



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 1, 2022 – 06:22 PM EDT

PDB ID : 7TII  
Title : Annealed structure of oxidized bovine cytochrome c oxidase with reduced metal centers induced by synchrotron X-ray exposure  
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.; Russi, S.; Cohen, A.  
Deposited on : 2022-01-13  
Resolution : 2.45 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	:	2.29
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)	:	2.29

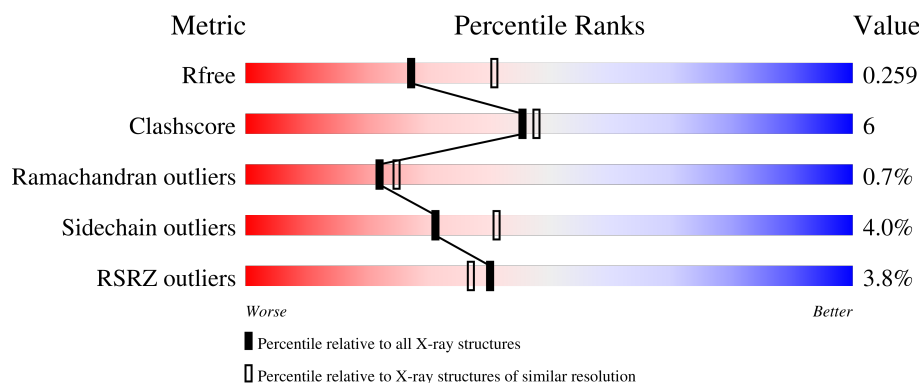
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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.





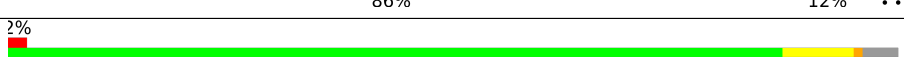


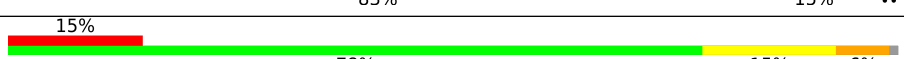


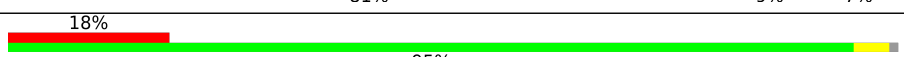





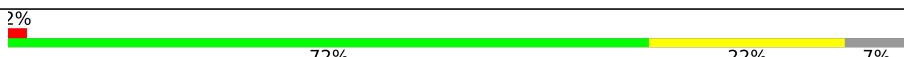
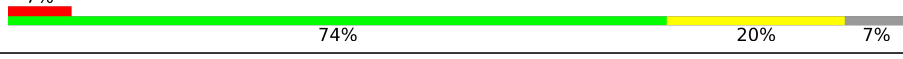

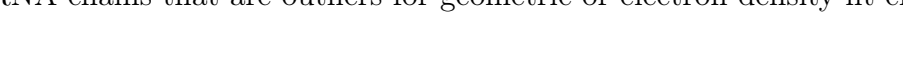
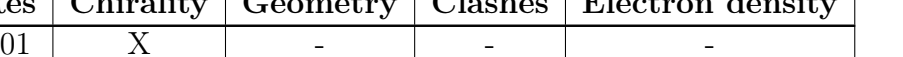
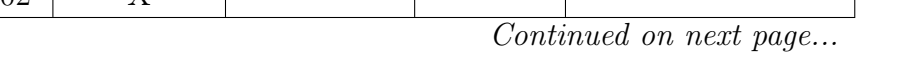

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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>84%</div> <div>15%</div> <div>.</div> </div>
1	N	514	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	227	<div> <div>81%</div> <div>18%</div> <div>.</div> </div>
2	O	227	<div> <div>3%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
3	C	261	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	261	
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	601	X	-	-	-
14	HEA	N	602	X	-	-	-
18	PGV	A	607	X	-	-	-
19	EDO	S	103	-	-	X	-
23	DMU	C	301	-	-	-	X
23	DMU	W	101	-	-	-	X
24	PEK	T	103	-	-	-	X
26	CHD	W	102	X	-	-	-
27	PSC	E	201	-	-	-	X
29	SAC	I	101	-	-	-	X
29	SAC	V	101	-	-	-	X



## 2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32401 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	20	0
			4181	2791	646	703	41			
1	N	514	Total	C	N	O	S	0	21	0
			4188	2795	647	704	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	6	0
			1874	1216	289	350	19			
2	O	227	Total	C	N	O	S	0	5	0
			1870	1215	289	348	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	8	0
			2174	1451	345	364	14			
3	P	259	Total	C	N	O	S	0	8	0
			2173	1451	344	363	15			

- 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	6	0
			1249	814	206	224	5			
4	Q	144	Total	C	N	O	S	0	1	0
			1203	782	197	219	5			

- 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
			863	550	148	163	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	98	Total	C	N	O	S	0	5	0
			789	489	142	152	6			
6	S	98	Total	C	N	O	S	0	1	0
			755	468	135	147	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 686	C 440	N 130	O 114	P 1	S 1	0	1	0
7	T	84	Total 706	C 454	N 133	O 117	P 1	S 1	0	3	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	1	0
			600	390	107	98	5			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

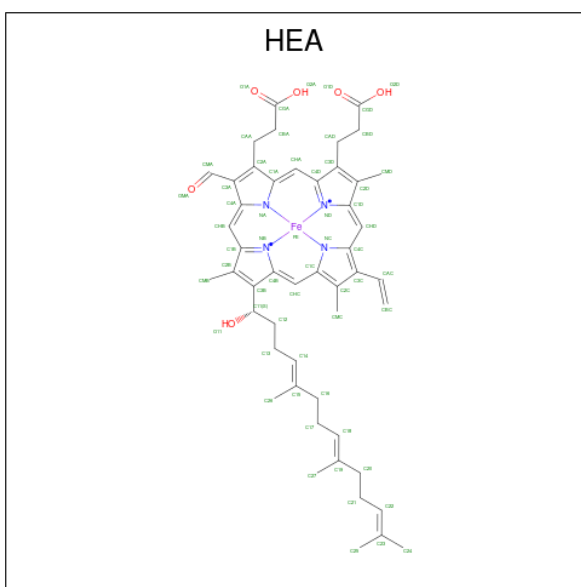
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



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

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

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

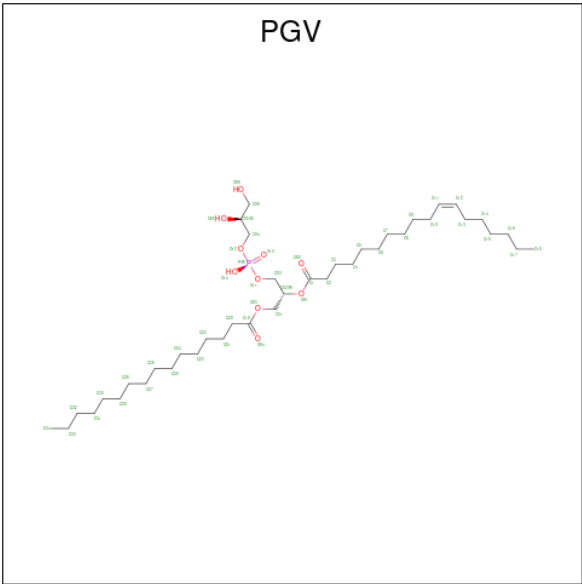
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- 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 (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



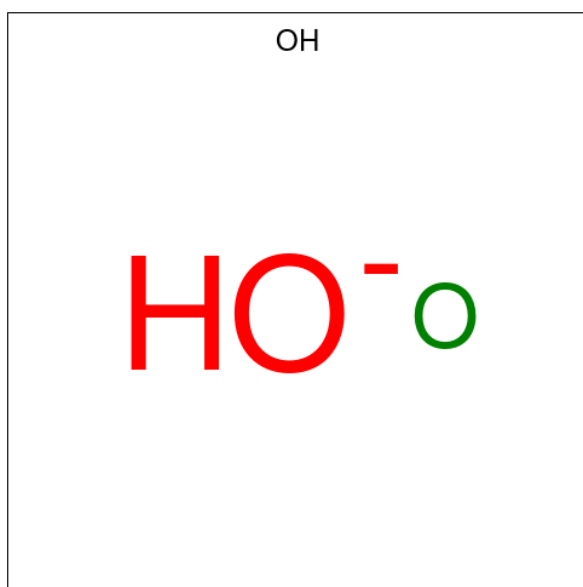
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	Z	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



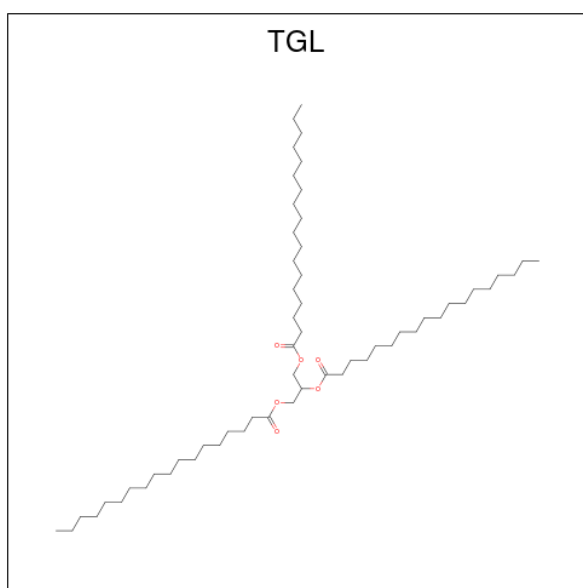
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		
19	C	1	Total	C	O	0	0
			4	2	2		
19	G	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



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

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



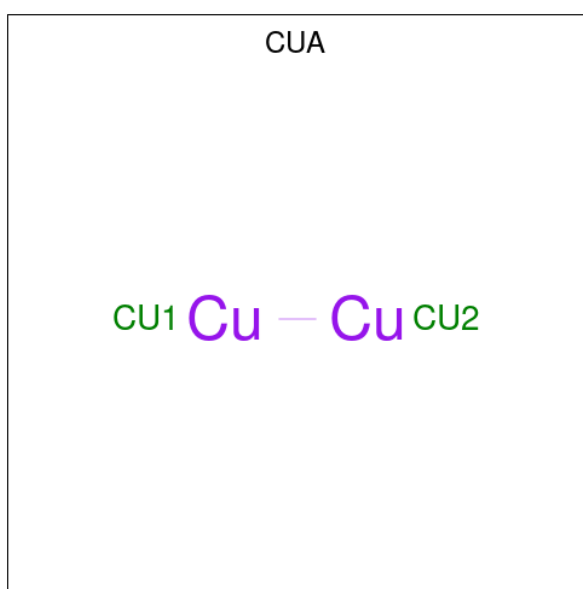
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		

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

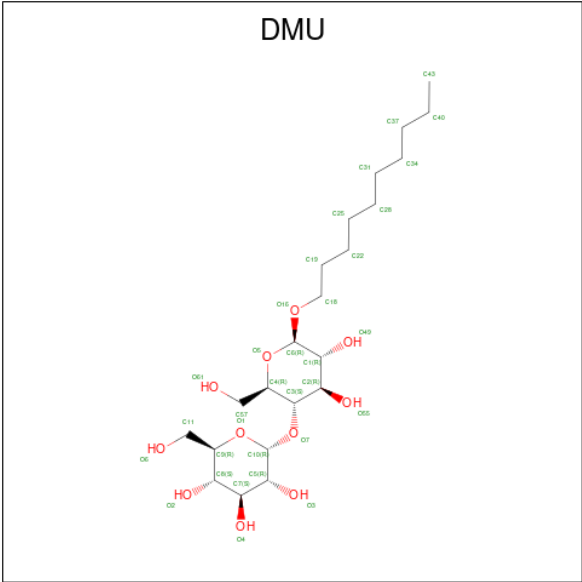
- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

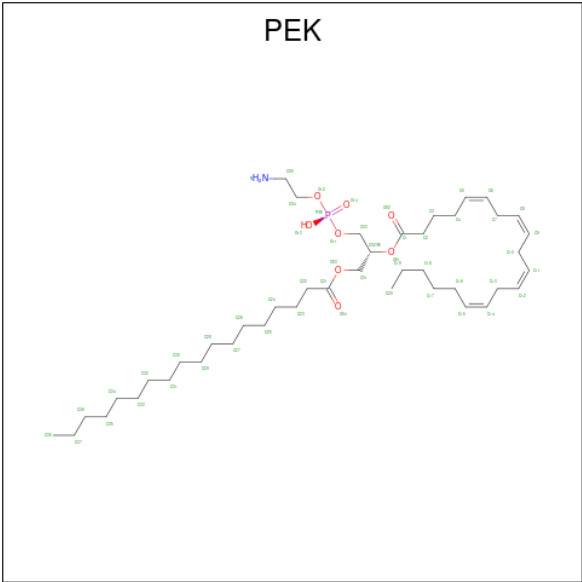
- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).





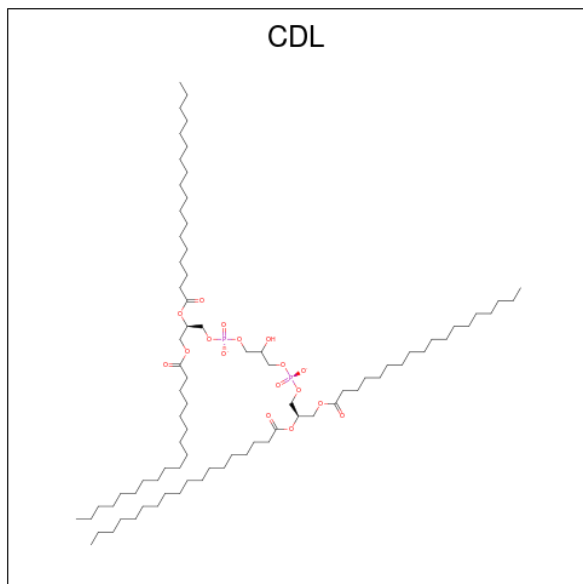
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			33	22	11		
23	D	1	Total	C	O	0	0
			33	22	11		
23	W	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



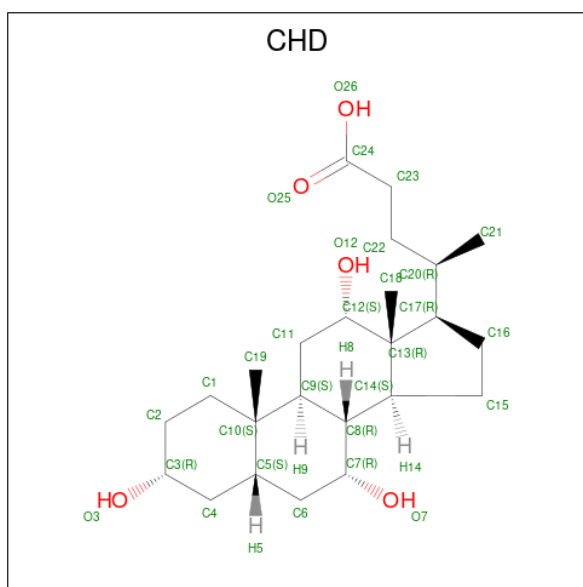
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



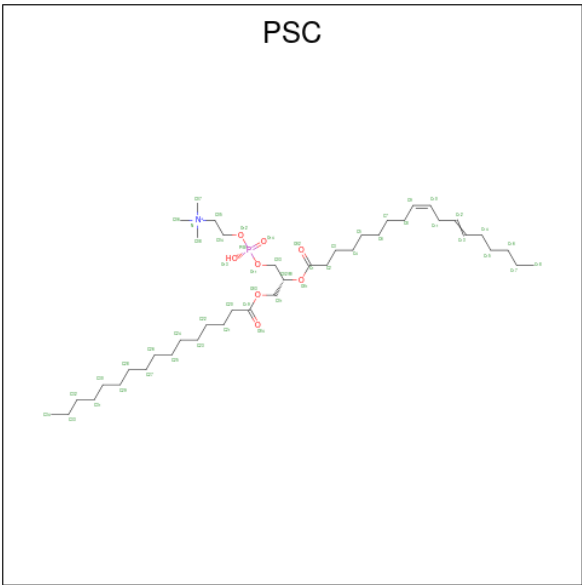
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	G	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).

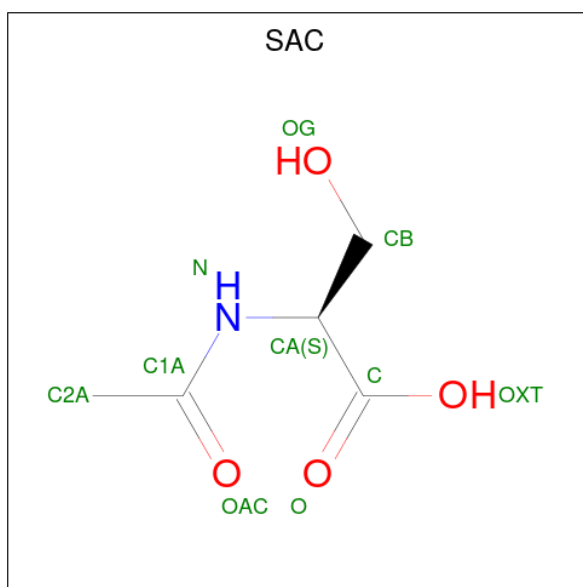


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
27	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	I	1	Total	C	N	O	0	0
			9	5	1	3		
29	V	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	130	Total	O	0	0
			130	130		
30	B	88	Total	O	0	0
			88	88		
30	C	54	Total	O	0	0
			54	54		
30	D	53	Total	O	0	0
			53	53		
30	E	35	Total	O	0	0
			35	35		
30	F	39	Total	O	0	0
			39	39		
30	G	31	Total	O	0	0
			31	31		
30	H	22	Total	O	0	0
			22	22		
30	I	19	Total	O	0	0
			19	19		
30	J	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	13	Total 13	O 13	0	0
30	L	14	Total 14	O 14	0	0
30	M	14	Total 14	O 14	0	0
30	N	114	Total 114	O 114	0	0
30	O	64	Total 64	O 64	0	0
30	P	54	Total 54	O 54	0	0
30	Q	16	Total 16	O 16	0	0
30	R	19	Total 19	O 19	0	0
30	S	41	Total 41	O 41	0	0
30	T	30	Total 30	O 30	0	0
30	U	18	Total 18	O 18	0	0
30	V	9	Total 9	O 9	0	0
30	W	10	Total 10	O 10	0	0
30	X	1	Total 1	O 1	0	0
30	Y	11	Total 11	O 11	0	0
30	Z	7	Total 7	O 7	0	0

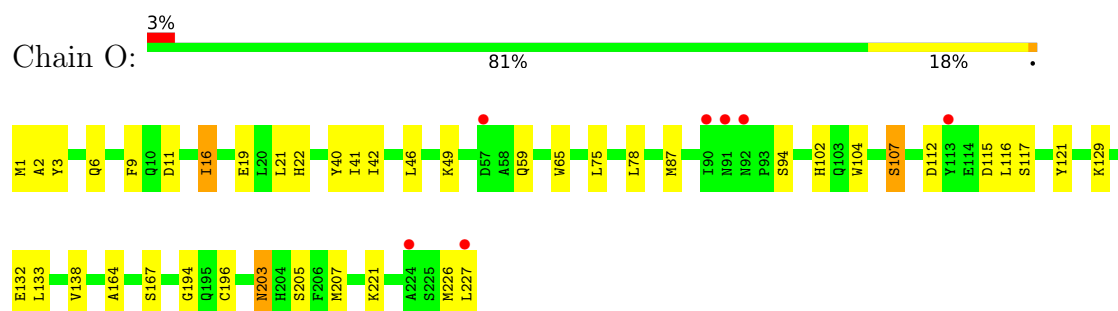
### 3 Residue-property plots [i](#)

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.

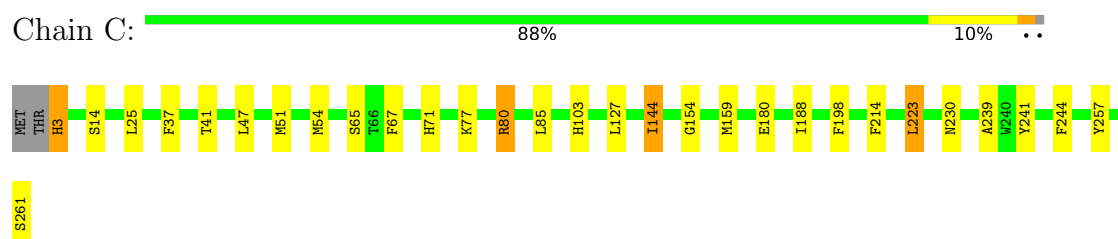
#### • Molecule 1: Cytochrome c oxidase subunit 1



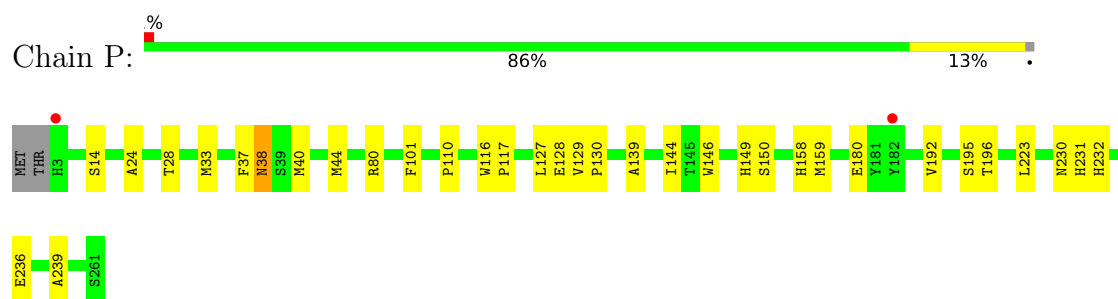
- Molecule 2: Cytochrome c oxidase subunit 2



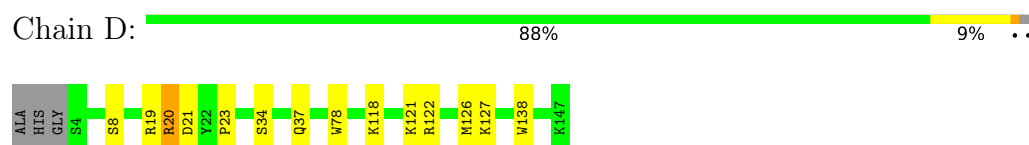
- Molecule 3: Cytochrome c oxidase subunit 3



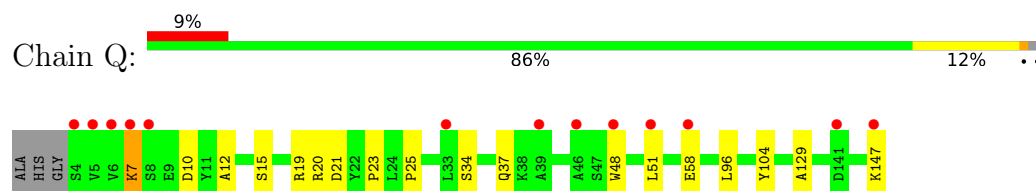
- Molecule 3: Cytochrome c oxidase subunit 3



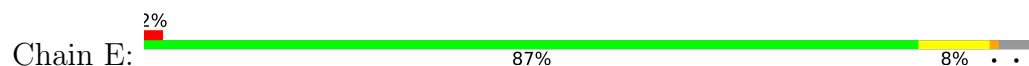
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



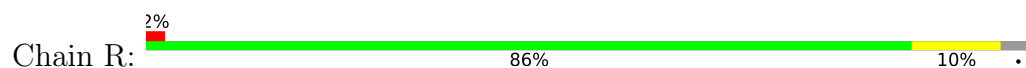
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



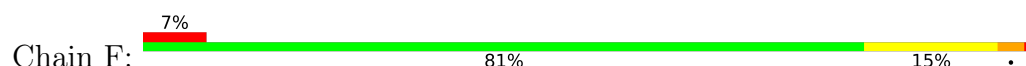




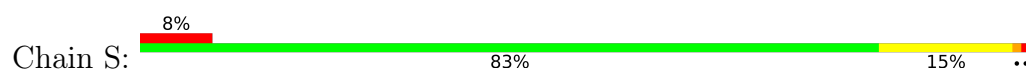
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



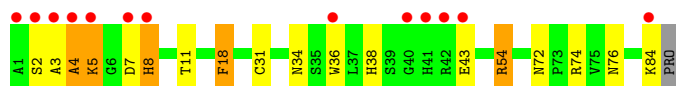
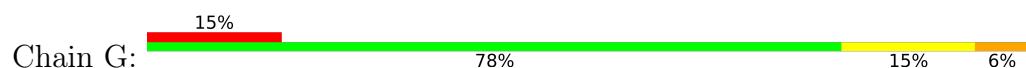
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



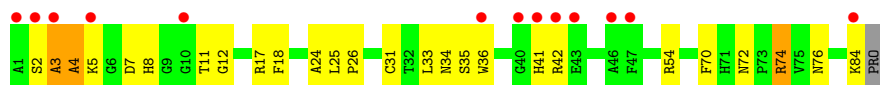
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



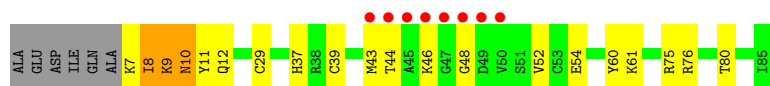
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



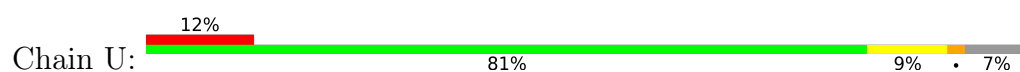
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



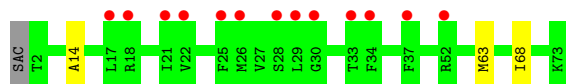
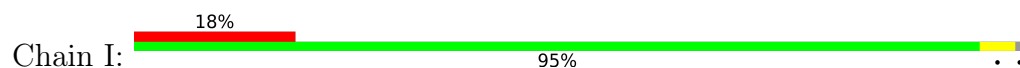
- Molecule 8: Cytochrome c oxidase subunit 6B1



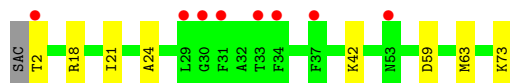
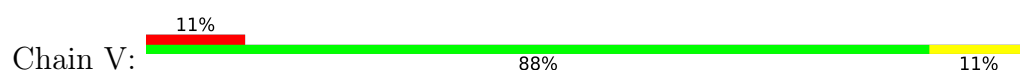
- Molecule 8: Cytochrome c oxidase subunit 6B1



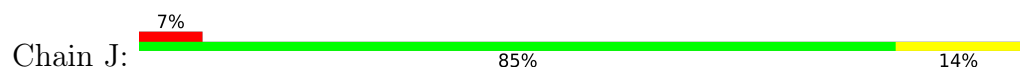
- Molecule 9: Cytochrome c oxidase subunit 6C



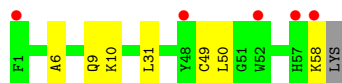
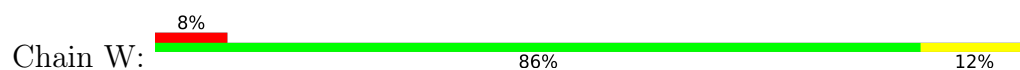
- Molecule 9: Cytochrome c oxidase subunit 6C



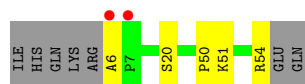
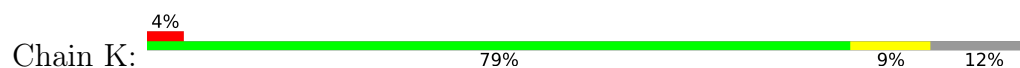
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



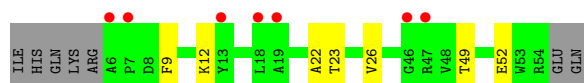
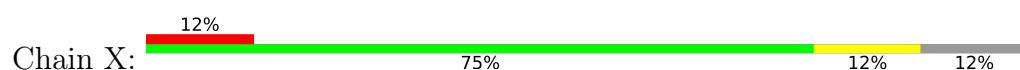
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial




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



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




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

Chain L:  77% 21% .



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

Chain Y:  2% 87% 11% .




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

Chain M:  2% 72% 22% 7%



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

Chain Z:  7% 74% 20% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.04Å 182.63Å 205.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 2.45 39.27 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.30-2.45) 99.9 (39.27-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.206 , 0.253 0.215 , 0.259	Depositor DCC
$R_{free}$ test set	12054 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: CHD, OH, TGL, ZN, DMU, CUA, PSC, SAC, MG, CU, CDL, HEA, TPO, PGV, FME, NA, PEK, EDO

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	0.67	0/4311	0.79	2/5884 (0.0%)
1	N	0.68	0/4318	0.77	1/5893 (0.0%)
2	B	0.70	0/1912	0.85	0/2603
2	O	0.68	0/1908	0.83	0/2599
3	C	0.65	0/2261	0.76	1/3090 (0.0%)
3	P	0.65	0/2260	0.77	0/3088
4	D	0.69	0/1284	0.80	0/1730
4	Q	0.67	0/1237	0.82	0/1668
5	E	0.68	0/882	0.78	0/1196
5	R	0.66	0/871	0.77	0/1182
6	F	0.73	0/806	0.90	0/1093
6	S	0.72	0/772	0.86	0/1048
7	G	0.66	0/702	0.82	0/953
7	T	0.65	0/724	0.83	0/984
8	H	0.66	0/682	0.85	0/921
8	U	0.69	0/682	0.83	0/921
9	I	0.67	0/605	0.83	0/802
9	V	0.67	0/613	0.81	0/812
10	J	0.67	0/471	0.79	0/636
10	W	0.68	0/471	0.76	0/636
11	K	0.68	0/405	0.80	0/556
11	X	0.67	0/405	0.76	0/556
12	L	0.62	0/393	0.81	0/526
12	Y	0.64	0/393	0.75	0/526
13	M	0.66	0/345	0.77	0/470
13	Z	0.66	0/345	0.78	0/470
All	All	0.67	0/30058	0.80	4/40843 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	512	ASN	CB-CA-C	-5.92	98.55	110.40
1	N	512	ASN	CB-CA-C	-5.73	98.93	110.40
3	C	80	ARG	CG-CD-NE	-5.58	100.08	111.80
1	A	439	ARG	CB-CA-C	5.54	121.48	110.40

There are no chirality outliers.

There are no planarity outliers.

## 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	4181	0	4161	69	0
1	N	4188	0	4166	76	0
2	B	1874	0	1869	22	0
2	O	1870	0	1867	33	0
3	C	2174	0	2082	23	0
3	P	2173	0	2083	25	0
4	D	1249	0	1242	12	0
4	Q	1203	0	1191	13	0
5	E	863	0	857	8	0
5	R	852	0	845	5	0
6	F	789	0	769	14	0
6	S	755	0	734	14	0
7	G	686	0	651	11	0
7	T	706	0	664	18	0
8	H	662	0	623	14	0
8	U	662	0	623	4	0
9	I	592	0	604	2	0
9	V	600	0	612	6	0
10	J	460	0	459	5	0
10	W	460	0	459	3	0
11	K	391	0	374	4	0
11	X	391	0	374	2	0
12	L	380	0	380	8	0
12	Y	380	0	380	3	0
13	M	335	0	352	7	0
13	Z	335	0	352	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	120	0	108	11	0
14	N	120	0	108	13	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	102	0	152	5	0
18	C	102	0	152	0	0
18	P	153	0	228	6	0
18	Z	51	0	76	2	0
19	A	8	0	12	0	0
19	C	4	0	6	1	0
19	G	4	0	6	1	0
19	N	4	0	6	0	0
19	S	8	0	12	5	0
19	T	4	0	6	0	0
20	A	1	0	0	1	0
20	N	1	0	0	1	0
21	B	63	0	110	0	0
21	D	63	0	110	4	0
21	L	63	0	110	4	0
21	N	63	0	110	0	0
21	Q	63	0	110	0	0
21	Y	63	0	110	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	C	33	0	42	6	0
23	D	33	0	42	0	0
23	W	33	0	42	7	0
23	Z	33	0	42	0	0
24	C	106	0	154	1	0
24	G	53	0	77	3	0
24	T	159	0	231	6	0
25	C	100	0	156	2	0
25	G	100	0	156	4	0
25	P	100	0	156	2	0
25	T	100	0	156	7	0
26	C	58	0	78	2	0
26	G	29	0	39	0	0
26	J	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	P	58	0	78	1	0
26	T	29	0	39	1	0
26	W	29	0	39	1	0
27	E	52	0	80	6	0
27	O	52	0	80	2	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	0	0
29	V	9	0	8	1	0
30	A	130	0	0	4	0
30	B	88	0	0	0	0
30	C	54	0	0	2	0
30	D	53	0	0	1	0
30	E	35	0	0	2	0
30	F	39	0	0	1	0
30	G	31	0	0	3	0
30	H	22	0	0	2	0
30	I	19	0	0	2	0
30	J	8	0	0	0	0
30	K	13	0	0	1	0
30	L	14	0	0	2	0
30	M	14	0	0	2	0
30	N	114	0	0	3	0
30	O	64	0	0	2	0
30	P	54	0	0	4	0
30	Q	16	0	0	0	0
30	R	19	0	0	0	0
30	S	41	0	0	1	0
30	T	30	0	0	5	0
30	U	18	0	0	0	0
30	V	9	0	0	0	0
30	W	10	0	0	0	0
30	X	1	0	0	0	0
30	Y	11	0	0	0	0
30	Z	7	0	0	0	0
All	All	32401	0	32047	404	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 6.

All (404) 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)
1:N:297[B]:MET:SD	1:N:302[B]:ARG:HG2	1.77	1.22
20:A:610:OH:O	30:A:701:HOH:O	1.67	1.12
3:P:40[B]:MET:O	3:P:44[B]:MET:HG3	1.57	1.03
1:A:51:ASP:OD2	1:A:441:SER:OG	1.78	0.99
8:H:9:LYS:HB3	30:H:121:HOH:O	1.65	0.95
1:N:297[B]:MET:SD	1:N:302[B]:ARG:CG	2.56	0.92
1:N:297[B]:MET:HG2	1:N:302[B]:ARG:HG3	1.52	0.91
1:A:379[A]:TYR:CG	1:A:383[A]:MET:HE3	2.09	0.87
12:L:2:HIS:HB3	30:L:213:HOH:O	1.76	0.85
3:P:33:MET:SD	23:W:101:DMU:H9	2.16	0.85
18:Z:101:PGV:H21	18:Z:101:PGV:H011	1.58	0.83
6:F:1:ALA:HB2	30:G:230:HOH:O	1.77	0.83
14:N:601:HEA:HBC1	14:N:601:HEA:HMC1	1.61	0.82
20:N:608:OH:O	30:N:701:HOH:O	1.99	0.81
6:F:92[A]:VAL:HG23	6:F:92[A]:VAL:O	1.83	0.79
24:C:302:PEK:HN2	7:G:76:ASN:HD21	1.29	0.79
4:Q:19:ARG:HG2	4:Q:21:ASP:OD1	1.83	0.78
1:A:379[A]:TYR:CD2	1:A:383[A]:MET:HE3	2.18	0.78
7:G:72:ASN:H	7:G:76:ASN:HD22	1.30	0.77
9:V:59:ASP:O	9:V:63[B]:MET:HG3	1.85	0.76
1:A:379[A]:TYR:HA	1:A:383[A]:MET:HE3	1.69	0.74
1:A:377:PHE:O	1:A:381[A]:LEU:HB3	1.89	0.73
7:T:5:LYS:NZ	30:T:201:HOH:O	2.21	0.73
1:A:380[A]:VAL:CG1	1:A:381[A]:LEU:N	2.51	0.73
1:N:297[B]:MET:CG	1:N:302[B]:ARG:HG3	2.19	0.72
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.30	0.71
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.70	0.71
12:L:20:ARG:HH22	21:L:101:TGL:HC41	1.53	0.71
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.74	0.70
13:M:32:TRP:CH2	30:M:113:HOH:O	2.45	0.68
1:N:400:PHE:HB3	21:Y:101:TGL:H283	1.76	0.68
7:G:31:CYS:SG	25:G:101:CDL:H532	2.34	0.67
14:A:602:HEA:HBD2	14:A:602:HEA:HMD1	1.76	0.67
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.30	0.67
25:C:304:CDL:HA31	30:C:422:HOH:O	1.95	0.67
9:V:73:LYS:HE2	9:V:73:LYS:HA	1.77	0.67
2:B:49:LYS:O	4:D:20:ARG:NH2	2.28	0.66
3:C:51[A]:MET:SD	3:C:54[A]:MET:HE1	2.35	0.66
3:C:51[A]:MET:SD	3:C:54[A]:MET:CE	2.83	0.66
1:N:377:PHE:O	1:N:381[A]:LEU:HB3	1.95	0.66
1:A:382[A]:SER:O	1:A:386[A]:VAL:HB	1.97	0.65
1:A:380[A]:VAL:HG12	1:A:381[A]:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.78	0.64
21:L:101:TGL:HC81	21:L:101:TGL:H332	1.79	0.64
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.79	0.64
21:D:201:TGL:HG32	30:D:333:HOH:O	1.96	0.64
1:A:406:ASN:HD21	18:A:607:PGV:H22	1.62	0.64
2:B:41:ILE:HD13	27:E:201:PSC:H342	1.79	0.63
18:P:301:PGV:C33	30:P:402:HOH:O	2.46	0.63
26:P:305:CHD:H183	26:P:305:CHD:H212	1.80	0.63
7:T:72:ASN:H	7:T:76:ASN:HD22	1.46	0.63
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.81	0.63
2:O:121:TYR:O	2:O:138:VAL:HA	1.99	0.63
7:T:11:TPO:O1P	7:T:11:TPO:HA	1.98	0.63
8:H:37:HIS:NE2	8:H:76:ARG:NH2	2.46	0.63
7:T:76:ASN:HD21	24:T:102:PEK:HN2	1.47	0.63
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.81	0.61
7:T:12:GLY:HA3	30:T:225:HOH:O	2.00	0.61
1:N:417[A]:MET:HE3	30:N:811:HOH:O	2.00	0.61
7:T:31:CYS:SG	25:T:105:CDL:H532	2.41	0.60
4:D:19[B]:ARG:HG2	4:D:21:ASP:OD1	2.01	0.60
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.36	0.60
1:N:347:LEU:HD13	1:N:383[B]:MET:SD	2.41	0.60
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.83	0.60
1:N:381[A]:LEU:HB2	14:N:602:HEA:CAC	2.32	0.60
2:B:18[A]:GLU:O	2:B:22[A]:HIS:CD2	2.55	0.59
19:C:309:EDO:O2	6:F:1:ALA:O	2.16	0.59
3:P:231:HIS:CG	18:P:303:PGV:H061	2.37	0.59
24:T:104:PEK:H383	25:T:105:CDL:H271	1.84	0.59
3:C:188[B]:ILE:HD12	3:C:188[B]:ILE:O	2.02	0.59
6:F:92[A]:VAL:O	6:F:92[A]:VAL:CG2	2.51	0.59
1:N:297[B]:MET:CG	1:N:302[B]:ARG:CG	2.78	0.59
1:N:379[A]:TYR:O	1:N:383[A]:MET:HB2	2.02	0.58
3:P:33:MET:SD	23:W:101:DMU:C19	2.90	0.58
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.86	0.58
1:N:417[A]:MET:CE	30:N:811:HOH:O	2.52	0.58
2:O:102:HIS:HE2	2:O:107:SER:HG	1.51	0.57
6:S:1:ALA:HA	19:S:103:EDO:H22	1.86	0.57
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.38	0.57
3:P:37:PHE:HD2	23:W:101:DMU:H11	1.69	0.57
2:B:58:ALA:O	2:B:62:GLU:HG3	2.04	0.57
24:G:102:PEK:H221	30:G:227:HOH:O	2.05	0.56
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:59:ASP:O	9:V:63[B]:MET:CG	2.53	0.56
1:A:87:ILE:O	1:A:173:PRO:HD3	2.05	0.56
7:G:3:ALA:O	7:G:4:ALA:HB2	2.06	0.56
2:O:102:HIS:NE2	2:O:107:SER:OG	2.37	0.56
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.06	0.56
1:N:381[A]:LEU:HA	14:N:602:HEA:CBC	2.36	0.55
18:A:607:PGV:H02	18:A:607:PGV:O14	2.06	0.55
1:A:347:LEU:HD13	1:A:383[B]:MET:SD	2.45	0.55
1:A:380[A]:VAL:HG13	1:A:381[A]:LEU:N	2.19	0.55
14:N:602:HEA:CBD	14:N:602:HEA:HMD1	2.35	0.55
6:F:64:GLU:O	6:F:65:ASP:HB2	2.06	0.55
6:S:75:HIS:H	6:S:80:GLN:HE22	1.53	0.55
1:A:297[A]:MET:O	1:A:302[A]:ARG:NE	2.33	0.55
2:B:121:TYR:O	2:B:138:VAL:HA	2.05	0.55
18:A:607:PGV:H201	30:A:825:HOH:O	2.07	0.55
18:A:607:PGV:H232	18:A:607:PGV:H31	1.89	0.55
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.88	0.54
1:N:152:LEU:HD21	3:P:28:THR:HG21	1.90	0.54
4:D:127:LYS:HD2	30:I:216:HOH:O	2.06	0.54
1:N:43:GLN:HE22	4:Q:104:TYR:HB3	1.73	0.53
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.90	0.53
27:E:201:PSC:C14	27:E:201:PSC:H343	2.39	0.53
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.91	0.53
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.90	0.53
18:P:301:PGV:H332	30:P:402:HOH:O	2.06	0.53
1:A:51:ASP:HB2	2:B:202:SER:O	2.07	0.53
1:A:411:LYS:NZ	30:A:702:HOH:O	2.30	0.53
2:B:18[A]:GLU:O	2:B:22[A]:HIS:HD2	1.92	0.53
3:C:67:PHE:HE2	25:C:304:CDL:H1	1.73	0.53
3:P:116:TRP:HA	3:P:117:PRO:C	2.29	0.53
2:B:56:MET:HA	27:E:201:PSC:H211	1.91	0.53
3:C:51[A]:MET:HA	3:C:54[A]:MET:HE2	1.92	0.52
3:P:128:GLU:OE1	7:T:42:ARG:NH2	2.42	0.52
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.91	0.52
1:N:87:ILE:O	1:N:173:PRO:HD3	2.09	0.52
11:K:6:ALA:N	30:K:101:HOH:O	2.42	0.52
2:O:1:FME:HE3	2:O:133:LEU:HD22	1.92	0.52
1:A:351:GLY:HA3	1:A:380[B]:VAL:HG23	1.91	0.52
1:A:379[A]:TYR:HA	1:A:383[A]:MET:CE	2.39	0.52
4:D:34:SER:H	4:D:37:GLN:HE21	1.57	0.51
8:H:9:LYS:CB	30:H:121:HOH:O	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:305:CHD:H212	26:C:305:CHD:H183	1.91	0.51
3:C:103:HIS:ND1	26:C:306:CHD:O26	2.40	0.51
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.92	0.51
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.91	0.51
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.43	0.51
27:E:201:PSC:H343	27:E:201:PSC:H141	1.93	0.51
1:A:381[A]:LEU:HD12	1:A:381[A]:LEU:C	2.30	0.51
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.93	0.50
24:T:102:PEK:C12	24:T:102:PEK:H161	2.42	0.50
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.47	0.50
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.46	0.50
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.47	0.50
1:A:397:PHE:N	1:A:398:PRO:CD	2.74	0.50
3:C:3:HIS:HB2	30:C:454:HOH:O	2.11	0.50
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.45	0.50
6:F:76:LYS:HD2	6:F:93:PRO:HG2	1.93	0.50
13:M:19:LEU:HD11	13:M:23:PHE:CE1	2.47	0.50
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.93	0.50
1:N:484:THR:HG23	13:Z:2:THR:OG1	2.11	0.50
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.12	0.50
3:P:158:HIS:CG	19:S:103:EDO:H11	2.46	0.50
2:O:16:ILE:O	2:O:19:GLU:HB2	2.12	0.49
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.93	0.49
5:E:52:LEU:O	5:E:55:CYS:HB2	2.13	0.49
3:P:192:VAL:HA	3:P:195:SER:HB2	1.94	0.49
2:O:40:TYR:CE2	9:V:24:ALA:HB2	2.47	0.49
1:A:380[A]:VAL:HG12	1:A:381[A]:LEU:N	2.22	0.49
6:F:1:ALA:HB1	6:S:65:ASP:OD2	2.11	0.49
7:T:3:ALA:O	7:T:4:ALA:CB	2.61	0.49
25:T:105:CDL:H531	25:T:105:CDL:H241	1.95	0.49
1:N:71:MET:CE	1:N:195:LEU:HD21	2.43	0.49
1:A:113[B]:LEU:HD22	1:A:117[B]:MET:SD	2.53	0.49
3:P:38:ASN:HB3	30:P:448:HOH:O	2.13	0.49
25:P:304:CDL:HB21	25:P:304:CDL:CB3	2.43	0.49
1:A:347:LEU:CD1	1:A:383[B]:MET:HB3	2.44	0.48
8:H:9:LYS:O	8:H:11:TYR:N	2.46	0.48
2:O:22[B]:HIS:CD2	30:O:439:HOH:O	2.66	0.48
1:N:489:THR:HA	6:S:71:TRP:O	2.13	0.48
3:P:80:ARG:NH2	3:P:236:GLU:OE1	2.45	0.48
8:H:54:GLU:OE1	8:H:54:GLU:HA	2.13	0.48
1:N:309:THR:HG22	14:N:602:HEA:HMB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:42:ILE:O	2:O:46:LEU:HG	2.13	0.48
10:W:49:CYS:HB3	23:W:101:DMU:H8	1.96	0.48
1:A:278:MET:HE1	30:T:210:HOH:O	2.13	0.48
1:A:481:GLU:HB2	13:M:4:LYS:HD2	1.95	0.48
1:N:336:PRO:HB2	1:N:394[B]:VAL:HG11	1.95	0.48
7:T:17:ARG:HD2	30:T:212:HOH:O	2.12	0.48
3:P:127[A]:LEU:N	3:P:127[A]:LEU:HD22	2.29	0.48
1:A:499:PRO:HD2	12:L:7:PRO:HD3	1.95	0.48
3:C:257:TYR:O	3:C:261:SER:HB3	2.14	0.48
1:N:377:PHE:HA	1:N:380[B]:VAL:HG22	1.95	0.48
13:M:32:TRP:HH2	30:M:113:HOH:O	1.89	0.48
5:E:82:TYR:N	5:E:83:PRO:CD	2.77	0.48
7:G:54:ARG:HH12	19:G:104:EDO:H21	1.79	0.48
2:O:116:LEU:HD12	2:O:117:SER:N	2.29	0.48
1:A:437:PRO:HG2	1:A:440:TYR:CE2	2.49	0.47
2:O:3:TYR:CZ	2:O:6:GLN:HG3	2.49	0.47
2:O:104:TRP:CG	2:O:203[A]:ASN:HB2	2.47	0.47
1:A:489:THR:HA	6:F:71:TRP:O	2.14	0.47
3:C:51[A]:MET:HA	3:C:54[A]:MET:CE	2.45	0.47
1:N:382[A]:SER:O	1:N:383[A]:MET:C	2.51	0.47
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	1.95	0.47
18:Z:101:PGV:H011	18:Z:101:PGV:C2	2.37	0.47
3:C:188[B]:ILE:HD13	3:C:198:PHE:HB2	1.96	0.47
1:N:152:LEU:HD23	1:N:152:LEU:N	2.30	0.47
1:N:362:SER:HA	2:O:87:MET:HE1	1.95	0.47
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.14	0.47
1:N:199:LEU:N	1:N:200:PRO:CD	2.78	0.47
1:N:343:GLY:O	1:N:347:LEU:HG	2.14	0.47
2:O:1:FME:CE	2:O:133:LEU:HD13	2.45	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.47
1:N:378:HIS:O	1:N:382[A]:SER:HB2	2.14	0.47
3:P:144[A]:ILE:CD1	3:P:239:ALA:HA	2.45	0.47
9:V:2:THR:HB	29:V:101:SAC:C	2.45	0.47
1:A:321:PHE:CD1	27:E:201:PSC:H341	2.50	0.47
3:C:37:PHE:HB3	23:C:301:DMU:O49	2.15	0.47
25:P:304:CDL:HB21	25:P:304:CDL:HB32	1.95	0.47
12:L:47:LYS:HD2	30:L:211:HOH:O	2.13	0.47
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.50	0.47
6:S:96:LEU:HA	30:S:232:HOH:O	2.14	0.47
11:X:22:ALA:O	11:X:26:VAL:HG23	2.15	0.47
1:N:24:ALA:HB2	14:N:601:HEA:H252	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379[B]:TYR:CE1	1:N:383[B]:MET:SD	3.08	0.47
25:T:105:CDL:H791	25:T:105:CDL:H832	1.96	0.47
1:N:43:GLN:NE2	4:Q:104:TYR:HB3	2.30	0.46
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.97	0.46
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.51	0.46
25:G:101:CDL:H241	25:G:101:CDL:H531	1.98	0.46
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.30	0.46
1:N:400:PHE:HB3	21:Y:101:TGL:C28	2.44	0.46
3:P:33:MET:CG	23:W:101:DMU:H9	2.45	0.46
2:B:122:MET:SD	2:B:135:LEU:HA	2.55	0.46
6:F:95:GLN:O	6:F:96:LEU:O	2.33	0.46
7:G:5:LYS:HG3	24:G:102:PEK:H383	1.96	0.46
1:N:68:PHE:O	1:N:72:PRO:HG2	2.16	0.46
1:N:101:SER:O	1:N:156:SER:OG	2.31	0.46
2:O:102:HIS:CD2	2:O:107:SER:HG	2.33	0.46
1:A:379[A]:TYR:CA	1:A:383[A]:MET:HE3	2.42	0.46
1:A:426:PHE:N	1:A:427:PRO:CD	2.79	0.46
1:N:44:PRO:HD3	1:N:448:THR:HG23	1.98	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.96	0.46
3:P:139:ALA:HA	7:T:24:ALA:HB1	1.96	0.46
1:A:115[B]:SER:O	1:A:121:GLY:HA2	2.16	0.46
1:N:347:LEU:CD1	1:N:383[B]:MET:HB3	2.46	0.46
1:A:424:THR:HG21	14:A:601:HEA:HMB2	1.96	0.46
5:E:36:LEU:HD21	5:E:43:PRO:HB3	1.98	0.46
2:O:102:HIS:O	2:O:104:TRP:HA	2.15	0.46
5:R:52:LEU:O	5:R:55:CYS:HB2	2.16	0.45
1:A:364:ASP:OD1	14:A:602:HEA:O1A	2.34	0.45
8:H:37:HIS:CD2	8:H:76:ARG:CZ	2.99	0.45
4:D:78:TRP:CB	21:D:201:TGL:HB22	2.45	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.16	0.45
8:H:39:CYS:O	8:H:43:MET:HG2	2.16	0.45
1:N:115[B]:SER:O	1:N:121:GLY:HA2	2.17	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.16	0.45
3:P:129:VAL:N	3:P:130:PRO:CD	2.80	0.45
6:S:1:ALA:HA	19:S:103:EDO:C2	2.45	0.45
3:P:33:MET:HB2	23:W:101:DMU:H10	1.98	0.45
1:A:242:GLU:HA	1:A:245:ILE:HD12	1.99	0.45
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.99	0.45
4:Q:7:LYS:HE3	4:Q:10:ASP:OD1	2.16	0.45
11:X:9:PHE:CD1	11:X:9:PHE:C	2.89	0.45
6:S:94:HIS:CG	6:S:95:GLN:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:602:HEA:HMD1	14:A:602:HEA:CBD	2.47	0.45
10:J:43:THR:O	10:J:46:SER:HB3	2.17	0.45
18:P:302:PGV:H012	30:P:433:HOH:O	2.16	0.45
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.99	0.45
2:B:42:ILE:HG22	2:B:43:SER:N	2.31	0.44
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.44
30:I:215:HOH:O	11:K:54:ARG:HD3	2.17	0.44
13:M:41:LYS:O	13:M:43:SER:N	2.50	0.44
3:P:37:PHE:CD2	23:W:101:DMU:H11	2.50	0.44
1:N:397:PHE:N	1:N:398:PRO:CD	2.80	0.44
3:P:149:HIS:CE1	7:T:11:TPO:HG22	2.53	0.44
7:T:72:ASN:N	7:T:76:ASN:HD22	2.13	0.44
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.99	0.44
8:H:52:VAL:O	8:U:46:LYS:NZ	2.37	0.44
14:N:602:HEA:HMD1	14:N:602:HEA:HBD2	1.97	0.44
1:A:379[A]:TYR:CD2	1:A:383[A]:MET:CE	2.97	0.44
4:D:19[B]:ARG:CG	4:D:21:ASP:OD1	2.65	0.44
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.17	0.44
2:B:143:VAL:HB	2:B:222:TRP:CE3	2.53	0.44
1:N:65:MET:HG3	14:N:601:HEA:C2C	2.48	0.44
2:O:1:FME:HE1	2:O:133:LEU:HD13	2.00	0.44
6:S:1:ALA:HB1	19:S:103:EDO:O2	2.17	0.44
1:A:381[A]:LEU:HD13	14:A:602:HEA:HBC2	1.98	0.44
2:O:11:ASP:HB2	4:Q:129:ALA:HA	2.00	0.44
6:S:96:LEU:HD11	19:S:102:EDO:O2	2.17	0.44
7:T:41:HIS:HB3	7:T:74:ARG:CZ	2.48	0.44
1:A:165:ILE:CG2	3:C:85:LEU:HD11	2.48	0.44
12:L:12:PRO:HB2	21:L:101:TGL:HG2	2.00	0.44
1:N:58:VAL:O	1:N:61:HIS:HB3	2.18	0.44
1:N:347:LEU:HD13	1:N:383[B]:MET:HB3	2.00	0.44
24:T:104:PEK:H383	25:T:105:CDL:C27	2.48	0.44
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.53	0.44
8:U:9:LYS:HA	8:U:9:LYS:HD3	1.66	0.44
1:A:205:GLY:O	1:A:208[B]:MET:HB2	2.17	0.43
8:H:9:LYS:O	8:H:10:ASN:C	2.56	0.43
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.00	0.43
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.00	0.43
1:A:65:MET:HB3	14:A:601:HEA:CAC	2.49	0.43
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.90	0.43
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.53	0.43
1:A:514:LYS:HA	6:F:38:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.00	0.43
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.00	0.43
1:A:382[B]:SER:OG	14:A:601:HEA:H121	2.18	0.43
1:A:383[A]:MET:O	1:A:384[A]:GLY:C	2.56	0.43
6:F:87:THR:HG22	30:F:222:HOH:O	2.18	0.43
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.43
18:P:301:PGV:H343	24:T:102:PEK:C37	2.48	0.43
1:N:113[A]:LEU:O	1:N:117[A]:MET:HG2	2.18	0.43
5:R:41:LEU:C	5:R:41:LEU:HD12	2.38	0.43
7:T:31:CYS:SG	25:T:105:CDL:H551	2.58	0.43
26:T:101:CHD:O7	26:T:101:CHD:H41	2.18	0.43
26:W:102:CHD:H9	26:W:102:CHD:H3	1.99	0.43
1:A:353:LEU:HB3	2:B:31:VAL:HG22	2.01	0.43
5:E:14[A]:ARG:NH2	30:E:301:HOH:O	2.32	0.43
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.19	0.43
7:T:33:LEU:O	7:T:34:ASN:C	2.57	0.43
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.89	0.43
3:C:37:PHE:CD2	23:C:301:DMU:H8	2.53	0.43
25:G:101:CDL:H212	1:N:311:ILE:HD12	2.01	0.43
1:A:380[B]:VAL:HG12	1:A:380[B]:VAL:O	2.19	0.42
2:B:78:LEU:CB	2:B:79:PRO:CD	2.97	0.42
2:B:102:HIS:O	2:B:104:TRP:HA	2.18	0.42
3:C:144[A]:ILE:CD1	3:C:239:ALA:HA	2.49	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.00	0.42
1:N:19:TYR:CG	1:N:76:GLY:HA3	2.54	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.96	0.42
1:A:178:GLN:HB3	30:T:223:HOH:O	2.18	0.42
12:L:14:SER:H	21:L:101:TGL:HC51	1.83	0.42
13:M:19:LEU:CD1	13:M:23:PHE:CE1	3.02	0.42
1:N:248:LEU:N	1:N:249:PRO:CD	2.82	0.42
1:N:65:MET:HB3	14:N:601:HEA:CAC	2.49	0.42
1:A:172:LYS:HD2	1:A:181:THR:CG2	2.49	0.42
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.68	0.42
3:P:101:PHE:HA	3:P:196:THR:HG21	2.01	0.42
7:G:34:ASN:HD21	7:G:38:HIS:CE1	2.37	0.42
1:N:381[A]:LEU:HB2	14:N:602:HEA:HAC	1.99	0.42
2:O:203[A]:ASN:N	2:O:203[A]:ASN:HD22	2.16	0.42
2:O:227:LEU:HB2	30:O:428:HOH:O	2.19	0.42
1:A:331:ASN:OD1	4:D:20:ARG:NH1	2.53	0.42
7:G:5:LYS:HB3	1:N:278[B]:MET:SD	2.60	0.42
8:H:8:ILE:HG13	8:H:9:LYS:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:67:ILE:O	5:R:71:VAL:HG23	2.19	0.42
7:T:25:LEU:N	7:T:26:PRO:CD	2.83	0.42
1:A:199:LEU:N	1:A:200:PRO:CD	2.82	0.42
18:A:607:PGV:H241	18:A:607:PGV:H52	2.00	0.42
27:E:201:PSC:C1	9:I:14:ALA:HB2	2.49	0.42
9:I:63:MET:HB3	9:I:68:ILE:HD11	2.01	0.42
1:A:297[B]:MET:HG2	1:A:302[B]:ARG:HG3	2.02	0.42
2:B:78:LEU:CB	2:B:79:PRO:HD3	2.50	0.42
1:N:169[A]:ILE:HD13	1:N:169[A]:ILE:HA	1.83	0.42
27:O:302:PSC:H012	27:O:302:PSC:O13	2.20	0.42
3:P:24:ALA:HB2	18:P:301:PGV:C11	2.49	0.42
3:P:127[A]:LEU:N	3:P:127[A]:LEU:CD2	2.83	0.42
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.68	0.42
1:A:113[B]:LEU:CD2	1:A:117[B]:MET:SD	3.08	0.42
14:A:601:HEA:H271	14:A:601:HEA:H212	1.83	0.42
24:G:102:PEK:C22	30:G:227:HOH:O	2.64	0.42
1:N:280:ILE:HG13	1:N:315:PRO:HB2	2.00	0.42
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.02	0.42
1:A:71:MET:CE	1:A:195:LEU:HD21	2.50	0.41
1:N:37:ILE:HD11	1:N:58:VAL:HA	2.02	0.41
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.41
1:N:379[B]:TYR:CD1	1:N:383[B]:MET:SD	3.13	0.41
2:O:41:ILE:HD13	27:O:302:PSC:H342	2.01	0.41
7:G:3:ALA:O	7:G:4:ALA:CB	2.69	0.41
7:G:18[A]:PHE:CZ	1:N:278[A]:MET:HE1	2.55	0.41
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.84	0.41
30:A:702:HOH:O	21:D:201:TGL:CG2	2.68	0.41
2:O:116:LEU:HD12	2:O:117:SER:H	1.85	0.41
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.21	0.41
1:A:140:GLY:O	1:A:213:ARG:NH2	2.53	0.41
4:D:118:LYS:HA	11:K:51:LYS:O	2.21	0.41
1:N:440:TYR:CZ	2:O:205:SER:HA	2.56	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.20	0.41
2:B:113:TYR:OH	8:H:12:GLN:HA	2.20	0.41
8:H:44:THR:O	8:H:44:THR:HG22	2.20	0.41
3:C:77:LYS:O	3:C:80:ARG:HB2	2.20	0.41
23:C:301:DMU:H10	10:J:49:CYS:HB3	2.02	0.41
1:N:113[B]:LEU:HD11	1:N:117[B]:MET:SD	2.60	0.41
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.03	0.41
1:N:486:ASP:OD2	4:Q:19:ARG:HD3	2.21	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ALA:HB1	2:B:18[A]:GLU:HG3	2.02	0.41
23:C:301:DMU:H36	23:C:301:DMU:O55	2.21	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.03	0.41
1:N:424:THR:HG21	14:N:601:HEA:HMB2	2.02	0.41
1:N:440:TYR:CE1	2:O:205:SER:HA	2.55	0.41
2:O:129:LYS:O	2:O:132:GLU:HB2	2.21	0.41
10:W:6:ALA:HA	10:W:9:GLN:OE1	2.21	0.41
2:B:98:LYS:HB2	2:B:109:GLU:HB2	2.03	0.41
8:U:85:ILE:OXT	8:U:85:ILE:HG22	2.21	0.41
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.93	0.41
1:A:44:PRO:HG3	1:A:448:THR:OG1	2.21	0.40
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.89	0.40
14:N:602:HEA:HMD1	14:N:602:HEA:HBD1	2.03	0.40
3:C:241:TYR:O	3:C:244:PHE:HB3	2.20	0.40
23:C:301:DMU:H21	10:J:50:LEU:HB2	2.02	0.40
25:G:101:CDL:H241	25:G:101:CDL:C53	2.51	0.40
10:J:6:ALA:HA	10:J:9:GLN:OE1	2.21	0.40
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.22	0.40
1:A:311[B]:ILE:HG22	25:T:105:CDL:H441	2.03	0.40
1:A:350:VAL:HG11	1:A:379[B]:TYR:CE2	2.56	0.40
2:B:222:TRP:CE2	2:B:226:MET:HG3	2.56	0.40
3:C:37:PHE:CE2	23:C:301:DMU:H12	2.56	0.40
3:C:51[A]:MET:SD	3:C:54[A]:MET:HE2	2.62	0.40
8:H:75:ARG:HG2	8:H:80:THR:OG1	2.22	0.40
1:N:240:HIS:CD2	1:N:240:HIS:C	2.94	0.40
1:N:324:LEU:HD13	2:O:41:ILE:HG22	2.02	0.40
9:V:21:ILE:HD13	9:V:21:ILE:HA	1.94	0.40
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.56	0.40
4:D:122:ARG:HG2	4:D:126:MET:CE	2.51	0.40
5:E:5:HIS:N	30:E:306:HOH:O	2.53	0.40
1:N:181:THR:HA	1:N:182:PRO:HD3	1.93	0.40
1:N:306:THR:O	1:N:310:MET:HG3	2.22	0.40
7:T:70[A]:PHE:O	24:T:102:PEK:N	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/514 (104%)	507 (95%)	24 (4%)	1 (0%)	47	57
1	N	533/514 (104%)	514 (96%)	19 (4%)	0	100	100
2	B	231/227 (102%)	218 (94%)	12 (5%)	1 (0%)	34	41
2	O	230/227 (101%)	213 (93%)	16 (7%)	1 (0%)	34	41
3	C	265/261 (102%)	258 (97%)	7 (3%)	0	100	100
3	P	265/261 (102%)	256 (97%)	7 (3%)	2 (1%)	19	22
4	D	148/147 (101%)	142 (96%)	6 (4%)	0	100	100
4	Q	143/147 (97%)	132 (92%)	11 (8%)	0	100	100
5	E	104/109 (95%)	103 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	101/98 (103%)	92 (91%)	4 (4%)	5 (5%)	2	0
6	S	97/98 (99%)	88 (91%)	8 (8%)	1 (1%)	15	16
7	G	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	1
7	T	84/85 (99%)	71 (84%)	9 (11%)	4 (5%)	2	1
8	H	77/85 (91%)	66 (86%)	9 (12%)	2 (3%)	5	3
8	U	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	12	11
9	I	70/73 (96%)	67 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
11	K	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
11	X	48/56 (86%)	45 (94%)	2 (4%)	1 (2%)	7	5
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3591/3614 (99%)	3393 (94%)	174 (5%)	24 (1%)	22	25

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
6	F	96	LEU
6	F	97	ALA
7	G	4	ALA
7	G	8	HIS
8	H	10	ASN
13	M	42	LYS
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
1	A	50	ASP
7	G	43	GLU
8	H	48	GLY
3	P	38	ASN
7	T	3	ALA
7	G	5	LYS
3	P	232	HIS
6	S	96	LEU
8	U	8	ILE
11	X	12	LYS
6	F	65	ASP
2	O	112	ASP
2	B	130	PRO
6	F	93	PRO

### 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	444/426 (104%)	435 (98%)	9 (2%)	55	67
1	N	445/426 (104%)	432 (97%)	13 (3%)	42	53
2	B	216/210 (103%)	202 (94%)	14 (6%)	17	21
2	O	215/210 (102%)	202 (94%)	13 (6%)	19	24
3	C	232/226 (103%)	220 (95%)	12 (5%)	23	30
3	P	232/226 (103%)	225 (97%)	7 (3%)	41	52
4	D	134/129 (104%)	131 (98%)	3 (2%)	52	64
4	Q	129/129 (100%)	125 (97%)	4 (3%)	40	52
5	E	93/95 (98%)	92 (99%)	1 (1%)	73	82
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	64
6	F	86/81 (106%)	83 (96%)	3 (4%)	36	47
6	S	82/81 (101%)	78 (95%)	4 (5%)	25	32
7	G	68/68 (100%)	59 (87%)	9 (13%)	4	3
7	T	70/68 (103%)	62 (89%)	8 (11%)	5	5
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	7
8	U	71/75 (95%)	64 (90%)	7 (10%)	8	7
9	I	57/57 (100%)	57 (100%)	0	100	100
9	V	58/57 (102%)	56 (97%)	2 (3%)	37	48
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	67
10	W	49/50 (98%)	46 (94%)	3 (6%)	18	24
11	K	40/46 (87%)	39 (98%)	1 (2%)	47	60
11	X	40/46 (87%)	37 (92%)	3 (8%)	13	16
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	31
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	58
13	M	37/38 (97%)	36 (97%)	1 (3%)	44	57
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	13
All	All	3125/3082 (101%)	2992 (96%)	133 (4%)	31	38

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	180	GLN
1	A	238	PHE

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Mol	Chain	Res	Type
1	A	290	HIS
1	A	369	ASP
1	A	380[A]	VAL
1	A	380[B]	VAL
1	A	381[A]	LEU
1	A	381[B]	LEU
2	B	42	ILE
2	B	60	GLU
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	115	ASP
2	B	130	PRO
2	B	167	SER
2	B	171	LYS
2	B	183	THR
2	B	187	SER
2	B	205	SER
2	B	225	SER
3	C	3	HIS
3	C	14	SER
3	C	41	THR
3	C	127	LEU
3	C	144[A]	ILE
3	C	144[B]	ILE
3	C	159	MET
3	C	180[A]	GLU
3	C	180[B]	GLU
3	C	214	PHE
3	C	223	LEU
3	C	230	ASN
4	D	8	SER
4	D	20	ARG
4	D	121	LYS
5	E	70	VAL
6	F	48	LEU
6	F	53	THR
6	F	96	LEU
7	G	2	SER
7	G	7	ASP
7	G	8	HIS

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Mol	Chain	Res	Type
7	G	18[A]	PHE
7	G	18[B]	PHE
7	G	36	TRP
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	46	LYS
8	H	60	TYR
8	H	61	LYS
10	J	27	THR
11	K	20	SER
12	L	26	THR
12	L	27	LEU
13	M	38	ASP
1	N	38	ARG
1	N	109	PHE
1	N	112	LEU
1	N	115[A]	SER
1	N	115[B]	SER
1	N	152	LEU
1	N	180	GLN
1	N	189	MET
1	N	338	MET
1	N	369	ASP
1	N	380[A]	VAL
1	N	380[B]	VAL
1	N	484	THR
2	O	16	ILE
2	O	59	GLN
2	O	65	TRP
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	107	SER
2	O	115	ASP
2	O	167	SER
2	O	203[A]	ASN
2	O	203[B]	ASN

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Mol	Chain	Res	Type
2	O	221	LYS
2	O	226	MET
3	P	14	SER
3	P	150	SER
3	P	159	MET
3	P	180[A]	GLU
3	P	180[B]	GLU
3	P	223	LEU
3	P	230	ASN
4	Q	7	LYS
4	Q	15	SER
4	Q	58	GLU
4	Q	147	LYS
5	R	7	THR
5	R	79	LYS
6	S	2	SER
6	S	54	ASN
6	S	95	GLN
6	S	96	LEU
7	T	2	SER
7	T	18	PHE
7	T	35	SER
7	T	36[A]	TRP
7	T	36[B]	TRP
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	7	LYS
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	49	ASP
8	U	60	TYR
8	U	84	LYS
9	V	18	ARG
9	V	42	LYS
10	W	10	LYS
10	W	50	LEU
10	W	58	LYS
11	X	23	THR
11	X	49	THR
11	X	52	GLU

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Mol	Chain	Res	Type
12	Y	20	ARG
13	Z	13	LYS
13	Z	19	LEU
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	68	GLN
3	C	76	GLN
3	C	230	ASN
4	D	32	ASN
4	D	37	GLN
5	E	94	ASN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
10	J	29	ASN
12	L	42	HIS
1	N	43	GLN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	92	ASN
3	P	68	GLN
3	P	70	HIS
4	Q	37	GLN
5	R	94	ASN

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Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
8	U	37	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	A	1	1	8,9,10	0.53	0	7,9,11	0.82	0
7	TPO	T	11	7	8,10,11	0.78	0	10,14,16	1.01	0
7	TPO	G	11	7	8,10,11	1.28	1 (12%)	10,14,16	0.85	0
2	FME	O	1	2	8,9,10	0.50	0	7,9,11	0.79	0
1	FME	N	1	1	8,9,10	0.45	0	7,9,11	0.84	0
2	FME	B	1	2	8,9,10	0.56	0	7,9,11	1.37	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
7	TPO	G	11	7	-	6/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
2	FME	B	1	2	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.15	1.65	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-2.70	118.68	122.82
2	B	1	FME	C-CA-N	2.15	113.62	109.73

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
2	B	1	FME	CB-CA-N-CN
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	CA-CB-OG1-P
7	G	11	TPO	CB-OG1-P-O1P
1	N	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CA-CB-OG1-P
1	A	1	FME	CB-CG-SD-CE
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CA-N-CN
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	2	0
2	O	1	FME	3	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 54 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	$\# Z  > 2$
19	EDO	G	104	-	3,3,3	0.16	0	2,2,2	0.12	0
25	CDL	G	101	-	99,99,99	0.40	0	105,111,111	0.51	1 (0%)
23	DMU	C	301	-	34,34,34	1.62	6 (17%)	45,45,45	1.49	7 (15%)
26	CHD	C	305	-	32,32,32	0.57	0	51,51,51	0.80	0
21	TGL	Y	101	-	62,62,62	0.33	0	65,65,65	0.30	0
23	DMU	D	202	-	34,34,34	1.00	1 (2%)	45,45,45	1.51	5 (11%)
26	CHD	T	101	-	32,32,32	0.57	0	51,51,51	0.93	0
25	CDL	T	105	-	99,99,99	0.33	0	105,111,111	0.41	0
19	EDO	S	103	-	3,3,3	0.18	0	2,2,2	0.15	0
26	CHD	J	101	-	32,32,32	0.71	0	51,51,51	1.10	3 (5%)
24	PEK	C	302	-	52,52,52	0.29	0	55,57,57	0.60	0
21	TGL	B	301	-	62,62,62	0.36	0	65,65,65	0.46	1 (1%)
24	PEK	G	102	-	52,52,52	0.33	0	55,57,57	0.46	0
14	HEA	A	601	1	57,67,67	2.15	17 (29%)	61,103,103	2.47	22 (36%)
18	PGV	P	303	-	50,50,50	0.31	0	53,56,56	0.49	0
26	CHD	P	306	-	32,32,32	0.64	0	51,51,51	1.03	5 (9%)
24	PEK	T	103	-	52,52,52	0.36	0	55,57,57	0.50	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-
18	PGV	A	606	-	50,50,50	0.38	0	53,56,56	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	CDL	P	304	-	99,99,99	0.37	0	105,111,111	0.45	1 (0%)
19	EDO	C	309	-	3,3,3	0.13	0	2,2,2	0.16	0
19	EDO	N	607	-	3,3,3	0.17	0	2,2,2	0.28	0
19	EDO	T	106	-	3,3,3	0.35	0	2,2,2	0.40	0
18	PGV	C	308	-	50,50,50	0.47	0	53,56,56	0.52	0
18	PGV	C	303	-	50,50,50	0.35	0	53,56,56	0.62	1 (1%)
21	TGL	N	606	-	62,62,62	0.34	0	65,65,65	0.42	0
22	CUA	O	301	2	0,1,1	-	-	-	-	-
27	PSC	E	201	-	51,51,51	0.33	0	57,59,59	0.42	0
14	HEA	N	602	1	57,67,67	1.96	13 (22%)	61,103,103	2.48	24 (39%)
21	TGL	L	101	-	62,62,62	0.36	0	65,65,65	0.47	0
21	TGL	Q	201	-	62,62,62	0.38	0	65,65,65	0.49	2 (3%)
14	HEA	A	602	1	57,67,67	1.95	16 (28%)	61,103,103	2.56	26 (42%)
18	PGV	A	607	-	50,50,50	0.36	0	53,56,56	0.50	0
24	PEK	T	102	-	52,52,52	0.27	0	55,57,57	0.62	2 (3%)
25	CDL	C	304	-	99,99,99	0.38	0	105,111,111	0.39	0
19	EDO	S	102	-	3,3,3	0.18	0	2,2,2	0.14	0
18	PGV	Z	101	-	50,50,50	0.39	0	53,56,56	0.77	1 (1%)
27	PSC	O	302	-	51,51,51	0.34	0	57,59,59	0.50	1 (1%)
19	EDO	A	608	-	3,3,3	0.23	0	2,2,2	0.20	0
18	PGV	P	301	-	50,50,50	0.32	0	53,56,56	0.52	0
14	HEA	N	601	1	57,67,67	1.96	14 (24%)	61,103,103	2.31	22 (36%)
19	EDO	A	609	-	3,3,3	0.08	0	2,2,2	0.34	0
18	PGV	P	302	-	50,50,50	0.39	0	53,56,56	0.44	0
26	CHD	C	306	-	32,32,32	0.50	0	51,51,51	0.64	0
24	PEK	T	104	-	52,52,52	0.41	0	55,57,57	0.56	1 (1%)
26	CHD	W	102	-	32,32,32	0.67	0	51,51,51	0.85	2 (3%)
29	SAC	V	101	-	7,8,9	0.52	0	8,9,11	0.92	1 (12%)
29	SAC	I	101	-	7,8,9	0.53	0	8,9,11	1.21	1 (12%)
21	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.64	2 (3%)
23	DMU	W	101	-	34,34,34	2.02	9 (26%)	45,45,45	1.78	12 (26%)
26	CHD	P	305	-	32,32,32	0.61	0	51,51,51	0.75	0
26	CHD	G	103	-	32,32,32	0.58	0	51,51,51	0.73	0
24	PEK	C	307	-	52,52,52	0.43	0	55,57,57	0.49	0
23	DMU	Z	102	-	34,34,34	1.09	3 (8%)	45,45,45	1.14	3 (6%)

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
19	EDO	G	104	-	-	1/1/1/1	-
25	CDL	G	101	-	-	60/110/110/110	-
23	DMU	C	301	-	-	12/19/59/59	0/2/2/2
26	CHD	C	305	-	-	5/9/74/74	0/4/4/4
21	TGL	Y	101	-	-	37/65/65/65	-
23	DMU	D	202	-	-	10/19/59/59	0/2/2/2
26	CHD	T	101	-	-	2/9/74/74	0/4/4/4
25	CDL	T	105	-	-	56/110/110/110	-
19	EDO	S	103	-	-	0/1/1/1	-
26	CHD	J	101	-	-	4/9/74/74	0/4/4/4
24	PEK	C	302	-	-	13/56/56/56	-
21	TGL	B	301	-	-	31/65/65/65	-
24	PEK	G	102	-	-	28/56/56/56	-
14	HEA	A	601	1	3/3/7/16	6/32/76/76	-
18	PGV	P	303	-	-	12/55/55/55	-
26	CHD	P	306	-	-	1/9/74/74	0/4/4/4
24	PEK	T	103	-	-	29/56/56/56	-
18	PGV	A	606	-	-	11/55/55/55	-
25	CDL	P	304	-	-	59/110/110/110	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	607	-	-	0/1/1/1	-
19	EDO	T	106	-	-	0/1/1/1	-
18	PGV	C	308	-	-	37/55/55/55	-
18	PGV	C	303	-	-	13/55/55/55	-
21	TGL	N	606	-	-	34/65/65/65	-
27	PSC	E	201	-	-	25/55/55/55	-
14	HEA	N	602	1	3/3/7/16	6/32/76/76	-
21	TGL	L	101	-	-	38/65/65/65	-
21	TGL	Q	201	-	-	33/65/65/65	-
18	PGV	A	607	-	1/1/5/7	34/55/55/55	-
14	HEA	A	602	1	3/3/7/16	4/32/76/76	-
24	PEK	T	102	-	-	17/56/56/56	-
25	CDL	C	304	-	-	69/110/110/110	-
19	EDO	S	102	-	-	0/1/1/1	-
18	PGV	Z	101	-	-	31/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PSC	O	302	-	-	23/55/55/55	-
19	EDO	A	608	-	-	1/1/1/1	-
18	PGV	P	301	-	-	13/55/55/55	-
14	HEA	N	601	1	3/3/7/16	8/32/76/76	-
19	EDO	A	609	-	-	0/1/1/1	-
18	PGV	P	302	-	-	22/55/55/55	-
26	CHD	C	306	-	-	0/9/74/74	0/4/4/4
26	CHD	W	102	-	1/1/12/12	4/9/74/74	0/4/4/4
24	PEK	T	104	-	-	23/56/56/56	-
29	SAC	V	101	-	-	3/7/8/10	-
29	SAC	I	101	-	-	4/7/8/10	-
21	TGL	D	201	-	-	36/65/65/65	-
23	DMU	W	101	-	-	4/19/59/59	0/2/2/2
26	CHD	P	305	-	-	6/9/74/74	0/4/4/4
26	CHD	G	103	-	-	4/9/74/74	0/4/4/4
24	PEK	C	307	-	-	24/56/56/56	-
23	DMU	Z	102	-	-	5/19/59/59	0/2/2/2

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	101	DMU	O16-C6	6.96	1.52	1.40
23	C	301	DMU	O16-C6	6.15	1.50	1.40
14	N	601	HEA	C3B-C2B	5.57	1.47	1.34
14	A	601	HEA	C3D-C2D	5.40	1.48	1.36
14	A	601	HEA	CHD-C1D	5.20	1.48	1.35
14	A	601	HEA	C3A-C2A	5.07	1.47	1.40
14	A	601	HEA	C4B-NB	-4.79	1.32	1.40
14	A	601	HEA	C3C-C2C	4.78	1.47	1.40
14	A	602	HEA	C1D-ND	-4.78	1.32	1.40
14	A	601	HEA	CHC-C4B	4.74	1.47	1.35
14	N	601	HEA	C3D-C2D	4.72	1.46	1.36
14	A	602	HEA	CHC-C4B	4.66	1.46	1.35
14	N	602	HEA	C3C-C2C	4.55	1.46	1.40
14	N	602	HEA	C3B-C2B	4.54	1.45	1.34
14	N	602	HEA	C3A-C2A	4.50	1.46	1.40
14	A	602	HEA	C3D-C2D	4.48	1.46	1.36
14	N	601	HEA	CHC-C4B	4.36	1.46	1.35
14	N	601	HEA	CHD-C1D	4.30	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C3D-C2D	4.30	1.45	1.36
14	N	602	HEA	C4B-NB	-4.20	1.33	1.40
14	N	602	HEA	CHC-C4B	4.19	1.45	1.35
14	N	602	HEA	C1D-ND	-4.19	1.33	1.40
14	A	601	HEA	C3B-C2B	4.13	1.44	1.34
14	A	602	HEA	C3B-C2B	4.13	1.44	1.34
14	N	602	HEA	CHD-C1D	4.11	1.45	1.35
14	N	601	HEA	C3A-C2A	4.08	1.46	1.40
14	A	602	HEA	C4B-NB	-4.06	1.33	1.40
14	A	602	HEA	C1B-NB	-4.05	1.30	1.38
23	W	101	DMU	O1-C10	3.94	1.51	1.41
14	N	601	HEA	C3C-C2C	3.93	1.45	1.40
14	A	602	HEA	CHD-C1D	3.79	1.44	1.35
23	W	101	DMU	C8-C9	3.70	1.60	1.53
14	N	601	HEA	C4B-NB	-3.54	1.34	1.40
23	Z	102	DMU	C8-C9	3.36	1.60	1.53
23	W	101	DMU	O1-C9	3.34	1.52	1.44
23	C	301	DMU	O5-C6	3.33	1.50	1.41
14	N	601	HEA	C1D-ND	-3.27	1.34	1.40
14	N	602	HEA	C4D-ND	-3.19	1.32	1.38
14	A	601	HEA	C4D-ND	-3.18	1.32	1.38
23	W	101	DMU	O7-C10	3.16	1.50	1.41
14	A	602	HEA	C3A-C2A	3.13	1.44	1.40
14	A	602	HEA	C4D-ND	-3.03	1.32	1.38
14	N	601	HEA	C2A-C1A	3.00	1.49	1.42
14	N	601	HEA	C4D-ND	-2.99	1.32	1.38
14	A	602	HEA	C2A-C1A	2.98	1.49	1.42
14	A	602	HEA	C3C-C2C	2.98	1.44	1.40
14	A	601	HEA	C4C-CHD	2.95	1.49	1.41
14	A	601	HEA	C2A-C1A	2.93	1.49	1.42
23	C	301	DMU	O7-C10	2.85	1.49	1.41
14	N	602	HEA	C2A-C1A	2.84	1.49	1.42
23	W	101	DMU	O5-C6	2.82	1.49	1.41
14	A	601	HEA	C1B-NB	-2.82	1.33	1.38
14	N	602	HEA	C1B-NB	-2.76	1.33	1.38
14	A	602	HEA	C1C-CHC	2.57	1.48	1.41
14	A	601	HEA	C1D-ND	-2.56	1.35	1.40
14	N	601	HEA	C4C-CHD	2.56	1.48	1.41
23	D	202	DMU	O1-C10	2.55	1.48	1.41
23	Z	102	DMU	O16-C6	2.52	1.44	1.40
14	N	601	HEA	FE-ND	2.52	2.09	1.96
14	N	601	HEA	FE-NB	2.47	2.09	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	101	DMU	O5-C4	2.32	1.50	1.44
14	A	601	HEA	C12-C11	-2.27	1.48	1.52
14	A	601	HEA	CHB-C1B	2.27	1.47	1.41
14	A	602	HEA	C4B-C3B	2.25	1.48	1.44
14	N	602	HEA	C4C-CHD	2.23	1.47	1.41
14	A	601	HEA	FE-NB	2.22	2.07	1.96
23	W	101	DMU	O16-C18	2.21	1.49	1.43
23	C	301	DMU	C6-C1	2.20	1.58	1.52
14	A	601	HEA	FE-ND	2.16	2.07	1.96
14	A	602	HEA	FE-NB	2.16	2.07	1.96
23	W	101	DMU	C6-C1	2.15	1.58	1.52
23	Z	102	DMU	O7-C10	2.15	1.47	1.41
14	N	602	HEA	FE-NB	2.12	2.07	1.96
23	C	301	DMU	O16-C18	2.10	1.48	1.43
23	C	301	DMU	O1-C10	2.08	1.47	1.41
14	A	602	HEA	C1B-C2B	2.07	1.48	1.44
14	N	601	HEA	C1C-CHC	2.05	1.46	1.41
14	A	601	HEA	C1B-C2B	2.03	1.48	1.44
14	A	602	HEA	CHA-C4D	2.02	1.46	1.41

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C13-C12-C11	-7.67	102.82	114.35
14	N	602	HEA	C3D-C4D-ND	7.05	117.18	110.36
14	A	602	HEA	C2B-C1B-NB	6.64	117.83	109.88
23	D	202	DMU	C18-O16-C6	5.83	123.51	113.84
14	N	602	HEA	C3B-C4B-NB	5.81	116.73	109.84
14	N	601	HEA	C1D-C2D-C3D	-5.61	101.06	106.96
14	N	601	HEA	C13-C12-C11	-5.60	105.94	114.35
14	N	602	HEA	C2B-C1B-NB	5.38	116.33	109.88
14	A	602	HEA	C3D-C4D-ND	5.35	115.54	110.36
14	A	602	HEA	C3B-C4B-NB	5.09	115.87	109.84
14	N	601	HEA	C2D-C1D-ND	5.02	115.79	109.84
14	A	602	HEA	CMB-C2B-C1B	5.00	132.65	125.04
14	N	601	HEA	C3D-C4D-ND	4.98	115.18	110.36
14	A	601	HEA	C3B-C4B-NB	4.94	115.70	109.84
14	A	601	HEA	C2B-C1B-NB	4.86	115.70	109.88
23	W	101	DMU	C18-O16-C6	4.79	121.78	113.84
14	N	601	HEA	C3B-C4B-NB	4.78	115.50	109.84
14	A	601	HEA	C3D-C4D-ND	4.75	114.96	110.36
14	A	602	HEA	C1B-C2B-C3B	-4.69	101.19	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C4A-CHB-C1B	4.69	128.75	122.56
14	N	602	HEA	CHA-C4D-C3D	-4.59	118.10	124.84
14	N	602	HEA	C2D-C1D-ND	4.58	115.26	109.84
14	A	602	HEA	CHA-C4D-C3D	-4.53	118.19	124.84
14	A	601	HEA	C1D-C2D-C3D	-4.41	102.31	106.96
23	W	101	DMU	C10-O1-C9	4.36	122.24	113.69
14	N	602	HEA	C1D-C2D-C3D	-4.29	102.45	106.96
14	A	602	HEA	C1D-C2D-C3D	-4.27	102.47	106.96
14	A	601	HEA	C1B-C2B-C3B	-4.25	101.71	106.80
14	A	602	HEA	C4D-CHA-C1A	4.19	128.08	122.56
14	A	601	HEA	C2D-C1D-ND	4.18	114.79	109.84
14	A	602	HEA	C2D-C1D-ND	4.00	114.58	109.84
23	C	301	DMU	C18-O16-C6	4.00	120.47	113.84
23	W	101	DMU	C6-O5-C4	3.98	121.49	113.69
14	N	601	HEA	C2B-C1B-NB	3.96	114.63	109.88
14	N	602	HEA	C4D-CHA-C1A	3.86	127.65	122.56
26	J	101	CHD	C5-C6-C7	3.85	118.71	114.46
14	A	601	HEA	C4A-CHB-C1B	3.76	127.51	122.56
14	N	602	HEA	C1B-C2B-C3B	-3.74	102.33	106.80
14	A	601	HEA	C26-C15-C16	3.65	121.41	115.27
14	A	601	HEA	CMC-C2C-C3C	3.62	131.46	124.68
14	A	602	HEA	CAD-C3D-C2D	3.58	134.54	127.88
14	N	602	HEA	C3C-C4C-NC	3.47	113.70	109.21
14	A	602	HEA	C3C-C4C-NC	3.43	113.64	109.21
14	N	602	HEA	CHB-C1B-C2B	-3.42	119.64	124.98
14	N	602	HEA	C4D-C3D-C2D	-3.39	101.96	106.90
14	A	601	HEA	C4D-CHA-C1A	3.37	127.00	122.56
14	A	602	HEA	C13-C12-C11	-3.34	109.33	114.35
14	N	601	HEA	C4D-CHA-C1A	3.33	126.95	122.56
14	A	601	HEA	CMB-C2B-C1B	3.33	130.11	125.04
14	A	601	HEA	CHA-C4D-C3D	-3.32	119.97	124.84
14	A	602	HEA	CHB-C1B-C2B	-3.25	119.90	124.98
14	N	602	HEA	OMA-CMA-C3A	-3.22	117.89	124.91
14	A	601	HEA	CAA-CBA-CGA	-3.15	104.92	113.76
23	W	101	DMU	O16-C6-C1	3.15	113.22	108.30
14	N	602	HEA	CAD-C3D-C2D	3.12	133.68	127.88
14	N	602	HEA	C4B-C3B-C2B	-3.10	102.11	107.41
14	A	601	HEA	C3C-C4C-NC	3.08	113.20	109.21
18	Z	101	PGV	O01-C1-C2	3.08	118.13	111.50
14	N	601	HEA	C27-C19-C20	3.06	120.42	115.27
14	N	601	HEA	C4B-C3B-C2B	-3.05	102.21	107.41
21	D	201	TGL	CG2-OG2-CB1	3.03	125.26	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601	HEA	C3C-C4C-NC	2.99	113.08	109.21
14	N	602	HEA	CAD-CBD-CGD	-2.98	107.19	113.60
14	A	602	HEA	C4D-C3D-C2D	-2.97	102.56	106.90
23	D	202	DMU	O16-C18-C19	-2.94	99.25	109.56
14	A	602	HEA	CMC-C2C-C3C	2.94	130.18	124.68
14	N	601	HEA	CHA-C4D-C3D	-2.92	120.55	124.84
14	N	601	HEA	C1B-C2B-C3B	-2.91	103.33	106.80
29	I	101	SAC	O-C-CA	-2.90	117.17	124.78
14	N	602	HEA	CMB-C2B-C1B	2.88	129.43	125.04
14	N	602	HEA	CMC-C2C-C3C	2.88	130.07	124.68
23	C	301	DMU	C6-C1-C2	2.85	115.93	110.00
14	N	601	HEA	C4A-CHB-C1B	2.80	126.25	122.56
14	A	602	HEA	CAD-CBD-CGD	-2.79	107.60	113.60
23	C	301	DMU	C25-C22-C19	-2.79	100.28	114.42
14	N	601	HEA	C26-C15-C16	2.78	119.94	115.27
14	A	602	HEA	CAA-CBA-CGA	-2.77	105.99	113.76
14	A	602	HEA	C4B-C3B-C2B	-2.75	102.70	107.41
14	N	601	HEA	CMB-C2B-C1B	2.74	129.21	125.04
23	W	101	DMU	O7-C10-O1	2.72	118.26	110.67
14	N	601	HEA	OMA-CMA-C3A	-2.67	119.10	124.91
14	A	601	HEA	C4D-C3D-C2D	-2.65	103.04	106.90
23	W	101	DMU	C28-C25-C22	-2.64	101.01	114.42
14	A	602	HEA	C4B-NB-C1B	-2.59	102.40	105.07
14	A	601	HEA	C17-C18-C19	-2.58	121.44	127.66
14	N	601	HEA	C17-C18-C19	-2.57	121.47	127.66
23	C	301	DMU	C10-O1-C9	2.56	118.70	113.69
23	C	301	DMU	C2-C3-C4	-2.55	105.09	110.93
24	T	104	PEK	O01-C1-C2	2.54	116.98	111.50
14	N	601	HEA	CAA-CBA-CGA	-2.54	106.64	113.76
14	N	602	HEA	C4B-NB-C1B	-2.50	102.49	105.07
23	Z	102	DMU	C22-C19-C18	-2.50	102.42	113.49
25	G	101	CDL	OB6-CB5-C51	2.47	116.82	111.50
23	W	101	DMU	O1-C9-C11	2.45	112.53	106.44
26	P	306	CHD	C13-C17-C20	2.44	122.41	119.50
14	A	601	HEA	CHB-C1B-C2B	-2.43	121.18	124.98
29	V	101	SAC	O-C-CA	-2.42	118.44	124.78
14	N	602	HEA	CHC-C4B-C3B	-2.41	119.59	125.80
23	D	202	DMU	O1-C9-C11	2.39	112.39	106.44
21	D	201	TGL	OG2-CG2-CG3	2.39	117.06	108.40
14	A	601	HEA	C4B-C3B-C2B	-2.39	103.33	107.41
21	B	301	TGL	OG2-CB1-CB2	2.37	116.61	111.50
14	N	601	HEA	CMC-C2C-C3C	2.37	129.10	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	303	PGV	O12-P-O13	-2.37	99.82	109.07
23	Z	102	DMU	O7-C10-C5	2.36	114.22	108.10
27	O	302	PSC	O01-C1-C2	2.36	116.58	111.50
14	A	601	HEA	CHC-C4B-C3B	-2.35	119.74	125.80
14	N	601	HEA	CHC-C4B-C3B	-2.35	119.75	125.80
14	N	602	HEA	C27-C19-C20	2.33	119.19	115.27
26	W	102	CHD	C9-C10-C5	2.29	111.80	108.58
26	P	306	CHD	C11-C12-C13	2.28	113.58	111.24
23	W	101	DMU	O49-C1-C2	-2.26	105.11	110.35
21	Q	201	TGL	OG2-CB1-CB2	2.26	116.37	111.50
23	W	101	DMU	O16-C18-C19	-2.25	101.67	109.56
14	N	601	HEA	C16-C15-C14	-2.25	116.56	121.12
23	W	101	DMU	O5-C4-C3	2.25	114.49	109.75
14	A	601	HEA	OMA-CMA-C3A	-2.24	120.02	124.91
23	W	101	DMU	C7-C8-C9	2.24	114.24	110.24
23	C	301	DMU	C10-O7-C3	-2.24	112.42	117.96
21	Q	201	TGL	OG2-CB1-OB1	-2.22	118.33	123.70
14	A	602	HEA	CMB-C2B-C3B	-2.19	126.16	130.34
23	C	301	DMU	O49-C1-C2	-2.18	105.30	110.35
26	P	306	CHD	C9-C11-C12	2.18	117.18	114.30
26	J	101	CHD	C14-C8-C9	2.18	112.70	109.71
26	P	306	CHD	C10-C9-C8	-2.18	109.48	111.82
14	N	602	HEA	C4A-CHB-C1B	2.18	125.43	122.56
25	P	304	CDL	OA6-CA5-C11	2.17	116.18	111.50
14	N	602	HEA	O2A-CGA-CBA	2.17	121.00	114.03
24	T	102	PEK	O13-P-O14	2.17	122.96	112.24
14	A	602	HEA	OMA-CMA-C3A	-2.16	120.20	124.91
26	P	306	CHD	C16-C17-C13	-2.13	101.46	103.55
23	W	101	DMU	C37-C34-C31	-2.12	103.65	114.42
14	A	601	HEA	CBA-CAA-C2A	2.12	116.17	112.60
14	N	602	HEA	C26-C15-C16	2.10	118.81	115.27
26	J	101	CHD	C6-C5-C10	2.10	114.89	112.66
14	A	602	HEA	CHB-C1B-NB	-2.10	122.15	124.43
23	D	202	DMU	O5-C4-C57	2.09	111.64	106.44
23	Z	102	DMU	C6-O5-C4	-2.09	109.58	113.69
23	D	202	DMU	O16-C6-C1	-2.09	105.04	108.30
26	W	102	CHD	C6-C5-C10	2.08	114.87	112.66
14	A	602	HEA	CHD-C1D-C2D	-2.05	121.06	126.72
14	A	602	HEA	C13-C14-C15	-2.04	122.75	127.66
24	T	102	PEK	O11-P-O14	-2.04	101.11	109.07
14	N	601	HEA	CHD-C1D-C2D	-2.03	121.09	126.72
14	A	602	HEA	CHC-C4B-C3B	-2.01	120.61	125.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C16-C15-C14	-2.00	117.06	121.12

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	NB
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	602	HEA	NB
14	A	602	HEA	ND
14	A	602	HEA	NA
14	N	601	HEA	NB
14	N	601	HEA	ND
14	N	601	HEA	NA
14	N	602	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NA
18	A	607	PGV	C05
26	W	102	CHD	C3

All (899) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	HEA	C26-C15-C16-C17
14	A	602	HEA	C2D-C3D-CAD-CBD
14	N	602	HEA	C4D-C3D-CAD-CBD
18	A	607	PGV	C04-O12-P-O13
18	A	607	PGV	C04-O12-P-O14
18	A	607	PGV	C02-C03-O11-P
18	A	607	PGV	C04-C05-C06-O06
18	A	607	PGV	O05-C05-C06-O06
18	A	607	PGV	O02-C1-O01-C02
18	A	607	PGV	C2-C1-O01-C02
18	C	308	PGV	C03-O11-P-O13
18	C	308	PGV	C04-O12-P-O14
18	C	308	PGV	O03-C01-C02-O01
18	Z	101	PGV	C03-O11-P-O13
18	Z	101	PGV	C04-O12-P-O13
18	Z	101	PGV	O02-C1-O01-C02
18	Z	101	PGV	C2-C1-O01-C02
21	L	101	TGL	CB2-CB1-OG2-CG2
21	Q	201	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	OC1-CC1-OG3-CG3
23	C	301	DMU	C1-C6-O16-C18
23	C	301	DMU	O5-C6-O16-C18
23	D	202	DMU	C19-C18-O16-C6
24	C	307	PEK	O12-C04-C05-N
24	C	307	PEK	C5-C6-C7-C8
24	G	102	PEK	C04-O12-P-O11
24	G	102	PEK	C04-O12-P-O13
24	G	102	PEK	C04-O12-P-O14
24	G	102	PEK	O12-C04-C05-N
24	G	102	PEK	C5-C6-C7-C8
24	T	102	PEK	O12-C04-C05-N
24	T	102	PEK	C12-C13-C14-C15
24	T	103	PEK	C03-O11-P-O12
24	T	103	PEK	C03-O11-P-O14
24	T	103	PEK	O03-C01-C02-O01
24	T	103	PEK	O12-C04-C05-N
24	T	103	PEK	C12-C13-C14-C15
24	T	104	PEK	C04-O12-P-O11
24	T	104	PEK	C04-O12-P-O14
24	T	104	PEK	O12-C04-C05-N
25	C	304	CDL	CB2-C1-CA2-OA2
25	C	304	CDL	CA2-OA2-PA1-OA3
25	C	304	CDL	CA2-OA2-PA1-OA4
25	C	304	CDL	CA2-OA2-PA1-OA5
25	C	304	CDL	CA3-OA5-PA1-OA4
25	C	304	CDL	C11-CA5-OA6-CA4
25	C	304	CDL	CB2-OB2-PB2-OB4
25	C	304	CDL	CB2-OB2-PB2-OB5
25	G	101	CDL	CB3-OB5-PB2-OB2
25	G	101	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	CB3-OB5-PB2-OB4
25	P	304	CDL	CA2-OA2-PA1-OA3
25	P	304	CDL	CA2-OA2-PA1-OA4
25	P	304	CDL	CA2-OA2-PA1-OA5
25	P	304	CDL	CA3-OA5-PA1-OA4
25	P	304	CDL	C11-CA5-OA6-CA4
25	P	304	CDL	CB2-OB2-PB2-OB4
25	P	304	CDL	CB2-OB2-PB2-OB5
25	T	105	CDL	CA2-OA2-PA1-OA3
25	T	105	CDL	CA2-OA2-PA1-OA4
25	T	105	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
25	T	105	CDL	C1-CB2-OB2-PB2
25	T	105	CDL	CB2-OB2-PB2-OB4
27	E	201	PSC	C03-O11-P-O14
27	E	201	PSC	O12-C04-C05-N
27	O	302	PSC	O12-C04-C05-N
29	I	101	SAC	C-CA-CB-OG
29	V	101	SAC	O-C-CA-CB
29	V	101	SAC	N-CA-CB-OG
29	V	101	SAC	C-CA-CB-OG
21	D	201	TGL	OC1-CC1-OG3-CG3
21	Y	101	TGL	OA1-CA1-OG1-CG1
21	Q	201	TGL	CC2-CC1-OG3-CG3
21	Y	101	TGL	CA2-CA1-OG1-CG1
18	A	607	PGV	O04-C19-O03-C01
18	Z	101	PGV	O04-C19-O03-C01
21	L	101	TGL	OA1-CA1-OG1-CG1
21	L	101	TGL	OB1-CB1-OG2-CG2
25	P	304	CDL	OA7-CA5-OA6-CA4
18	A	607	PGV	C20-C19-O03-C01
18	Z	101	PGV	C20-C19-O03-C01
21	D	201	TGL	CC2-CC1-OG3-CG3
21	L	101	TGL	CC2-CC1-OG3-CG3
25	P	304	CDL	C31-CA7-OA8-CA6
21	Q	201	TGL	CB2-CB1-OG2-CG2
14	N	602	HEA	C2D-C3D-CAD-CBD
14	A	601	HEA	C14-C15-C16-C17
26	W	102	CHD	C20-C22-C23-C24
21	L	101	TGL	CA2-CA1-OG1-CG1
24	T	103	PEK	C22-C21-O03-C01
25	T	105	CDL	C71-CB7-OB8-CB6
23	C	301	DMU	O6-C11-C9-O1
14	A	602	HEA	C4D-C3D-CAD-CBD
25	C	304	CDL	OA7-CA5-OA6-CA4
25	T	105	CDL	OA7-CA5-OA6-CA4
24	T	103	PEK	O04-C21-O03-C01
25	P	304	CDL	OA9-CA7-OA8-CA6
25	T	105	CDL	OB9-CB7-OB8-CB6
25	C	304	CDL	C71-CB7-OB8-CB6
25	C	304	CDL	C51-CB5-OB6-CB4
25	T	105	CDL	C55-C56-C57-C58
25	T	105	CDL	C40-C41-C42-C43
23	W	101	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
18	C	308	PGV	C2-C3-C4-C5
21	L	101	TGL	CA2-CA3-CA4-CA5
21	L	101	TGL	OC1-CC1-OG3-CG3
25	C	304	CDL	OB9-CB7-OB8-CB6
14	N	601	HEA	C26-C15-C16-C17
14	N	601	HEA	C14-C15-C16-C17
27	O	302	PSC	O04-C19-O03-C01
14	N	601	HEA	C19-C20-C21-C22
27	O	302	PSC	C20-C19-O03-C01
26	P	305	CHD	C17-C20-C22-C23
21	D	201	TGL	OA1-CA1-OG1-CG1
25	T	105	CDL	C79-C80-C81-C82
25	P	304	CDL	CB2-C1-CA2-OA2
25	C	304	CDL	OB7-CB5-OB6-CB4
23	C	301	DMU	O6-C11-C9-C8
21	D	201	TGL	CA2-CA1-OG1-CG1
25	G	101	CDL	C31-CA7-OA8-CA6
25	G	101	CDL	C71-CB7-OB8-CB6
27	E	201	PSC	C20-C19-O03-C01
23	D	202	DMU	O6-C11-C9-O1
26	G	103	CHD	C17-C20-C22-C23
18	A	607	PGV	C20-C21-C22-C23
21	L	101	TGL	C18-C19-C33-C34
23	W	101	DMU	O5-C4-C57-O61
25	T	105	CDL	C62-C63-C64-C65
27	O	302	PSC	C19-C20-C21-C22
25	G	101	CDL	OA9-CA7-OA8-CA6
25	G	101	CDL	OB9-CB7-OB8-CB6
24	C	302	PEK	C22-C21-O03-C01
25	G	101	CDL	CB7-C71-C72-C73
27	E	201	PSC	C1-C2-C3-C4
27	O	302	PSC	C1-C2-C3-C4
26	P	305	CHD	C21-C20-C22-C23
21	B	301	TGL	CA1-CA2-CA3-CA4
25	P	304	CDL	CA7-C31-C32-C33
29	I	101	SAC	N-CA-CB-OG
27	E	201	PSC	C2-C1-O01-C02
21	N	606	TGL	C11-C12-C13-C14
21	L	101	TGL	C23-C24-C25-C26
25	C	304	CDL	O1-C1-CA2-OA2
25	P	304	CDL	O1-C1-CA2-OA2
27	E	201	PSC	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
27	E	201	PSC	O04-C19-O03-C01
23	D	202	DMU	O16-C18-C19-C22
25	G	101	CDL	C11-CA5-OA6-CA4
25	P	304	CDL	C51-CB5-OB6-CB4
18	A	607	PGV	C04-O12-P-O11
18	C	308	PGV	C04-O12-P-O11
18	P	302	PGV	C04-O12-P-O11
18	Z	101	PGV	C04-O12-P-O11
25	T	105	CDL	CA2-OA2-PA1-OA5
25	T	105	CDL	CA3-OA5-PA1-OA2
25	T	105	CDL	CB2-OB2-PB2-OB5
27	E	201	PSC	C04-O12-P-O11
18	A	607	PGV	C1-C2-C3-C4
23	Z	102	DMU	O16-C18-C19-C22
23	W	101	DMU	O1-C10-O7-C3
21	Y	101	TGL	OB1-CB1-OG2-CG2
24	T	104	PEK	O02-C1-O01-C02
25	G	101	CDL	OA7-CA5-OA6-CA4
18	P	301	PGV	C4-C5-C6-C7
26	P	305	CHD	C20-C22-C23-C24
18	C	308	PGV	C11-C10-C9-C8
18	P	301	PGV	C12-C13-C14-C15
18	P	302	PGV	C1-C2-C3-C4
25	T	105	CDL	CA7-C31-C32-C33
25	C	304	CDL	C40-C41-C42-C43
25	G	101	CDL	C43-C44-C45-C46
25	G	101	CDL	C81-C82-C83-C84
27	O	302	PSC	C2-C3-C4-C5
21	Y	101	TGL	CB2-CB1-OG2-CG2
24	T	104	PEK	C2-C1-O01-C02
18	A	607	PGV	C28-C29-C30-C31
18	C	303	PGV	C7-C8-C9-C10
18	C	308	PGV	C28-C29-C30-C31
21	D	201	TGL	CC6-CC7-CC8-CC9
21	N	606	TGL	CB4-CB5-CB6-CB7
23	Z	102	DMU	C22-C25-C28-C31
24	T	103	PEK	C34-C35-C36-C37
25	C	304	CDL	C42-C43-C44-C45
25	T	105	CDL	C14-C15-C16-C17
27	O	302	PSC	C25-C26-C27-C28
24	C	302	PEK	O04-C21-O03-C01
21	B	301	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
21	D	201	TGL	CA3-CA4-CA5-CA6
21	Q	201	TGL	CC6-CC7-CC8-CC9
21	Y	101	TGL	CB9-C10-C11-C12
25	C	304	CDL	C23-C24-C25-C26
25	C	304	CDL	C60-C61-C62-C63
25	G	101	CDL	C80-C81-C82-C83
25	P	304	CDL	C37-C38-C39-C40
18	A	607	PGV	C03-C02-O01-C1
21	B	301	TGL	OB1-CB1-OG2-CG2
25	P	304	CDL	OB7-CB5-OB6-CB4
21	L	101	TGL	CB3-CB4-CB5-CB6
23	W	101	DMU	C19-C22-C25-C28
25	P	304	CDL	C58-C59-C60-C61
25	P	304	CDL	C74-C75-C76-C77
25	P	304	CDL	C76-C77-C78-C79
18	P	302	PGV	C20-C21-C22-C23
18	Z	101	PGV	C3-C4-C5-C6
21	D	201	TGL	C11-C10-CB9-CB8
21	Q	201	TGL	C11-C10-CB9-CB8
21	Q	201	TGL	C21-C22-C23-C24
21	Q	201	TGL	C23-C24-C25-C26
21	Y	101	TGL	C19-C33-C34-C35
23	C	301	DMU	C25-C28-C31-C34
25	T	105	CDL	C34-C35-C36-C37
25	T	105	CDL	C59-C60-C61-C62
26	P	305	CHD	C13-C17-C20-C21
25	P	304	CDL	O1-C1-CB2-OB2
21	B	301	TGL	CA5-CA6-CA7-CA8
21	Y	101	TGL	CC4-CC5-CC6-CC7
25	P	304	CDL	C79-C80-C81-C82
25	T	105	CDL	CA5-C11-C12-C13
18	P	302	PGV	C3-C4-C5-C6
18	Z	101	PGV	C2-C3-C4-C5
21	D	201	TGL	C16-C15-CC9-CC8
21	N	606	TGL	C12-C13-C14-C29
21	Q	201	TGL	C24-C25-C26-C27
25	G	101	CDL	C62-C63-C64-C65
25	P	304	CDL	C57-C58-C59-C60
18	P	302	PGV	C25-C26-C27-C28
21	B	301	TGL	CB4-CB5-CB6-CB7
21	B	301	TGL	C15-C16-C17-C18
21	Y	101	TGL	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
24	C	307	PEK	C25-C26-C27-C28
24	C	307	PEK	C28-C29-C30-C31
25	C	304	CDL	C56-C57-C58-C59
18	A	607	PGV	C19-C20-C21-C22
24	T	103	PEK	C1-C2-C3-C4
21	D	201	TGL	C23-C24-C25-C26
21	L	101	TGL	CB4-CB5-CB6-CB7
21	L	101	TGL	CC9-C15-C16-C17
21	Q	201	TGL	CA3-CA4-CA5-CA6
21	Y	101	TGL	CA5-CA6-CA7-CA8
23	C	301	DMU	C22-C25-C28-C31
24	T	103	PEK	C32-C33-C34-C35
25	P	304	CDL	C38-C39-C40-C41
25	T	105	CDL	C17-C18-C19-C20
25	T	105	CDL	C19-C20-C21-C22
18	Z	101	PGV	C4-C5-C6-C7
21	L	101	TGL	C11-C10-CB9-CB8
24	G	102	PEK	C27-C28-C29-C30
25	G	101	CDL	C11-C12-C13-C14
18	P	302	PGV	C04-C05-C06-O06
26	C	305	CHD	C13-C17-C20-C21
21	B	301	TGL	CB2-CB1-OG2-CG2
18	A	607	PGV	C30-C31-C32-C33
18	P	302	PGV	C6-C7-C8-C9
21	D	201	TGL	CC3-CC4-CC5-CC6
21	L	101	TGL	CC7-CC8-CC9-C15
21	L	101	TGL	C22-C23-C24-C25
21	Q	201	TGL	CA9-C20-C21-C22
25	C	304	CDL	C37-C38-C39-C40
25	C	304	CDL	C61-C62-C63-C64
25	G	101	CDL	C23-C24-C25-C26
25	G	101	CDL	C52-C53-C54-C55
25	G	101	CDL	C55-C56-C57-C58
24	G	102	PEK	C2-C3-C4-C5
18	P	302	PGV	C26-C27-C28-C29
21	B	301	TGL	C11-C12-C13-C14
21	L	101	TGL	C10-C11-C12-C13
21	L	101	TGL	C19-C33-C34-C35
21	N	606	TGL	CB9-C10-C11-C12
21	Y	101	TGL	C23-C24-C25-C26
25	C	304	CDL	C58-C59-C60-C61
25	C	304	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C12-C13-C14-C15
25	G	101	CDL	C20-C21-C22-C23
25	P	304	CDL	C56-C57-C58-C59
25	P	304	CDL	C83-C84-C85-C86
25	T	105	CDL	C21-C22-C23-C24
25	T	105	CDL	C33-C34-C35-C36
18	Z	101	PGV	C14-C15-C16-C17
21	D	201	TGL	CC7-CC8-CC9-C15
21	N	606	TGL	C23-C24-C25-C26
21	Y	101	TGL	CB7-CB8-CB9-C10
24	C	307	PEK	C31-C32-C33-C34
25	C	304	CDL	C79-C80-C81-C82
25	G	101	CDL	C72-C73-C74-C75
25	T	105	CDL	C11-C12-C13-C14
18	A	606	PGV	C23-C24-C25-C26
18	P	301	PGV	C23-C24-C25-C26
18	P	301	PGV	C25-C26-C27-C28
18	P	302	PGV	C29-C30-C31-C32
21	D	201	TGL	C11-C12-C13-C14
21	D	201	TGL	CC2-CC3-CC4-CC5
21	N	606	TGL	CB6-CB7-CB8-CB9
21	Q	201	TGL	C19-C33-C34-C35
25	C	304	CDL	C74-C75-C76-C77
25	G	101	CDL	C59-C60-C61-C62
25	T	105	CDL	C77-C78-C79-C80
24	T	104	PEK	C1-C2-C3-C4
18	A	606	PGV	C24-C25-C26-C27
18	C	303	PGV	C13-C14-C15-C16
21	Q	201	TGL	CA5-CA6-CA7-CA8
25	C	304	CDL	C83-C84-C85-C86
21	B	301	TGL	CC2-CC1-OG3-CG3
21	N	606	TGL	CA4-CA5-CA6-CA7
21	Q	201	TGL	C10-C11-C12-C13
24	G	102	PEK	C25-C26-C27-C28
24	T	104	PEK	C25-C26-C27-C28
25	G	101	CDL	C36-C37-C38-C39
25	P	304	CDL	C60-C61-C62-C63
23	D	202	DMU	C18-C19-C22-C25
18	C	308	PGV	C6-C7-C8-C9
25	G	101	CDL	C42-C43-C44-C45
25	T	105	CDL	C54-C55-C56-C57
18	P	302	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	CA9-C20-C21-C22
21	L	101	TGL	C14-C29-C30-C31
24	T	102	PEK	C25-C26-C27-C28
24	T	104	PEK	O03-C01-C02-C03
25	G	101	CDL	CA3-CA4-CA6-OA8
24	G	102	PEK	O02-C1-O01-C02
24	C	302	PEK	C10-C11-C12-C13
24	T	104	PEK	C28-C29-C30-C31
25	T	105	CDL	C16-C17-C18-C19
18	Z	101	PGV	C7-C8-C9-C10
23	Z	102	DMU	C25-C28-C31-C34
25	P	304	CDL	C42-C43-C44-C45
24	G	102	PEK	C2-C1-O01-C02
18	P	302	PGV	O05-C05-C06-O06
24	C	302	PEK	C24-C25-C26-C27
27	O	302	PSC	C27-C28-C29-C30
27	O	302	PSC	C23-C24-C25-C26
18	Z	101	PGV	O12-C04-C05-O05
24	T	103	PEK	C24-C25-C26-C27
25	T	105	CDL	C43-C44-C45-C46
25	G	101	CDL	C75-C76-C77-C78
25	T	105	CDL	C58-C59-C60-C61
21	D	201	TGL	CB4-CB5-CB6-CB7
21	N	606	TGL	CC7-CC8-CC9-C15
21	B	301	TGL	CB6-CB7-CB8-CB9
21	Y	101	TGL	C10-C11-C12-C13
21	Y	101	TGL	C16-C15-CC9-CC8
25	T	105	CDL	C36-C37-C38-C39
21	B	301	TGL	OC1-CC1-OG3-CG3
24	C	307	PEK	C16-C17-C18-C19
25	C	304	CDL	C21-C22-C23-C24
25	C	304	CDL	C57-C58-C59-C60
21	B	301	TGL	C24-C25-C26-C27
21	D	201	TGL	CB2-CB1-OG2-CG2
18	Z	101	PGV	C6-C7-C8-C9
21	N	606	TGL	CC3-CC4-CC5-CC6
21	N	606	TGL	CC4-CC5-CC6-CC7
24	T	104	PEK	C34-C35-C36-C37
25	G	101	CDL	C33-C34-C35-C36
25	G	101	CDL	CA7-C31-C32-C33
21	L	101	TGL	CC5-CC6-CC7-CC8
21	Q	201	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	O	302	PSC	C5-C6-C7-C8
24	T	103	PEK	C10-C11-C12-C13
21	Q	201	TGL	C20-C21-C22-C23
21	Y	101	TGL	CC3-CC4-CC5-CC6
18	A	606	PGV	C11-C10-C9-C8
18	C	303	PGV	C12-C13-C14-C15
18	P	302	PGV	C11-C10-C9-C8
18	Z	101	PGV	C11-C10-C9-C8
24	C	307	PEK	C2-C3-C4-C5
24	G	102	PEK	C15-C16-C17-C18
25	C	304	CDL	CA5-C11-C12-C13
21	Y	101	TGL	C14-C29-C30-C31
21	Q	201	TGL	C16-C15-CC9-CC8
21	B	301	TGL	C12-C13-C14-C29
21	N	606	TGL	CA6-CA7-CA8-CA9
27	E	201	PSC	C22-C23-C24-C25
27	E	201	PSC	C28-C29-C30-C31
21	Y	101	TGL	CA1-CA2-CA3-CA4
21	D	201	TGL	C17-C18-C19-C33
21	L	101	TGL	CC3-CC4-CC5-CC6
25	G	101	CDL	C77-C78-C79-C80
25	G	101	CDL	C79-C80-C81-C82
25	P	304	CDL	C72-C73-C74-C75
18	A	607	PGV	C14-C15-C16-C17
18	C	308	PGV	C27-C28-C29-C30
18	C	308	PGV	C20-C19-O03-C01
21	D	201	TGL	CB5-CB6-CB7-CB8
21	L	101	TGL	CB6-CB7-CB8-CB9
21	N	606	TGL	CB2-CB1-OG2-CG2
18	C	308	PGV	C3-C4-C5-C6
25	P	304	CDL	C52-C53-C54-C55
25	P	304	CDL	C78-C79-C80-C81
27	E	201	PSC	C29-C30-C31-C32
18	C	308	PGV	O12-C04-C05-O05
21	D	201	TGL	OB1-CB1-OG2-CG2
21	Q	201	TGL	CA4-CA5-CA6-CA7
18	P	302	PGV	O03-C01-C02-O01
21	Q	201	TGL	OG1-CG1-CG2-OG2
24	C	307	PEK	O03-C01-C02-O01
24	T	104	PEK	O03-C01-C02-O01
25	G	101	CDL	OB6-CB4-CB6-OB8
18	P	302	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	A	607	PGV	C5-C6-C7-C8
18	P	303	PGV	C13-C14-C15-C16
25	C	304	CDL	C17-C18-C19-C20
18	A	607	PGV	C12-C13-C14-C15
24	T	103	PEK	C2-C3-C4-C5
24	T	103	PEK	C15-C16-C17-C18
24	T	104	PEK	C2-C3-C4-C5
24	T	104	PEK	C24-C25-C26-C27
18	C	308	PGV	C24-C25-C26-C27
21	D	201	TGL	CA9-C20-C21-C22
21	Y	101	TGL	C24-C25-C26-C27
21	N	606	TGL	C15-C16-C17-C18
25	P	304	CDL	C40-C41-C42-C43
21	N	606	TGL	OB1-CB1-OG2-CG2
25	T	105	CDL	C20-C21-C22-C23
25	P	304	CDL	CA3-OA5-PA1-OA2
24	G	102	PEK	C30-C31-C32-C33
23	D	202	DMU	O6-C11-C9-C8
25	C	304	CDL	C51-C52-C53-C54
25	C	304	CDL	C31-CA7-OA8-CA6
18	C	308	PGV	C01-C02-C03-O11
18	Z	101	PGV	C01-C02-C03-O11
25	G	101	CDL	OB5-CB3-CB4-CB6
25	P	304	CDL	OA5-CA3-CA4-CA6
25	P	304	CDL	OB5-CB3-CB4-CB6
21	L	101	TGL	C33-C34-C35-C36
24	C	307	PEK	C33-C34-C35-C36
21	Q	201	TGL	CB1-CB2-CB3-CB4
25	T	105	CDL	CB7-C71-C72-C73
18	C	303	PGV	C24-C25-C26-C27
25	C	304	CDL	C15-C16-C17-C18
26	C	305	CHD	C16-C17-C20-C22
18	C	308	PGV	C14-C15-C16-C17
27	E	201	PSC	C13-C14-C15-C16
18	C	308	PGV	C26-C27-C28-C29
25	G	101	CDL	C60-C61-C62-C63
25	P	304	CDL	CA2-C1-CB2-OB2
21	D	201	TGL	C14-C29-C30-C31
21	Q	201	TGL	C15-C16-C17-C18
25	G	101	CDL	C37-C38-C39-C40
18	P	301	PGV	C26-C27-C28-C29
21	L	101	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
21	N	606	TGL	CA5-CA6-CA7-CA8
23	Z	102	DMU	C19-C22-C25-C28
25	P	304	CDL	C43-C44-C45-C46
18	C	308	PGV	O04-C19-O03-C01
25	C	304	CDL	O1-C1-CB2-OB2
25	T	105	CDL	O1-C1-CB2-OB2
23	D	202	DMU	C19-C22-C25-C28
25	P	304	CDL	C11-C12-C13-C14
18	P	302	PGV	O03-C01-C02-C03
24	C	302	PEK	O03-C01-C02-C03
24	C	307	PEK	O03-C01-C02-C03
25	P	304	CDL	CB3-CB4-CB6-OB8
26	P	305	CHD	C16-C17-C20-C22
24	T	102	PEK	C4-C5-C6-C7
21	D	201	TGL	C15-C16-C17-C18
21	L	101	TGL	C29-C30-C31-C32
23	C	301	DMU	O16-C18-C19-C22
25	C	304	CDL	C18-C19-C20-C21
21	N	606	TGL	C16-C17-C18-C19
21	L	101	TGL	CB7-CB8-CB9-C10
25	P	304	CDL	C23-C24-C25-C26
24	G	102	PEK	C3-C4-C5-C6
25	C	304	CDL	CB4-CB6-OB8-CB7
18	P	301	PGV	C31-C32-C33-C34
18	P	303	PGV	C25-C26-C27-C28
21	B	301	TGL	CC4-CC5-CC6-CC7
25	P	304	CDL	C73-C74-C75-C76
18	A	607	PGV	C11-C10-C9-C8
24	G	102	PEK	C31-C32-C33-C34
27	E	201	PSC	C20-C21-C22-C23
21	B	301	TGL	C21-C20-CA9-CA8
27	E	201	PSC	C27-C28-C29-C30
21	L	101	TGL	CC2-CC3-CC4-CC5
25	C	304	CDL	C24-C25-C26-C27
21	Y	101	TGL	CA3-CA4-CA5-CA6
24	T	102	PEK	C35-C36-C37-C38
24	G	102	PEK	C23-C24-C25-C26
25	C	304	CDL	C62-C63-C64-C65
18	P	302	PGV	C11-C12-C13-C14
25	G	101	CDL	C54-C55-C56-C57
24	T	103	PEK	C13-C14-C15-C16
23	C	301	DMU	C4-C3-O7-C10

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Mol	Chain	Res	Type	Atoms
25	C	304	CDL	C44-C45-C46-C47
21	L	101	TGL	C21-C22-C23-C24
18	Z	101	PGV	C31-C32-C33-C34
21	L	101	TGL	CA4-CA5-CA6-CA7
24	G	102	PEK	C29-C30-C31-C32
25	P	304	CDL	C62-C63-C64-C65
27	E	201	PSC	O03-C01-C02-O01
21	B	301	TGL	C29-C30-C31-C32
25	G	101	CDL	C41-C42-C43-C44
25	P	304	CDL	C53-C54-C55-C56
21	N	606	TGL	C13-C14-C29-C30
23	D	202	DMU	C22-C25-C28-C31
18	Z	101	PGV	C25-C26-C27-C28
21	Y	101	TGL	C22-C23-C24-C25
25	G	101	CDL	C22-C23-C24-C25
27	O	302	PSC	C31-C32-C33-C34
25	G	101	CDL	C19-C20-C21-C22
25	C	304	CDL	CA2-C1-CB2-OB2
24	T	102	PEK	C33-C34-C35-C36
25	P	304	CDL	C75-C76-C77-C78
25	C	304	CDL	CB5-C51-C52-C53
25	T	105	CDL	C22-C23-C24-C25
25	G	101	CDL	C39-C40-C41-C42
25	P	304	CDL	C16-C17-C18-C19
25	G	101	CDL	OA5-CA3-CA4-CA6
25	T	105	CDL	OB5-CB3-CB4-CB6
24	C	302	PEK	O12-C04-C05-N
25	T	105	CDL	C23-C24-C25-C26
23	C	301	DMU	C2-C3-O7-C10
25	T	105	CDL	C18-C19-C20-C21
21	D	201	TGL	CA2-CA3-CA4-CA5
25	T	105	CDL	C24-C25-C26-C27
21	Q	201	TGL	CB9-C10-C11-C12
18	A	606	PGV	C31-C32-C33-C34
27	E	201	PSC	C4-C5-C6-C7
18	C	308	PGV	C31-C32-C33-C34
21	Q	201	TGL	CC5-CC6-CC7-CC8
25	C	304	CDL	C84-C85-C86-C87
18	P	303	PGV	C14-C15-C16-C17
18	C	308	PGV	O03-C01-C02-C03
18	Z	101	PGV	O03-C01-C02-C03
21	D	201	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
21	Q	201	TGL	OG1-CG1-CG2-CG3
24	T	103	PEK	O03-C01-C02-C03
25	C	304	CDL	CA3-CA4-CA6-OA8
25	C	304	CDL	CB3-CB4-CB6-OB8
25	G	101	CDL	CB3-CB4-CB6-OB8
25	T	105	CDL	CA3-CA4-CA6-OA8
21	Y	101	TGL	CC7-CC8-CC9-C15
24	C	307	PEK	C10-C11-C12-C13
21	D	201	TGL	CC1-CC2-CC3-CC4
21	Y	101	TGL	C16-C17-C18-C19
25	C	304	CDL	C12-C13-C14-C15
18	Z	101	PGV	C03-O11-P-O12
24	G	102	PEK	C11-C10-C9-C8
24	G	102	PEK	C11-C12-C13-C14
24	G	102	PEK	C12-C13-C14-C15
24	T	102	PEK	C11-C10-C9-C8
24	T	103	PEK	C5-C6-C7-C8
24	T	103	PEK	C11-C10-C9-C8
26	W	102	CHD	C17-C20-C22-C23
27	E	201	PSC	C9-C10-C11-C12
27	E	201	PSC	C10-C11-C12-C13
27	O	302	PSC	C9-C10-C11-C12
18	A	606	PGV	C19-C20-C21-C22
18	C	303	PGV	C21-C22-C23-C24
21	L	101	TGL	CC4-CC5-CC6-CC7
25	G	101	CDL	OA5-CA3-CA4-OA6
25	P	304	CDL	OA5-CA3-CA4-OA6
18	C	308	PGV	C7-C8-C9-C10
18	Z	101	PGV	C23-C24-C25-C26
21	D	201	TGL	CA6-CA7-CA8-CA9
27	E	201	PSC	C31-C32-C33-C34
25	C	304	CDL	OA9-CA7-OA8-CA6
18	A	607	PGV	O03-C01-C02-O01
18	Z	101	PGV	O03-C01-C02-O01
25	P	304	CDL	OB6-CB4-CB6-OB8
21	N	606	TGL	CB3-CB4-CB5-CB6
21	N	606	TGL	C17-C18-C19-C33
21	Y	101	TGL	C33-C34-C35-C36
23	Z	102	DMU	C34-C37-C40-C43
24	G	102	PEK	C16-C17-C18-C19
25	G	101	CDL	C16-C17-C18-C19
18	C	308	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
25	T	105	CDL	CA2-C1-CB2-OB2
18	C	303	PGV	C02-C03-O11-P
25	P	304	CDL	C1-CA2-OA2-PA1
21	L	101	TGL	CA5-CA6-CA7-CA8
25	C	304	CDL	C34-C35-C36-C37
25	C	304	CDL	C43-C44-C45-C46
25	C	304	CDL	C53-C54-C55-C56
21	D	201	TGL	CA1-CA2-CA3-CA4
25	C	304	CDL	C31-C32-C33-C34
18	C	303	PGV	C11-C12-C13-C14
21	Q	201	TGL	C33-C34-C35-C36
25	C	304	CDL	C72-C73-C74-C75
25	C	304	CDL	C14-C15-C16-C17
25	G	101	CDL	C34-C35-C36-C37
18	C	308	PGV	C13-C14-C15-C16
25	G	101	CDL	CB5-C51-C52-C53
25	G	101	CDL	C78-C79-C80-C81
18	A	607	PGV	C01-C02-C03-O11
25	C	304	CDL	OA5-CA3-CA4-CA6
18	P	303	PGV	C11-C12-C13-C14
21	N	606	TGL	CC5-CC6-CC7-CC8
24	T	102	PEK	C28-C29-C30-C31
25	T	105	CDL	C37-C38-C39-C40
21	Y	101	TGL	CB5-CB6-CB7-CB8
21	N	606	TGL	CC2-CC3-CC4-CC5
21	N	606	TGL	C29-C30-C31-C32
18	C	308	PGV	C23-C24-C25-C26
21	D	201	TGL	C10-C11-C12-C13
18	P	302	PGV	C30-C31-C32-C33
24	T	104	PEK	C29-C30-C31-C32
18	A	607	PGV	C24-C25-C26-C27
23	D	202	DMU	O5-C6-O16-C18
18	P	303	PGV	C23-C24-C25-C26
18	P	302	PGV	C02-C03-O11-P
21	L	101	TGL	CG1-CG2-CG3-OG3
25	C	304	CDL	C1-CA2-OA2-PA1
25	G	101	CDL	C1-CB2-OB2-PB2
18	C	308	PGV	O01-C02-C03-O11
24	G	102	PEK	O01-C02-C03-O11
25	C	304	CDL	OA5-CA3-CA4-OA6
25	G	101	CDL	OB5-CB3-CB4-OB6
21	D	201	TGL	C21-C20-CA9-CA8

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Mol	Chain	Res	Type	Atoms
26	J	101	CHD	C17-C20-C22-C23
24	C	307	PEK	C35-C36-C37-C38
23	C	301	DMU	C18-C19-C22-C25
24	T	102	PEK	C29-C30-C31-C32
21	L	101	TGL	OG2-CG2-CG3-OG3
21	Y	101	TGL	OG1-CG1-CG2-OG2
25	C	304	CDL	OA6-CA4-CA6-OA8
25	C	304	CDL	OB6-CB4-CB6-OB8
25	T	105	CDL	OA6-CA4-CA6-OA8
18	P	301	PGV	C29-C30-C31-C32
21	B	301	TGL	C16-C15-CC9-CC8
24	T	102	PEK	C26-C27-C28-C29
18	A	607	PGV	C23-C24-C25-C26
24	T	103	PEK	C31-C32-C33-C34
25	G	101	CDL	OB7-CB5-OB6-CB4
25	T	105	CDL	OB7-CB5-OB6-CB4
21	N	606	TGL	OC1-CC1-OG3-CG3
25	T	105	CDL	C32-C33-C34-C35
18	A	607	PGV	C26-C27-C28-C29
25	T	105	CDL	C12-C13-C14-C15
21	L	101	TGL	C20-C21-C22-C23
29	I	101	SAC	CB-CA-N-C1A
18	Z	101	PGV	C13-C14-C15-C16
18	C	308	PGV	C03-O11-P-O12
24	C	307	PEK	C04-O12-P-O11
25	C	304	CDL	CA3-OA5-PA1-OA2
27	E	201	PSC	C03-O11-P-O12
25	G	101	CDL	C82-C83-C84-C85
25	G	101	CDL	O1-C1-CA2-OA2
18	P	303	PGV	C02-C03-O11-P
25	P	304	CDL	C71-C72-C73-C74
18	C	308	PGV	C04-O12-P-O13
18	P	302	PGV	C04-O12-P-O13
18	Z	101	PGV	C03-O11-P-O14
18	Z	101	PGV	C04-O12-P-O14
25	C	304	CDL	CA3-OA5-PA1-OA3
25	C	304	CDL	CB2-OB2-PB2-OB3
25	P	304	CDL	CA3-OA5-PA1-OA3
25	P	304	CDL	CB2-OB2-PB2-OB3
25	T	105	CDL	CA3-OA5-PA1-OA3
27	E	201	PSC	C04-O12-P-O14
21	Y	101	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
24	G	102	PEK	C01-C02-C03-O11
25	C	304	CDL	OB5-CB3-CB4-CB6
18	A	606	PGV	C26-C27-C28-C29
25	T	105	CDL	C73-C74-C75-C76
24	G	102	PEK	C32-C33-C34-C35
25	P	304	CDL	C77-C78-C79-C80
14	N	602	HEA	C3B-C11-C12-C13
24	C	302	PEK	C34-C35-C36-C37
25	C	304	CDL	C19-C20-C21-C22
18	P	303	PGV	C11-C10-C9-C8
21	B	301	TGL	CA7-CA8-CA9-C20
24	C	302	PEK	C33-C34-C35-C36
26	P	305	CHD	C16-C17-C20-C21
18	A	607	PGV	O01-C02-C03-O11
18	P	303	PGV	C19-C20-C21-C22
18	Z	101	PGV	O01-C02-C03-O11
25	P	304	CDL	OB5-CB3-CB4-OB6
25	T	105	CDL	OB5-CB3-CB4-OB6
27	E	201	PSC	C5-C6-C7-C8
25	T	105	CDL	C51-CB5-OB6-CB4
27	E	201	PSC	C24-C25-C26-C27
26	C	305	CHD	C16-C17-C20-C21
27	O	302	PSC	C15-C16-C17-C18
18	A	607	PGV	O03-C01-C02-C03
21	Y	101	TGL	OG1-CG1-CG2-CG3
21	D	201	TGL	OG2-CG2-CG3-OG3
24	C	302	PEK	O03-C01-C02-O01
25	G	101	CDL	OA6-CA4-CA6-OA8
21	D	201	TGL	C18-C19-C33-C34
21	L	101	TGL	C15-C16-C17-C18
21	Y	101	TGL	CA7-CA8-CA9-C20
27	O	302	PSC	C02-C03-O11-P
21	B	301	TGL	OA1-CA1-OG1-CG1
25	T	105	CDL	C35-C36-C37-C38
18	A	607	PGV	C7-C8-C9-C10
18	P	302	PGV	C31-C32-C33-C34
21	Q	201	TGL	C16-C17-C18-C19
24	T	103	PEK	C25-C26-C27-C28
18	C	308	PGV	C25-C26-C27-C28
25	P	304	CDL	C81-C82-C83-C84
24	T	102	PEK	C23-C24-C25-C26
25	C	304	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	CA2-CA1-OG1-CG1
18	P	303	PGV	C20-C21-C22-C23
21	D	201	TGL	CB2-CB3-CB4-CB5
21	L	101	TGL	CA3-CA4-CA5-CA6
24	T	103	PEK	C23-C24-C25-C26
21	B	301	TGL	CG1-CG2-OG2-CB1
21	D	201	TGL	CG3-CG2-OG2-CB1
21	Y	101	TGL	C29-C30-C31-C32
26	G	103	CHD	C21-C20-C22-C23
25	P	304	CDL	C59-C60-C61-C62
21	B	301	TGL	C22-C23-C24-C25
18	C	308	PGV	C4-C5-C6-C7
21	B	301	TGL	C17-C18-C19-C33
21	N	606	TGL	CC9-C15-C16-C17
19	A	608	EDO	O1-C1-C2-O2
24	T	103	PEK	C29-C30-C31-C32
25	C	304	CDL	C36-C37-C38-C39
18	A	607	PGV	C03-O11-P-O12
24	C	307	PEK	C03-O11-P-O12
24	G	102	PEK	C03-O11-P-O12
25	G	101	CDL	CB2-OB2-PB2-OB5
27	O	302	PSC	C03-O11-P-O12
25	P	304	CDL	C14-C15-C16-C17
18	Z	101	PGV	C20-C21-C22-C23
27	E	201	PSC	O03-C01-C02-C03
24	T	102	PEK	C27-C28-C29-C30
26	P	306	CHD	C16-C17-C20-C22
24	G	102	PEK	C17-C18-C19-C20
18	C	308	PGV	C05-C04-O12-P
25	G	101	CDL	CB4-CB3-OB5-PB2
25	T	105	CDL	CB4-CB3-OB5-PB2
24	C	307	PEK	C14-C15-C16-C17
24	T	104	PEK	C3-C4-C5-C6
18	A	607	PGV	O12-C04-C05-C06
18	P	301	PGV	C30-C31-C32-C33
21	B	301	TGL	C16-C17-C18-C19
21	N	606	TGL	CC2-CC1-OG3-CG3
24	T	102	PEK	C13-C14-C15-C16
18	C	303	PGV	C19-C20-C21-C22
25	T	105	CDL	C81-C82-C83-C84
18	C	303	PGV	C1-C2-C3-C4
14	N	602	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	C33-C34-C35-C36
18	C	308	PGV	C22-C23-C24-C25
21	Q	201	TGL	CB4-CB5-CB6-CB7
25	C	304	CDL	C38-C39-C40-C41
25	T	105	CDL	C53-C54-C55-C56
24	C	307	PEK	C23-C24-C25-C26
18	A	606	PGV	O03-C19-C20-C21
18	P	301	PGV	C11-C10-C9-C8
21	N	606	TGL	C24-C25-C26-C27
14	A	602	HEA	CAA-CBA-CGA-O1A
23	D	202	DMU	C1-C6-O16-C18
21	N	606	TGL	OG1-CG1-CG2-OG2
24	C	307	PEK	C24-C25-C26-C27
21	L	101	TGL	CC6-CC7-CC8-CC9
18	A	606	PGV	C25-C26-C27-C28
26	G	103	CHD	C22-C23-C24-O26
21	Q	201	TGL	CA2-CA3-CA4-CA5
21	N	606	TGL	C16-C15-CC9-CC8
21	N	606	TGL	CA7-CA8-CA9-C20
18	Z	101	PGV	O12-C04-C05-C06
24	C	307	PEK	O02-C1-O01-C02
21	N	606	TGL	CC6-CC7-CC8-CC9
14	N	602	HEA	CAA-CBA-CGA-O2A
18	A	606	PGV	C6-C7-C8-C9
26	T	101	CHD	C22-C23-C24-O25
26	T	101	CHD	C22-C23-C24-O26
21	Y	101	TGL	CC5-CC6-CC7-CC8
25	G	101	CDL	C76-C77-C78-C79
21	Y	101	TGL	C11-C12-C13-C14
21	Y	101	TGL	CC2-CC3-CC4-CC5
27	O	302	PSC	O01-C1-C2-C3
26	C	305	CHD	C22-C23-C24-O25
24	C	307	PEK	C6-C7-C8-C9
24	T	102	PEK	C11-C12-C13-C14
24	T	104	PEK	C9-C10-C11-C12
24	T	104	PEK	C11-C12-C13-C14
26	W	102	CHD	C22-C23-C24-O25
24	T	104	PEK	C35-C36-C37-C38
25	C	304	CDL	C41-C42-C43-C44
25	P	304	CDL	C31-C32-C33-C34
18	A	607	PGV	C05-C04-O12-P
26	J	101	CHD	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	C	307	PEK	O01-C02-C03-O11
24	G	102	PEK	C26-C27-C28-C29
21	N	606	TGL	C25-C26-C27-C28
18	A	607	PGV	O12-C04-C05-O05
18	P	303	PGV	C15-C16-C17-C18
18	A	606	PGV	C28-C29-C30-C31
21	B	301	TGL	CA2-CA3-CA4-CA5
21	Y	101	TGL	C13-C14-C29-C30
21	B	301	TGL	CB1-CB2-CB3-CB4
25	G	101	CDL	C31-C32-C33-C34
24	T	102	PEK	C10-C11-C12-C13
24	T	103	PEK	C7-C8-C9-C10
21	Y	101	TGL	CA2-CA3-CA4-CA5
25	C	304	CDL	C75-C76-C77-C78
24	C	302	PEK	C31-C32-C33-C34
24	C	302	PEK	C22-C23-C24-C25
21	Y	101	TGL	C25-C26-C27-C28
14	A	602	HEA	CAA-CBA-CGA-O2A
26	W	102	CHD	C22-C23-C24-O26
24	C	302	PEK	C25-C26-C27-C28
25	G	101	CDL	C61-C62-C63-C64
25	G	101	CDL	C51-CB5-OB6-CB4
14	N	601	HEA	CAD-CBD-CGD-O1D
21	B	301	TGL	C21-C22-C23-C24
25	T	105	CDL	C15-C16-C17-C18
24	G	102	PEK	C7-C8-C9-C10
18	P	301	PGV	C15-C16-C17-C18
24	T	104	PEK	O01-C02-C03-O11
25	C	304	CDL	OB5-CB3-CB4-OB6
21	D	201	TGL	OG2-CB1-CB2-CB3
24	C	307	PEK	C32-C33-C34-C35
25	C	304	CDL	C64-C65-C66-C67
18	C	308	PGV	C29-C30-C31-C32
18	C	303	PGV	C9-C10-C11-C12
24	C	307	PEK	C3-C4-C5-C6
24	T	104	PEK	C21-C22-C23-C24
25	G	101	CDL	C32-C33-C34-C35
18	Z	101	PGV	O03-C19-C20-C21
26	G	103	CHD	C22-C23-C24-O25
24	T	104	PEK	C03-O11-P-O12
27	O	302	PSC	C28-C29-C30-C31
18	P	301	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
14	A	601	HEA	CAD-CBD-CGD-O1D
27	O	302	PSC	C22-C23-C24-C25
14	A	601	HEA	CAA-CBA-CGA-O1A
21	N	606	TGL	CG1-CG2-OG2-CB1
18	P	302	PGV	O02-C1-O01-C02
18	C	308	PGV	O01-C1-C2-C3
18	C	308	PGV	C9-C10-C11-C12
24	T	103	PEK	C3-C4-C5-C6
27	E	201	PSC	C6-C7-C8-C9
21	N	606	TGL	CA2-CA3-CA4-CA5
23	C	301	DMU	C28-C31-C34-C37
25	T	105	CDL	OA5-CA3-CA4-OA6
18	C	303	PGV	O03-C19-C20-C21
24	T	102	PEK	C31-C32-C33-C34
19	C	309	EDO	O1-C1-C2-O2
14	N	601	HEA	CAD-CBD-CGD-O2D
24	T	104	PEK	C01-C02-C03-O11
14	N	601	HEA	CAA-CBA-CGA-O1A
21	Q	201	TGL	OG3-CC1-CC2-CC3
18	P	301	PGV	C22-C23-C24-C25
21	B	301	TGL	OG1-CG1-CG2-OG2
26	C	305	CHD	C22-C23-C24-O26
21	D	201	TGL	OG1-CA1-CA2-CA3
21	N	606	TGL	OG3-CC1-CC2-CC3
14	A	601	HEA	CAD-CBD-CGD-O2D
24	C	307	PEK	C27-C28-C29-C30
21	Y	101	TGL	OC1-CC1-OG3-CG3
18	P	303	PGV	C05-C04-O12-P
27	O	302	PSC	C7-C8-C9-C10
18	A	607	PGV	C21-C22-C23-C24
24	C	307	PEK	C2-C1-O01-C02
18	Z	101	PGV	O04-C19-C20-C21
18	A	607	PGV	C9-C10-C11-C12
21	Y	101	TGL	CC2-CC1-OG3-CG3
26	J	101	CHD	C22-C23-C24-O26
18	C	308	PGV	O02-C1-C2-C3
21	Y	101	TGL	CA9-C20-C21-C22
18	C	308	PGV	C04-C05-C06-O06
21	L	101	TGL	C16-C15-CC9-CC8
29	I	101	SAC	C-CA-N-C1A
18	P	303	PGV	C1-C2-C3-C4
18	C	308	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
14	N	601	HEA	C16-C17-C18-C19
18	C	303	PGV	O04-C19-C20-C21
24	T	103	PEK	O01-C1-C2-C3
24	T	104	PEK	C17-C18-C19-C20
18	A	606	PGV	C02-C01-O03-C19
18	C	308	PGV	C02-C03-O11-P
27	O	302	PSC	C26-C27-C28-C29
23	D	202	DMU	C34-C37-C40-C43
27	O	302	PSC	C03-O11-P-O14
21	D	201	TGL	OA1-CA1-CA2-CA3
21	Q	201	TGL	CC2-CC3-CC4-CC5
19	G	104	EDO	O1-C1-C2-O2
14	N	602	HEA	O11-C11-C12-C13
21	Q	201	TGL	OC1-CC1-CC2-CC3
27	O	302	PSC	C12-C13-C14-C15
14	A	601	HEA	CAA-CBA-CGA-O2A
26	J	101	CHD	C22-C23-C24-O25
21	Q	201	TGL	C25-C26-C27-C28
18	P	302	PGV	C27-C28-C29-C30
21	Q	201	TGL	C21-C20-CA9-CA8
24	T	102	PEK	C05-C04-O12-P
24	T	103	PEK	O02-C1-C2-C3
21	B	301	TGL	C23-C24-C25-C26
24	G	102	PEK	C28-C29-C30-C31
24	C	302	PEK	O03-C21-C22-C23
25	P	304	CDL	C52-C51-CB5-OB6
14	N	601	HEA	CAA-CBA-CGA-O2A
21	L	101	TGL	C24-C25-C26-C27
24	T	103	PEK	O03-C21-C22-C23
25	G	101	CDL	C32-C31-CA7-OA8
27	O	302	PSC	C3-C4-C5-C6
18	C	303	PGV	C05-C04-O12-P
25	P	304	CDL	CA4-CA3-OA5-PA1
18	P	301	PGV	O03-C19-C20-C21
23	C	301	DMU	C19-C18-O16-C6
24	T	103	PEK	C27-C28-C29-C30
25	P	304	CDL	C52-C51-CB5-OB7
18	Z	101	PGV	C24-C25-C26-C27
24	T	103	PEK	O04-C21-C22-C23
21	D	201	TGL	OG3-CC1-CC2-CC3

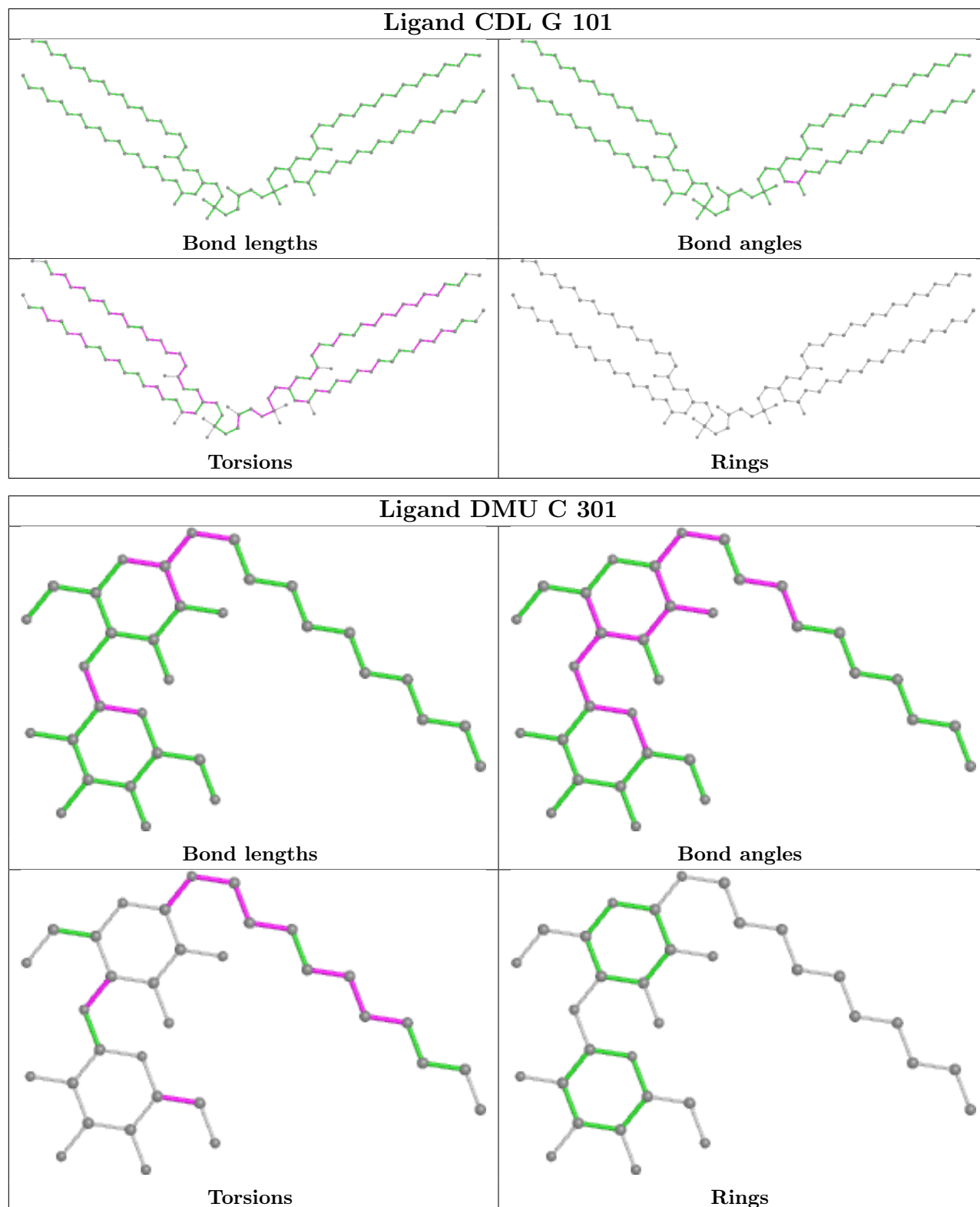
There are no ring outliers.

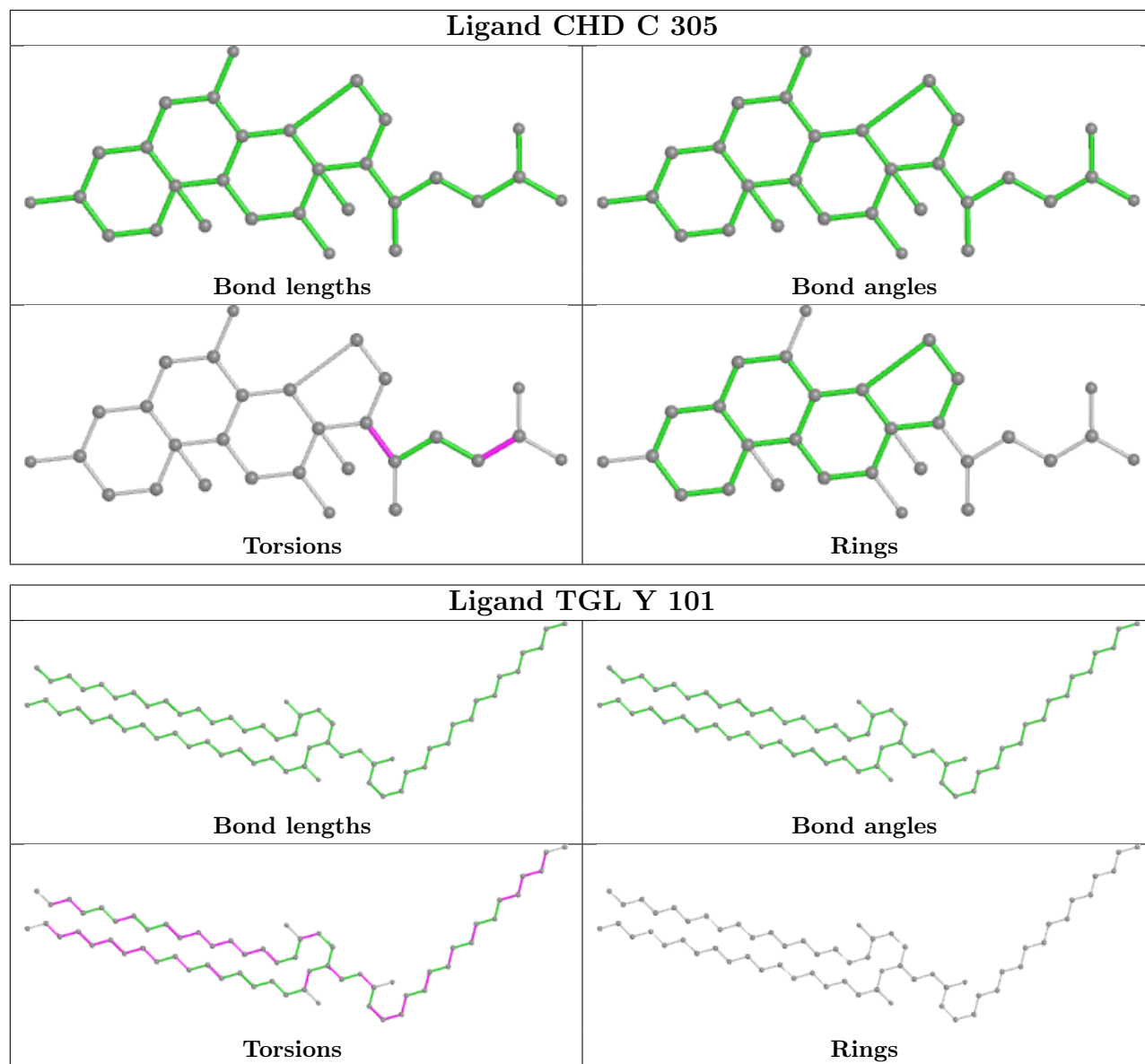
34 monomers are involved in 103 short contacts:

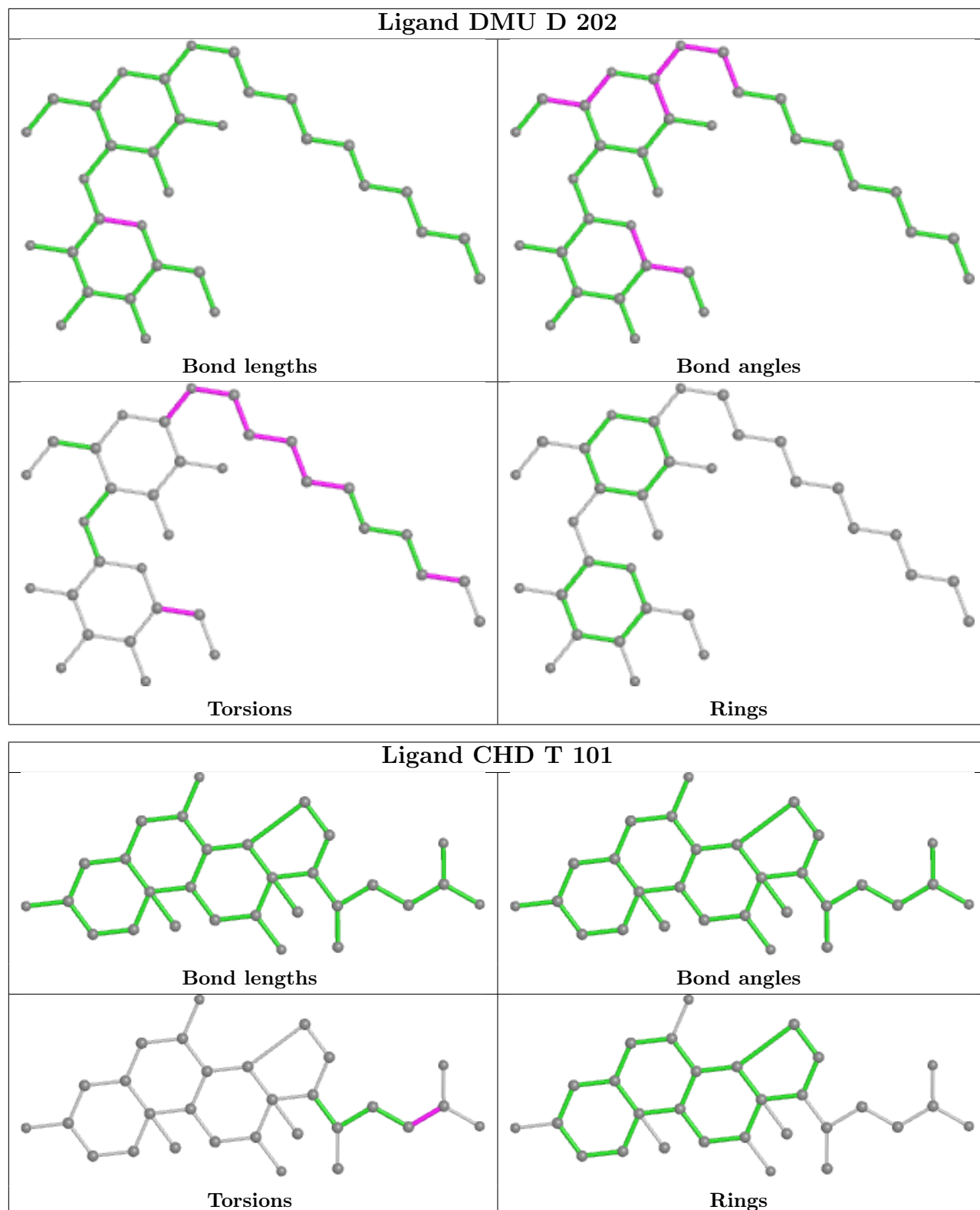
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	G	104	EDO	1	0
25	G	101	CDL	4	0
23	C	301	DMU	6	0
26	C	305	CHD	1	0
21	Y	101	TGL	2	0
26	T	101	CHD	1	0
25	T	105	CDL	7	0
19	S	103	EDO	4	0
24	C	302	PEK	1	0
24	G	102	PEK	3	0
14	A	601	HEA	5	0
18	P	303	PGV	1	0
25	P	304	CDL	2	0
19	C	309	EDO	1	0
27	E	201	PSC	6	0
14	N	602	HEA	8	0
21	L	101	TGL	4	0
14	A	602	HEA	6	0
18	A	607	PGV	5	0
24	T	102	PEK	4	0
25	C	304	CDL	2	0
19	S	102	EDO	1	0
18	Z	101	PGV	2	0
27	O	302	PSC	2	0
18	P	301	PGV	4	0
14	N	601	HEA	5	0
18	P	302	PGV	1	0
26	C	306	CHD	1	0
24	T	104	PEK	2	0
26	W	102	CHD	1	0
29	V	101	SAC	1	0
21	D	201	TGL	4	0
23	W	101	DMU	7	0
26	P	305	CHD	1	0

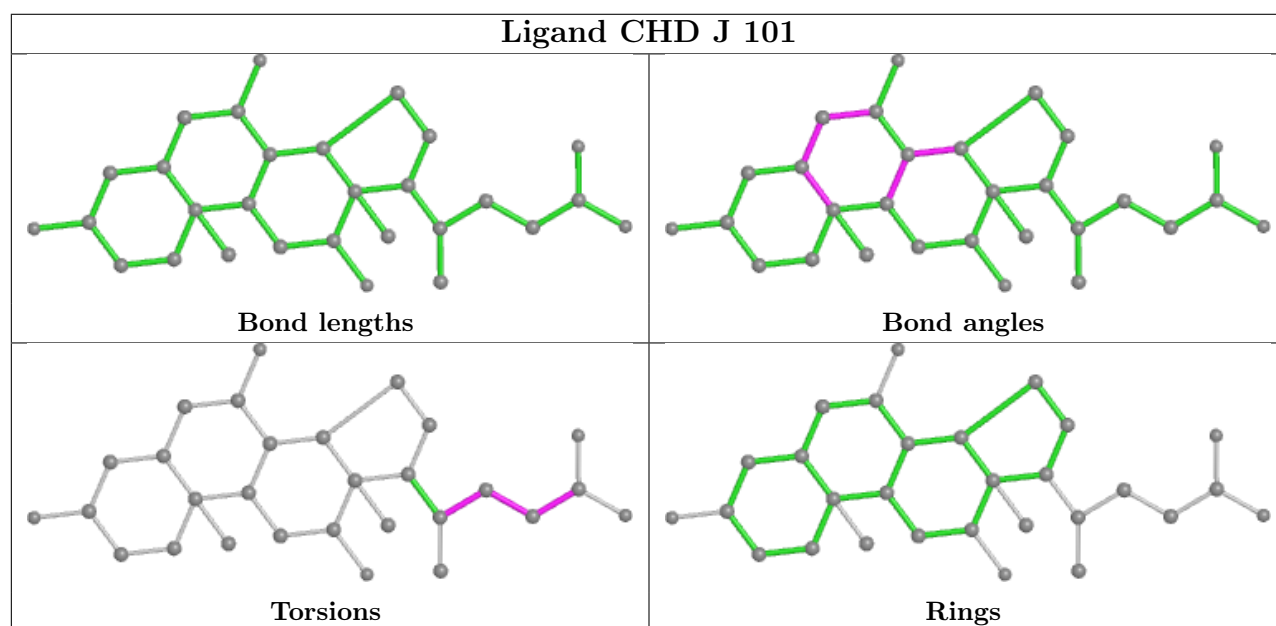
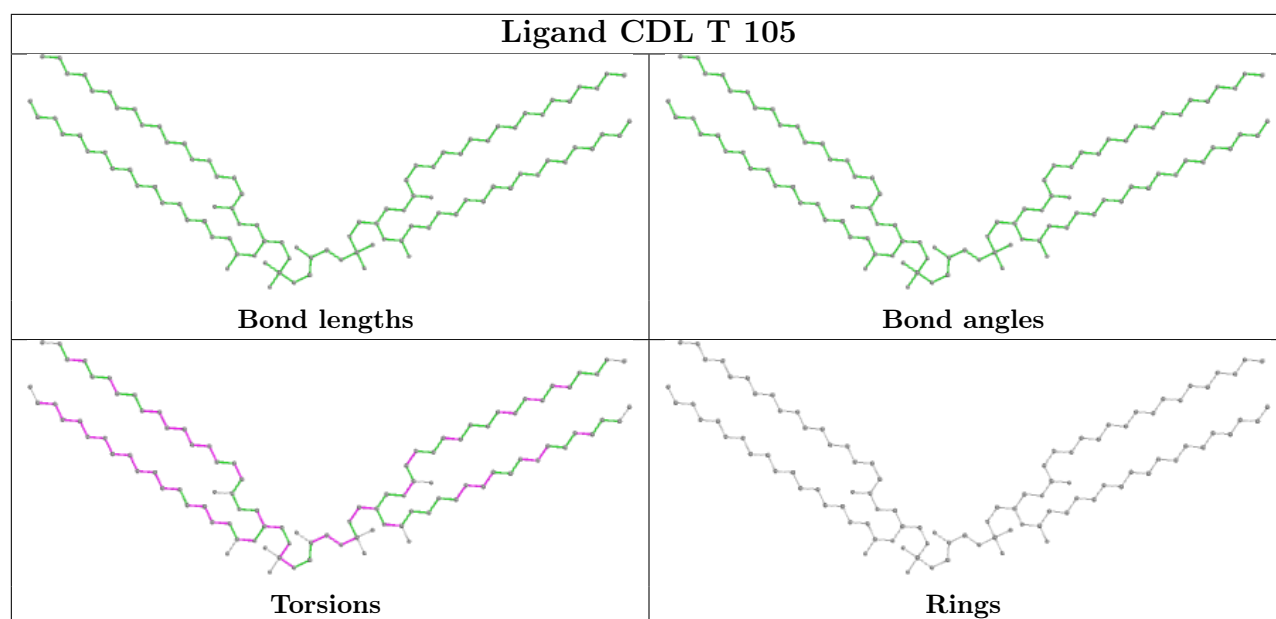
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

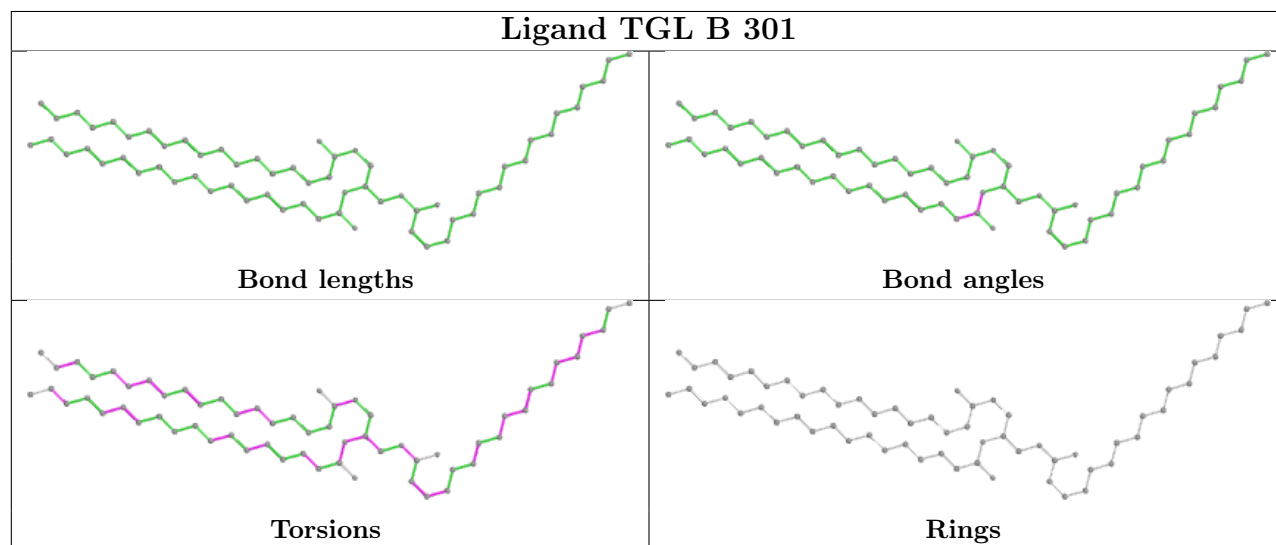
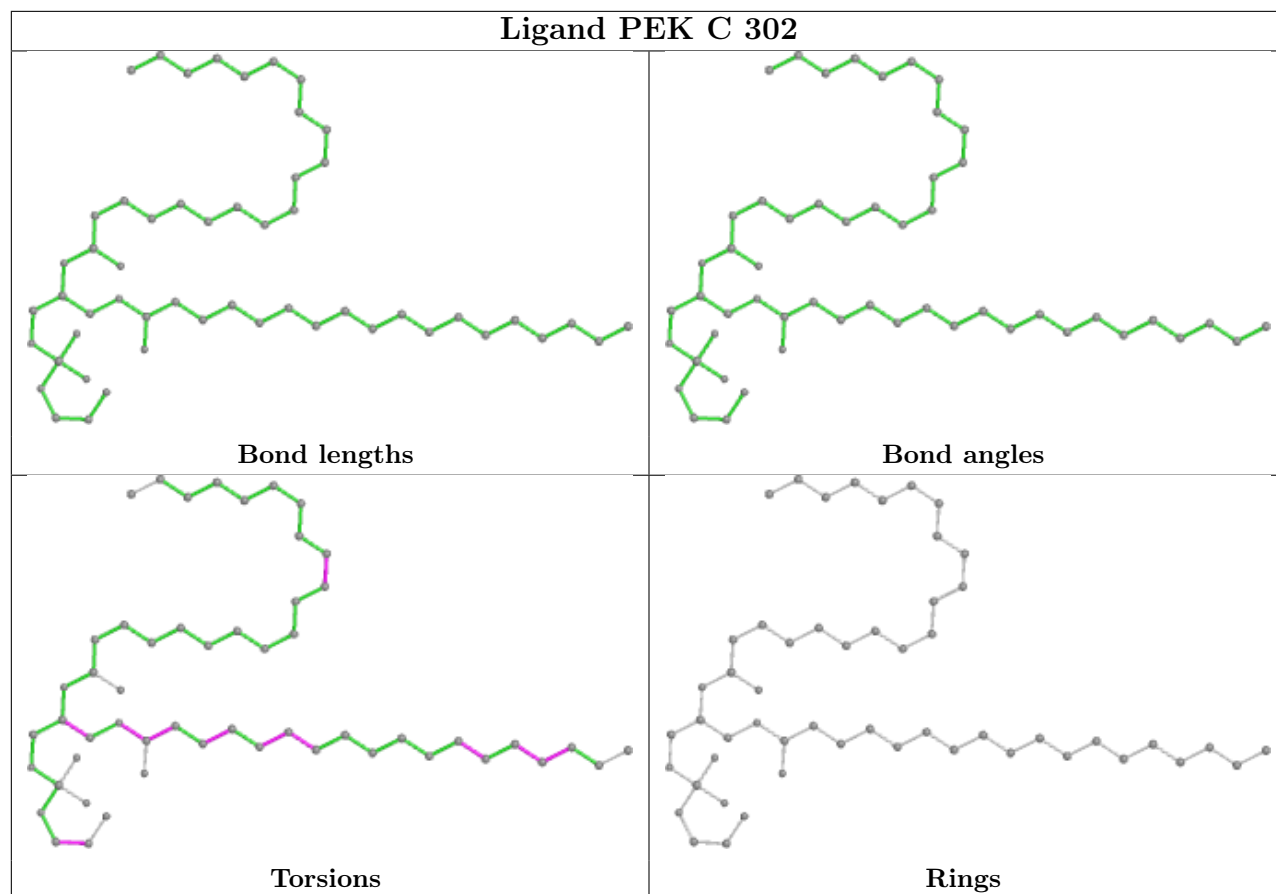
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



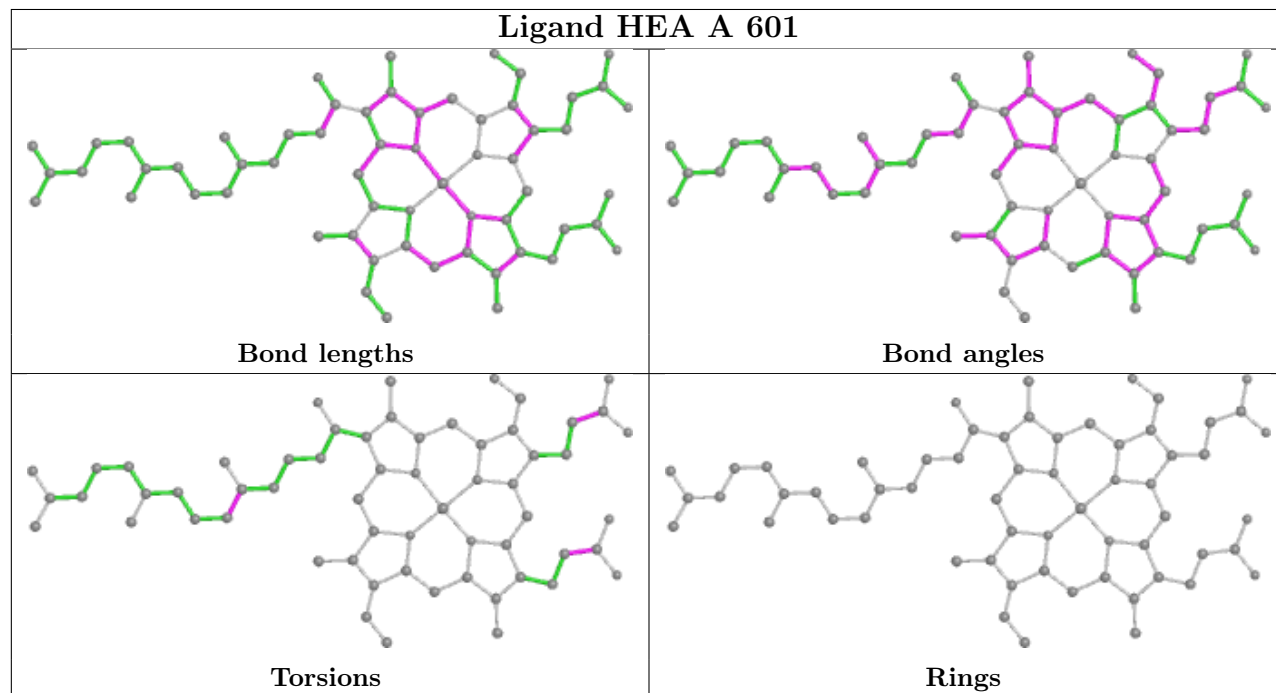
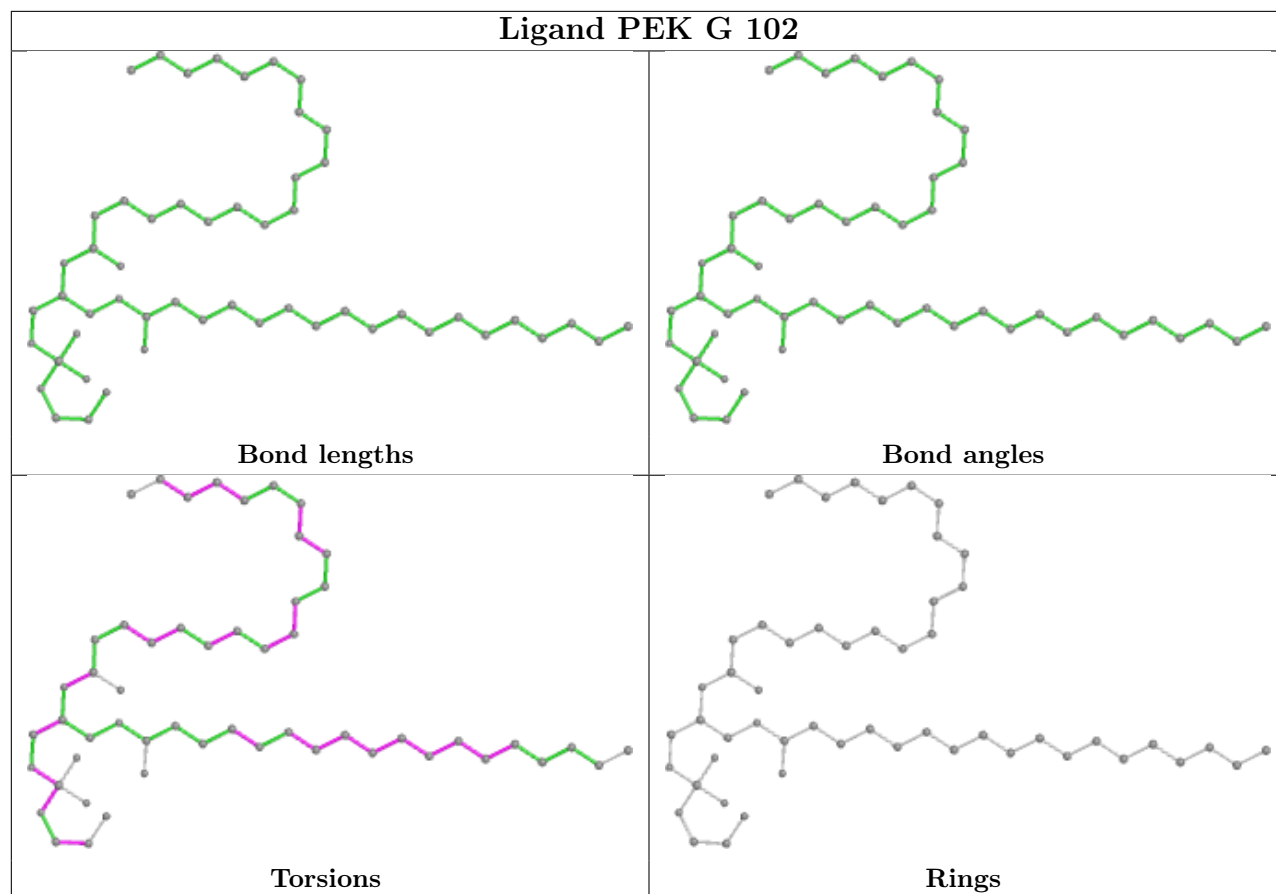




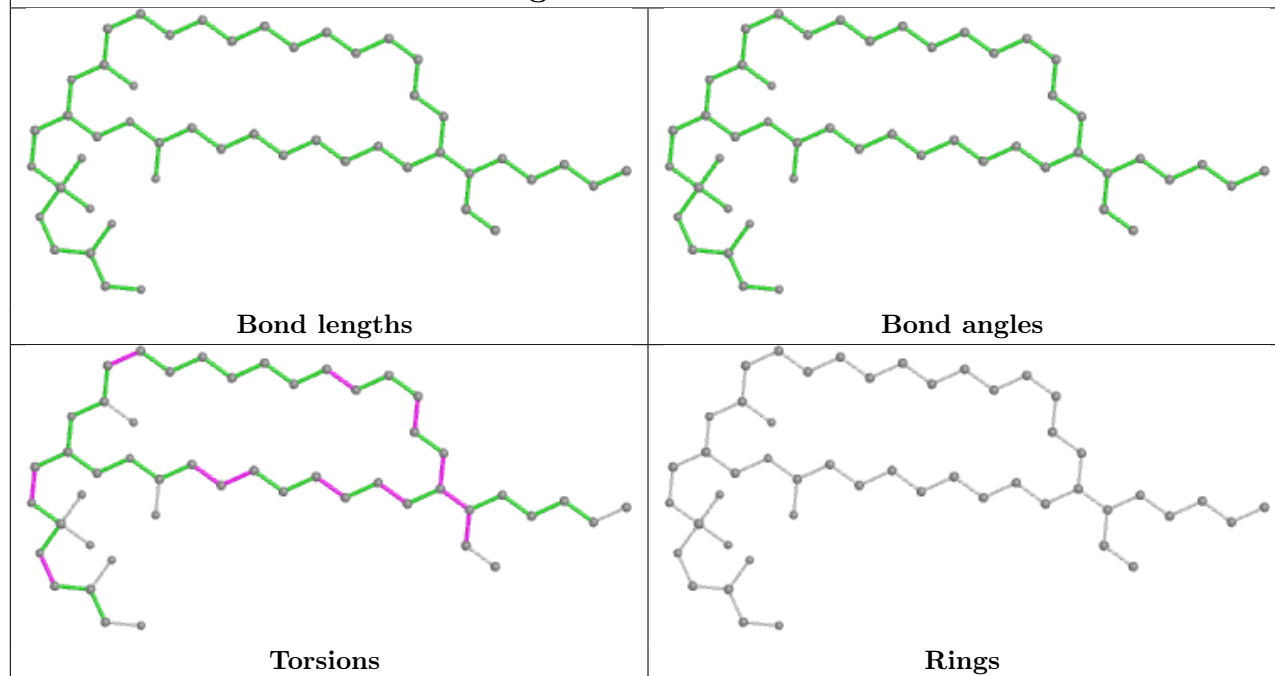




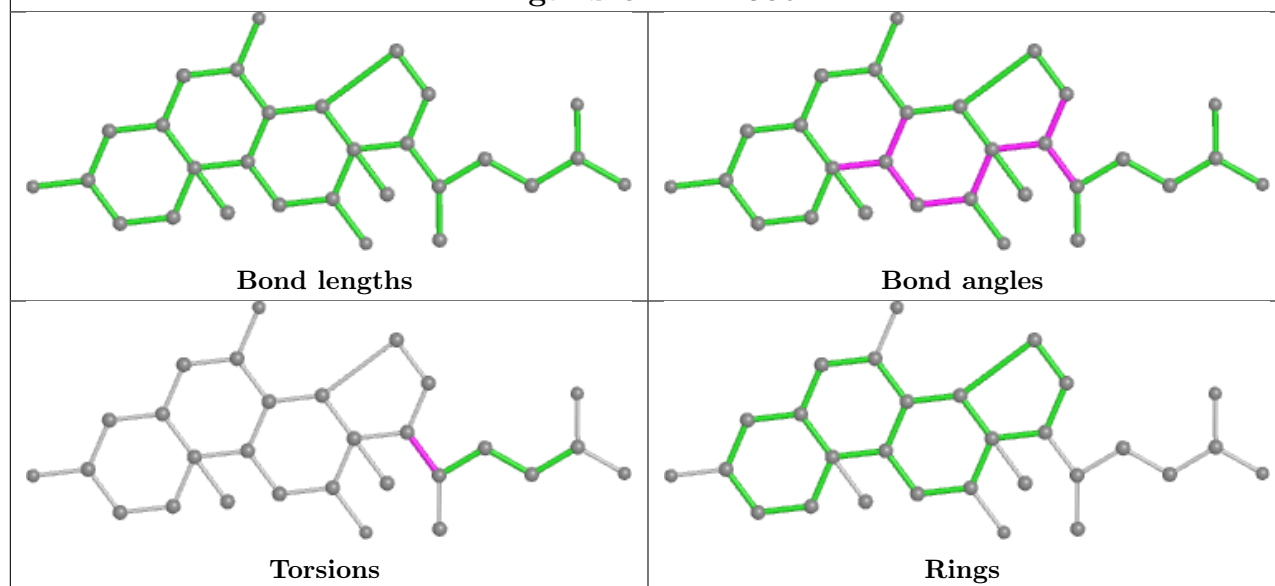


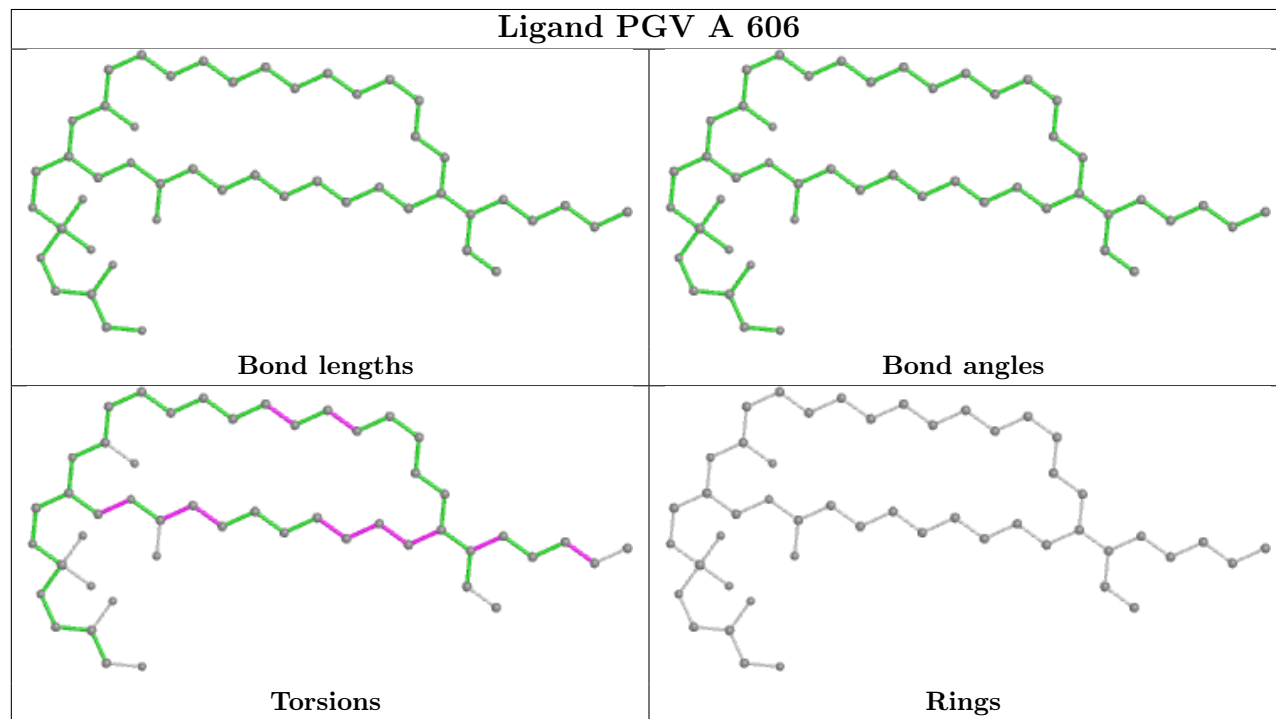
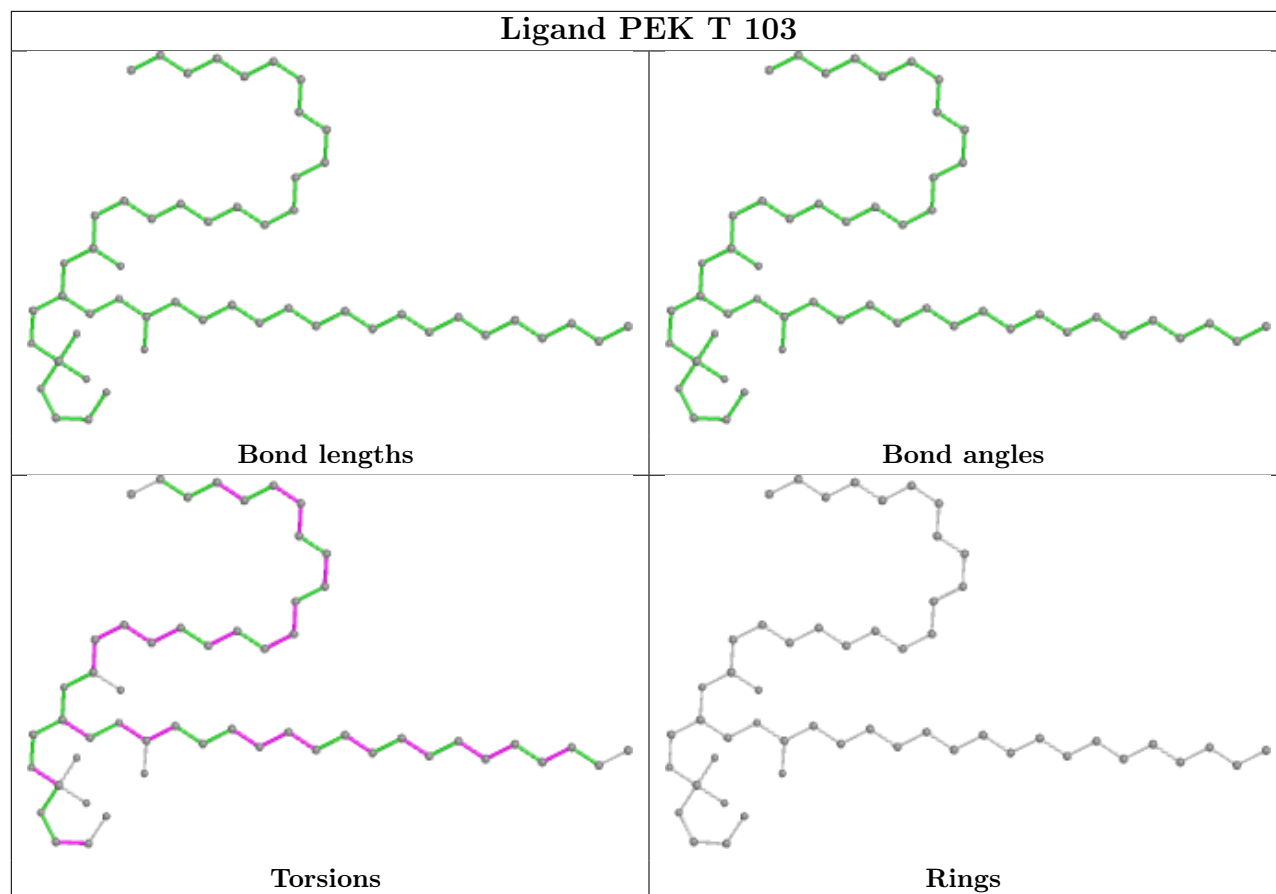


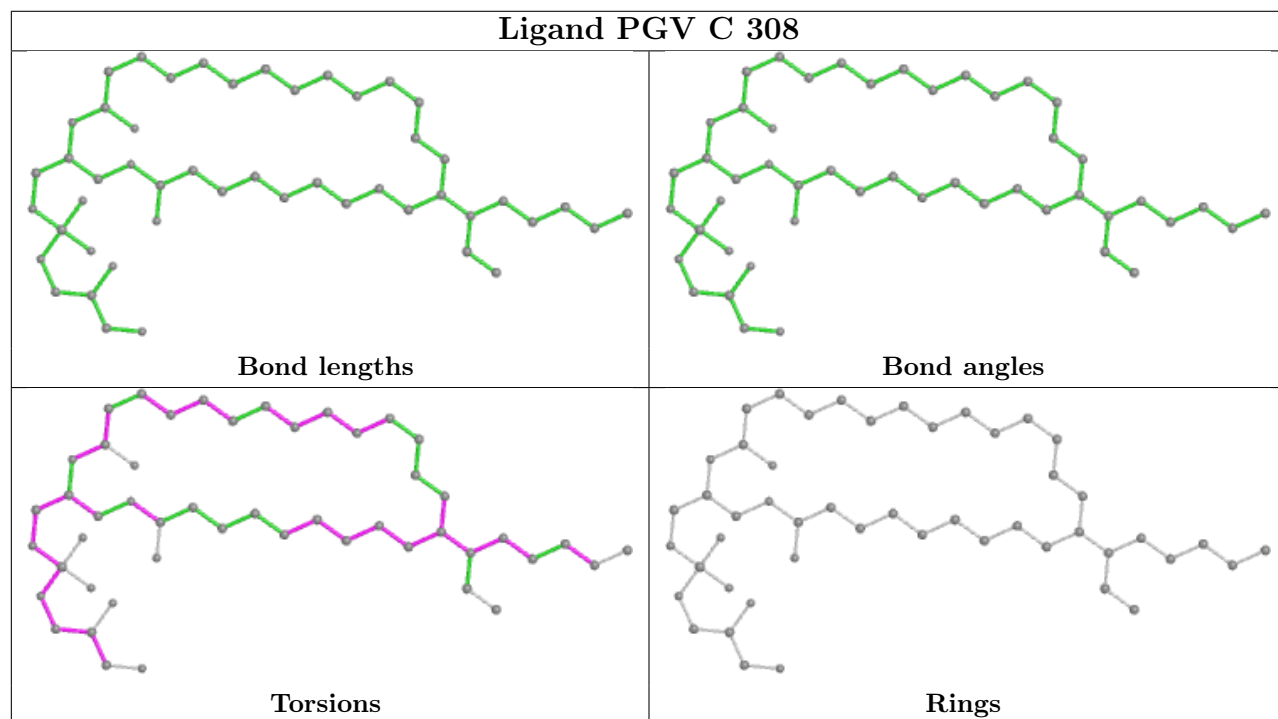
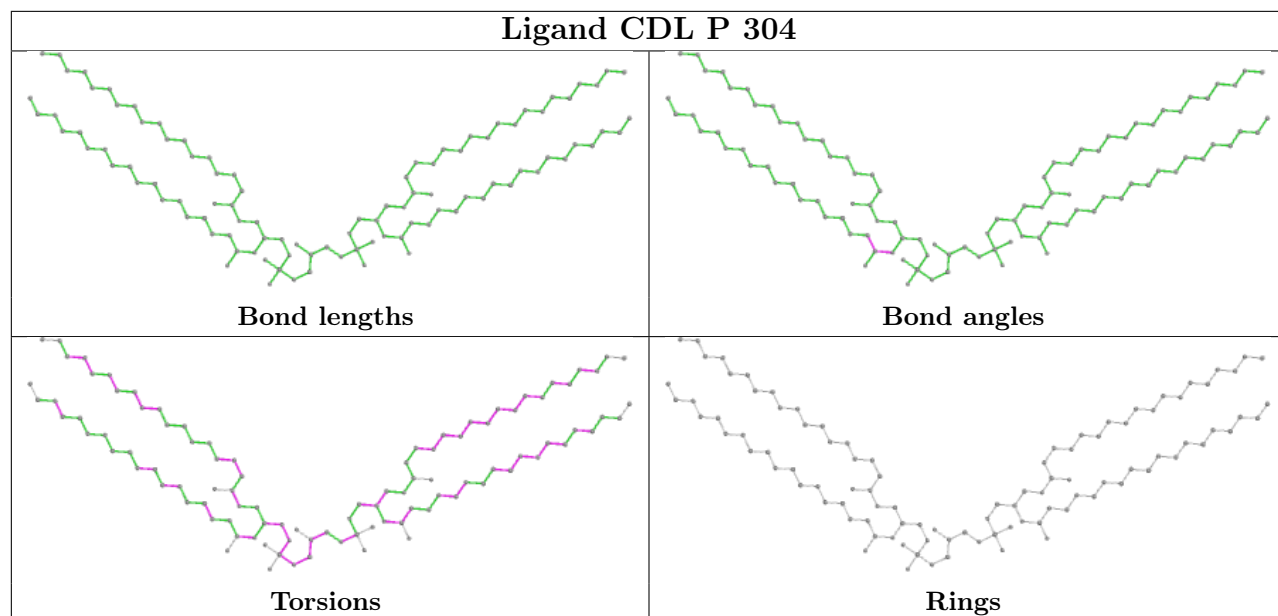
## Ligand PGV P 303

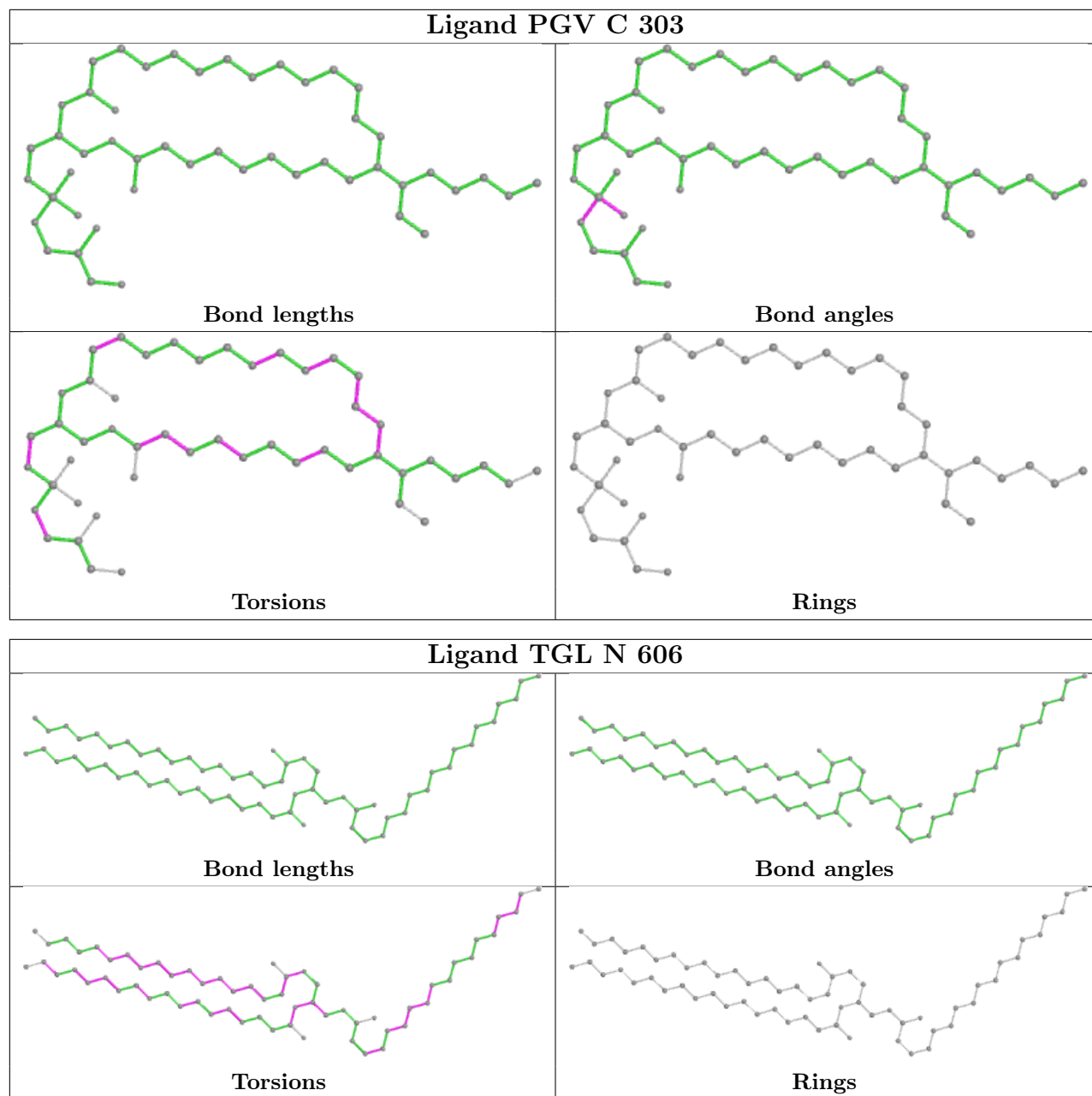


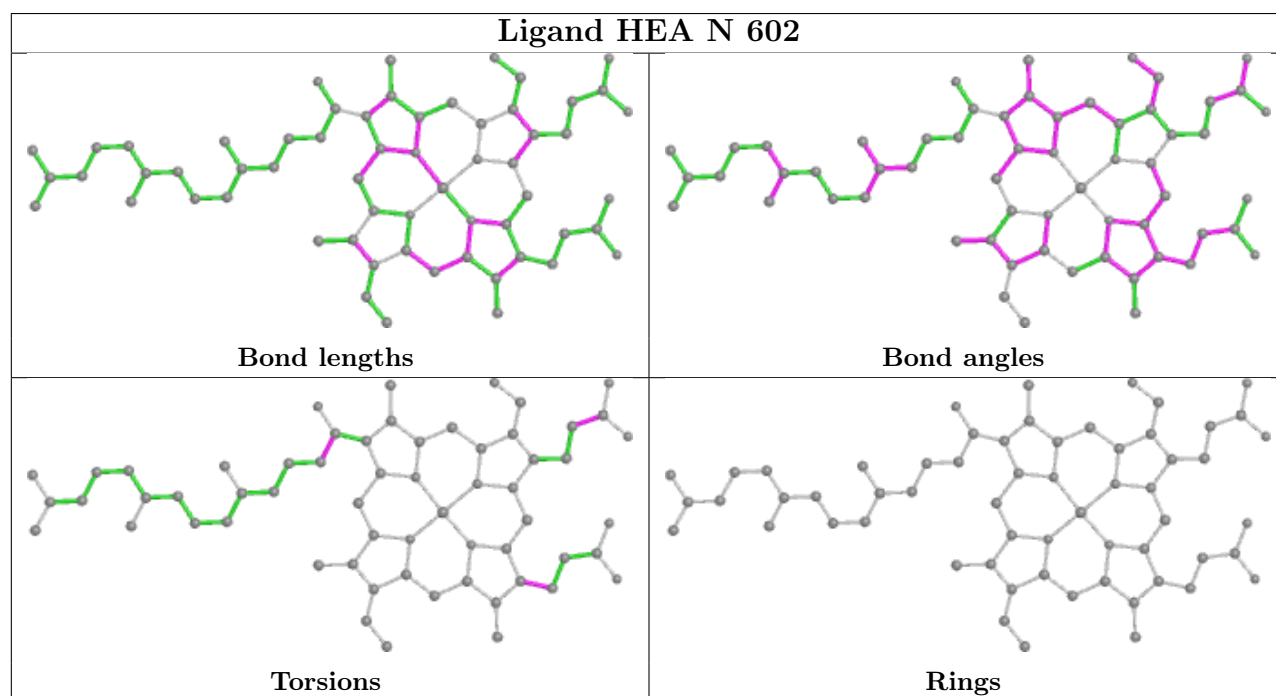
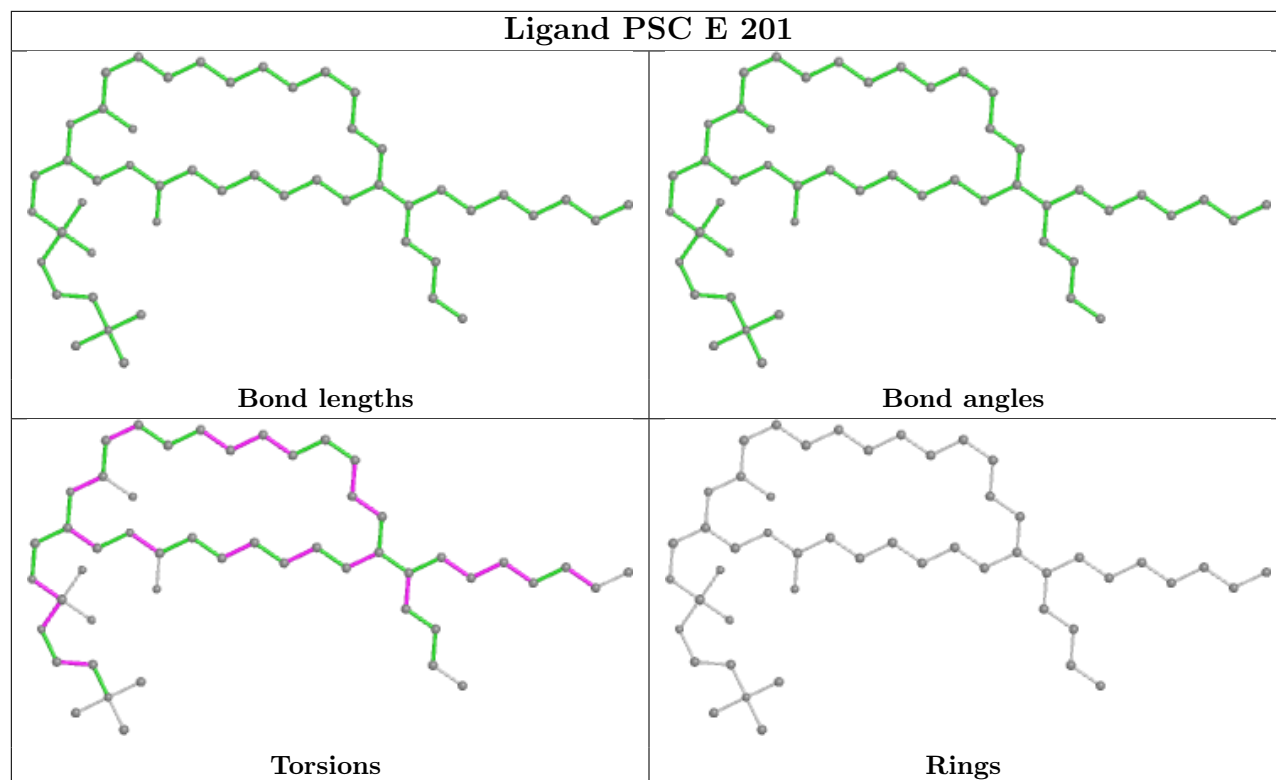
## Ligand CHD P 306

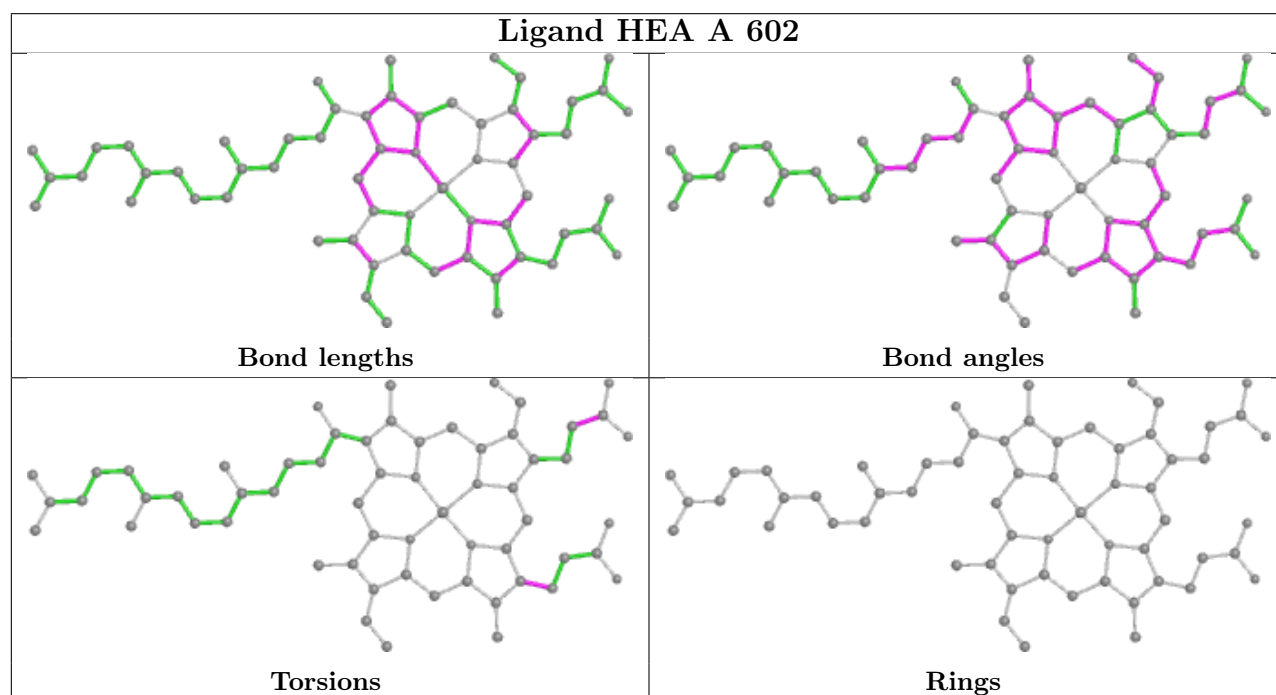
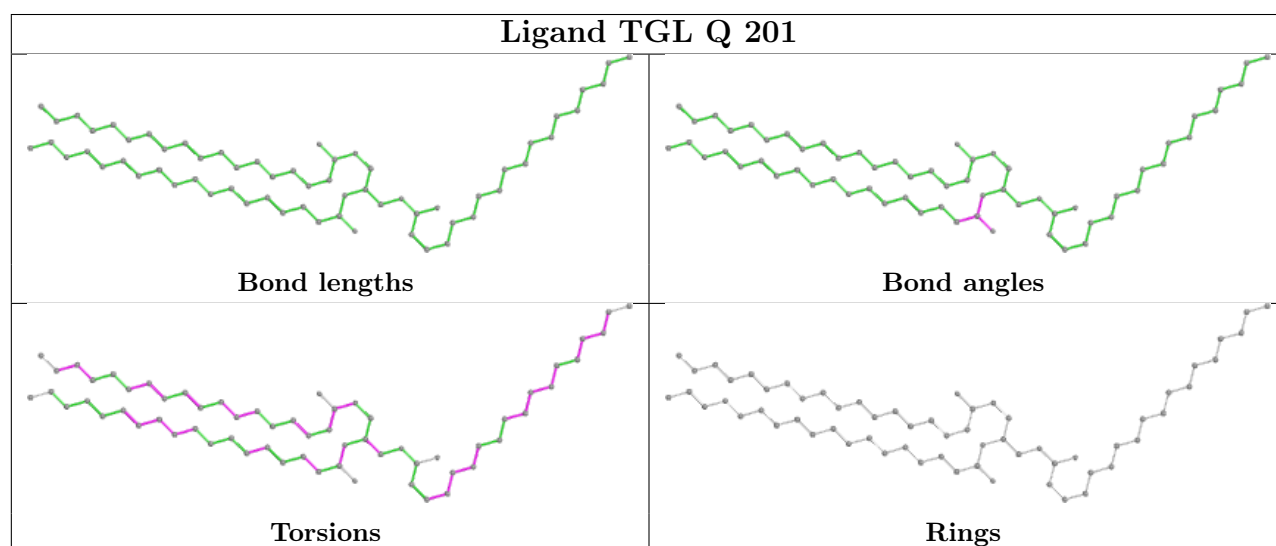
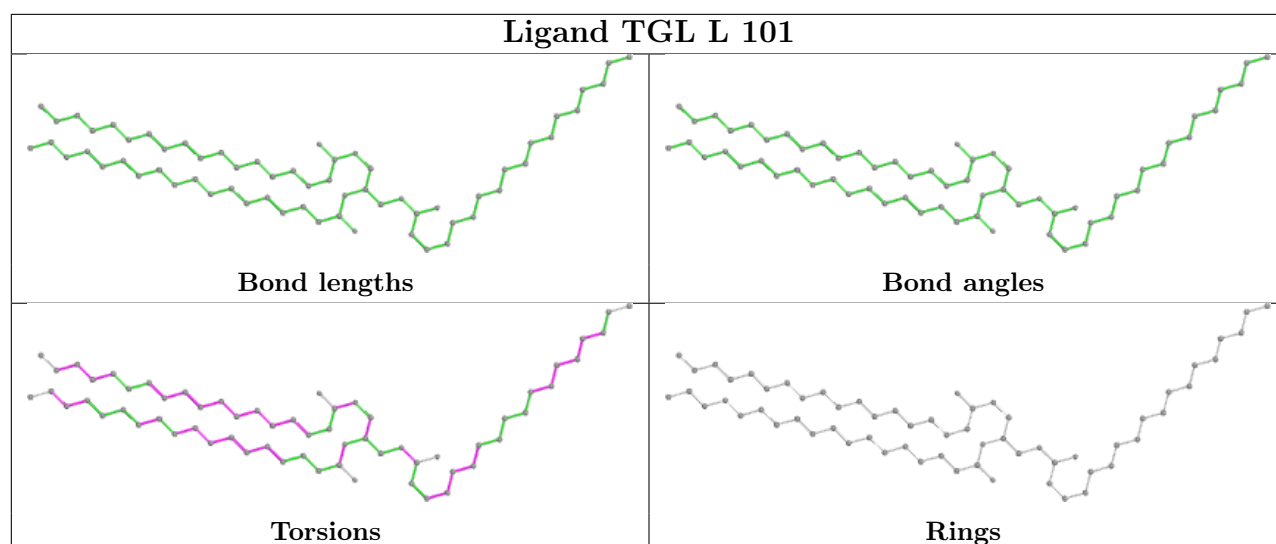


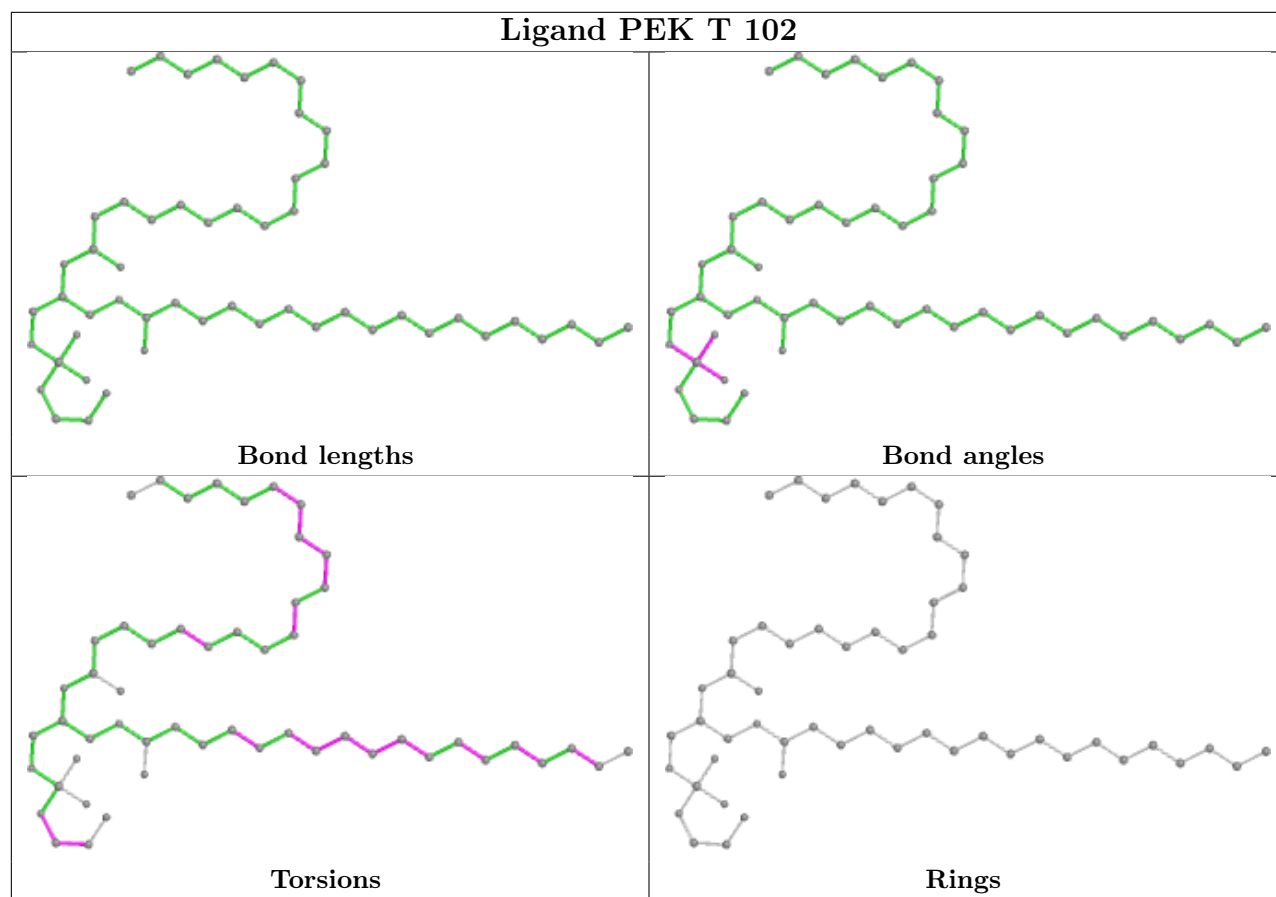
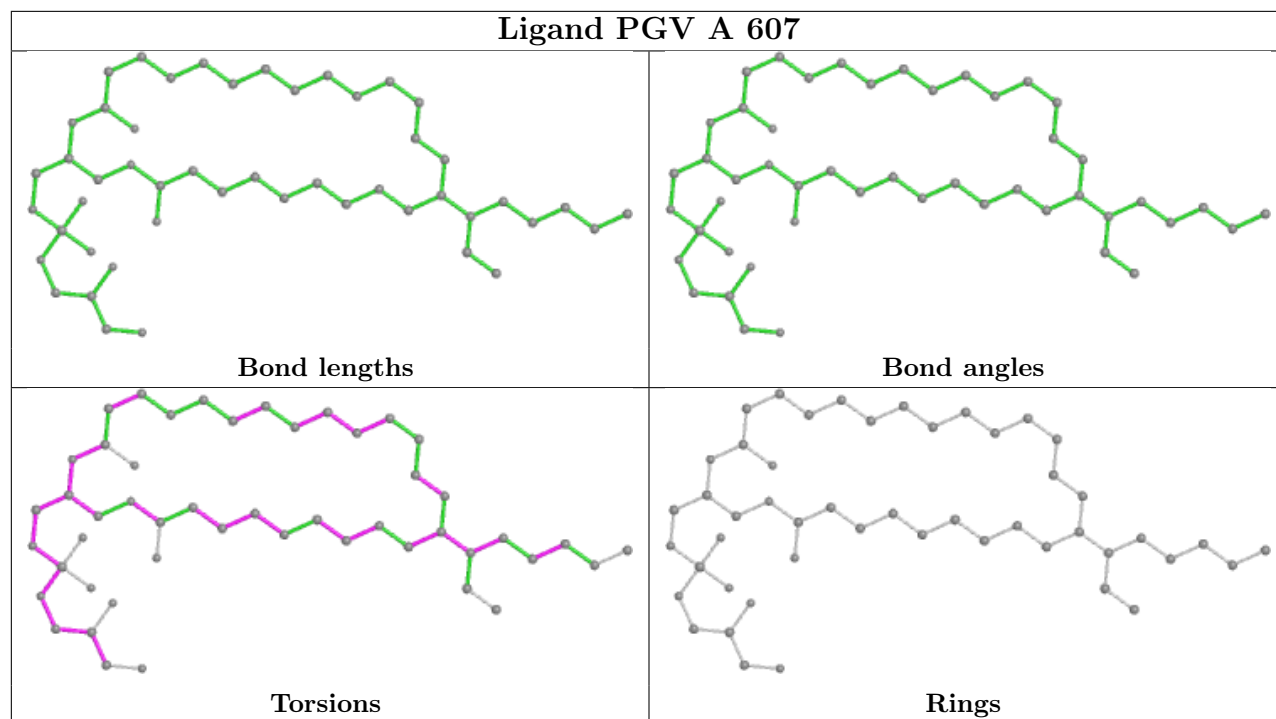




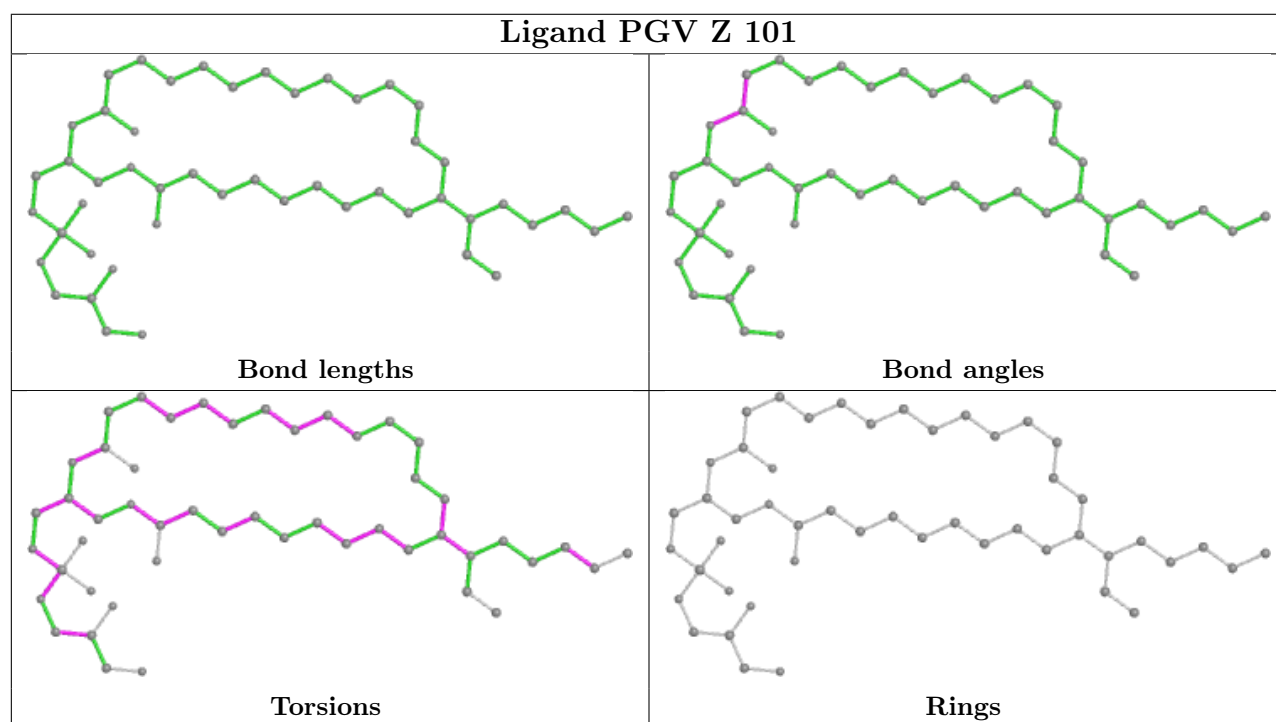
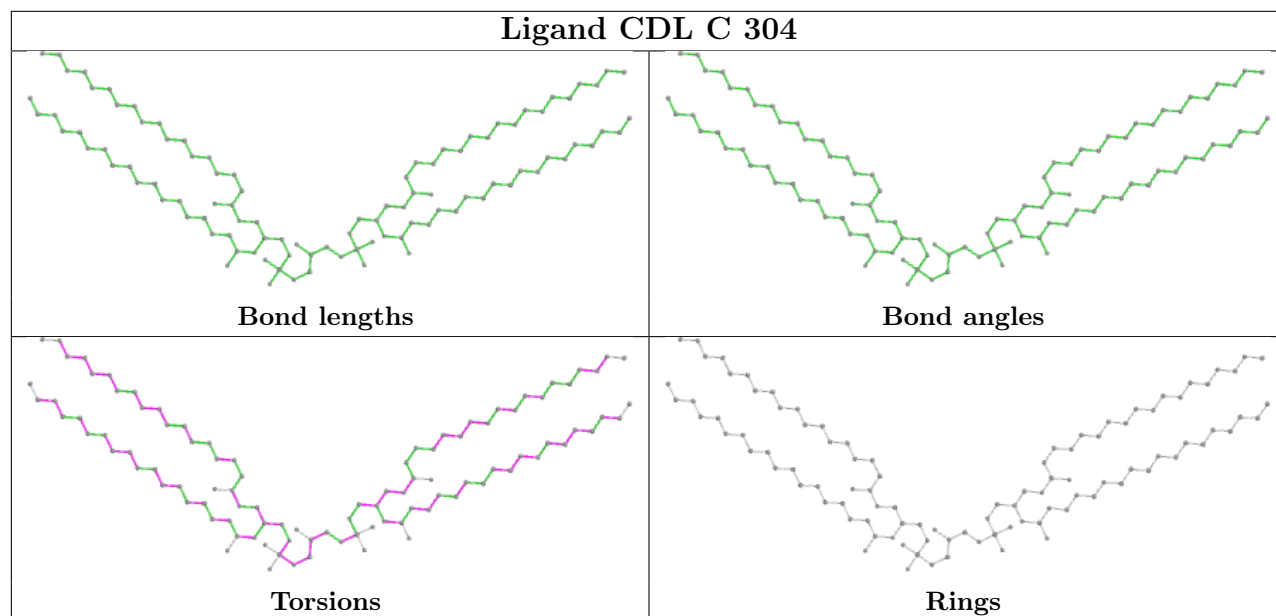




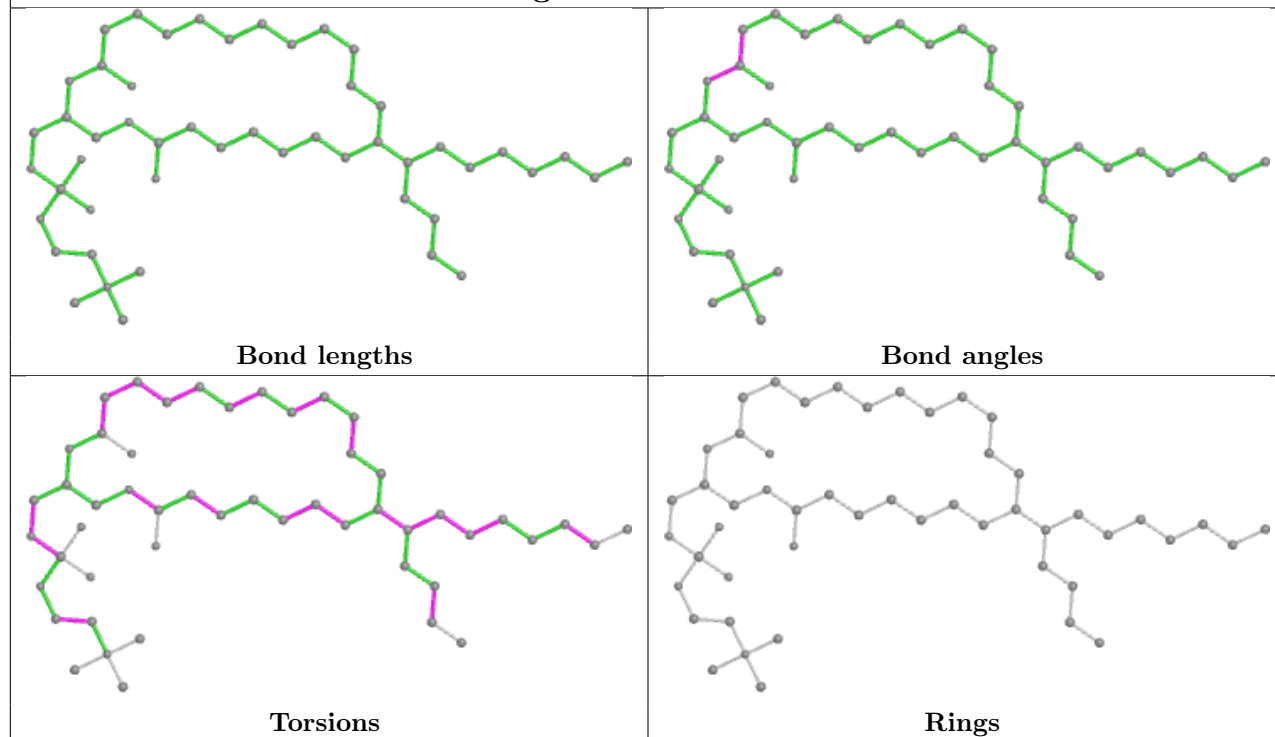




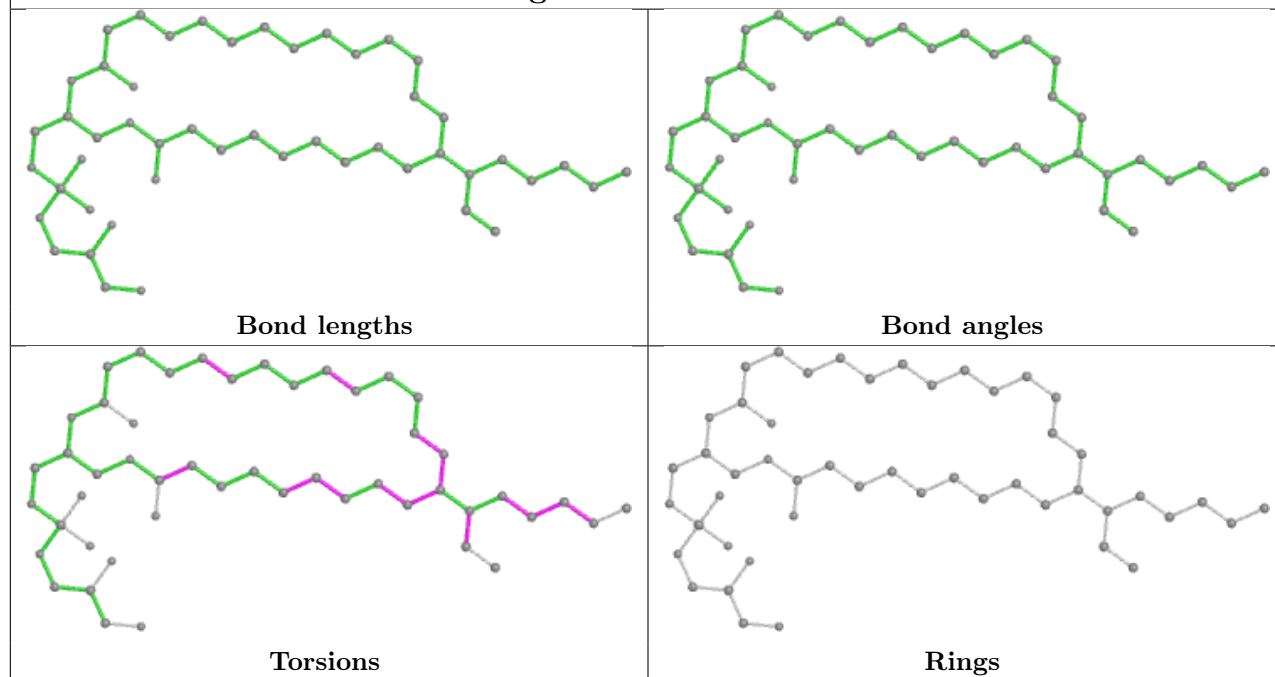


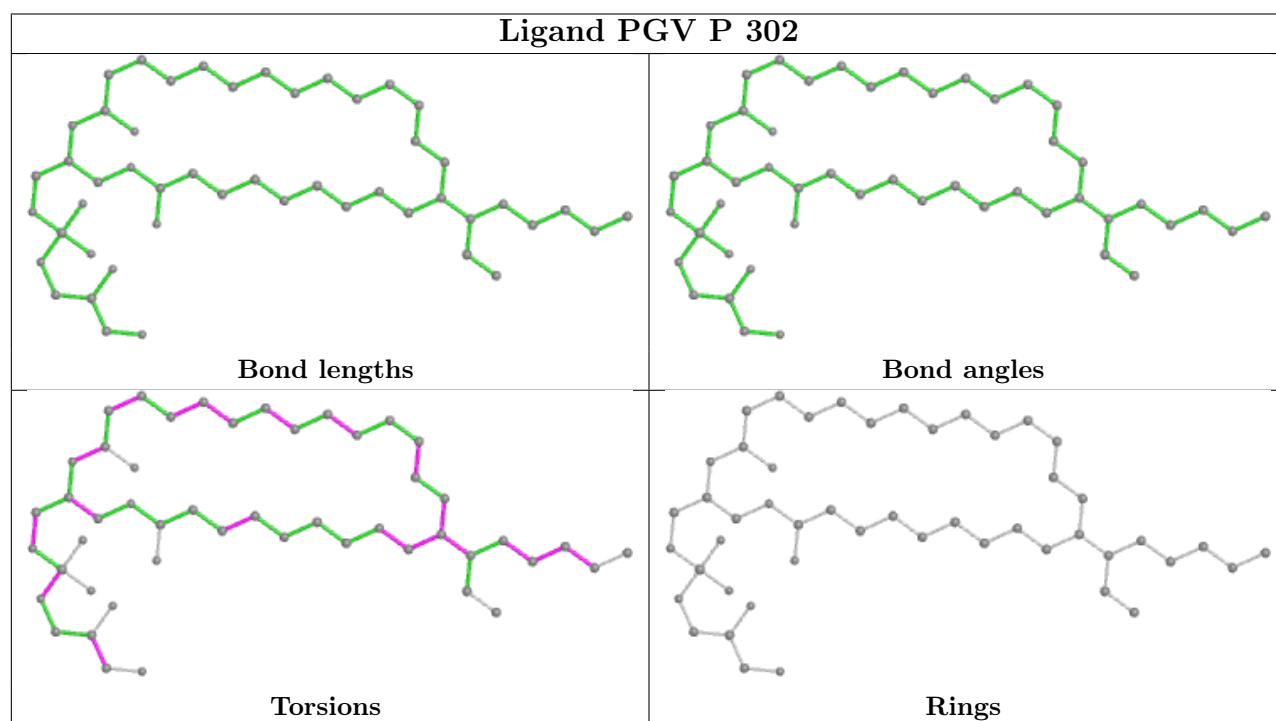
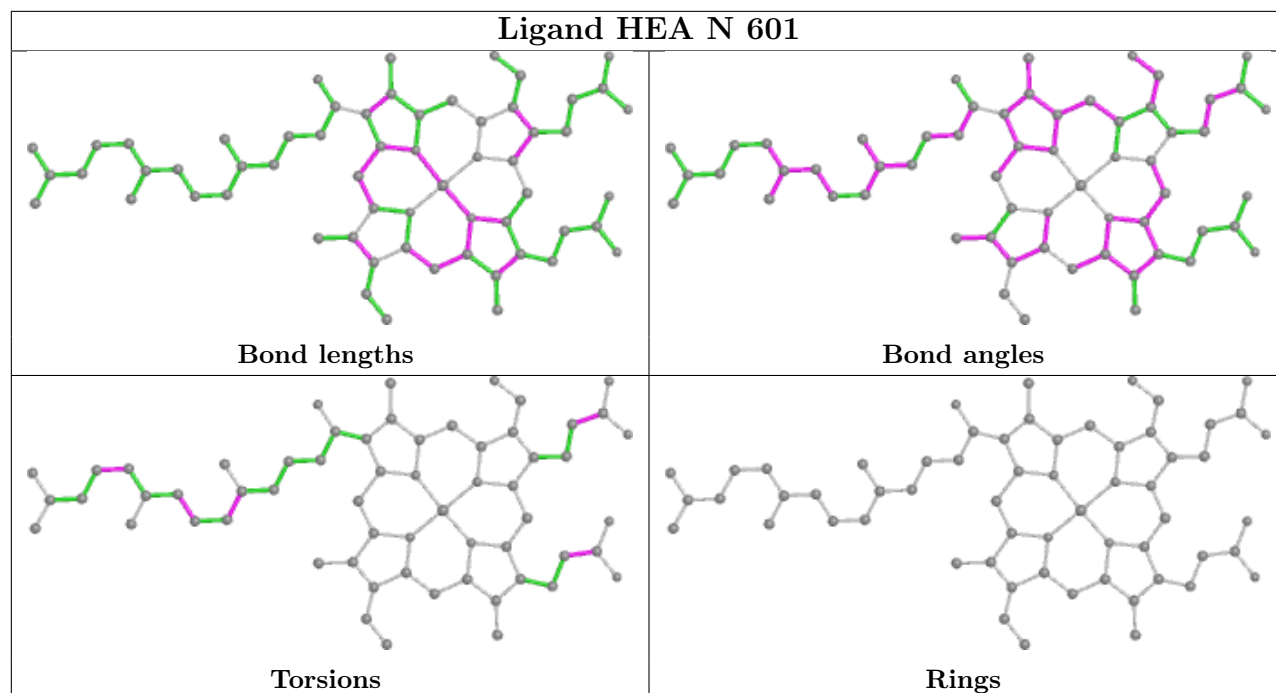


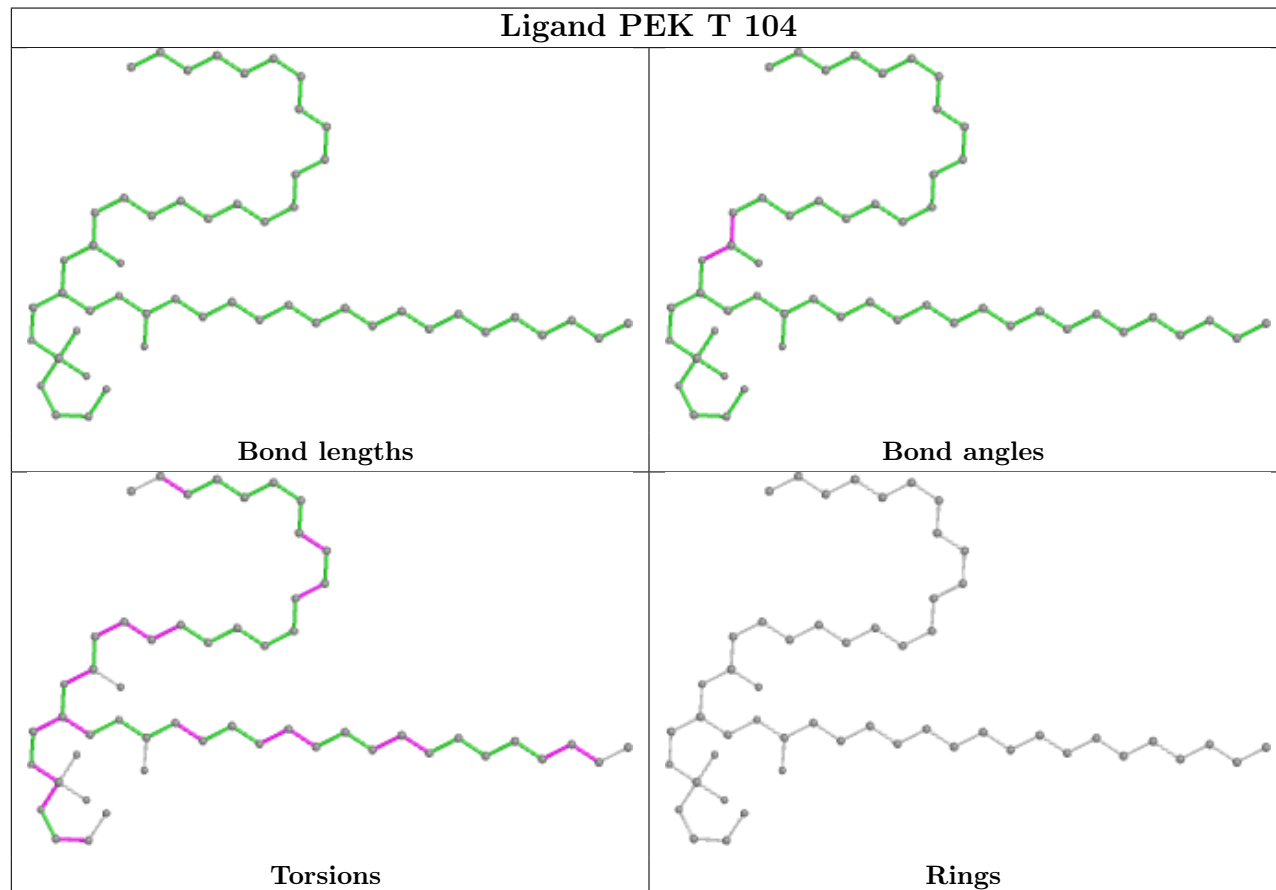
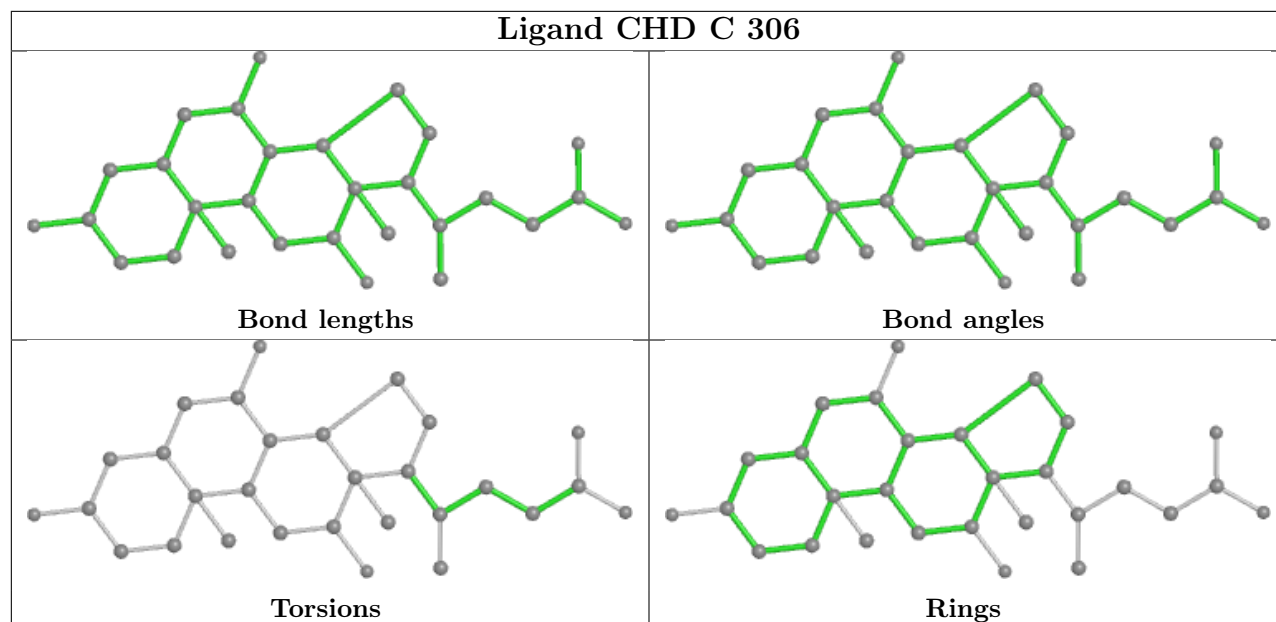
## Ligand PSC O 302

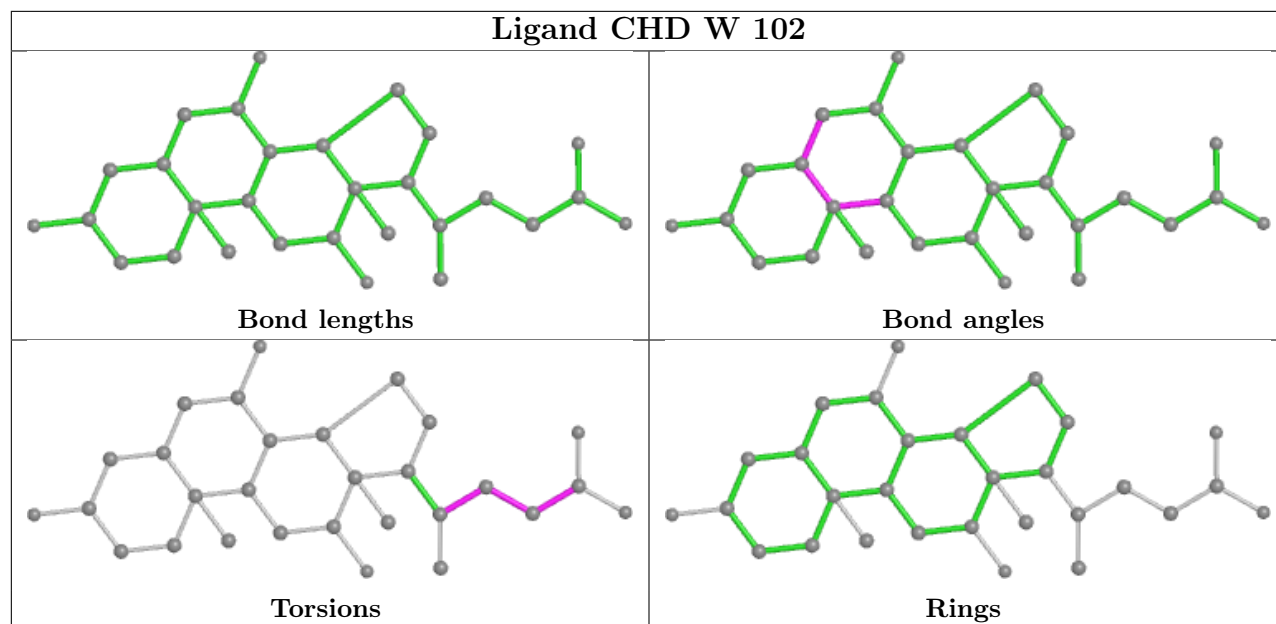


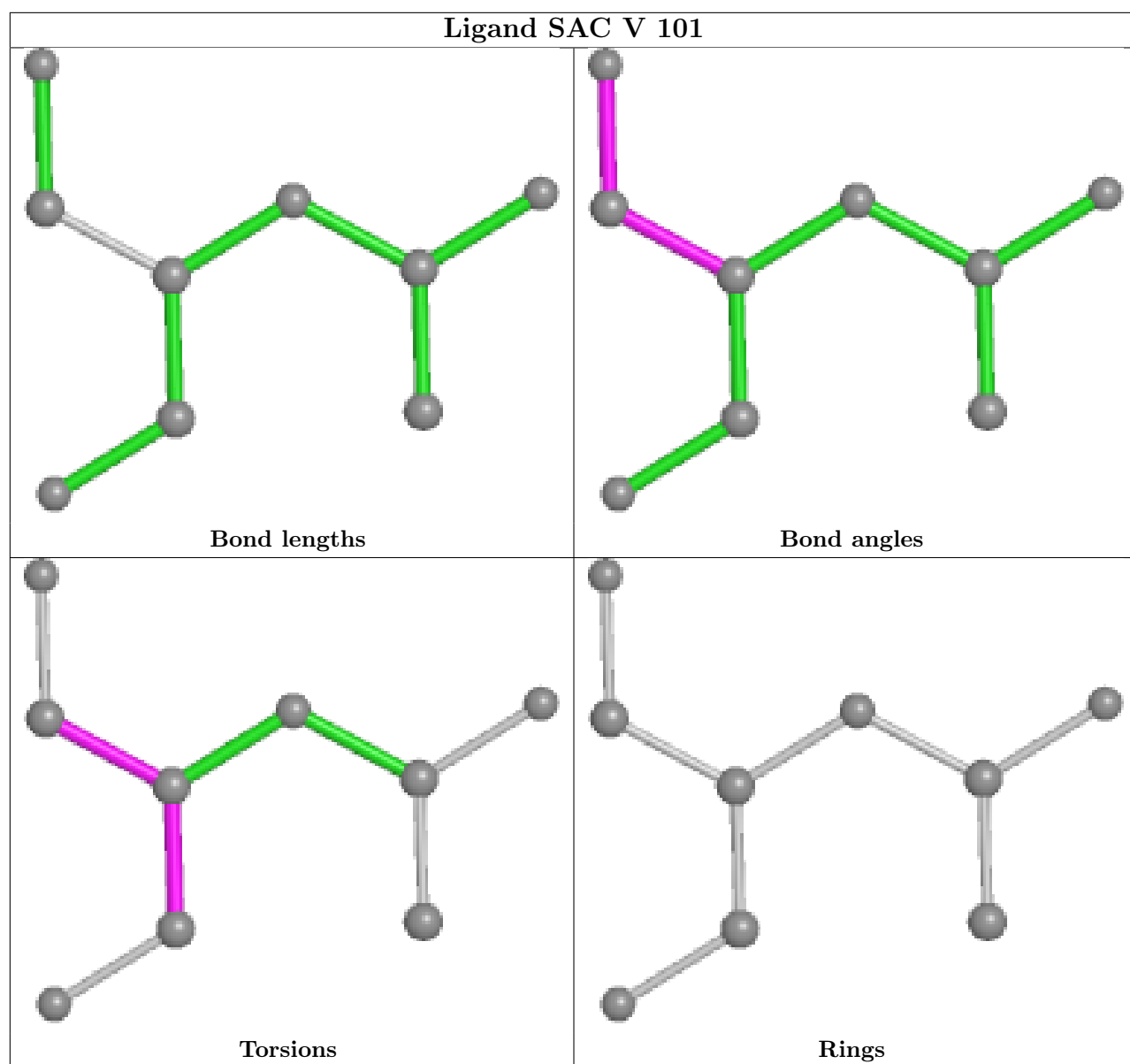
## Ligand PGV P 301

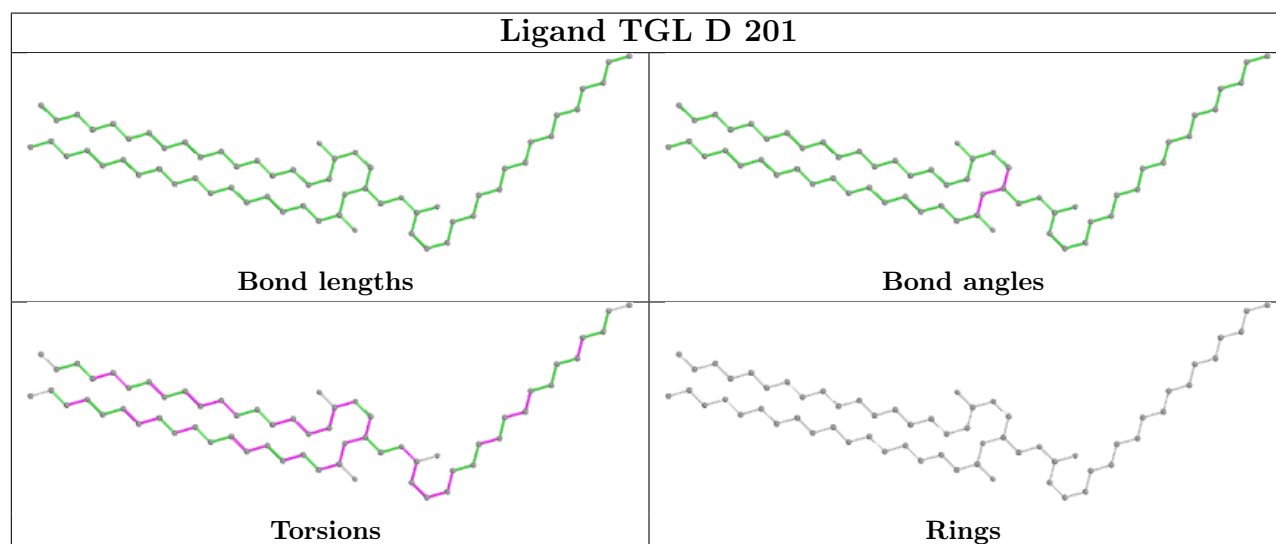
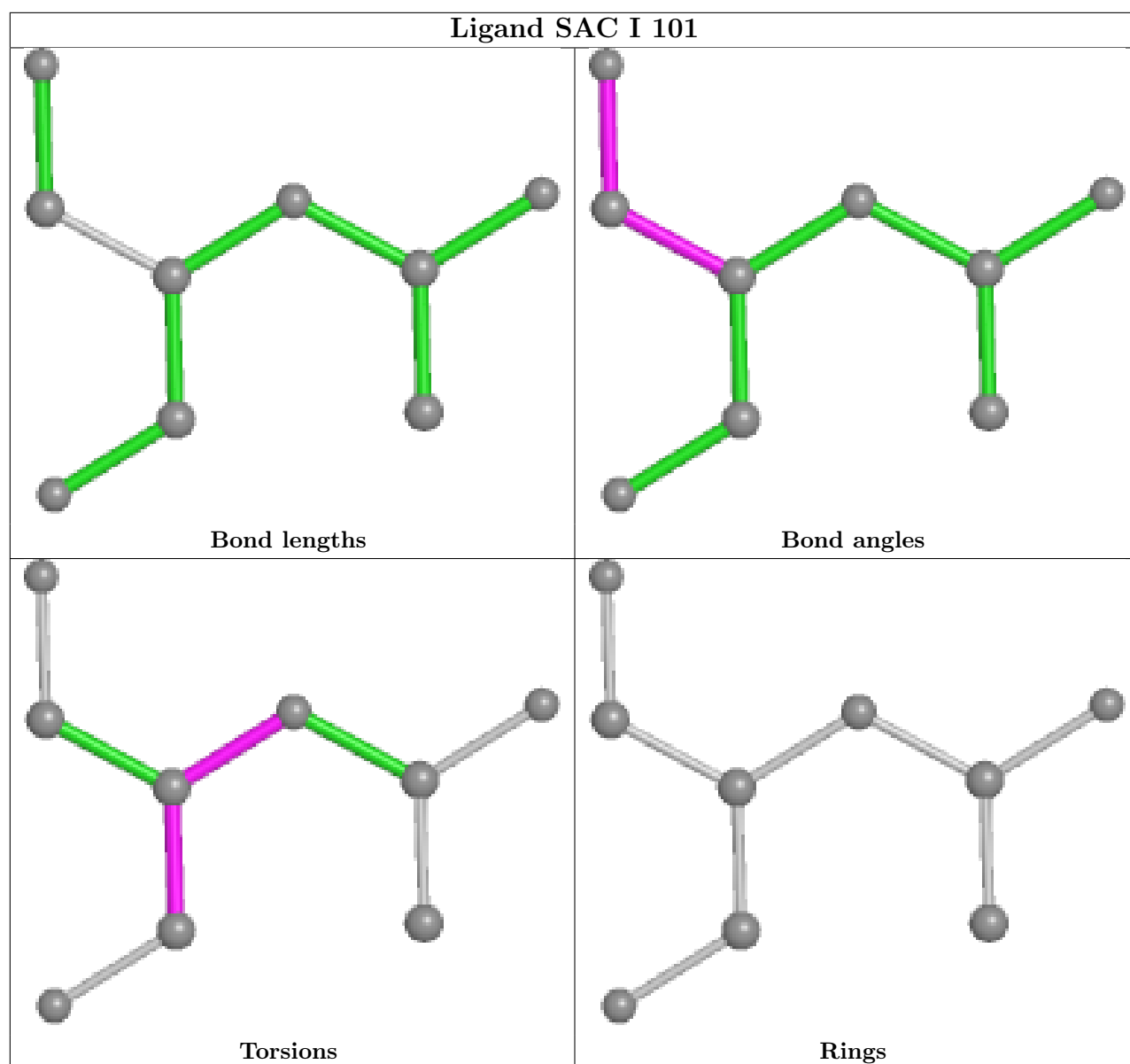




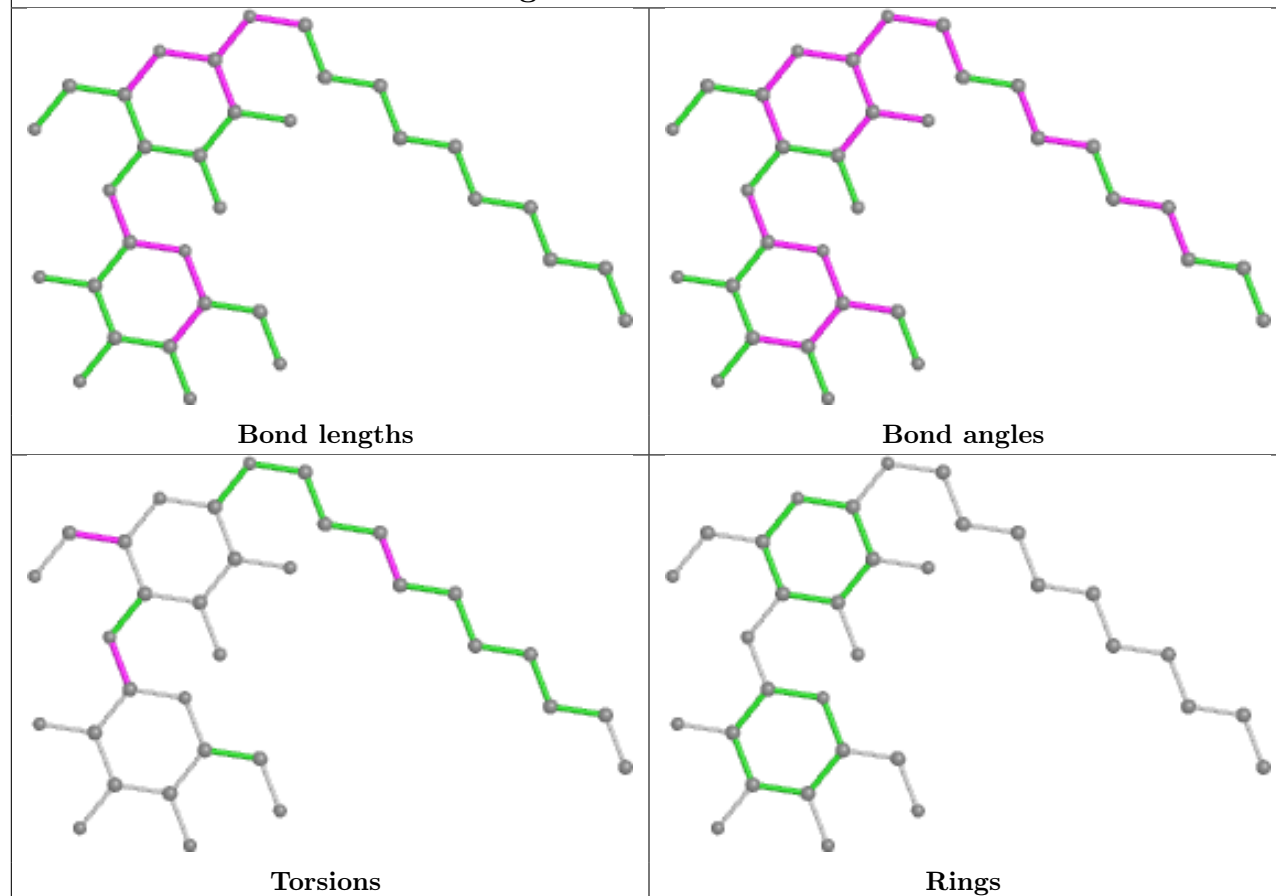




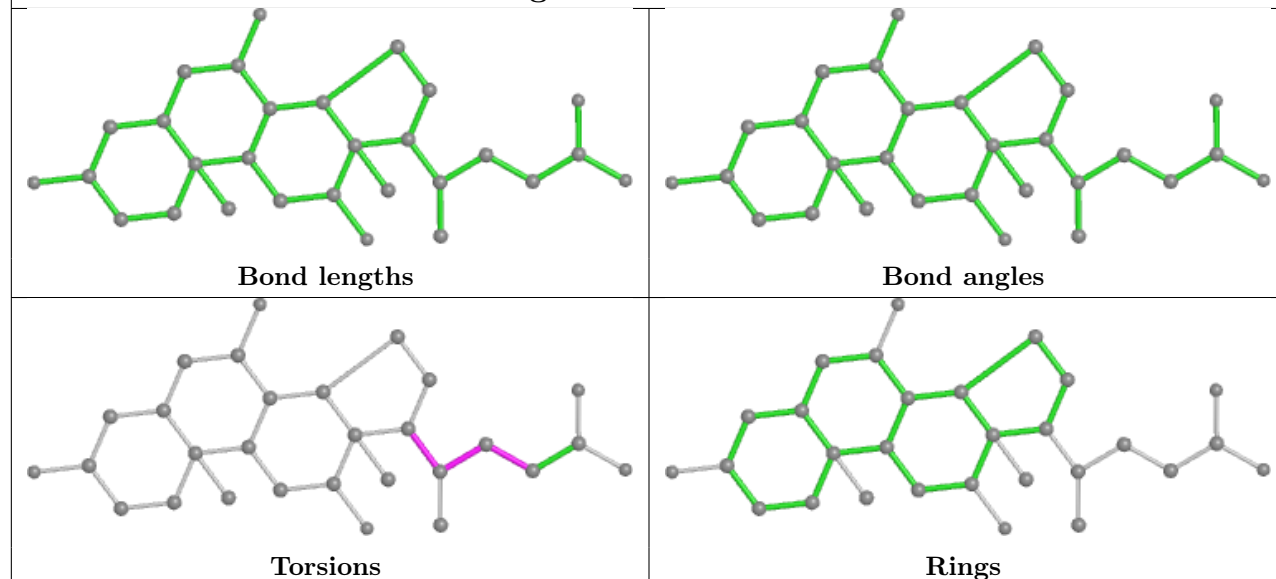




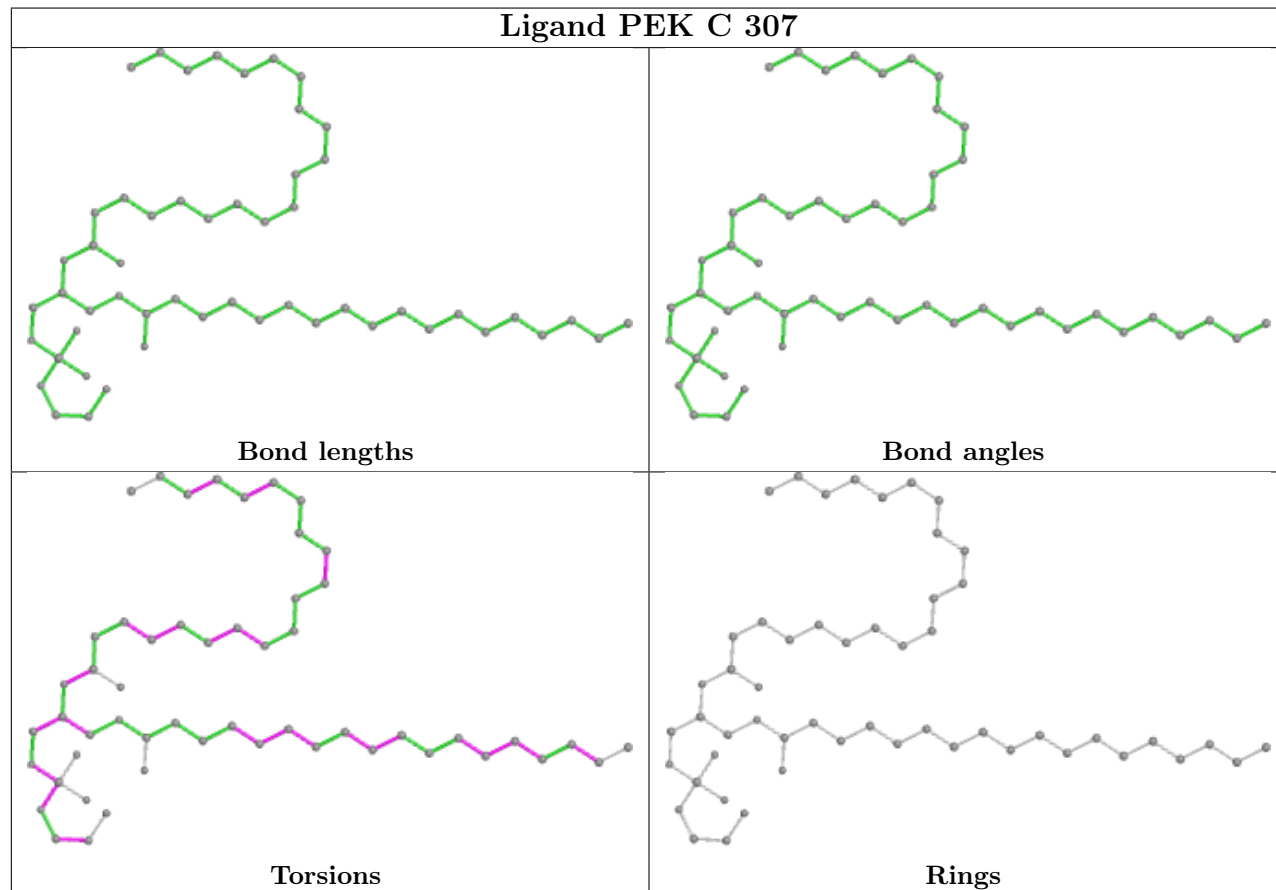
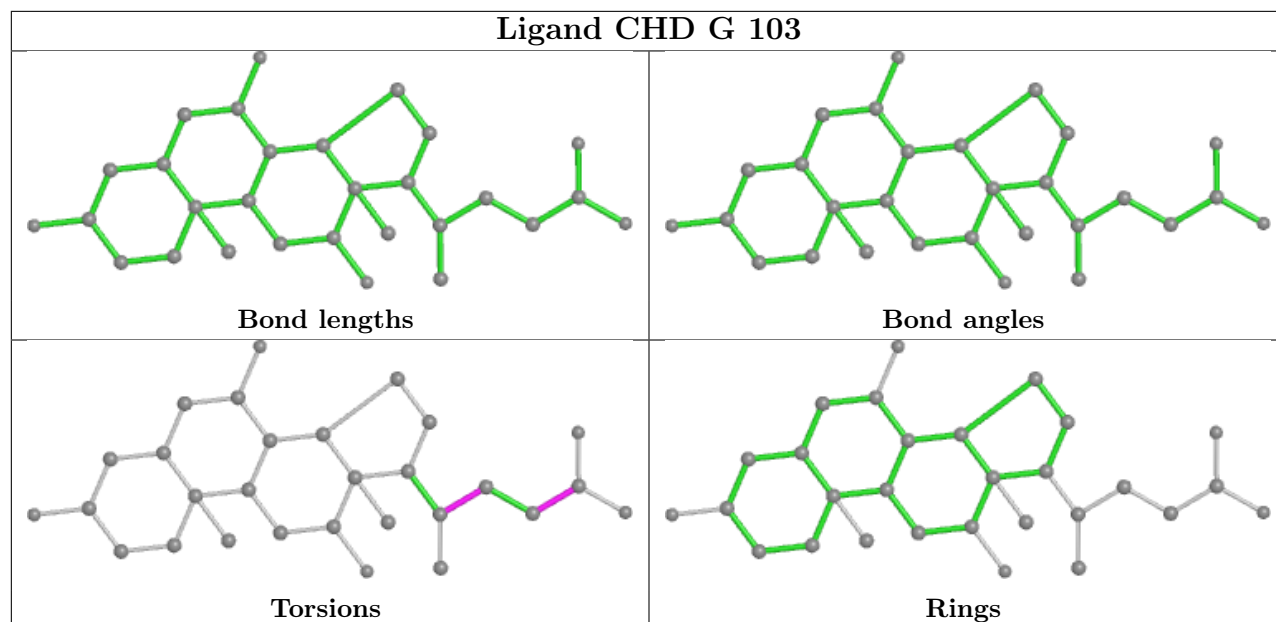
## Ligand DMU W 101

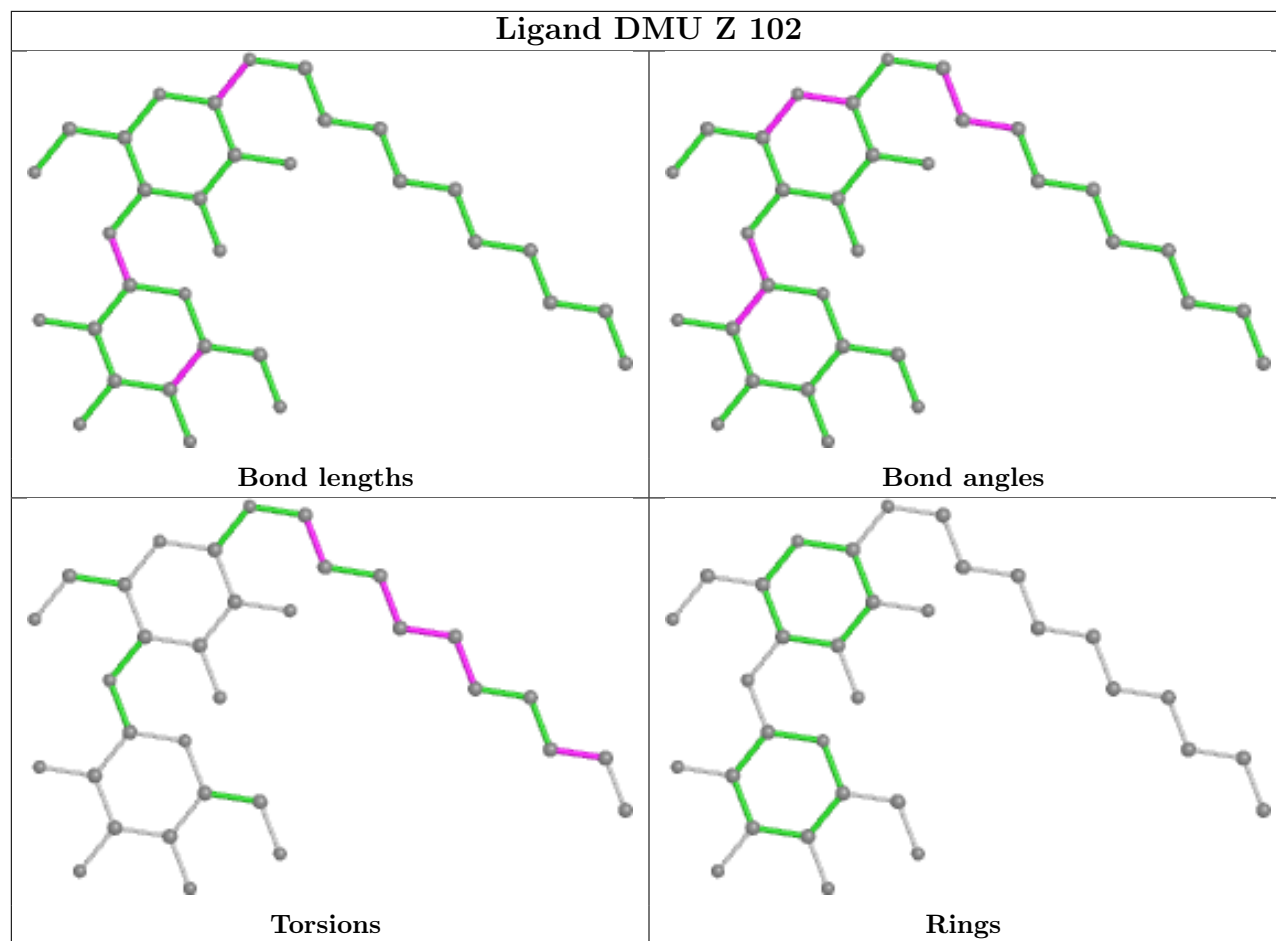


## Ligand CHD P 305









## 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%)	-0.30	4 (0%) 86 86	24, 33, 42, 77	0
1	N	513/514 (99%)	-0.31	1 (0%) 95 95	28, 37, 48, 84	0
2	B	226/227 (99%)	-0.50	1 (0%) 92 93	26, 42, 77, 117	0
2	O	226/227 (99%)	-0.36	7 (3%) 49 45	31, 48, 79, 118	0
3	C	259/261 (99%)	-0.70	0 100 100	26, 37, 52, 96	0
3	P	259/261 (99%)	-0.62	2 (0%) 86 86	29, 38, 55, 94	0
4	D	144/147 (97%)	-0.53	0 100 100	32, 43, 63, 83	0
4	Q	144/147 (97%)	0.42	13 (9%) 9 6	41, 59, 90, 149	0
5	E	105/109 (96%)	-0.44	2 (1%) 66 64	33, 45, 75, 122	0
5	R	105/109 (96%)	-0.28	2 (1%) 66 64	41, 52, 74, 119	0
6	F	98/98 (100%)	0.15	7 (7%) 16 12	30, 43, 111, 165	0
6	S	98/98 (100%)	0.18	8 (8%) 11 8	33, 44, 133, 189	0
7	G	83/85 (97%)	0.34	13 (15%) 2 1	31, 47, 124, 150	0
7	T	83/85 (97%)	0.42	13 (15%) 2 1	34, 49, 111, 135	0
8	H	79/85 (92%)	0.32	8 (10%) 7 4	35, 47, 114, 130	0
8	U	79/85 (92%)	0.39	10 (12%) 3 2	35, 52, 116, 152	0
9	I	72/73 (98%)	0.45	13 (18%) 1 0	36, 53, 92, 107	0
9	V	72/73 (98%)	0.29	8 (11%) 5 3	40, 62, 93, 107	0
10	J	58/59 (98%)	-0.11	4 (6%) 16 13	36, 47, 82, 128	0
10	W	58/59 (98%)	-0.04	5 (8%) 10 7	38, 52, 84, 138	0
11	K	49/56 (87%)	-0.33	2 (4%) 37 34	33, 48, 62, 76	0
11	X	49/56 (87%)	0.37	7 (14%) 2 1	43, 57, 82, 100	0
12	L	46/47 (97%)	-0.66	0 100 100	33, 39, 56, 106	0
12	Y	46/47 (97%)	-0.47	1 (2%) 62 58	36, 49, 71, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.36	1 (2%) 60 56	30, 39, 69, 97	0
13	Z	43/46 (93%)	0.08	3 (6%) 16 13	43, 51, 95, 138	0
All	All	3550/3614 (98%)	-0.23	135 (3%) 40 37	24, 42, 82, 189	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	16.3
4	Q	6	VAL	13.2
4	Q	4	SER	11.9
8	U	45	ALA	11.3
4	Q	5	VAL	11.0
6	F	97	ALA	10.7
13	Z	42	LYS	9.7
6	F	1	ALA	8.6
8	H	45	ALA	8.4
6	F	98	HIS	7.9
10	J	58	LYS	7.8
6	S	1	ALA	7.8
2	O	90	ILE	7.5
4	Q	7	LYS	7.4
8	H	44	THR	6.9
13	Z	43	SER	6.9
7	G	3	ALA	6.8
6	S	98	HIS	6.6
10	W	58	LYS	6.6
5	R	5	HIS	6.6
10	J	57	HIS	6.5
9	I	37	PHE	6.4
8	H	46	LYS	6.2
5	R	109	VAL	6.0
8	U	44	THR	5.9
4	Q	8	SER	5.9
7	G	2	SER	5.8
7	T	1	ALA	5.6
7	G	36	TRP	5.4
7	T	36[A]	TRP	5.4
9	V	37	PHE	5.2
7	T	3	ALA	5.2
8	U	48	GLY	5.2
6	S	96	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
6	S	94	HIS	4.9
12	Y	47	LYS	4.8
6	S	95	GLN	4.7
9	V	34	PHE	4.7
8	U	47	GLY	4.7
2	O	227	LEU	4.7
10	J	1	PHE	4.5
4	Q	147	LYS	4.5
7	T	84	LYS	4.4
5	E	5	HIS	4.4
5	E	109	VAL	4.3
8	U	10	ASN	4.2
6	F	94	HIS	4.2
10	W	48	TYR	4.1
3	P	3	HIS	4.0
10	W	57	HIS	4.0
8	H	48	GLY	4.0
8	U	49	ASP	3.9
7	G	42	ARG	3.9
2	O	113	TYR	3.9
9	I	29	LEU	3.9
9	I	30	GLY	3.8
6	F	96	LEU	3.8
7	G	40	GLY	3.7
7	T	5	LYS	3.6
6	F	2	SER	3.5
7	G	8	HIS	3.5
7	G	41	HIS	3.4
7	G	84	LYS	3.4
8	H	47	GLY	3.4
9	V	33	THR	3.3
13	Z	41	LYS	3.3
9	V	30	GLY	3.3
7	G	5	LYS	3.3
8	U	46	LYS	3.2
8	H	49	ASP	3.2
8	H	43	MET	3.1
7	T	42	ARG	3.1
9	V	2	THR	3.1
11	X	6	ALA	3.1
2	B	90	ILE	3.0
11	X	7	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
7	T	40	GLY	3.0
7	T	2	SER	3.0
9	V	53	ASN	2.9
7	T	46	ALA	2.9
4	Q	58	GLU	2.9
2	O	57	ASP	2.9
9	I	33	THR	2.9
13	M	43	SER	2.9
4	Q	39	ALA	2.9
8	H	50	VAL	2.8
10	J	52	TRP	2.8
10	W	1	PHE	2.8
11	X	18	LEU	2.8
1	N	382[A]	SER	2.7
7	T	43	GLU	2.7
7	T	41	HIS	2.7
7	G	7	ASP	2.6
9	I	34	PHE	2.6
1	A	377	PHE	2.5
9	I	22	VAL	2.5
1	A	66	ILE	2.5
8	U	51	SER	2.5
1	A	374	VAL	2.5
2	O	92	ASN	2.5
1	A	382[A]	SER	2.5
11	X	13	TYR	2.5
2	O	224	ALA	2.5
7	G	1	ALA	2.5
7	G	4	ALA	2.5
11	X	19	ALA	2.4
4	Q	51	LEU	2.4
7	T	47	PHE	2.4
6	F	95	GLN	2.3
9	I	52	ARG	2.3
4	Q	46	ALA	2.3
10	W	52	TRP	2.3
8	U	43	MET	2.3
6	S	2	SER	2.3
3	P	182	TYR	2.3
4	Q	48	TRP	2.3
9	I	21	ILE	2.3
11	X	46	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	91	ASN	2.2
9	I	25	PHE	2.2
6	S	93	PRO	2.2
9	V	29	LEU	2.2
11	X	47	ARG	2.1
8	U	8	ILE	2.1
7	G	43	GLU	2.1
9	I	17	LEU	2.1
9	V	31	PHE	2.1
9	I	18	ARG	2.1
11	K	6	ALA	2.0
11	K	7	PRO	2.0
4	Q	33	LEU	2.0
9	I	26	MET	2.0
9	I	28	SER	2.0
7	T	10	GLY	2.0
4	Q	141	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
7	TPO	G	11	11/12	0.68	0.30	110,125,150,150	0
7	TPO	T	11	11/12	0.79	0.24	116,120,142,143	0
1	FME	N	1	10/11	0.95	0.25	51,63,84,88	0
1	FME	A	1	10/11	0.95	0.21	55,60,85,92	0
2	FME	O	1	10/11	0.96	0.14	41,48,54,55	0
2	FME	B	1	10/11	0.97	0.14	33,40,47,61	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
29	SAC	I	101	9/10	0.22	0.59	80,104,115,123	0
29	SAC	V	101	9/10	0.32	0.49	118,130,141,147	0
27	PSC	E	201	52/52	0.58	0.46	66,112,177,181	0
21	TGL	Q	201	63/63	0.59	0.28	69,98,120,131	0
24	PEK	C	307	53/53	0.60	0.30	57,90,174,186	0
21	TGL	Y	101	63/63	0.61	0.38	55,84,128,139	0
24	PEK	T	103	53/53	0.64	0.41	54,124,165,170	0
24	PEK	G	102	53/53	0.66	0.32	56,120,164,170	0
27	PSC	O	302	52/52	0.68	0.37	54,111,177,203	0
25	CDL	G	101	100/100	0.68	0.33	70,109,164,179	0
23	DMU	W	101	33/33	0.68	0.50	59,104,124,144	0
25	CDL	P	304	100/100	0.70	0.32	58,109,142,159	0
18	PGV	P	302	51/51	0.71	0.33	69,104,137,150	0
24	PEK	T	104	53/53	0.71	0.34	51,98,170,183	0
23	DMU	C	301	33/33	0.72	0.50	60,111,136,138	0
21	TGL	N	606	63/63	0.73	0.32	61,94,161,172	0
25	CDL	T	105	100/100	0.73	0.29	76,115,154,202	0
25	CDL	C	304	100/100	0.74	0.33	52,101,131,139	0
18	PGV	C	308	51/51	0.74	0.28	60,93,116,126	0
18	PGV	Z	101	51/51	0.75	0.34	51,98,124,137	0
21	TGL	B	301	63/63	0.79	0.29	61,88,159,165	0
21	TGL	L	101	63/63	0.80	0.25	47,73,104,111	0
18	PGV	A	607	51/51	0.82	0.26	52,87,123,134	0
21	TGL	D	201	63/63	0.82	0.22	52,80,107,110	0
23	DMU	Z	102	33/33	0.85	0.24	55,63,88,90	0
26	CHD	W	102	29/29	0.85	0.24	64,77,91,94	0
26	CHD	J	101	29/29	0.86	0.30	59,70,95,96	0
23	DMU	D	202	33/33	0.88	0.18	44,50,69,72	0
19	EDO	T	106	4/4	0.91	0.28	42,51,51,56	0
24	PEK	T	102	53/53	0.91	0.21	34,56,92,98	0
19	EDO	A	608	4/4	0.92	0.21	31,37,38,43	0
19	EDO	C	309	4/4	0.92	0.14	54,54,57,61	0
26	CHD	C	305	29/29	0.93	0.26	52,63,72,74	0
19	EDO	G	104	4/4	0.94	0.20	51,58,59,59	0
26	CHD	P	305	29/29	0.95	0.24	53,61,66,72	0
16	MG	N	604	1/1	0.95	0.10	34,34,34,34	0
19	EDO	A	609	4/4	0.95	0.17	54,57,57,58	0
16	MG	A	604	1/1	0.95	0.13	29,29,29,29	0
24	PEK	C	302	53/53	0.95	0.19	38,57,85,94	0
18	PGV	C	303	51/51	0.95	0.21	31,45,80,81	0

*Continued on next page...*



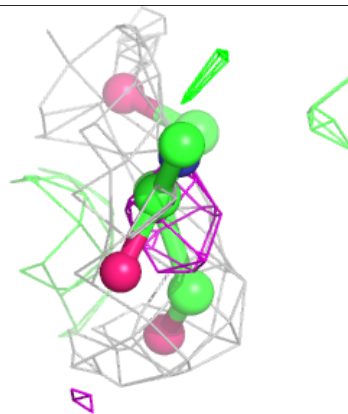
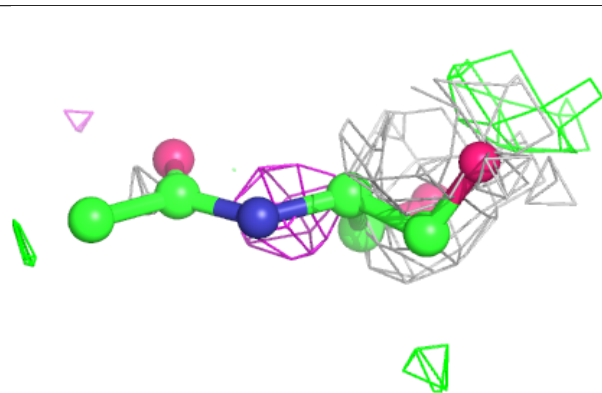
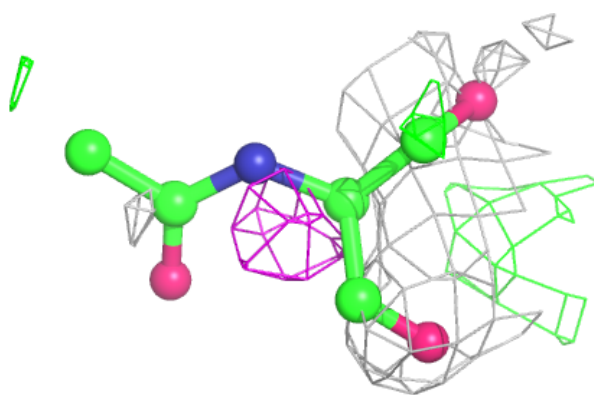
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
26	CHD	P	306	29/29	0.96	0.10	32,38,42,43	0
18	PGV	P	303	51/51	0.96	0.18	29,47,84,86	0
19	EDO	S	102	4/4	0.96	0.20	59,59,60,61	0
14	HEA	N	602	60/60	0.97	0.15	30,34,47,52	0
26	CHD	C	306	29/29	0.97	0.10	31,37,41,41	0
26	CHD	G	103	29/29	0.97	0.09	34,36,39,41	0
14	HEA	A	601	60/60	0.97	0.19	29,35,47,50	0
18	PGV	P	301	51/51	0.97	0.22	30,50,72,75	0
19	EDO	N	607	4/4	0.97	0.15	37,37,37,38	0
26	CHD	T	101	29/29	0.97	0.10	32,36,40,49	0
14	HEA	A	602	60/60	0.97	0.17	25,32,40,42	0
19	EDO	S	103	4/4	0.97	0.14	45,49,49,51	0
17	NA	A	605	1/1	0.97	0.07	32,32,32,32	0
18	PGV	A	606	51/51	0.97	0.22	27,41,71,81	0
14	HEA	N	601	60/60	0.97	0.19	31,39,53,57	0
22	CUA	B	302	2/2	0.98	0.07	29,29,29,31	0
22	CUA	O	301	2/2	0.98	0.06	36,36,36,38	0
17	NA	N	605	1/1	0.99	0.04	35,35,35,35	0
20	OH	A	610	1/1	0.99	0.24	26,26,26,26	1
15	CU	A	603	1/1	1.00	0.12	32,32,32,32	0
28	ZN	F	101	1/1	1.00	0.07	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.05	40,40,40,40	0
20	OH	N	608	1/1	1.00	0.26	27,27,27,27	1
15	CU	N	603	1/1	1.00	0.13	36,36,36,36	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.

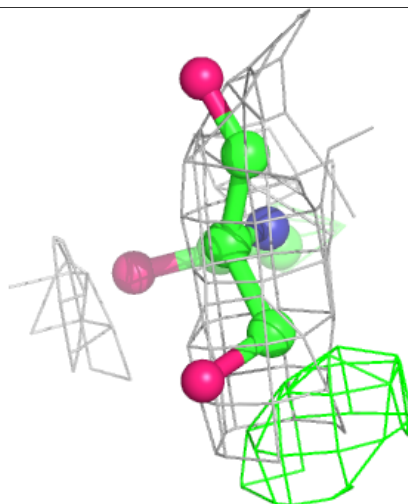
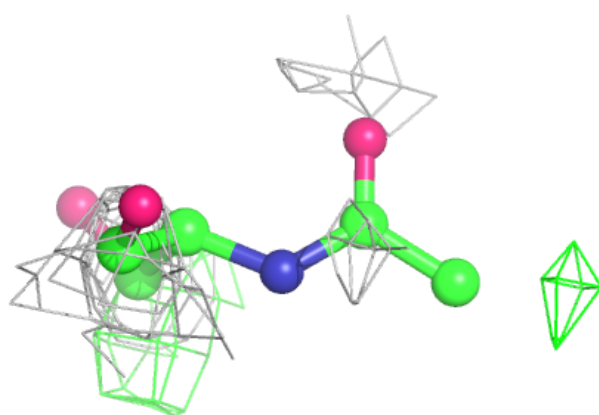
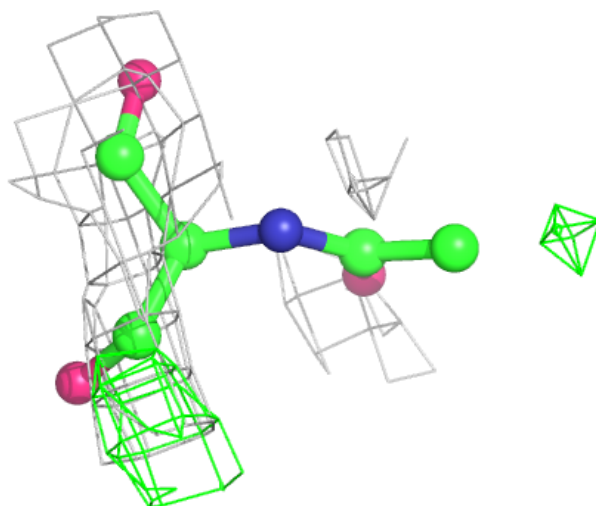
**Electron density around SAC I 101:**

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



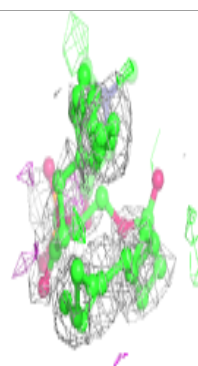
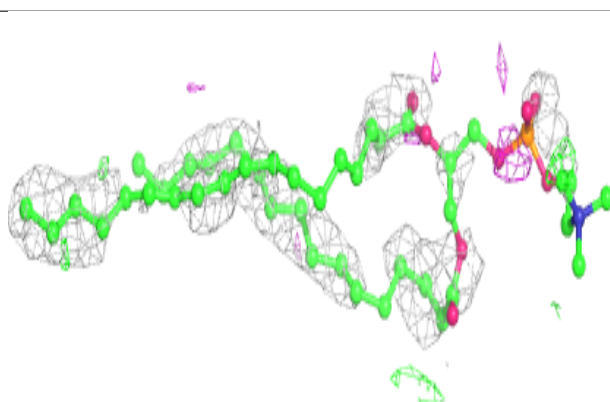
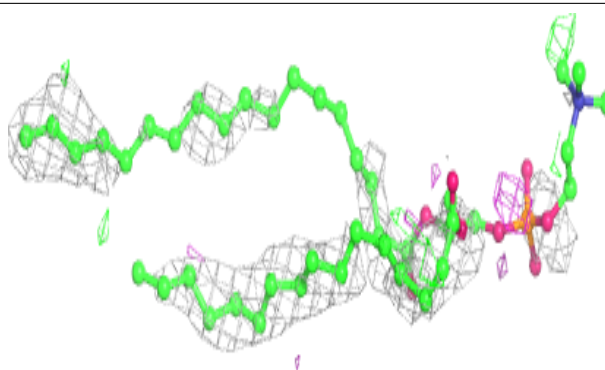
**Electron density around SAC V 101:**

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

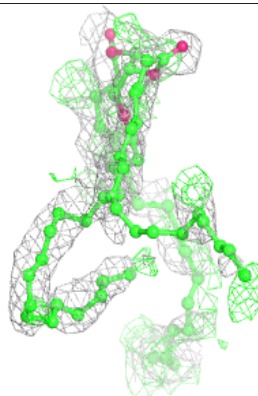
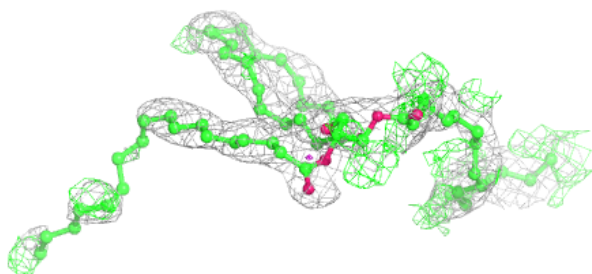
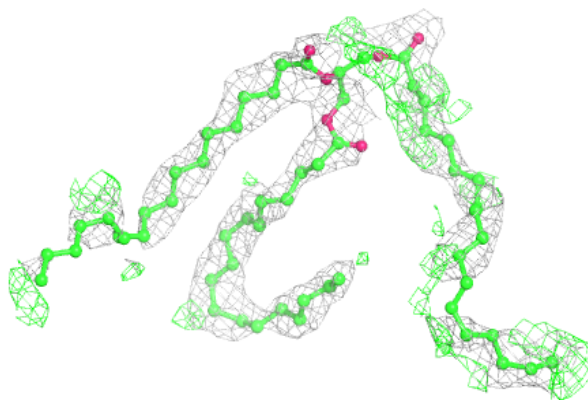


**Electron density around PSC E 201:**

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

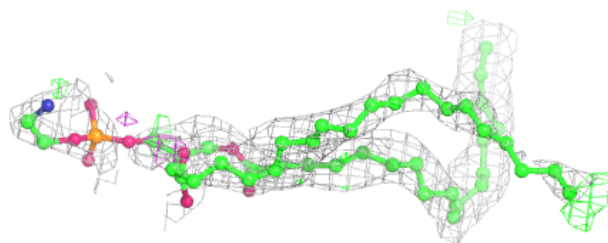
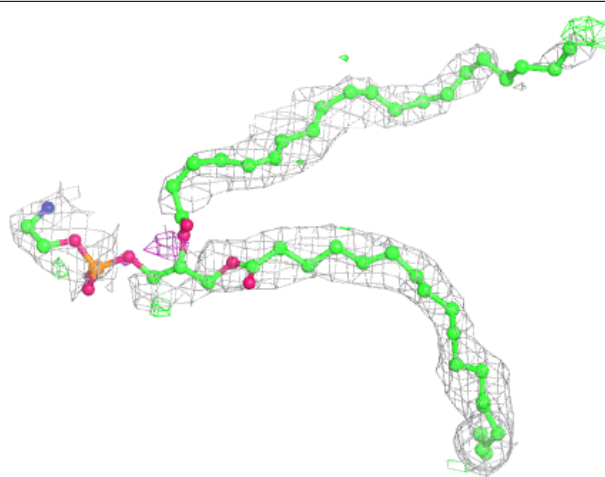
**Electron density around TGL Q 201:**

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



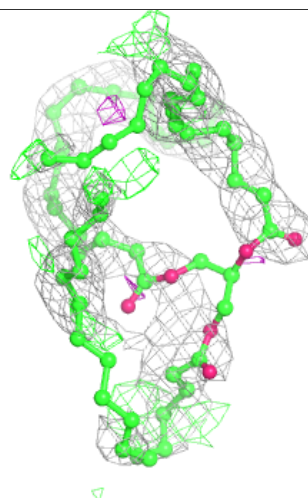
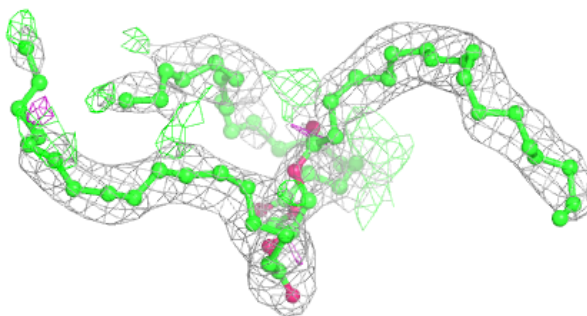
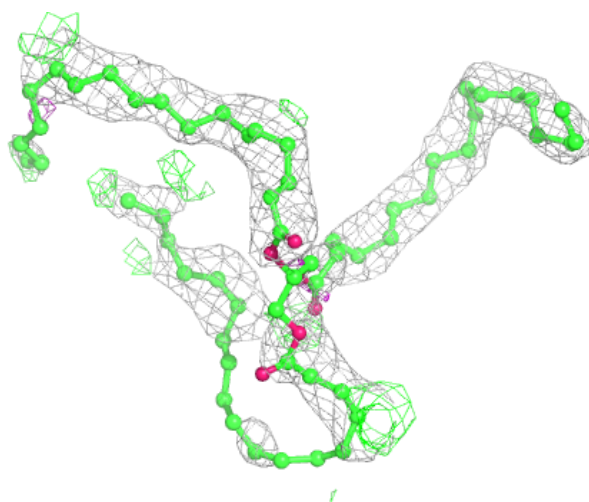
**Electron density around PEK C 307:**

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



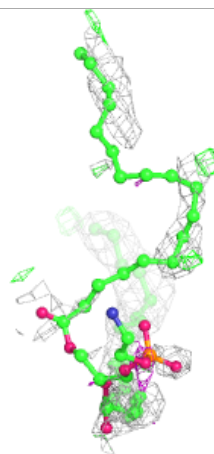
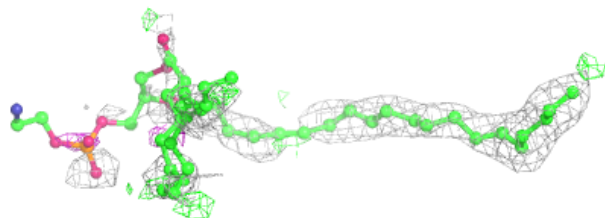
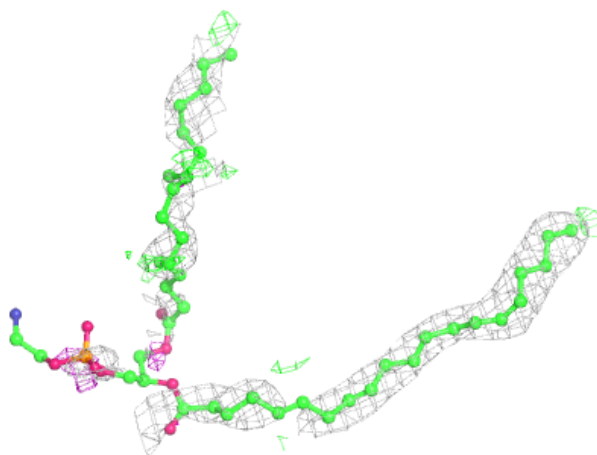
**Electron density around TGL Y 101:**

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



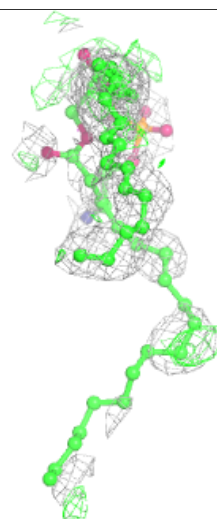
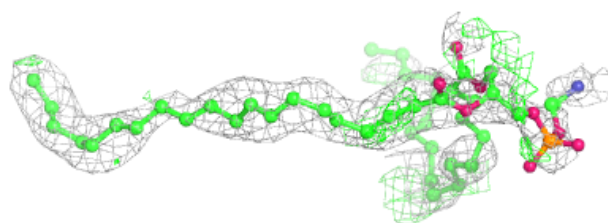
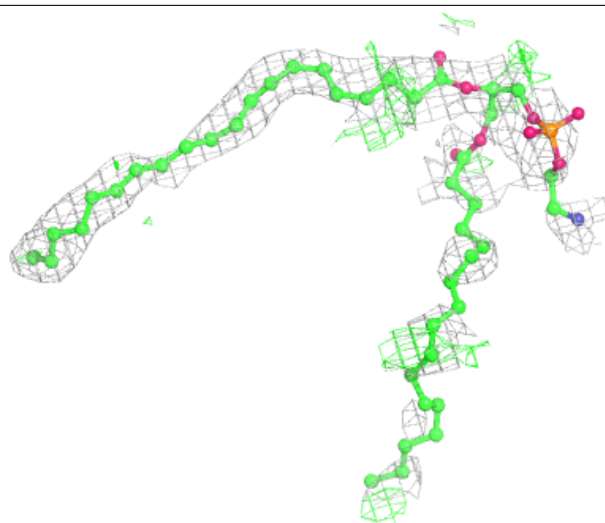
**Electron density around PEK T 103:**

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



**Electron density around PEK G 102:**

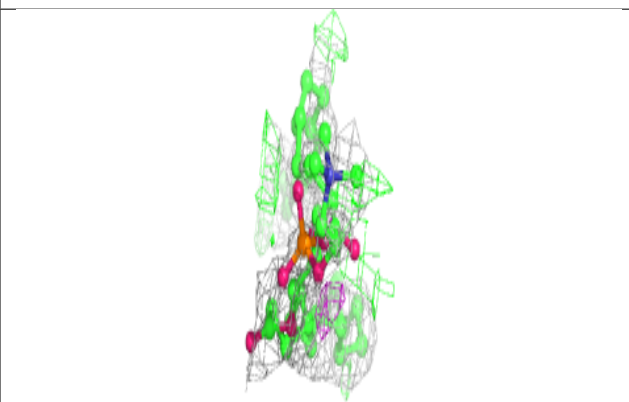
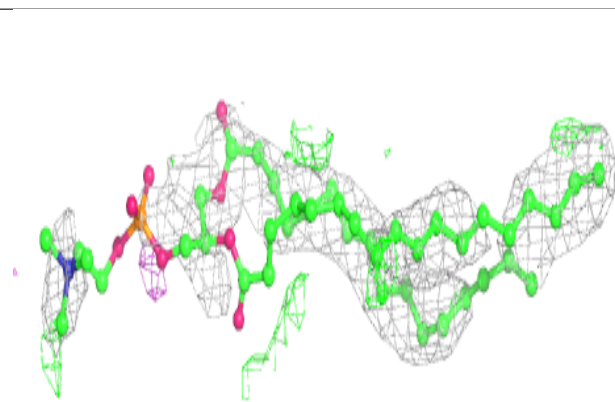
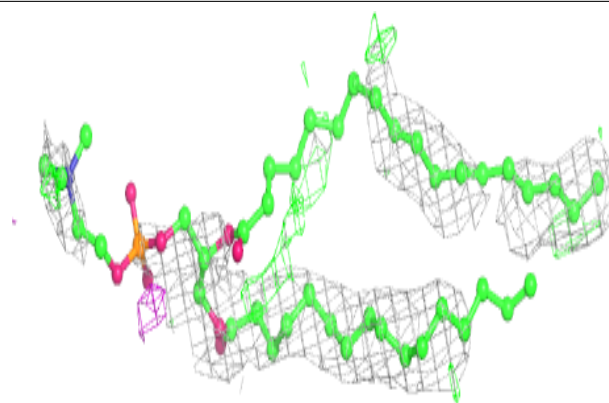
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



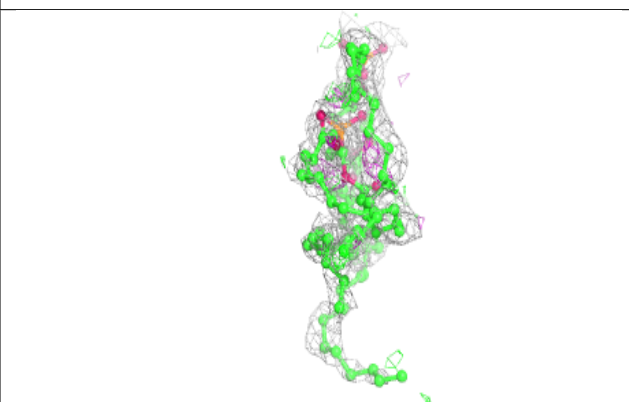
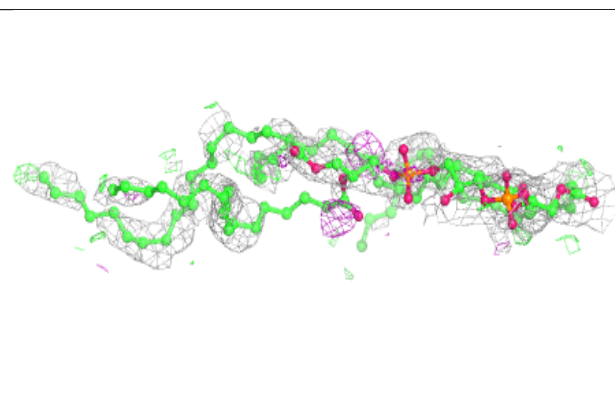
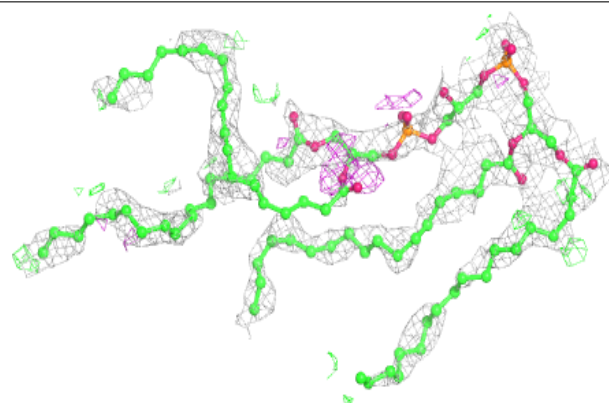


**Electron density around PSC O 302:**

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

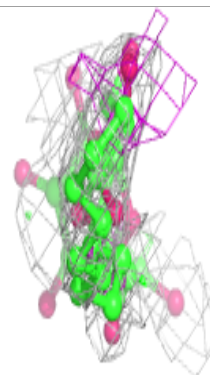
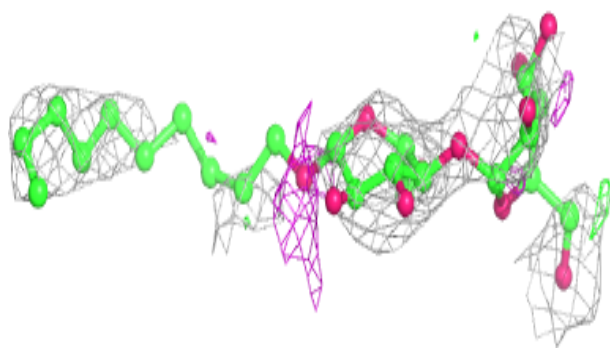
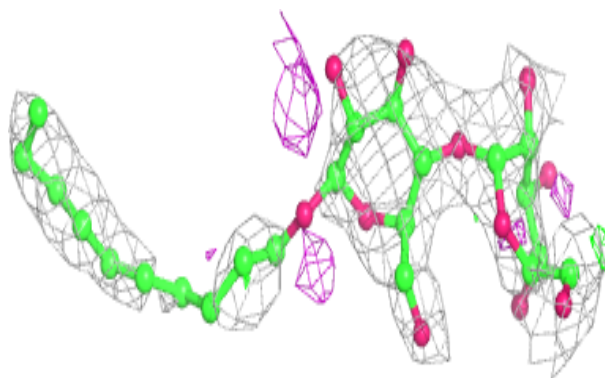
**Electron density around CDL G 101:**

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



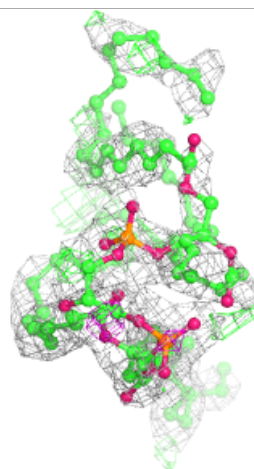
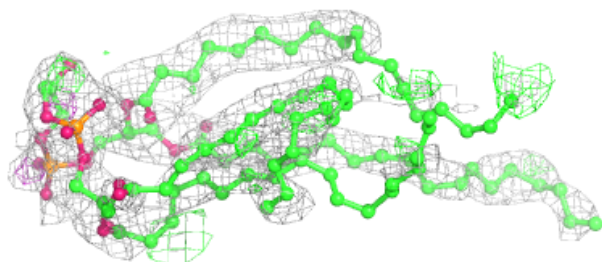
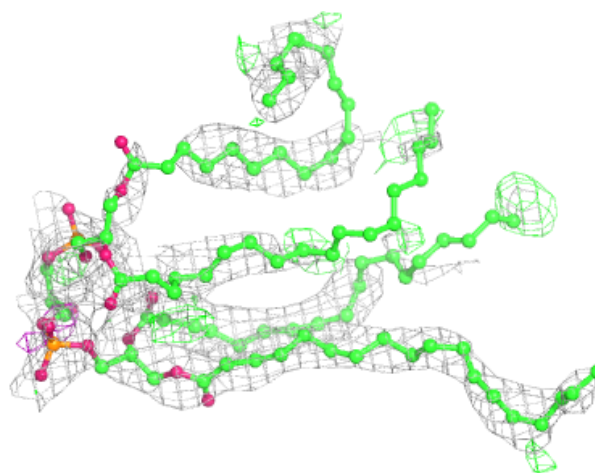
**Electron density around DMU W 101:**

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



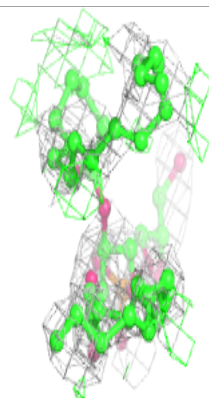
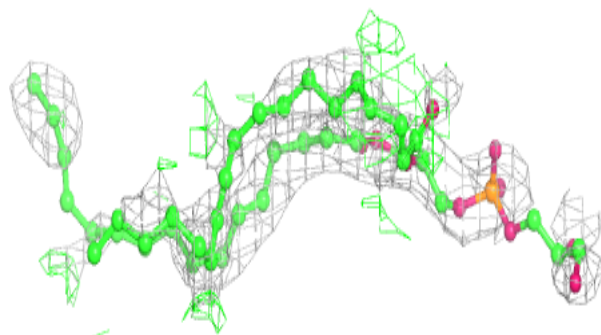
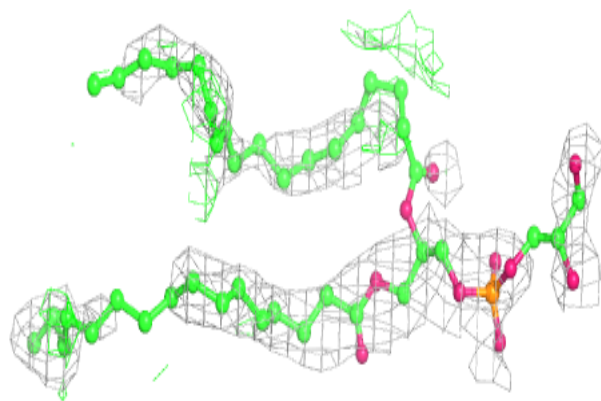
**Electron density around CDL P 304:**

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



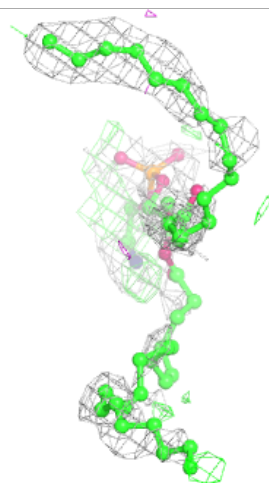
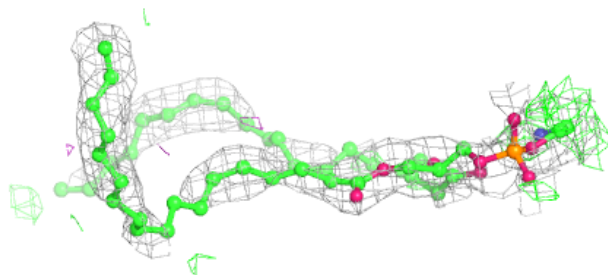
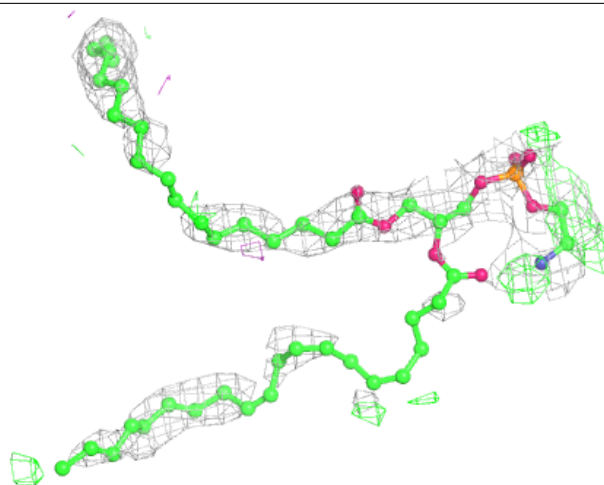
**Electron density around PGV P 302:**

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



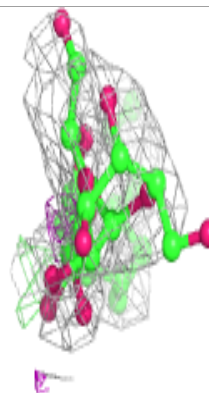
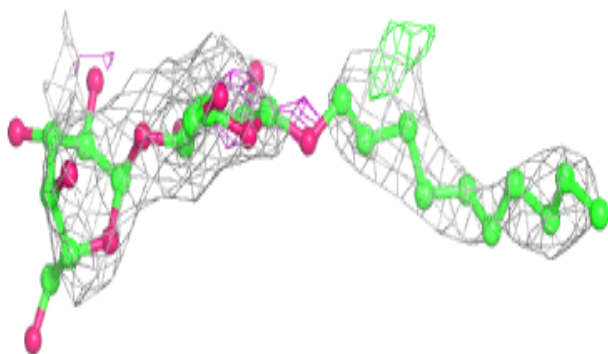
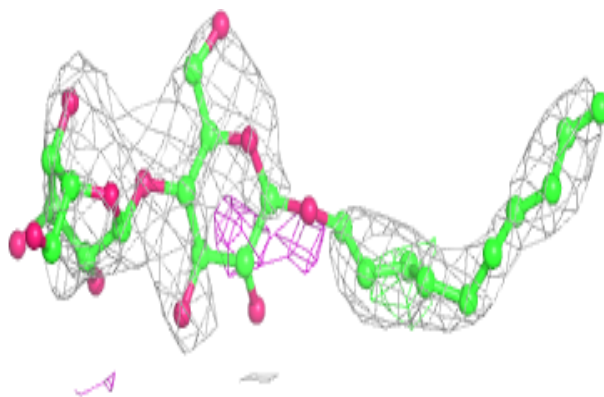
**Electron density around PEK T 104:**

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

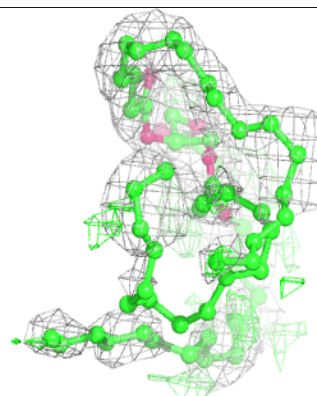
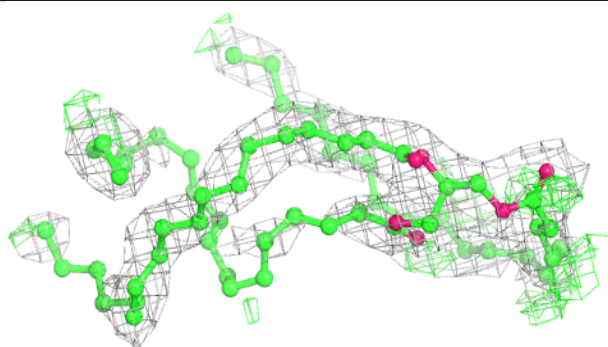
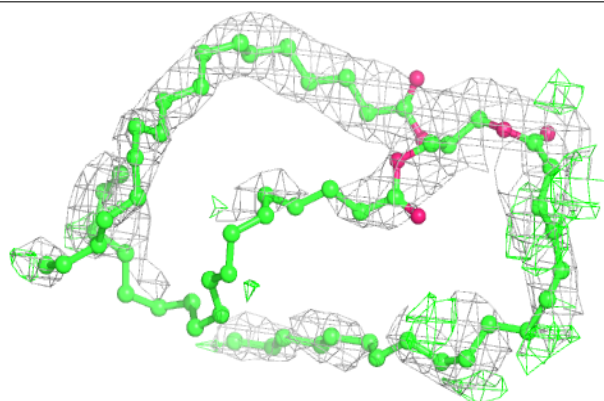


**Electron density around DMU C 301:**

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

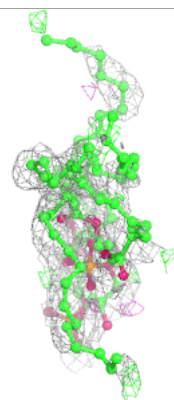
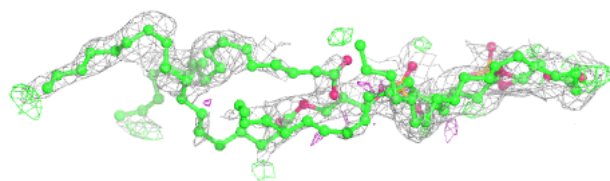
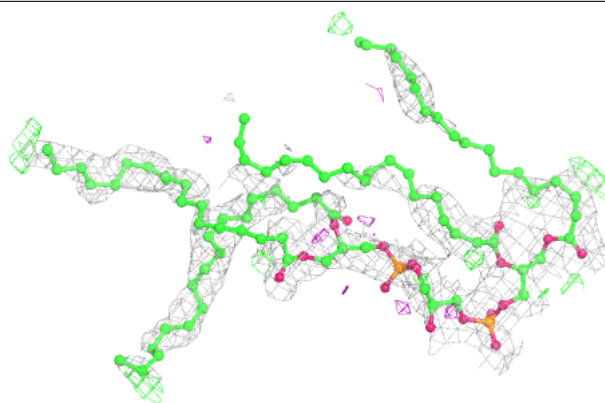
**Electron density around TGL N 606:**

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



**Electron density around CDL T 105:**

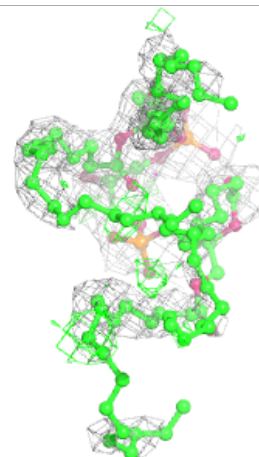
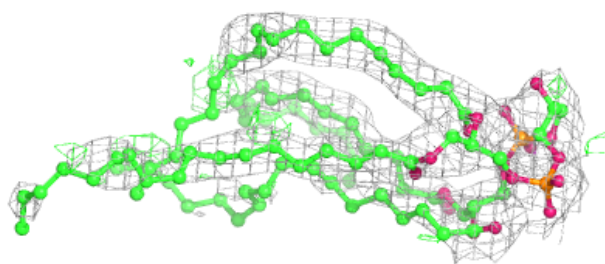
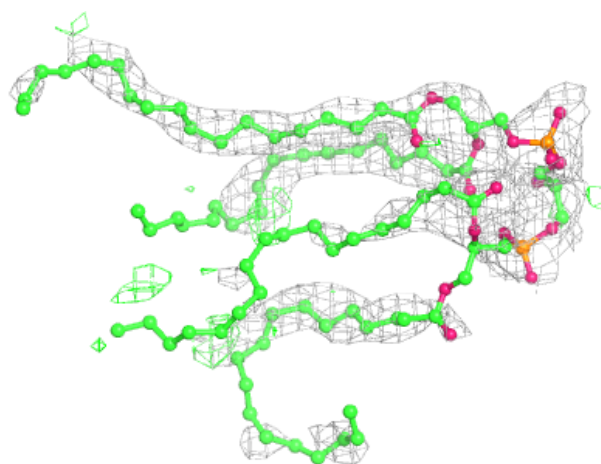
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CDL C 304:**

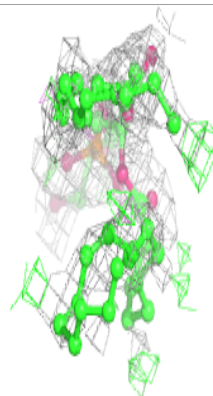
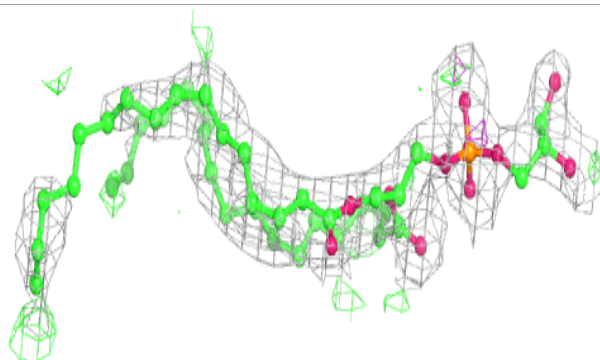
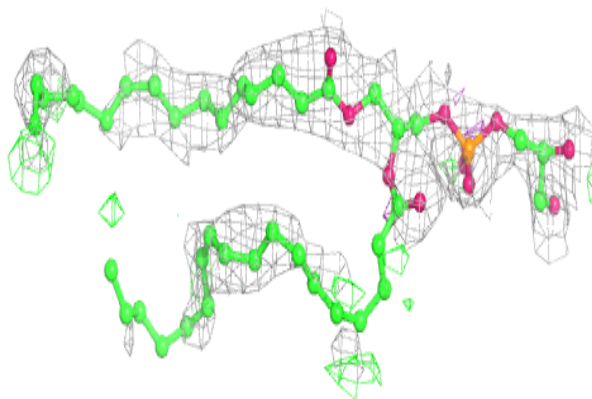
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



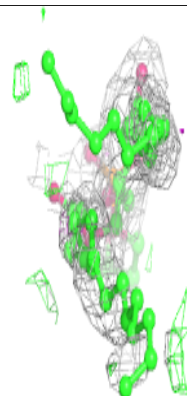
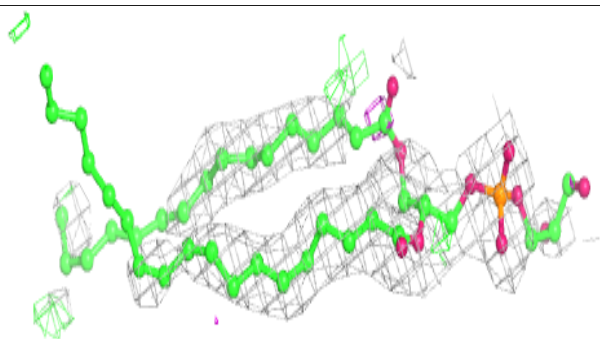
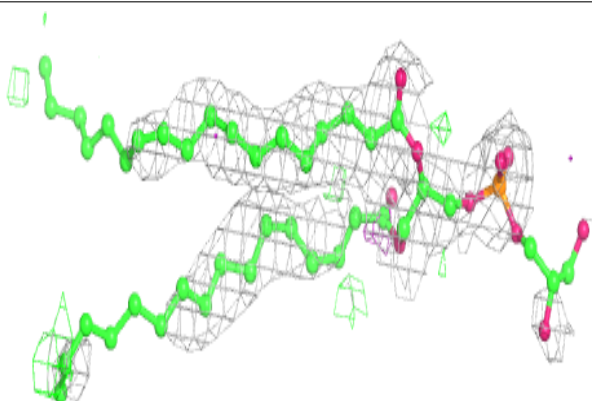


**Electron density around PGV C 308:**

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

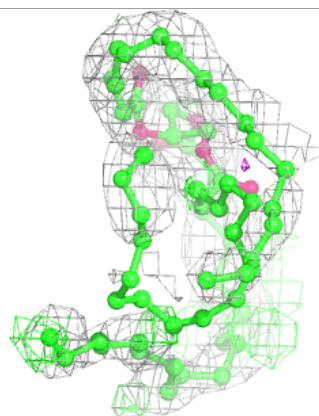
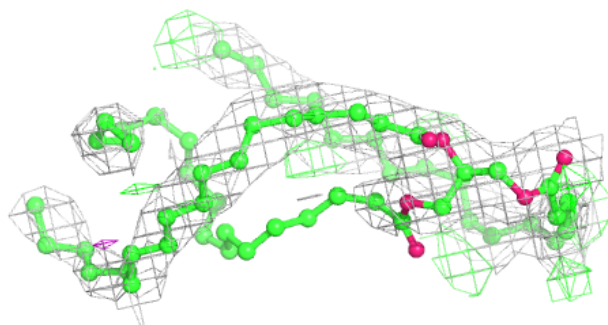
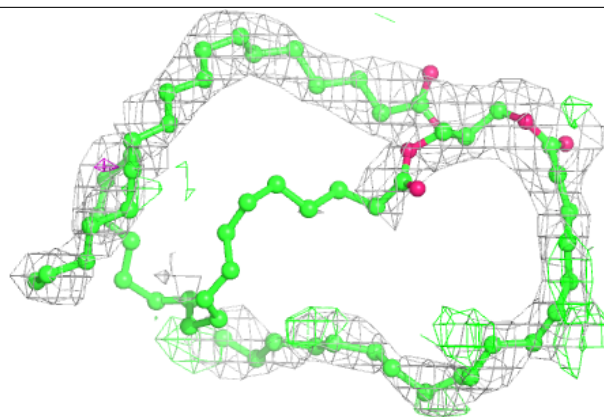
**Electron density around PGV Z 101:**

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



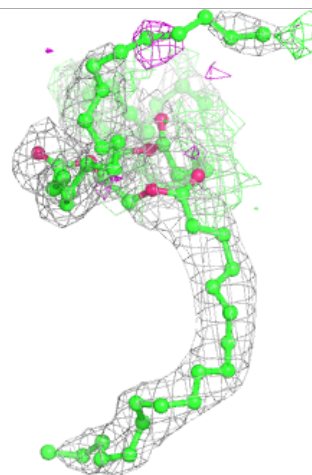
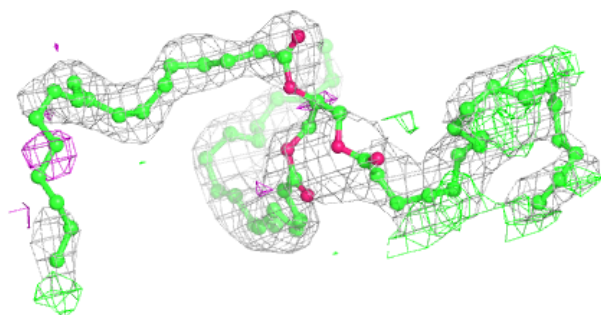
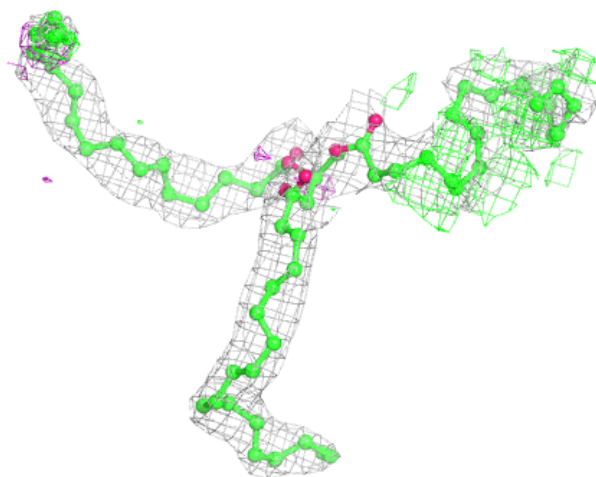
**Electron density around TGL B 301:**

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



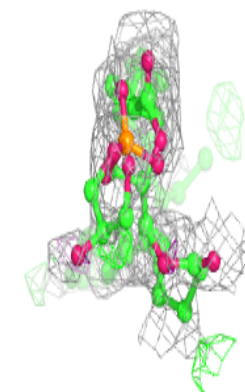
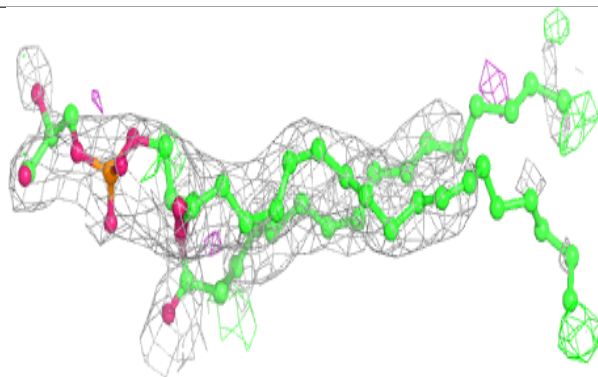
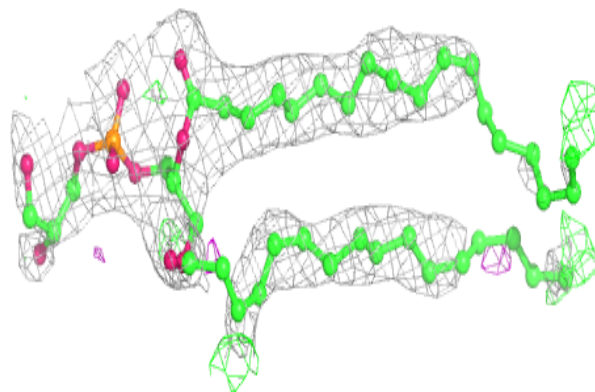
**Electron density around TGL L 101:**

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

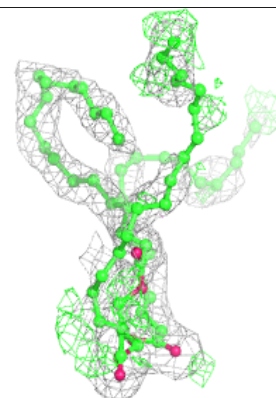
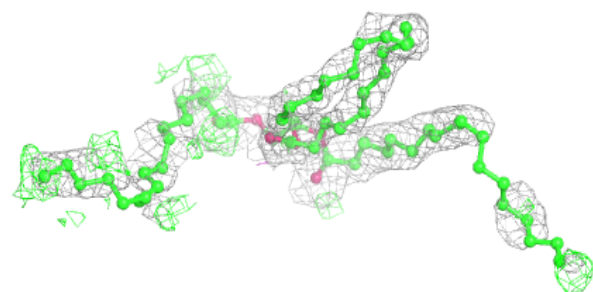
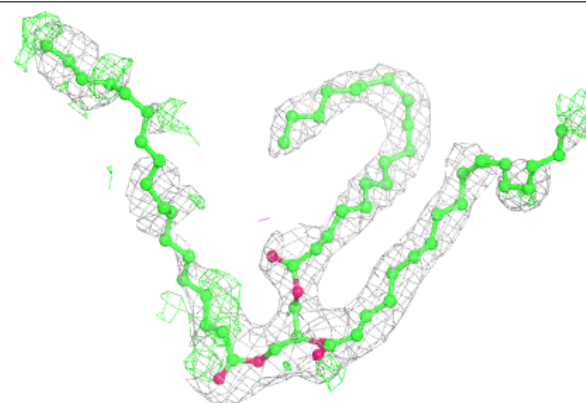


**Electron density around PGV A 607:**

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

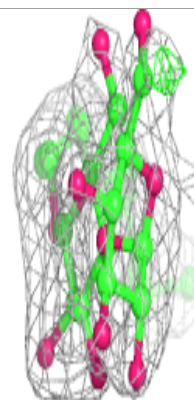
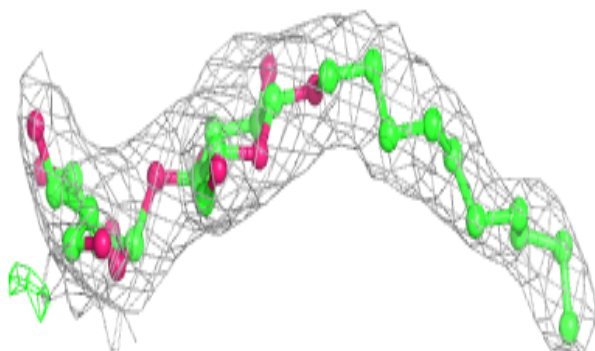
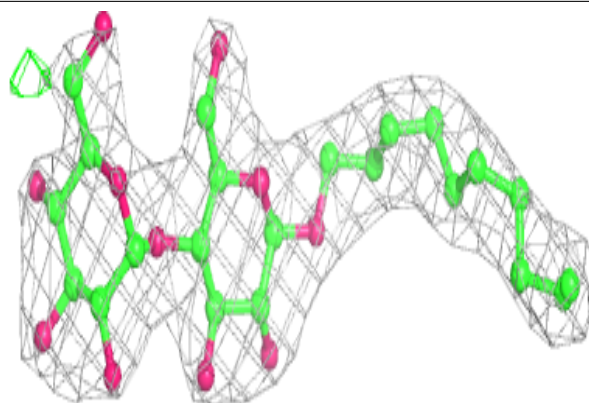
**Electron density around TGL D 201:**

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

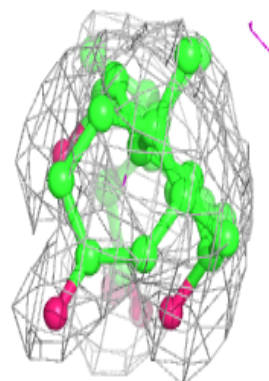
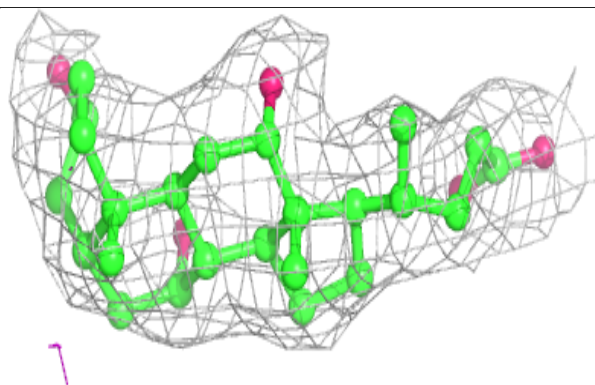
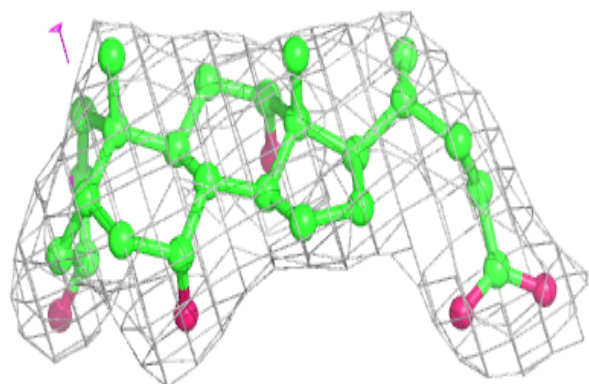


**Electron density around DMU Z 102:**

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

**Electron density around CHD W 102:**

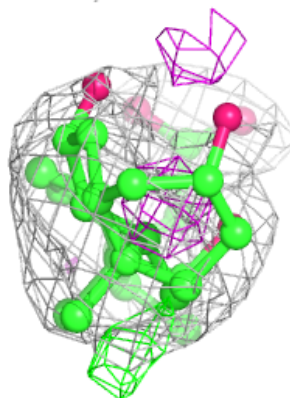
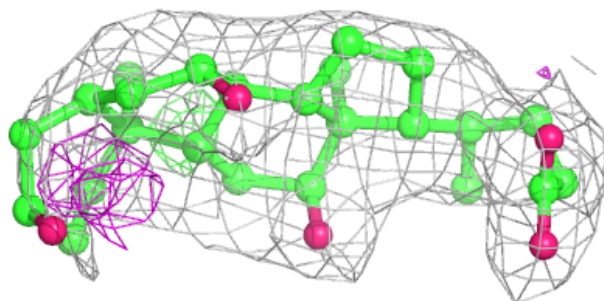
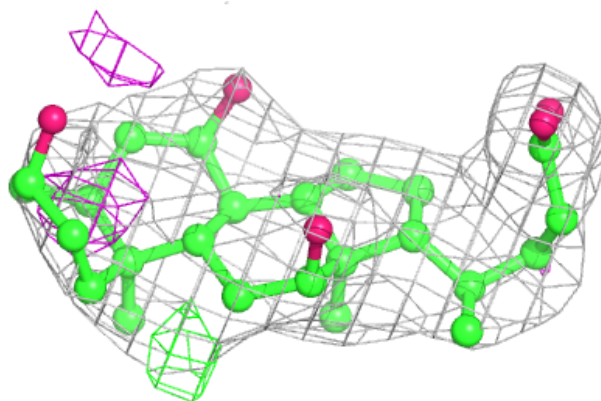
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



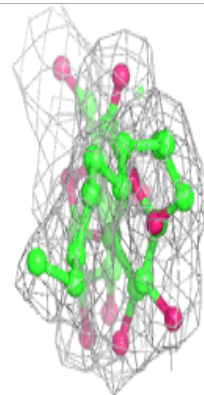
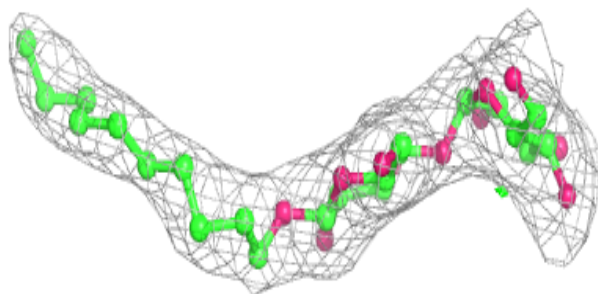
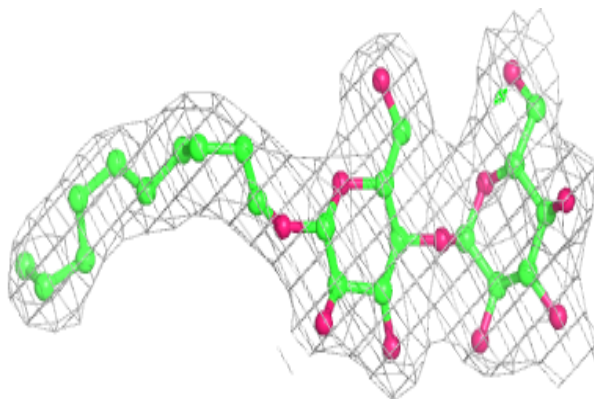


**Electron density around CHD J 101:**

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

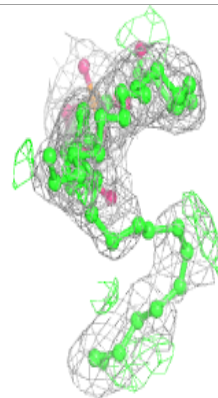
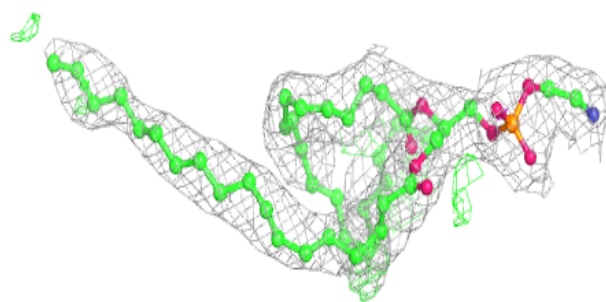
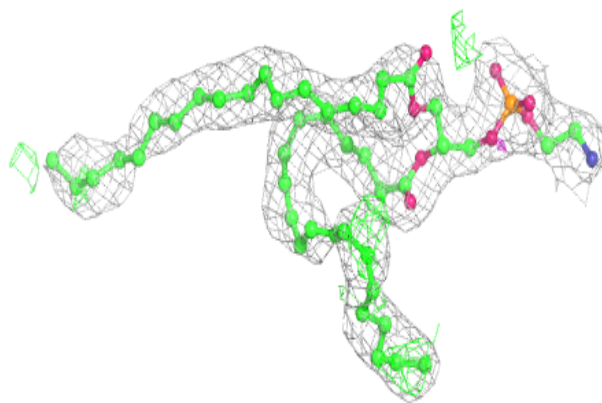
**Electron density around DMU D 202:**

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

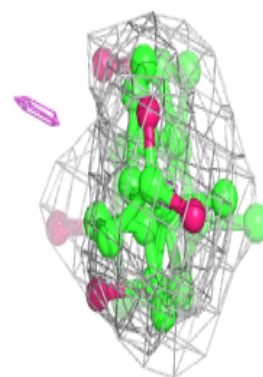
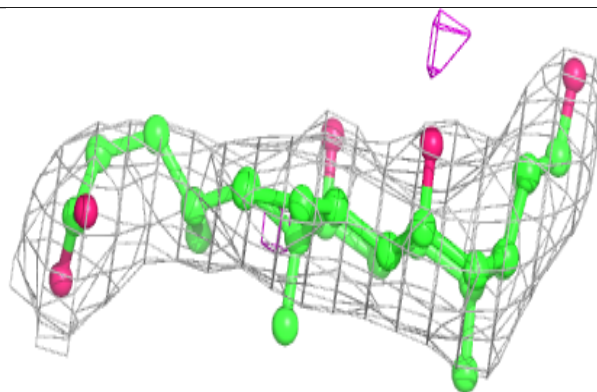
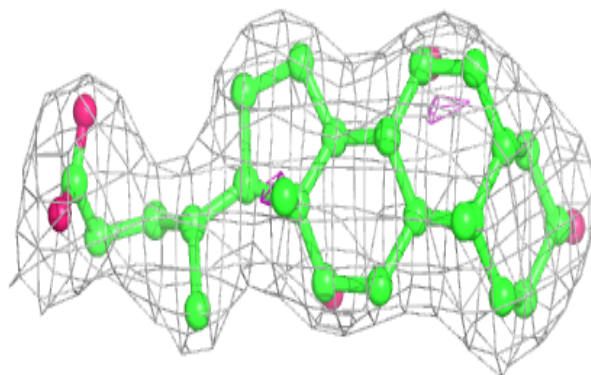


**Electron density around PEK T 102:**

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

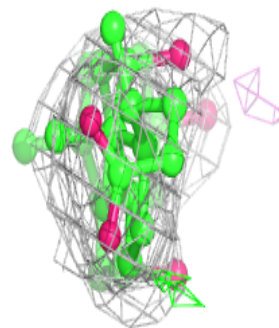
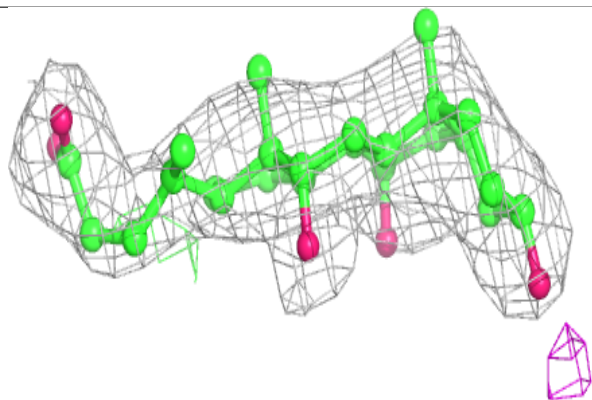
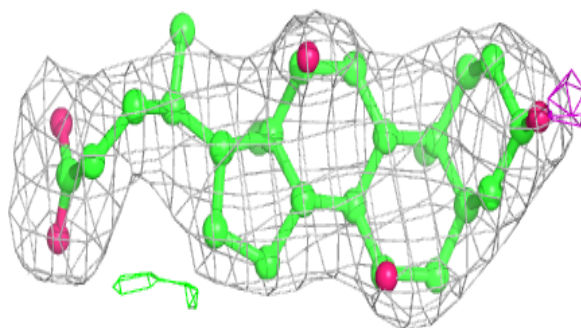
**Electron density around CHD C 305:**

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

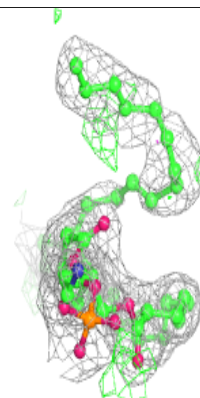
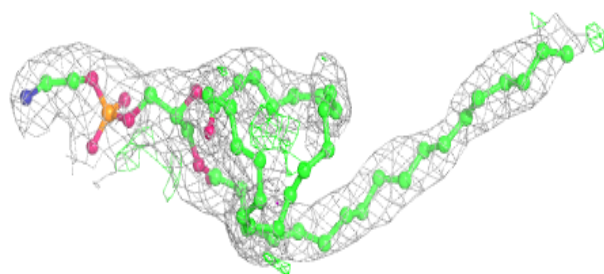
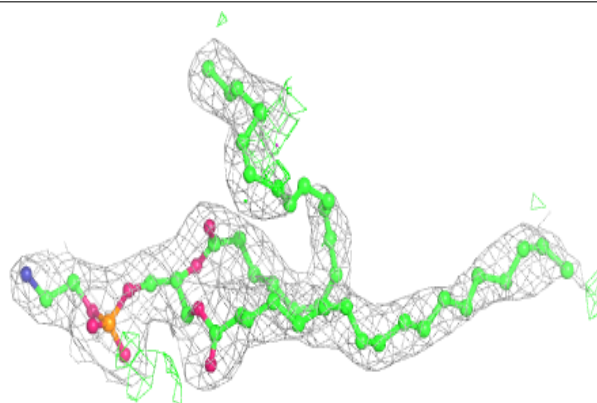


**Electron density around CHD P 305:**

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

**Electron density around PEK C 302:**

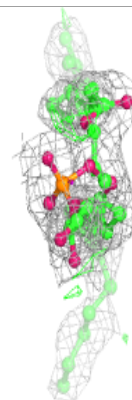
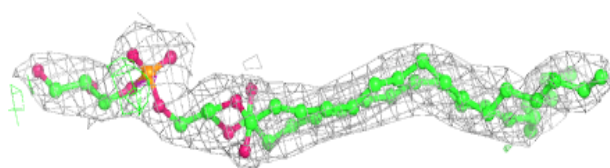
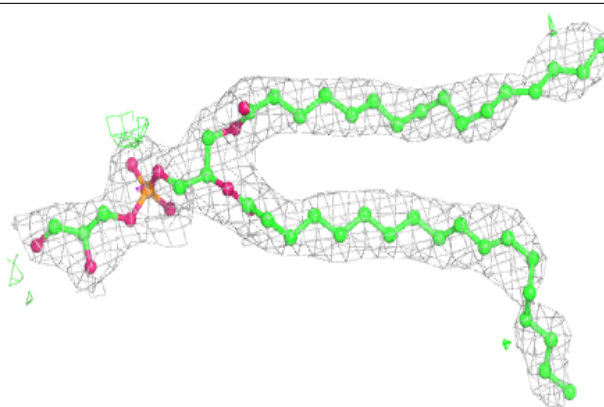
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



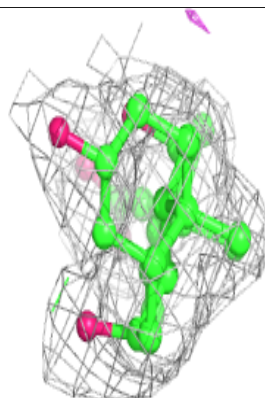
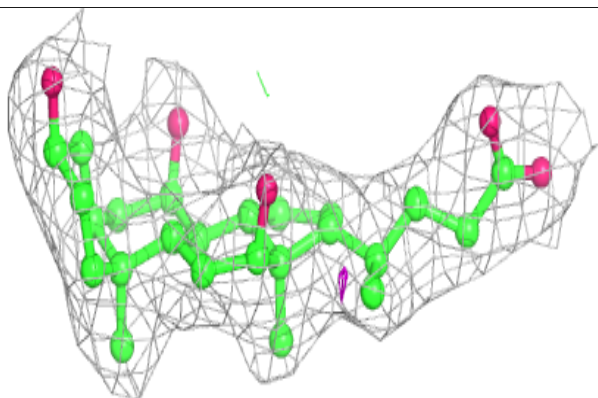
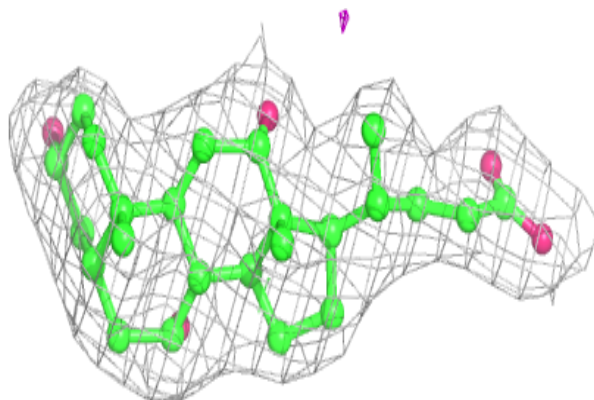


**Electron density around PGV C 303:**

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

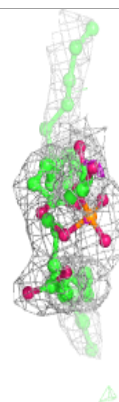
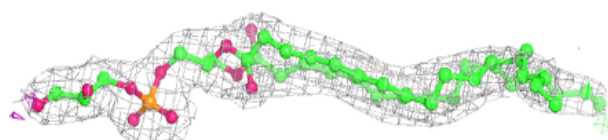
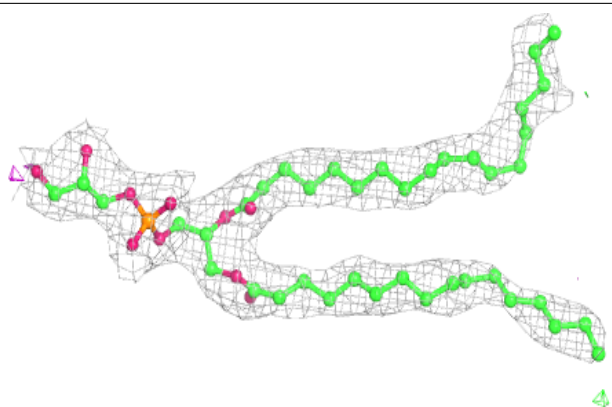
**Electron density around CHD P 306:**

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

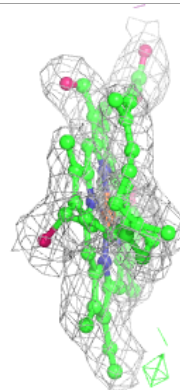
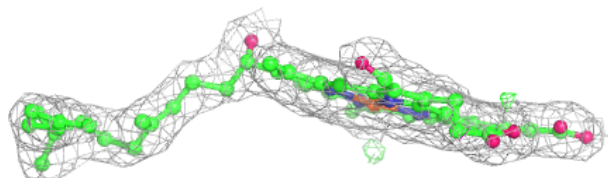
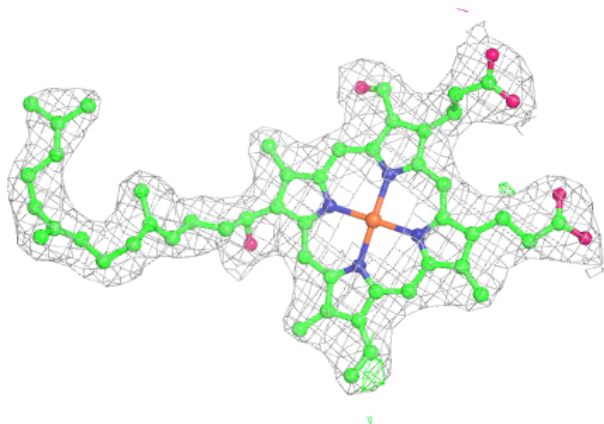


**Electron density around PGV P 303:**

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

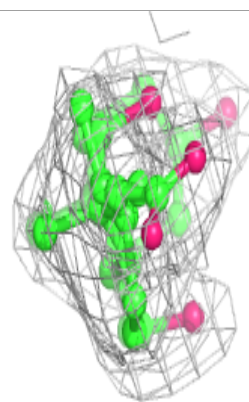
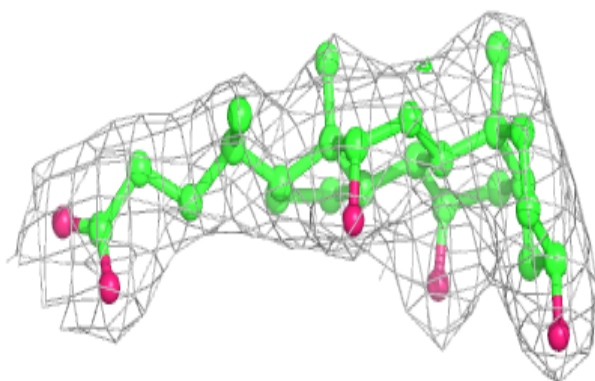
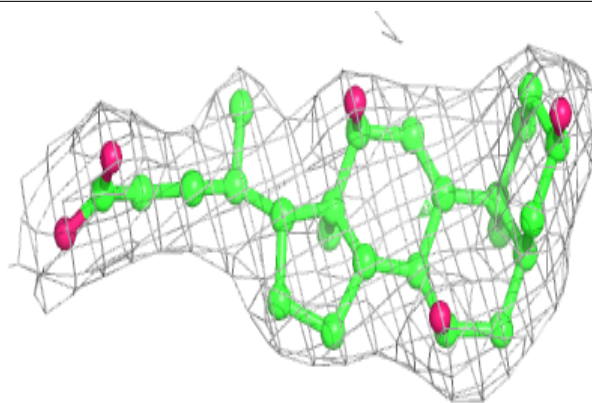
**Electron density around HEA N 602:**

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

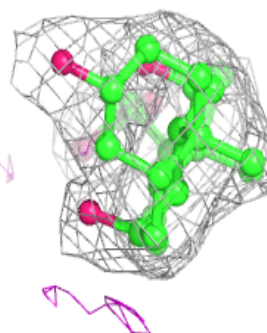
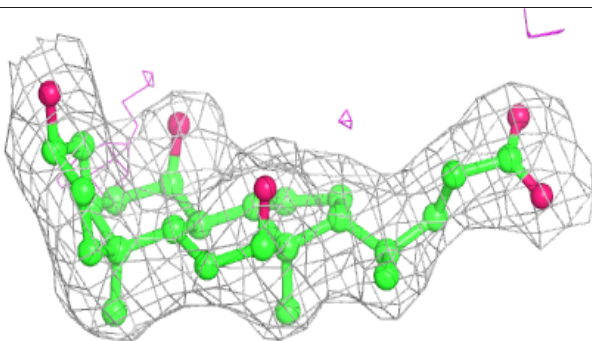
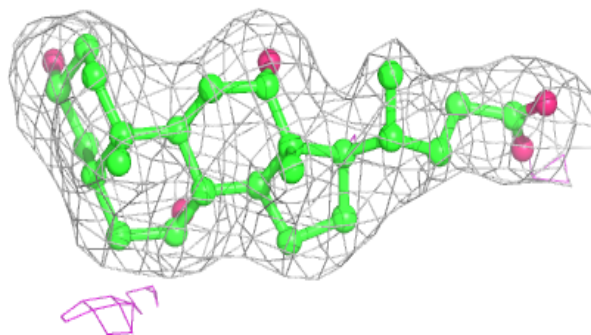


**Electron density around CHD C 306:**

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

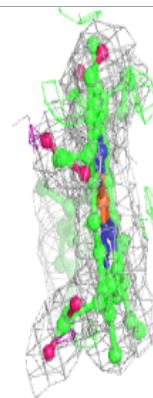
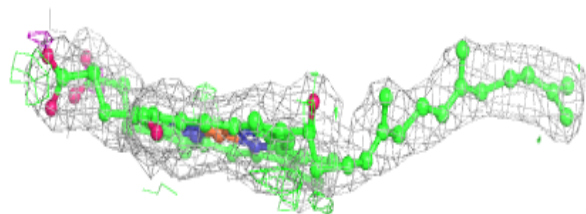
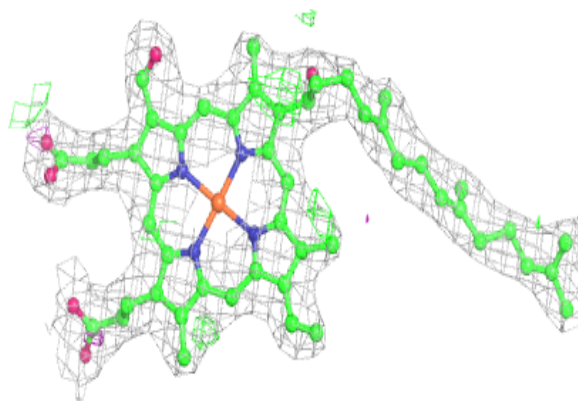
**Electron density around CHD G 103:**

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

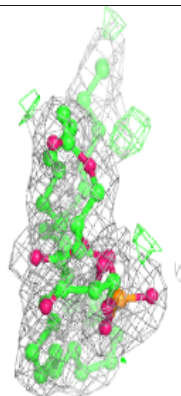
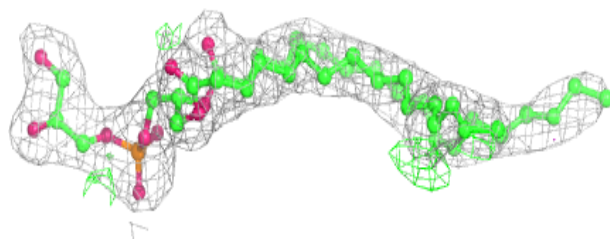
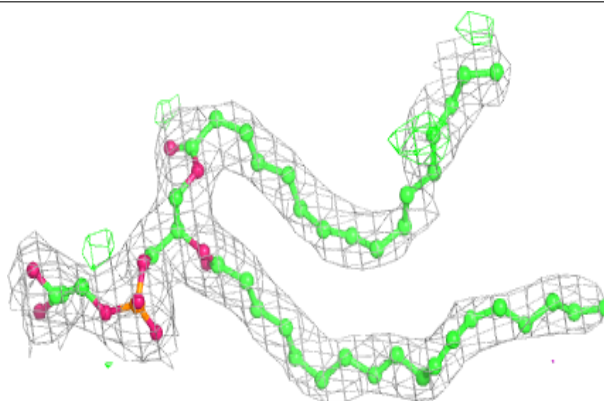


**Electron density around HEA A 601:**

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

**Electron density around PGV P 301:**

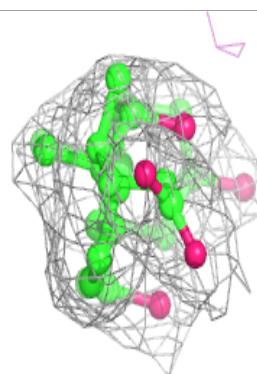
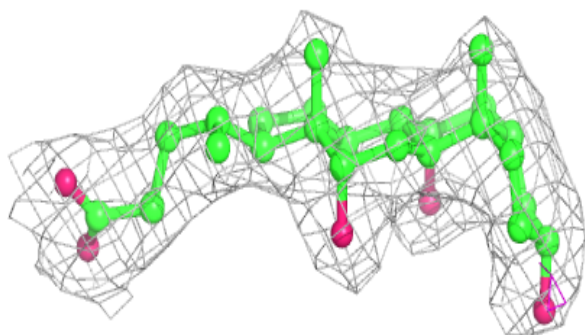
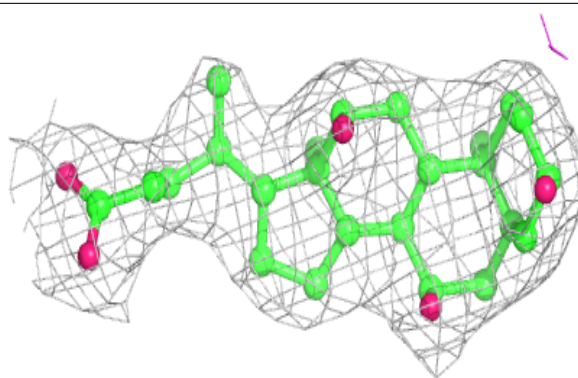
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



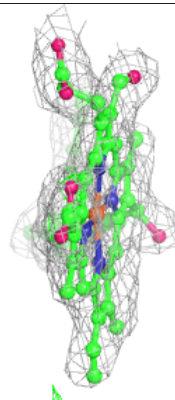
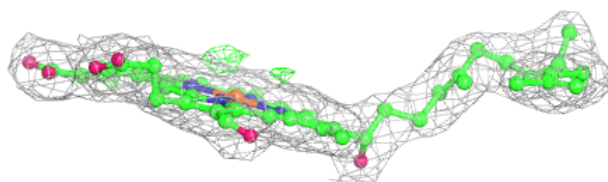
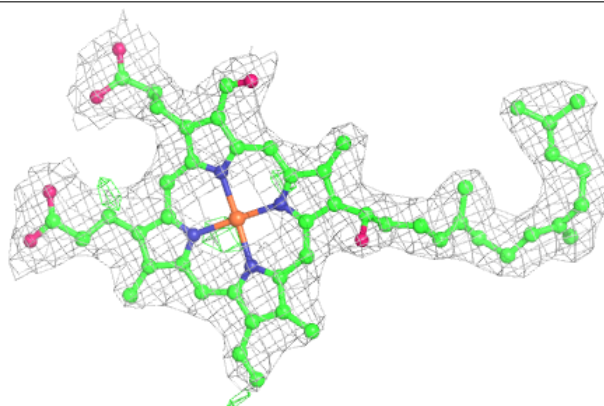


**Electron density around CHD T 101:**

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

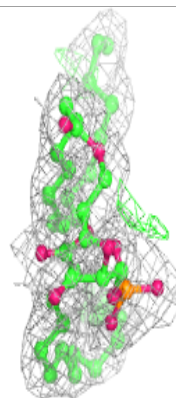
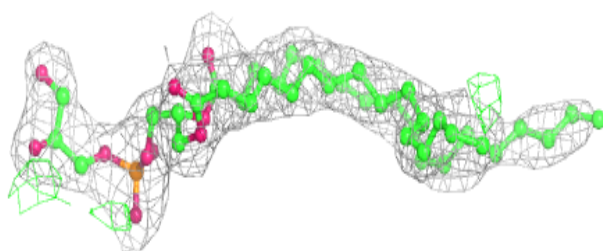
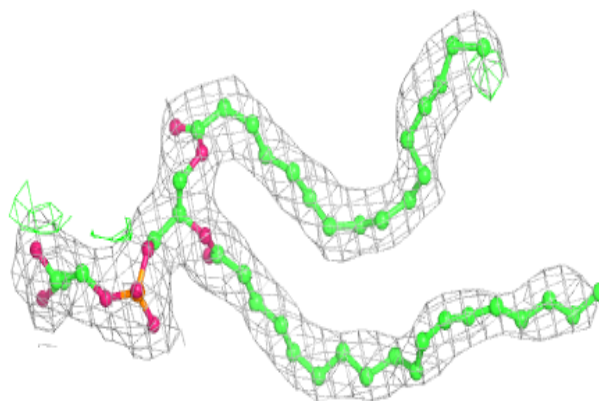
**Electron density around HEA A 602:**

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

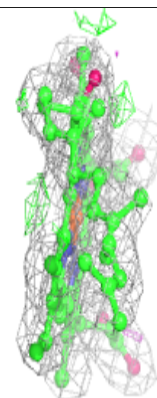
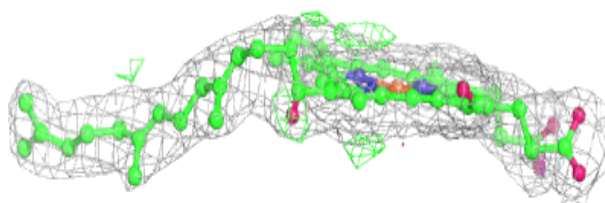
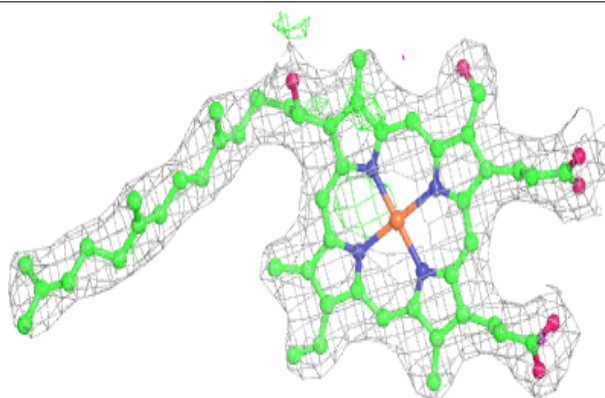


**Electron density around PGV A 606:**

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

**Electron density around HEA N 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.