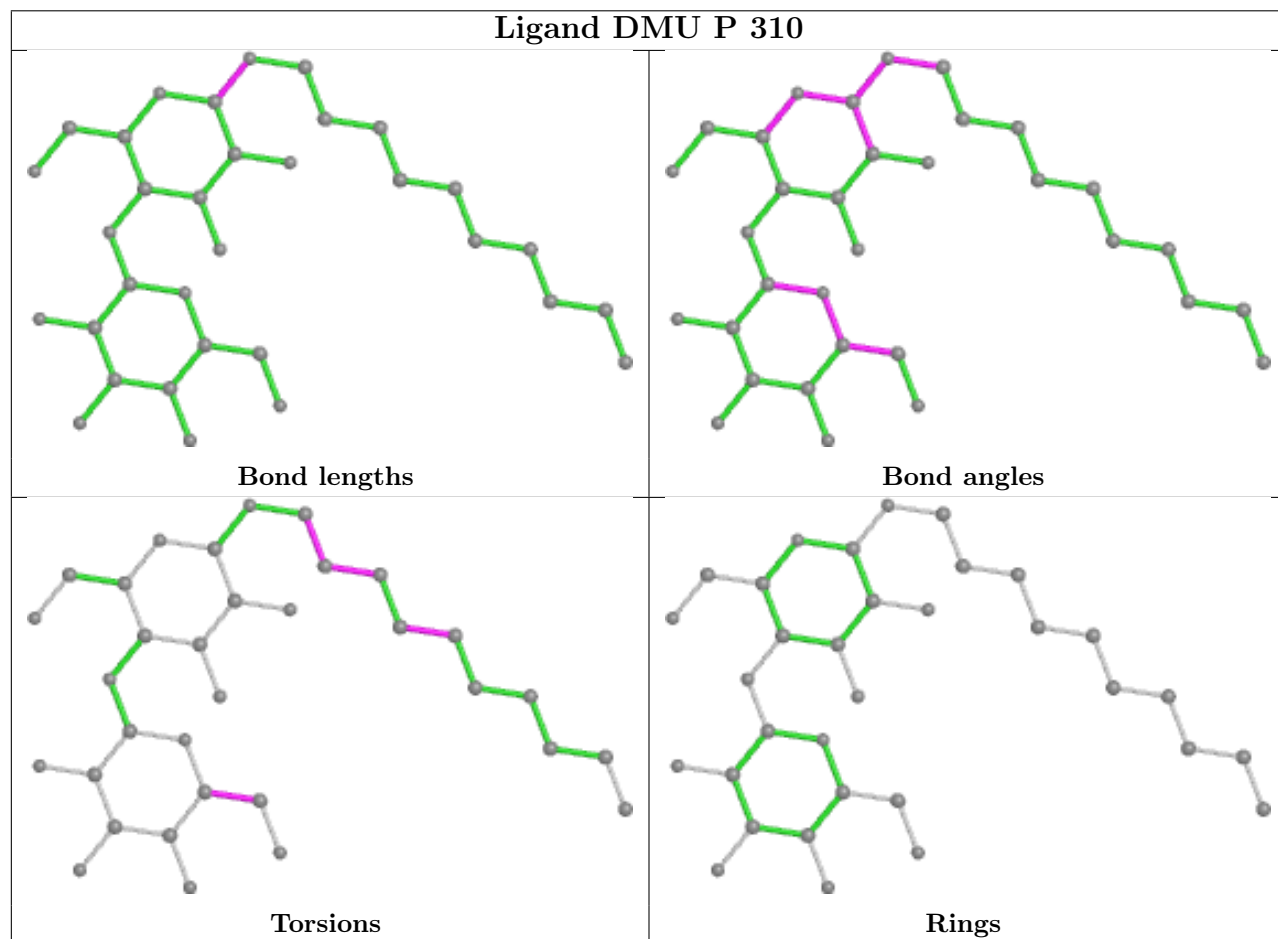
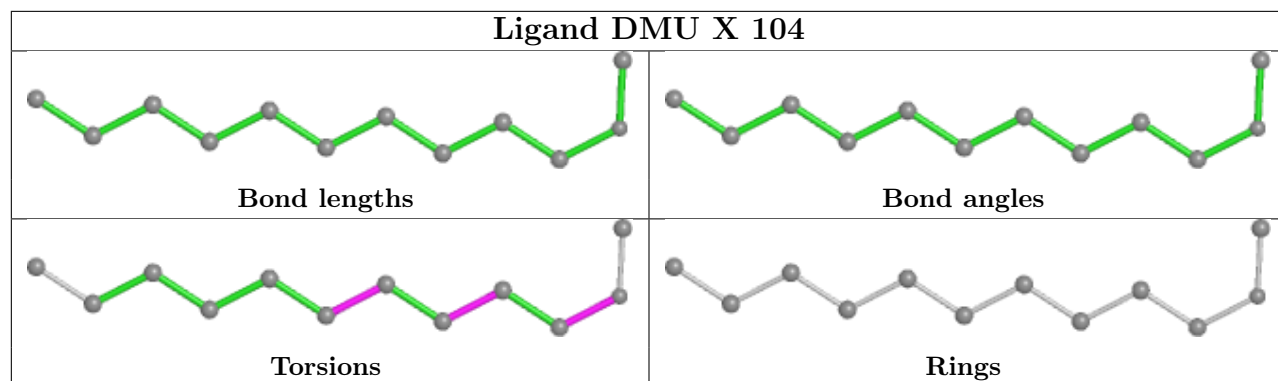




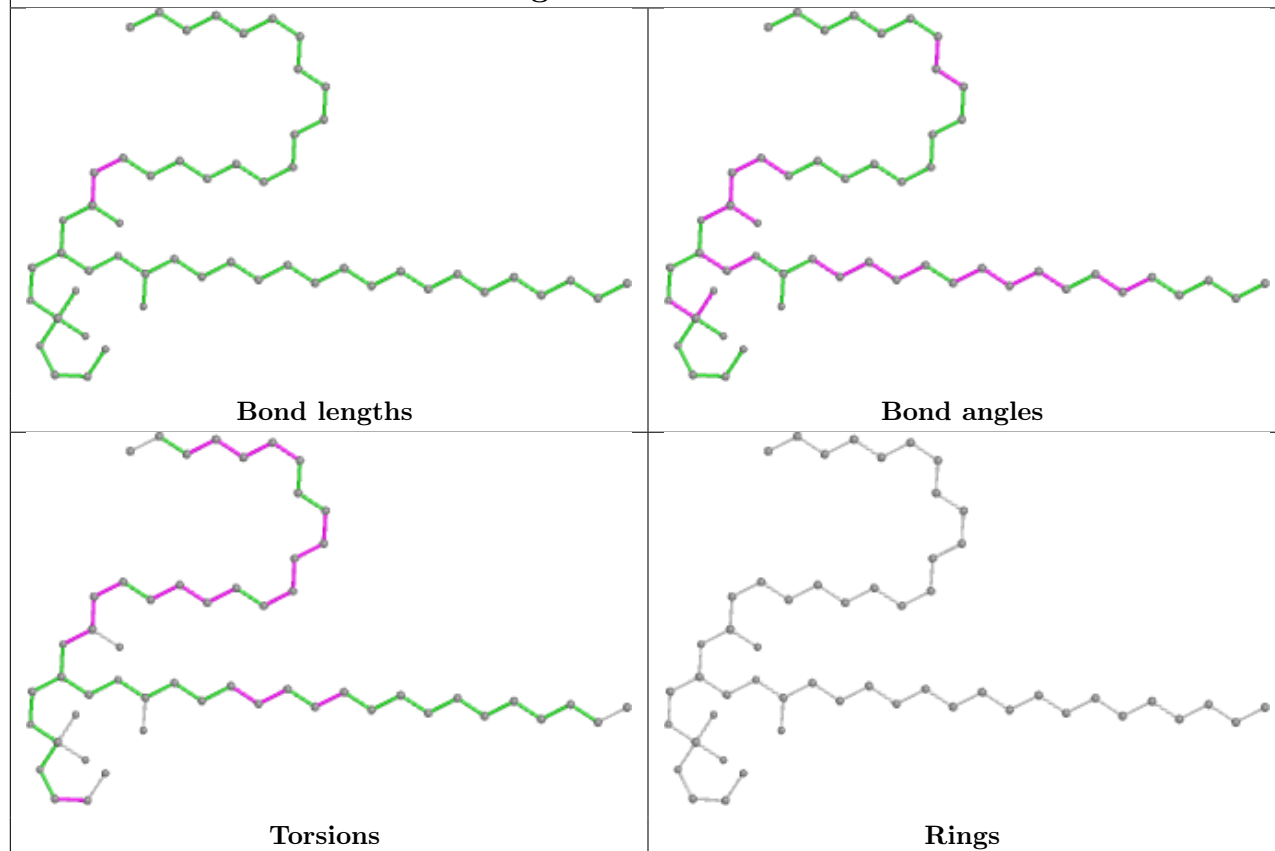




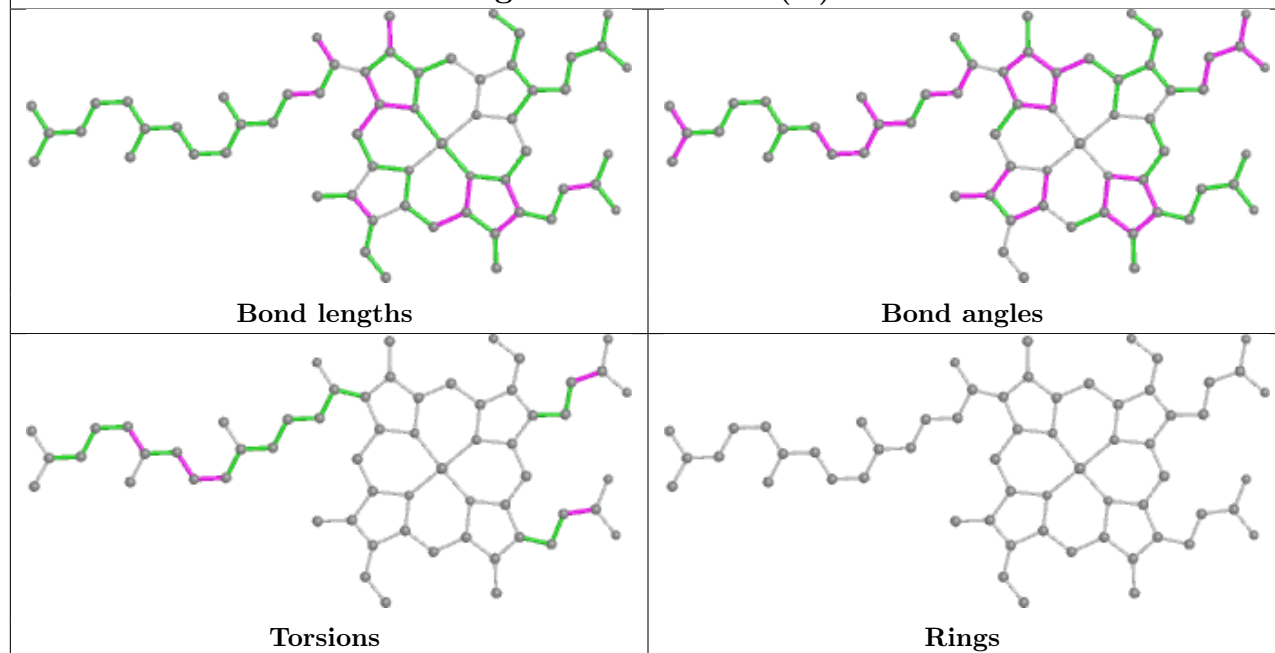


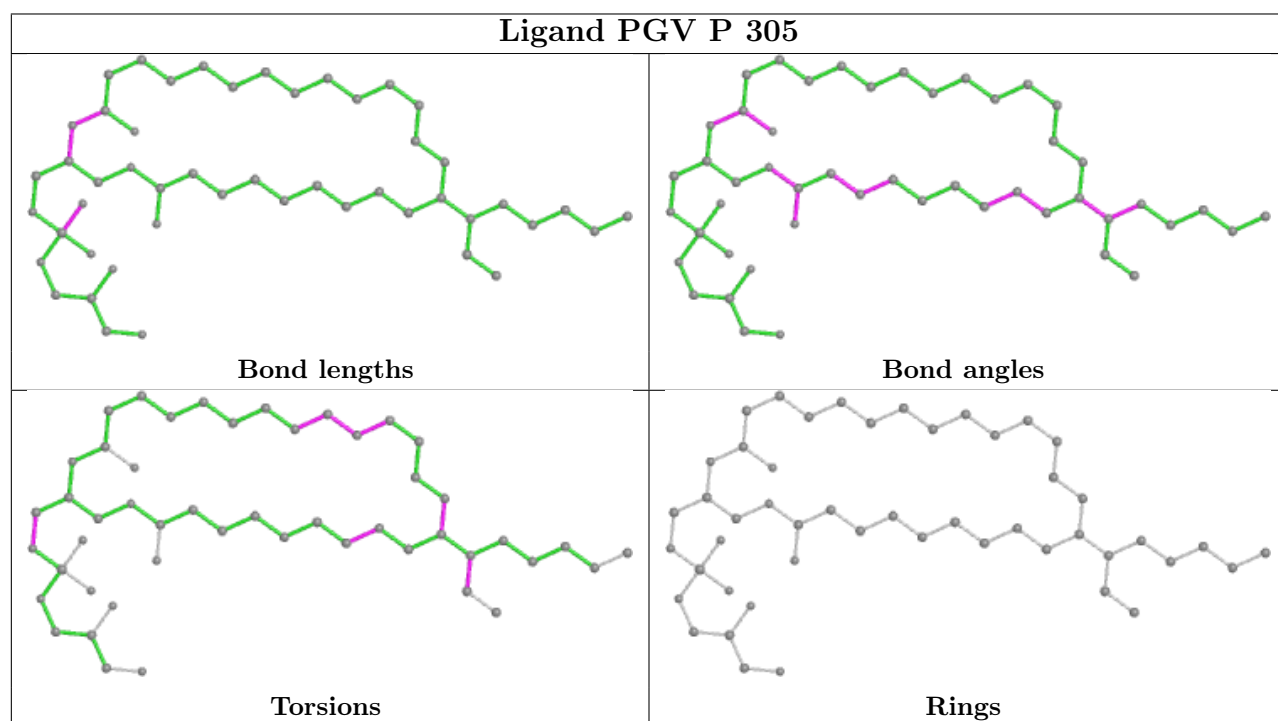
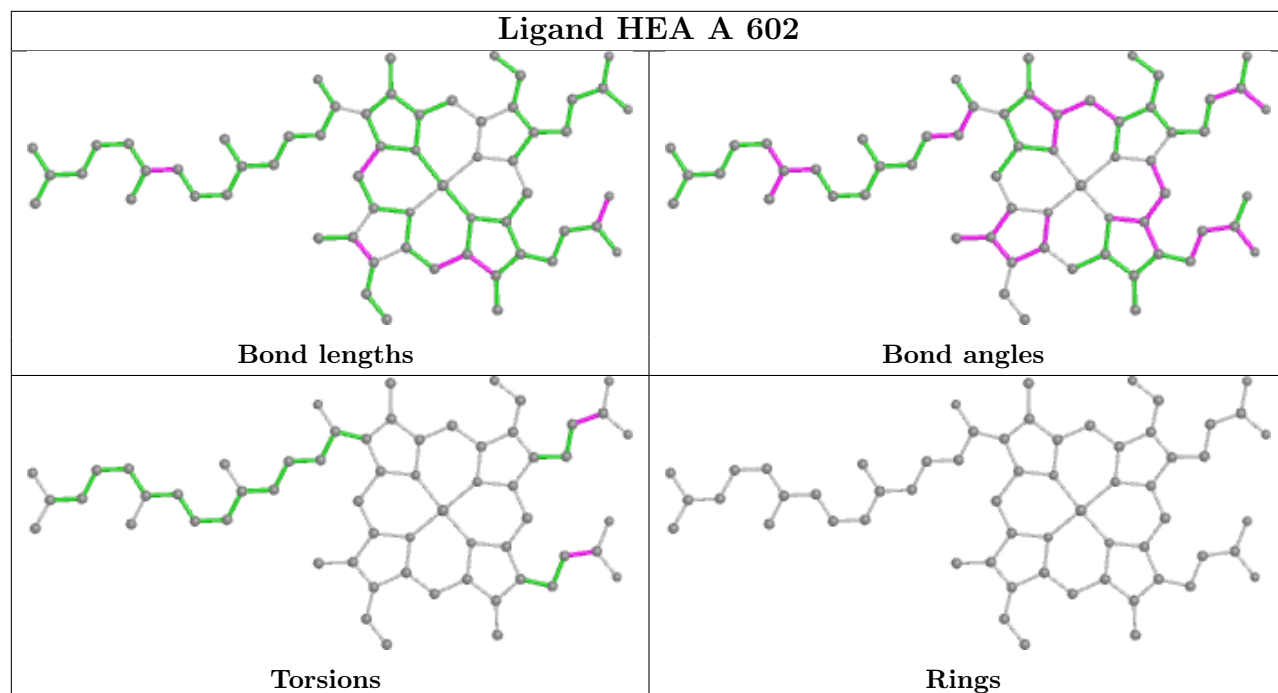


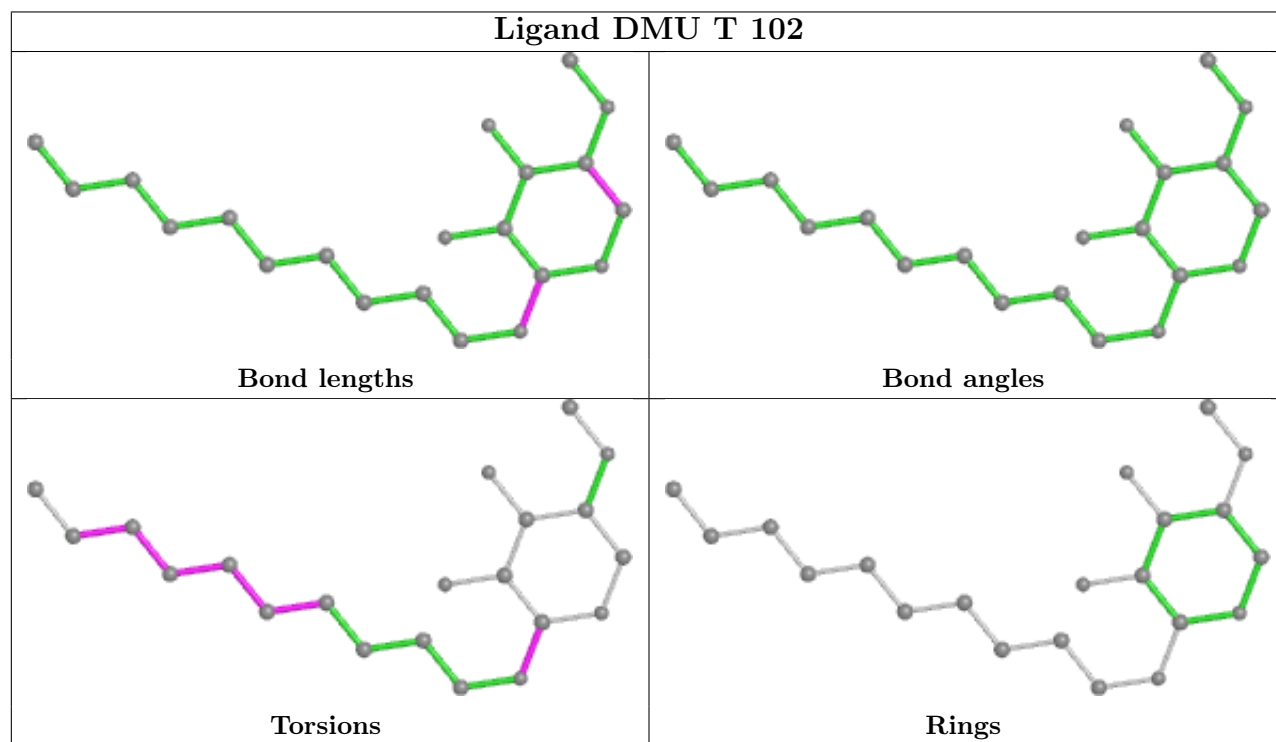
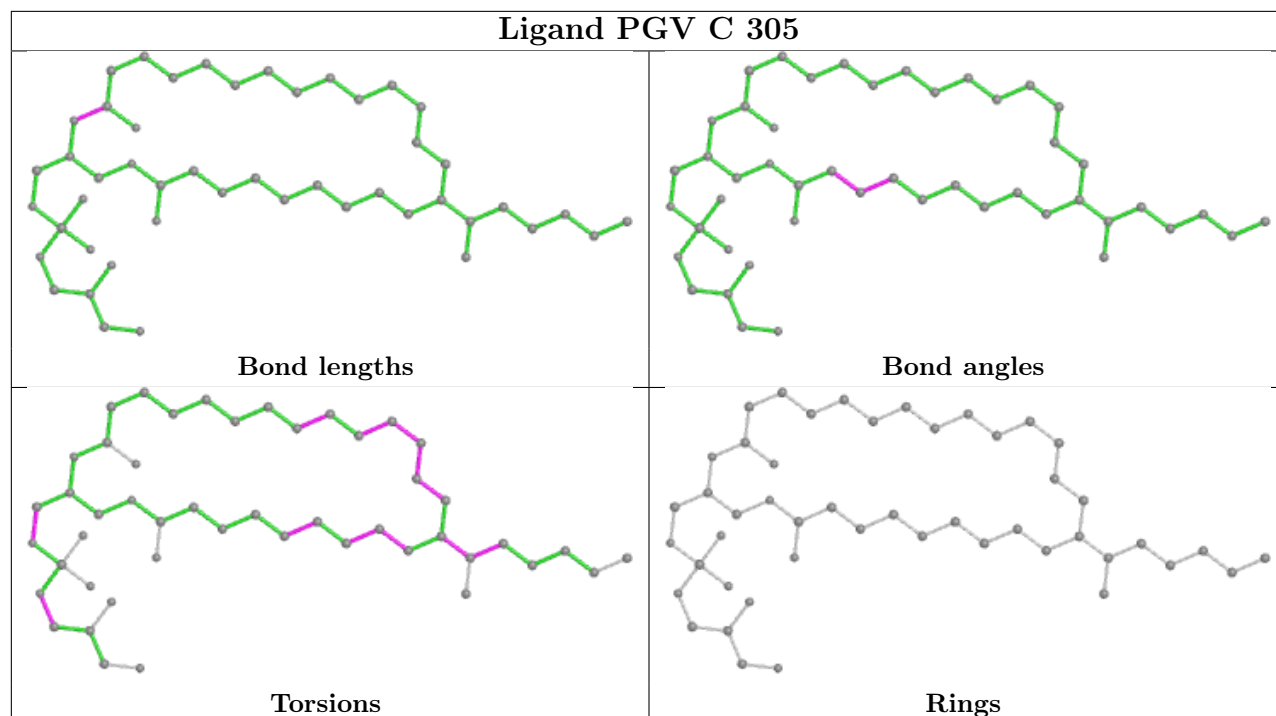
## Ligand PEK P 303

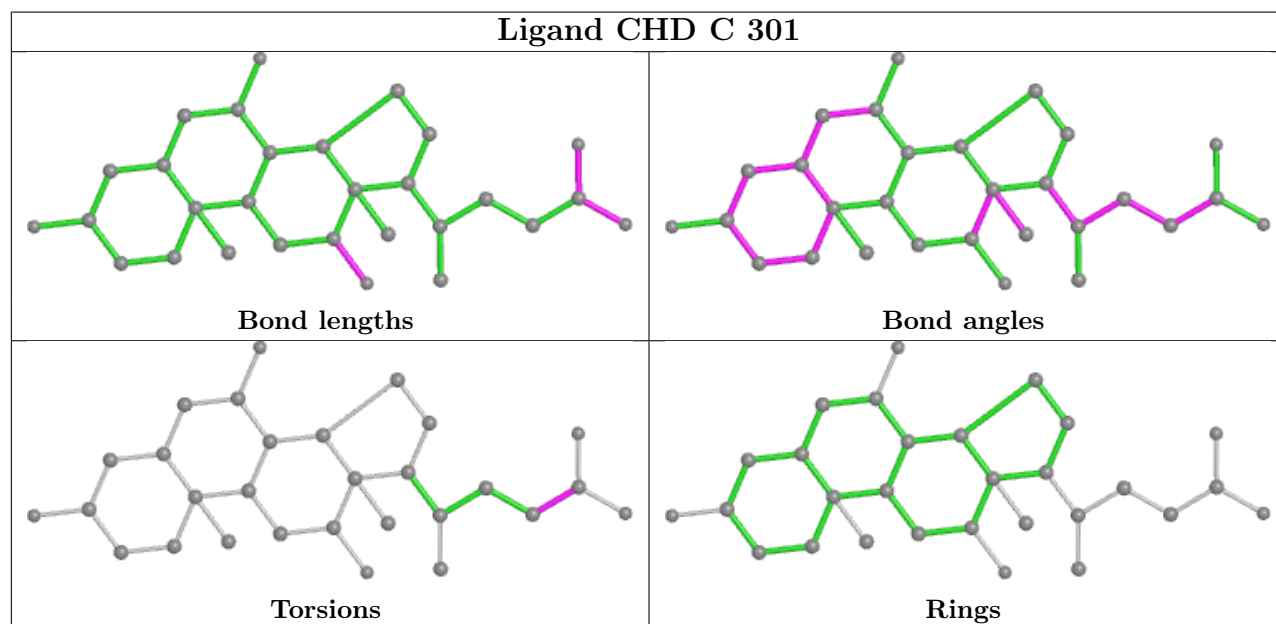
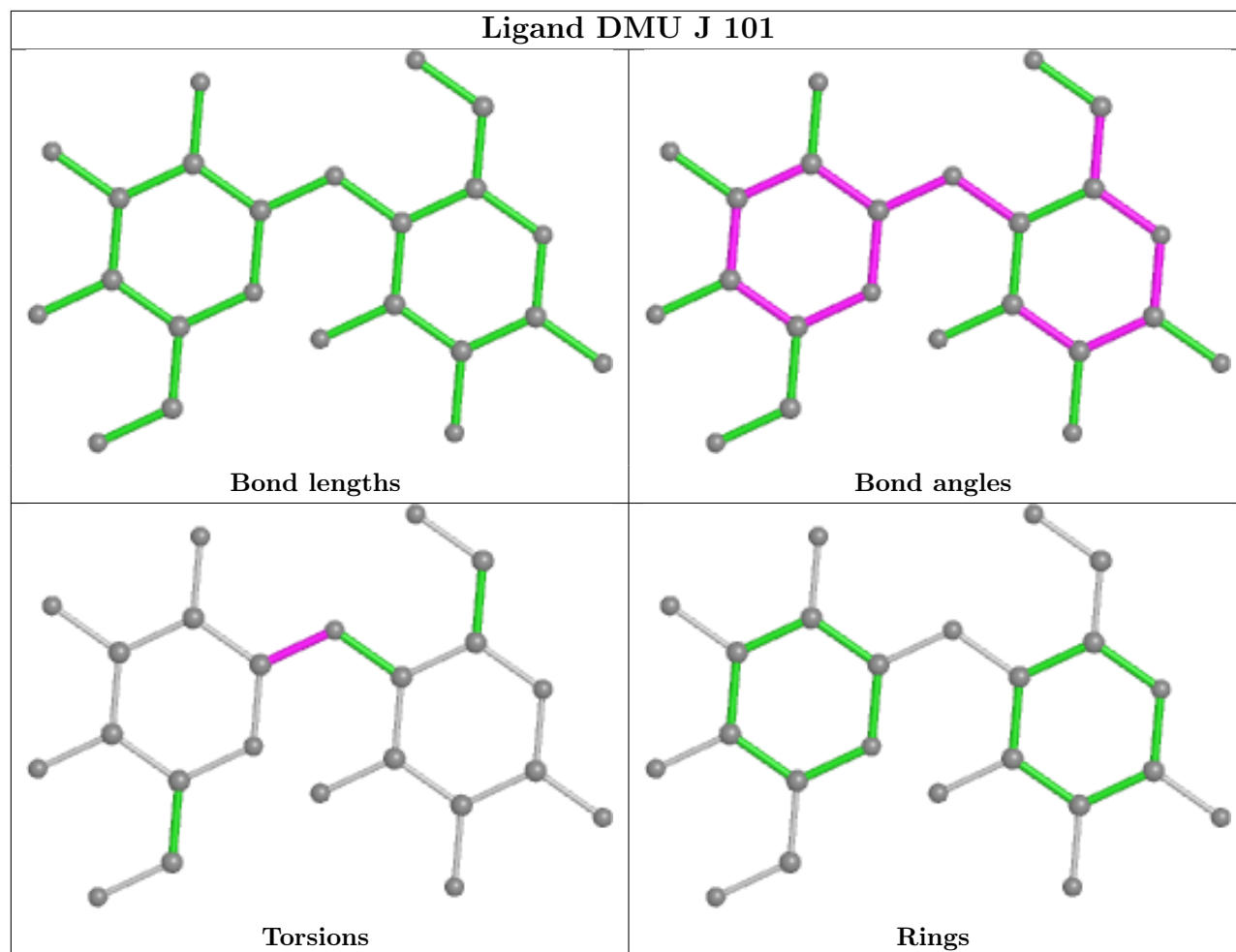


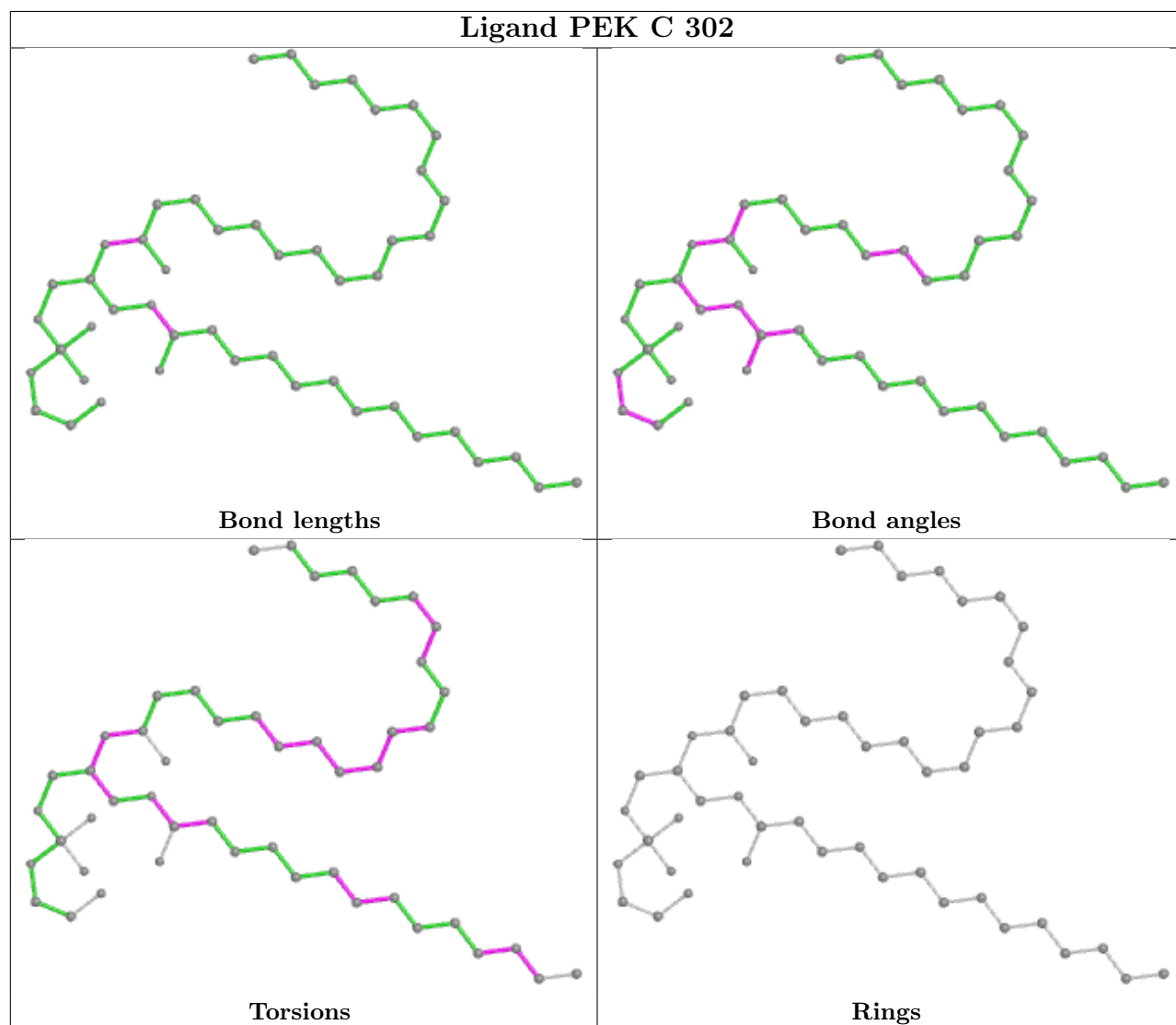
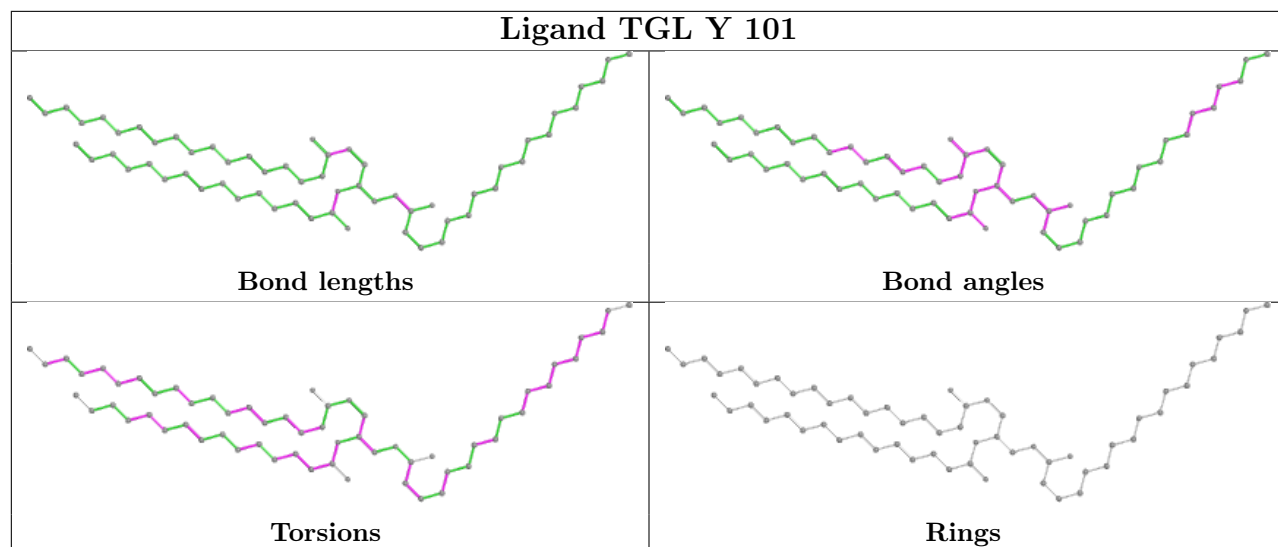
## Ligand HEA A 601 (A)

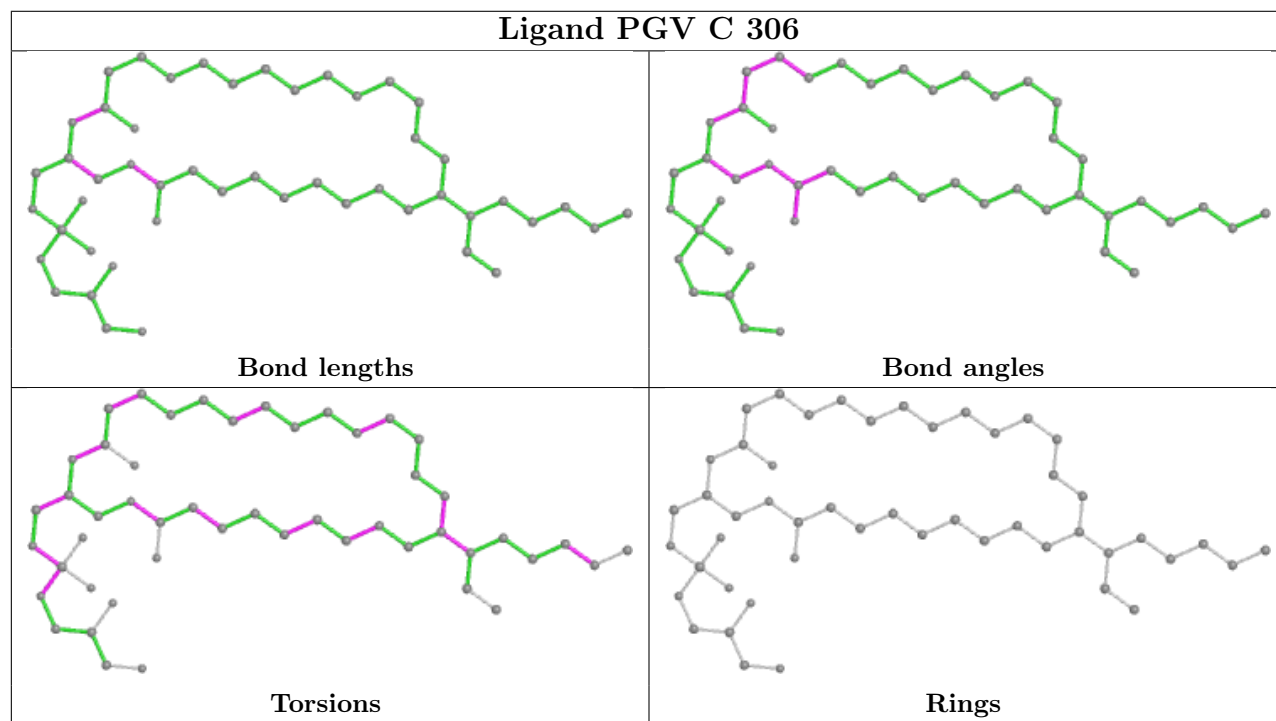
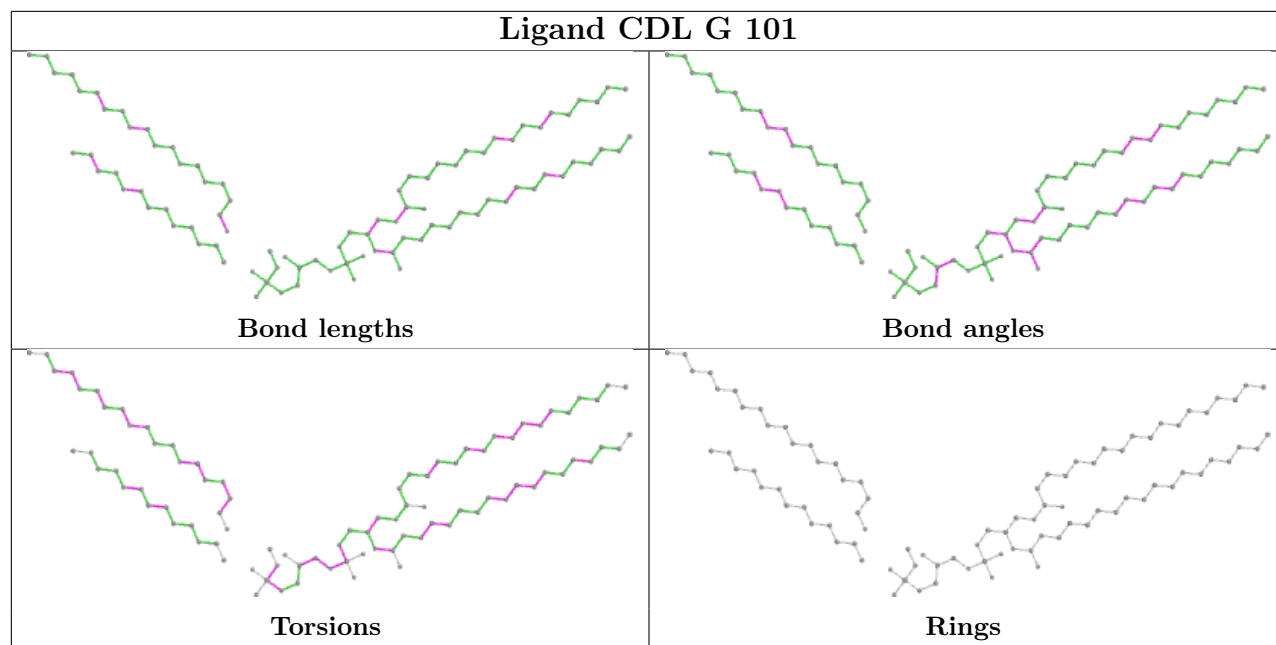




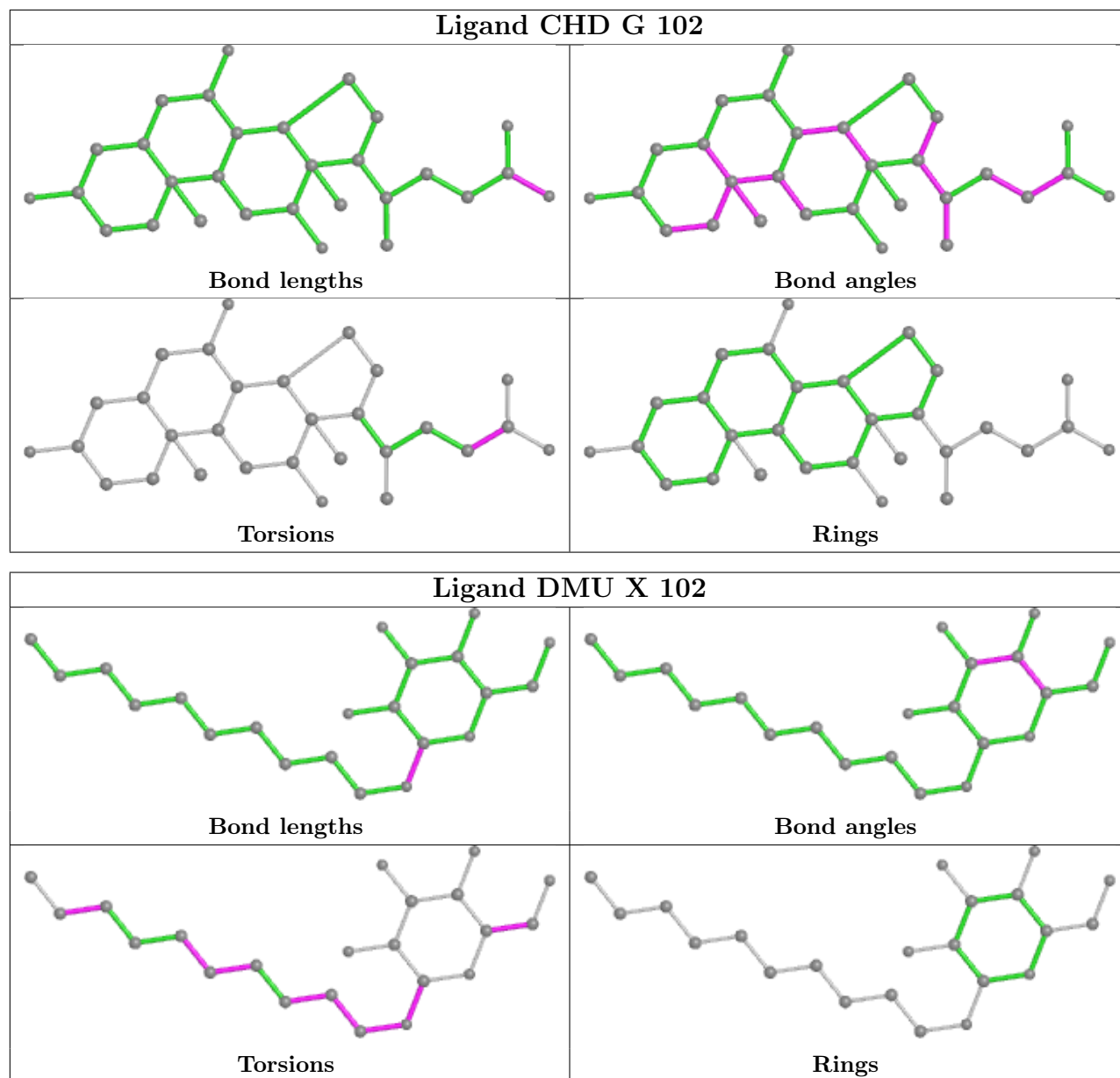


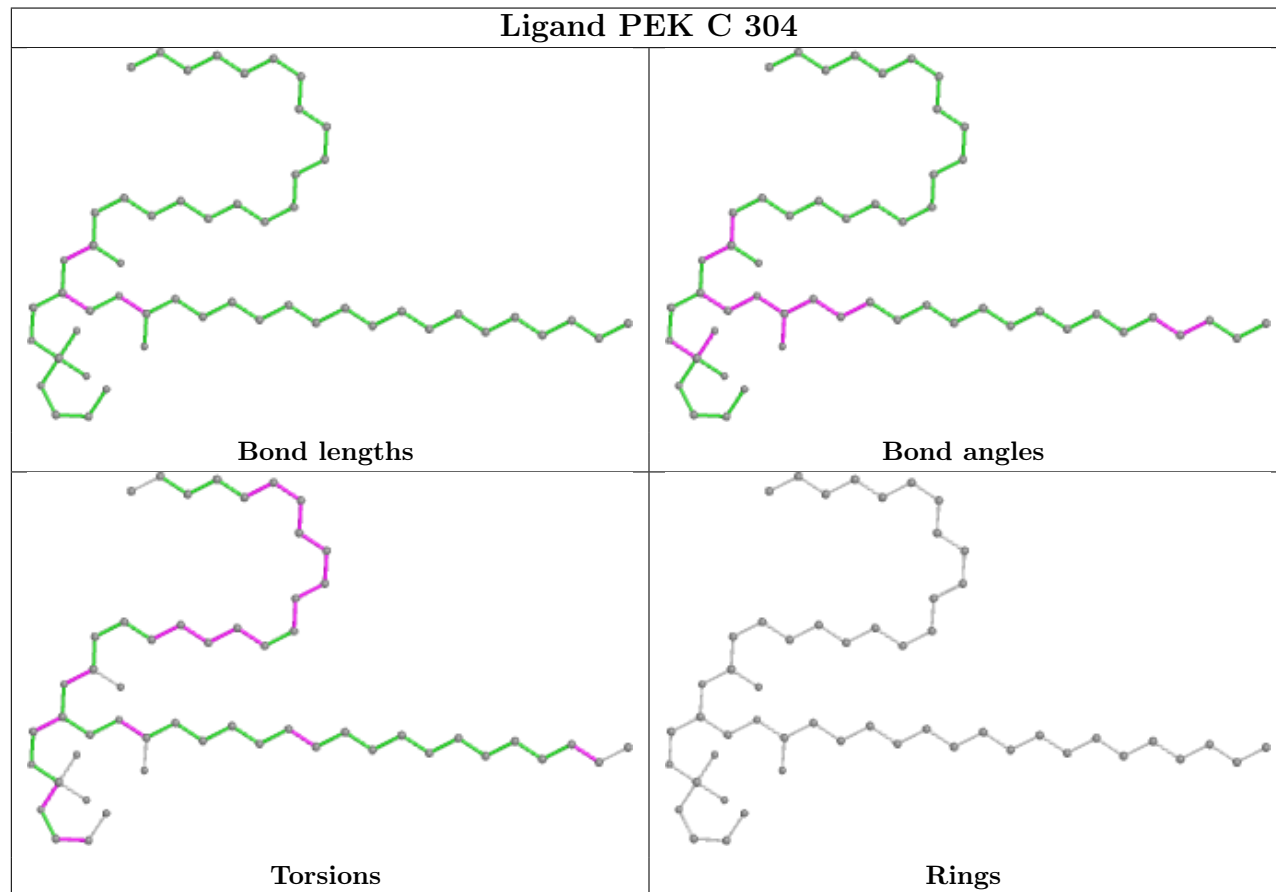
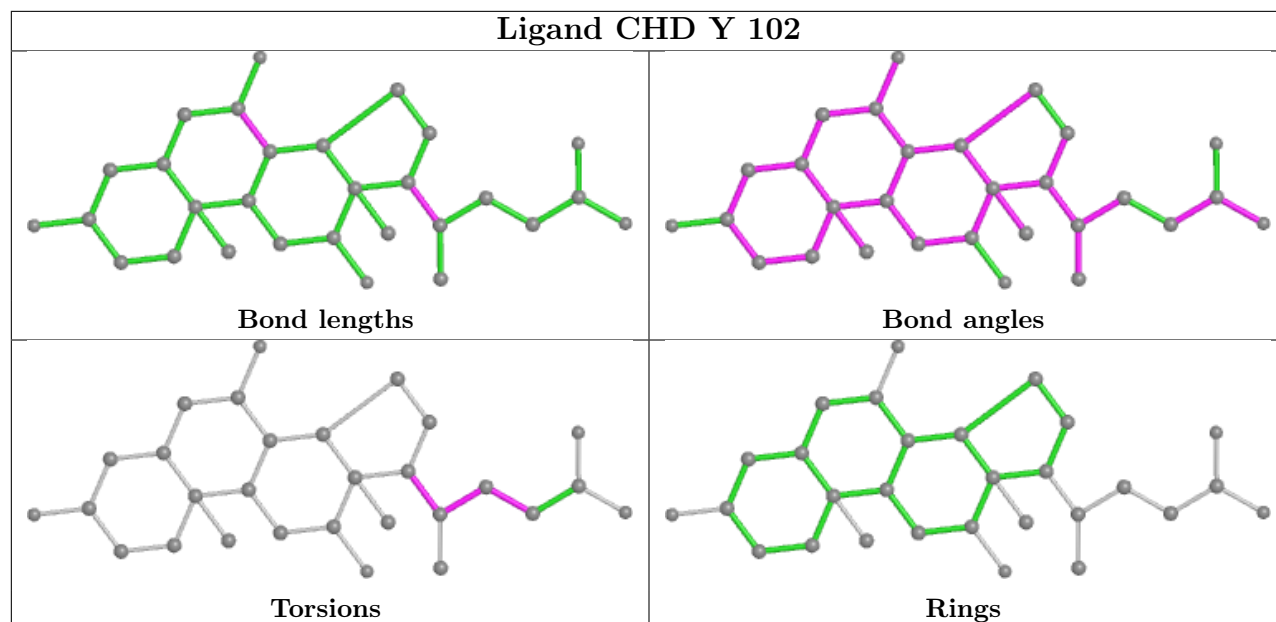


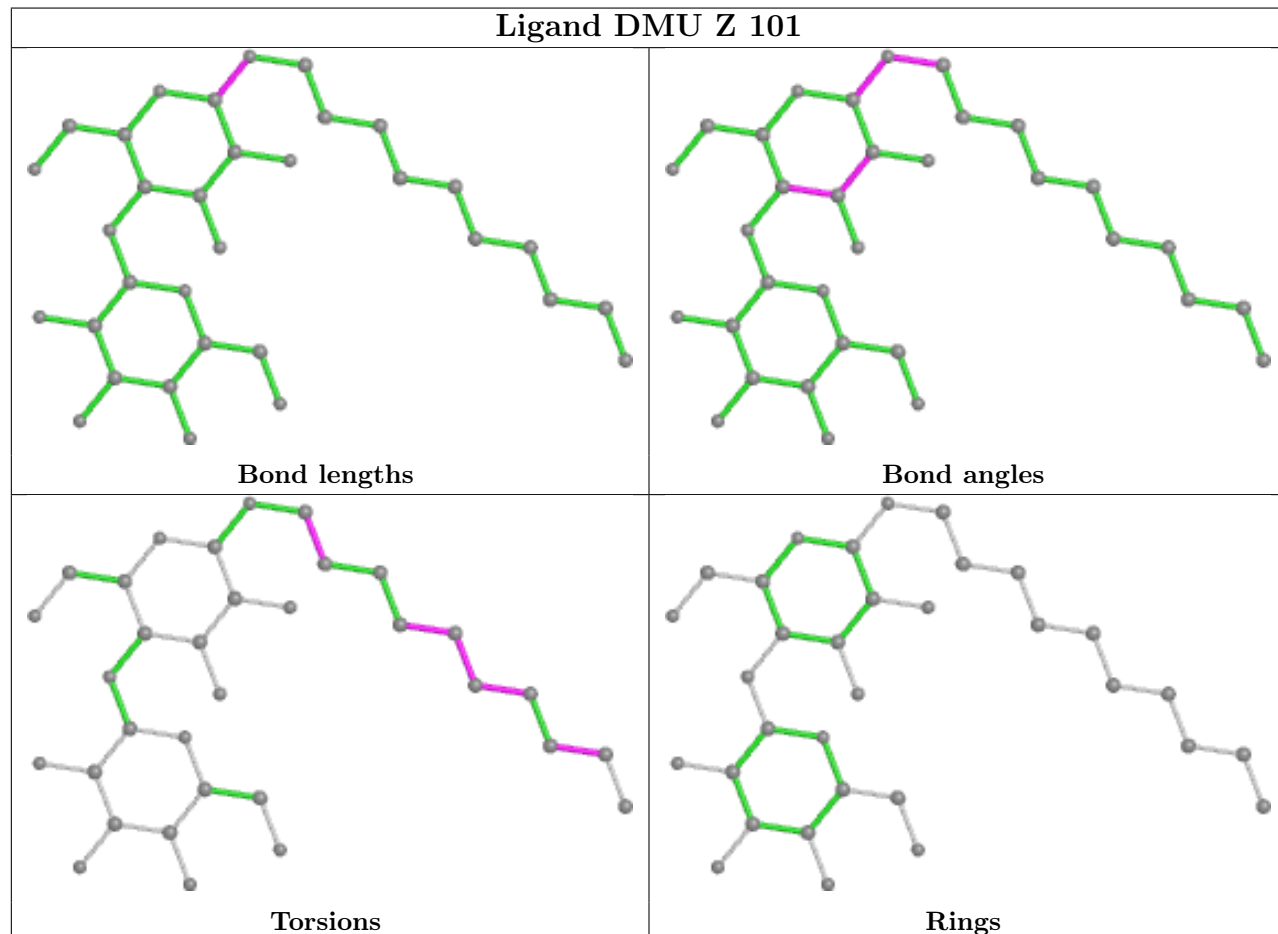
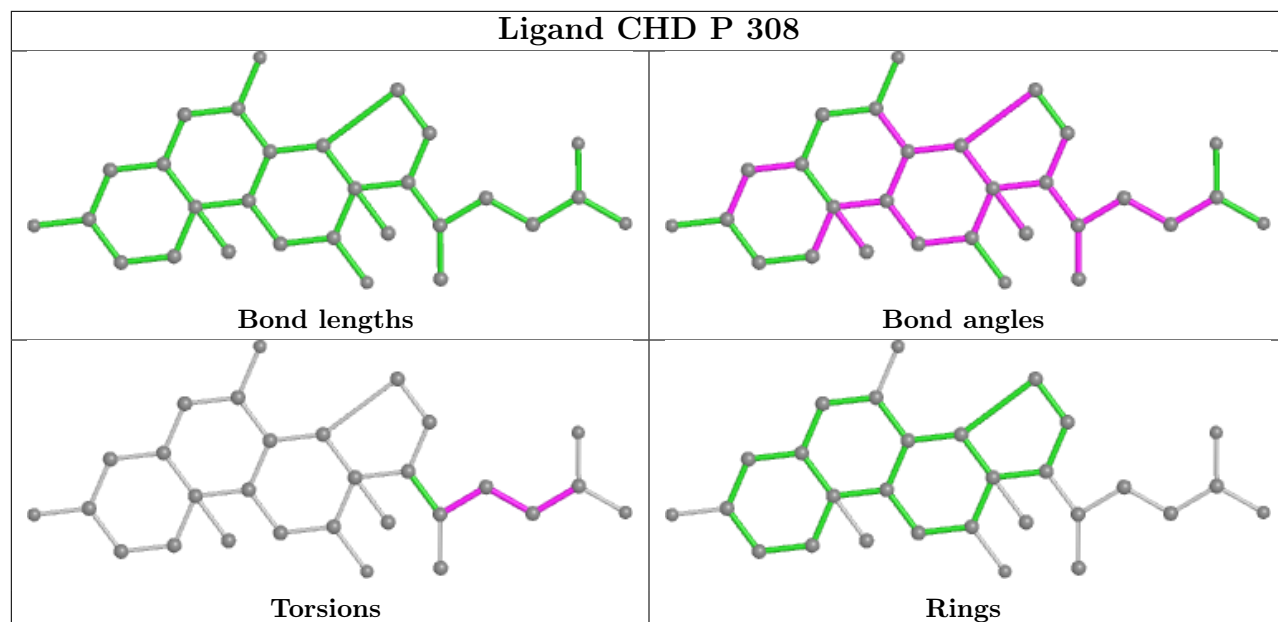


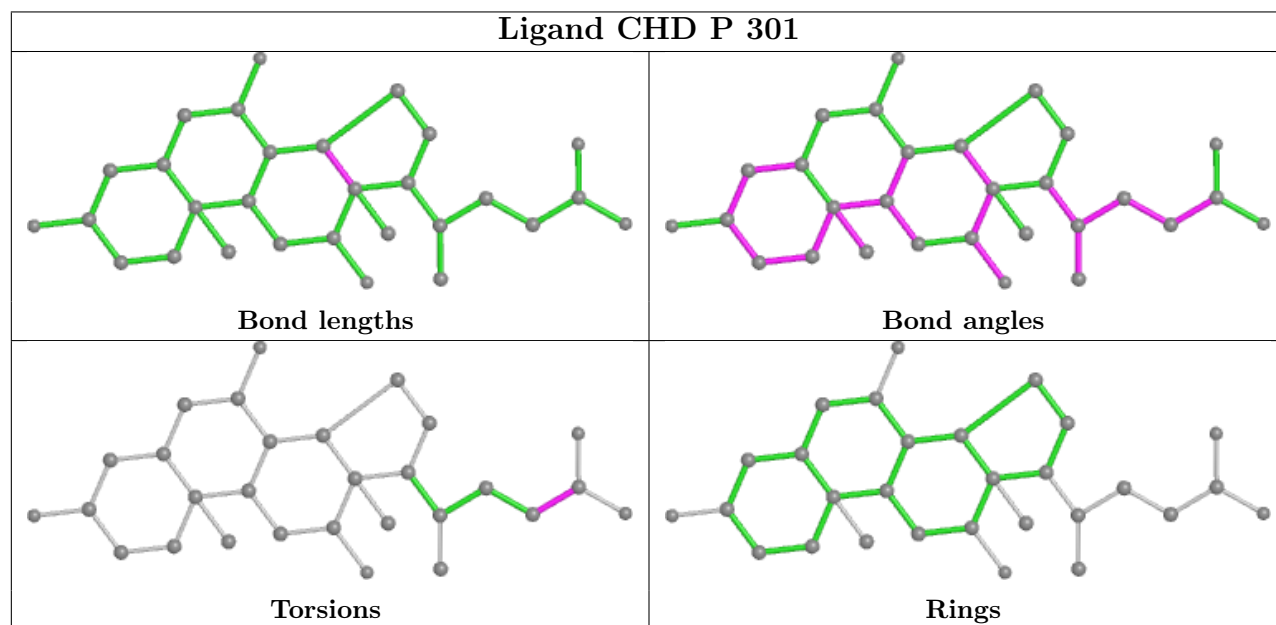
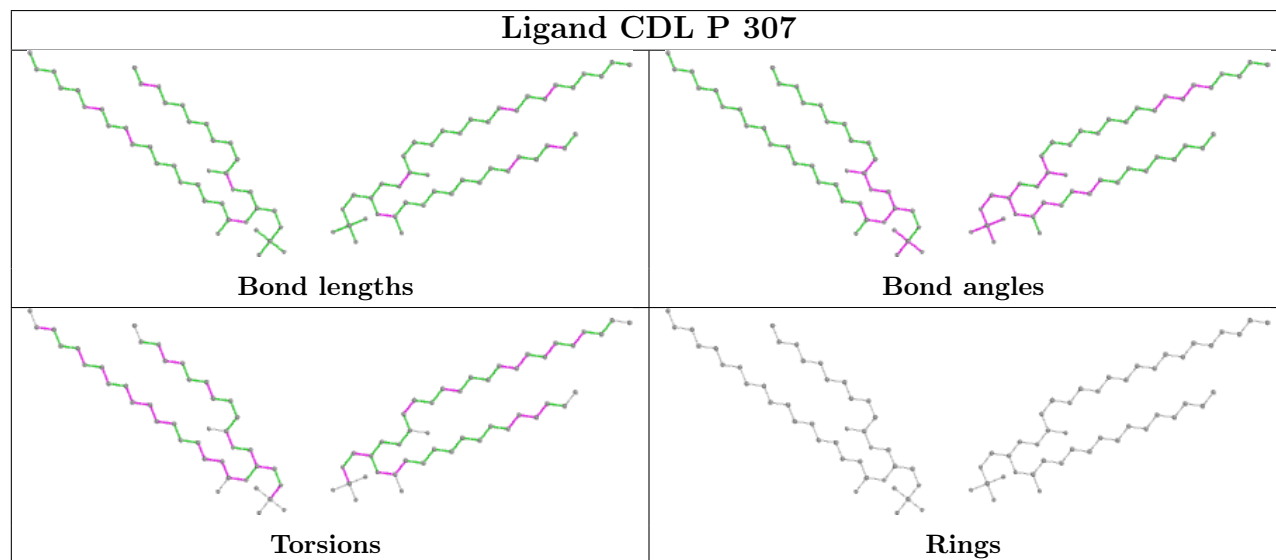
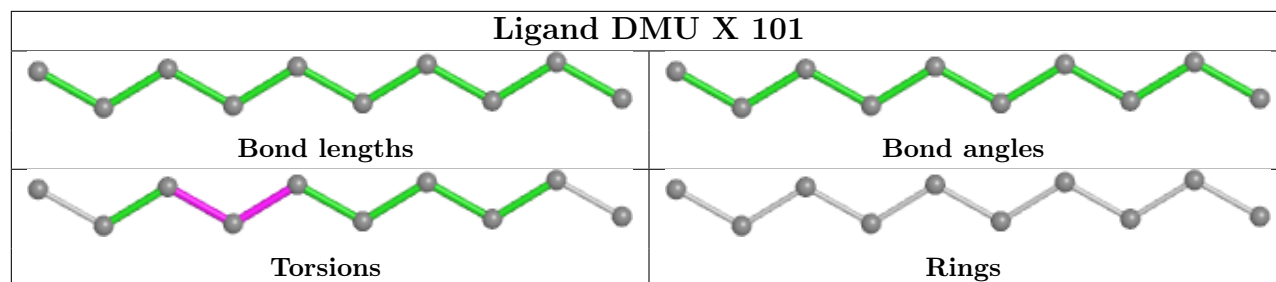




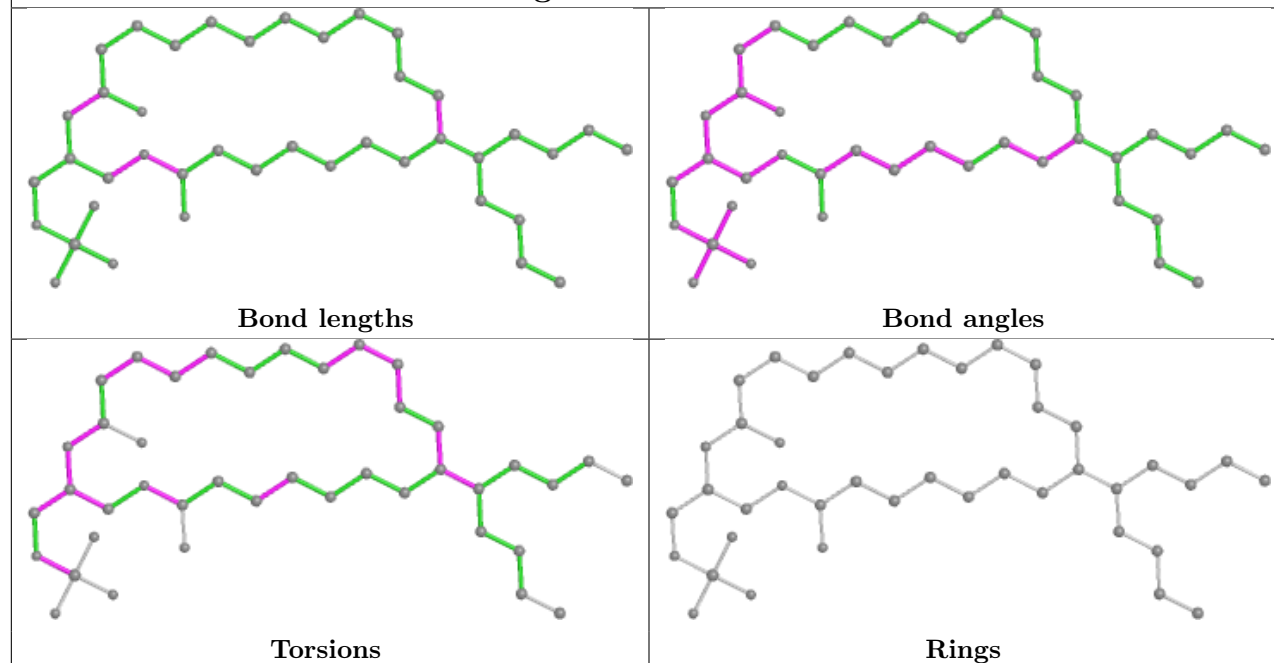




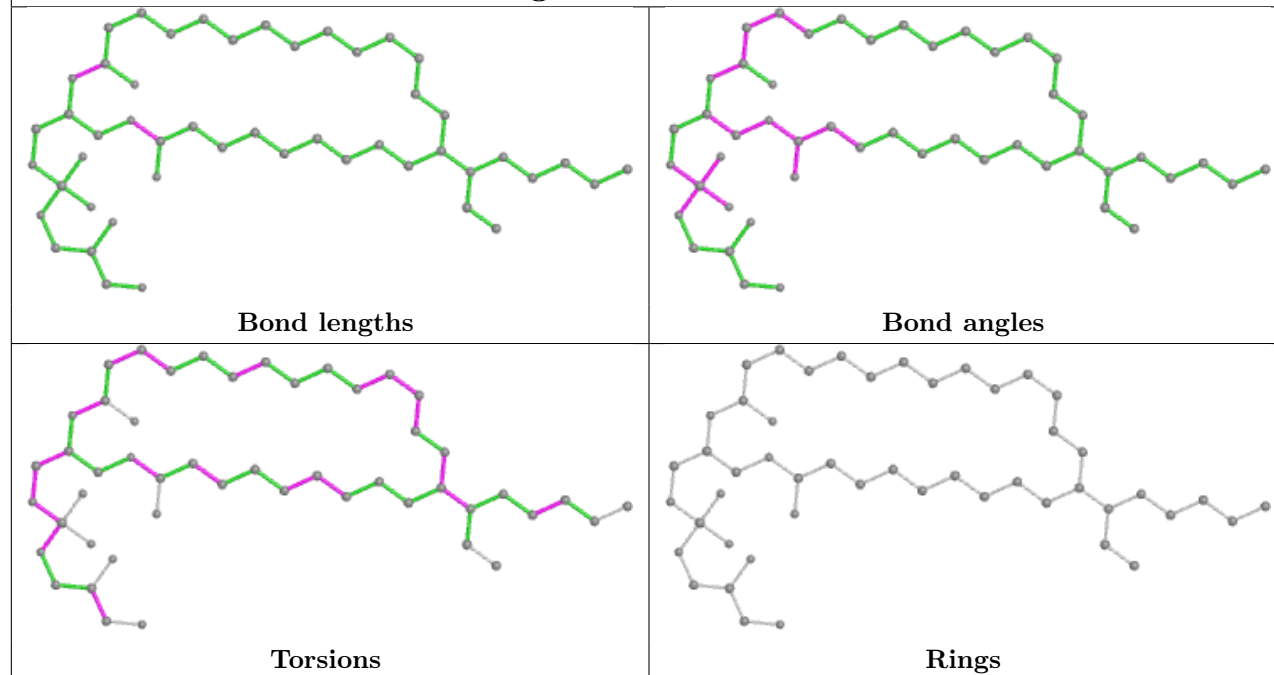


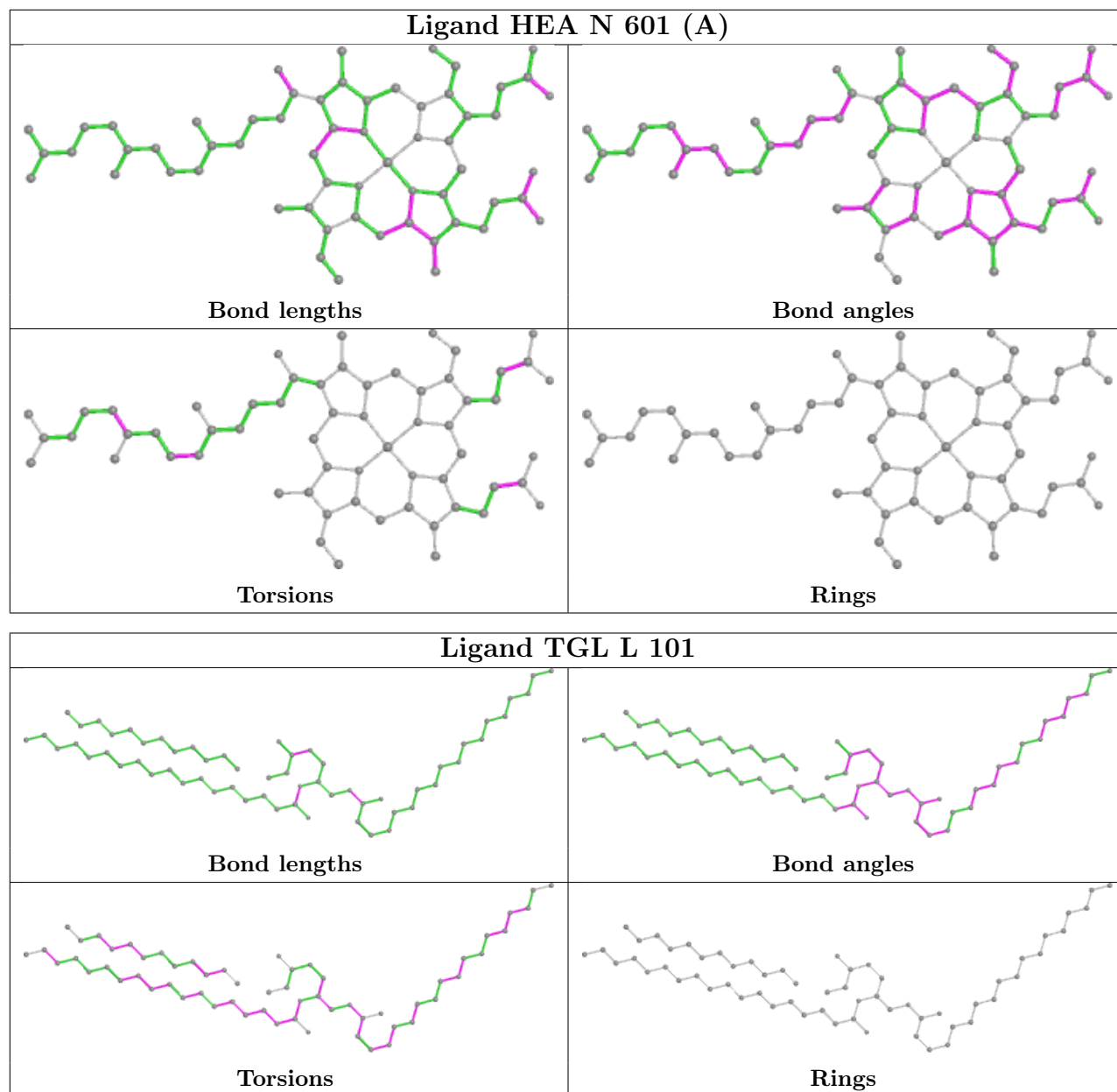


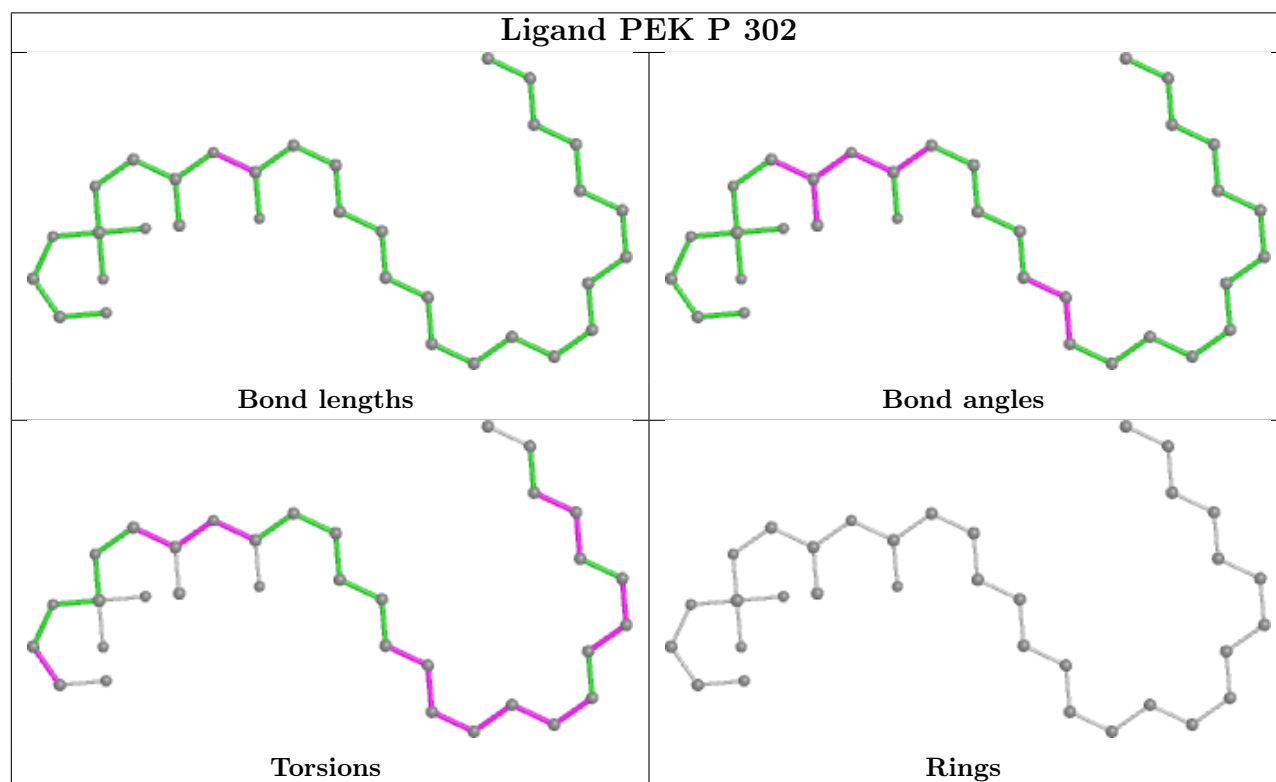
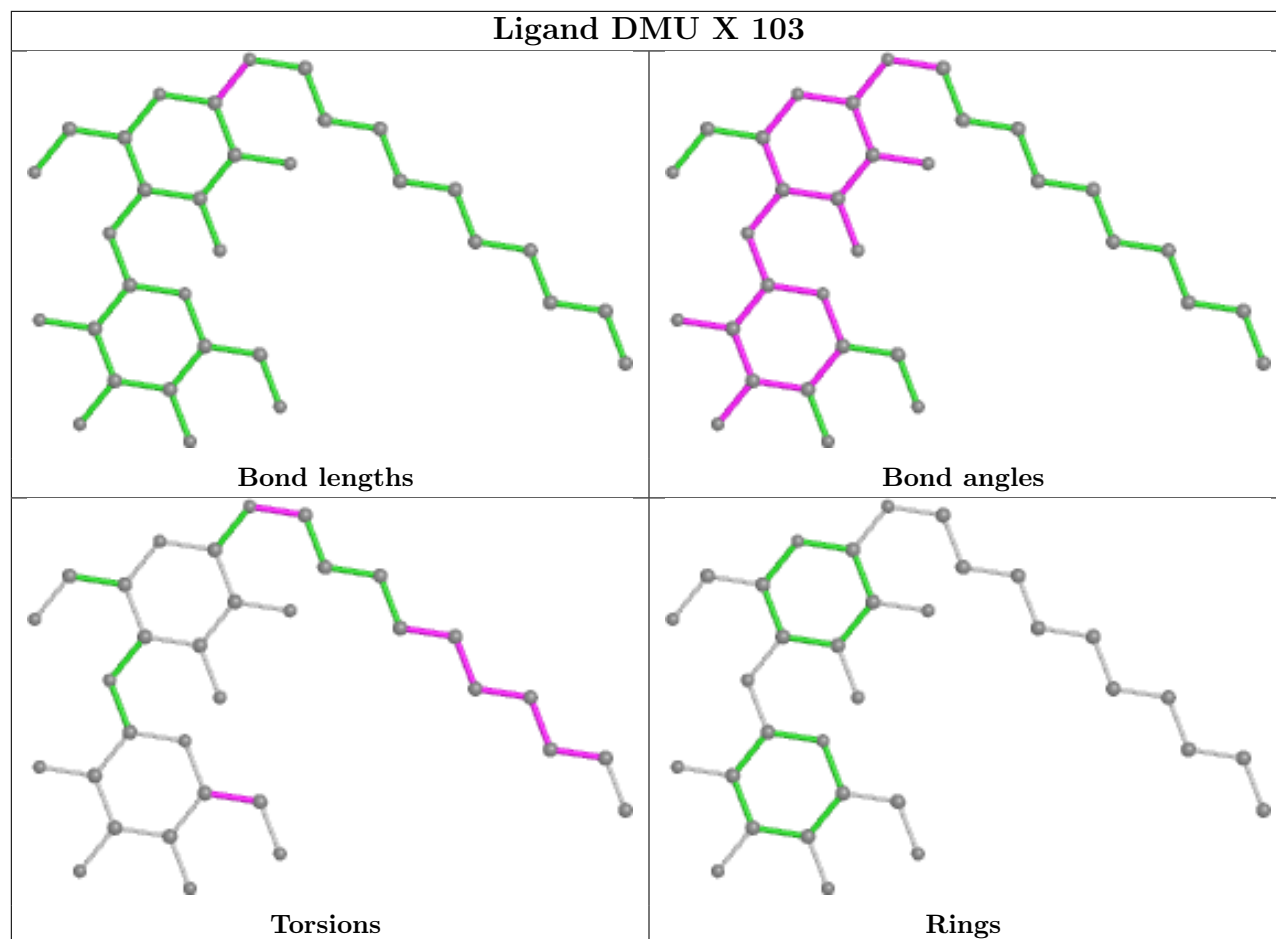
## Ligand PSC O 302

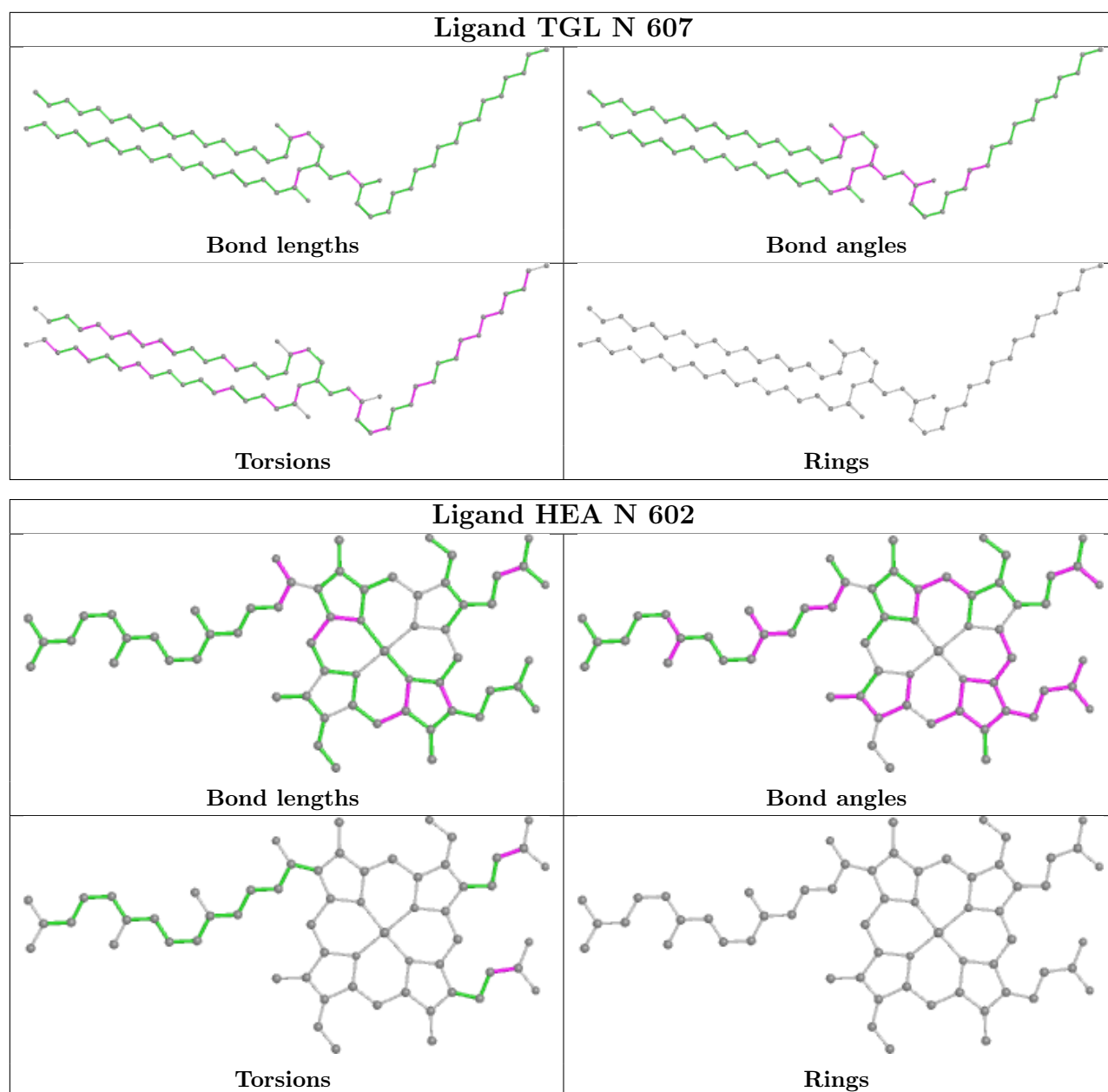


## Ligand PGV P 306









## 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%)	-0.35	0 100 100	18, 22, 29, 77	0
1	N	512/514 (99%)	-0.41	0 100 100	19, 25, 34, 77	0
2	B	226/227 (99%)	-0.40	0 100 100	20, 28, 49, 91	0
2	O	226/227 (99%)	-0.37	2 (0%) 84 84	25, 34, 62, 102	0
3	C	259/259 (100%)	-0.39	0 100 100	20, 26, 37, 75	0
3	P	259/259 (100%)	-0.40	1 (0%) 92 92	21, 27, 40, 85	0
4	D	144/144 (100%)	-0.54	0 100 100	23, 30, 51, 83	0
4	Q	138/144 (95%)	-0.05	1 (0%) 87 87	30, 42, 74, 101	0
5	E	105/105 (100%)	-0.51	1 (0%) 82 82	24, 30, 56, 134	0
5	R	105/105 (100%)	-0.42	2 (1%) 66 65	26, 37, 63, 149	0
6	F	94/94 (100%)	-0.24	3 (3%) 47 44	21, 31, 63, 144	0
6	S	94/94 (100%)	-0.22	4 (4%) 35 32	22, 32, 60, 141	0
7	G	83/84 (98%)	0.45	13 (15%) 2 1	24, 34, 122, 164	0
7	T	83/84 (98%)	0.50	14 (16%) 1 1	23, 37, 114, 175	0
8	H	79/79 (100%)	0.14	7 (8%) 9 8	26, 35, 101, 127	0
8	U	79/79 (100%)	0.04	6 (7%) 13 12	31, 40, 108, 151	0
9	I	72/73 (98%)	-0.10	2 (2%) 53 50	27, 41, 71, 88	0
9	V	72/73 (98%)	0.01	3 (4%) 36 33	27, 49, 77, 156	0
10	J	58/58 (100%)	-0.14	2 (3%) 45 42	25, 36, 70, 142	0
10	W	58/58 (100%)	-0.19	4 (6%) 16 15	28, 39, 77, 170	0
11	K	49/49 (100%)	-0.42	0 100 100	27, 35, 51, 58	0
11	X	49/49 (100%)	-0.17	1 (2%) 65 64	35, 46, 73, 99	0
12	L	46/46 (100%)	-0.36	0 100 100	23, 27, 58, 87	0
12	Y	46/46 (100%)	-0.34	1 (2%) 62 60	28, 35, 62, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/43 (100%)	-0.10	3 (6%) 16 15	24, 28, 67, 122	0
13	Z	43/43 (100%)	-0.05	3 (6%) 16 15	32, 38, 82, 225	0
All	All	3535/3550 (99%)	-0.28	73 (2%) 63 62	18, 29, 65, 225	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	12.3
7	T	3	ALA	10.8
6	S	1	ALA	10.6
8	H	8	ILE	9.7
6	F	2	SER	9.0
7	T	8	HIS	8.1
6	F	1	ALA	7.7
8	U	8	ILE	7.6
8	H	45	ALA	7.1
7	T	10	GLY	6.7
8	U	7	LYS	6.3
5	R	5	HIS	5.6
7	G	8	HIS	5.6
8	H	44	THR	5.5
8	H	46	LYS	5.1
7	T	2	SER	5.0
13	Z	42	LYS	4.9
7	G	42	ARG	4.8
13	M	42	LYS	4.7
8	H	47	GLY	4.6
6	S	94	HIS	4.4
9	I	37	PHE	4.3
9	V	37	PHE	4.3
10	W	58	LYS	4.2
12	Y	47	LYS	4.1
6	S	2	SER	4.1
7	T	36	TRP	3.9
7	G	9	GLY	3.9
7	G	36	TRP	3.8
7	T	42	ARG	3.8
10	J	58	LYS	3.8
2	O	113	TYR	3.7
5	R	109	VAL	3.7
10	J	1	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
13	Z	43	SER	3.7
7	G	2	SER	3.6
7	G	7	ASP	3.5
7	T	7	ASP	3.5
7	G	5	LYS	3.4
13	M	43	SER	3.4
10	W	57	HIS	3.3
9	I	25	PHE	3.3
10	W	1	PHE	3.3
9	V	2	THR	3.2
6	F	3	GLY	3.2
7	T	40	GLY	3.1
8	H	7	LYS	3.0
11	X	6	ALA	3.0
7	T	1	ALA	2.9
2	O	90	ILE	2.9
5	E	5	HIS	2.9
9	V	34	PHE	2.9
7	T	5	LYS	2.9
8	U	44	THR	2.9
4	Q	147	LYS	2.8
7	G	4	ALA	2.8
7	G	40	GLY	2.7
7	T	9	GLY	2.7
7	T	39	SER	2.7
7	G	6	GLY	2.6
8	U	45	ALA	2.6
7	G	84	LYS	2.6
13	M	40	TYR	2.4
7	T	6	GLY	2.3
7	T	84	LYS	2.3
6	S	93	PRO	2.2
10	W	52	TRP	2.2
8	H	48	GLY	2.2
8	U	47	GLY	2.2
3	P	3	HIS	2.1
8	U	10	ASN	2.1
13	Z	40	TYR	2.1
7	G	39	SER	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	0.34	0.34	188,205,220,225	0
7	TPO	G	11	11/12	0.69	0.30	61,113,143,248	0
7	TPO	T	11	11/12	0.75	0.31	66,125,184,270	0
9	SAC	I	1	9/10	0.78	0.28	94,112,142,154	0
1	FME	N	1	10/11	0.88	0.14	35,44,82,153	0
1	FME	A	1	10/11	0.94	0.10	34,43,84,159	0
2	FME	B	1	10/11	0.95	0.11	18,28,34,66	0
2	FME	O	1	10/11	0.98	0.08	32,35,40,95	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
27	DMU	O	303	33/33	0.25	0.34	64,83,90,92	0
20	EDO	A	622	4/4	0.30	0.36	59,70,82,92	0
27	DMU	N	610	17/33	0.35	0.34	68,77,89,90	0
20	EDO	E	211	4/4	0.35	0.18	52,60,66,70	0
20	EDO	K	102	4/4	0.37	0.17	60,65,68,71	0
20	EDO	Y	105	4/4	0.40	0.21	65,68,73,78	0
20	EDO	Q	203	4/4	0.45	0.17	62,62,66,70	0
20	EDO	L	106	4/4	0.45	0.14	49,65,74,75	0
20	EDO	V	103	4/4	0.46	0.30	66,79,84,85	0
20	EDO	D	212	4/4	0.46	0.22	59,68,73,78	0
20	EDO	N	623	4/4	0.47	0.28	72,78,84,92	0
27	DMU	C	310	33/33	0.47	0.26	63,80,88,93	0
20	EDO	D	207	4/4	0.52	0.23	66,68,71,76	0
27	DMU	P	310	33/33	0.53	0.30	39,78,84,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	D	213	4/4	0.57	0.19	74,75,78,80	0
20	EDO	J	102	4/4	0.57	0.12	61,69,75,83	0
20	EDO	D	221	4/4	0.58	0.27	50,66,71,82	0
20	EDO	O	308	4/4	0.60	0.24	62,66,67,68	0
25	PEK	C	302	49/53	0.60	0.37	46,72,108,213	0
27	DMU	T	102	21/33	0.61	0.21	56,74,95,104	0
27	DMU	X	103	33/33	0.61	0.32	66,80,88,96	0
20	EDO	A	637[A]	3/4	0.62	0.26	29,29,60,70	0
20	EDO	D	211	4/4	0.62	0.16	68,69,75,85	0
27	DMU	P	309	33/33	0.62	0.20	67,80,87,88	0
20	EDO	M	102	4/4	0.63	0.22	68,73,75,86	0
20	EDO	N	627	4/4	0.63	0.32	50,58,69,82	0
20	EDO	C	315	4/4	0.64	0.15	66,71,73,75	0
20	EDO	B	309	4/4	0.65	0.17	46,57,62,68	0
20	EDO	K	103	4/4	0.65	0.13	63,66,69,73	0
24	CHD	Y	102	29/29	0.66	0.34	72,81,86,89	0
20	EDO	N	615	4/4	0.66	0.22	61,63,64,70	0
27	DMU	C	309	22/33	0.66	0.19	53,68,95,98	0
20	EDO	N	633	4/4	0.66	0.29	45,45,45,50	0
27	DMU	X	102	22/33	0.66	0.33	75,83,87,98	0
20	EDO	B	320	4/4	0.66	0.17	63,64,76,91	0
20	EDO	P	316	4/4	0.67	0.14	41,60,70,80	0
25	PEK	C	304	53/53	0.68	0.24	35,67,94,199	0
25	PEK	P	302	33/53	0.68	0.23	48,69,94,166	0
25	PEK	P	304	52/53	0.68	0.27	36,67,109,179	0
26	CDL	T	101	92/100	0.69	0.26	46,72,99,186	0
20	EDO	U	101	4/4	0.69	0.37	45,54,59,81	0
19	PGV	N	608	42/51	0.69	0.27	43,66,100,164	0
20	EDO	H	101	4/4	0.69	0.17	58,63,69,71	0
20	EDO	Q	207	4/4	0.69	0.45	53,76,85,89	0
20	EDO	P	319	4/4	0.70	0.15	47,68,77,77	0
20	EDO	C	317	4/4	0.70	0.28	40,60,65,86	0
23	PSC	B	304	48/52	0.70	0.27	35,73,104,190	0
20	EDO	F	107	4/4	0.71	0.20	52,69,70,76	0
20	EDO	U	102	4/4	0.71	0.37	46,53,76,87	0
20	EDO	O	305	4/4	0.71	0.19	65,74,78,79	0
20	EDO	A	615	4/4	0.71	0.23	54,54,56,62	0
20	EDO	P	313	4/4	0.71	0.14	67,67,72,74	0
26	CDL	G	101	90/100	0.72	0.28	47,69,97,194	0
20	EDO	C	322	4/4	0.72	0.15	42,54,61,91	0
20	EDO	I	103	4/4	0.72	0.21	45,61,67,75	0
24	CHD	P	308	29/29	0.72	0.27	51,64,81,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
27	DMU	J	101	23/33	0.72	0.28	55,78,86,89	0
19	PGV	P	306	51/51	0.72	0.26	43,70,94,168	0
21	TGL	Y	101	60/63	0.73	0.22	39,62,90,109	0
20	EDO	D	204	4/4	0.73	0.30	45,63,84,94	0
19	PGV	C	306	51/51	0.73	0.24	39,69,92,152	0
20	EDO	P	327	4/4	0.73	0.16	50,63,64,69	0
27	DMU	X	101	10/33	0.74	0.16	57,77,79,81	0
20	EDO	R	204	4/4	0.74	0.16	38,59,60,65	0
21	TGL	Q	201	63/63	0.74	0.19	47,67,87,109	0
20	EDO	I	104	4/4	0.75	0.20	40,49,55,83	0
20	EDO	L	103	4/4	0.75	0.13	44,55,66,76	0
20	EDO	Q	208	4/4	0.75	0.17	50,68,70,75	0
20	EDO	N	614	4/4	0.76	0.12	62,64,73,87	0
20	EDO	O	309	4/4	0.76	0.12	48,53,60,69	0
20	EDO	D	214	4/4	0.77	0.50	48,50,64,77	0
21	TGL	B	302	62/63	0.77	0.18	36,62,84,94	0
20	EDO	B	319	4/4	0.77	0.21	59,64,73,89	0
27	DMU	X	104	12/33	0.77	0.21	72,78,81,86	0
23	PSC	O	302	43/52	0.78	0.20	34,67,94,178	0
20	EDO	C	320	4/4	0.78	0.12	44,60,64,71	0
20	EDO	C	314	4/4	0.78	0.10	55,57,67,69	0
20	EDO	A	630	4/4	0.79	0.24	38,42,72,79	0
20	EDO	B	311	4/4	0.79	0.27	49,60,76,83	0
20	EDO	Y	107	4/4	0.79	0.14	58,67,70,82	0
20	EDO	A	631	4/4	0.79	0.19	40,56,68,78	0
20	EDO	R	205	4/4	0.79	0.38	61,70,72,80	0
20	EDO	I	102	4/4	0.79	0.16	45,50,56,67	0
20	EDO	A	625	4/4	0.79	0.10	54,58,62,75	0
20	EDO	L	104	4/4	0.80	0.13	53,56,61,77	0
26	CDL	P	307	85/100	0.80	0.21	37,70,101,147	0
20	EDO	P	315	4/4	0.80	0.12	54,64,70,78	0
20	EDO	V	101	4/4	0.81	0.18	50,53,67,70	0
20	EDO	C	325	4/4	0.81	0.44	47,71,79,84	0
26	CDL	C	307	96/100	0.81	0.23	40,70,100,148	0
20	EDO	E	212	4/4	0.81	0.16	58,59,62,67	0
24	CHD	C	308	29/29	0.81	0.26	48,62,79,84	0
20	EDO	O	315	4/4	0.81	0.23	47,55,68,80	0
20	EDO	D	215	4/4	0.81	0.23	58,59,61,69	0
21	TGL	L	101	60/63	0.81	0.20	29,60,97,128	0
20	EDO	A	624	4/4	0.81	0.13	56,73,74,80	0
20	EDO	E	205	4/4	0.82	0.22	43,51,67,87	0
20	EDO	C	313	4/4	0.82	0.15	48,55,62,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	D	209	4/4	0.82	0.45	64,66,72,82	0
20	EDO	Y	104	4/4	0.82	0.10	59,65,70,72	0
20	EDO	M	103	4/4	0.82	0.22	44,49,66,67	0
20	EDO	S	111	4/4	0.82	0.28	40,52,67,76	0
20	EDO	M	105	4/4	0.82	0.11	54,58,64,78	0
20	EDO	N	629	4/4	0.83	0.13	64,70,72,75	0
20	EDO	T	107	4/4	0.83	0.34	48,51,66,80	0
20	EDO	A	634	4/4	0.83	0.17	41,51,56,63	0
20	EDO	Y	103	4/4	0.83	0.17	51,65,74,77	0
20	EDO	Q	206	4/4	0.84	0.34	49,69,79,82	0
20	EDO	D	202	4/4	0.84	0.13	47,57,64,76	0
20	EDO	D	203	4/4	0.84	0.28	44,50,53,98	0
20	EDO	E	208	4/4	0.84	0.23	50,51,83,89	0
20	EDO	E	209	4/4	0.84	0.13	34,52,58,59	0
20	EDO	B	312	4/4	0.84	0.31	41,44,46,64	0
20	EDO	C	323	4/4	0.84	0.09	56,59,65,75	0
19	PGV	A	607	47/51	0.84	0.21	26,61,97,181	0
20	EDO	G	105	4/4	0.84	0.12	47,61,74,76	0
20	EDO	N	630	4/4	0.84	0.12	57,63,68,79	0
20	EDO	D	218	4/4	0.84	0.34	43,48,57,89	0
20	EDO	L	105	4/4	0.85	0.10	55,63,73,78	0
20	EDO	S	112	4/4	0.85	0.20	45,52,70,86	0
20	EDO	S	114	4/4	0.85	0.17	55,65,65,68	0
20	EDO	T	105	4/4	0.85	0.21	51,60,72,75	0
20	EDO	I	105	4/4	0.85	0.21	60,65,68,73	0
21	TGL	N	607	63/63	0.85	0.19	42,68,82,87	0
20	EDO	L	102	4/4	0.85	0.23	41,43,54,70	0
20	EDO	D	201	4/4	0.85	0.09	50,63,65,66	0
20	EDO	A	621	4/4	0.85	0.22	39,51,55,62	0
20	EDO	O	311	4/4	0.85	0.23	79,80,83,86	0
20	EDO	S	103	4/4	0.85	0.14	39,41,54,54	0
20	EDO	H	104	4/4	0.86	0.26	37,42,56,62	0
20	EDO	J	103	4/4	0.86	0.23	48,52,53,84	0
20	EDO	K	104	4/4	0.86	0.10	61,68,75,91	0
20	EDO	P	312	4/4	0.86	0.10	50,55,68,69	0
20	EDO	N	624	4/4	0.86	0.33	55,57,57,83	0
20	EDO	U	103	4/4	0.86	0.31	49,52,68,75	0
20	EDO	K	105	4/4	0.86	0.17	60,75,75,83	0
27	DMU	Z	101	33/33	0.86	0.12	41,50,63,68	0
20	EDO	C	319	4/4	0.87	0.15	50,70,76,78	0
20	EDO	N	635	4/4	0.87	0.18	42,63,66,73	0
20	EDO	T	106	4/4	0.87	0.26	33,52,57,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
20	EDO	B	322	4/4	0.87	0.22	33,44,71,93	0
20	EDO	K	101	4/4	0.87	0.10	40,46,49,68	0
20	EDO	B	323	4/4	0.87	0.37	52,53,73,86	0
20	EDO	C	318	4/4	0.87	0.15	57,64,74,84	0
20	EDO	L	110	4/4	0.87	0.33	36,37,49,104	0
20	EDO	O	317	4/4	0.87	0.37	45,60,73,74	0
20	EDO	N	628	4/4	0.87	0.36	51,68,72,74	0
20	EDO	E	201	4/4	0.87	0.15	28,40,52,59	0
20	EDO	S	107	4/4	0.87	0.17	58,61,69,70	0
20	EDO	P	314	4/4	0.87	0.07	59,60,75,85	0
21	TGL	B	301	63/63	0.87	0.17	31,61,82,89	0
20	EDO	C	324	4/4	0.87	0.17	37,44,66,84	0
20	EDO	S	113	4/4	0.88	0.41	69,72,73,97	0
20	EDO	G	104	4/4	0.88	0.22	48,63,68,73	0
20	EDO	C	312	4/4	0.88	0.28	40,53,65,65	0
20	EDO	E	210	4/4	0.88	0.27	29,45,48,82	0
20	EDO	P	317	4/4	0.88	0.09	46,57,57,79	0
20	EDO	A	609	4/4	0.88	0.20	42,44,45,64	0
20	EDO	O	318	4/4	0.88	0.17	38,60,61,75	0
20	EDO	B	318	4/4	0.88	0.11	58,63,74,77	0
20	EDO	A	628	4/4	0.88	0.15	47,52,64,65	0
27	DMU	M	101	33/33	0.88	0.10	33,40,53,62	0
20	EDO	I	101	4/4	0.89	0.19	47,47,54,75	0
20	EDO	A	635	4/4	0.89	0.58	50,58,61,66	0
20	EDO	F	108	4/4	0.89	0.40	45,66,67,87	0
20	EDO	N	618	4/4	0.89	0.16	30,42,51,77	0
20	EDO	R	203	4/4	0.89	0.12	39,40,51,53	0
20	EDO	H	103	4/4	0.89	0.26	43,49,53,58	0
20	EDO	C	326	4/4	0.89	0.14	29,38,38,43	0
20	EDO	P	322	4/4	0.89	0.15	39,52,70,73	0
20	EDO	P	324	4/4	0.89	0.14	68,69,70,71	0
20	EDO	N	626	4/4	0.89	0.09	51,51,60,74	0
20	EDO	W	102	4/4	0.89	0.27	52,58,70,72	0
20	EDO	Q	202	4/4	0.89	0.23	58,67,68,68	0
20	EDO	P	326	4/4	0.90	0.31	35,54,67,73	0
20	EDO	O	312	4/4	0.90	0.22	39,45,58,85	0
20	EDO	O	304	4/4	0.90	0.17	53,55,71,86	0
20	EDO	S	108	4/4	0.90	0.36	43,68,69,77	0
20	EDO	O	316	4/4	0.90	0.49	49,64,85,98	0
20	EDO	C	316	4/4	0.90	0.06	64,68,68,81	0
20	EDO	D	217	4/4	0.90	0.19	46,56,67,92	0
20	EDO	P	321	4/4	0.90	0.32	51,64,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	T	103	4/4	0.90	0.09	46,70,82,83	0
20	EDO	A	610	4/4	0.90	0.20	56,58,63,70	0
20	EDO	D	219	4/4	0.90	0.18	34,59,69,79	0
20	EDO	N	619	4/4	0.91	0.25	56,61,73,76	0
20	EDO	O	313	4/4	0.91	0.41	42,62,72,86	0
20	EDO	N	620	4/4	0.91	0.22	38,70,78,90	0
20	EDO	N	634	4/4	0.91	0.17	57,58,71,82	0
20	EDO	A	636	4/4	0.91	0.26	36,39,48,56	0
20	EDO	H	102	4/4	0.91	0.27	43,53,76,81	0
20	EDO	E	206	4/4	0.91	0.25	53,56,64,65	0
20	EDO	E	207	4/4	0.91	0.16	58,60,69,72	0
20	EDO	I	106	4/4	0.91	0.36	41,54,72,76	0
20	EDO	A	623	4/4	0.91	0.27	36,73,79,80	0
20	EDO	R	202	4/4	0.92	0.18	53,58,71,81	0
20	EDO	O	314	4/4	0.92	0.31	38,54,61,77	0
20	EDO	A	613	4/4	0.92	0.10	25,25,28,31	0
20	EDO	D	208	4/4	0.92	0.20	36,52,85,98	0
20	EDO	B	313	4/4	0.92	0.26	47,56,57,60	0
20	EDO	L	111	4/4	0.92	0.14	38,62,63,74	0
20	EDO	D	210	4/4	0.92	0.30	63,66,88,89	0
20	EDO	S	109	4/4	0.92	0.41	43,50,54,69	0
24	CHD	C	301	29/29	0.92	0.07	23,27,32,33	0
20	EDO	W	101	4/4	0.92	0.12	47,63,63,65	0
20	EDO	C	321	4/4	0.92	0.19	36,56,61,71	0
20	EDO	B	317	4/4	0.92	0.30	46,57,74,87	0
20	EDO	M	106	4/4	0.92	0.29	38,40,61,78	0
20	EDO	D	206	4/4	0.92	0.12	48,48,53,74	0
20	EDO	Y	106	4/4	0.92	0.23	39,60,74,79	0
20	EDO	E	203	4/4	0.92	0.09	44,46,53,57	0
20	EDO	Z	102	4/4	0.92	0.22	66,71,77,83	0
20	EDO	N	622	4/4	0.93	0.19	36,61,75,79	0
20	EDO	D	220	4/4	0.93	0.21	36,50,64,75	0
20	EDO	P	325	4/4	0.93	0.23	41,53,75,93	0
20	EDO	L	108	4/4	0.93	0.15	35,53,72,83	0
20	EDO	N	625	4/4	0.93	0.08	43,58,61,66	0
20	EDO	N	611	4/4	0.93	0.10	35,38,38,42	0
20	EDO	W	103	4/4	0.93	0.22	44,48,72,88	0
20	EDO	A	620	4/4	0.93	0.17	37,60,63,67	0
20	EDO	Q	205	4/4	0.93	0.15	52,58,65,71	0
20	EDO	B	306	4/4	0.93	0.09	34,41,44,52	0
20	EDO	B	307	4/4	0.93	0.11	27,41,45,46	0
20	EDO	F	105	4/4	0.93	0.18	42,43,59,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	Y	108	4/4	0.93	0.12	55,56,62,64	0
20	EDO	N	632	4/4	0.93	0.17	33,41,45,65	0
20	EDO	P	320	4/4	0.93	0.08	56,70,71,85	0
20	EDO	M	104	4/4	0.93	0.10	55,59,66,68	0
29	PO4	U	104	5/5	0.93	0.34	54,56,61,69	0
25	PEK	P	303	53/53	0.94	0.13	27,48,81,88	0
20	EDO	L	107	4/4	0.94	0.17	48,53,74,85	0
20	EDO	B	316	4/4	0.94	0.11	48,53,53,78	0
20	EDO	Q	204	4/4	0.94	0.14	54,57,59,73	0
20	EDO	A	626	4/4	0.94	0.26	34,37,70,89	0
20	EDO	T	104	4/4	0.94	0.08	29,32,37,37	0
20	EDO	A	632	4/4	0.94	0.20	31,33,62,80	0
20	EDO	O	306	4/4	0.94	0.19	49,52,55,56	0
20	EDO	O	307	4/4	0.94	0.14	42,50,53,59	0
20	EDO	R	201	4/4	0.94	0.10	45,62,62,78	0
20	EDO	A	617	4/4	0.94	0.17	41,45,46,72	0
20	EDO	A	618	4/4	0.94	0.17	40,53,60,63	0
20	EDO	D	205	4/4	0.94	0.12	45,52,57,65	0
20	EDO	V	102	4/4	0.94	0.30	56,65,68,77	0
20	EDO	E	213	4/4	0.94	0.19	42,43,70,81	0
20	EDO	F	104	4/4	0.94	0.09	32,35,41,46	0
20	EDO	B	314	4/4	0.94	0.09	37,39,41,60	0
20	EDO	B	315	4/4	0.94	0.20	36,49,52,63	0
20	EDO	W	104	4/4	0.94	0.18	48,52,61,65	0
20	EDO	D	216	4/4	0.94	0.12	35,59,61,89	0
20	EDO	G	103	4/4	0.94	0.07	29,30,34,34	0
20	EDO	O	319	4/4	0.95	0.50	44,50,74,103	0
24	CHD	P	301	29/29	0.95	0.06	23,28,32,34	0
20	EDO	P	311	4/4	0.95	0.10	28,33,40,54	0
20	EDO	F	106	4/4	0.95	0.16	36,43,68,82	0
20	EDO	S	110	4/4	0.95	0.13	30,44,53,57	0
20	EDO	E	204	4/4	0.95	0.20	37,49,53,69	0
20	EDO	A	633	4/4	0.95	0.17	30,35,36,47	0
18	CYN	N	606	2/2	0.95	0.11	17,17,17,29	0
20	EDO	A	627	4/4	0.95	0.41	36,50,50,82	0
20	EDO	A	616	4/4	0.95	0.10	49,53,62,74	0
20	EDO	P	318	4/4	0.95	0.27	42,70,82,83	0
20	EDO	R	206	4/4	0.95	0.09	36,36,38,41	0
20	EDO	B	310	4/4	0.95	0.12	42,62,63,65	0
29	PO4	H	105	5/5	0.95	0.26	55,55,64,66	0
20	EDO	S	105	4/4	0.95	0.13	37,51,64,77	0
20	EDO	L	109	4/4	0.96	0.28	44,44,78,80	0

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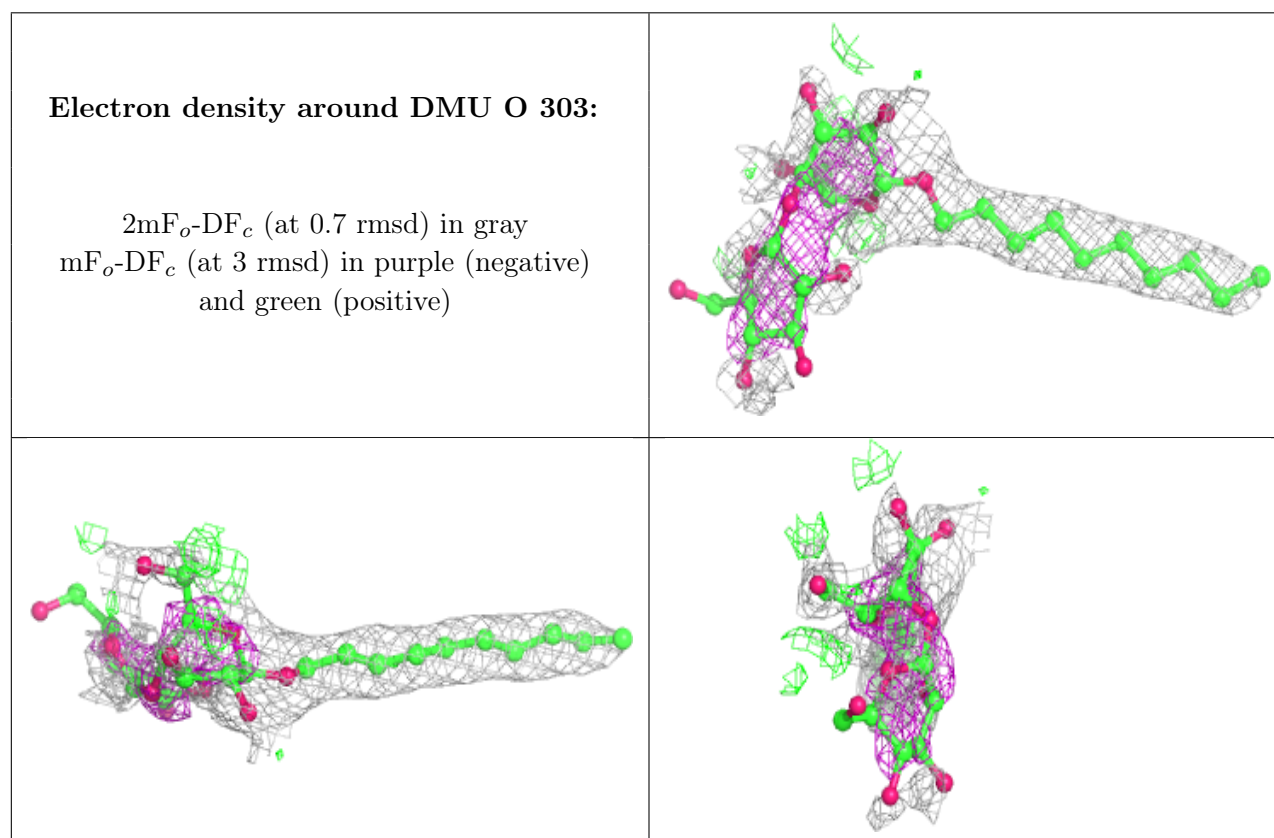
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	EDO	B	324	4/4	0.96	0.10	30,32,44,63	0
20	EDO	P	323	4/4	0.96	0.17	34,37,37,41	0
25	PEK	C	303	53/53	0.96	0.11	25,41,74,96	0
20	EDO	N	616	4/4	0.96	0.12	27,50,57,61	0
20	EDO	F	109	4/4	0.96	0.19	28,32,60,95	0
20	EDO	C	311	4/4	0.96	0.07	31,32,32,32	0
20	EDO	J	104	4/4	0.96	0.25	44,55,57,59	0
18	CYN	A	606	2/2	0.96	0.11	14,14,14,25	0
20	EDO	S	102	4/4	0.96	0.08	28,28,29,33	0
17	NA	N	605	1/1	0.96	0.09	29,29,29,29	0
20	EDO	A	619	4/4	0.96	0.11	29,37,44,72	0
20	EDO	A	612	4/4	0.96	0.12	37,38,42,48	0
20	EDO	N	612	4/4	0.96	0.10	23,26,28,30	0
20	EDO	A	629	4/4	0.97	0.18	28,36,37,75	0
20	EDO	N	621	4/4	0.97	0.13	34,34,51,61	0
20	EDO	N	613	4/4	0.97	0.10	36,38,41,42	0
20	EDO	O	310	4/4	0.97	0.06	29,30,31,32	0
19	PGV	N	609	51/51	0.97	0.10	23,31,61,77	0
20	EDO	S	104	4/4	0.97	0.07	32,34,39,41	0
19	PGV	P	305	51/51	0.97	0.10	21,30,73,85	0
20	EDO	B	321	4/4	0.97	0.22	30,53,63,69	0
20	EDO	Q	209	4/4	0.97	0.14	29,48,53,63	0
24	CHD	B	305	29/29	0.97	0.06	21,25,32,40	0
20	EDO	N	617	4/4	0.97	0.06	26,26,28,30	0
19	PGV	C	305	50/51	0.97	0.10	21,27,74,83	0
24	CHD	G	102	29/29	0.97	0.08	21,25,29,37	0
20	EDO	E	202	4/4	0.97	0.07	34,37,40,41	0
20	EDO	S	106	4/4	0.98	0.07	23,23,23,23	0
14	HEA	A	601[A]	60/60	0.98	0.08	17,19,31,39	9
20	EDO	A	614	4/4	0.98	0.12	28,36,74,76	0
14	HEA	A	601[B]	60/60	0.98	0.08	17,19,32,44	9
20	EDO	B	308	4/4	0.98	0.08	22,24,24,26	0
14	HEA	A	602	60/60	0.98	0.08	16,18,24,30	0
14	HEA	N	601[A]	60/60	0.98	0.08	21,24,35,43	9
19	PGV	A	608	51/51	0.98	0.10	21,28,64,68	0
20	EDO	F	102	4/4	0.98	0.11	28,29,30,32	0
14	HEA	N	601[B]	60/60	0.98	0.08	21,24,35,38	9
14	HEA	N	602	60/60	0.98	0.09	19,21,27,29	0
20	EDO	N	631	4/4	0.98	0.17	28,29,69,73	0
20	EDO	F	103	4/4	0.99	0.08	22,23,23,23	0
16	MG	N	604	1/1	0.99	0.08	25,25,25,25	0
17	NA	A	605	1/1	0.99	0.06	23,23,23,23	0

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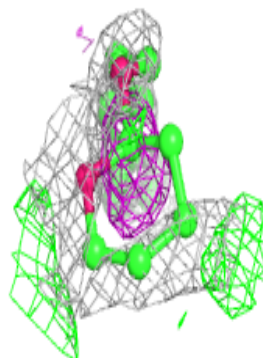
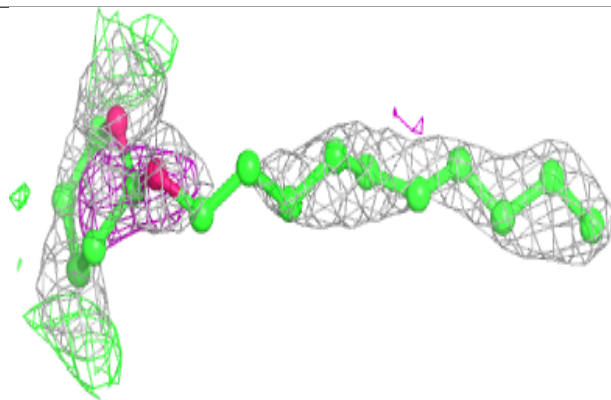
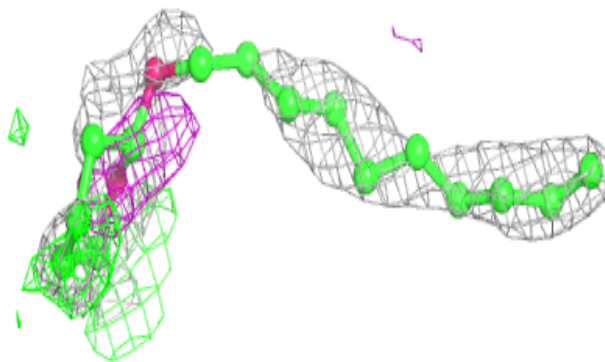
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	CU	N	603	1/1	0.99	0.13	21,21,21,21	0
20	EDO	A	611	4/4	0.99	0.08	21,22,24,25	0
16	MG	A	604	1/1	0.99	0.06	20,20,20,20	0
22	CUA	O	301	2/2	0.99	0.10	26,26,26,26	0
28	ZN	F	101	1/1	1.00	0.10	25,25,25,25	0
28	ZN	S	101	1/1	1.00	0.09	25,25,25,25	0
15	CU	A	603	1/1	1.00	0.13	19,19,19,19	0
22	CUA	B	303	2/2	1.00	0.13	21,21,21,21	0

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

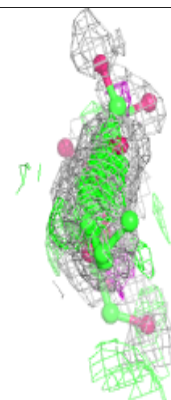
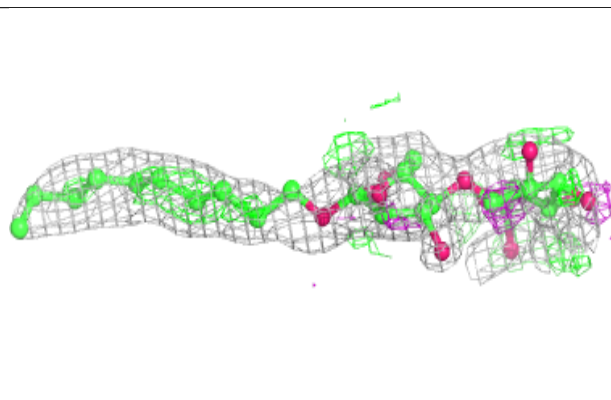
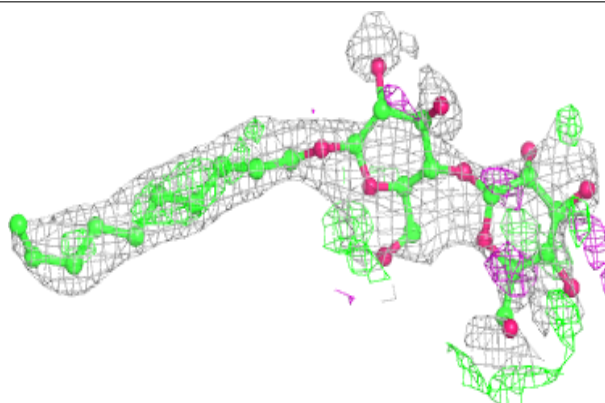


**Electron density around DMU N 610:**

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

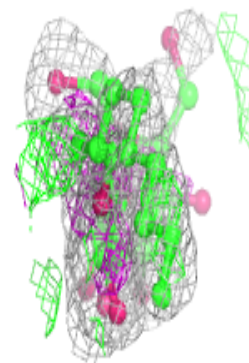
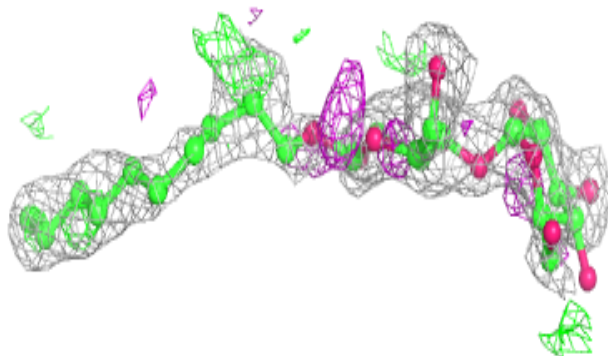
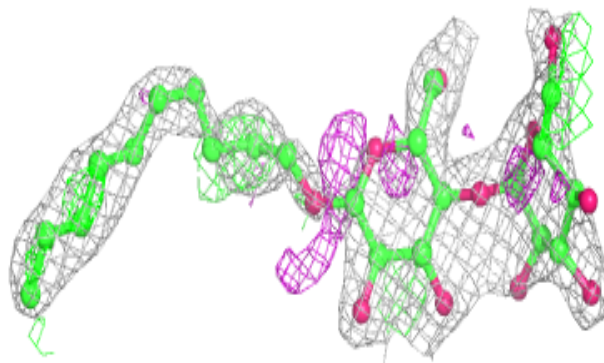
**Electron density around DMU C 310:**

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

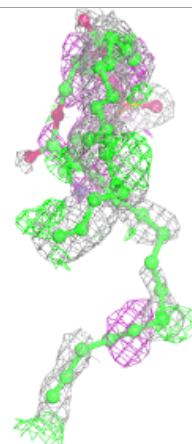
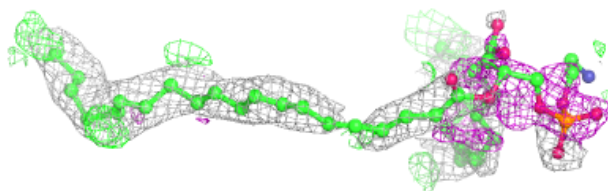
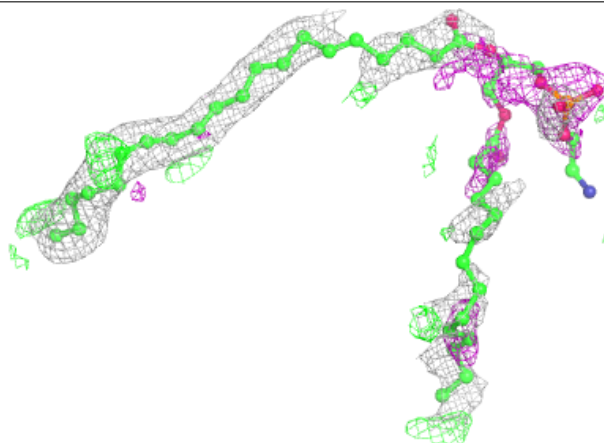


**Electron density around DMU P 310:**

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

**Electron density around PEK C 302:**

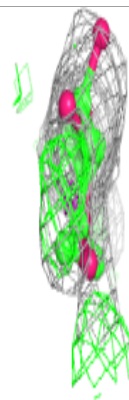
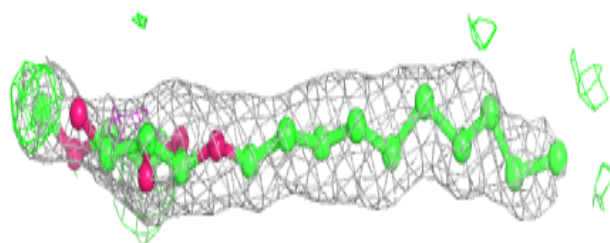
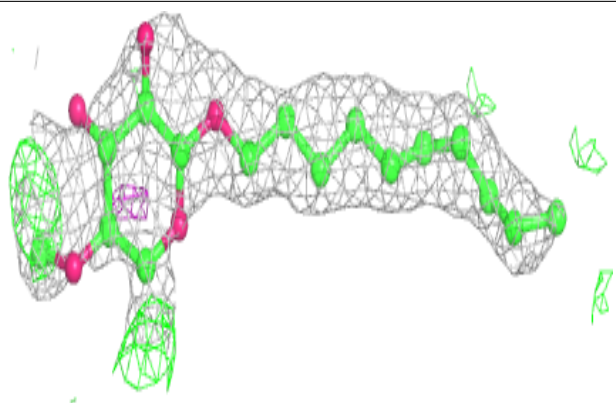
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



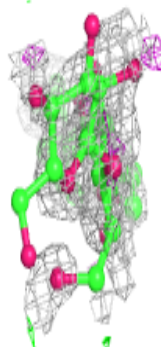
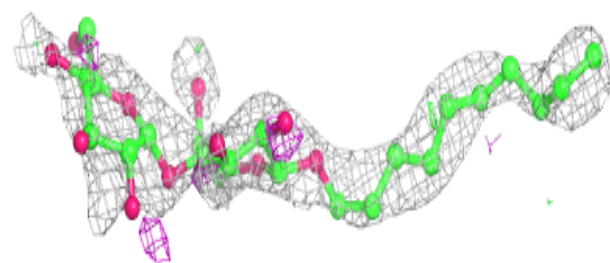
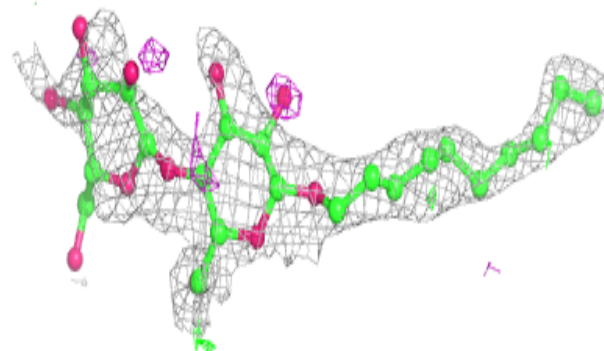


**Electron density around DMU T 102:**

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

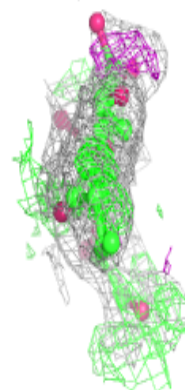
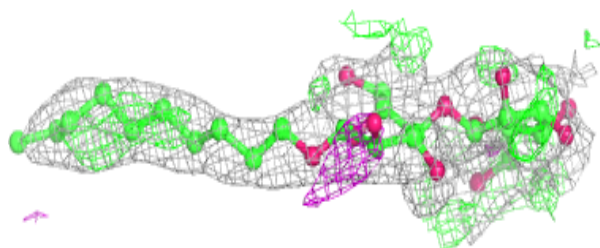
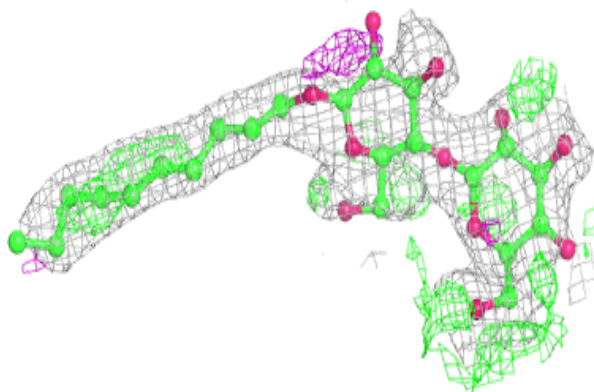
**Electron density around DMU X 103:**

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

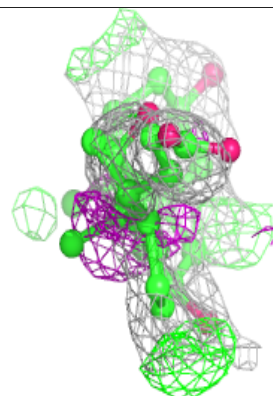
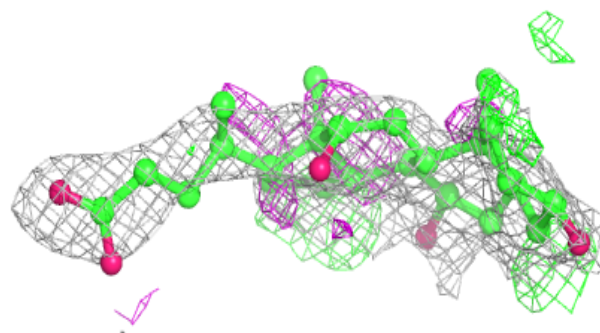
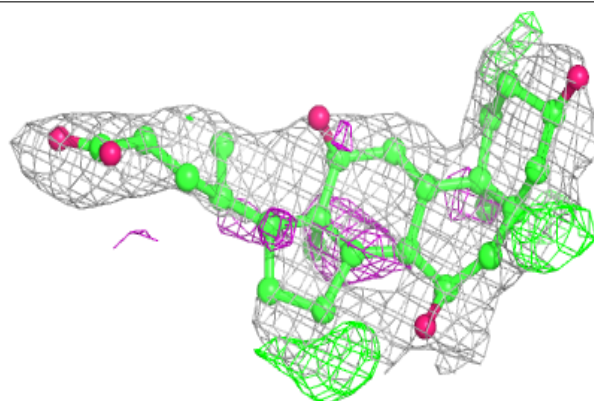


**Electron density around DMU P 309:**

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

**Electron density around CHD Y 102:**

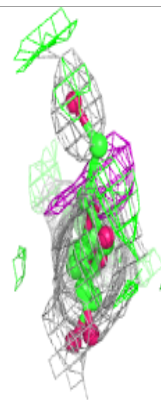
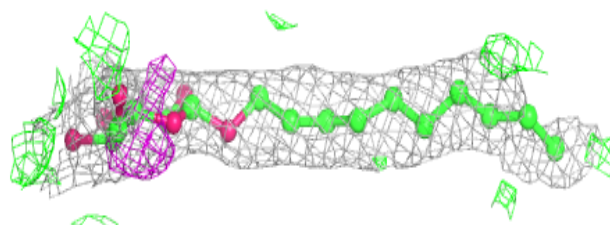
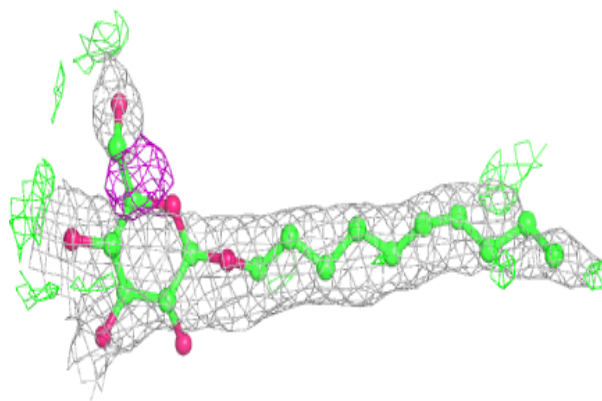
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



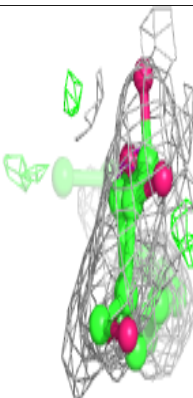
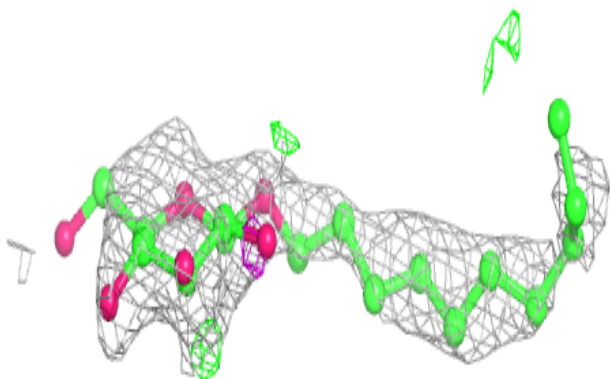
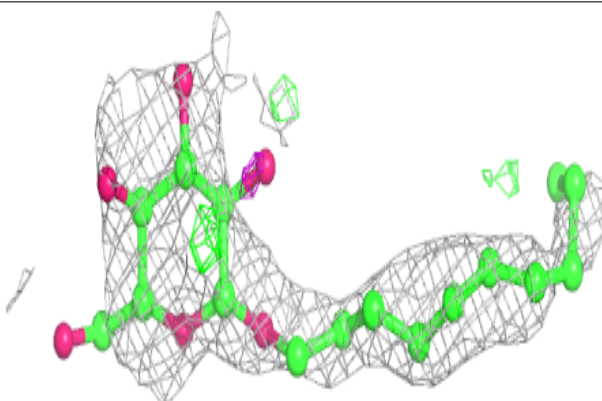


**Electron density around DMU C 309:**

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

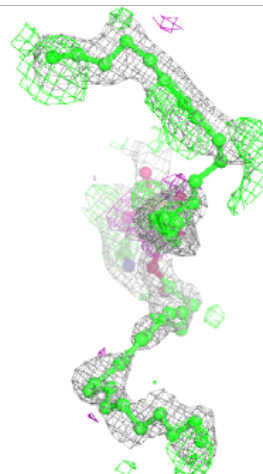
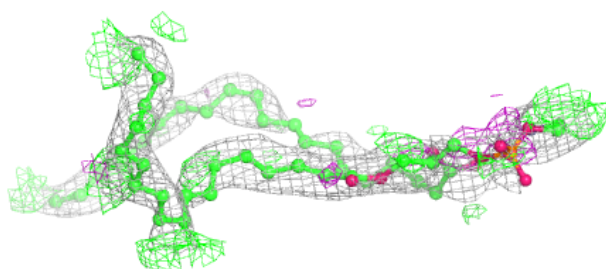
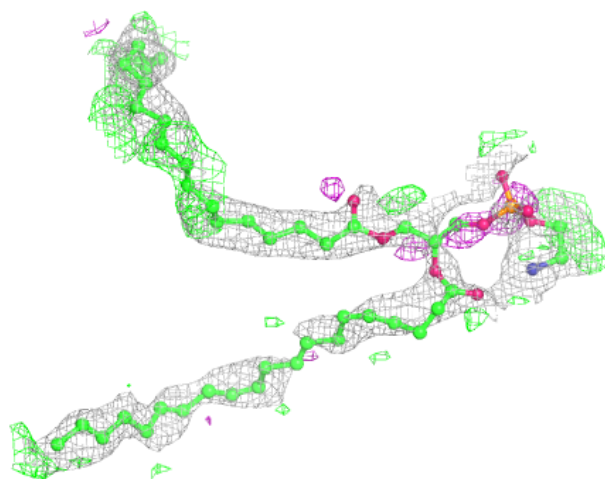
**Electron density around DMU X 102:**

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



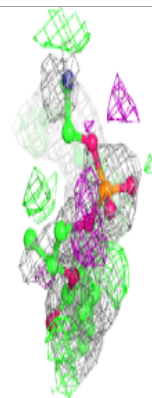
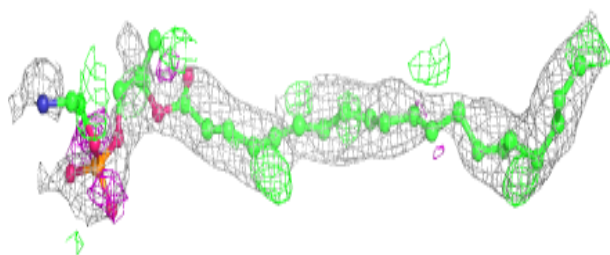
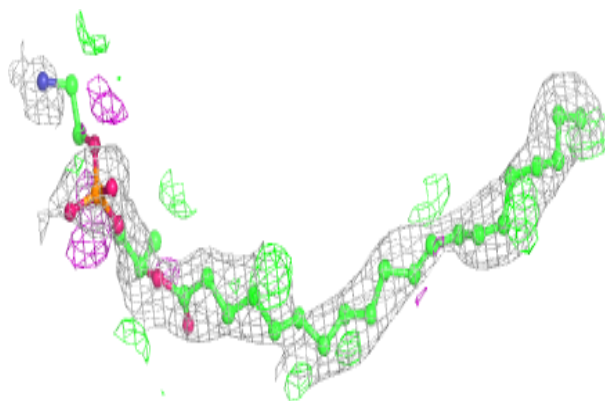
**Electron density around PEK C 304:**

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

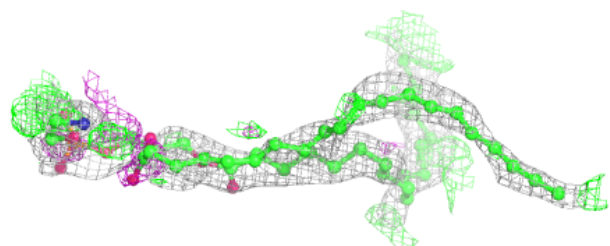
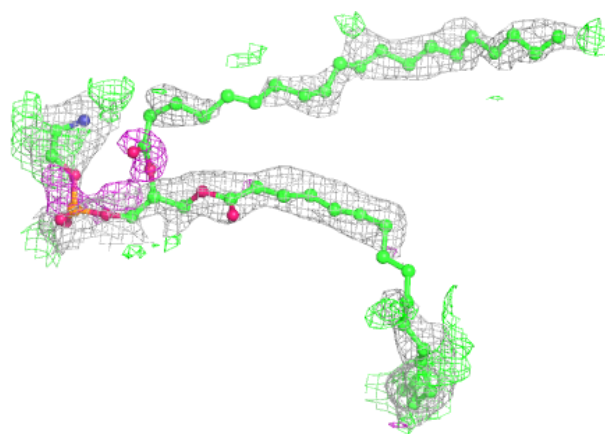


**Electron density around PEK P 302:**

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

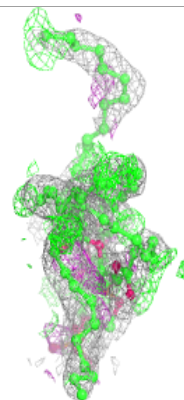
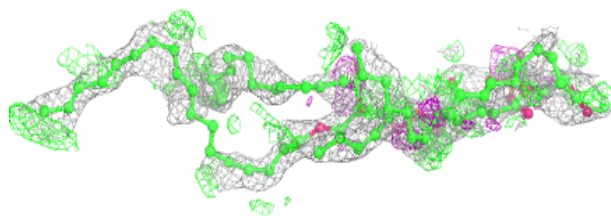
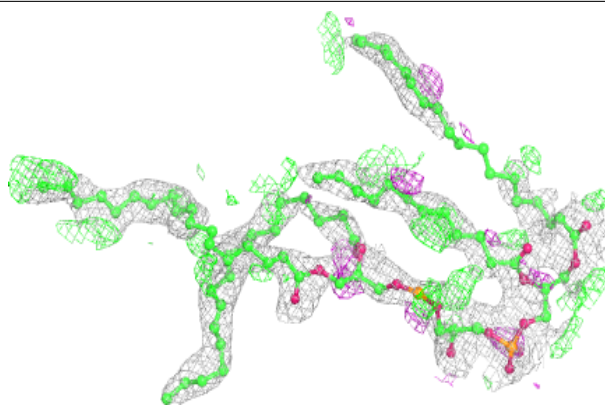
**Electron density around PEK P 304:**

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

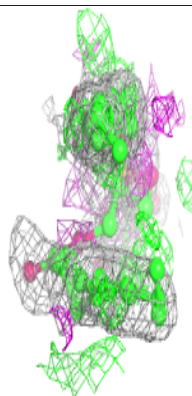
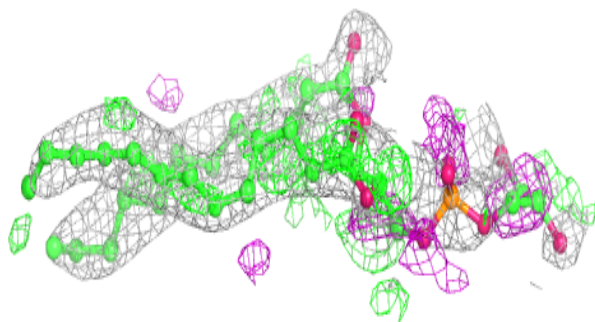
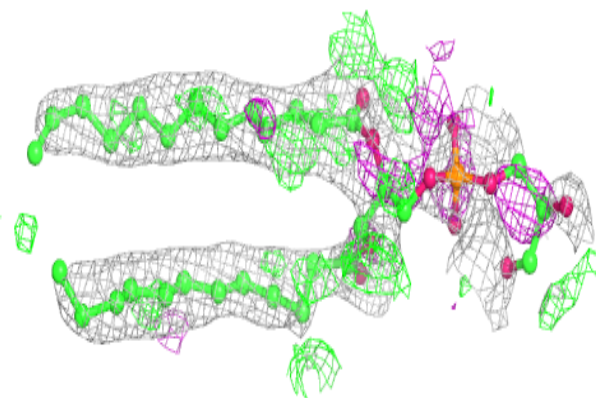


**Electron density around CDL T 101:**

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

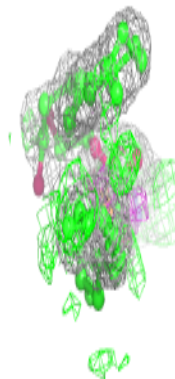
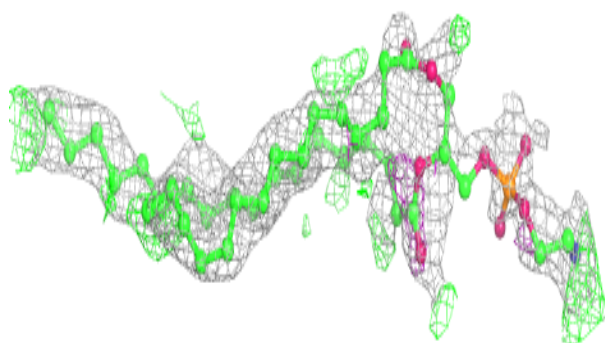
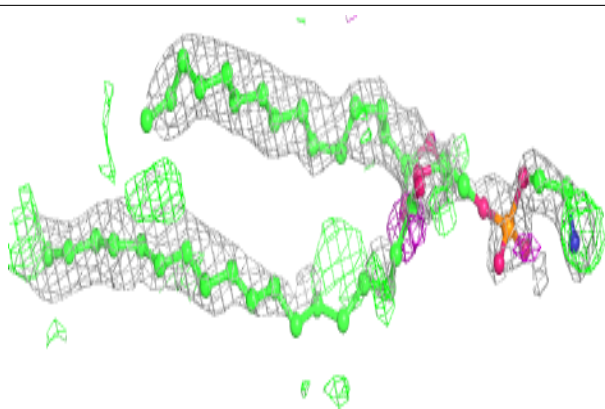
**Electron density around PGV N 608:**

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

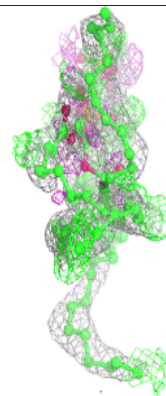
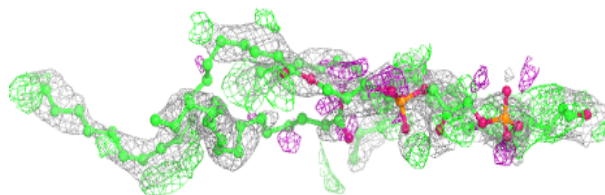
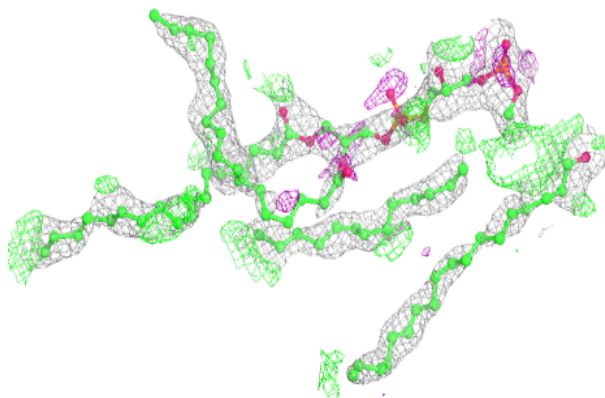


**Electron density around PSC B 304:**

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

**Electron density around CDL G 101:**

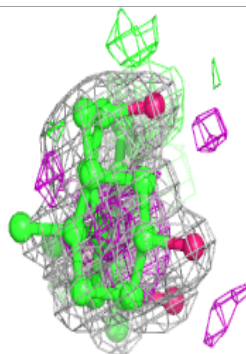
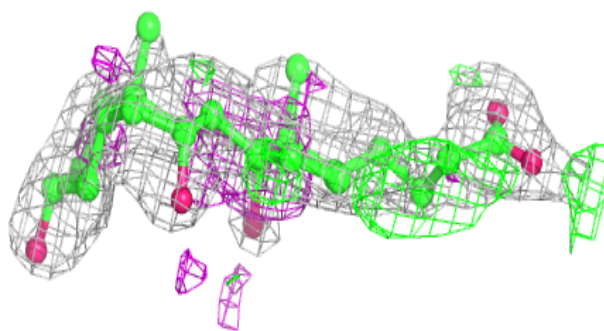
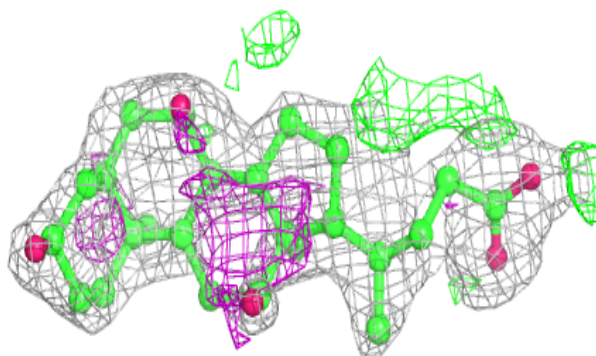
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



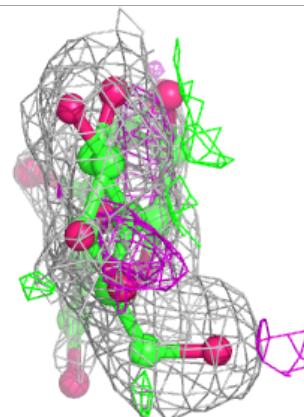
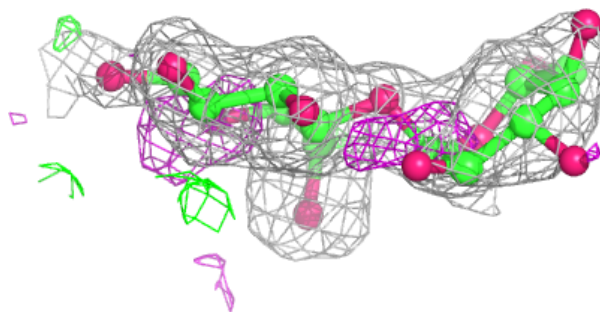
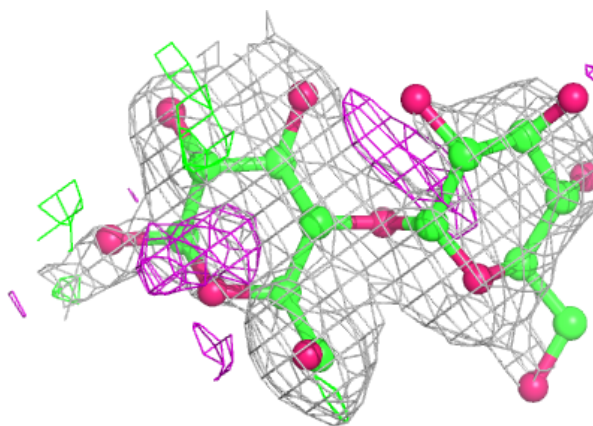


**Electron density around CHD P 308:**

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

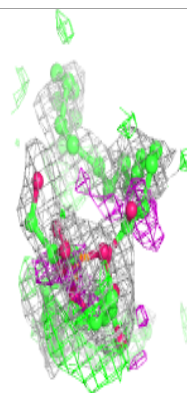
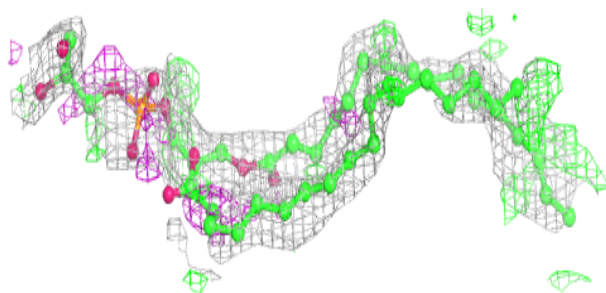
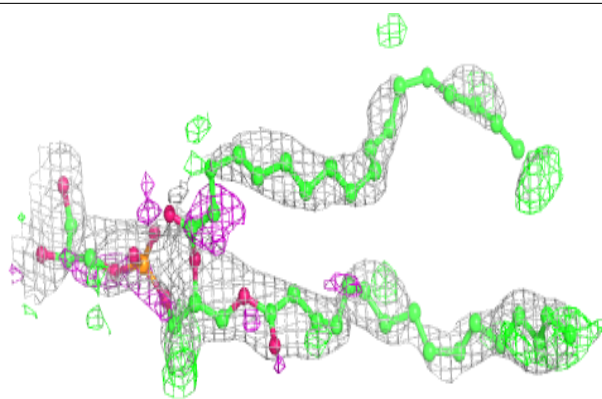
**Electron density around DMU J 101:**

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



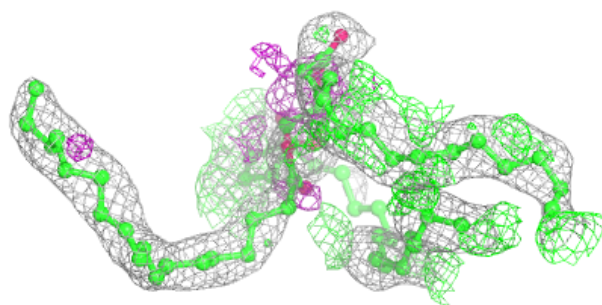
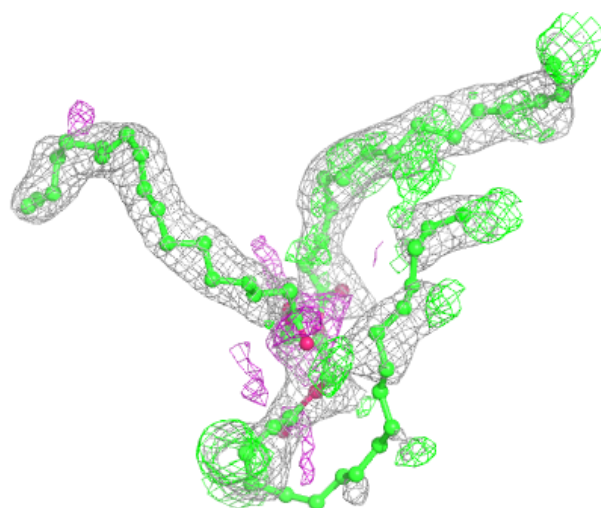
**Electron density around PGV P 306:**

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



**Electron density around TGL Y 101:**

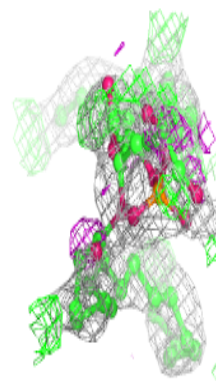
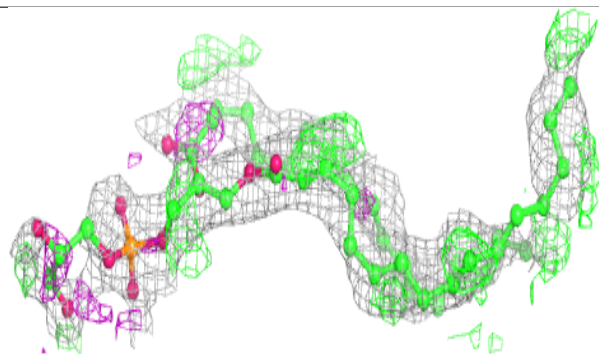
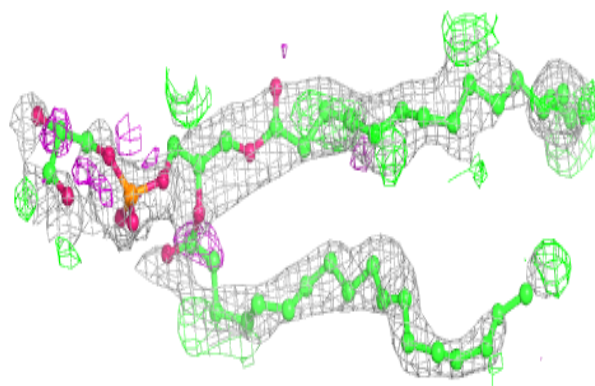
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



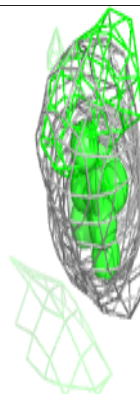
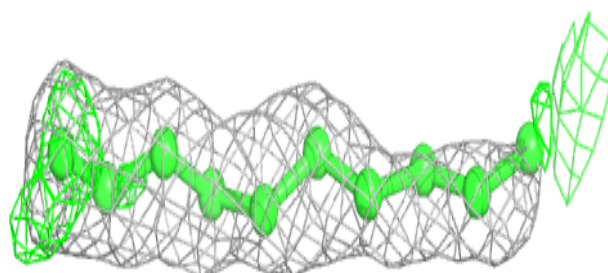
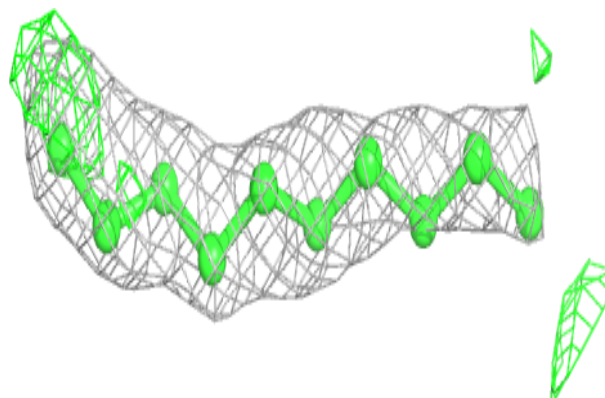


**Electron density around PGV C 306:**

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

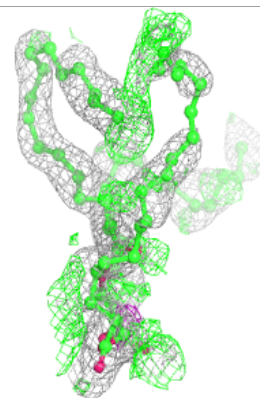
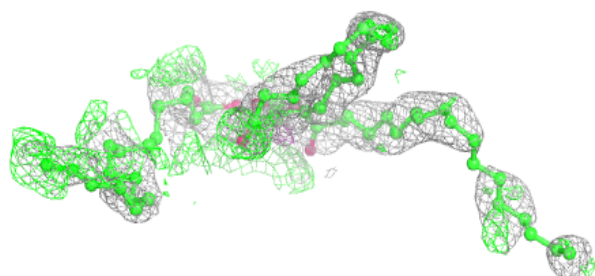
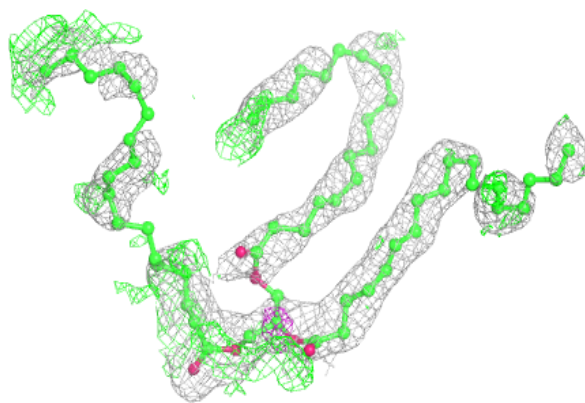
**Electron density around DMU X 101:**

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

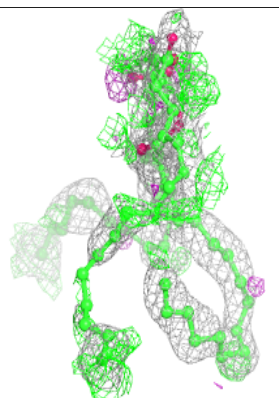
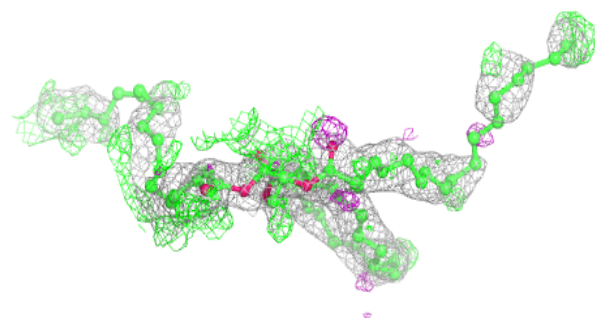
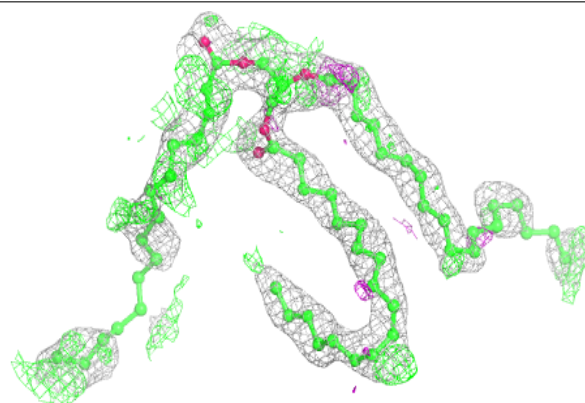


**Electron density around TGL Q 201:**

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

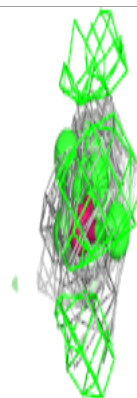
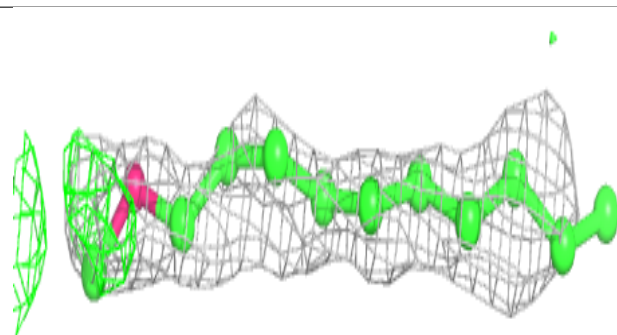
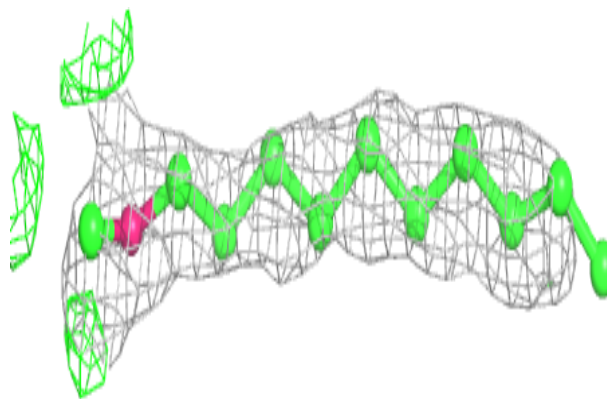
**Electron density around TGL B 302:**

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

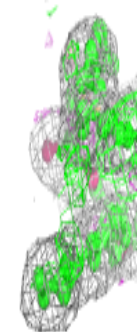
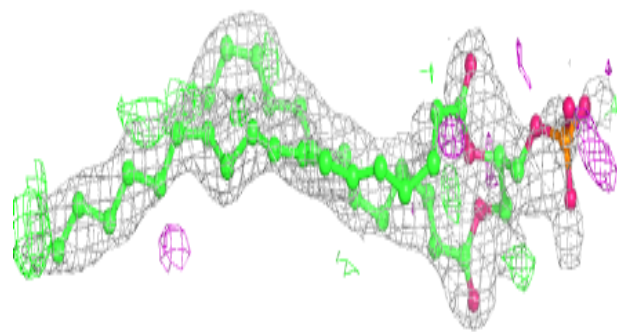
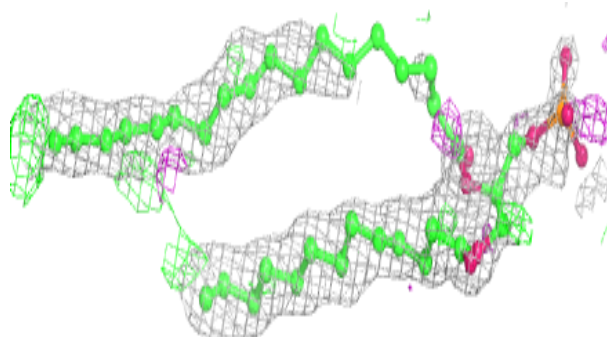


**Electron density around DMU X 104:**

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

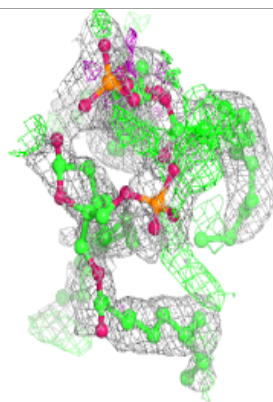
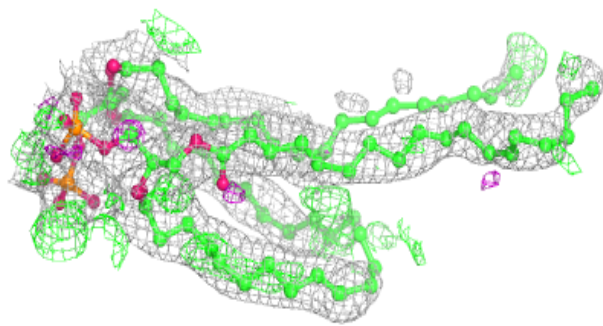
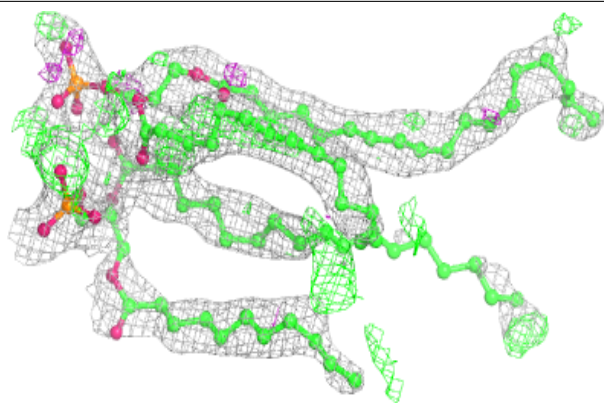
**Electron density around PSC O 302:**

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



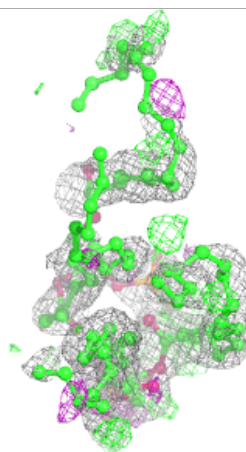
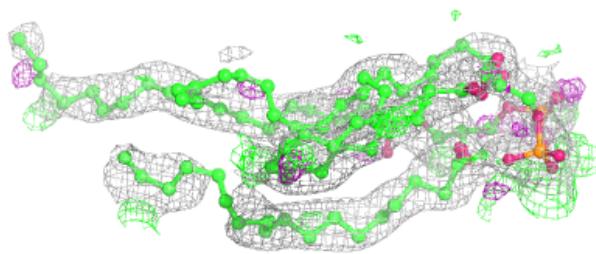
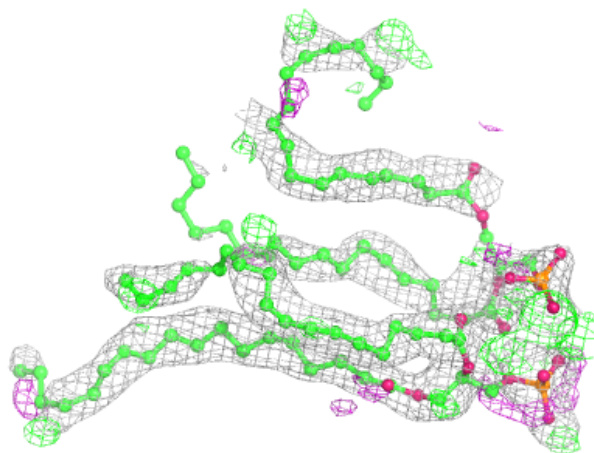
**Electron density around CDL P 307:**

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



**Electron density around CDL C 307:**

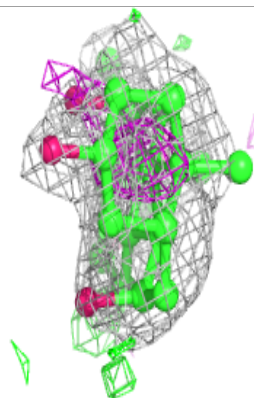
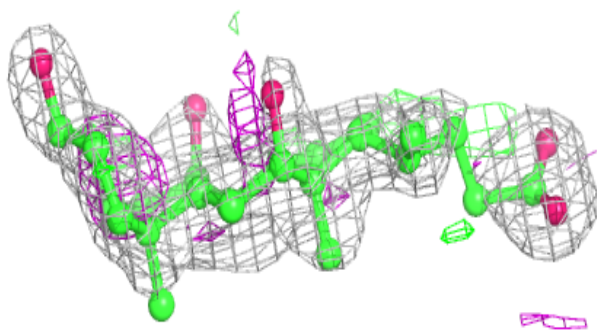
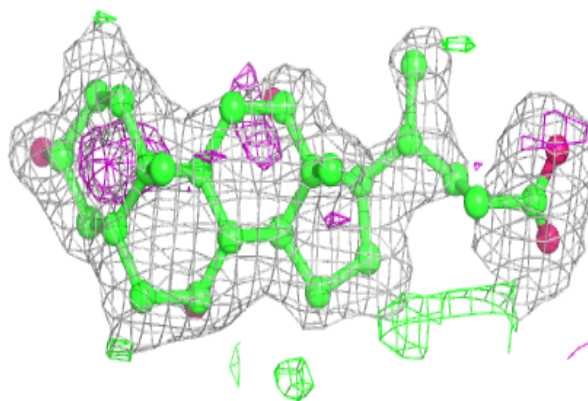
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





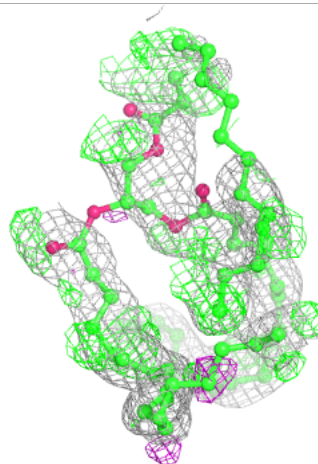
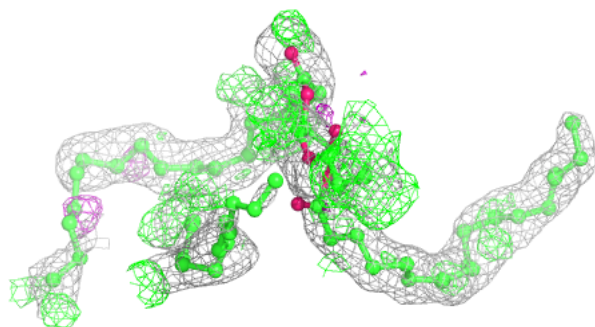
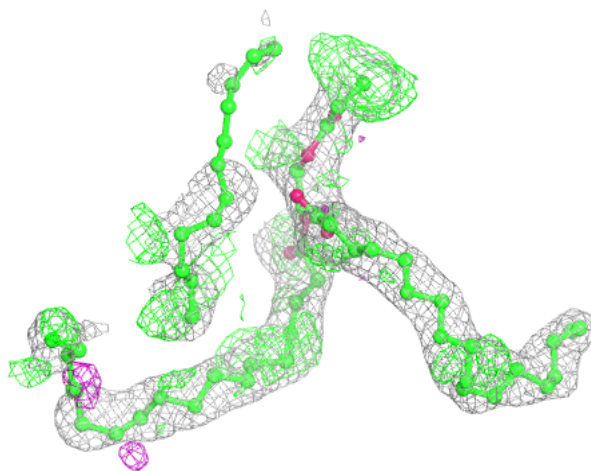
**Electron density around CHD C 308:**

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



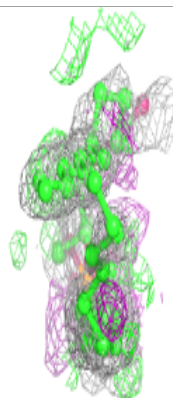
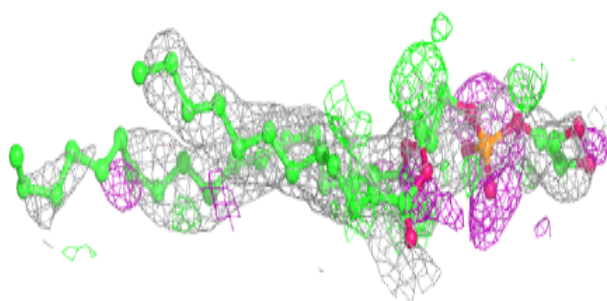
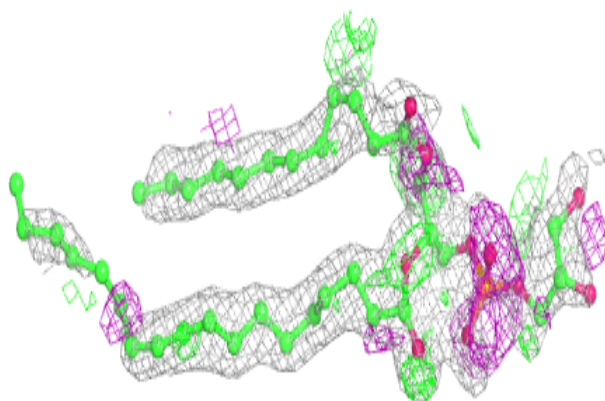
**Electron density around TGL L 101:**

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

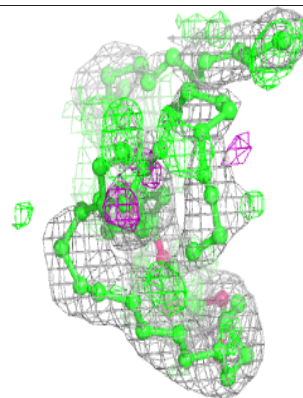
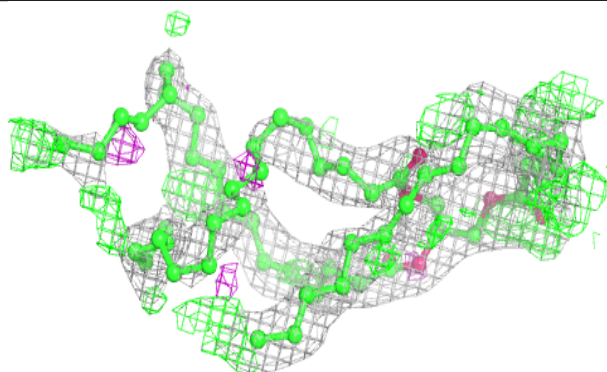
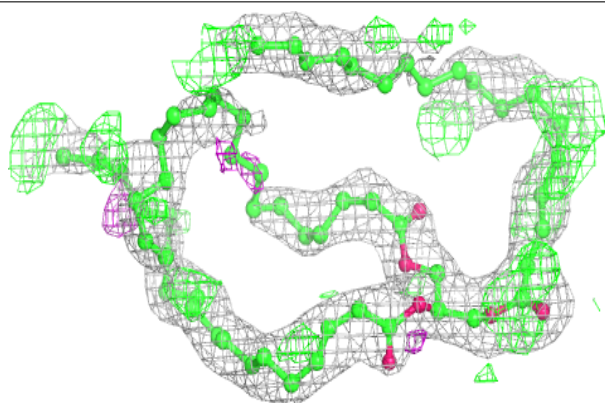


**Electron density around PGV A 607:**

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

**Electron density around TGL N 607:**

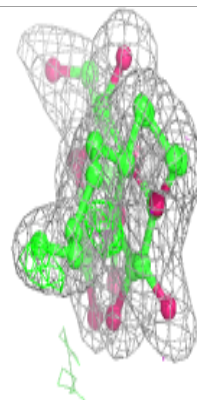
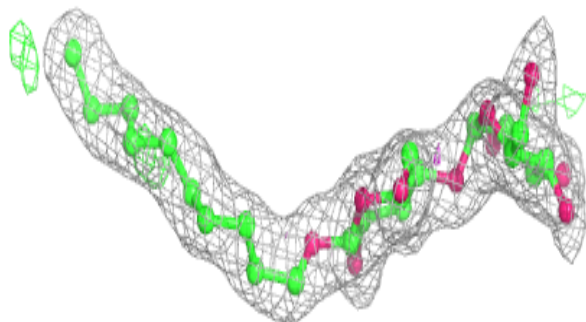
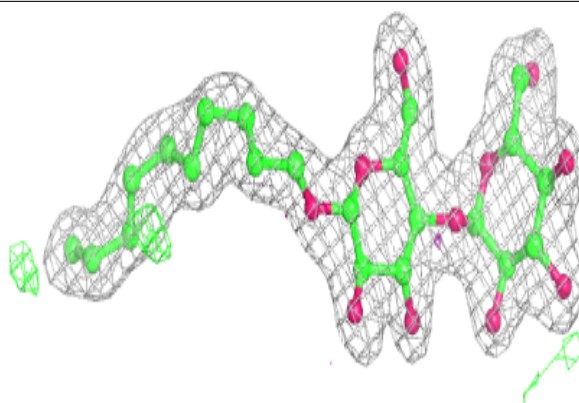
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



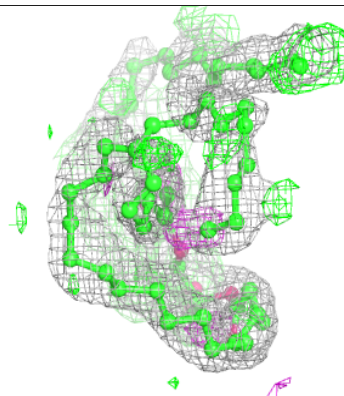
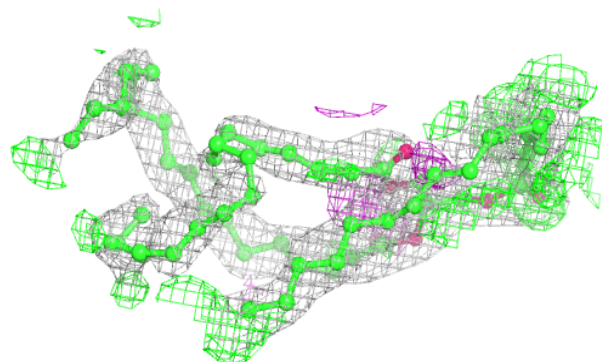
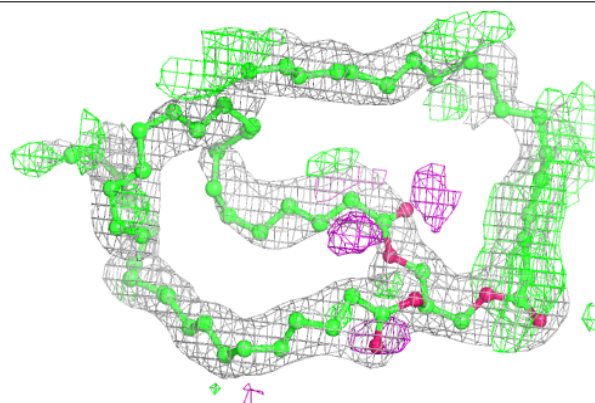


**Electron density around DMU Z 101:**

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

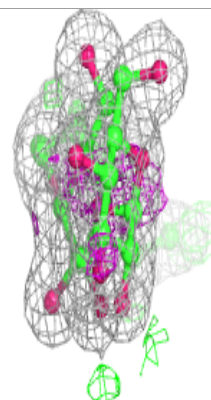
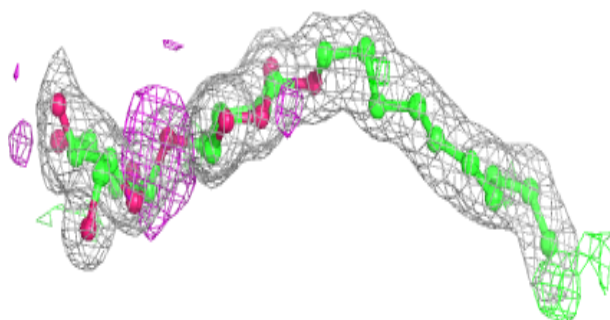
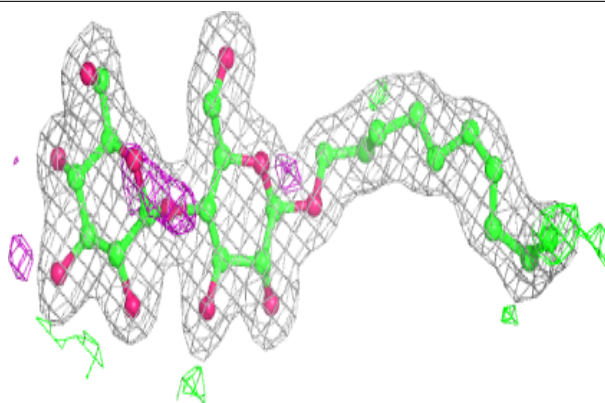
**Electron density around TGL B 301:**

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

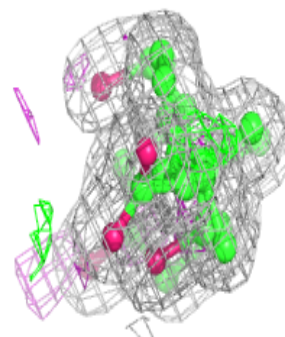
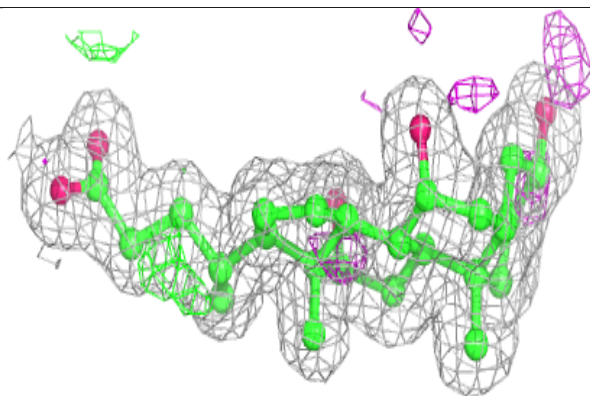
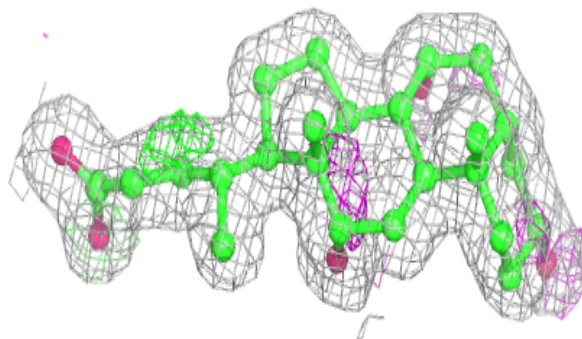


**Electron density around DMU M 101:**

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

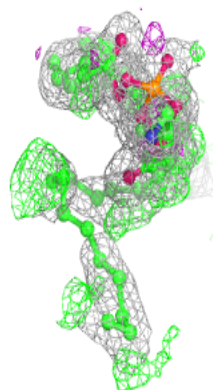
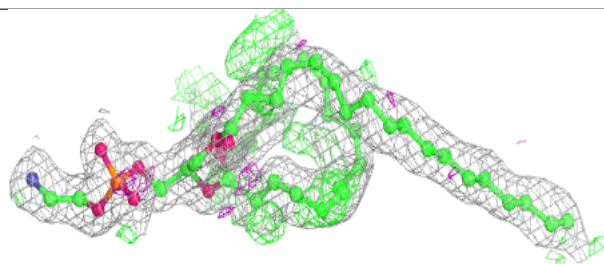
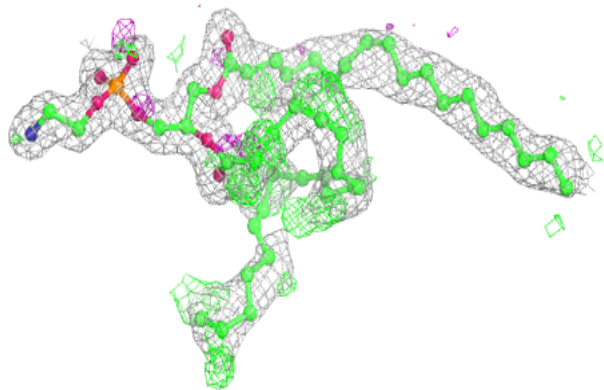
**Electron density around CHD C 301:**

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

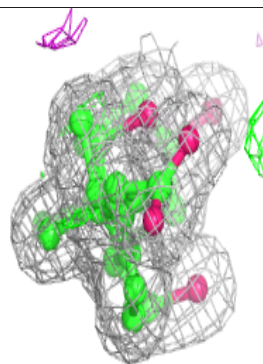
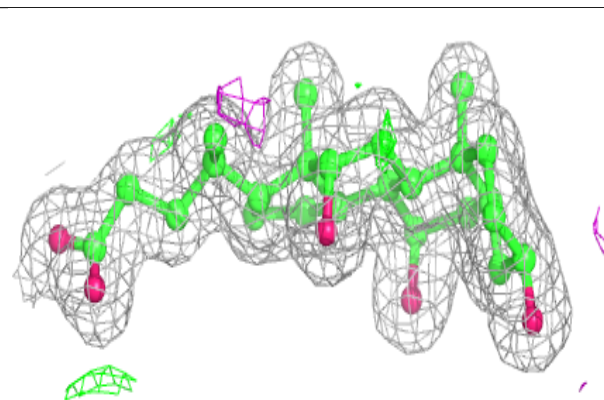
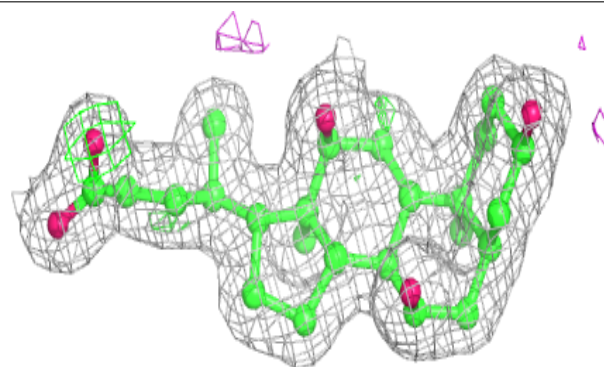


**Electron density around PEK P 303:**

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

**Electron density around CHD P 301:**

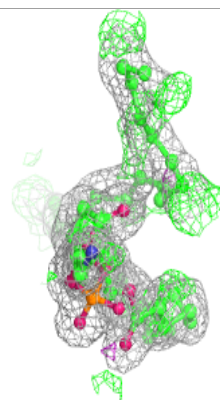
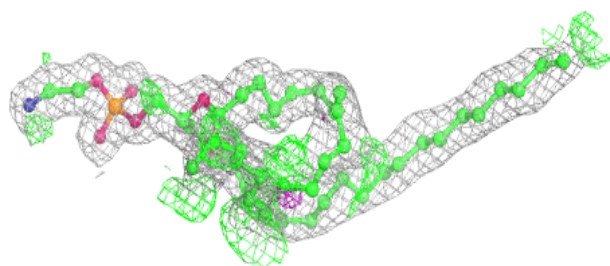
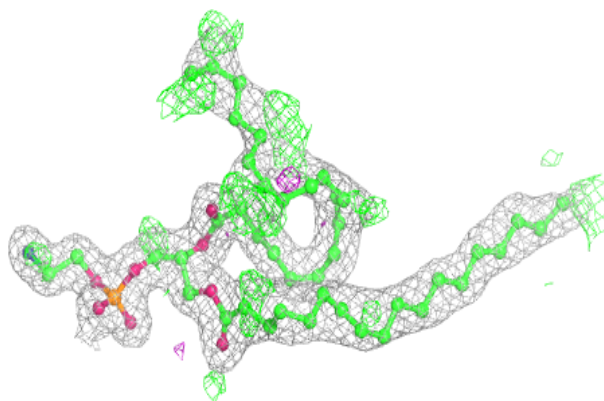
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



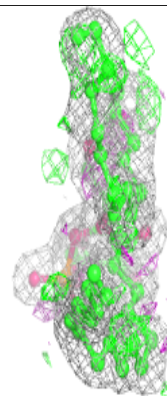
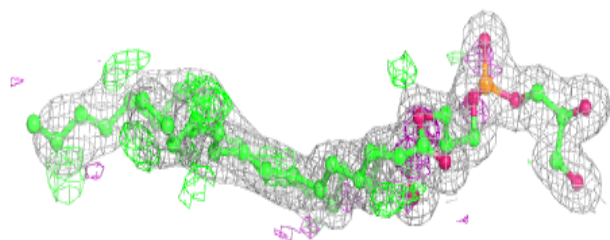
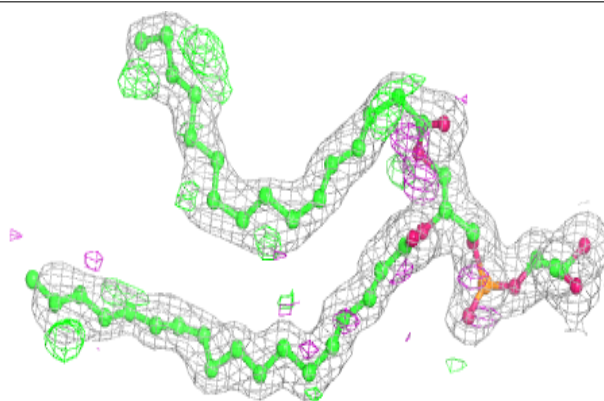


**Electron density around PEK C 303:**

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

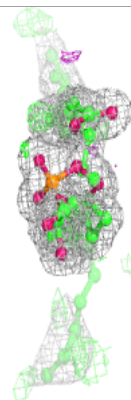
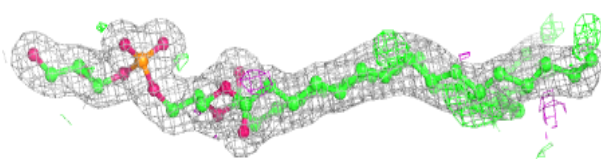
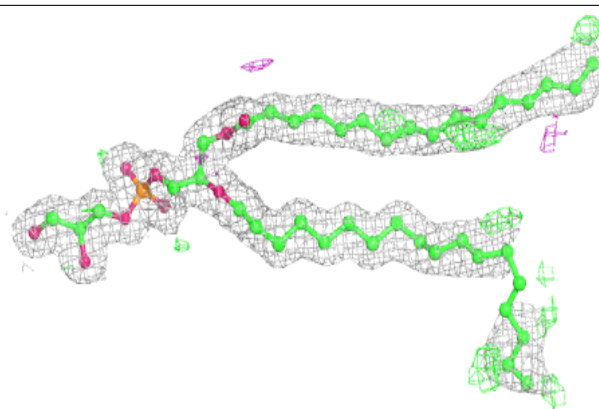
**Electron density around PGV N 609:**

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

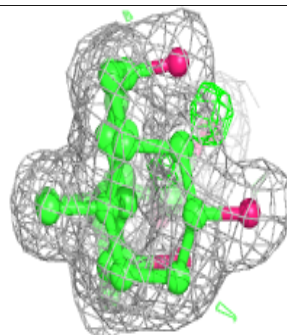
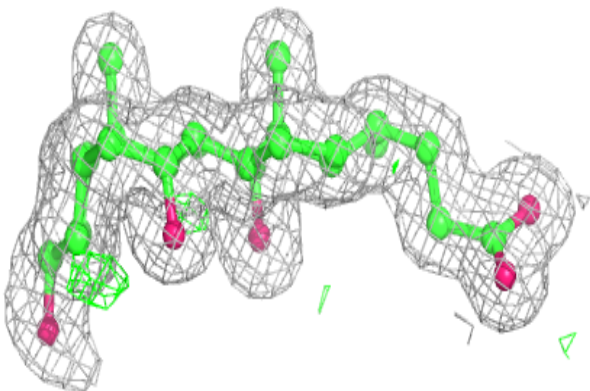
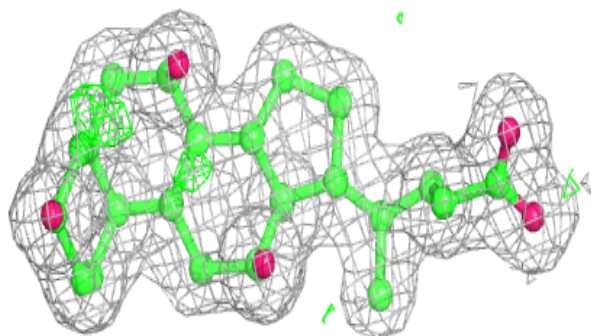


**Electron density around PGV P 305:**

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

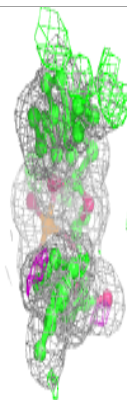
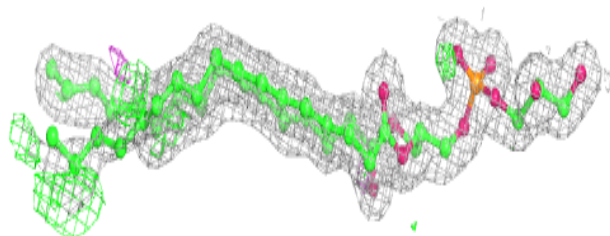
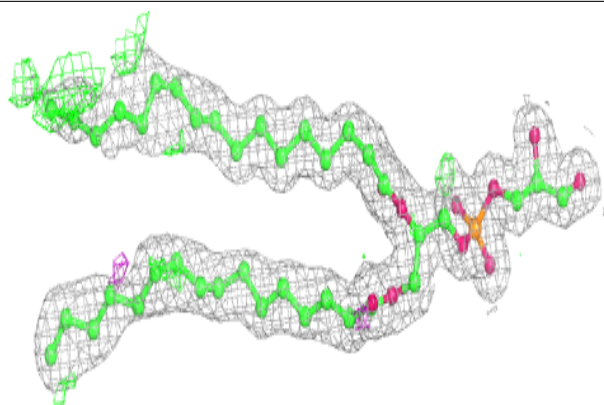
**Electron density around CHD B 305:**

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

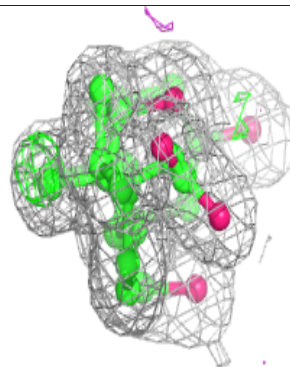
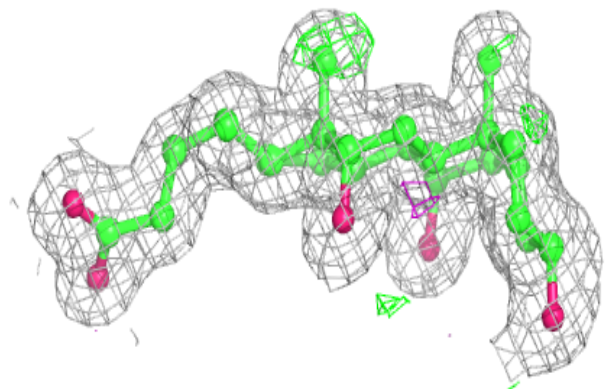
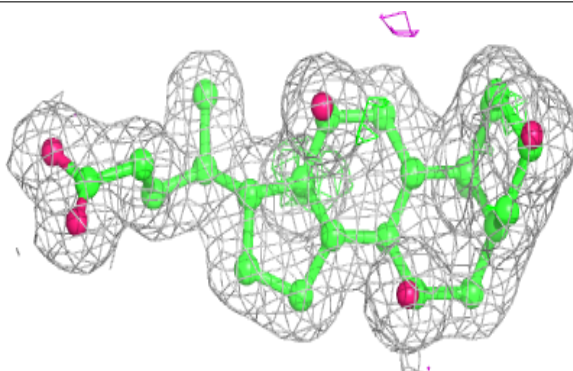


**Electron density around PGV C 305:**

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

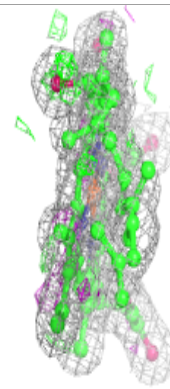
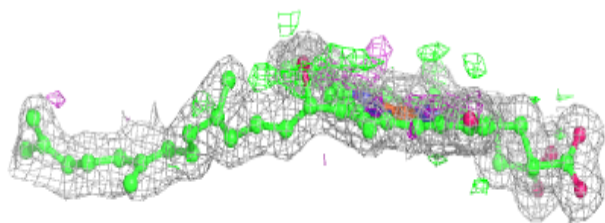
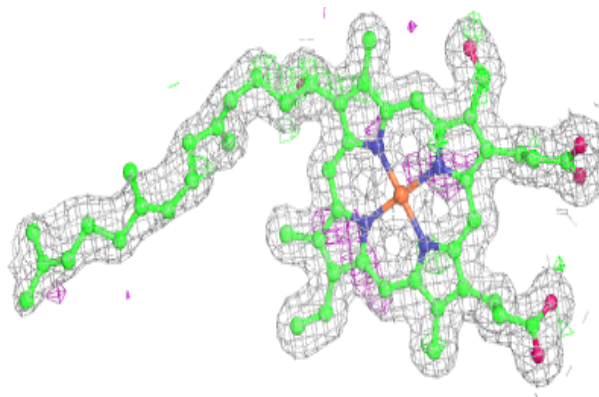
**Electron density around CHD G 102:**

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

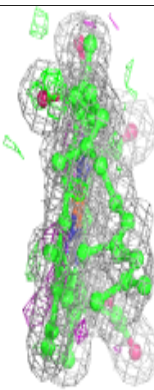
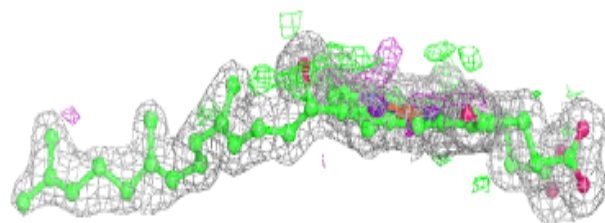
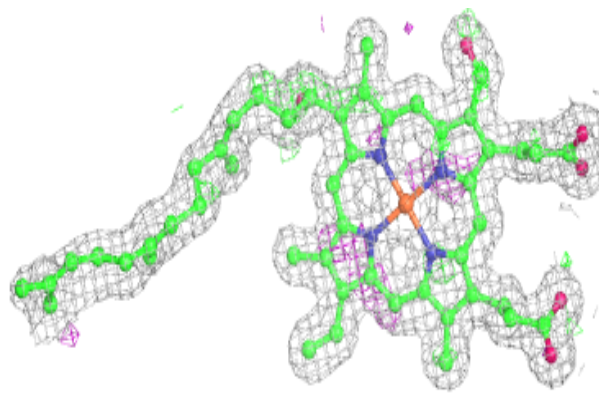


**Electron density around HEA A 601 (A):**

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

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

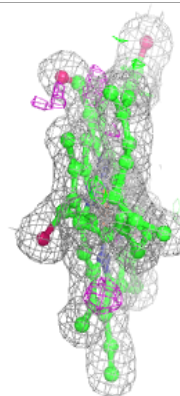
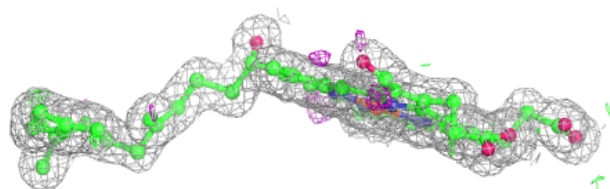
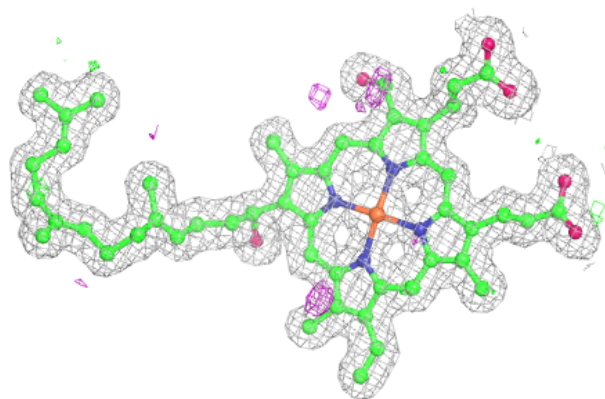
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



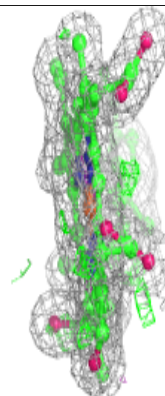
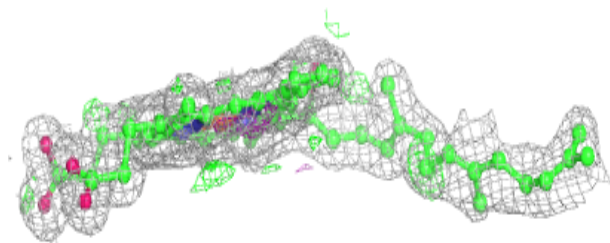
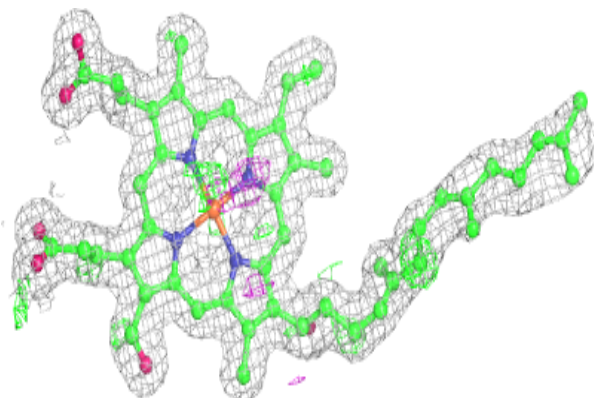


**Electron density around HEA A 602:**

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

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

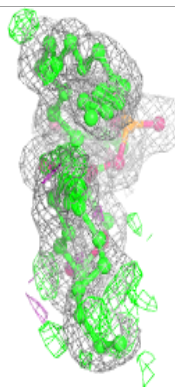
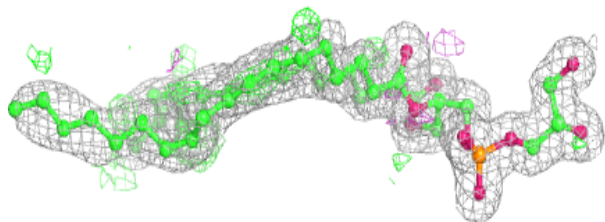
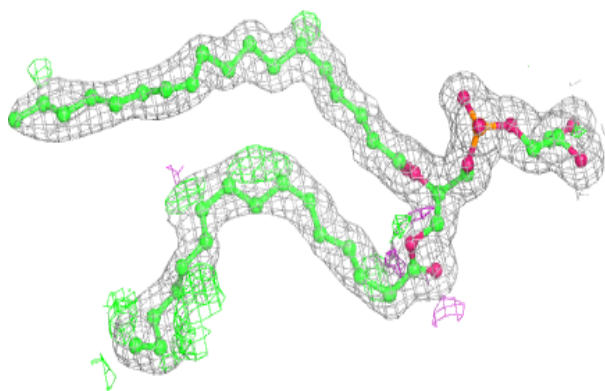
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



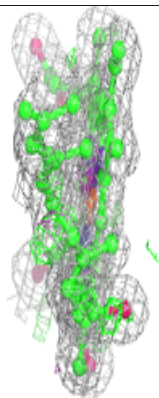
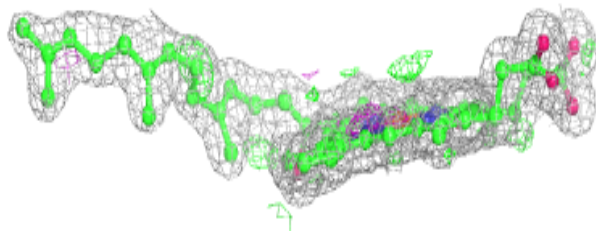
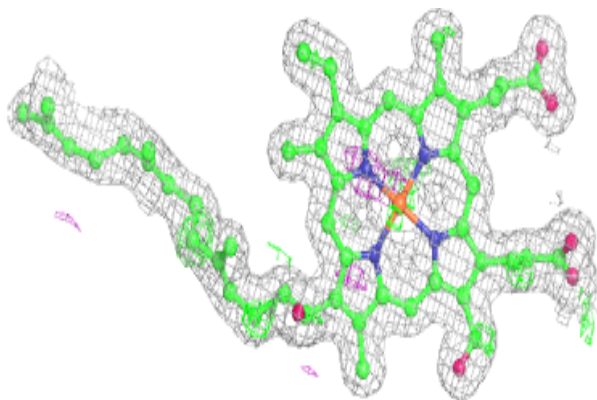


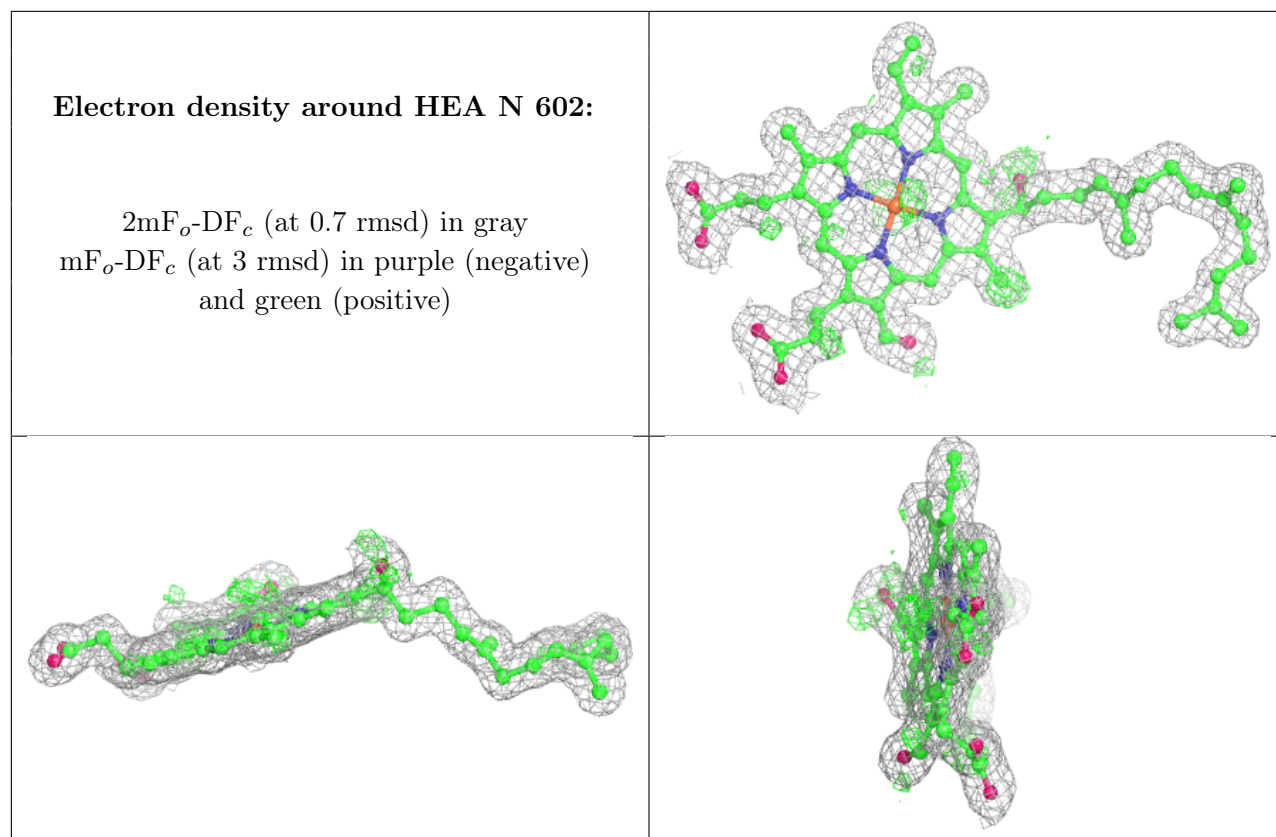
**Electron density around PGV A 608:**

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

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

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.