



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2022 – 06:34 PM JST

PDB ID : 8GVM
Title : The structure of azide-bound cytochrome C oxidase determined using the crystals exposed to 20 mM azide solution for 4 days
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2022-09-15
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

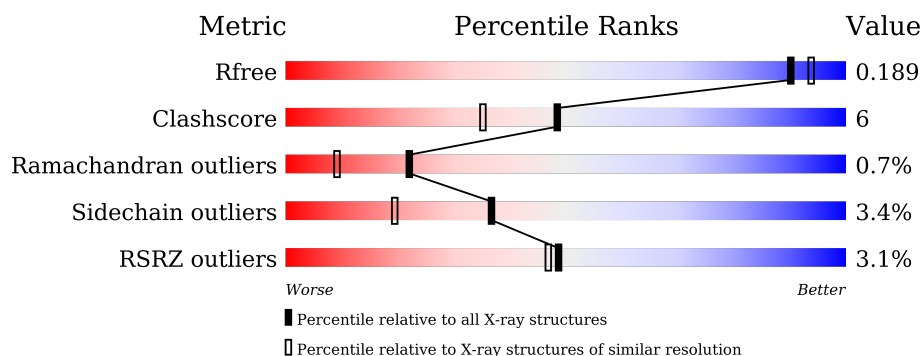
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>89%</div> <div>11%</div> <div>.</div> </div>
1	N	514	<div> <div>89%</div> <div>11%</div> <div>.</div> </div>
2	B	227	<div> <div>84%</div> <div>15%</div> <div>.</div> </div>
2	O	227	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
3	C	261	<div> <div>89%</div> <div>10%</div> <div>.</div> </div>
3	P	261	<div> <div>90%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
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[A]	X	-	-	-
14	HEA	A	602[B]	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	N	602	X	-	-	-
14	HEA	N	603[A]	X	-	-	-
14	HEA	N	603[B]	X	-	-	-
18	AZI	A	607[A]	-	-	X	-
18	AZI	A	607[B]	-	-	X	-
18	AZI	N	608[A]	-	-	X	-
20	EDO	C	317	-	-	-	X
20	EDO	S	101	-	-	X	-
22	CHD	W	101	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33558 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
			4125	2753	637	694	41			
1	N	514	Total	C	N	O	S	0	18	0
			4122	2753	634	694	41			

- 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	23	0
			1996	1304	304	368	20			
2	O	227	Total	C	N	O	S	0	20	0
			1975	1289	301	365	20			

- 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
			2152	1437	345	356	14			
3	P	259	Total	C	N	O	S	0	9	0
			2173	1449	348	361	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	2	0
			1198	779	197	218	4			
4	Q	144	Total	C	N	O	S	0	2	0
			1213	791	198	220	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	4	0
			773	478	138	151	6			
6	S	98	Total	C	N	O	S	0	2	0
			763	473	136	148	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	1
			681	438	129	112	1	1		

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

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

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

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

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

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	1	0
			469	302	79	85	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	1	0
			391	255	66	68	2			

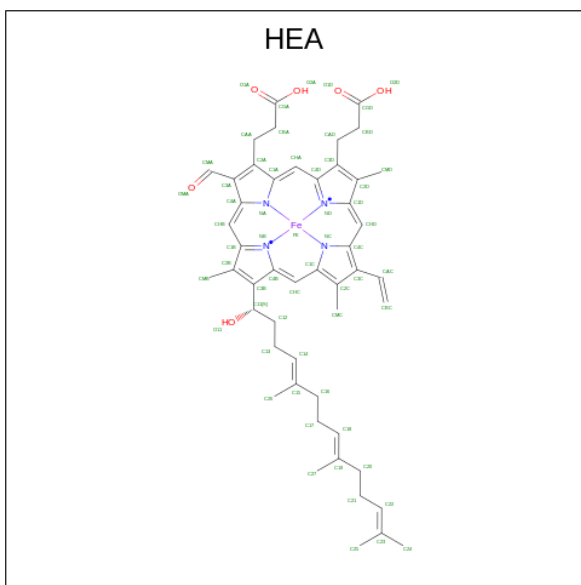
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			
12	Y	46	Total	C	N	O	S	0	1	0
			383	256	64	60	3			

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

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	A	1	Total 120	C 98	Fe 2	N 8	O 12	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 120	C 98	Fe 2	N 8	O 12	0	1

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

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

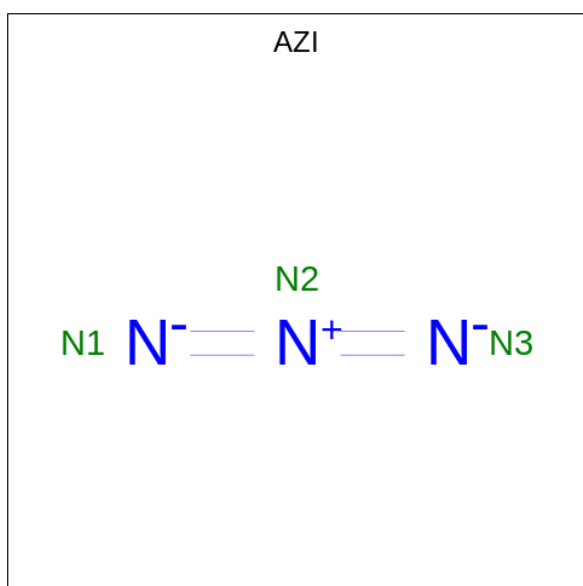
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

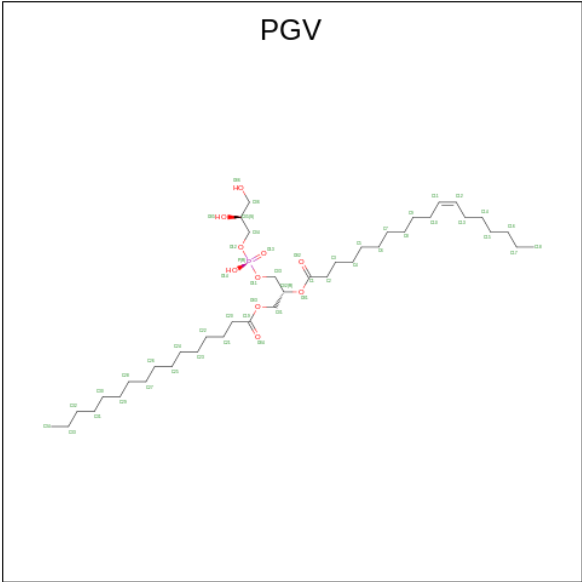
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

- Molecule 18 is AZIDE ION (three-letter code: AZI) (formula: N₃).



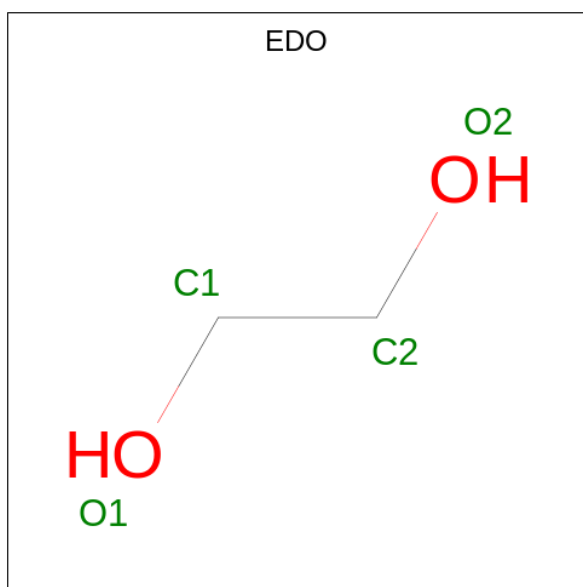
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total N 3 3	0	1
18	A	1	Total N 6 6	0	1
18	N	1	Total N 3 3	0	1
18	N	1	Total N 6 6	0	1

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			49	39	9	1		
19	G	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

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

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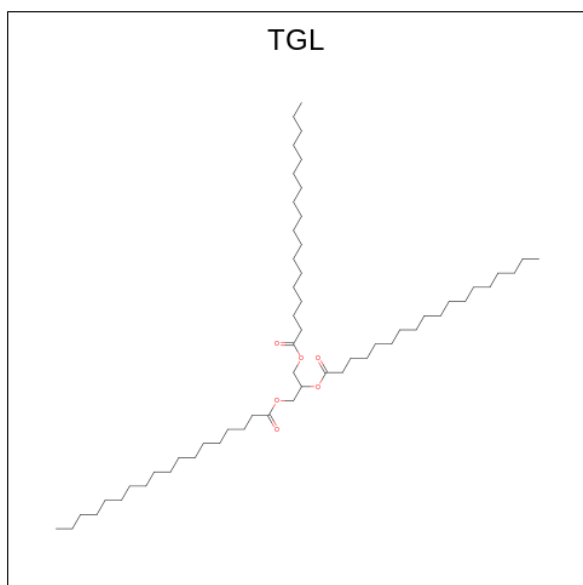
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	G	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	H	1	Total 4	C 2	O 2	0	0
20	L	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0

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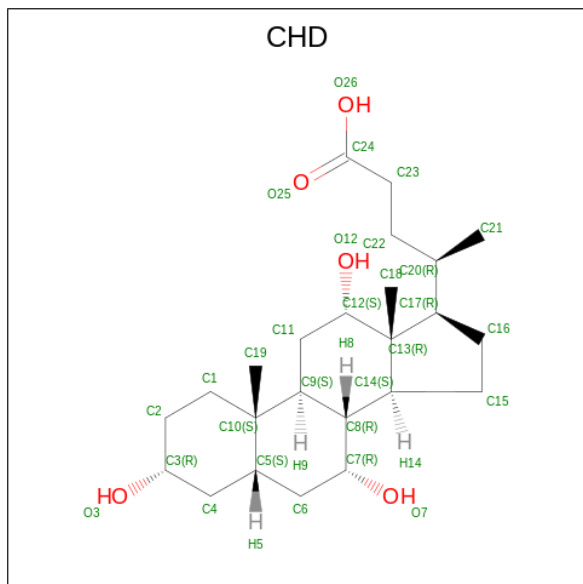
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	R	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20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

- 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		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			61	55	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 CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



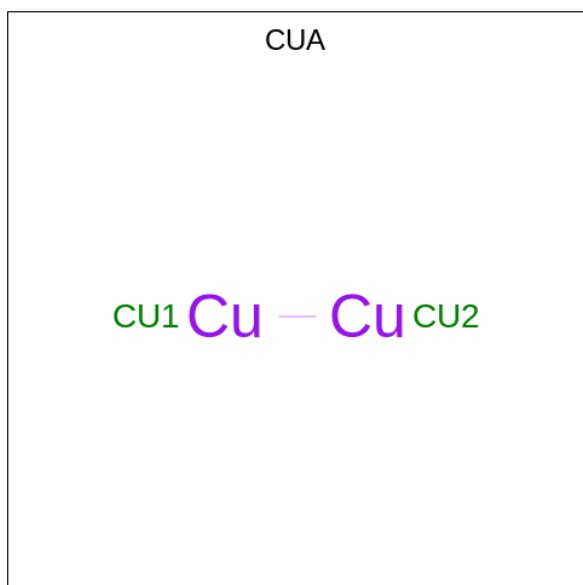
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	C	1	Total	C	O	0	0
			29	24	5		
22	G	1	Total	C	O	0	0
			29	24	5		
22	J	1	Total	C	O	0	0
			29	24	5		
22	P	1	Total	C	O	0	0
			29	24	5		

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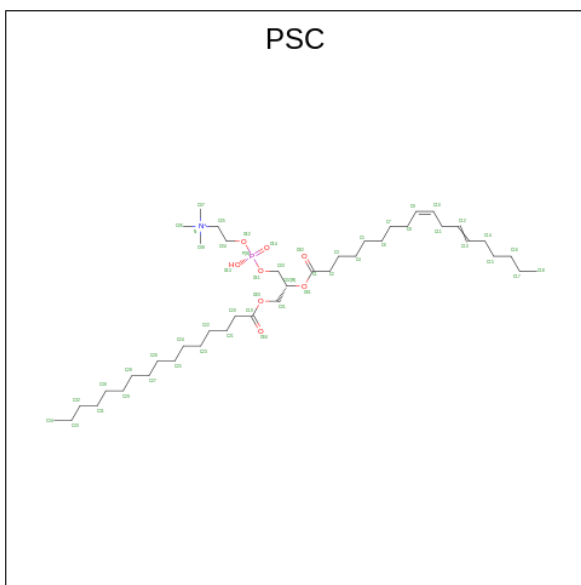
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	P	1	Total	C	O	0	0
			29	24	5		
22	W	1	Total	C	O	0	0
			29	24	5		

- Molecule 23 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



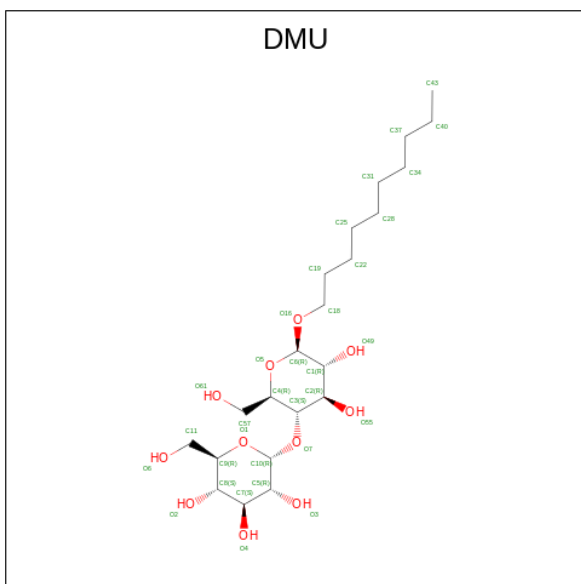
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

- Molecule 24 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total 50	C 40	N 1	O 8	P 1	0	0
24	O	1	Total 51	C 41	N 1	O 8	P 1	0	0

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



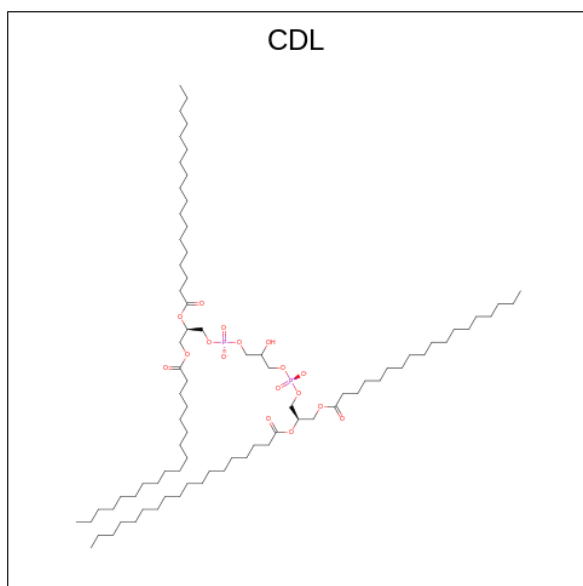
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			33	22	11		
25	C	1	Total	C	O	0	0
			22	16	6		
25	L	1	Total	C	O	0	0
			30	19	11		
25	M	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	P	1	Total	C	O	0	0
			33	22	11		
25	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



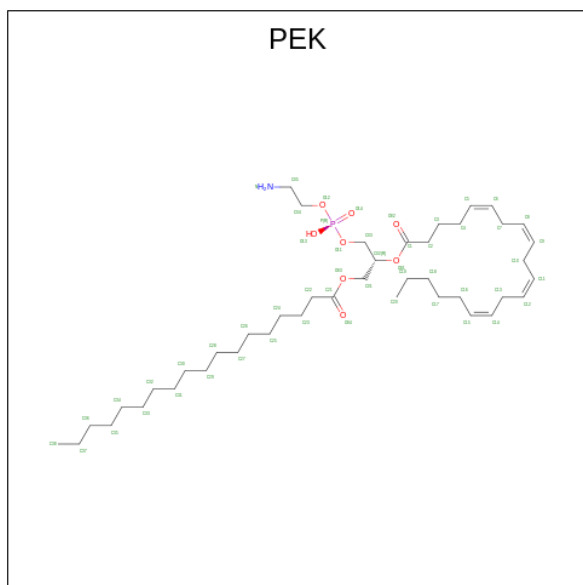
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			89	71	16	2		
26	N	1	Total	C	O	P	0	0
			96	77	17	2		
26	P	1	Total	C	O	P	0	0
			80	62	16	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	T	1	Total	C	O	P	0	0
			97	78	17	2		

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	C	1	Total	C	N	O	P	0	0
			44	34	1	8	1		
27	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	G	1	Total	C	O	P		0	0
			44	35	8	1			
27	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
27	T	1	Total	C	O	P		0	0
			50	41	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		

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	222	Total 222	O 222	0	1
29	B	133	Total 134	O 134	0	2
29	C	99	Total 99	O 99	0	0
29	D	108	Total 108	O 108	0	0
29	E	82	Total 82	O 82	0	0
29	F	79	Total 79	O 79	0	0
29	G	52	Total 52	O 52	0	0
29	H	44	Total 44	O 44	0	0
29	I	27	Total 27	O 27	0	0
29	J	27	Total 27	O 27	0	0
29	K	20	Total 20	O 20	0	0
29	L	26	Total 26	O 26	0	0
29	M	24	Total 24	O 24	0	0
29	N	209	Total 209	O 209	0	1
29	O	111	Total 112	O 112	0	1
29	P	90	Total 90	O 90	0	0
29	Q	38	Total 38	O 38	0	0
29	R	39	Total 39	O 39	0	0

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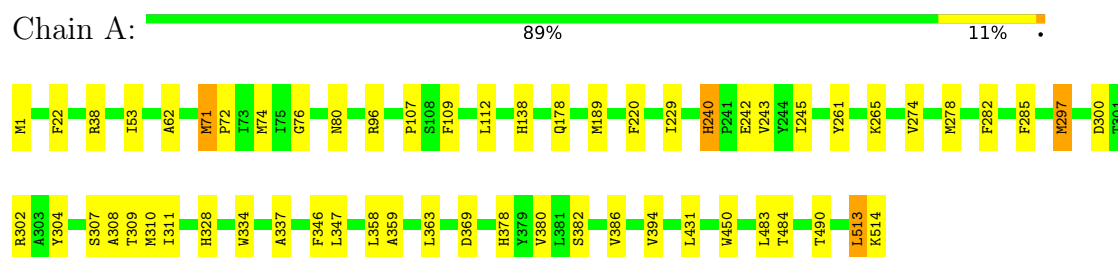
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	S	59	Total 59	O 59	0	0
29	T	35	Total 35	O 35	0	0
29	U	33	Total 33	O 33	0	0
29	V	14	Total 14	O 14	0	0
29	W	12	Total 12	O 12	0	0
29	X	11	Total 11	O 11	0	0
29	Y	13	Total 13	O 13	0	0
29	Z	16	Total 16	O 16	0	0

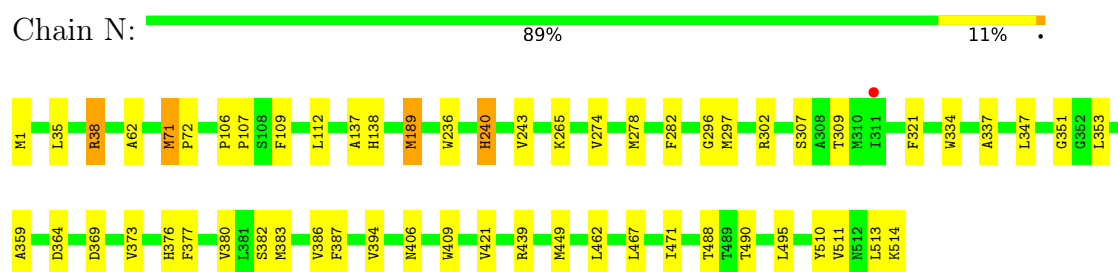
3 Residue-property plots

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

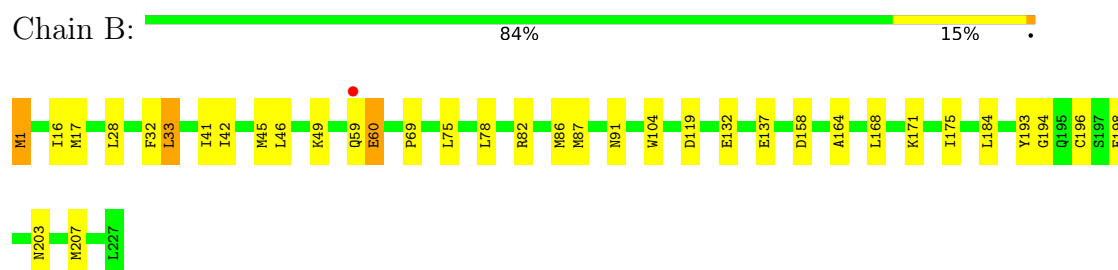
• Molecule 1: Cytochrome c oxidase subunit 1



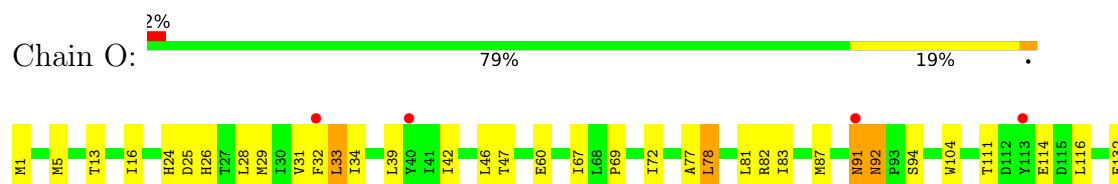
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



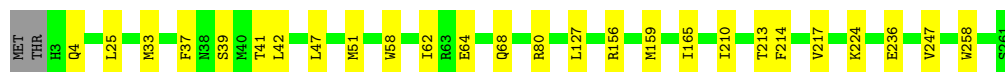
• Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 89% 10% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 90% 10% .



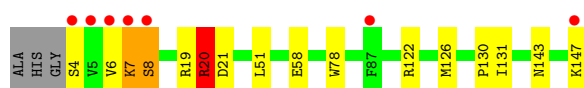
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 93% 5% .



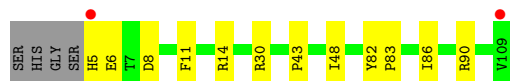
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 87% 5% 9% ...



- Molecule 5: Cytochrome c oxidase subunit 5A

Chain E: 85% 2% 11% .

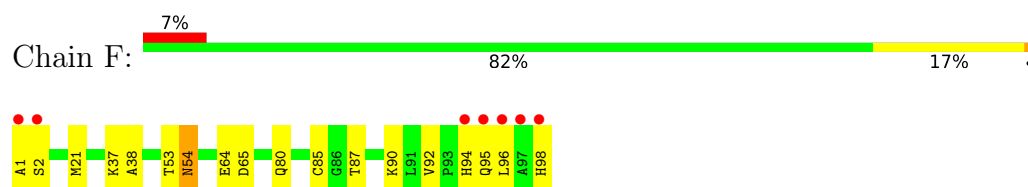


- Molecule 5: Cytochrome c oxidase subunit 5A

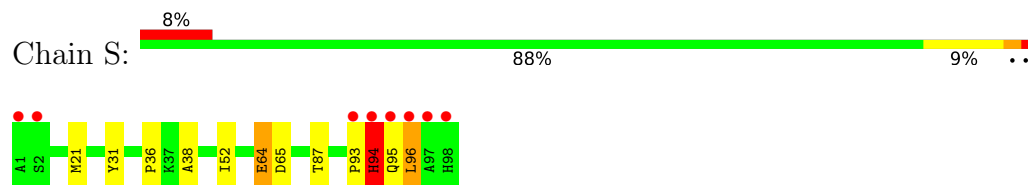
Chain R: 90% 2% 5% . .



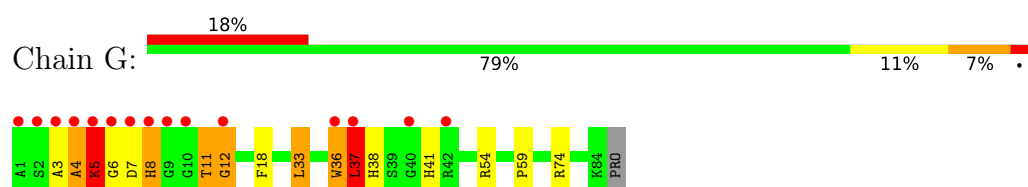
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



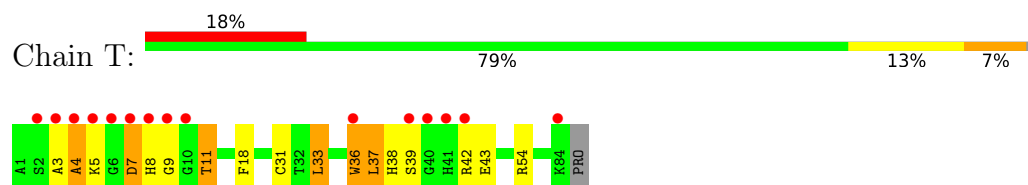
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



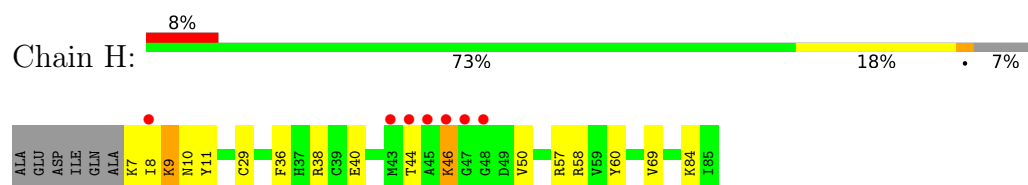
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



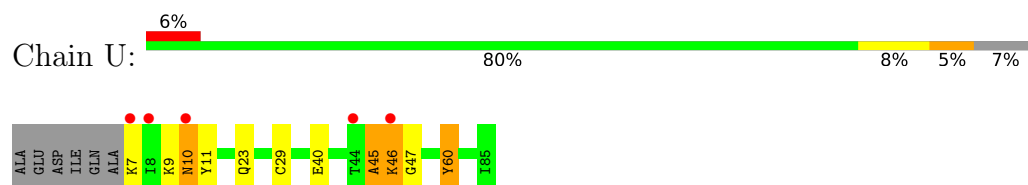
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



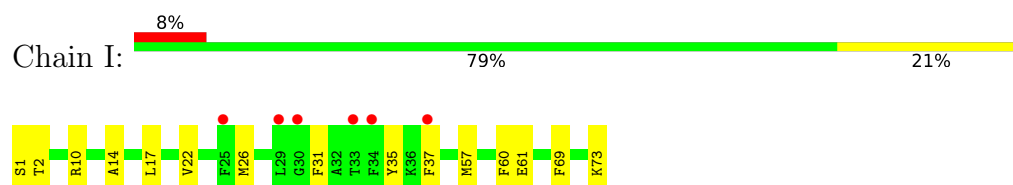
- Molecule 8: Cytochrome c oxidase subunit 6B1



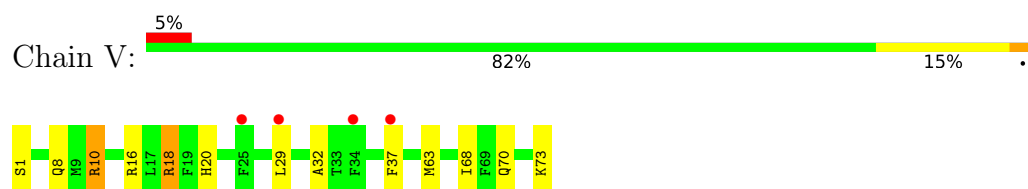
- Molecule 8: Cytochrome c oxidase subunit 6B1



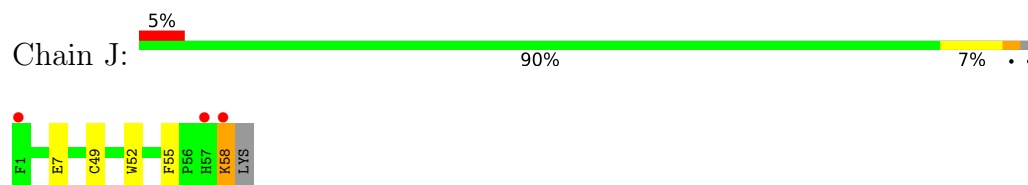
- Molecule 9: Cytochrome c oxidase subunit 6C



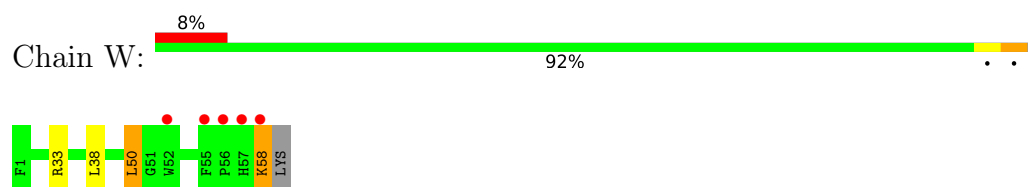
- Molecule 9: Cytochrome c oxidase subunit 6C



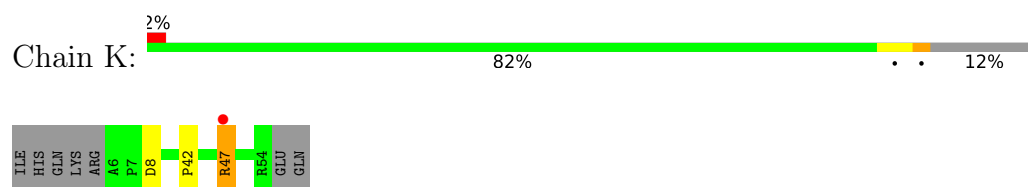
- Molecule 10: Cytochrome c oxidase subunit 7A1



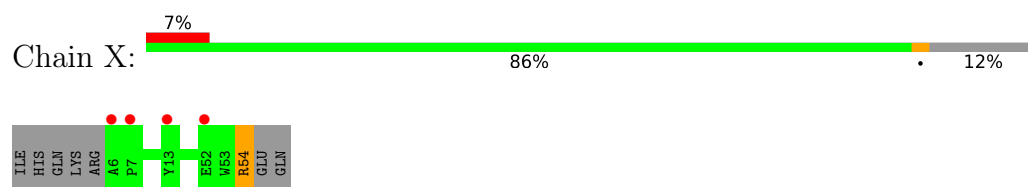
- Molecule 10: Cytochrome c oxidase subunit 7A1



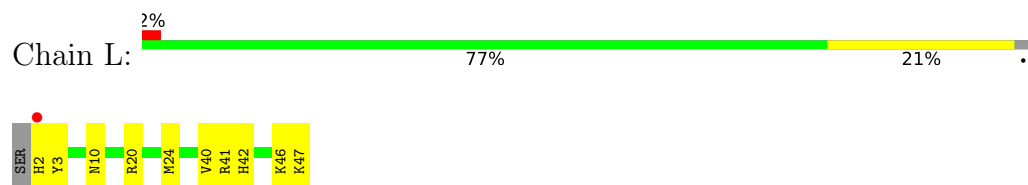
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



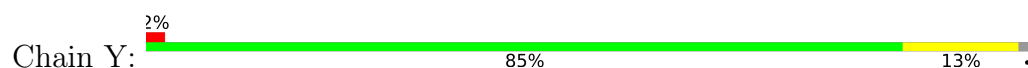
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

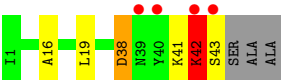
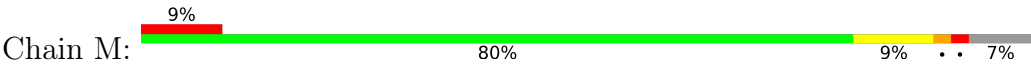


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

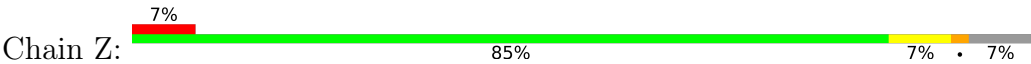




● Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.41Å 206.27Å 177.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 1.85 134.59 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.97-1.85) 99.4 (134.59-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 1.86Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.164 , 0.188 0.164 , 0.189	Depositor DCC
R_{free} test set	28371 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33558	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.08	6/4308 (0.1%)	0.93	11/5878 (0.2%)
1	N	0.88	0/4288	0.82	3/5852 (0.1%)
2	B	0.90	2/2047 (0.1%)	0.90	6/2790 (0.2%)
2	O	0.68	0/2024	0.77	2/2757 (0.1%)
3	C	0.90	1/2263 (0.0%)	0.74	0/3090
3	P	0.85	0/2272	0.73	0/3102
4	D	0.90	0/1245	0.79	0/1679
4	Q	0.54	0/1248	0.67	1/1684 (0.1%)
5	E	0.81	0/871	0.76	1/1182 (0.1%)
5	R	0.65	0/871	0.73	0/1182
6	F	0.86	0/795	0.81	0/1079
6	S	0.71	1/780 (0.1%)	0.82	0/1058
7	G	0.85	1/690 (0.1%)	0.86	1/937 (0.1%)
7	T	0.76	1/701 (0.1%)	0.84	1/951 (0.1%)
8	H	0.88	2/682 (0.3%)	0.78	1/921 (0.1%)
8	U	0.66	0/682	0.68	0/921
9	I	0.78	2/605 (0.3%)	0.75	0/802
9	V	0.53	0/605	0.73	1/802 (0.1%)
10	J	0.62	0/471	0.65	0/636
10	W	0.57	0/480	0.63	0/648
11	K	0.79	0/398	0.77	1/546 (0.2%)
11	X	0.47	0/405	0.55	0/556
12	L	0.85	0/401	0.74	0/536
12	Y	0.61	0/401	0.63	0/536
13	M	0.83	0/345	0.75	0/470
13	Z	0.51	0/345	0.58	0/470
All	All	0.84	16/30223 (0.1%)	0.79	29/41065 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
6	S	0	1
12	Y	0	1
All	All	0	4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	193	TYR	CD1-CE1	6.55	1.49	1.39
7	T	36	TRP	CB-CG	6.20	1.61	1.50
1	A	346	PHE	CD2-CE2	6.20	1.51	1.39
1	A	74	MET	CB-CG	6.13	1.71	1.51
1	A	220	PHE	CE1-CZ	5.88	1.48	1.37
2	B	198	GLU	CD-OE2	-5.87	1.19	1.25
7	G	36	TRP	CB-CG	5.70	1.60	1.50
8	H	69	VAL	CB-CG1	5.66	1.64	1.52
6	S	31	TYR	CD2-CE2	5.62	1.47	1.39
1	A	74	MET	CG-SD	-5.53	1.66	1.81
1	A	304	TYR	CD2-CE2	5.37	1.47	1.39
1	A	261	TYR	CE2-CZ	5.37	1.45	1.38
9	I	60	PHE	CE1-CZ	5.37	1.47	1.37
3	C	58	TRP	CE3-CZ3	5.22	1.47	1.38
9	I	69	PHE	CG-CD1	5.17	1.46	1.38
8	H	11	TYR	CD2-CE2	5.04	1.47	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-11.24	82.22	100.20
1	N	71	MET	CG-SD-CE	-9.71	84.67	100.20
1	A	96	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	A	189	MET	CG-SD-CE	-7.65	87.96	100.20
2	B	45	MET	CG-SD-CE	7.17	111.67	100.20
7	G	12	GLY	N-CA-C	6.66	129.75	113.10
11	K	47	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	N	189	MET	CG-SD-CE	-6.18	90.31	100.20
1	A	38	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	N	38	ARG	NE-CZ-NH1	6.09	123.35	120.30
2	B	82	ARG	NE-CZ-NH2	-6.06	117.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	MET	CG-SD-CE	-5.96	90.66	100.20
8	H	58	ARG	NE-CZ-NH2	-5.82	117.39	120.30
4	Q	20	ARG	NE-CZ-NH2	-5.75	117.42	120.30
2	O	82	ARG	NE-CZ-NH2	-5.72	117.44	120.30
5	E	30	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	B	87[A]	MET	CA-CB-CG	-5.58	103.81	113.30
2	B	87[B]	MET	CA-CB-CG	-5.58	103.81	113.30
9	V	10	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	A	74	MET	CB-CG-SD	-5.36	96.33	112.40
2	B	119	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	300	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	347	LEU	CA-CB-CG	-5.21	103.31	115.30
2	B	158	ASP	CB-CG-OD1	5.15	122.94	118.30
7	T	33	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	38	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	363	LEU	CA-CB-CG	5.06	126.95	115.30
2	O	139	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	513	LEU	CA-CB-CG	-5.04	103.72	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide
12	Y	46	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4125	0	4107	38	0
1	N	4122	0	4101	52	0
2	B	1996	0	2031	24	0
2	O	1975	0	2000	33	0
3	C	2152	0	2068	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	2173	0	2081	20	0
4	D	1198	0	1179	7	0
4	Q	1213	0	1199	7	0
5	E	852	0	845	7	0
5	R	852	0	845	3	0
6	F	773	0	751	12	0
6	S	763	0	742	8	0
7	G	675	0	643	12	0
7	T	681	0	648	10	0
8	H	662	0	623	7	0
8	U	662	0	623	5	0
9	I	601	0	613	9	0
9	V	601	0	613	11	0
10	J	460	0	459	7	0
10	W	469	0	463	7	0
11	K	384	0	366	2	0
11	X	391	0	374	1	0
12	L	383	0	385	7	0
12	Y	383	0	385	5	0
13	M	335	0	352	4	0
13	Z	335	0	352	3	0
14	A	180	0	162	17	0
14	N	180	0	162	20	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	9	0	0	7	0
18	N	9	0	0	6	0
19	A	102	0	152	6	0
19	C	100	0	148	3	0
19	G	51	0	76	4	0
19	N	102	0	152	9	0
19	P	51	0	76	1	0
20	A	40	0	60	3	0
20	B	8	0	12	0	0
20	C	32	0	48	2	0
20	D	16	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	E	20	0	30	0	0
20	F	20	0	30	0	0
20	G	8	0	12	1	0
20	H	8	0	12	2	0
20	L	4	0	6	0	0
20	N	32	0	48	1	0
20	O	12	0	18	1	0
20	P	12	0	18	0	0
20	Q	8	0	12	0	0
20	R	24	0	36	2	0
20	S	12	0	18	5	0
20	T	4	0	6	0	0
20	U	4	0	6	0	0
20	V	4	0	6	0	0
21	B	63	0	110	7	0
21	D	63	0	110	11	0
21	L	63	0	110	4	0
21	N	61	0	102	0	0
21	Q	63	0	110	7	0
21	Y	63	0	110	7	0
22	B	29	0	39	0	0
22	C	58	0	78	4	0
22	G	29	0	39	1	0
22	J	29	0	39	1	0
22	P	58	0	78	3	0
22	W	29	0	37	4	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	50	0	72	10	0
24	O	51	0	75	6	0
25	C	88	0	115	10	0
25	L	30	0	33	4	0
25	M	33	0	42	1	0
25	P	99	0	126	9	0
25	Z	33	0	42	1	0
26	C	89	0	133	13	0
26	N	96	0	140	10	0
26	P	80	0	106	8	0
26	T	97	0	146	11	0
27	C	97	0	133	4	0
27	G	97	0	131	3	0
27	P	53	0	77	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	T	50	0	71	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	222	0	0	1	0
29	B	134	0	0	2	0
29	C	99	0	0	0	0
29	D	108	0	0	2	0
29	E	82	0	0	1	0
29	F	79	0	0	2	0
29	G	52	0	0	1	0
29	H	44	0	0	0	0
29	I	27	0	0	2	0
29	J	27	0	0	1	0
29	K	20	0	0	1	0
29	L	26	0	0	0	0
29	M	24	0	0	0	0
29	N	209	0	0	0	0
29	O	112	0	0	0	0
29	P	90	0	0	1	0
29	Q	38	0	0	1	0
29	R	39	0	0	0	0
29	S	59	0	0	1	0
29	T	35	0	0	0	0
29	U	33	0	0	0	0
29	V	14	0	0	0	0
29	W	12	0	0	0	0
29	X	11	0	0	0	0
29	Y	13	0	0	0	0
29	Z	16	0	0	1	0
All	All	33558	0	32582	387	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 (387) 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)
6:F:85:CYS:SG	6:F:87[B]:THR:HG23	2.09	0.93
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.61	0.82
26:N:601:CDL:H371	2:O:78:LEU:HD12	1.63	0.79
1:N:309:THR:HG22	14:N:603[B]:HEA:HMB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:7:ASP:O	7:T:9:GLY:N	2.17	0.78
3:P:161[A]:GLN:HE22	27:T:101:PEK:H22	1.49	0.77
10:W:33:ARG:HG2	22:W:101:CHD:H152	1.67	0.76
19:G:104:PGV:H22	19:G:104:PGV:H71	1.69	0.74
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.70	0.74
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.71	0.73
6:F:94:HIS:HD2	29:F:219:HOH:O	1.70	0.73
1:N:406:ASN:HD21	19:N:619:PGV:H21	1.53	0.73
27:T:101:PEK:H383	26:T:102:CDL:H273	1.68	0.72
3:C:51[B]:MET:HE3	26:C:305:CDL:H392	1.72	0.72
3:P:161[A]:GLN:NE2	27:T:101:PEK:H22	2.05	0.71
14:A:601:HEA:HMC1	14:A:601:HEA:HBC1	1.72	0.70
2:O:34[C]:ILE:HD11	2:O:72:ILE:HG21	1.74	0.69
4:Q:78:TRP:HA	21:Q:201:TGL:HB22	1.75	0.69
7:T:37:LEU:HD23	26:T:102:CDL:H381	1.73	0.69
2:O:33[C]:LEU:HD21	9:V:32:ALA:HB2	1.74	0.69
12:L:42:HIS:ND1	25:L:102:DMU:O49	2.24	0.68
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.76	0.68
12:L:24[B]:MET:HG2	21:L:101:TGL:HA22	1.75	0.68
2:O:47:THR:HB	21:Q:201:TGL:H181	1.75	0.68
4:Q:78:TRP:CA	21:Q:201:TGL:HB22	2.24	0.67
14:N:603[B]:HEA:HBC1	14:N:603[B]:HEA:HMC1	1.76	0.67
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.35	0.67
1:N:359:ALA:HA	14:N:603[B]:HEA:OMA	1.94	0.66
26:N:601:CDL:H382	2:O:81:LEU:HD12	1.78	0.66
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.76	0.66
2:O:16:ILE:HD12	2:O:87[A]:MET:HG2	1.75	0.66
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.78	0.66
4:D:78:TRP:CB	21:D:201:TGL:HB22	2.24	0.66
1:A:359:ALA:HA	14:A:602[B]:HEA:OMA	1.95	0.66
13:M:41:LYS:O	13:M:43:SER:N	2.29	0.65
2:B:32[A]:PHE:HZ	21:B:301:TGL:HA22	1.61	0.65
6:S:52:ILE:O	6:S:94:HIS:NE2	2.29	0.65
19:A:609:PGV:H311	13:M:19:LEU:HD23	1.77	0.65
3:C:213:THR:HG23	26:C:305:CDL:H771	1.79	0.64
25:C:302:DMU:H7	10:J:49:CYS:HB3	1.81	0.63
21:B:301:TGL:HC22	29:I:124:HOH:O	1.97	0.62
5:E:90:ARG:HD2	29:E:359:HOH:O	1.98	0.62
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.82	0.62
7:T:11:TPO:HA	7:T:11:TPO:O3P	1.97	0.62
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:LYS:CD	26:C:305:CDL:HB32	2.30	0.61
19:A:608:PGV:H343	27:G:101:PEK:H382	1.82	0.61
4:Q:20:ARG:HG2	29:Q:332:HOH:O	2.00	0.61
3:C:224:LYS:HD3	26:C:305:CDL:HB32	1.83	0.61
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC1	1.84	0.60
1:A:243:VAL:HG11	14:A:602[B]:HEA:HMD2	1.85	0.59
3:C:33[B]:MET:HE1	3:C:41:THR:HB	1.84	0.59
19:N:619:PGV:H22	19:N:619:PGV:H011	1.84	0.59
7:T:31:CYS:SG	26:T:102:CDL:H532	2.43	0.59
1:A:309:THR:HG22	14:A:602[B]:HEA:HMB2	1.84	0.58
21:D:201:TGL:H242	21:D:201:TGL:HA91	1.84	0.58
1:N:510:TYR:HA	20:S:101:EDO:H21	1.85	0.58
24:B:304:PSC:C1	9:I:14:ALA:HB2	2.34	0.58
2:O:28[C]:LEU:HG	2:O:32[C]:PHE:CE2	2.39	0.58
24:O:302:PSC:C07	9:V:10:ARG:HH21	2.17	0.58
3:P:210:ILE:HD13	19:P:303:PGV:H301	1.86	0.57
7:G:12:GLY:HA3	29:G:236:HOH:O	2.03	0.57
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.38	0.57
24:B:304:PSC:H51	29:I:105:HOH:O	2.04	0.57
3:P:224:LYS:HZ1	26:P:304:CDL:H112	1.70	0.57
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.35	0.56
19:C:308:PGV:H72	19:C:308:PGV:H21	1.87	0.56
14:N:603[B]:HEA:HBD1	14:N:603[B]:HEA:HMD1	1.86	0.56
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.05	0.56
6:F:90:LYS:HD2	29:F:277:HOH:O	2.05	0.56
25:P:306:DMU:H35	25:P:306:DMU:H29	1.88	0.56
3:P:142:VAL:HG21	26:T:102:CDL:H822	1.87	0.56
4:D:78:TRP:CA	21:D:201:TGL:HB22	2.36	0.56
19:N:619:PGV:H22	19:N:619:PGV:H202	1.87	0.56
1:A:334:TRP:CZ3	21:D:201:TGL:HA52	2.41	0.55
3:C:33[B]:MET:CE	3:C:41:THR:HB	2.37	0.55
6:S:36:PRO:HD3	20:S:101:EDO:C1	2.36	0.55
14:N:603[A]:HEA:HMC1	14:N:603[A]:HEA:HBC1	1.88	0.55
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.89	0.54
1:A:297[A]:MET:HG2	1:A:302[A]:ARG:HG3	1.88	0.54
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.90	0.54
6:S:87[A]:THR:HG21	29:S:241:HOH:O	2.07	0.54
12:Y:20:ARG:HH12	21:Y:101:TGL:HC32	1.71	0.54
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.08	0.54
18:N:607[A]:AZI:N1	18:N:608[A]:AZI:N1	2.55	0.54
26:T:102:CDL:HA4	26:T:102:CDL:H311	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.90	0.54
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.88	0.54
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.43	0.53
4:D:65:LYS:HE3	29:D:398:HOH:O	2.07	0.53
3:C:33[B]:MET:HE1	3:C:42:LEU:H	1.74	0.53
7:G:41:HIS:HB3	7:G:74:ARG:CZ	2.38	0.53
14:A:602[B]:HEA:HMC1	14:A:602[B]:HEA:HBC1	1.91	0.53
2:O:26:HIS:HA	2:O:29[C]:MET:HE3	1.90	0.53
4:D:121:LYS:NZ	20:D:204:EDO:H22	2.23	0.53
1:A:358:LEU:HB3	14:A:602[A]:HEA:HMA	1.90	0.53
8:H:38:ARG:HH22	20:H:101:EDO:H22	1.74	0.53
7:G:11:TPO:HA	7:G:11:TPO:O3P	2.09	0.53
1:N:377:PHE:HB2	14:N:603[B]:HEA:HMD3	1.90	0.53
26:N:601:CDL:H161	26:N:601:CDL:OB3	2.10	0.52
1:A:62:ALA:HB2	14:A:601:HEA:HBD1	1.91	0.52
1:A:112:LEU:C	1:A:112:LEU:HD23	2.29	0.52
19:C:308:PGV:H21	19:C:308:PGV:C7	2.40	0.52
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.91	0.52
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.91	0.52
3:C:156:ARG:HE	22:C:306:CHD:C24	2.23	0.52
1:N:364:ASP:OD1	14:N:603[B]:HEA:O1A	2.27	0.52
1:N:243:VAL:HG11	14:N:603[B]:HEA:HMD2	1.92	0.52
12:L:41:ARG:HH22	25:L:102:DMU:H30	1.74	0.52
8:U:10:ASN:N	8:U:10:ASN:OD1	2.41	0.52
1:A:378:HIS:HA	1:A:382[B]:SER:HB2	1.92	0.51
27:C:307:PEK:H041	6:F:1:ALA:H1	1.76	0.51
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.91	0.51
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.46	0.51
1:A:22:PHE:HA	21:L:101:TGL:HB71	1.92	0.51
24:B:304:PSC:H31	9:I:17:LEU:HD23	1.91	0.51
1:A:282:PHE:HA	7:T:4:ALA:CB	2.38	0.51
19:G:104:PGV:H292	3:P:95:THR:HG21	1.93	0.51
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.93	0.51
14:N:603[A]:HEA:NB	18:N:608[A]:AZI:N2	2.59	0.50
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.91	0.50
1:N:386:VAL:HG21	14:N:602:HEA:H261	1.93	0.50
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.11	0.50
26:T:102:CDL:H511	26:T:102:CDL:H202	1.93	0.50
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.12	0.50
14:A:602[A]:HEA:NB	18:A:607[A]:AZI:N2	2.58	0.50
1:A:307:SER:CB	26:T:102:CDL:H171	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:377:PHE:CD2	14:N:603[B]:HEA:HBD2	2.46	0.50
3:C:165:ILE:HG12	27:C:307:PEK:H9	1.93	0.50
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.11	0.49
1:A:243:VAL:HB	14:A:602[B]:HEA:HAC	1.95	0.49
2:B:33[A]:LEU:HD13	9:I:31:PHE:CD1	2.47	0.49
5:E:86:ILE:O	5:E:90:ARG:HG2	2.12	0.49
12:L:20:ARG:NH2	21:L:101:TGL:OC1	2.45	0.49
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.49
1:N:307:SER:HB3	26:N:601:CDL:H191	1.94	0.49
12:Y:13:PHE:HB3	21:Y:101:TGL:HA22	1.94	0.49
26:C:305:CDL:H521	26:C:305:CDL:OB9	2.12	0.49
21:Q:201:TGL:H362	9:V:20:HIS:CE1	2.47	0.49
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.43	0.49
7:G:11:TPO:O2P	7:G:12:GLY:N	2.39	0.48
2:O:83:ILE:O	2:O:87[A]:MET:HG3	2.13	0.48
3:C:224:LYS:HE3	26:C:305:CDL:HB32	1.95	0.48
3:P:62:ILE:CD1	26:P:304:CDL:H522	2.44	0.48
1:N:351:GLY:HA3	1:N:380[B]:VAL:HB	1.95	0.48
3:P:80[B]:ARG:HG2	3:P:233:PHE:CE1	2.48	0.48
7:G:59:PRO:O	20:G:105:EDO:H22	2.13	0.48
1:N:240:HIS:HE1	18:N:608[A]:AZI:N2	2.11	0.48
3:C:224:LYS:CE	26:C:305:CDL:HB32	2.44	0.48
1:N:321:PHE:CZ	24:O:302:PSC:H162	2.49	0.48
1:A:483:LEU:O	20:A:616:EDO:H12	2.14	0.48
2:B:16[B]:ILE:HG13	2:B:17:MET:N	2.29	0.48
2:O:67:ILE:HD11	20:O:305:EDO:O2	2.14	0.48
14:A:602[A]:HEA:H243	2:B:69:PRO:HB3	1.95	0.48
21:D:201:TGL:H302	21:D:201:TGL:H131	1.74	0.48
24:B:304:PSC:H072	5:E:11:PHE:HB2	1.96	0.47
2:B:49:LYS:HD3	21:D:201:TGL:HC71	1.95	0.47
3:C:247:VAL:HG12	27:C:319:PEK:H132	1.96	0.47
2:B:16[B]:ILE:HG23	29:B:507:HOH:O	2.13	0.47
21:B:301:TGL:H272	21:B:301:TGL:H242	1.53	0.47
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.34	0.47
11:K:42:PRO:O	11:K:47:ARG:NH2	2.48	0.47
7:T:36:TRP:CE3	7:T:39:SER:HB3	2.50	0.47
12:Y:14:SER:H	21:Y:101:TGL:HC31	1.80	0.47
1:A:380[A]:VAL:HG21	14:A:602[A]:HEA:C3C	2.44	0.47
8:H:7:LYS:NZ	8:U:46:LYS:HG3	2.30	0.47
1:N:297[B]:MET:SD	1:N:302:ARG:CG	3.03	0.47
1:N:488:THR:HB	1:N:495:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:301:TGL:HA21	21:B:301:TGL:HB21	1.96	0.47
1:N:511:VAL:H	20:S:101:EDO:H22	1.79	0.47
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.73	0.47
29:A:701:HOH:O	21:D:201:TGL:HG11	2.15	0.47
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.96	0.47
1:N:409:TRP:CE2	19:N:619:PGV:H61	2.49	0.47
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.97	0.47
2:O:164:ALA:O	2:O:194:GLY:HA3	2.14	0.47
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.45	0.47
1:N:240:HIS:CE1	18:N:608[A]:AZI:N2	2.83	0.47
25:P:306:DMU:H23	10:W:50:LEU:HG	1.97	0.47
10:W:33:ARG:HG2	22:W:101:CHD:H7	1.96	0.47
12:Y:24[B]:MET:HG2	21:Y:101:TGL:HA21	1.97	0.47
12:L:2:HIS:CG	12:L:3:TYR:H	2.32	0.46
1:N:35:LEU:HB3	25:Z:101:DMU:H24	1.97	0.46
26:N:601:CDL:H411	2:O:77:ALA:CB	2.45	0.46
8:H:84:LYS:HG3	20:H:102:EDO:H12	1.98	0.46
24:O:302:PSC:H071	9:V:10:ARG:HE	1.80	0.46
5:R:25:ASP:HB3	20:R:205:EDO:H11	1.97	0.46
21:Y:101:TGL:HC22	21:Y:101:TGL:HC81	1.97	0.46
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.97	0.46
1:A:240:HIS:HE1	18:A:607[A]:AZI:N2	2.14	0.46
20:A:610:EDO:H22	12:L:10:ASN:HB2	1.98	0.46
2:B:49:LYS:HD3	21:D:201:TGL:CC7	2.46	0.46
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.98	0.46
2:B:60:GLU:H	2:B:60:GLU:CD	2.18	0.46
26:C:305:CDL:H621	26:C:305:CDL:H591	1.79	0.46
1:N:347:LEU:HD13	1:N:383[A]:MET:HB3	1.97	0.46
2:B:32[A]:PHE:CZ	21:B:301:TGL:HA22	2.45	0.46
3:C:4:GLN:HG2	20:C:314:EDO:H12	1.98	0.46
27:C:307:PEK:H331	27:C:307:PEK:H362	1.78	0.46
5:E:43:PRO:HB2	5:E:48:ILE:HD11	1.98	0.46
1:N:467:LEU:O	1:N:471:ILE:HG13	2.16	0.46
2:B:42[A]:ILE:HG22	2:B:46:LEU:HD12	1.98	0.45
19:N:609:PGV:H342	19:N:609:PGV:H311	1.68	0.45
3:P:246:ASP:HB2	29:P:480:HOH:O	2.16	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.45
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.81	0.45
6:F:64:GLU:O	6:F:65:ASP:HB2	2.16	0.45
27:G:103:PEK:H261	27:G:103:PEK:H222	1.98	0.45
26:T:102:CDL:H451	26:T:102:CDL:H421	1.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:58:LYS:HB3	10:W:58:LYS:HE2	1.77	0.45
3:C:258:TRP:CZ3	25:C:309:DMU:H12	2.51	0.45
7:G:37:LEU:HD21	26:N:601:CDL:H372	1.98	0.45
10:J:58:LYS:HB2	10:J:58:LYS:HE2	1.68	0.45
3:C:80[A]:ARG:NH2	3:C:236:GLU:OE1	2.41	0.45
26:P:304:CDL:H521	26:P:304:CDL:OB9	2.16	0.45
7:G:5:LYS:HB3	1:N:278[B]:MET:HE3	1.98	0.45
1:N:236:TRP:CH2	14:N:603[A]:HEA:HBD1	2.52	0.45
2:O:25:ASP:O	2:O:29[C]:MET:N	2.48	0.45
25:P:307:DMU:H34	25:P:307:DMU:H36	1.77	0.45
19:A:608:PGV:H183	27:G:101:PEK:H322	1.98	0.45
4:D:98:TRP:CE2	25:M:101:DMU:H11	2.52	0.45
10:J:7:GLU:HG3	29:J:218:HOH:O	2.17	0.45
1:N:353:LEU:HB3	2:O:31[A]:VAL:HG22	1.99	0.45
24:O:302:PSC:H071	9:V:10:ARG:HH21	1.82	0.45
3:P:261:SER:OXT	25:P:307:DMU:H40	2.17	0.45
25:C:302:DMU:H4	10:J:52:TRP:CZ2	2.52	0.45
2:O:39[A]:LEU:HD11	21:Q:201:TGL:H221	1.97	0.45
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.99	0.45
22:J:101:CHD:H213	22:J:101:CHD:H232	1.64	0.45
3:P:259:TRP:CD1	25:P:307:DMU:H30	2.51	0.45
22:P:305:CHD:H162	22:P:305:CHD:C23	2.47	0.45
5:R:5:HIS:O	5:R:6:GLU:HB3	2.16	0.45
26:T:102:CDL:H311	26:T:102:CDL:OA7	2.17	0.45
21:B:301:TGL:H211	21:B:301:TGL:HA81	1.76	0.45
24:B:304:PSC:C06	9:I:10:ARG:HH21	2.30	0.45
3:C:210:ILE:HG21	19:C:304:PGV:H282	1.98	0.45
10:W:33:ARG:HE	22:W:101:CHD:H7	1.82	0.45
7:T:31:CYS:SG	26:T:102:CDL:H552	2.58	0.44
11:X:54:ARG:HE	11:X:54:ARG:HB3	1.76	0.44
7:G:38:HIS:CE1	26:N:601:CDL:H141	2.52	0.44
1:N:71:MET:HB2	1:N:72:PRO:HD3	1.99	0.44
22:C:306:CHD:H162	22:C:306:CHD:C23	2.48	0.44
25:P:308:DMU:H22	10:W:38:LEU:HD23	1.99	0.44
3:C:37:PHE:CB	25:C:302:DMU:H8	2.48	0.44
10:J:55:PHE:HE1	25:L:102:DMU:H2	1.81	0.44
2:O:42[A]:ILE:O	2:O:46:LEU:HG	2.18	0.44
2:B:28[C]:LEU:HG	2:B:32[C]:PHE:CE2	2.53	0.44
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.98	0.44
9:I:57:MET:O	9:I:61:GLU:HG2	2.17	0.44
8:U:45:ALA:O	8:U:47:GLY:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:304:PSC:H262	24:B:304:PSC:H62	1.99	0.44
6:F:37:LYS:HD2	6:F:37:LYS:HA	1.83	0.44
11:K:8:ASP:HB2	29:K:111:HOH:O	2.17	0.44
19:N:619:PGV:H251	13:Z:12:PRO:HB3	2.00	0.44
24:O:302:PSC:H073	9:V:10:ARG:HH21	1.81	0.44
14:A:602[B]:HEA:ND	18:A:607[B]:AZI:N2	2.65	0.44
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.99	0.44
1:N:62:ALA:HB2	14:N:602:HEA:HBD1	2.00	0.44
6:S:52:ILE:HA	6:S:94:HIS:CD2	2.53	0.44
1:N:373:VAL:HG13	14:N:603[A]:HEA:HBA1	1.99	0.44
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.83	0.44
7:G:7:ASP:CG	7:G:8:HIS:N	2.69	0.43
22:G:102:CHD:H12	22:G:102:CHD:H212	2.00	0.43
3:P:62:ILE:HD12	26:P:304:CDL:H522	2.00	0.43
1:A:386:VAL:HG21	14:A:601:HEA:H261	1.99	0.43
2:B:69:PRO:HG2	29:B:429:HOH:O	2.18	0.43
19:G:104:PGV:H22	19:G:104:PGV:C7	2.44	0.43
26:N:601:CDL:OA7	26:N:601:CDL:H311	2.17	0.43
22:C:306:CHD:H112	22:C:306:CHD:H12A	1.81	0.43
1:N:137:ALA:O	20:N:613:EDO:H21	2.19	0.43
27:T:101:PEK:C38	26:T:102:CDL:H273	2.41	0.43
24:B:304:PSC:H081	5:E:8:ASP:OD1	2.18	0.43
7:G:33:LEU:O	7:G:37:LEU:HB2	2.18	0.43
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.54	0.43
9:I:22:VAL:O	9:I:26:MET:HG2	2.18	0.43
2:O:111:THR:HA	2:O:114:GLU:O	2.19	0.43
6:S:36:PRO:HD3	20:S:101:EDO:H11	1.99	0.43
1:A:240:HIS:CE1	18:A:607[B]:AZI:N1	2.87	0.43
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.99	0.43
19:A:609:PGV:H312	13:M:16:ALA:HA	2.01	0.43
2:B:32[A]:PHE:HE1	21:B:301:TGL:HA52	1.84	0.43
19:N:619:PGV:H011	19:N:619:PGV:C2	2.48	0.43
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.43
6:S:36:PRO:HD3	20:S:101:EDO:H12	2.01	0.43
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.54	0.43
13:M:38:ASP:OD2	13:M:42:LYS:HD3	2.18	0.43
2:B:49:LYS:HE2	29:D:391:HOH:O	2.18	0.43
26:P:304:CDL:OA7	26:P:304:CDL:H162	2.19	0.43
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.01	0.42
3:C:62:ILE:CD1	26:C:305:CDL:H522	2.49	0.42
8:H:46:LYS:HZ2	8:H:46:LYS:HG2	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383[B]:MET:SD	1:N:421:VAL:HG11	2.59	0.42
20:C:318:EDO:O1	6:F:1:ALA:HA	2.19	0.42
13:Z:38:ASP:HB2	29:Z:207:HOH:O	2.20	0.42
1:A:240:HIS:CE1	18:A:607[A]:AZI:N2	2.88	0.42
6:F:92:VAL:HG23	6:F:92:VAL:O	2.19	0.42
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.00	0.42
14:N:603[A]:HEA:C1B	18:N:608[A]:AZI:N2	2.82	0.42
3:P:164:PHE:CD1	22:P:305:CHD:H192	2.55	0.42
14:N:603[A]:HEA:C1B	18:N:608[A]:AZI:N3	2.83	0.42
1:A:274:VAL:O	1:A:278[A]:MET:HG3	2.19	0.42
3:C:37:PHE:CG	25:C:302:DMU:H8	2.55	0.42
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.84	0.42
19:N:619:PGV:H312	13:Z:19:LEU:HD23	2.02	0.42
1:A:76:GLY:O	1:A:80:ASN:HB2	2.20	0.42
14:A:602[B]:HEA:HMB1	14:A:602[B]:HEA:H11	1.86	0.42
14:N:602:HEA:HHC	14:N:602:HEA:H122	2.01	0.42
19:A:609:PGV:C19	19:A:609:PGV:H231	2.49	0.42
26:C:305:CDL:H191	26:C:305:CDL:H752	2.01	0.42
26:N:601:CDL:H221	26:N:601:CDL:H511	2.01	0.42
1:N:380[A]:VAL:HG21	14:N:603[A]:HEA:C3C	2.49	0.42
14:N:603[A]:HEA:H243	2:O:69:PRO:HB3	2.02	0.42
3:C:51[B]:MET:HB3	26:C:305:CDL:H381	2.02	0.42
25:C:309:DMU:H29	25:C:309:DMU:H32	2.02	0.42
2:O:28[C]:LEU:HD12	2:O:28[C]:LEU:HA	1.89	0.42
26:P:304:CDL:H821	26:P:304:CDL:H851	1.38	0.42
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	2.01	0.42
10:W:33:ARG:CG	22:W:101:CHD:H152	2.41	0.42
2:B:60:GLU:CD	2:B:60:GLU:N	2.74	0.41
24:O:302:PSC:H251	24:O:302:PSC:H221	1.77	0.41
3:C:217:VAL:HG22	26:C:305:CDL:H732	2.02	0.41
6:S:64:GLU:O	6:S:65:ASP:HB2	2.20	0.41
21:Y:101:TGL:OC1	21:Y:101:TGL:HC41	2.18	0.41
9:I:31:PHE:CD1	9:I:31:PHE:C	2.94	0.41
2:O:24:HIS:CE1	2:O:28[C]:LEU:HD22	2.56	0.41
9:V:18:ARG:HG2	9:V:18:ARG:NH1	2.28	0.41
12:Y:24[B]:MET:SD	21:Y:101:TGL:HC21	2.61	0.41
26:P:304:CDL:H521	26:P:304:CDL:HB62	2.02	0.41
4:Q:21:ASP:OD1	4:Q:21:ASP:N	2.53	0.41
4:Q:122:ARG:O	4:Q:126:MET:HG2	2.20	0.41
3:C:33[B]:MET:CE	3:C:42:LEU:H	2.32	0.41
25:C:302:DMU:H7	10:J:49:CYS:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:D:201:TGL:H242	21:D:201:TGL:H212	1.82	0.41
9:I:31:PHE:CZ	9:I:35:TYR:HB2	2.55	0.41
26:N:601:CDL:H371	2:O:78:LEU:CD1	2.43	0.41
3:P:156:ARG:HE	22:P:305:CHD:C24	2.33	0.41
8:U:60:TYR:CD1	8:U:60:TYR:C	2.93	0.41
2:B:41[C]:ILE:HD13	24:B:304:PSC:H342	2.02	0.41
1:N:449:MET:SD	2:O:5:MET:HG2	2.61	0.41
7:T:36:TRP:HE3	7:T:39:SER:HB3	1.84	0.41
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.02	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
1:A:334:TRP:HZ3	21:D:201:TGL:HA72	1.86	0.41
2:B:1:FME:HE2	2:B:1:FME:HB3	1.90	0.41
6:F:21[B]:MET:HE2	6:F:21[B]:MET:HB2	1.87	0.41
2:B:28[C]:LEU:HD12	2:B:28[C]:LEU:HA	1.79	0.41
6:F:54[A]:ASN:C	6:F:54[A]:ASN:HD22	2.23	0.41
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.56	0.41
18:A:606[A]:AZI:N1	18:A:607[A]:AZI:N1	2.69	0.41
19:G:104:PGV:H71	19:G:104:PGV:C2	2.44	0.41
2:O:91:ASN:HD22	2:O:92:ASN:N	2.18	0.41
3:P:133:ASN:HD21	3:P:176:LEU:HB2	1.85	0.41
27:P:312:PEK:H203	27:P:312:PEK:H171	1.88	0.41
5:R:14:ARG:NH1	20:R:202:EDO:O2	2.48	0.41
1:A:328:HIS:NE2	24:B:304:PSC:H22	2.36	0.41
14:A:602[A]:HEA:C1B	18:A:607[A]:AZI:N2	2.83	0.41
14:A:602[B]:HEA:HMD1	14:A:602[B]:HEA:CBD	2.51	0.41
19:A:609:PGV:H131	19:A:609:PGV:H302	2.02	0.41
26:C:305:CDL:H111	26:C:305:CDL:HA62	2.03	0.41
8:H:40:GLU:OE1	8:H:50:VAL:HG11	2.21	0.40
10:J:55:PHE:CE1	25:L:102:DMU:H36	2.56	0.40
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.03	0.40
1:N:513:LEU:O	1:N:514:LYS:HB2	2.21	0.40
25:P:306:DMU:H29	25:P:306:DMU:C9	2.50	0.40
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.56	0.40
24:B:304:PSC:O01	9:I:14:ALA:HB2	2.22	0.40
1:N:112:LEU:HD23	1:N:112:LEU:C	2.42	0.40
19:N:609:PGV:H21	3:P:57:TRP:CZ2	2.56	0.40
26:P:304:CDL:OA7	26:P:304:CDL:H132	2.21	0.40
21:Q:201:TGL:H362	9:V:20:HIS:HE1	1.86	0.40
1:A:484:THR:HA	20:A:616:EDO:H12	2.03	0.40
22:C:306:CHD:H162	22:C:306:CHD:H231	2.04	0.40
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383[A]:MET:HA	1:N:387:PHE:CD1	2.57	0.40
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.03	0.40
1:N:274:VAL:O	1:N:278[A]:MET:HG3	2.22	0.40
21:L:101:TGL:H262	21:L:101:TGL:H231	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	532/514 (104%)	514 (97%)	18 (3%)	0	100	100
1	N	530/514 (103%)	517 (98%)	13 (2%)	0	100	100
2	B	248/227 (109%)	242 (98%)	6 (2%)	0	100	100
2	O	245/227 (108%)	239 (98%)	5 (2%)	1 (0%)	34	19
3	C	265/261 (102%)	260 (98%)	5 (2%)	0	100	100
3	P	266/261 (102%)	261 (98%)	5 (2%)	0	100	100
4	D	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
4	Q	144/147 (98%)	138 (96%)	4 (3%)	2 (1%)	11	3
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	0	1 (1%)	15	5
6	F	100/98 (102%)	96 (96%)	2 (2%)	2 (2%)	7	1
6	S	98/98 (100%)	92 (94%)	3 (3%)	3 (3%)	4	0
7	G	81/85 (95%)	70 (86%)	5 (6%)	6 (7%)	1	0
7	T	82/85 (96%)	68 (83%)	10 (12%)	4 (5%)	2	0
8	H	77/85 (91%)	72 (94%)	5 (6%)	0	100	100
8	U	77/85 (91%)	72 (94%)	2 (3%)	3 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	42 (93%)	2 (4%)	1 (2%)	6	1
12	Y	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	1 (2%)	1 (2%)	6	1
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3617/3614 (100%)	3494 (97%)	99 (3%)	24 (1%)	22	9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	8	HIS
13	M	42	LYS
4	Q	7	LYS
4	Q	8	SER
5	R	6	GLU
6	S	94	HIS
7	T	3	ALA
7	T	4	ALA
7	T	5	LYS
7	T	8	HIS
6	F	96	LEU
7	G	37	LEU
6	S	96	LEU
6	F	2	SER
7	G	3	ALA
7	G	5	LYS
8	U	46	LYS
7	G	6	GLY
12	L	46	LYS
2	O	92	ASN
6	S	95	GLN
8	U	45	ALA
8	U	11	TYR

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	445/426 (104%)	440 (99%)	5 (1%)	73	65
1	N	443/426 (104%)	436 (98%)	7 (2%)	62	49
2	B	233/210 (111%)	224 (96%)	9 (4%)	32	15
2	O	230/210 (110%)	222 (96%)	8 (4%)	36	18
3	C	232/226 (103%)	229 (99%)	3 (1%)	69	58
3	P	233/226 (103%)	228 (98%)	5 (2%)	53	38
4	D	130/129 (101%)	129 (99%)	1 (1%)	81	76
4	Q	130/129 (101%)	121 (93%)	9 (7%)	15	4
5	E	92/95 (97%)	91 (99%)	1 (1%)	73	65
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	12
6	F	85/81 (105%)	80 (94%)	5 (6%)	19	6
6	S	83/81 (102%)	78 (94%)	5 (6%)	19	5
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	1
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	0
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	1
8	U	71/75 (95%)	65 (92%)	6 (8%)	10	2
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	8
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	1
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	40
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	14
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	40/46 (87%)	39 (98%)	1 (2%)	47	31
12	L	40/40 (100%)	39 (98%)	1 (2%)	47	31
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	31
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	8
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3151/3082 (102%)	3043 (97%)	108 (3%)	37 19

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	138	HIS
1	A	297[A]	MET
1	A	297[B]	MET
1	A	369	ASP
2	B	33[A]	LEU
2	B	33[C]	LEU
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	147	LYS
5	E	5	HIS
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80	GLN
6	F	95	GLN
6	F	98	HIS
7	G	5	LYS
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
8	H	8	ILE
8	H	9	LYS
8	H	10	ASN
8	H	29	CYS
8	H	44	THR
8	H	46	LYS
8	H	60	TYR

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Mol	Chain	Res	Type
9	I	2	THR
9	I	37	PHE
9	I	73	LYS
10	J	58	LYS
12	L	47	LYS
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	138	HIS
1	N	189	MET
1	N	369	ASP
1	N	382[A]	SER
1	N	382[B]	SER
2	O	33[A]	LEU
2	O	33[C]	LEU
2	O	60	GLU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	171	LYS
2	O	226	MET
3	P	40	MET
3	P	76	GLN
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	6	VAL
4	Q	7	LYS
4	Q	8	SER
4	Q	20	ARG
4	Q	51	LEU
4	Q	58	GLU
4	Q	143	ASN
4	Q	147	LYS
5	R	5	HIS
5	R	79	LYS
5	R	90	ARG
5	R	109	VAL
6	S	21[A]	MET
6	S	21[B]	MET

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Mol	Chain	Res	Type
6	S	64	GLU
6	S	94	HIS
6	S	96	LEU
7	T	7	ASP
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
8	U	7	LYS
8	U	9	LYS
8	U	10	ASN
8	U	29	CYS
8	U	40	GLU
8	U	60	TYR
9	V	8	GLN
9	V	18	ARG
9	V	29	LEU
9	V	37	PHE
9	V	70	GLN
9	V	73	LYS
10	W	50	LEU
10	W	58	LYS
11	X	54	ARG
12	Y	47	LYS
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
4	D	101	HIS
4	D	143	ASN
5	E	94	ASN
6	F	95	GLN
8	H	37	HIS
2	O	24	HIS

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Mol	Chain	Res	Type
2	O	52	HIS
2	O	195	GLN
3	P	133	ASN
4	Q	101	HIS
8	U	22	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.62	2 (25%)	10,14,16	1.13	1 (10%)
7	TPO	T	11	7	8,10,11	1.47	1 (12%)	10,14,16	1.35	1 (10%)
2	FME	O	1	2	8,9,10	0.59	0	7,9,11	1.44	2 (28%)
1	FME	N	1	1	8,9,10	0.43	0	7,9,11	1.42	1 (14%)
1	FME	A	1	1	8,9,10	0.56	0	7,9,11	1.79	1 (14%)
9	SAC	V	1	9	7,8,9	0.55	0	8,9,11	1.05	1 (12%)
9	SAC	I	1	9	7,8,9	0.59	0	8,9,11	1.15	1 (12%)
2	FME	B	1	2	8,9,10	0.85	0	7,9,11	1.97	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
7	TPO	G	11	7	-	5/9/11/13	-

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.88	1.59	1.50
7	G	11	TPO	P-O1P	2.84	1.59	1.50
7	G	11	TPO	P-OG1	2.61	1.64	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.15	101.42	112.95
7	T	11	TPO	CG2-CB-CA	3.02	119.12	113.16
1	A	1	FME	C-CA-N	2.91	114.99	109.73
2	O	1	FME	CG-CB-CA	-2.70	105.45	112.95
1	N	1	FME	O-C-CA	-2.61	117.94	124.78
7	G	11	TPO	O3P-P-OG1	2.56	117.46	105.99
9	I	1	SAC	C-CA-N	2.38	114.02	109.73
9	V	1	SAC	O-C-CA	-2.32	118.69	124.78
2	B	1	FME	C-CA-N	-2.22	105.72	109.73
2	O	1	FME	CA-N-CN	2.11	126.07	122.82

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	N-CA-CB-OG

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 10 are monoatomic - leaving 124 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	$\# Z > 2$
25	DMU	M	101	-	34,34,34	0.45	0	45,45,45	1.35	4 (8%)
20	EDO	A	615	-	3,3,3	0.80	0	2,2,2	0.71	0
18	AZI	A	606[A]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	C	312	-	3,3,3	0.48	0	2,2,2	0.42	0
20	EDO	R	202	-	3,3,3	0.36	0	2,2,2	0.51	0
22	CHD	G	102	-	32,32,32	0.83	0	51,51,51	1.29	7 (13%)
20	EDO	D	203	-	3,3,3	0.39	0	2,2,2	0.30	0
18	AZI	N	608[B]	15,14	0,2,2	-	-	0,1,1	-	-
20	EDO	N	612	-	3,3,3	0.49	0	2,2,2	0.24	0
14	HEA	A	602[A]	18,1	57,67,67	1.62	11 (19%)	61,103,103	2.08	16 (26%)
22	CHD	J	101	-	32,32,32	0.79	1 (3%)	51,51,51	1.27	5 (9%)
25	DMU	C	310	-	22,22,34	0.46	0	27,27,45	0.97	1 (3%)
20	EDO	C	315	-	3,3,3	0.53	0	2,2,2	0.18	0
22	CHD	W	101	10	32,32,32	0.82	1 (3%)	51,51,51	2.51	19 (37%)
20	EDO	T	103	-	3,3,3	0.93	0	2,2,2	0.59	0
22	CHD	C	306	-	32,32,32	0.93	0	51,51,51	2.14	16 (31%)
20	EDO	F	106	-	3,3,3	0.42	0	2,2,2	0.71	0
25	DMU	P	307	-	34,34,34	0.63	0	45,45,45	1.94	10 (22%)
20	EDO	S	104	-	3,3,3	0.70	0	2,2,2	0.54	0
20	EDO	H	102	-	3,3,3	0.45	0	2,2,2	0.58	0
20	EDO	R	201	-	3,3,3	0.69	0	2,2,2	0.52	0
20	EDO	O	304	-	3,3,3	0.49	0	2,2,2	0.48	0
27	PEK	C	307	-	52,52,52	1.08	2 (3%)	55,57,57	1.57	10 (18%)
20	EDO	A	610	-	3,3,3	0.36	0	2,2,2	0.77	0
19	PGV	A	608	-	50,50,50	1.03	3 (6%)	53,56,56	0.93	3 (5%)
14	HEA	N	603[A]	18,1	57,67,67	1.53	10 (17%)	61,103,103	2.04	23 (37%)
25	DMU	P	308	-	34,34,34	0.65	1 (2%)	45,45,45	0.98	1 (2%)
20	EDO	E	201	-	3,3,3	0.73	0	2,2,2	0.24	0
20	EDO	Q	202	-	3,3,3	0.45	0	2,2,2	0.60	0
22	CHD	P	301	-	32,32,32	0.83	0	51,51,51	1.45	7 (13%)
20	EDO	O	303	-	3,3,3	0.59	0	2,2,2	0.94	0
20	EDO	A	614	-	3,3,3	0.92	0	2,2,2	0.27	0
27	PEK	P	312	-	52,52,52	0.86	3 (5%)	55,57,57	2.31	9 (16%)
20	EDO	A	618	-	3,3,3	0.35	0	2,2,2	0.46	0
19	PGV	C	304	-	50,50,50	0.87	3 (6%)	53,56,56	1.13	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	618	-	3,3,3	0.44	0	2,2,2	0.39	0
22	CHD	B	302	-	32,32,32	1.15	2 (6%)	51,51,51	1.46	9 (17%)
19	PGV	P	303	-	50,50,50	0.70	2 (4%)	53,56,56	1.08	5 (9%)
20	EDO	D	202	-	3,3,3	0.45	0	2,2,2	0.79	0
24	PSC	B	304	-	48,48,51	1.31	4 (8%)	53,55,59	1.28	4 (7%)
20	EDO	S	103	-	3,3,3	0.96	0	2,2,2	0.48	0
19	PGV	C	308	-	48,48,50	1.22	3 (6%)	51,53,56	1.33	4 (7%)
20	EDO	E	204	-	3,3,3	0.74	0	2,2,2	0.11	0
20	EDO	C	311	-	3,3,3	0.76	0	2,2,2	0.33	0
20	EDO	G	106	-	3,3,3	0.67	0	2,2,2	0.38	0
20	EDO	B	305	-	3,3,3	0.61	0	2,2,2	0.14	0
20	EDO	O	305	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	P	309	-	3,3,3	0.51	0	2,2,2	0.70	0
20	EDO	A	612	-	3,3,3	1.13	0	2,2,2	0.87	0
26	CDL	N	601	-	93,93,99	1.43	12 (12%)	97,103,111	1.19	11 (11%)
20	EDO	A	616	-	3,3,3	0.99	0	2,2,2	0.89	0
18	AZI	N	608[A]	14	0,2,2	-	-	0,1,1	-	-
26	CDL	P	304	-	77,77,99	1.48	10 (12%)	84,85,111	1.68	13 (15%)
27	PEK	G	101	-	52,52,52	0.85	4 (7%)	55,57,57	1.13	5 (9%)
20	EDO	F	104	-	3,3,3	0.38	0	2,2,2	0.48	0
20	EDO	Q	203	-	3,3,3	0.55	0	2,2,2	0.18	0
19	PGV	G	104	-	50,50,50	1.08	2 (4%)	53,56,56	1.54	10 (18%)
20	EDO	P	311	-	3,3,3	0.58	0	2,2,2	0.46	0
20	EDO	R	203	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	C	314	-	3,3,3	0.48	0	2,2,2	0.56	0
21	TGL	B	301	-	62,62,62	1.20	3 (4%)	65,65,65	1.38	6 (9%)
14	HEA	A	602[B]	18,1	57,67,67	1.51	9 (15%)	61,103,103	2.09	18 (29%)
20	EDO	N	614	-	3,3,3	1.22	0	2,2,2	0.59	0
21	TGL	Q	201	-	62,62,62	1.06	4 (6%)	65,65,65	0.90	5 (7%)
20	EDO	E	202	-	3,3,3	0.49	0	2,2,2	0.57	0
20	EDO	L	103	-	3,3,3	0.41	0	2,2,2	0.49	0
18	AZI	N	607[A]	15	0,2,2	-	-	0,1,1	-	-
20	EDO	C	318	-	3,3,3	0.67	0	2,2,2	0.79	0
27	PEK	T	101	-	49,49,52	1.13	3 (6%)	53,54,57	1.58	9 (16%)
14	HEA	A	601	1	57,67,67	1.77	13 (22%)	61,103,103	2.33	24 (39%)
20	EDO	H	101	-	3,3,3	0.32	0	2,2,2	0.86	0
25	DMU	P	306	-	34,34,34	0.67	1 (2%)	45,45,45	0.88	2 (4%)
14	HEA	N	603[B]	18,1	57,67,67	1.55	10 (17%)	61,103,103	2.04	20 (32%)
21	TGL	D	201	-	62,62,62	1.24	4 (6%)	65,65,65	1.21	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.44	0
25	DMU	C	302	-	34,34,34	0.69	0	45,45,45	1.66	8 (17%)
21	TGL	N	610	-	59,59,62	1.14	3 (5%)	61,61,65	1.39	7 (11%)
20	EDO	N	611	-	3,3,3	0.38	0	2,2,2	0.54	0
20	EDO	E	203	-	3,3,3	0.42	0	2,2,2	0.46	0
18	AZI	A	607[B]	15,14	0,2,2	-	-	0,1,1	-	-
25	DMU	L	102	-	31,31,34	0.91	0	42,42,45	1.83	12 (28%)
20	EDO	R	206	-	3,3,3	0.63	0	2,2,2	0.25	0
20	EDO	A	613	-	3,3,3	0.95	0	2,2,2	0.59	0
19	PGV	N	609	-	50,50,50	0.94	3 (6%)	53,56,56	1.38	7 (13%)
20	EDO	C	316	-	3,3,3	0.55	0	2,2,2	0.32	0
23	CUA	O	301	2	0,1,1	-	-	-	-	-
21	TGL	L	101	-	62,62,62	1.60	5 (8%)	65,65,65	1.99	15 (23%)
20	EDO	P	310	-	3,3,3	0.58	0	2,2,2	0.32	0
20	EDO	F	103	-	3,3,3	0.59	0	2,2,2	0.49	0
20	EDO	F	102	-	3,3,3	0.83	0	2,2,2	0.66	0
20	EDO	N	617	-	3,3,3	0.57	0	2,2,2	0.22	0
20	EDO	V	101	-	3,3,3	0.46	0	2,2,2	0.54	0
25	DMU	Z	101	-	34,34,34	0.44	0	45,45,45	0.86	1 (2%)
23	CUA	B	303	2	0,1,1	-	-	-	-	-
24	PSC	O	302	-	50,50,51	1.16	3 (6%)	56,58,59	1.31	5 (8%)
20	EDO	N	616	-	3,3,3	0.77	0	2,2,2	0.09	0
20	EDO	R	204	-	3,3,3	0.68	0	2,2,2	0.41	0
20	EDO	E	205	-	3,3,3	0.48	0	2,2,2	0.44	0
20	EDO	R	205	-	3,3,3	0.45	0	2,2,2	0.59	0
22	CHD	C	301	-	32,32,32	1.01	2 (6%)	51,51,51	1.77	12 (23%)
20	EDO	U	101	-	3,3,3	0.49	0	2,2,2	0.22	0
20	EDO	A	619	-	3,3,3	0.47	0	2,2,2	0.40	0
20	EDO	A	617	-	3,3,3	0.68	0	2,2,2	0.47	0
21	TGL	Y	101	-	62,62,62	1.18	3 (4%)	65,65,65	1.45	11 (16%)
20	EDO	B	306	-	3,3,3	1.03	0	2,2,2	0.27	0
20	EDO	C	317	-	3,3,3	0.57	0	2,2,2	0.34	0
27	PEK	C	319	-	43,43,52	1.15	2 (4%)	46,48,57	1.67	8 (17%)
20	EDO	F	105	-	3,3,3	0.36	0	2,2,2	0.77	0
20	EDO	A	611	-	3,3,3	0.57	0	2,2,2	0.64	0
14	HEA	N	602	1	57,67,67	1.45	8 (14%)	61,103,103	2.20	24 (39%)
22	CHD	P	305	-	32,32,32	0.77	0	51,51,51	1.89	11 (21%)
26	CDL	C	305	-	87,87,99	1.48	14 (16%)	95,97,111	1.73	22 (23%)
20	EDO	D	204	-	3,3,3	0.36	0	2,2,2	0.64	0
25	DMU	C	309	-	34,34,34	0.69	1 (2%)	45,45,45	1.66	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PEK	G	103	-	43,43,52	1.09	2 (4%)	46,48,57	1.59	9 (19%)
20	EDO	D	205	-	3,3,3	0.58	0	2,2,2	0.36	0
20	EDO	G	105	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	C	313	-	3,3,3	0.53	0	2,2,2	0.36	0
20	EDO	S	101	-	3,3,3	0.55	0	2,2,2	0.18	0
20	EDO	N	615	-	3,3,3	0.51	0	2,2,2	0.66	0
19	PGV	N	619	-	50,50,50	1.04	2 (4%)	53,56,56	1.22	6 (11%)
18	AZI	A	607[A]	14	0,2,2	-	-	0,1,1	-	-
26	CDL	T	102	-	95,95,99	1.40	12 (12%)	100,106,111	1.48	13 (13%)
19	PGV	A	609	-	50,50,50	1.25	4 (8%)	53,56,56	1.64	10 (18%)

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
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
20	EDO	A	615	-	-	1/1/1/1	-
20	EDO	C	312	-	-	1/1/1/1	-
20	EDO	R	202	-	-	1/1/1/1	-
22	CHD	G	102	-	-	3/9/74/74	0/4/4/4
20	EDO	D	203	-	-	1/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
14	HEA	A	602[A]	18,1	3/3/7/16	6/32/76/76	-
22	CHD	J	101	-	-	4/9/74/74	0/4/4/4
25	DMU	C	310	-	-	4/13/33/59	0/1/1/2
20	EDO	C	315	-	-	1/1/1/1	-
22	CHD	W	101	10	-	8/9/74/74	0/4/4/4
20	EDO	T	103	-	-	0/1/1/1	-
22	CHD	C	306	-	-	6/9/74/74	0/4/4/4
20	EDO	F	106	-	-	0/1/1/1	-
25	DMU	P	307	-	-	8/19/59/59	0/2/2/2
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	O	304	-	-	1/1/1/1	-
27	PEK	C	307	-	-	27/56/56/56	-
20	EDO	A	610	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	A	608	-	-	7/55/55/55	-
14	HEA	N	603[A]	18,1	3/3/7/16	6/32/76/76	-
25	DMU	P	308	-	-	6/19/59/59	0/2/2/2
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	0/1/1/1	-
22	CHD	P	301	-	-	2/9/74/74	0/4/4/4
20	EDO	O	303	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
27	PEK	P	312	-	-	19/56/56/56	-
20	EDO	A	618	-	-	1/1/1/1	-
19	PGV	C	304	-	-	12/55/55/55	-
20	EDO	N	618	-	-	0/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
19	PGV	P	303	-	-	7/55/55/55	-
20	EDO	D	202	-	-	1/1/1/1	-
24	PSC	B	304	-	-	21/50/50/55	-
20	EDO	S	103	-	-	0/1/1/1	-
19	PGV	C	308	-	-	21/52/52/55	-
20	EDO	E	204	-	-	1/1/1/1	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	G	106	-	-	1/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
20	EDO	O	305	-	-	0/1/1/1	-
20	EDO	P	309	-	-	1/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
26	CDL	N	601	-	-	47/100/100/110	-
20	EDO	A	616	-	-	0/1/1/1	-
26	CDL	P	304	-	-	25/75/77/110	-
27	PEK	G	101	-	-	10/56/56/56	-
20	EDO	F	104	-	-	1/1/1/1	-
20	EDO	Q	203	-	-	0/1/1/1	-
19	PGV	G	104	-	-	28/55/55/55	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
21	TGL	B	301	-	-	30/65/65/65	-
14	HEA	A	602[B]	18,1	3/3/7/16	5/32/76/76	-
20	EDO	N	614	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	TGL	Q	201	-	-	30/65/65/65	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	C	318	-	-	1/1/1/1	-
27	PEK	T	101	-	-	21/51/51/56	-
14	HEA	A	601	1	3/3/7/16	4/32/76/76	-
20	EDO	H	101	-	-	1/1/1/1	-
25	DMU	P	306	-	-	7/19/59/59	0/2/2/2
14	HEA	N	603[B]	18,1	3/3/7/16	5/32/76/76	-
21	TGL	D	201	-	-	36/65/65/65	-
20	EDO	N	613	-	-	1/1/1/1	-
25	DMU	C	302	-	-	5/19/59/59	0/2/2/2
21	TGL	N	610	-	-	29/60/60/65	-
20	EDO	N	611	-	-	1/1/1/1	-
20	EDO	E	203	-	-	0/1/1/1	-
25	DMU	L	102	-	-	10/16/56/59	0/2/2/2
20	EDO	R	206	-	-	1/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
19	PGV	N	609	-	-	9/55/55/55	-
20	EDO	C	316	-	-	1/1/1/1	-
21	TGL	L	101	-	-	37/65/65/65	-
20	EDO	P	310	-	-	0/1/1/1	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
20	EDO	V	101	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	5/19/59/59	0/2/2/2
24	PSC	O	302	-	-	30/54/54/55	-
20	EDO	N	616	-	-	0/1/1/1	-
20	EDO	E	205	-	-	0/1/1/1	-
20	EDO	R	205	-	-	0/1/1/1	-
22	CHD	C	301	-	-	3/9/74/74	0/4/4/4
20	EDO	U	101	-	-	1/1/1/1	-
20	EDO	A	619	-	-	0/1/1/1	-
20	EDO	A	617	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	30/65/65/65	-
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	C	317	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PEK	C	319	-	-	28/47/47/56	-
20	EDO	F	105	-	-	1/1/1/1	-
20	EDO	A	611	-	-	1/1/1/1	-
14	HEA	N	602	1	3/3/7/16	7/32/76/76	-
22	CHD	P	305	-	-	5/9/74/74	0/4/4/4
26	CDL	C	305	-	-	51/91/91/110	-
20	EDO	D	204	-	-	1/1/1/1	-
25	DMU	C	309	-	-	8/19/59/59	0/2/2/2
27	PEK	G	103	-	-	23/47/47/56	-
20	EDO	D	205	-	-	0/1/1/1	-
20	EDO	G	105	-	-	1/1/1/1	-
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	S	101	-	-	1/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
19	PGV	N	619	-	-	23/55/55/55	-
20	EDO	R	204	-	-	0/1/1/1	-
26	CDL	T	102	-	-	52/104/104/110	-
19	PGV	A	609	-	-	21/55/55/55	-

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG3-CC1	7.63	1.55	1.33
21	L	101	TGL	OG2-CB1	7.07	1.54	1.34
21	B	301	TGL	OG2-CB1	5.54	1.49	1.34
19	C	308	PGV	O03-C19	5.51	1.49	1.33
21	Y	101	TGL	OG2-CB1	5.34	1.49	1.34
24	B	304	PSC	O01-C1	5.29	1.49	1.34
19	C	308	PGV	O01-C1	5.25	1.49	1.34
19	A	609	PGV	O01-C1	5.16	1.48	1.34
27	C	319	PEK	O03-C21	5.15	1.48	1.33
27	C	307	PEK	O03-C21	5.11	1.48	1.33
21	Y	101	TGL	OG3-CC1	5.11	1.48	1.33
26	N	601	CDL	OB6-CB5	5.09	1.48	1.34
26	T	102	CDL	OB6-CB5	5.07	1.48	1.34
19	N	619	PGV	O03-C19	5.03	1.48	1.33
14	A	601	HEA	CHD-C1D	5.01	1.47	1.35
26	N	601	CDL	OB8-CB7	5.01	1.48	1.33
26	C	305	CDL	OA8-CA7	5.00	1.48	1.33
21	D	201	TGL	OG1-CA1	4.99	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	102	CDL	OB8-CB7	4.96	1.47	1.33
21	N	610	TGL	OG2-CB1	4.94	1.48	1.34
26	C	305	CDL	OB8-CB7	4.93	1.47	1.33
19	G	104	PGV	O01-C1	4.93	1.48	1.34
14	A	602[B]	HEA	CHD-C1D	4.92	1.47	1.35
26	P	304	CDL	OA8-CA7	4.87	1.47	1.33
27	T	101	PEK	O03-C21	4.83	1.47	1.33
19	A	609	PGV	O03-C19	4.81	1.47	1.33
24	O	302	PSC	O01-C1	4.77	1.47	1.34
26	P	304	CDL	OB8-CB7	4.74	1.47	1.33
21	D	201	TGL	OB1-CB1	4.72	1.36	1.22
21	B	301	TGL	OG1-CA1	4.69	1.47	1.33
19	G	104	PGV	O03-C19	4.69	1.47	1.33
21	B	301	TGL	OG3-CC1	4.66	1.47	1.33
14	A	602[A]	HEA	CHD-C1D	4.66	1.46	1.35
27	G	103	PEK	O03-C21	4.65	1.46	1.33
26	T	102	CDL	OA8-CA7	4.63	1.46	1.33
27	G	103	PEK	O01-C1	4.60	1.47	1.34
21	N	610	TGL	OG1-CA1	4.60	1.46	1.33
26	P	304	CDL	OA6-CA5	4.58	1.47	1.34
26	N	601	CDL	OA8-CA7	4.53	1.46	1.33
21	N	610	TGL	OG3-CC1	4.50	1.46	1.33
14	A	602[A]	HEA	C4D-C3D	-4.47	1.37	1.45
27	T	101	PEK	O01-C1	4.43	1.46	1.34
26	C	305	CDL	OA6-CA5	4.43	1.46	1.34
21	L	101	TGL	OG1-CA1	4.39	1.46	1.33
21	Q	201	TGL	OG1-CA1	4.38	1.46	1.33
26	T	102	CDL	OA6-CA5	4.36	1.46	1.34
19	N	619	PGV	O01-C1	4.36	1.46	1.34
21	D	201	TGL	OG2-CB1	4.36	1.46	1.34
14	N	603[B]	HEA	C1D-ND	-4.36	1.32	1.40
27	C	307	PEK	O01-C1	4.32	1.46	1.34
26	N	601	CDL	OA6-CA5	4.28	1.46	1.34
27	C	319	PEK	O01-C1	4.25	1.46	1.34
21	Y	101	TGL	OG1-CA1	4.16	1.45	1.33
21	Q	201	TGL	OG3-CC1	4.08	1.45	1.33
21	Q	201	TGL	OG2-CB1	4.07	1.45	1.34
24	B	304	PSC	O03-C19	4.06	1.45	1.33
14	N	603[A]	HEA	C4D-C3D	-4.00	1.38	1.45
24	O	302	PSC	O03-C19	4.00	1.45	1.33
14	A	602[A]	HEA	CHC-C4B	3.95	1.45	1.35
26	P	304	CDL	OB6-CB5	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	HEA	CHC-C4B	3.88	1.44	1.35
24	O	302	PSC	C13-C12	3.88	1.54	1.31
14	A	601	HEA	C3A-C2A	-3.88	1.35	1.40
14	N	602	HEA	CHC-C4B	3.85	1.44	1.35
26	C	305	CDL	C79-C78	-3.79	1.30	1.51
24	B	304	PSC	C13-C12	3.75	1.53	1.31
14	N	603[A]	HEA	C4B-NB	-3.70	1.33	1.40
14	N	603[A]	HEA	CHD-C1D	3.60	1.44	1.35
21	D	201	TGL	OG3-CC1	3.55	1.43	1.33
14	A	601	HEA	CBD-CGD	3.52	1.58	1.50
26	C	305	CDL	C82-C81	-3.50	1.32	1.51
27	G	101	PEK	O03-C21	3.49	1.43	1.33
14	A	602[B]	HEA	CHC-C4B	3.47	1.43	1.35
26	C	305	CDL	C59-C58	-3.47	1.32	1.51
14	N	603[A]	HEA	CHC-C4B	3.46	1.43	1.35
26	C	305	CDL	OB6-CB5	3.42	1.43	1.34
26	N	601	CDL	C82-C81	-3.37	1.32	1.51
14	N	603[B]	HEA	CHD-C1D	3.34	1.43	1.35
14	N	602	HEA	CHD-C1D	3.33	1.43	1.35
14	A	602[A]	HEA	C4B-C3B	-3.30	1.39	1.44
22	B	302	CHD	C11-C12	3.29	1.58	1.53
26	P	304	CDL	C82-C81	-3.28	1.33	1.51
26	T	102	CDL	C59-C58	-3.27	1.33	1.51
26	N	601	CDL	C22-C21	-3.26	1.33	1.51
26	P	304	CDL	C19-C18	-3.26	1.33	1.51
14	N	603[B]	HEA	CHC-C4B	3.23	1.43	1.35
26	C	305	CDL	PA1-OA2	3.23	1.67	1.54
14	N	603[B]	HEA	C4B-C3B	-3.22	1.39	1.44
26	P	304	CDL	C22-C21	-3.22	1.33	1.51
14	A	601	HEA	C4B-C3B	-3.18	1.39	1.44
26	C	305	CDL	C62-C61	-3.18	1.33	1.51
14	N	603[B]	HEA	C4B-NB	-3.16	1.34	1.40
14	N	603[A]	HEA	C4B-C3B	-3.15	1.39	1.44
26	P	304	CDL	C59-C58	-3.14	1.33	1.51
26	N	601	CDL	C59-C58	-3.14	1.34	1.51
14	N	603[B]	HEA	FE-ND	3.13	2.12	1.96
26	N	601	CDL	C62-C61	-3.12	1.34	1.51
26	N	601	CDL	C42-C41	-3.11	1.34	1.51
14	N	603[B]	HEA	C4D-C3D	-3.10	1.39	1.45
26	T	102	CDL	C82-C81	-3.09	1.34	1.51
26	T	102	CDL	C42-C41	-3.08	1.34	1.51
26	P	304	CDL	C79-C78	-3.08	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	102	CDL	C39-C38	-3.07	1.34	1.51
26	T	102	CDL	C62-C61	-3.06	1.34	1.51
26	T	102	CDL	C22-C21	-3.06	1.34	1.51
21	L	101	TGL	CG3-CG2	3.06	1.60	1.50
26	N	601	CDL	C19-C18	-3.04	1.34	1.51
14	A	602[B]	HEA	C4B-NB	-3.03	1.35	1.40
26	C	305	CDL	C39-C38	-3.03	1.34	1.51
25	P	306	DMU	O16-C6	3.03	1.45	1.40
26	T	102	CDL	C19-C18	-3.03	1.34	1.51
14	A	601	HEA	C4D-C3D	-3.02	1.39	1.45
19	N	609	PGV	O03-C19	3.01	1.42	1.33
19	A	608	PGV	O03-C01	3.01	1.52	1.45
14	A	602[B]	HEA	C4B-C3B	-3.01	1.39	1.44
27	P	312	PEK	O03-C21	3.01	1.42	1.33
19	A	608	PGV	O01-C1	2.98	1.42	1.34
26	N	601	CDL	C39-C38	-2.94	1.35	1.51
14	N	602	HEA	CBD-CGD	2.93	1.57	1.50
26	C	305	CDL	C42-C41	-2.93	1.35	1.51
19	N	609	PGV	O01-C1	2.92	1.42	1.34
14	A	601	HEA	CBA-CGA	2.91	1.57	1.50
25	P	308	DMU	O16-C6	2.86	1.45	1.40
21	L	101	TGL	OG3-CG3	2.86	1.51	1.45
19	C	304	PGV	O01-C02	-2.80	1.39	1.46
26	P	304	CDL	PA1-OA2	2.76	1.65	1.54
14	N	603[A]	HEA	O11-C11	2.75	1.48	1.42
27	P	312	PEK	C2-C1	2.74	1.58	1.50
27	G	101	PEK	O01-C1	2.73	1.42	1.34
24	B	304	PSC	C2-C1	2.72	1.58	1.50
14	N	602	HEA	C4B-NB	-2.71	1.35	1.40
14	A	602[A]	HEA	C1D-C2D	-2.70	1.39	1.44
19	A	608	PGV	O03-C19	2.69	1.41	1.33
25	C	309	DMU	O16-C6	2.69	1.44	1.40
14	A	601	HEA	C3C-C2C	-2.68	1.36	1.40
14	A	601	HEA	CAD-C3D	2.65	1.58	1.51
14	N	603[B]	HEA	C1B-C2B	-2.60	1.39	1.44
26	N	601	CDL	C78-C79	-2.59	1.33	1.51
14	A	602[A]	HEA	O11-C11	2.59	1.48	1.42
22	W	101	CHD	C19-C10	2.54	1.58	1.54
14	A	602[A]	HEA	C1D-ND	-2.53	1.35	1.40
14	A	602[B]	HEA	C1D-ND	-2.53	1.35	1.40
26	C	305	CDL	C19-C18	-2.52	1.33	1.51
26	T	102	CDL	C78-C79	-2.49	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	O1A-CGA	2.48	1.30	1.22
14	N	603[A]	HEA	C1B-C2B	-2.47	1.39	1.44
14	A	602[B]	HEA	C4D-C3D	-2.46	1.40	1.45
14	N	603[A]	HEA	C1D-ND	-2.39	1.36	1.40
22	C	301	CHD	C11-C12	2.38	1.57	1.53
14	A	602[B]	HEA	C1B-C2B	-2.37	1.40	1.44
14	A	602[B]	HEA	C1B-NB	-2.36	1.33	1.38
22	B	302	CHD	C10-C9	-2.34	1.51	1.56
14	N	603[A]	HEA	C1D-C2D	-2.33	1.40	1.44
19	A	609	PGV	O02-C1	2.31	1.29	1.22
14	N	603[A]	HEA	C4D-ND	-2.30	1.34	1.38
19	C	304	PGV	O01-C1	2.30	1.40	1.34
21	Q	201	TGL	OB1-CB1	2.27	1.29	1.22
14	A	602[A]	HEA	C1B-NB	-2.25	1.34	1.38
27	T	101	PEK	P-O12	2.25	1.63	1.54
14	A	602[A]	HEA	C4B-NB	-2.24	1.36	1.40
27	P	312	PEK	C05-C04	2.22	1.59	1.50
14	A	601	HEA	C12-C11	-2.22	1.49	1.52
19	A	609	PGV	C2-C1	-2.18	1.44	1.50
19	P	303	PGV	O03-C19	2.17	1.39	1.33
19	N	609	PGV	O03-C01	2.15	1.50	1.45
14	A	601	HEA	C12-C13	2.14	1.60	1.53
14	N	602	HEA	C1D-ND	-2.13	1.36	1.40
14	N	602	HEA	C3A-CMA	2.13	1.51	1.46
19	C	308	PGV	C01-C02	2.13	1.57	1.50
22	C	301	CHD	O25-C24	2.13	1.29	1.22
19	P	303	PGV	O01-C1	2.12	1.40	1.34
26	C	305	CDL	PB2-OB2	2.11	1.63	1.54
22	J	101	CHD	C13-C14	-2.10	1.51	1.55
26	C	305	CDL	PB2-OB3	2.09	1.57	1.50
14	A	602[A]	HEA	C2A-C1A	-2.08	1.37	1.42
14	N	603[B]	HEA	C1D-C2D	-2.08	1.40	1.44
14	A	601	HEA	C1D-ND	-2.07	1.36	1.40
19	C	304	PGV	C03-C02	2.07	1.57	1.50
14	A	602[A]	HEA	C1B-C2B	-2.07	1.40	1.44
27	G	101	PEK	P-O13	-2.02	1.45	1.55
27	G	101	PEK	C05-C04	2.02	1.58	1.50
14	A	602[B]	HEA	CAA-C2A	2.02	1.55	1.52
14	N	603[B]	HEA	C4D-ND	-2.01	1.34	1.38
14	N	602	HEA	C4D-C3D	-2.01	1.41	1.45
14	A	601	HEA	CMB-C2B	2.00	1.55	1.50

All (477) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	312	PEK	C2-C3-C4	11.86	134.37	113.23
21	L	101	TGL	OG2-CB1-CB2	8.28	129.34	111.50
22	C	306	CHD	C23-C22-C20	-7.67	100.50	114.52
27	P	312	PEK	O01-C1-O02	-7.62	105.29	123.70
21	B	301	TGL	OG2-CB1-CB2	7.06	126.72	111.50
21	N	610	TGL	OG2-CB1-CB2	6.52	125.55	111.50
26	T	102	CDL	OB6-CB5-C51	6.45	125.40	111.50
14	N	602	HEA	C13-C14-C15	-6.35	112.36	127.66
21	Y	101	TGL	OG2-CB1-CB2	6.32	125.12	111.50
14	A	602[A]	HEA	OMA-CMA-C3A	-6.20	111.40	124.91
26	P	304	CDL	OA6-CA5-C11	6.10	124.64	111.50
22	W	101	CHD	C13-C17-C20	6.06	126.73	119.50
22	W	101	CHD	C11-C12-C13	6.05	117.46	111.24
27	C	319	PEK	O01-C1-C2	6.02	124.47	111.50
25	P	307	DMU	O16-C6-C1	5.92	117.55	108.30
19	G	104	PGV	O01-C1-C2	5.78	123.96	111.50
14	A	601	HEA	C13-C12-C11	-5.77	105.68	114.35
14	A	601	HEA	C3D-C4D-ND	5.69	115.87	110.36
19	A	609	PGV	O03-C19-C20	5.63	129.57	111.91
22	P	305	CHD	C13-C17-C20	-5.43	113.02	119.50
14	A	602[B]	HEA	C3D-C4D-ND	5.41	115.60	110.36
21	L	101	TGL	CG2-OG2-CB1	5.36	131.00	117.79
21	L	101	TGL	OG3-CG3-CG2	5.36	124.04	108.43
22	P	305	CHD	C23-C22-C20	-5.31	104.83	114.52
25	C	309	DMU	O16-C6-C1	5.28	116.55	108.30
27	G	103	PEK	O03-C21-C22	5.27	128.43	111.91
22	W	101	CHD	C14-C13-C12	5.25	112.29	107.40
22	W	101	CHD	C6-C5-C4	-5.17	105.23	111.19
27	T	101	PEK	O01-C1-C2	5.07	122.44	111.50
25	M	101	DMU	C18-O16-C6	-4.93	105.66	113.84
14	N	603[A]	HEA	C13-C12-C11	-4.93	106.95	114.35
19	G	104	PGV	O03-C19-C20	4.92	127.36	111.91
24	O	302	PSC	O01-C1-C2	4.91	122.09	111.50
14	A	601	HEA	C13-C14-C15	-4.91	115.84	127.66
14	A	602[A]	HEA	CHA-C4D-C3D	-4.91	117.62	124.84
26	T	102	CDL	OA6-CA5-C11	4.90	122.07	111.50
14	N	603[B]	HEA	OMA-CMA-C3A	-4.89	114.25	124.91
26	C	305	CDL	CB4-OB6-CB5	-4.87	105.80	117.79
14	A	602[B]	HEA	CBA-CAA-C2A	-4.86	104.42	112.60
22	C	306	CHD	C13-C17-C20	-4.82	113.74	119.50
27	C	307	PEK	O03-C21-C22	4.81	126.99	111.91
21	D	201	TGL	CB3-CB2-CB1	4.75	130.89	113.62
14	A	602[A]	HEA	CHA-C4D-ND	4.70	129.54	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	103	PEK	O01-C1-C2	4.65	121.52	111.50
26	N	601	CDL	OB6-CB5-C51	4.63	123.73	110.80
14	A	602[B]	HEA	CHA-C4D-C3D	-4.61	118.07	124.84
25	P	307	DMU	C10-O1-C9	-4.60	104.66	113.69
14	A	601	HEA	C4B-NB-C1B	-4.57	100.35	105.07
26	P	304	CDL	CA4-OA6-CA5	-4.56	106.55	117.79
21	D	201	TGL	OG2-CB1-CB2	-4.55	101.69	111.50
14	A	601	HEA	C17-C18-C19	-4.55	116.71	127.66
22	W	101	CHD	C11-C9-C10	-4.54	109.05	113.73
14	A	602[A]	HEA	C13-C12-C11	-4.50	107.59	114.35
25	P	307	DMU	C18-O16-C6	-4.47	106.43	113.84
25	C	309	DMU	O7-C10-C5	4.41	119.52	108.10
14	N	602	HEA	C12-C13-C14	4.35	123.73	112.23
25	P	307	DMU	O7-C10-C5	4.34	119.34	108.10
27	C	307	PEK	O03-C21-O04	-4.32	112.69	123.59
19	A	609	PGV	O03-C19-O04	-4.30	112.75	123.59
19	N	609	PGV	O03-C19-O04	-4.28	112.79	123.59
14	N	603[A]	HEA	CAD-CBD-CGD	-4.26	104.43	113.60
26	P	304	CDL	OB8-CB7-C71	4.24	125.21	111.91
25	L	102	DMU	O5-C4-C3	4.22	118.64	109.75
14	N	603[B]	HEA	C3D-C4D-ND	4.21	114.43	110.36
22	W	101	CHD	C22-C20-C17	4.21	118.98	110.28
26	P	304	CDL	OA8-CA7-C31	4.21	125.11	111.91
25	L	102	DMU	C10-O1-C9	4.20	121.94	113.69
25	C	302	DMU	O1-C9-C8	4.17	117.26	109.69
27	C	319	PEK	O03-C21-C22	4.14	124.91	111.91
22	C	301	CHD	C18-C13-C12	4.12	113.26	109.07
19	C	308	PGV	O03-C19-C20	4.10	124.78	111.91
14	N	603[A]	HEA	OMA-CMA-C3A	-4.09	116.00	124.91
22	P	301	CHD	C21-C20-C22	-4.07	103.98	110.36
26	C	305	CDL	C78-C77-C76	-4.06	93.81	114.42
19	A	609	PGV	C4-C3-C2	-4.04	98.67	113.19
14	A	602[B]	HEA	C27-C19-C20	4.03	122.06	115.27
26	C	305	CDL	OA6-CA5-C11	4.01	120.15	111.50
14	A	601	HEA	CAD-CBD-CGD	-4.01	104.97	113.60
22	C	301	CHD	C1-C2-C3	-3.97	105.37	110.47
24	B	304	PSC	O01-C1-C2	3.96	120.03	111.50
24	B	304	PSC	C03-C02-C01	-3.96	102.43	111.79
25	P	307	DMU	O7-C3-C4	-3.95	98.63	109.45
22	W	101	CHD	C17-C13-C14	-3.91	96.15	100.09
25	C	302	DMU	O1-C10-C5	-3.91	102.08	110.35
26	C	305	CDL	C81-C80-C79	-3.90	94.64	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	305	CHD	C16-C17-C20	3.90	118.18	112.15
22	W	101	CHD	C19-C10-C9	-3.88	105.84	111.18
14	N	603[B]	HEA	CMC-C2C-C3C	3.87	131.92	124.68
14	N	602	HEA	C2D-C1D-ND	3.87	114.42	109.84
25	C	302	DMU	C18-O16-C6	-3.86	107.43	113.84
21	B	301	TGL	OG2-CG2-CG3	3.86	122.39	108.40
27	C	307	PEK	O01-C1-C2	3.86	119.82	111.50
27	T	101	PEK	P-O11-C03	3.85	128.89	118.30
26	C	305	CDL	OB8-CB7-C71	3.84	123.96	111.91
25	C	309	DMU	C10-O1-C9	-3.84	106.16	113.69
14	A	601	HEA	C2B-C1B-NB	3.83	114.47	109.88
14	A	601	HEA	C20-C19-C18	3.81	128.82	121.12
14	N	602	HEA	C3D-C4D-ND	3.78	114.02	110.36
14	N	602	HEA	C2B-C1B-NB	3.77	114.40	109.88
22	W	101	CHD	C14-C8-C9	-3.76	104.55	109.71
27	T	101	PEK	O03-C21-C22	3.76	123.70	111.91
22	P	305	CHD	C14-C13-C12	3.75	110.89	107.40
19	N	609	PGV	O03-C19-C20	3.75	123.67	111.91
27	C	319	PEK	C02-O01-C1	-3.75	108.56	117.79
21	L	101	TGL	OC1-CC1-CC2	-3.69	109.34	123.73
14	N	603[A]	HEA	CHA-C4D-C3D	-3.68	119.43	124.84
19	A	609	PGV	C02-O01-C1	3.68	126.85	117.79
14	A	601	HEA	C1D-ND-C4D	-3.66	101.29	105.07
14	A	602[B]	HEA	CAD-C3D-C2D	3.66	134.69	127.88
19	A	609	PGV	O01-C1-O02	3.63	132.48	123.70
22	B	302	CHD	C19-C10-C1	-3.62	102.43	108.26
27	G	103	PEK	O03-C21-O04	-3.61	114.48	123.59
22	W	101	CHD	C19-C10-C5	3.61	116.49	110.36
26	T	102	CDL	CA4-OA6-CA5	-3.58	108.98	117.79
22	P	301	CHD	C22-C20-C17	-3.57	102.91	110.28
14	A	602[A]	HEA	CMB-C2B-C3B	-3.57	123.54	130.34
14	N	603[A]	HEA	CAD-C3D-C2D	3.55	134.50	127.88
25	L	102	DMU	O7-C10-C5	3.55	117.31	108.10
26	P	304	CDL	OB4-PB2-OB3	3.54	124.55	110.68
25	C	302	DMU	C7-C8-C9	3.52	116.53	110.24
26	P	304	CDL	OA6-CA5-OA7	-3.52	115.20	123.70
22	C	306	CHD	C15-C14-C13	3.51	106.99	103.55
14	N	603[B]	HEA	CMB-C2B-C1B	3.50	130.37	125.04
27	P	312	PEK	C14-C13-C12	-3.49	94.82	112.02
25	L	102	DMU	C8-C7-C5	-3.49	104.73	110.82
22	C	306	CHD	C22-C23-C24	-3.47	103.30	112.51
27	P	312	PEK	O01-C1-C2	3.46	118.97	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	307	PEK	P-O12-C04	-3.46	104.54	121.59
14	A	602[B]	HEA	CAA-CBA-CGA	-3.46	104.07	113.76
19	N	619	PGV	O03-C19-C20	3.45	122.75	111.91
22	J	101	CHD	C11-C9-C10	-3.45	110.17	113.73
19	C	308	PGV	O01-C1-C2	3.45	118.93	111.50
14	A	602[B]	HEA	CMB-C2B-C3B	-3.45	123.77	130.34
22	C	306	CHD	C21-C20-C17	3.44	118.19	112.92
22	C	301	CHD	C23-C22-C20	-3.44	108.24	114.52
14	N	603[B]	HEA	CMC-C2C-C1C	-3.42	123.22	128.46
21	L	101	TGL	CG3-OG3-CC1	3.41	129.74	117.12
14	N	602	HEA	O2A-CGA-CBA	3.41	124.98	114.03
14	N	603[B]	HEA	C27-C19-C20	3.40	120.99	115.27
22	B	302	CHD	C11-C9-C10	-3.39	110.23	113.73
27	T	101	PEK	O03-C21-O04	-3.39	115.04	123.59
26	C	305	CDL	OA8-CA7-C31	3.38	122.53	111.91
14	N	603[B]	HEA	C3B-C4B-NB	3.36	113.82	109.84
19	C	308	PGV	O03-C01-C02	3.36	118.20	108.43
27	T	101	PEK	C02-O01-C1	-3.35	109.55	117.79
26	P	304	CDL	OA2-PA1-OA5	3.35	115.64	106.73
22	C	306	CHD	C11-C9-C10	-3.34	110.28	113.73
14	N	602	HEA	C1D-ND-C4D	-3.33	101.63	105.07
22	W	101	CHD	C9-C11-C12	3.31	118.67	114.30
14	A	602[B]	HEA	CMB-C2B-C1B	3.31	130.07	125.04
21	Y	101	TGL	OG2-CB1-OB1	-3.29	115.75	123.70
25	L	102	DMU	O3-C5-C10	3.29	118.04	110.05
14	N	603[A]	HEA	C3D-C4D-ND	3.29	113.54	110.36
14	A	602[A]	HEA	CAD-CBD-CGD	-3.29	106.53	113.60
14	N	603[A]	HEA	CMC-C2C-C3C	3.29	130.83	124.68
14	A	602[A]	HEA	C26-C15-C16	3.28	120.78	115.27
25	M	101	DMU	O16-C6-C1	3.27	113.42	108.30
27	T	101	PEK	C2-C3-C4	-3.27	107.39	113.23
14	A	602[A]	HEA	C27-C19-C20	3.26	120.75	115.27
21	N	610	TGL	CG3-CG2-CG1	-3.25	104.10	111.79
14	N	603[B]	HEA	C2B-C1B-NB	3.25	113.78	109.88
14	A	602[A]	HEA	CAD-C3D-C2D	3.25	133.93	127.88
21	Q	201	TGL	OG1-CA1-CA2	3.22	122.01	111.91
14	N	602	HEA	C16-C17-C18	-3.21	101.32	111.88
26	C	305	CDL	C76-C75-C74	-3.21	98.12	114.42
22	C	301	CHD	C22-C20-C17	-3.21	103.66	110.28
14	A	602[A]	HEA	C12-C13-C14	-3.20	103.78	112.23
24	B	304	PSC	O01-C1-O02	-3.20	115.96	123.70
26	T	102	CDL	CB6-CB4-CB3	-3.20	104.22	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Y	101	TGL	OG3-CC1-CC2	3.19	121.91	111.91
25	P	307	DMU	O49-C1-C2	-3.18	103.00	110.35
21	L	101	TGL	OG1-CA1-CA2	3.17	121.85	111.91
14	N	603[B]	HEA	CMD-C2D-C1D	-3.17	120.22	125.04
27	P	312	PEK	O03-C21-C22	3.15	121.78	111.91
14	A	602[A]	HEA	CMB-C2B-C1B	3.13	129.81	125.04
26	T	102	CDL	OB6-CB4-CB3	3.13	119.74	108.40
14	A	602[B]	HEA	C1D-ND-C4D	-3.13	101.84	105.07
26	C	305	CDL	OB2-PB2-OB5	-3.12	98.44	106.73
26	C	305	CDL	OA2-PA1-OA5	3.11	115.02	106.73
22	B	302	CHD	C16-C17-C13	3.11	106.60	103.55
22	C	301	CHD	C5-C6-C7	3.11	117.89	114.46
21	N	610	TGL	OG3-CC1-CC2	3.09	121.62	111.91
14	A	601	HEA	CHA-C4D-ND	-3.09	121.08	124.43
25	C	302	DMU	C10-C5-C7	-3.08	103.58	110.00
21	N	610	TGL	OG1-CA1-CA2	3.07	121.54	111.91
14	N	602	HEA	CHB-C1B-C2B	-3.06	120.19	124.98
27	P	312	PEK	O02-C1-C2	3.06	135.68	123.73
22	C	306	CHD	C1-C10-C5	3.06	112.29	107.77
22	P	305	CHD	C17-C13-C12	-3.05	114.88	117.67
19	P	303	PGV	O01-C1-O02	-3.05	116.33	123.70
14	N	602	HEA	C3C-C4C-NC	3.05	113.15	109.21
14	N	603[B]	HEA	C4D-C3D-C2D	-3.03	102.48	106.90
22	C	306	CHD	C17-C13-C12	-3.03	114.90	117.67
14	N	603[B]	HEA	CAD-C3D-C2D	3.03	133.52	127.88
22	P	301	CHD	C18-C13-C17	-3.03	106.48	111.21
27	C	319	PEK	O01-C1-O02	-3.02	116.40	123.70
14	N	602	HEA	C17-C18-C19	-3.00	120.45	127.66
21	B	301	TGL	CG3-OG3-CC1	2.99	128.18	117.12
22	C	301	CHD	C5-C4-C3	-2.98	108.38	112.76
21	L	101	TGL	OB1-CB1-CB2	-2.97	112.15	123.73
21	Y	101	TGL	OG3-CC1-OC1	-2.95	116.15	123.59
14	N	603[A]	HEA	CAD-C3D-C4D	-2.94	119.52	124.66
22	C	301	CHD	C14-C13-C12	-2.94	104.67	107.40
22	C	301	CHD	C16-C17-C20	-2.94	107.60	112.15
14	A	602[B]	HEA	C2D-C1D-ND	2.93	113.31	109.84
14	N	602	HEA	OMA-CMA-C3A	-2.93	118.53	124.91
25	P	308	DMU	O16-C6-C1	2.92	112.87	108.30
27	C	319	PEK	O03-C01-C02	2.92	116.94	108.43
19	A	608	PGV	O03-C19-C20	2.92	121.08	111.91
14	A	601	HEA	O1A-CGA-CBA	-2.91	113.73	123.08
14	A	601	HEA	CAA-CBA-CGA	-2.91	105.60	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[B]	HEA	O2A-CGA-O1A	-2.91	116.05	123.30
14	N	603[B]	HEA	CMB-C2B-C3B	-2.91	124.80	130.34
26	T	102	CDL	C58-C57-C56	-2.90	99.69	114.42
14	A	601	HEA	C3C-C4C-NC	2.89	112.95	109.21
14	N	602	HEA	C27-C19-C18	-2.89	116.26	123.68
19	N	619	PGV	C01-O03-C19	2.89	127.82	117.12
26	N	601	CDL	CB6-OB8-CB7	2.89	127.81	117.12
25	L	102	DMU	C7-C8-C9	-2.88	105.11	110.24
14	N	602	HEA	C1B-C2B-C3B	-2.88	103.36	106.80
19	A	609	PGV	C3-C2-C1	2.87	124.07	113.62
22	C	301	CHD	C11-C9-C10	-2.87	110.77	113.73
25	C	309	DMU	C10-C5-C7	-2.86	104.04	110.00
22	W	101	CHD	C17-C13-C12	2.86	120.28	117.67
14	N	603[B]	HEA	C4B-NB-C1B	-2.86	102.12	105.07
21	L	101	TGL	OG2-CG2-CG3	2.85	118.73	108.40
19	G	104	PGV	C03-C02-C01	-2.84	105.06	111.79
14	N	603[B]	HEA	CAA-CBA-CGA	-2.84	105.81	113.76
21	L	101	TGL	OG3-CC1-CC2	2.83	120.80	111.91
14	A	601	HEA	C2D-C1D-ND	2.83	113.20	109.84
21	Q	201	TGL	CG2-OG2-CB1	-2.83	110.82	117.79
14	A	602[B]	HEA	C3B-C4B-NB	2.81	113.17	109.84
26	C	305	CDL	OB4-PB2-OB3	2.81	121.67	110.68
19	N	609	PGV	C03-C02-C01	-2.80	105.16	111.79
14	A	601	HEA	O2A-CGA-CBA	2.80	123.03	114.03
14	A	602[B]	HEA	O2A-CGA-CBA	2.78	122.96	114.03
14	N	603[B]	HEA	O2A-CGA-CBA	2.78	122.95	114.03
26	C	305	CDL	OA8-CA6-CA4	2.77	116.51	108.43
22	C	301	CHD	C21-C20-C22	-2.77	106.02	110.36
22	W	101	CHD	C9-C8-C7	2.77	115.19	111.88
22	B	302	CHD	C16-C17-C20	-2.77	107.86	112.15
14	N	602	HEA	O2D-CGD-CBD	2.77	122.92	114.03
26	C	305	CDL	OA5-PA1-OA3	-2.77	98.72	106.47
22	W	101	CHD	C14-C8-C7	2.76	115.47	111.81
19	G	104	PGV	O03-C01-C02	2.76	116.47	108.43
19	C	304	PGV	O03-C19-O04	-2.76	116.63	123.59
14	N	603[A]	HEA	CHB-C1B-C2B	-2.76	120.67	124.98
21	L	101	TGL	C20-CA9-CA8	-2.75	100.46	114.42
25	L	102	DMU	O16-C6-C1	-2.75	104.01	108.30
26	C	305	CDL	OB6-CB5-C51	2.74	117.40	111.50
25	L	102	DMU	O1-C10-C5	2.73	116.13	110.35
14	N	602	HEA	CHD-C1D-C2D	-2.73	119.17	126.72
19	A	608	PGV	O03-C19-O04	-2.72	116.72	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[A]	HEA	C2B-C1B-NB	2.71	113.13	109.88
19	N	609	PGV	O12-P-O13	2.71	119.65	109.07
26	N	601	CDL	OA6-CA5-C11	2.71	117.33	111.50
22	W	101	CHD	C10-C9-C8	2.70	114.72	111.82
25	L	102	DMU	O5-C6-O16	2.70	116.36	109.97
21	D	201	TGL	CC3-CC2-CC1	-2.70	103.81	113.62
14	N	603[A]	HEA	CAA-CBA-CGA	-2.69	106.21	113.76
22	P	305	CHD	C19-C10-C9	-2.69	107.48	111.18
25	C	302	DMU	C8-C7-C5	-2.69	106.13	110.82
22	P	305	CHD	O12-C12-C11	2.68	114.59	109.12
14	A	601	HEA	C4D-C3D-C2D	-2.68	102.99	106.90
21	B	301	TGL	OB1-CB1-CB2	-2.67	113.30	123.73
19	P	303	PGV	O03-C19-O04	-2.67	116.86	123.59
22	B	302	CHD	C6-C5-C4	-2.66	108.12	111.19
24	B	304	PSC	C04-C05-N	-2.66	106.89	115.78
27	G	101	PEK	C02-O01-C1	-2.65	111.26	117.79
26	P	304	CDL	OB8-CB7-OB9	-2.65	116.90	123.59
25	C	309	DMU	C18-O16-C6	-2.64	109.46	113.84
27	G	103	PEK	C02-O01-C1	-2.64	111.30	117.79
22	C	306	CHD	C14-C8-C9	-2.63	106.09	109.71
26	C	305	CDL	C42-C41-C40	2.63	127.80	114.42
27	G	101	PEK	C24-C23-C22	-2.63	103.72	113.19
14	A	601	HEA	C4D-CHA-C1A	2.63	126.03	122.56
14	N	602	HEA	CHA-C4D-ND	-2.62	121.59	124.43
22	C	306	CHD	C16-C17-C20	2.61	116.18	112.15
26	P	304	CDL	OA8-CA7-OA9	-2.60	117.03	123.59
21	L	101	TGL	C25-C24-C23	-2.60	101.23	114.42
27	C	307	PEK	O12-P-O14	-2.60	98.91	109.07
14	N	603[A]	HEA	C26-C15-C16	2.60	119.64	115.27
14	N	603[B]	HEA	CBA-CAA-C2A	-2.60	108.23	112.60
26	C	305	CDL	OB5-PB2-OB3	2.59	113.75	106.47
27	C	307	PEK	C2-C3-C4	2.58	117.83	113.23
26	N	601	CDL	O1-C1-CA2	-2.58	100.50	109.56
14	A	602[B]	HEA	C4A-CHB-C1B	2.58	125.97	122.56
14	N	603[B]	HEA	CHA-C4D-ND	-2.58	121.63	124.43
19	N	619	PGV	O01-C1-C2	2.57	117.03	111.50
14	N	603[B]	HEA	C4A-CHB-C1B	2.56	125.93	122.56
26	T	102	CDL	OB6-CB5-OB7	-2.55	117.54	123.70
14	N	602	HEA	CAD-CBD-CGD	-2.55	108.12	113.60
21	D	201	TGL	OG1-CA1-CA2	2.54	119.89	111.91
19	A	609	PGV	O12-P-O13	2.54	118.98	109.07
22	J	101	CHD	C13-C17-C20	-2.54	116.47	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603[B]	HEA	CMD-C2D-C3D	2.53	133.00	126.12
22	C	306	CHD	C14-C13-C12	2.53	109.76	107.40
25	C	309	DMU	O7-C10-O1	2.53	117.74	110.67
14	A	602[B]	HEA	C4D-C3D-C2D	-2.52	103.22	106.90
21	D	201	TGL	OG2-CB1-OB1	2.52	129.78	123.70
14	N	603[A]	HEA	CBD-CAD-C3D	2.51	119.61	112.63
26	P	304	CDL	OA6-CA4-CA3	2.51	117.49	108.40
21	L	101	TGL	C26-C25-C24	-2.50	101.71	114.42
26	N	601	CDL	C60-C59-C58	2.50	127.12	114.42
25	C	310	DMU	C18-O16-C6	-2.50	109.69	113.84
22	B	302	CHD	C2-C1-C10	-2.49	108.50	112.78
26	N	601	CDL	OA8-CA7-C31	2.49	119.73	111.91
14	N	602	HEA	C1D-C2D-C3D	-2.49	104.34	106.96
14	A	602[A]	HEA	CMC-C2C-C3C	2.49	129.33	124.68
26	C	305	CDL	CB6-CB4-CB3	2.49	117.67	111.79
21	Q	201	TGL	OG1-CA1-OA1	-2.49	117.32	123.59
26	C	305	CDL	C54-C53-C52	-2.48	101.82	114.42
22	C	306	CHD	C5-C6-C7	2.48	117.20	114.46
19	C	304	PGV	C21-C20-C19	-2.48	104.60	113.62
21	Y	101	TGL	CC3-CC2-CC1	2.48	122.63	113.62
27	G	103	PEK	C3-C4-C5	-2.47	98.25	112.43
25	Z	101	DMU	C10-O7-C3	-2.47	111.85	117.96
25	C	302	DMU	O3-C5-C10	2.47	116.05	110.05
14	A	602[A]	HEA	CAD-C3D-C4D	-2.47	120.34	124.66
27	C	307	PEK	O01-C1-O02	-2.47	117.74	123.70
14	N	602	HEA	O2A-CGA-O1A	-2.46	117.16	123.30
19	G	104	PGV	O03-C19-O04	-2.46	117.37	123.59
14	N	603[A]	HEA	CBA-CAA-C2A	-2.46	108.46	112.60
21	L	101	TGL	OG3-CC1-OC1	2.46	129.79	123.59
27	T	101	PEK	C11-C10-C9	-2.46	99.92	112.02
22	J	101	CHD	C17-C13-C14	2.45	102.56	100.09
26	N	601	CDL	C84-C83-C82	-2.45	101.98	114.42
22	G	102	CHD	C2-C1-C10	-2.45	108.58	112.78
14	A	602[B]	HEA	CMC-C2C-C3C	2.45	129.25	124.68
22	B	302	CHD	O12-C12-C13	-2.44	106.90	111.03
19	N	619	PGV	O03-C19-O04	-2.44	117.43	123.59
19	P	303	PGV	C22-C21-C20	-2.44	104.42	113.19
26	N	601	CDL	C81-C80-C79	-2.44	102.05	114.42
19	N	609	PGV	O01-C1-O02	-2.43	117.82	123.70
21	Y	101	TGL	CA4-CA3-CA2	-2.43	104.46	113.19
14	A	601	HEA	C12-C13-C14	2.43	118.64	112.23
27	G	103	PEK	C03-C02-C01	-2.42	106.06	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	306	DMU	O16-C18-C19	2.41	118.02	109.56
27	C	319	PEK	O13-P-O14	2.41	124.14	112.24
19	A	609	PGV	C01-O03-C19	2.41	126.03	117.12
21	B	301	TGL	OG3-CC1-OC1	-2.41	117.52	123.59
22	J	101	CHD	C1-C10-C5	2.40	111.32	107.77
14	N	602	HEA	C13-C12-C11	-2.40	110.75	114.35
22	G	102	CHD	C5-C4-C3	-2.40	109.24	112.76
22	W	101	CHD	C5-C4-C3	2.40	116.28	112.76
22	G	102	CHD	C4-C3-C2	-2.40	107.69	110.55
19	N	619	PGV	O14-P-O13	2.39	124.08	112.24
27	P	312	PEK	C3-C2-C1	-2.39	104.92	113.62
21	Y	101	TGL	CG3-CG2-CG1	-2.39	106.15	111.79
14	N	602	HEA	C27-C19-C20	2.38	119.28	115.27
14	A	602[A]	HEA	C3D-C4D-ND	2.38	112.66	110.36
14	A	602[A]	HEA	CHC-C4B-NB	2.38	127.32	124.38
19	C	308	PGV	C21-C20-C19	-2.37	105.00	113.62
22	C	301	CHD	C22-C23-C24	-2.37	106.22	112.51
26	T	102	CDL	OB8-CB7-C71	2.37	119.34	111.91
14	A	602[B]	HEA	C13-C12-C11	-2.37	110.79	114.35
19	N	609	PGV	C9-C10-C11	-2.36	98.91	112.43
26	T	102	CDL	OB8-CB6-CB4	2.35	115.28	108.43
19	N	619	PGV	C28-C27-C26	-2.35	102.51	114.42
22	P	301	CHD	C10-C9-C8	-2.35	109.30	111.82
22	J	101	CHD	C13-C14-C8	-2.35	111.74	114.74
27	G	103	PEK	O01-C1-O02	-2.34	118.05	123.70
26	T	102	CDL	OA8-CA7-C31	2.34	119.24	111.91
19	C	304	PGV	C30-C29-C28	-2.33	102.58	114.42
21	N	610	TGL	CG3-OG3-CC1	2.33	125.75	117.12
24	O	302	PSC	C28-C27-C26	-2.32	102.65	114.42
27	C	319	PEK	C03-C02-C01	2.32	117.27	111.79
19	G	104	PGV	C21-C20-C19	-2.32	105.19	113.62
14	A	601	HEA	C27-C19-C18	-2.31	117.74	123.68
22	P	305	CHD	C21-C20-C17	2.31	116.46	112.92
14	N	603[A]	HEA	CMC-C2C-C1C	-2.31	124.91	128.46
14	N	603[A]	HEA	O1A-CGA-CBA	-2.30	115.68	123.08
27	T	101	PEK	O01-C1-O02	-2.30	118.15	123.70
27	P	312	PEK	O03-C21-O04	-2.30	117.80	123.59
27	P	312	PEK	C03-C02-C01	-2.29	106.36	111.79
14	N	603[A]	HEA	CHA-C4D-ND	2.29	126.92	124.43
19	A	609	PGV	O02-C1-C2	-2.29	114.81	123.73
26	T	102	CDL	OA6-CA5-OA7	-2.28	118.18	123.70
26	P	304	CDL	CB4-OB6-CB5	-2.28	109.54	116.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	101	CHD	O7-C7-C8	2.28	114.52	109.43
14	N	603[A]	HEA	C2D-C1D-ND	2.28	112.54	109.84
14	A	601	HEA	CHB-C1B-NB	-2.28	121.96	124.43
19	N	609	PGV	O01-C02-C03	2.27	116.62	108.40
27	G	101	PEK	O11-P-O14	-2.27	100.21	109.07
14	A	602[B]	HEA	C3C-C4C-NC	2.26	112.14	109.21
22	B	302	CHD	C22-C20-C17	2.26	114.95	110.28
22	G	102	CHD	C23-C22-C20	-2.26	110.39	114.52
19	A	609	PGV	O14-P-O11	-2.26	97.25	107.75
19	C	304	PGV	O03-C01-C02	-2.26	101.86	108.43
22	C	301	CHD	C16-C17-C13	-2.25	101.34	103.55
22	W	101	CHD	C4-C5-C10	2.25	115.05	112.66
25	P	306	DMU	O16-C6-C1	2.25	111.82	108.30
21	Y	101	TGL	C20-CA9-CA8	-2.25	102.99	114.42
22	C	306	CHD	C4-C5-C10	2.25	115.05	112.66
14	N	603[A]	HEA	O2A-CGA-CBA	2.25	121.26	114.03
14	N	602	HEA	C4A-CHB-C1B	2.24	125.52	122.56
27	C	319	PEK	O03-C21-O04	-2.24	117.93	123.59
25	P	307	DMU	O5-C6-O16	-2.24	104.66	109.97
14	A	601	HEA	CBD-CAD-C3D	-2.24	106.40	112.63
22	P	301	CHD	C19-C10-C1	-2.24	104.66	108.26
25	L	102	DMU	O7-C3-C2	2.23	113.22	107.28
19	C	304	PGV	O03-C19-C20	2.23	118.90	111.91
21	L	101	TGL	CA4-CA3-CA2	-2.23	105.19	113.19
14	N	603[A]	HEA	CMB-C2B-C1B	2.23	128.43	125.04
25	C	302	DMU	O7-C10-C5	2.22	113.86	108.10
25	P	307	DMU	O5-C4-C57	2.22	111.96	106.44
22	B	302	CHD	C9-C11-C12	-2.22	111.37	114.30
21	N	610	TGL	OG1-CG1-CG2	2.22	114.89	108.43
22	G	102	CHD	C16-C17-C20	-2.21	108.72	112.15
21	Y	101	TGL	OG1-CA1-CA2	2.21	118.85	111.91
22	G	102	CHD	C6-C5-C4	-2.21	108.65	111.19
26	C	305	CDL	OB8-CB7-OB9	-2.21	118.03	123.59
25	M	101	DMU	C22-C19-C18	-2.20	103.72	113.49
22	P	301	CHD	C4-C5-C10	-2.20	110.32	112.66
21	N	610	TGL	OG2-CB1-OB1	-2.20	118.38	123.70
22	P	305	CHD	C14-C8-C9	-2.20	106.69	109.71
14	A	601	HEA	C20-C21-C22	-2.19	104.67	111.88
24	O	302	PSC	C29-C28-C27	-2.19	103.29	114.42
19	G	104	PGV	O04-C19-C20	-2.19	115.18	123.73
22	P	305	CHD	C14-C8-C7	-2.19	108.91	111.81
22	W	101	CHD	C4-C3-C2	-2.18	107.95	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	Q	201	TGL	OG3-CC1-CC2	2.18	118.75	111.91
21	L	101	TGL	OG2-CB1-OB1	-2.18	118.43	123.70
19	P	303	PGV	O12-P-O13	-2.18	100.55	109.07
14	N	603[A]	HEA	C1B-C2B-C3B	-2.18	104.20	106.80
14	A	601	HEA	C21-C20-C19	2.18	120.13	112.98
26	T	102	CDL	C52-C51-CB5	-2.17	105.72	113.62
27	G	101	PEK	C3-C2-C1	-2.16	105.76	113.62
26	C	305	CDL	OA6-CA4-CA3	2.15	116.20	108.40
14	A	602[A]	HEA	C13-C14-C15	-2.15	122.48	127.66
27	G	101	PEK	C27-C26-C25	-2.15	103.52	114.42
27	G	103	PEK	C01-O03-C21	2.15	125.07	117.12
26	C	305	CDL	OA8-CA7-OA9	-2.14	118.18	123.59
27	T	101	PEK	O13-P-O11	2.13	112.40	106.73
19	G	104	PGV	C02-O01-C1	-2.13	112.55	117.79
24	O	302	PSC	C26-C25-C24	-2.13	103.62	114.42
26	N	601	CDL	C82-C81-C80	2.13	125.22	114.42
26	P	304	CDL	OB5-PB2-OB2	-2.12	96.48	105.99
19	G	104	PGV	O01-C1-O02	-2.12	118.58	123.70
14	A	602[B]	HEA	C2B-C1B-NB	2.12	112.42	109.88
26	C	305	CDL	C82-C81-C80	2.11	125.14	114.42
25	P	307	DMU	C6-O5-C4	-2.11	109.56	113.69
27	G	103	PEK	O13-P-O14	2.10	122.63	112.24
22	C	306	CHD	O25-C24-C23	-2.10	116.34	123.08
21	Y	101	TGL	OG3-CG3-CG2	2.10	114.53	108.43
21	Q	201	TGL	OG2-CB1-CB2	-2.09	106.99	111.50
26	N	601	CDL	C19-C18-C17	2.09	125.03	114.42
25	C	309	DMU	C10-O7-C3	2.08	123.12	117.96
19	A	608	PGV	O01-C1-C2	2.08	115.99	111.50
19	C	304	PGV	O12-P-O13	-2.08	100.96	109.07
14	N	602	HEA	C25-C23-C24	-2.07	110.02	114.60
26	P	304	CDL	C22-C21-C20	2.07	124.94	114.42
19	G	104	PGV	O14-P-O13	2.07	122.45	112.24
21	Y	101	TGL	CG2-OG2-CB1	2.06	122.87	117.79
26	C	305	CDL	C58-C57-C56	-2.06	103.95	114.42
27	C	307	PEK	O01-C02-C01	2.06	115.85	108.40
22	P	305	CHD	O25-C24-C23	-2.05	116.48	123.08
25	P	307	DMU	C10-C5-C7	-2.05	105.72	110.00
27	C	307	PEK	C24-C23-C22	2.05	120.55	113.19
22	C	306	CHD	C13-C14-C8	-2.04	112.13	114.74
24	O	302	PSC	C21-C20-C19	-2.04	106.20	113.62
26	N	601	CDL	OA8-CA7-OA9	-2.04	118.44	123.59
19	P	303	PGV	C27-C26-C25	-2.03	104.11	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601	HEA	C17-C16-C15	-2.03	106.30	112.98
22	P	301	CHD	C18-C13-C12	2.03	111.13	109.07
19	C	304	PGV	O14-P-O13	2.03	122.26	112.24
21	B	301	TGL	OG1-CA1-CA2	2.03	118.26	111.91
14	N	603[A]	HEA	C3B-C4B-NB	2.03	112.24	109.84
25	L	102	DMU	O2-C8-C9	2.02	114.31	109.30
14	N	603[A]	HEA	CMD-C2D-C1D	2.02	128.11	125.04
25	C	309	DMU	O55-C2-C1	2.01	115.00	110.35
25	L	102	DMU	O55-C2-C3	2.01	115.27	109.94
26	T	102	CDL	CB6-OB8-CB7	2.01	124.56	117.12
22	G	102	CHD	C19-C10-C1	-2.01	105.03	108.26
22	C	306	CHD	O26-C24-O25	2.00	128.29	123.30
27	C	307	PEK	O13-P-O14	2.00	122.14	112.24
25	M	101	DMU	O3-C5-C10	-2.00	105.18	110.05

All (18) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	601	HEA	ND
14	A	601	HEA	NA
14	A	601	HEA	NB
14	A	602[A]	HEA	ND
14	A	602[A]	HEA	NA
14	A	602[A]	HEA	NB
14	A	602[B]	HEA	ND
14	A	602[B]	HEA	NA
14	A	602[B]	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB
14	N	603[A]	HEA	ND
14	N	603[A]	HEA	NA
14	N	603[A]	HEA	NB
14	N	603[B]	HEA	ND
14	N	603[B]	HEA	NA
14	N	603[B]	HEA	NB

All (824) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	602[B]	HEA	C4D-C3D-CAD-CBD
14	N	603[B]	HEA	C4D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
19	A	609	PGV	C04-C05-C06-O06
19	A	609	PGV	O05-C05-C06-O06
19	A	609	PGV	C2-C1-O01-C02
19	C	308	PGV	C03-O11-P-O14
19	C	308	PGV	C04-O12-P-O14
19	C	308	PGV	O12-C04-C05-O05
19	G	104	PGV	C03-O11-P-O12
19	G	104	PGV	C03-O11-P-O13
19	G	104	PGV	C03-O11-P-O14
19	G	104	PGV	C04-O12-P-O14
19	N	619	PGV	C04-O12-P-O14
19	N	619	PGV	O02-C1-O01-C02
19	N	619	PGV	C2-C1-O01-C02
19	N	619	PGV	O04-C19-O03-C01
19	N	619	PGV	C20-C19-O03-C01
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	L	101	TGL	CC2-CC1-OG3-CG3
21	L	101	TGL	OC1-CC1-OG3-CG3
21	Y	101	TGL	CB2-CB1-OG2-CG2
21	Y	101	TGL	OB1-CB1-OG2-CG2
22	P	305	CHD	C20-C22-C23-C24
22	W	101	CHD	C13-C17-C20-C21
22	W	101	CHD	C13-C17-C20-C22
22	W	101	CHD	C16-C17-C20-C21
22	W	101	CHD	C16-C17-C20-C22
24	B	304	PSC	C03-O11-P-O12
24	B	304	PSC	C04-O12-P-O13
24	B	304	PSC	O12-C04-C05-N
24	O	302	PSC	C03-O11-P-O12
24	O	302	PSC	C04-O12-P-O14
24	O	302	PSC	C2-C1-O01-C02
25	C	302	DMU	C19-C18-O16-C6
25	L	102	DMU	C1-C6-O16-C18
25	L	102	DMU	O5-C6-O16-C18
25	P	306	DMU	O5-C6-O16-C18
25	P	308	DMU	O5-C6-O16-C18
26	C	305	CDL	CA3-OA5-PA1-OA3
26	C	305	CDL	OA7-CA5-OA6-CA4
26	C	305	CDL	C11-CA5-OA6-CA4
26	C	305	CDL	CB3-OB5-PB2-OB2
26	N	601	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
26	N	601	CDL	OB6-CB4-CB6-OB8
26	P	304	CDL	CB2-OB2-PB2-OB3
26	T	102	CDL	CA2-OA2-PA1-OA3
26	T	102	CDL	CA3-OA5-PA1-OA3
26	T	102	CDL	CB2-OB2-PB2-OB3
26	T	102	CDL	CB2-OB2-PB2-OB4
26	T	102	CDL	CB3-OB5-PB2-OB3
27	C	307	PEK	C03-O11-P-O13
27	C	307	PEK	C2-C1-O01-C02
27	C	307	PEK	C4-C5-C6-C7
27	C	319	PEK	C03-O11-P-O13
27	C	319	PEK	C03-O11-P-O14
27	C	319	PEK	C04-O12-P-O11
27	C	319	PEK	C04-O12-P-O13
27	C	319	PEK	C04-O12-P-O14
27	C	319	PEK	C2-C1-O01-C02
27	C	319	PEK	C11-C10-C9-C8
27	G	103	PEK	C03-O11-P-O12
27	G	103	PEK	C03-O11-P-O13
27	G	103	PEK	C03-O11-P-O14
27	G	103	PEK	C2-C1-O01-C02
27	G	103	PEK	C7-C8-C9-C10
27	P	312	PEK	C9-C10-C11-C12
27	P	312	PEK	C12-C13-C14-C15
21	D	201	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	OC1-CC1-OG3-CG3
24	B	304	PSC	O04-C19-O03-C01
26	T	102	CDL	OA9-CA7-OA8-CA6
27	G	103	PEK	O04-C21-O03-C01
25	C	309	DMU	C5-C10-O7-C3
25	L	102	DMU	C2-C3-O7-C10
21	D	201	TGL	CC2-CC1-OG3-CG3
21	Q	201	TGL	CC2-CC1-OG3-CG3
26	T	102	CDL	C31-CA7-OA8-CA6
27	G	103	PEK	C22-C21-O03-C01
19	A	609	PGV	O04-C19-O03-C01
24	O	302	PSC	O04-C19-O03-C01
26	C	305	CDL	OA9-CA7-OA8-CA6
26	N	601	CDL	OA9-CA7-OA8-CA6
27	C	319	PEK	O04-C21-O03-C01
25	P	307	DMU	C5-C10-O7-C3
24	O	302	PSC	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
27	C	307	PEK	O02-C1-O01-C02
27	C	319	PEK	O02-C1-O01-C02
27	G	103	PEK	O02-C1-O01-C02
21	D	201	TGL	CG2-CG1-OG1-CA1
19	A	609	PGV	C20-C19-O03-C01
24	O	302	PSC	C20-C19-O03-C01
26	N	601	CDL	C31-CA7-OA8-CA6
27	C	307	PEK	C22-C21-O03-C01
27	C	319	PEK	C22-C21-O03-C01
14	A	602[B]	HEA	C2D-C3D-CAD-CBD
14	N	603[B]	HEA	C2D-C3D-CAD-CBD
22	C	306	CHD	C20-C22-C23-C24
26	C	305	CDL	C80-C81-C82-C83
21	B	301	TGL	CC2-CC1-OG3-CG3
21	Y	101	TGL	CA2-CA1-OG1-CG1
24	B	304	PSC	C20-C19-O03-C01
26	C	305	CDL	C31-CA7-OA8-CA6
19	N	619	PGV	C10-C11-C12-C13
24	O	302	PSC	C11-C10-C9-C8
24	O	302	PSC	C11-C12-C13-C14
27	G	101	PEK	C10-C11-C12-C13
27	G	101	PEK	C13-C14-C15-C16
27	P	312	PEK	C4-C5-C6-C7
21	B	301	TGL	C21-C20-CA9-CA8
26	T	102	CDL	C42-C43-C44-C45
19	A	609	PGV	O02-C1-O01-C02
27	C	307	PEK	O04-C21-O03-C01
21	L	101	TGL	CA9-C20-C21-C22
24	O	302	PSC	C29-C30-C31-C32
26	T	102	CDL	C60-C61-C62-C63
22	P	305	CHD	C17-C20-C22-C23
22	W	101	CHD	C17-C20-C22-C23
19	A	609	PGV	C20-C21-C22-C23
21	Y	101	TGL	OA1-CA1-OG1-CG1
21	B	301	TGL	OC1-CC1-OG3-CG3
14	A	601	HEA	C15-C16-C17-C18
21	D	201	TGL	C21-C22-C23-C24
19	A	609	PGV	C10-C11-C12-C13
26	P	304	CDL	OA9-CA7-OA8-CA6
24	O	302	PSC	C04-C05-N-C06
26	P	304	CDL	C31-CA7-OA8-CA6
26	P	304	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	C22-C21-O03-C01
26	C	305	CDL	CB5-C51-C52-C53
24	O	302	PSC	C20-C21-C22-C23
22	P	305	CHD	C21-C20-C22-C23
21	B	301	TGL	CB1-CB2-CB3-CB4
26	P	304	CDL	CB5-C51-C52-C53
25	P	308	DMU	C1-C6-O16-C18
26	N	601	CDL	OA7-CA5-OA6-CA4
21	B	301	TGL	CA2-CA1-OG1-CG1
21	B	301	TGL	CA1-CA2-CA3-CA4
19	P	303	PGV	C10-C11-C12-C13
27	T	101	PEK	C4-C5-C6-C7
21	D	201	TGL	CB1-CB2-CB3-CB4
21	N	610	TGL	CC1-CC2-CC3-CC4
26	T	102	CDL	CA7-C31-C32-C33
27	P	312	PEK	C1-C2-C3-C4
22	C	306	CHD	C17-C20-C22-C23
25	C	302	DMU	O6-C11-C9-O1
25	L	102	DMU	O5-C4-C57-O61
24	O	302	PSC	C04-C05-N-C08
21	D	201	TGL	CA1-CA2-CA3-CA4
26	N	601	CDL	C11-CA5-OA6-CA4
25	P	308	DMU	O16-C18-C19-C22
26	P	304	CDL	OB7-CB5-OB6-CB4
27	T	101	PEK	O04-C21-O03-C01
26	N	601	CDL	CA5-C11-C12-C13
27	T	101	PEK	O02-C1-O01-C02
19	G	104	PGV	O04-C19-O03-C01
26	C	305	CDL	CA5-C11-C12-C13
27	P	312	PEK	C13-C14-C15-C16
27	T	101	PEK	C10-C11-C12-C13
22	C	306	CHD	C21-C20-C22-C23
21	B	301	TGL	OA1-CA1-OG1-CG1
26	C	305	CDL	C51-CB5-OB6-CB4
25	L	102	DMU	O16-C18-C19-C22
19	C	308	PGV	C04-O12-P-O11
19	N	619	PGV	C04-O12-P-O11
24	B	304	PSC	C04-O12-P-O11
26	T	102	CDL	CA2-OA2-PA1-OA5
26	T	102	CDL	CB2-OB2-PB2-OB5
26	T	102	CDL	CB3-OB5-PB2-OB2
27	C	307	PEK	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
27	C	307	PEK	C04-O12-P-O11
27	C	319	PEK	C03-O11-P-O12
27	G	103	PEK	C21-C22-C23-C24
26	C	305	CDL	OB7-CB5-OB6-CB4
19	G	104	PGV	C20-C19-O03-C01
21	D	201	TGL	CA2-CA1-OG1-CG1
21	L	101	TGL	CA2-CA1-OG1-CG1
21	N	610	TGL	CC2-CC1-OG3-CG3
26	P	304	CDL	C82-C83-C84-C85
21	N	610	TGL	CB7-CB8-CB9-C10
25	C	310	DMU	C19-C22-C25-C28
25	P	307	DMU	C19-C22-C25-C28
26	C	305	CDL	C43-C44-C45-C46
21	N	610	TGL	CB2-CB1-OG2-CG2
27	T	101	PEK	C2-C1-O01-C02
22	J	101	CHD	C17-C20-C22-C23
19	C	304	PGV	C7-C8-C9-C10
19	G	104	PGV	C13-C14-C15-C16
19	P	303	PGV	C7-C8-C9-C10
21	B	301	TGL	CA4-CA5-CA6-CA7
21	Y	101	TGL	CA5-CA6-CA7-CA8
21	Y	101	TGL	CB5-CB6-CB7-CB8
26	C	305	CDL	C58-C59-C60-C61
21	Q	201	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	CB6-CB7-CB8-CB9
26	P	304	CDL	C77-C78-C79-C80
26	T	102	CDL	C14-C15-C16-C17
21	B	301	TGL	OB1-CB1-OG2-CG2
21	N	610	TGL	OB1-CB1-OG2-CG2
26	C	305	CDL	CA7-C31-C32-C33
19	C	308	PGV	C13-C14-C15-C16
21	B	301	TGL	C23-C24-C25-C26
21	Q	201	TGL	C10-C11-C12-C13
26	C	305	CDL	C38-C39-C40-C41
26	T	102	CDL	C1-CB2-OB2-PB2
25	L	102	DMU	O6-C11-C9-O1
21	D	201	TGL	C17-C18-C19-C33
21	Q	201	TGL	CC9-C15-C16-C17
21	Y	101	TGL	CA2-CA3-CA4-CA5
25	L	102	DMU	C19-C22-C25-C28
26	P	304	CDL	C58-C59-C60-C61
26	T	102	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
25	Z	101	DMU	O16-C18-C19-C22
26	C	305	CDL	C78-C79-C80-C81
26	P	304	CDL	C81-C82-C83-C84
22	W	101	CHD	C21-C20-C22-C23
25	P	306	DMU	C1-C6-O16-C18
21	D	201	TGL	CC5-CC6-CC7-CC8
21	N	610	TGL	CB6-CB7-CB8-CB9
21	Q	201	TGL	CB4-CB5-CB6-CB7
21	Q	201	TGL	C19-C33-C34-C35
21	Y	101	TGL	CA3-CA4-CA5-CA6
21	Y	101	TGL	CB3-CB4-CB5-CB6
26	C	305	CDL	C41-C42-C43-C44
26	N	601	CDL	C61-C62-C63-C64
26	T	102	CDL	C61-C62-C63-C64
21	N	610	TGL	OC1-CC1-OG3-CG3
21	L	101	TGL	CA3-CA4-CA5-CA6
26	C	305	CDL	C36-C37-C38-C39
19	C	308	PGV	C28-C29-C30-C31
25	M	101	DMU	C19-C22-C25-C28
21	B	301	TGL	C12-C13-C14-C29
26	C	305	CDL	C82-C83-C84-C85
26	N	601	CDL	C11-C12-C13-C14
19	G	104	PGV	C04-C05-C06-O06
21	L	101	TGL	C12-C13-C14-C29
26	C	305	CDL	C42-C43-C44-C45
26	N	601	CDL	C42-C43-C44-C45
27	C	307	PEK	C25-C26-C27-C28
21	B	301	TGL	C20-C21-C22-C23
21	D	201	TGL	C18-C19-C33-C34
21	Q	201	TGL	CA2-CA3-CA4-CA5
21	Q	201	TGL	C22-C23-C24-C25
25	C	310	DMU	C22-C25-C28-C31
25	M	101	DMU	C28-C31-C34-C37
26	C	305	CDL	C57-C58-C59-C60
26	N	601	CDL	C14-C15-C16-C17
26	N	601	CDL	C35-C36-C37-C38
26	P	304	CDL	C57-C58-C59-C60
21	L	101	TGL	CC6-CC7-CC8-CC9
21	Q	201	TGL	CA6-CA7-CA8-CA9
26	N	601	CDL	C31-C32-C33-C34
21	N	610	TGL	CC9-C15-C16-C17
25	C	302	DMU	C19-C22-C25-C28

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Mol	Chain	Res	Type	Atoms
25	P	308	DMU	C19-C22-C25-C28
26	T	102	CDL	C56-C57-C58-C59
27	G	101	PEK	C34-C35-C36-C37
27	G	103	PEK	C24-C25-C26-C27
19	C	304	PGV	C14-C15-C16-C17
26	N	601	CDL	C80-C81-C82-C83
19	C	304	PGV	C20-C21-C22-C23
21	B	301	TGL	CA2-CA3-CA4-CA5
21	B	301	TGL	C24-C25-C26-C27
21	L	101	TGL	C21-C20-CA9-CA8
21	N	610	TGL	C16-C15-CC9-CC8
24	O	302	PSC	C25-C26-C27-C28
26	T	102	CDL	C59-C60-C61-C62
25	L	102	DMU	C3-C4-C57-O61
21	D	201	TGL	C21-C20-CA9-CA8
21	N	610	TGL	CC6-CC7-CC8-CC9
26	C	305	CDL	C76-C77-C78-C79
26	C	305	CDL	C79-C80-C81-C82
26	N	601	CDL	C81-C82-C83-C84
26	T	102	CDL	C52-C53-C54-C55
25	C	302	DMU	C18-C19-C22-C25
21	B	301	TGL	C10-C11-C12-C13
21	L	101	TGL	CB3-CB4-CB5-CB6
26	N	601	CDL	C78-C79-C80-C81
21	D	201	TGL	OA1-CA1-OG1-CG1
21	B	301	TGL	CB2-CB1-OG2-CG2
21	D	201	TGL	CB2-CB1-OG2-CG2
21	Q	201	TGL	CB2-CB1-OG2-CG2
26	T	102	CDL	C11-CA5-OA6-CA4
26	C	305	CDL	C72-C73-C74-C75
19	C	308	PGV	C6-C7-C8-C9
19	N	619	PGV	C11-C10-C9-C8
21	L	101	TGL	OA1-CA1-OG1-CG1
21	Q	201	TGL	C17-C18-C19-C33
26	N	601	CDL	C60-C61-C62-C63
24	O	302	PSC	C3-C4-C5-C6
26	T	102	CDL	C34-C35-C36-C37
21	D	201	TGL	OB1-CB1-OG2-CG2
21	Q	201	TGL	OB1-CB1-OG2-CG2
26	T	102	CDL	OB7-CB5-OB6-CB4
25	P	306	DMU	O6-C11-C9-C8
26	N	601	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	O	302	PSC	C04-C05-N-C07
20	A	610	EDO	O1-C1-C2-O2
20	C	315	EDO	O1-C1-C2-O2
20	C	317	EDO	O1-C1-C2-O2
20	D	204	EDO	O1-C1-C2-O2
20	O	304	EDO	O1-C1-C2-O2
19	N	619	PGV	C24-C25-C26-C27
21	Q	201	TGL	CC5-CC6-CC7-CC8
26	C	305	CDL	C73-C74-C75-C76
24	B	304	PSC	C2-C1-O01-C02
21	D	201	TGL	C11-C10-CB9-CB8
26	T	102	CDL	C80-C81-C82-C83
21	Y	101	TGL	CC1-CC2-CC3-CC4
27	C	319	PEK	C21-C22-C23-C24
21	Y	101	TGL	C10-C11-C12-C13
26	P	304	CDL	OB6-CB4-CB6-OB8
21	L	101	TGL	CB7-CB8-CB9-C10
21	L	101	TGL	C10-C11-C12-C13
24	B	304	PSC	C11-C10-C9-C8
27	C	319	PEK	C10-C11-C12-C13
21	Y	101	TGL	C11-C12-C13-C14
27	P	312	PEK	C16-C17-C18-C19
19	N	619	PGV	C12-C13-C14-C15
19	C	308	PGV	O02-C1-O01-C02
26	T	102	CDL	OA7-CA5-OA6-CA4
19	N	609	PGV	C30-C31-C32-C33
21	L	101	TGL	C20-C21-C22-C23
26	T	102	CDL	C13-C14-C15-C16
27	G	101	PEK	C26-C27-C28-C29
19	G	104	PGV	C6-C7-C8-C9
21	N	610	TGL	C13-C14-C29-C30
21	Q	201	TGL	CB9-C10-C11-C12
21	Q	201	TGL	C20-C21-C22-C23
27	C	319	PEK	C22-C23-C24-C25
27	G	101	PEK	C16-C17-C18-C19
19	C	304	PGV	C24-C25-C26-C27
21	Y	101	TGL	CC4-CC5-CC6-CC7
24	O	302	PSC	C23-C24-C25-C26
19	C	308	PGV	C2-C1-O01-C02
26	T	102	CDL	C51-CB5-OB6-CB4
27	P	312	PEK	C26-C27-C28-C29
21	B	301	TGL	CB9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	N	601	CDL	C59-C60-C61-C62
24	B	304	PSC	O02-C1-O01-C02
19	C	308	PGV	C23-C24-C25-C26
21	Y	101	TGL	C21-C20-CA9-CA8
26	T	102	CDL	OB6-CB4-CB6-OB8
21	Y	101	TGL	CC3-CC4-CC5-CC6
24	O	302	PSC	C24-C25-C26-C27
25	Z	101	DMU	C25-C28-C31-C34
19	C	304	PGV	C12-C13-C14-C15
19	C	308	PGV	C12-C13-C14-C15
21	Y	101	TGL	C18-C19-C33-C34
25	Z	101	DMU	C28-C31-C34-C37
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
14	N	603[A]	HEA	C4D-C3D-CAD-CBD
21	D	201	TGL	C16-C17-C18-C19
21	N	610	TGL	C11-C10-CB9-CB8
25	P	308	DMU	C22-C25-C28-C31
27	C	307	PEK	C16-C17-C18-C19
21	B	301	TGL	CB4-CB5-CB6-CB7
19	N	619	PGV	C19-C20-C21-C22
25	P	307	DMU	O6-C11-C9-O1
26	N	601	CDL	C43-C44-C45-C46
27	T	101	PEK	C1-C2-C3-C4
25	C	309	DMU	C19-C22-C25-C28
21	Q	201	TGL	C12-C13-C14-C29
24	O	302	PSC	C26-C27-C28-C29
19	N	609	PGV	C31-C32-C33-C34
21	Y	101	TGL	CC5-CC6-CC7-CC8
26	T	102	CDL	C16-C17-C18-C19
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
14	N	603[A]	HEA	C2D-C3D-CAD-CBD
19	G	104	PGV	O03-C01-C02-C03
21	D	201	TGL	CG1-CG2-CG3-OG3
26	T	102	CDL	CB3-CB4-CB6-OB8
27	C	307	PEK	O03-C01-C02-C03
27	C	307	PEK	C10-C11-C12-C13
27	G	103	PEK	C4-C5-C6-C7
19	A	608	PGV	C31-C32-C33-C34
21	N	610	TGL	CA3-CA4-CA5-CA6
26	T	102	CDL	C77-C78-C79-C80
19	G	104	PGV	O05-C05-C06-O06
27	P	312	PEK	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	D	201	TGL	CC6-CC7-CC8-CC9
21	L	101	TGL	C25-C26-C27-C28
26	C	305	CDL	C37-C38-C39-C40
19	G	104	PGV	C31-C32-C33-C34
21	B	301	TGL	CA7-CA8-CA9-C20
21	B	301	TGL	CC6-CC7-CC8-CC9
21	L	101	TGL	C11-C12-C13-C14
21	N	610	TGL	CB1-CB2-CB3-CB4
26	T	102	CDL	CB5-C51-C52-C53
27	C	307	PEK	C35-C36-C37-C38
21	L	101	TGL	C11-C10-CB9-CB8
21	N	610	TGL	CA9-C20-C21-C22
24	O	302	PSC	C03-C02-O01-C1
26	N	601	CDL	OB7-CB5-OB6-CB4
19	C	304	PGV	C27-C28-C29-C30
26	C	305	CDL	CB3-OB5-PB2-OB3
19	A	609	PGV	C21-C22-C23-C24
26	C	305	CDL	OB5-CB3-CB4-OB6
26	T	102	CDL	OA5-CA3-CA4-OA6
27	C	307	PEK	C13-C14-C15-C16
27	P	312	PEK	C10-C11-C12-C13
24	B	304	PSC	C4-C5-C6-C7
20	G	105	EDO	O1-C1-C2-O2
24	O	302	PSC	C1-C2-C3-C4
19	C	304	PGV	C28-C29-C30-C31
25	C	309	DMU	O16-C18-C19-C22
21	L	101	TGL	OG2-CG2-CG3-OG3
26	C	305	CDL	OB6-CB4-CB6-OB8
21	D	201	TGL	C20-C21-C22-C23
25	Z	101	DMU	C19-C22-C25-C28
21	L	101	TGL	CC2-CC3-CC4-CC5
26	N	601	CDL	C18-C19-C20-C21
25	C	309	DMU	C25-C28-C31-C34
25	C	310	DMU	C18-C19-C22-C25
21	Y	101	TGL	C12-C13-C14-C29
21	D	201	TGL	CC2-CC3-CC4-CC5
21	Q	201	TGL	CB5-CB6-CB7-CB8
21	Y	101	TGL	C29-C30-C31-C32
27	G	101	PEK	C4-C5-C6-C7
27	G	101	PEK	C7-C8-C9-C10
21	Y	101	TGL	CA1-CA2-CA3-CA4
27	G	103	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
21	N	610	TGL	CC4-CC5-CC6-CC7
19	N	619	PGV	C01-C02-C03-O11
26	N	601	CDL	OB5-CB3-CB4-CB6
27	C	319	PEK	C01-C02-C03-O11
21	Q	201	TGL	C16-C17-C18-C19
19	C	304	PGV	C1-C2-C3-C4
19	P	303	PGV	C24-C25-C26-C27
21	B	301	TGL	CA3-CA4-CA5-CA6
21	D	201	TGL	C13-C14-C29-C30
25	M	101	DMU	C31-C34-C37-C40
26	N	601	CDL	C20-C21-C22-C23
21	D	201	TGL	C10-C11-C12-C13
26	C	305	CDL	C71-CB7-OB8-CB6
19	A	609	PGV	O03-C01-C02-C03
21	B	301	TGL	OG1-CG1-CG2-CG3
24	O	302	PSC	O03-C01-C02-C03
26	N	601	CDL	CB3-CB4-CB6-OB8
19	C	304	PGV	C10-C11-C12-C13
21	D	201	TGL	CA7-CA8-CA9-C20
26	C	305	CDL	C61-C62-C63-C64
21	B	301	TGL	CA9-C20-C21-C22
19	G	104	PGV	C04-O12-P-O11
24	B	304	PSC	C9-C10-C11-C12
24	B	304	PSC	C10-C11-C12-C13
24	O	302	PSC	C9-C10-C11-C12
27	C	307	PEK	C5-C6-C7-C8
27	C	307	PEK	C6-C7-C8-C9
27	C	307	PEK	C9-C10-C11-C12
27	C	307	PEK	C11-C12-C13-C14
27	C	307	PEK	C12-C13-C14-C15
27	C	319	PEK	C6-C7-C8-C9
27	C	319	PEK	C9-C10-C11-C12
27	C	319	PEK	C12-C13-C14-C15
27	G	101	PEK	C11-C10-C9-C8
27	G	103	PEK	C6-C7-C8-C9
27	G	103	PEK	C11-C10-C9-C8
27	G	103	PEK	C11-C12-C13-C14
27	G	103	PEK	C12-C13-C14-C15
27	P	312	PEK	C5-C6-C7-C8
27	T	101	PEK	C6-C7-C8-C9
27	T	101	PEK	C11-C10-C9-C8
27	T	101	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	C12-C13-C14-C15
25	L	102	DMU	O6-C11-C9-C8
26	T	102	CDL	C21-C22-C23-C24
19	N	619	PGV	O01-C02-C03-O11
26	N	601	CDL	OB5-CB3-CB4-OB6
26	T	102	CDL	OB5-CB3-CB4-OB6
26	C	305	CDL	OB9-CB7-OB8-CB6
26	T	102	CDL	C64-C65-C66-C67
26	C	305	CDL	C62-C63-C64-C65
19	G	104	PGV	O03-C01-C02-O01
19	N	619	PGV	O03-C01-C02-O01
21	D	201	TGL	OG2-CG2-CG3-OG3
21	L	101	TGL	OG1-CG1-CG2-OG2
21	Q	201	TGL	CC2-CC3-CC4-CC5
26	N	601	CDL	C51-CB5-OB6-CB4
19	G	104	PGV	O12-C04-C05-C06
26	N	601	CDL	C77-C78-C79-C80
21	B	301	TGL	C29-C30-C31-C32
19	N	609	PGV	C27-C28-C29-C30
26	T	102	CDL	C19-C20-C21-C22
20	A	615	EDO	O1-C1-C2-O2
19	G	104	PGV	C4-C5-C6-C7
19	C	308	PGV	C01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-CA6
26	P	304	CDL	OA5-CA3-CA4-CA6
21	D	201	TGL	CC7-CC8-CC9-C15
21	D	201	TGL	C16-C15-CC9-CC8
21	L	101	TGL	CC7-CC8-CC9-C15
26	N	601	CDL	C41-C42-C43-C44
27	G	103	PEK	C23-C24-C25-C26
26	C	305	CDL	CA3-OA5-PA1-OA2
26	C	305	CDL	CB3-OB5-PB2-OB4
19	P	303	PGV	C20-C21-C22-C23
21	N	610	TGL	CA2-CA1-OG1-CG1
27	C	307	PEK	C01-C02-O01-C1
27	T	101	PEK	C29-C30-C31-C32
21	Q	201	TGL	CA4-CA5-CA6-CA7
21	Q	201	TGL	C13-C14-C29-C30
27	T	101	PEK	C35-C36-C37-C38
19	C	308	PGV	C02-C03-O11-P
19	N	619	PGV	O03-C01-C02-C03
21	L	101	TGL	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
21	Y	101	TGL	OG1-CG1-CG2-CG3
26	C	305	CDL	CB3-CB4-CB6-OB8
27	G	103	PEK	O03-C01-C02-C03
19	A	609	PGV	O01-C02-C03-O11
27	C	319	PEK	O01-C02-C03-O11
26	P	304	CDL	C73-C74-C75-C76
26	T	102	CDL	O1-C1-CB2-OB2
27	C	307	PEK	C24-C25-C26-C27
27	C	319	PEK	C17-C18-C19-C20
19	A	609	PGV	O03-C01-C02-O01
21	N	610	TGL	OG2-CG2-CG3-OG3
21	Q	201	TGL	OG2-CG2-CG3-OG3
21	Y	101	TGL	OG1-CG1-CG2-OG2
21	Y	101	TGL	OG2-CG2-CG3-OG3
24	O	302	PSC	O03-C01-C02-O01
26	N	601	CDL	OA6-CA4-CA6-OA8
26	T	102	CDL	OA6-CA4-CA6-OA8
27	C	319	PEK	O03-C01-C02-O01
19	A	609	PGV	C14-C15-C16-C17
25	C	309	DMU	O6-C11-C9-C8
27	P	312	PEK	C30-C31-C32-C33
21	B	301	TGL	CA5-CA6-CA7-CA8
21	B	301	TGL	C13-C14-C29-C30
19	G	104	PGV	C12-C13-C14-C15
19	A	609	PGV	C04-O12-P-O11
19	C	308	PGV	C03-O11-P-O12
26	T	102	CDL	CA3-OA5-PA1-OA2
19	A	609	PGV	C31-C32-C33-C34
21	Y	101	TGL	CA7-CA8-CA9-C20
19	P	303	PGV	C02-C03-O11-P
19	A	609	PGV	C04-O12-P-O14
19	C	308	PGV	C03-O11-P-O13
19	G	104	PGV	C04-O12-P-O13
24	B	304	PSC	C03-O11-P-O13
24	O	302	PSC	C03-O11-P-O13
26	T	102	CDL	CA2-OA2-PA1-OA4
26	T	102	CDL	CB3-OB5-PB2-OB4
27	C	307	PEK	C03-O11-P-O14
27	C	307	PEK	C04-O12-P-O14
21	Y	101	TGL	C11-C10-CB9-CB8
19	A	609	PGV	C01-C02-C03-O11
26	C	305	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
14	N	602	HEA	C15-C16-C17-C18
27	G	101	PEK	O12-C04-C05-N
21	N	610	TGL	OA1-CA1-OG1-CG1
20	C	316	EDO	O1-C1-C2-O2
20	E	204	EDO	O1-C1-C2-O2
20	N	613	EDO	O1-C1-C2-O2
20	R	202	EDO	O1-C1-C2-O2
22	J	101	CHD	C20-C22-C23-C24
21	N	610	TGL	C12-C13-C14-C29
26	C	305	CDL	C13-C14-C15-C16
21	L	101	TGL	CA6-CA7-CA8-CA9
19	A	608	PGV	C11-C10-C9-C8
26	P	304	CDL	C51-C52-C53-C54
21	D	201	TGL	C12-C13-C14-C29
19	C	308	PGV	O01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-OA6
26	P	304	CDL	OA5-CA3-CA4-OA6
27	T	101	PEK	O01-C02-C03-O11
25	P	307	DMU	C18-C19-C22-C25
25	P	307	DMU	C28-C31-C34-C37
26	N	601	CDL	C21-C22-C23-C24
26	P	304	CDL	C31-C32-C33-C34
19	G	104	PGV	O12-C04-C05-O05
21	N	610	TGL	CG1-CG2-CG3-OG3
21	Q	201	TGL	CG1-CG2-CG3-OG3
21	Y	101	TGL	CG1-CG2-CG3-OG3
25	P	306	DMU	C19-C22-C25-C28
26	N	601	CDL	CA3-CA4-CA6-OA8
27	G	103	PEK	O03-C01-C02-O01
19	G	104	PGV	C24-C25-C26-C27
25	P	307	DMU	O1-C10-O7-C3
19	N	609	PGV	C29-C30-C31-C32
19	C	308	PGV	C5-C6-C7-C8
19	C	304	PGV	C02-C03-O11-P
19	C	308	PGV	C4-C5-C6-C7
24	B	304	PSC	C3-C4-C5-C6
19	G	104	PGV	C29-C30-C31-C32
21	Y	101	TGL	C16-C17-C18-C19
26	T	102	CDL	C18-C19-C20-C21
21	L	101	TGL	C17-C18-C19-C33
19	N	609	PGV	C10-C11-C12-C13
26	P	304	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
21	N	610	TGL	CA1-CA2-CA3-CA4
27	T	101	PEK	C14-C15-C16-C17
25	L	102	DMU	C22-C25-C28-C31
26	P	304	CDL	C78-C79-C80-C81
26	T	102	CDL	C22-C23-C24-C25
26	T	102	CDL	C32-C33-C34-C35
27	T	101	PEK	C01-C02-C03-O11
21	L	101	TGL	C22-C23-C24-C25
27	C	319	PEK	C13-C14-C15-C16
26	C	305	CDL	C40-C41-C42-C43
26	T	102	CDL	C12-C13-C14-C15
20	A	618	EDO	O1-C1-C2-O2
20	N	612	EDO	O1-C1-C2-O2
20	U	101	EDO	O1-C1-C2-O2
21	B	301	TGL	CC9-C15-C16-C17
27	P	312	PEK	C3-C4-C5-C6
19	N	609	PGV	C28-C29-C30-C31
26	N	601	CDL	C17-C18-C19-C20
26	N	601	CDL	C57-C58-C59-C60
19	N	619	PGV	C03-O11-P-O12
24	O	302	PSC	C04-O12-P-O11
26	N	601	CDL	CA2-OA2-PA1-OA5
26	N	601	CDL	CA3-OA5-PA1-OA2
26	N	601	CDL	CB2-OB2-PB2-OB5
26	N	601	CDL	CB3-OB5-PB2-OB2
21	L	101	TGL	CG1-CG2-CG3-OG3
26	P	304	CDL	C11-C12-C13-C14
27	G	103	PEK	O03-C21-C22-C23
26	N	601	CDL	C34-C35-C36-C37
19	N	609	PGV	C11-C12-C13-C14
26	T	102	CDL	CA2-C1-CB2-OB2
21	D	201	TGL	OG2-CB1-CB2-CB3
26	N	601	CDL	C64-C65-C66-C67
21	N	610	TGL	CC5-CC6-CC7-CC8
27	C	319	PEK	C7-C8-C9-C10
27	P	312	PEK	C7-C8-C9-C10
21	L	101	TGL	C24-C25-C26-C27
25	P	307	DMU	C25-C28-C31-C34
19	P	303	PGV	C1-C2-C3-C4
27	P	312	PEK	O12-C04-C05-N
26	C	305	CDL	C51-C52-C53-C54
26	N	601	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
27	T	101	PEK	C21-C22-C23-C24
25	C	310	DMU	C28-C31-C34-C37
19	N	619	PGV	C02-C03-O11-P
25	C	302	DMU	C22-C25-C28-C31
14	N	602	HEA	CAD-CBD-CGD-O1D
22	G	102	CHD	C22-C23-C24-O26
21	L	101	TGL	C14-C29-C30-C31
26	C	305	CDL	C12-C13-C14-C15
21	Q	201	TGL	OG1-CA1-CA2-CA3
26	P	304	CDL	C18-C19-C20-C21
14	A	601	HEA	CAD-CBD-CGD-O1D
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
21	L	101	TGL	CC1-CC2-CC3-CC4
26	P	304	CDL	C22-C23-C24-C25
22	G	102	CHD	C22-C23-C24-O25
27	T	101	PEK	C30-C31-C32-C33
27	G	103	PEK	C04-O12-P-O13
21	B	301	TGL	CB5-CB6-CB7-CB8
14	A	602[B]	HEA	CAA-CBA-CGA-O2A
14	N	602	HEA	CAD-CBD-CGD-O2D
22	B	302	CHD	C22-C23-C24-O25
22	B	302	CHD	C22-C23-C24-O26
19	A	609	PGV	C11-C10-C9-C8
26	T	102	CDL	C81-C82-C83-C84
14	N	603[A]	HEA	CAA-CBA-CGA-O1A
14	N	603[A]	HEA	CAA-CBA-CGA-O2A
22	P	305	CHD	C22-C23-C24-O25
19	N	619	PGV	C01-C02-O01-C1
19	N	619	PGV	C03-C02-O01-C1
21	L	101	TGL	CG1-CG2-OG2-CB1
21	L	101	TGL	CG3-CG2-OG2-CB1
21	D	201	TGL	C25-C26-C27-C28
24	O	302	PSC	C10-C11-C12-C13
27	C	307	PEK	C11-C10-C9-C8
27	C	319	PEK	C5-C6-C7-C8
27	G	103	PEK	C9-C10-C11-C12
27	T	101	PEK	C5-C6-C7-C8
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
14	A	602[B]	HEA	CAA-CBA-CGA-O1A
19	G	104	PGV	C7-C8-C9-C10
21	Q	201	TGL	CB2-CB3-CB4-CB5
26	N	601	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	OA5-CA3-CA4-CA6
22	G	102	CHD	C17-C20-C22-C23
27	P	312	PEK	C2-C1-O01-C02
14	N	603[A]	HEA	CAD-CBD-CGD-O2D
22	C	306	CHD	C22-C23-C24-O26
26	P	304	CDL	C71-CB7-OB8-CB6
21	N	610	TGL	CB9-C10-C11-C12
24	B	304	PSC	O01-C1-C2-C3
19	N	619	PGV	O12-C04-C05-O05
26	T	102	CDL	C15-C16-C17-C18
14	N	603[A]	HEA	CAD-CBD-CGD-O1D
14	N	603[B]	HEA	CAA-CBA-CGA-O1A
21	L	101	TGL	OG1-CA1-CA2-CA3
21	N	610	TGL	OG3-CC1-CC2-CC3
20	C	318	EDO	O1-C1-C2-O2
20	H	101	EDO	O1-C1-C2-O2
20	P	309	EDO	O1-C1-C2-O2
20	R	206	EDO	O1-C1-C2-O2
25	P	306	DMU	O6-C11-C9-O1
14	N	602	HEA	C26-C15-C16-C17
22	P	301	CHD	C22-C23-C24-O26
22	C	306	CHD	C13-C17-C20-C21
21	Y	101	TGL	CA6-CA7-CA8-CA9
19	N	609	PGV	C12-C13-C14-C15
19	P	303	PGV	C12-C13-C14-C15
19	G	104	PGV	C11-C12-C13-C14
24	B	304	PSC	C7-C8-C9-C10
24	O	302	PSC	C12-C13-C14-C15
27	C	307	PEK	O01-C02-C03-O11
25	P	306	DMU	C18-C19-C22-C25
19	G	104	PGV	C23-C24-C25-C26
21	L	101	TGL	C16-C15-CC9-CC8
27	G	101	PEK	C35-C36-C37-C38
22	J	101	CHD	C21-C20-C22-C23
24	O	302	PSC	C22-C23-C24-C25
19	C	308	PGV	C24-C25-C26-C27
25	Z	101	DMU	C31-C34-C37-C40
24	B	304	PSC	O03-C19-C20-C21
26	N	601	CDL	C52-C51-CB5-OB6
19	A	608	PGV	O03-C19-C20-C21
21	L	101	TGL	CB5-CB6-CB7-CB8
14	A	602[A]	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
27	C	319	PEK	C14-C15-C16-C17
21	L	101	TGL	CB2-CB3-CB4-CB5
26	C	305	CDL	CA3-OA5-PA1-OA4
14	N	603[B]	HEA	C26-C15-C16-C17
25	P	307	DMU	O16-C18-C19-C22
21	B	301	TGL	CA6-CA7-CA8-CA9
19	G	104	PGV	C20-C21-C22-C23
21	D	201	TGL	OG1-CA1-CA2-CA3
19	N	619	PGV	C9-C10-C11-C12
24	O	302	PSC	C7-C8-C9-C10
27	C	307	PEK	C3-C4-C5-C6
22	C	306	CHD	C22-C23-C24-O25
22	P	305	CHD	C22-C23-C24-O26
19	N	619	PGV	O03-C19-C20-C21
21	D	201	TGL	OG3-CC1-CC2-CC3
27	P	312	PEK	O01-C1-C2-C3
21	B	301	TGL	C25-C26-C27-C28
14	N	602	HEA	C27-C19-C20-C21
14	N	602	HEA	C14-C15-C16-C17
19	C	308	PGV	C9-C10-C11-C12
19	G	104	PGV	C9-C10-C11-C12
27	C	307	PEK	C2-C3-C4-C5
21	N	610	TGL	C22-C23-C24-C25
24	B	304	PSC	O03-C01-C02-C03
27	C	319	PEK	O03-C01-C02-C03
26	N	601	CDL	OA5-CA3-CA4-OA6
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
22	J	101	CHD	C22-C23-C24-O25
22	W	101	CHD	C22-C23-C24-O26
25	P	306	DMU	C22-C25-C28-C31
21	L	101	TGL	C29-C30-C31-C32
24	O	302	PSC	C27-C28-C29-C30
22	P	301	CHD	C22-C23-C24-O25
21	D	201	TGL	C11-C12-C13-C14
26	T	102	CDL	C63-C64-C65-C66
21	N	610	TGL	C20-C21-C22-C23
26	C	305	CDL	C17-C18-C19-C20
26	P	304	CDL	C53-C54-C55-C56
24	B	304	PSC	O03-C01-C02-O01
25	C	309	DMU	O6-C11-C9-O1
27	G	103	PEK	C04-O12-P-O14
19	A	609	PGV	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	G	104	PGV	C3-C4-C5-C6
22	C	301	CHD	C16-C17-C20-C22
21	Q	201	TGL	OG3-CC1-CC2-CC3
27	C	319	PEK	O03-C21-C22-C23
21	D	201	TGL	CB7-CB8-CB9-C10
25	C	309	DMU	C18-C19-C22-C25
27	P	312	PEK	O02-C1-O01-C02
19	A	609	PGV	C11-C12-C13-C14
19	C	304	PGV	C9-C10-C11-C12
19	C	304	PGV	C11-C12-C13-C14
26	C	305	CDL	C52-C51-CB5-OB6
22	C	301	CHD	C22-C23-C24-O25
14	A	601	HEA	CAD-CBD-CGD-O2D
21	Q	201	TGL	OG2-CB1-CB2-CB3
21	D	201	TGL	OC1-CC1-CC2-CC3
19	A	608	PGV	C11-C12-C13-C14
19	N	619	PGV	O04-C19-C20-C21
25	P	308	DMU	C31-C34-C37-C40
24	B	304	PSC	C12-C13-C14-C15
24	B	304	PSC	O04-C19-C20-C21
19	A	608	PGV	C23-C24-C25-C26
21	D	201	TGL	OA1-CA1-CA2-CA3
27	P	312	PEK	O02-C1-C2-C3
22	W	101	CHD	C20-C22-C23-C24
26	C	305	CDL	C63-C64-C65-C66
26	N	601	CDL	C55-C56-C57-C58
26	C	305	CDL	C12-C11-CA5-OA6
21	D	201	TGL	CA9-C20-C21-C22
26	C	305	CDL	C12-C11-CA5-OA7
26	C	305	CDL	C53-C54-C55-C56
14	N	603[B]	HEA	CAA-CBA-CGA-O2A
25	C	309	DMU	C28-C31-C34-C37
26	P	304	CDL	C35-C36-C37-C38
26	N	601	CDL	CA2-OA2-PA1-OA3
26	N	601	CDL	CB2-OB2-PB2-OB3
27	T	101	PEK	C28-C29-C30-C31
21	Q	201	TGL	OC1-CC1-CC2-CC3
20	A	611	EDO	O1-C1-C2-O2
20	B	306	EDO	O1-C1-C2-O2
20	C	312	EDO	O1-C1-C2-O2
20	D	202	EDO	O1-C1-C2-O2
20	D	203	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	F	104	EDO	O1-C1-C2-O2
20	F	105	EDO	O1-C1-C2-O2
20	G	106	EDO	O1-C1-C2-O2
20	N	611	EDO	O1-C1-C2-O2
20	S	101	EDO	O1-C1-C2-O2
22	C	301	CHD	C22-C23-C24-O26
21	Q	201	TGL	C16-C15-CC9-CC8
14	A	602[B]	HEA	C26-C15-C16-C17
27	P	312	PEK	C05-C04-O12-P
19	A	608	PGV	C19-C20-C21-C22
21	N	610	TGL	CA2-CA3-CA4-CA5
21	Y	101	TGL	CC2-CC3-CC4-CC5
14	N	602	HEA	CAA-CBA-CGA-O2A
14	A	601	HEA	CAA-CBA-CGA-O1A
19	A	609	PGV	C05-C04-O12-P
19	A	608	PGV	C26-C27-C28-C29
27	C	319	PEK	O04-C21-C22-C23
19	N	609	PGV	O03-C19-C20-C21
21	N	610	TGL	OG1-CA1-CA2-CA3
19	C	308	PGV	O04-C19-O03-C01
19	G	104	PGV	C25-C26-C27-C28
26	T	102	CDL	C40-C41-C42-C43
26	C	305	CDL	C52-C51-CB5-OB7
27	T	101	PEK	O01-C1-C2-C3

There are no ring outliers.

62 monomers are involved in 225 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	101	DMU	1	0
18	A	606[A]	AZI	1	0
20	R	202	EDO	1	0
22	G	102	CHD	1	0
14	A	602[A]	HEA	6	0
22	J	101	CHD	1	0
22	W	101	CHD	4	0
22	C	306	CHD	4	0
25	P	307	DMU	3	0
20	H	102	EDO	1	0
27	C	307	PEK	3	0
20	A	610	EDO	1	0
19	A	608	PGV	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	N	603[A]	HEA	8	0
25	P	308	DMU	1	0
27	P	312	PEK	1	0
19	C	304	PGV	1	0
19	P	303	PGV	1	0
24	B	304	PSC	10	0
19	C	308	PGV	2	0
20	O	305	EDO	1	0
26	N	601	CDL	10	0
20	A	616	EDO	2	0
18	N	608[A]	AZI	6	0
26	P	304	CDL	8	0
27	G	101	PEK	2	0
19	G	104	PGV	4	0
20	C	314	EDO	1	0
21	B	301	TGL	7	0
14	A	602[B]	HEA	8	0
21	Q	201	TGL	7	0
18	N	607[A]	AZI	1	0
20	C	318	EDO	1	0
27	T	101	PEK	4	0
14	A	601	HEA	3	0
20	H	101	EDO	1	0
25	P	306	DMU	5	0
14	N	603[B]	HEA	8	0
21	D	201	TGL	11	0
20	N	613	EDO	1	0
25	C	302	DMU	8	0
18	A	607[B]	AZI	2	0
25	L	102	DMU	4	0
19	N	609	PGV	2	0
21	L	101	TGL	4	0
25	Z	101	DMU	1	0
24	O	302	PSC	6	0
20	R	205	EDO	1	0
21	Y	101	TGL	7	0
27	C	319	PEK	1	0
14	N	602	HEA	4	0
22	P	305	CHD	3	0
26	C	305	CDL	13	0
20	D	204	EDO	1	0
25	C	309	DMU	2	0

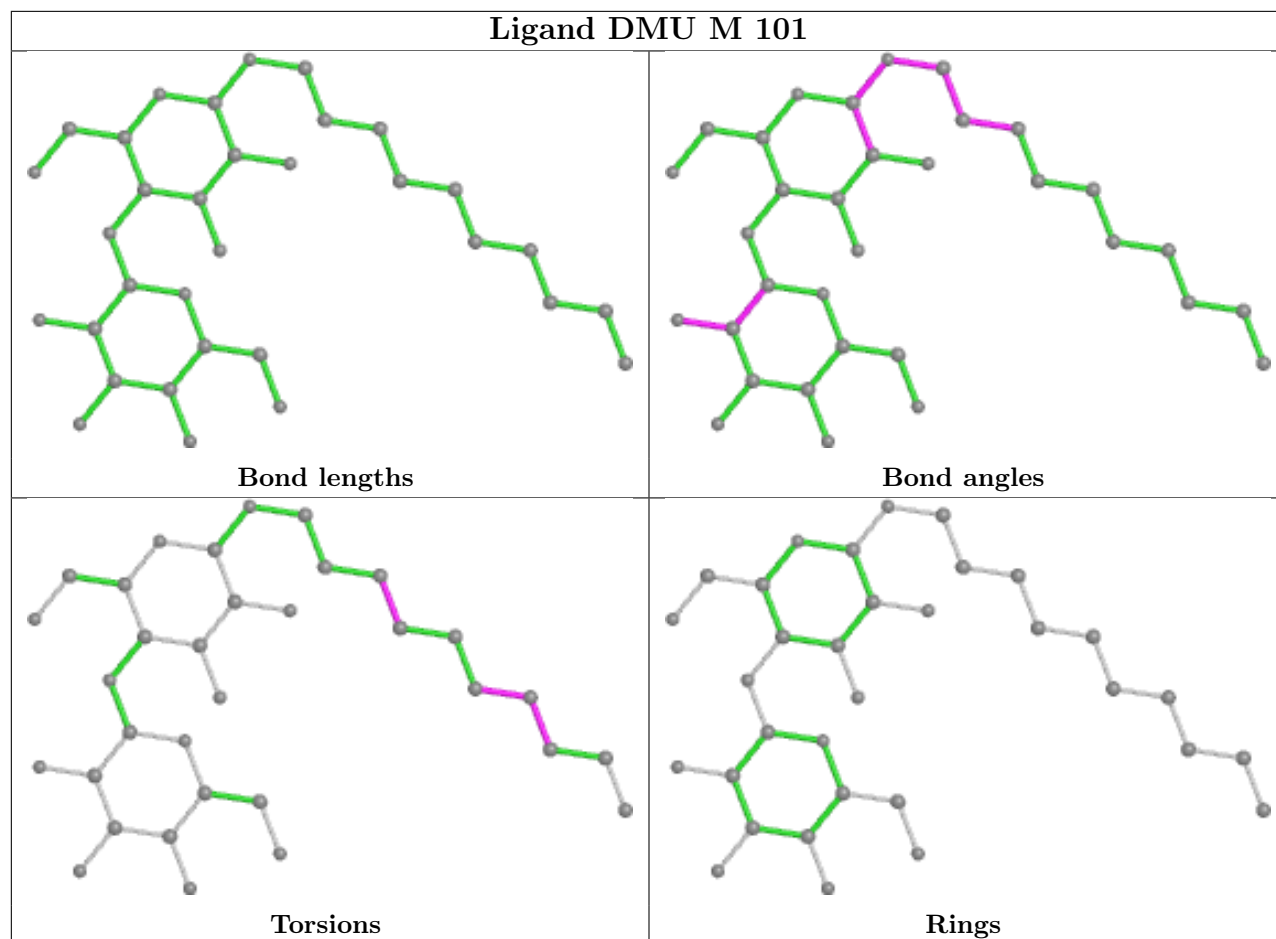
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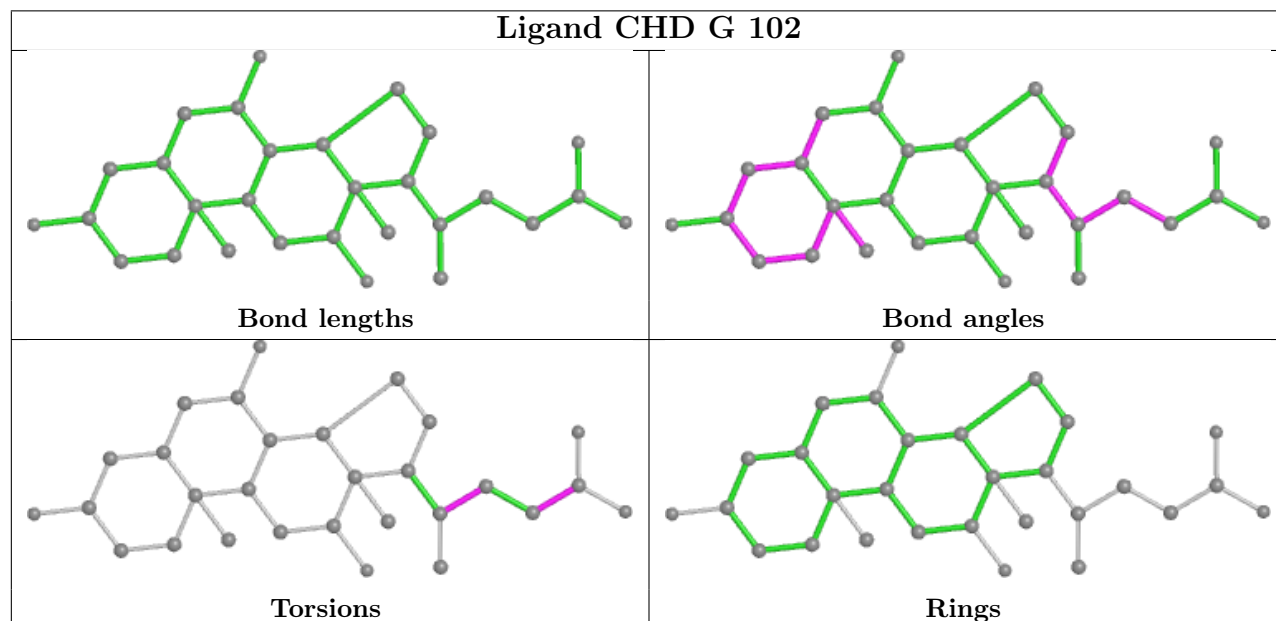
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	G	103	PEK	1	0
20	G	105	EDO	1	0
20	S	101	EDO	5	0
19	N	619	PGV	7	0
18	A	607[A]	AZI	5	0
26	T	102	CDL	11	0
19	A	609	PGV	4	0

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

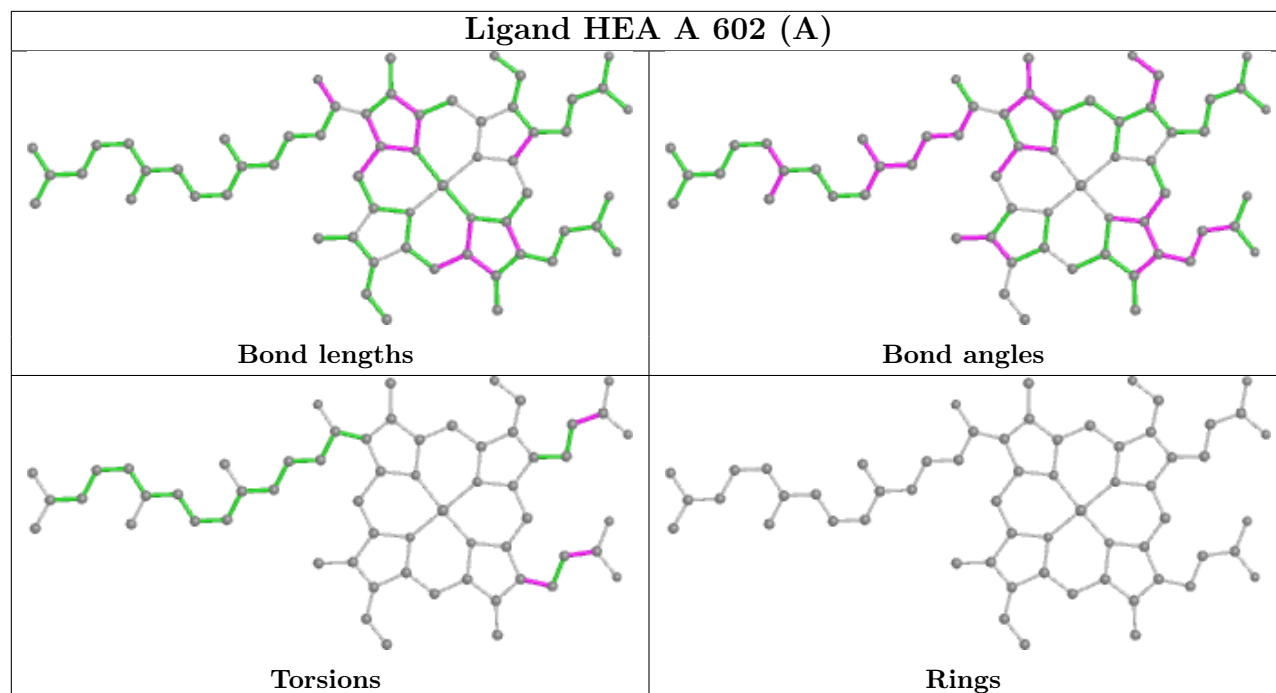
Ligand DMU M 101



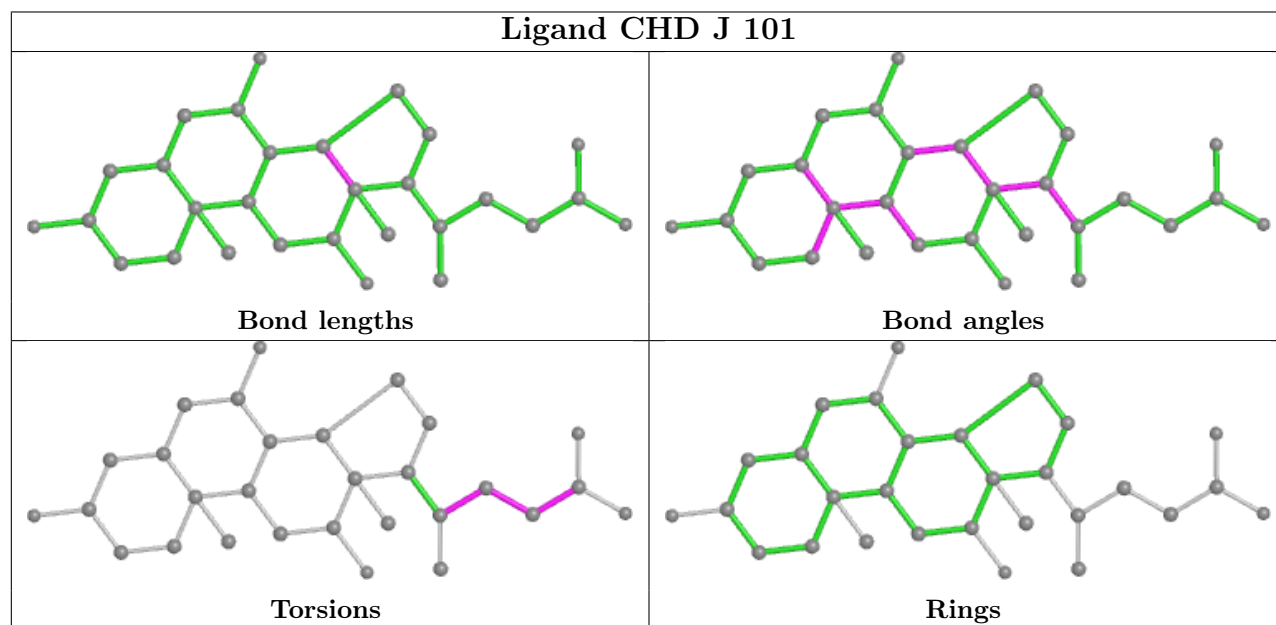
Ligand CHD G 102

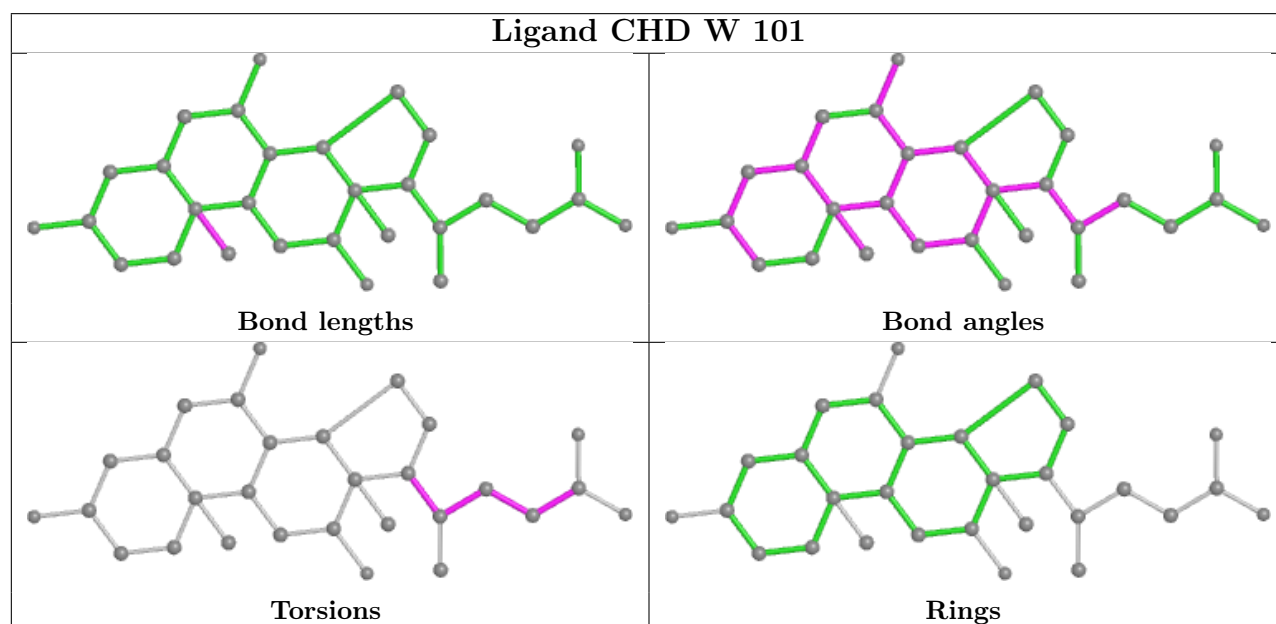
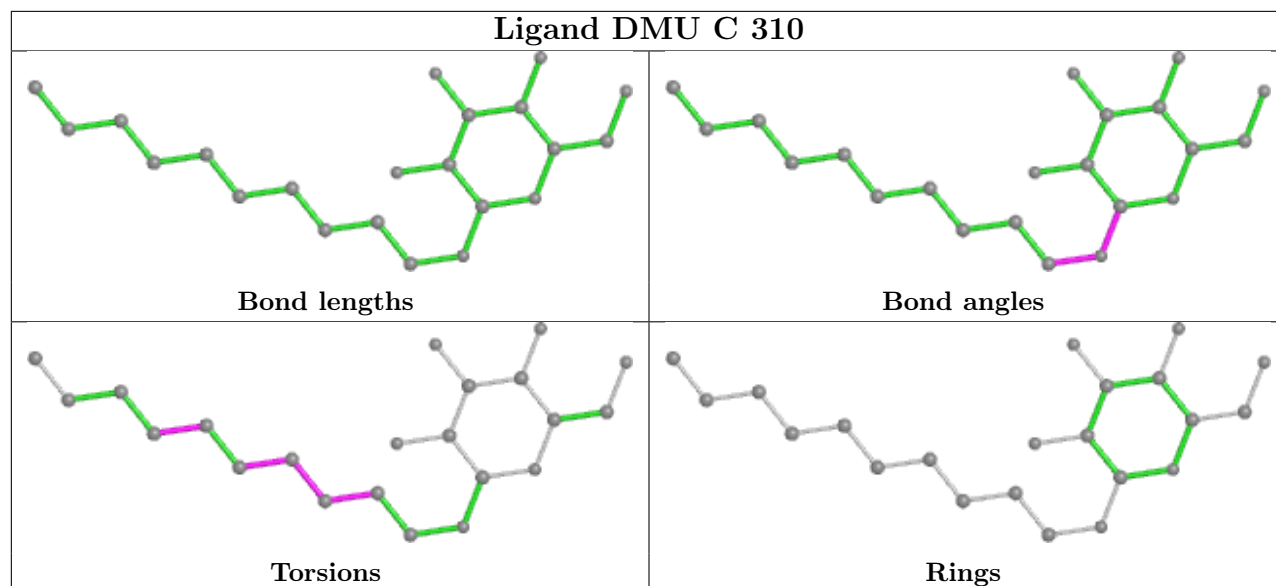


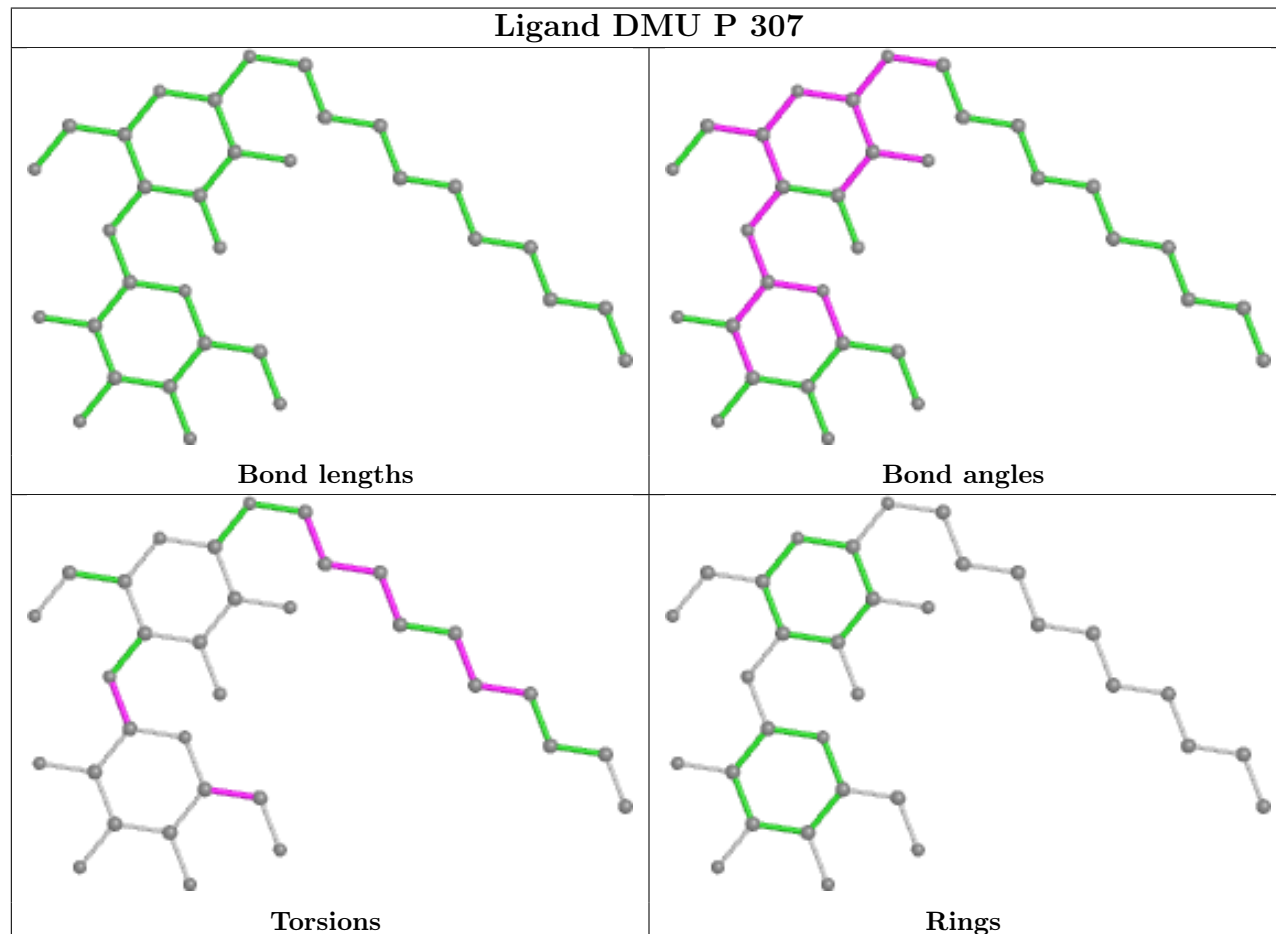
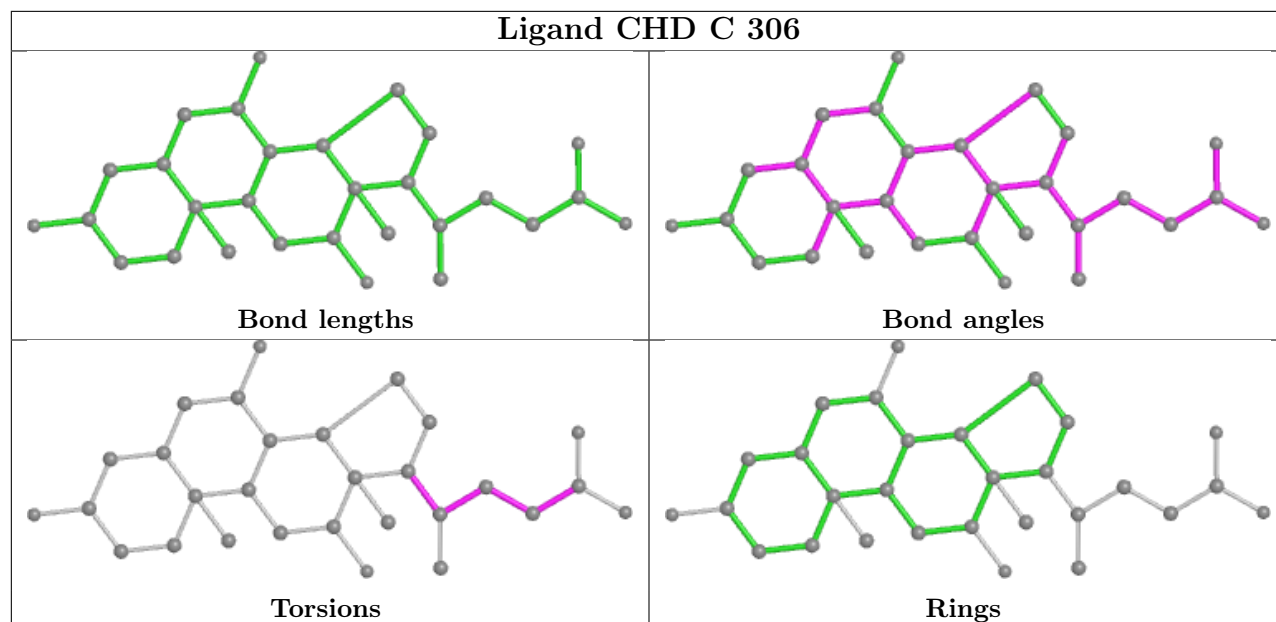
Ligand HEA A 602 (A)

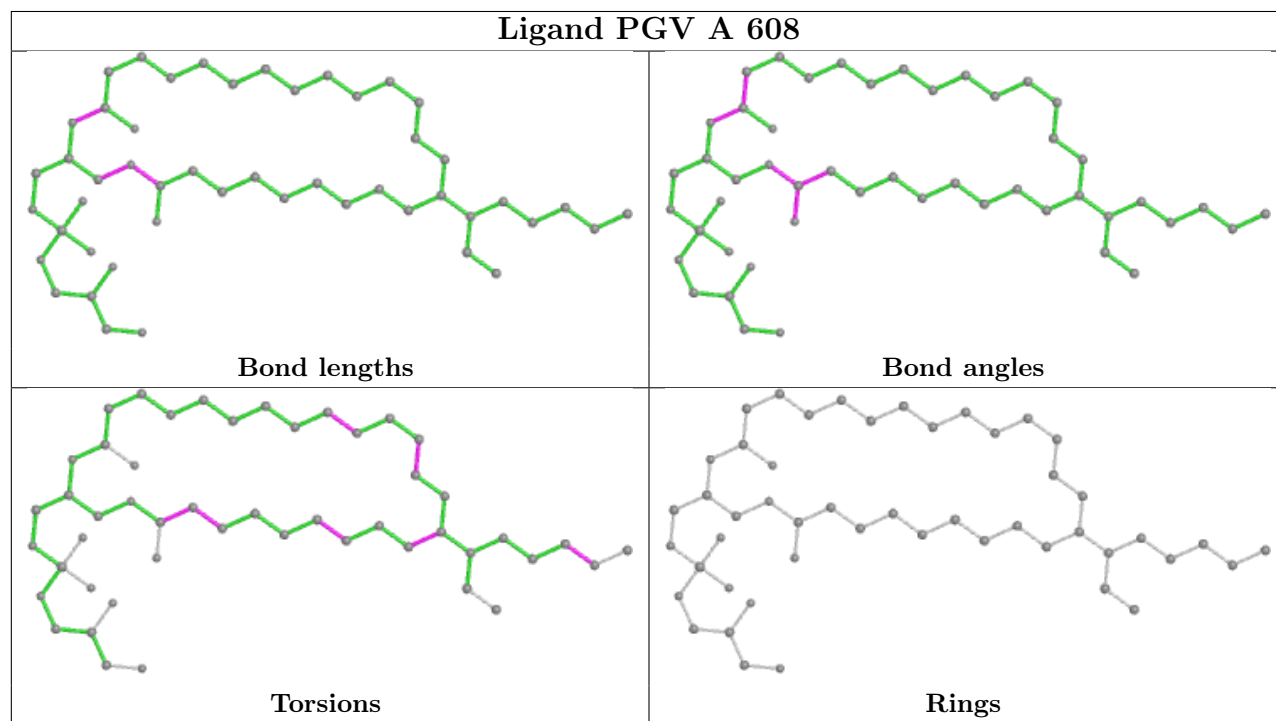
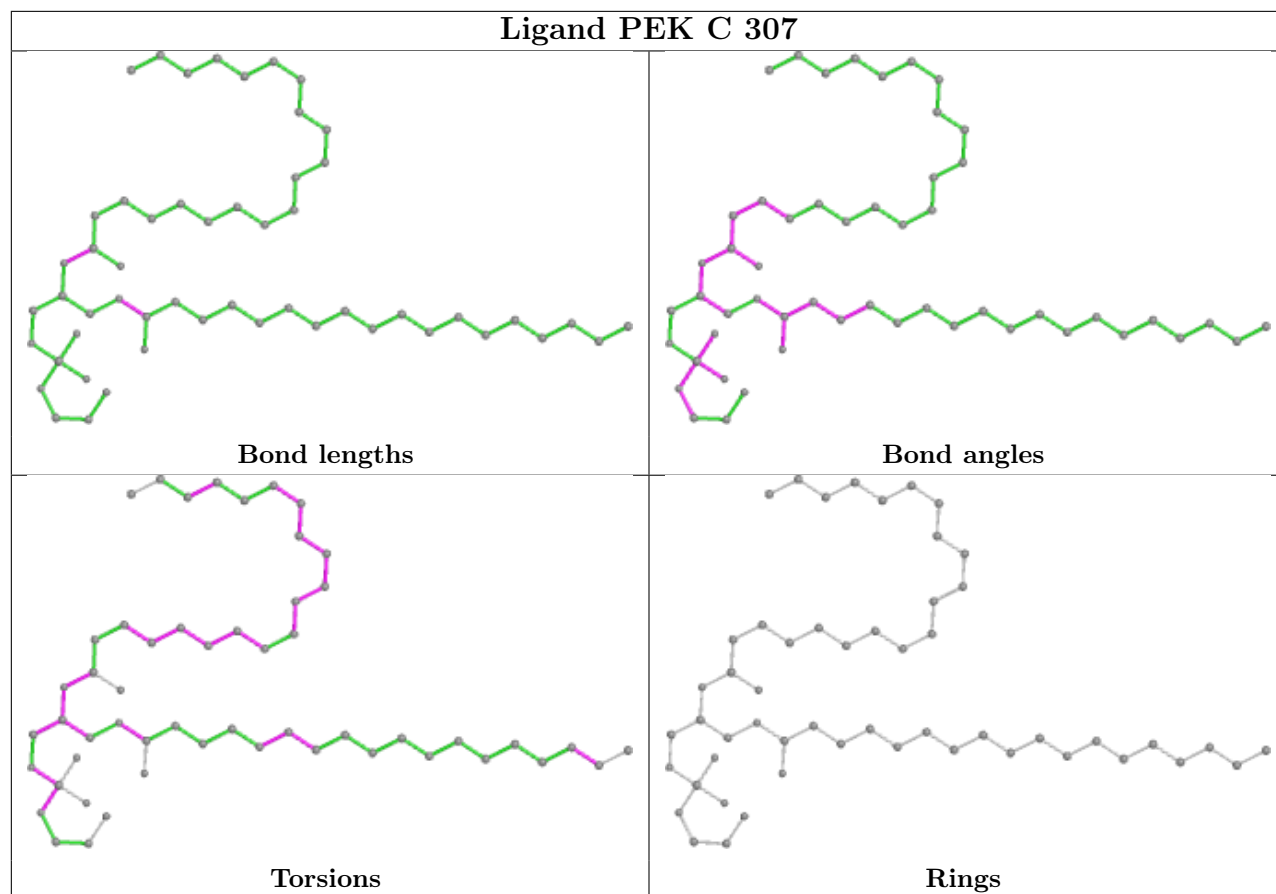


Ligand CHD J 101

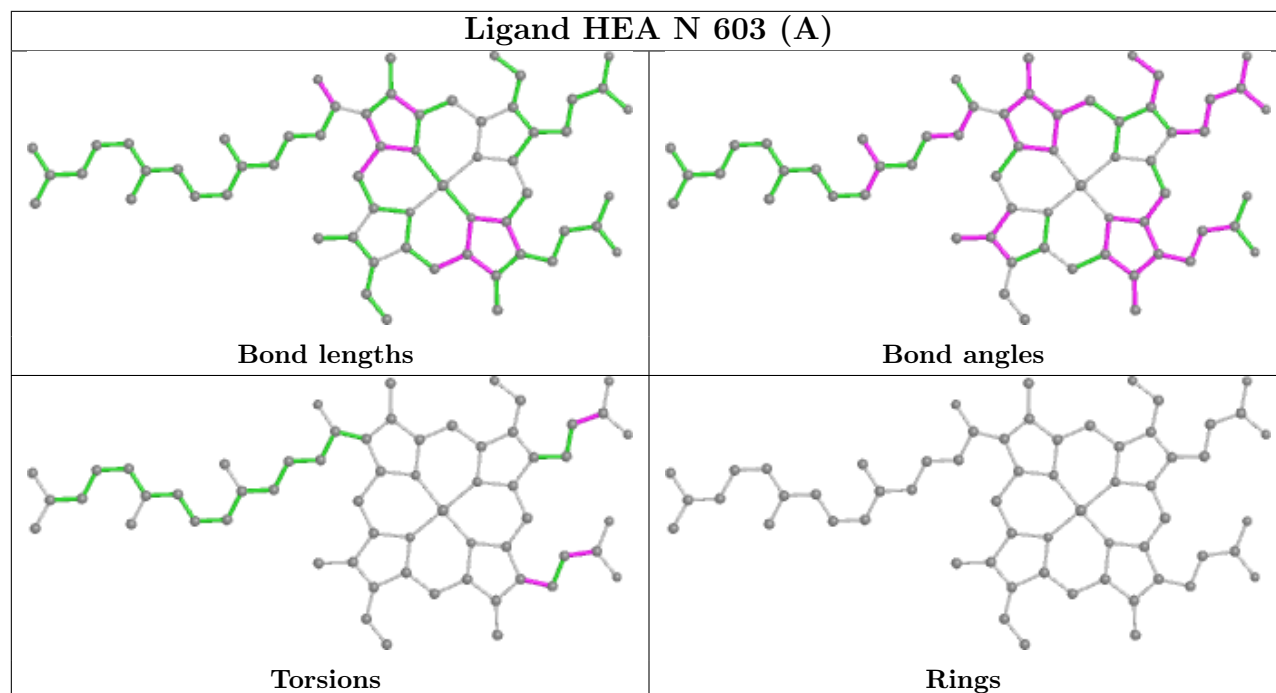




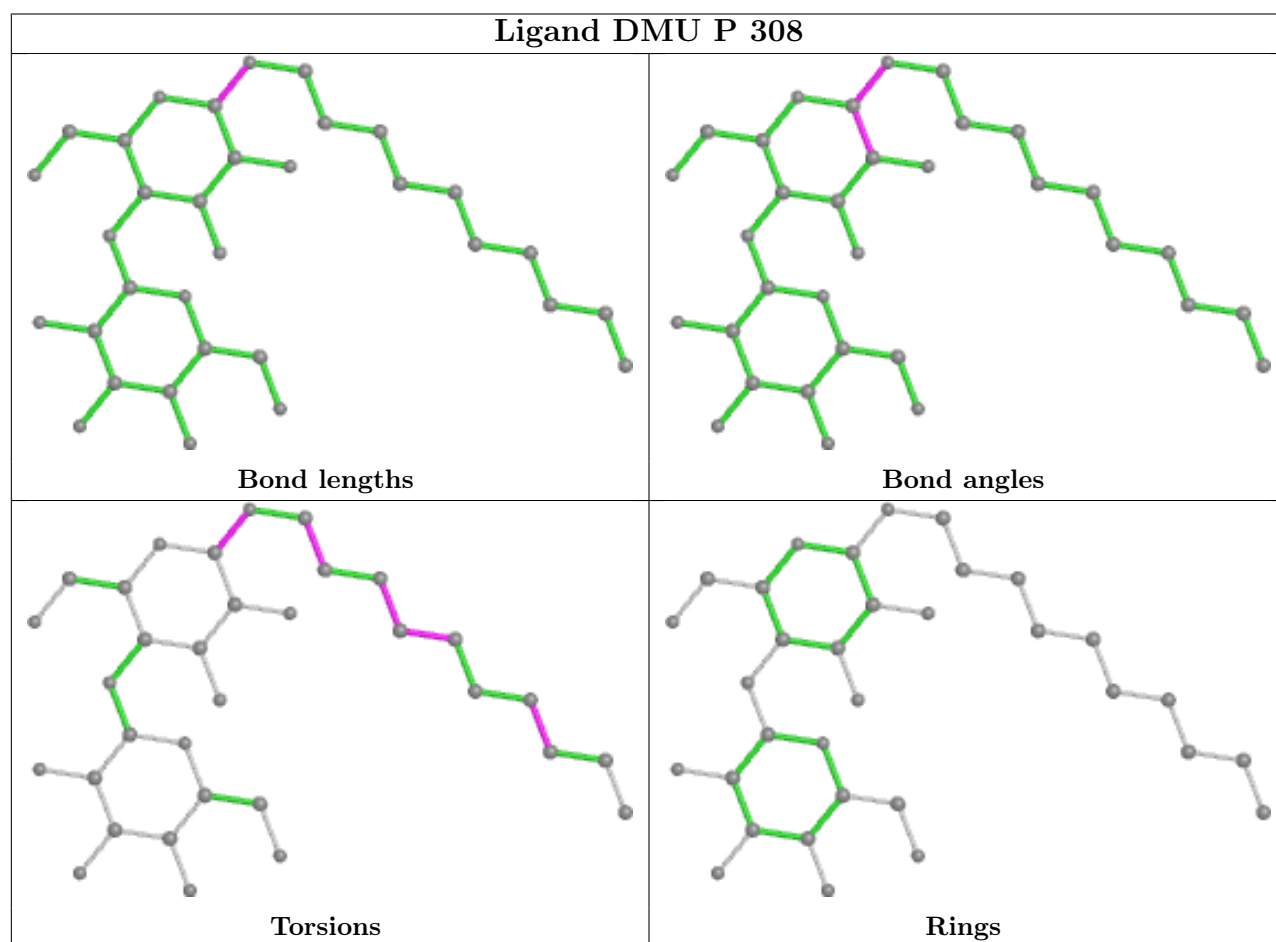


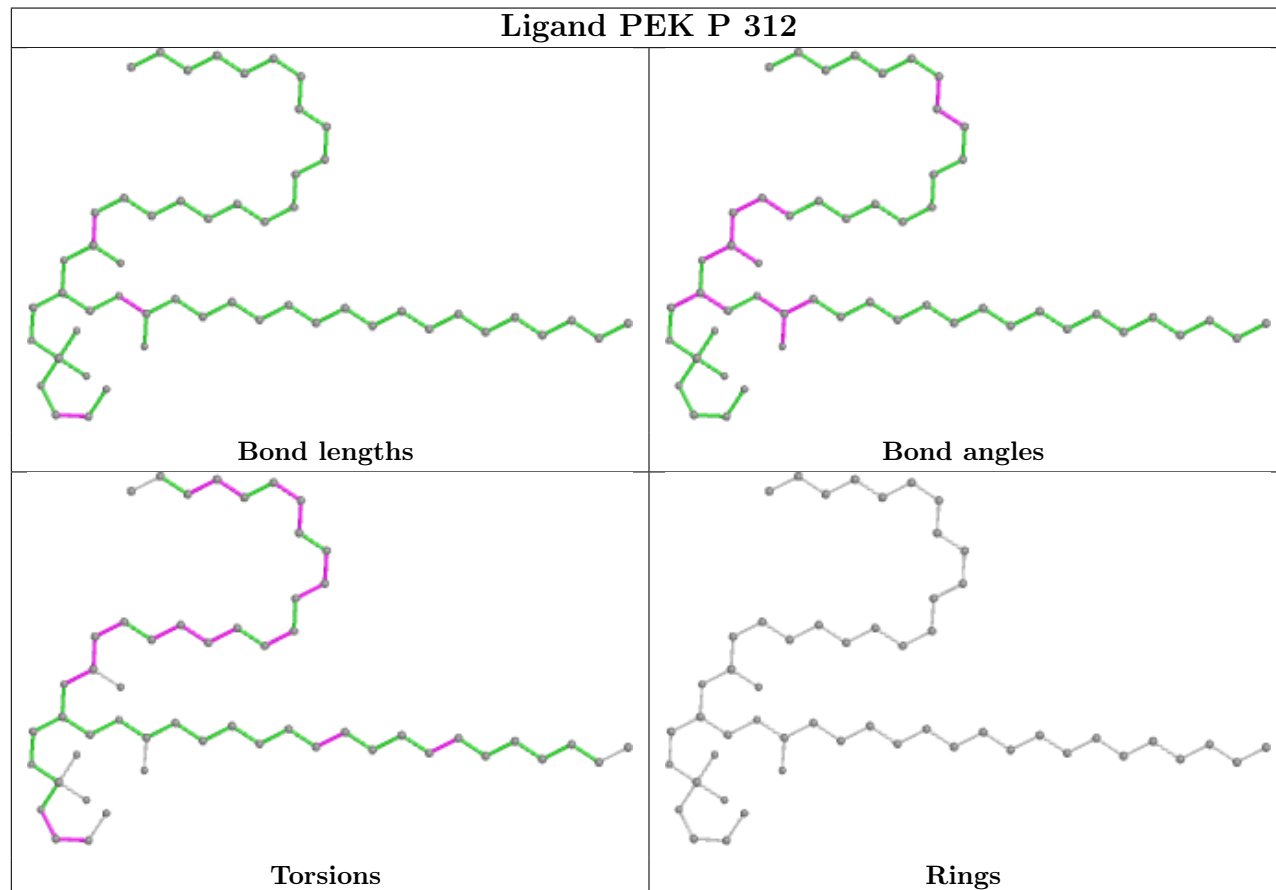
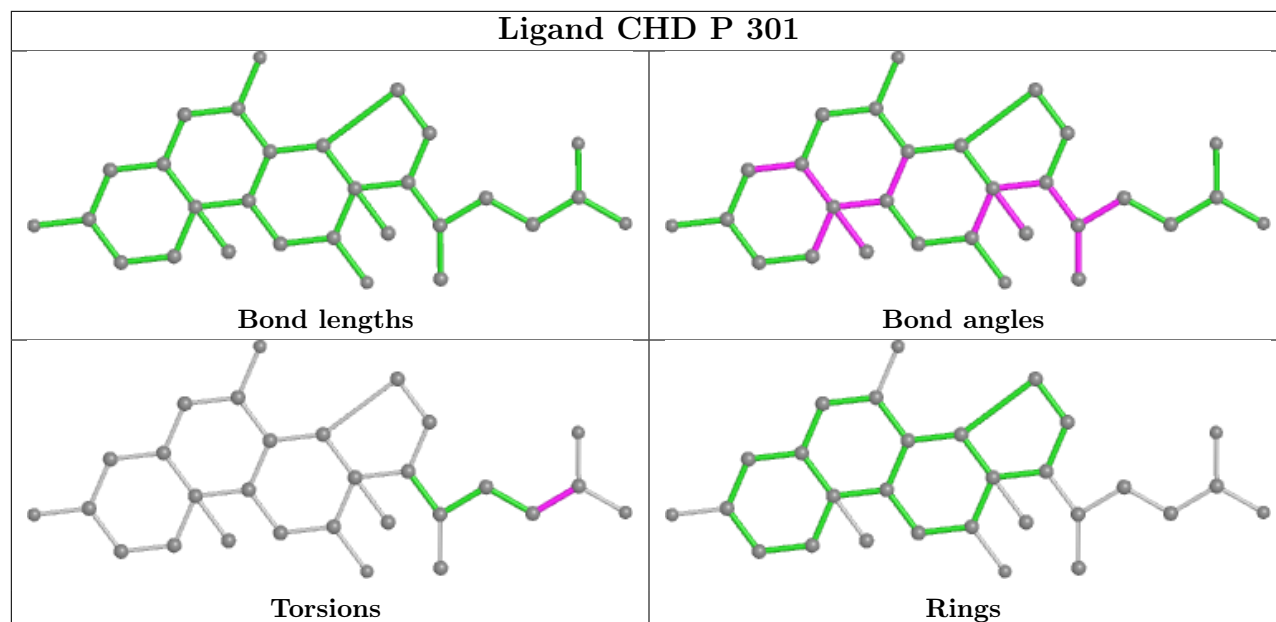


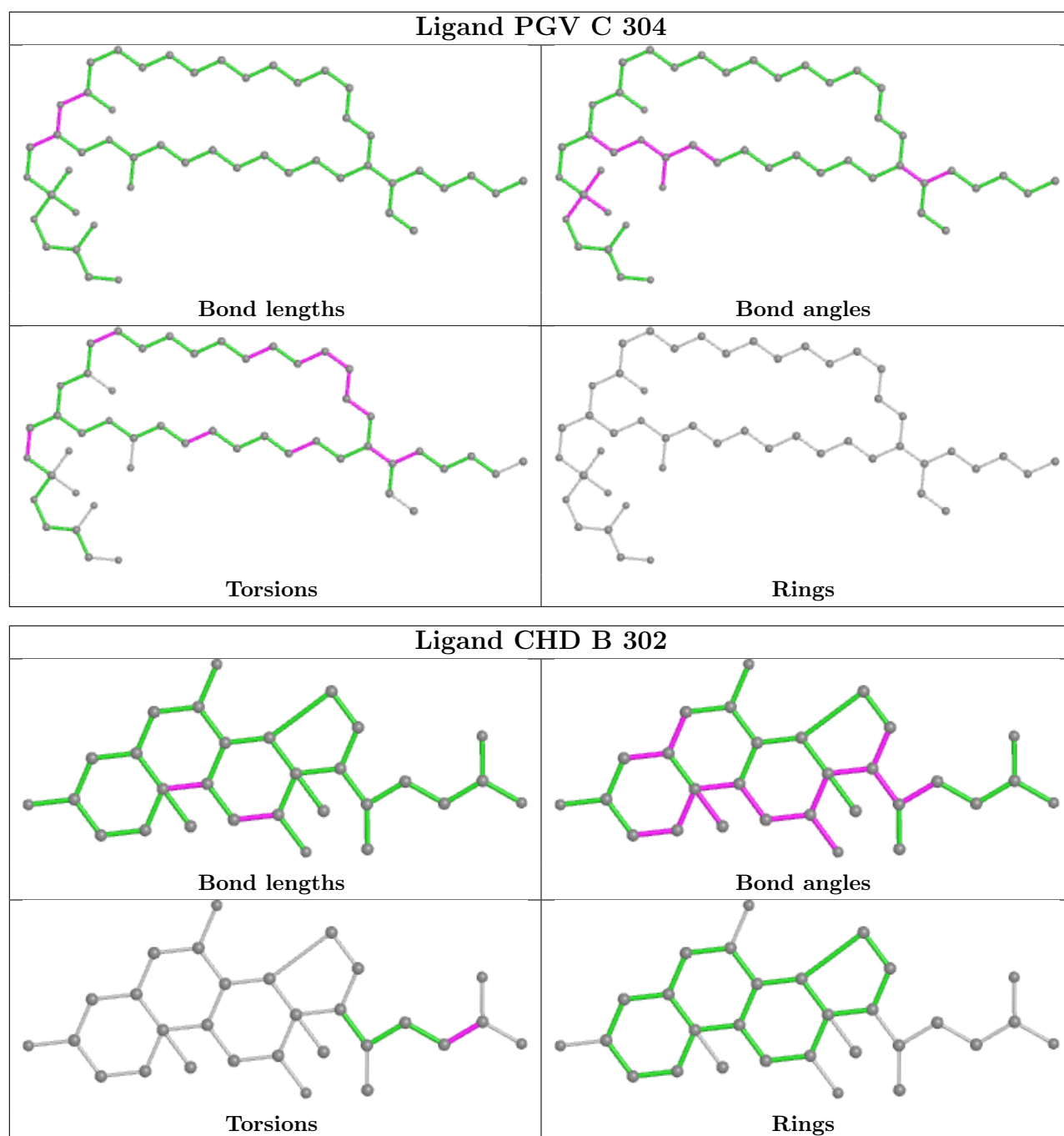
Ligand HEA N 603 (A)



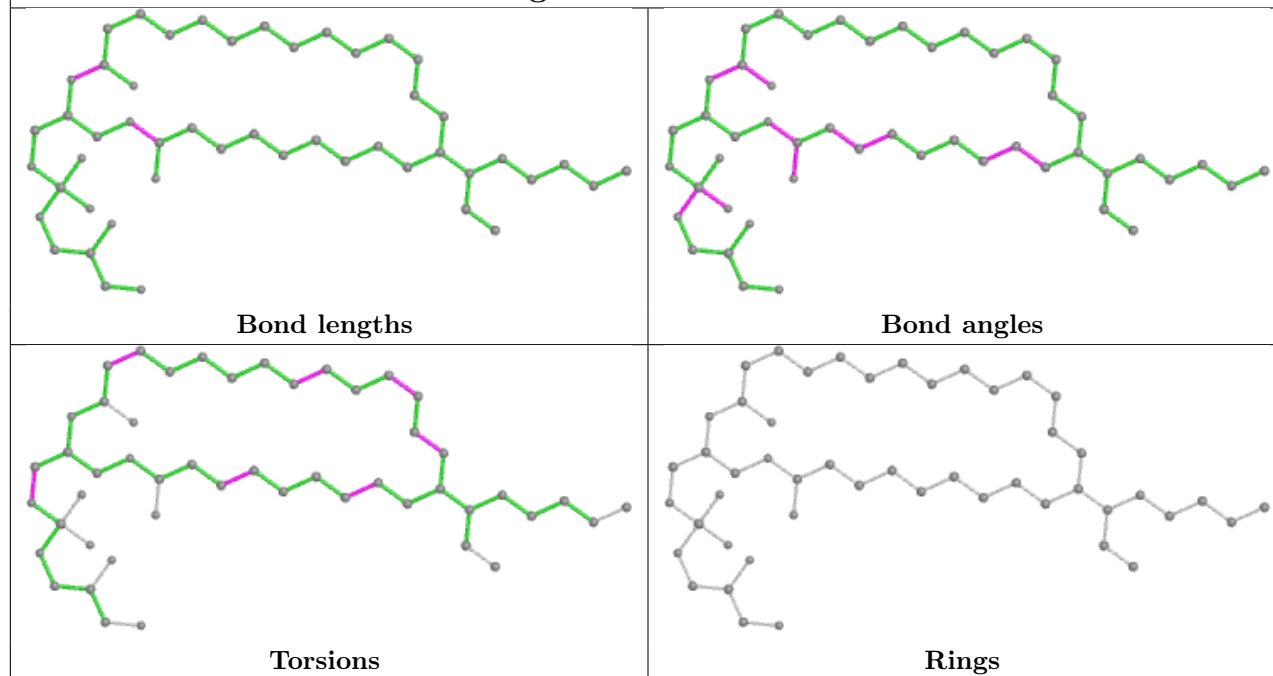
Ligand DMU P 308



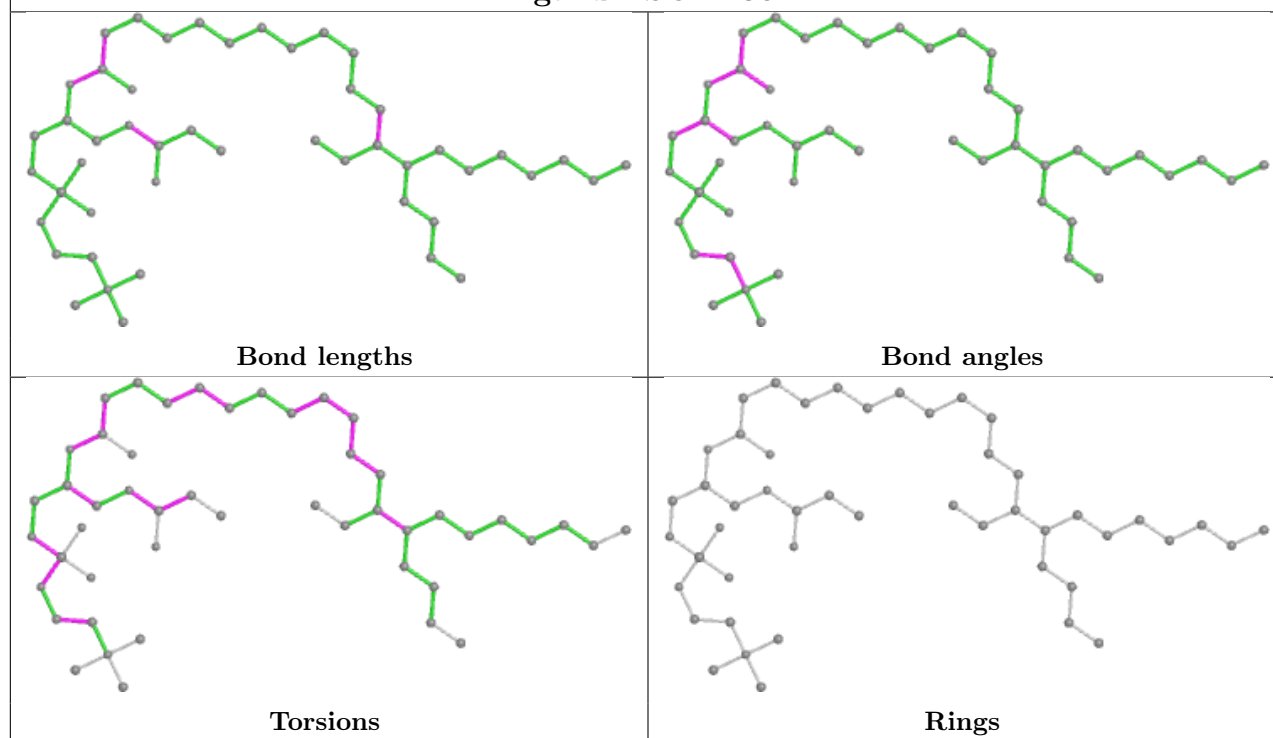


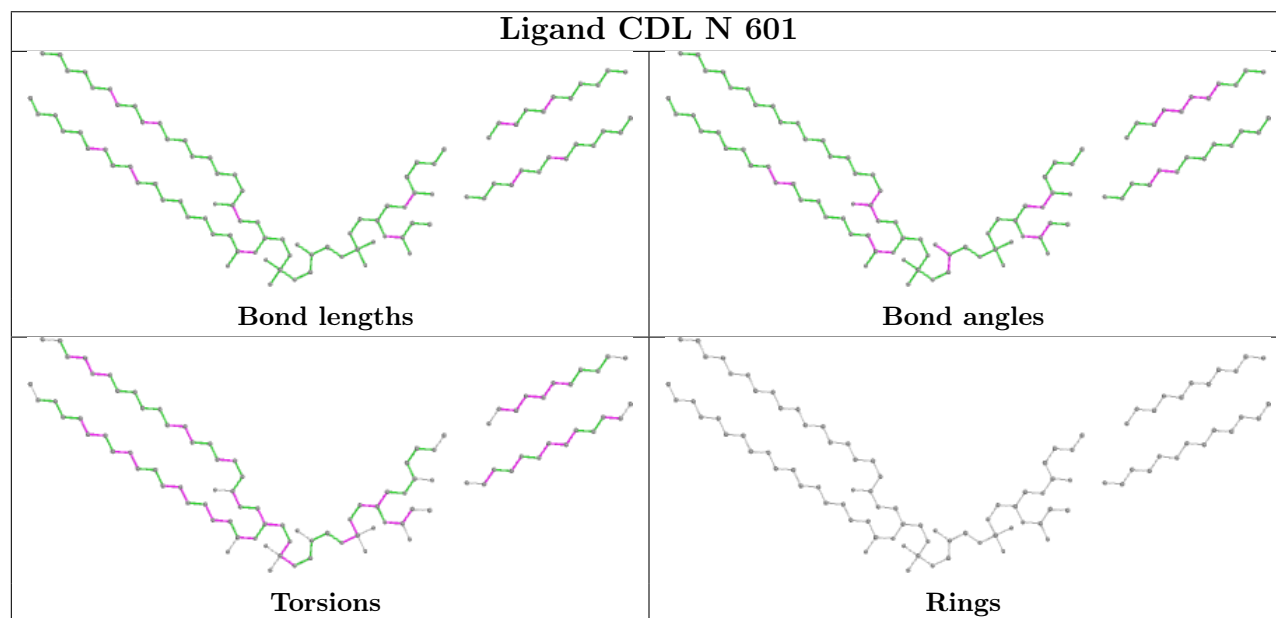
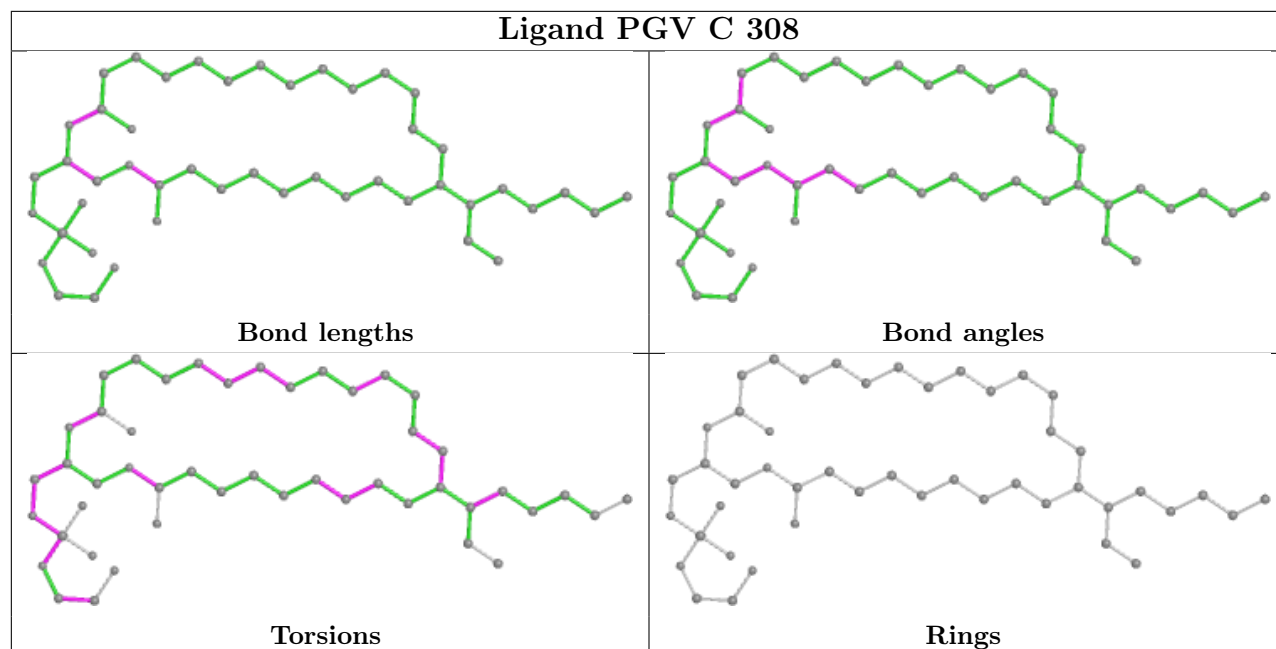


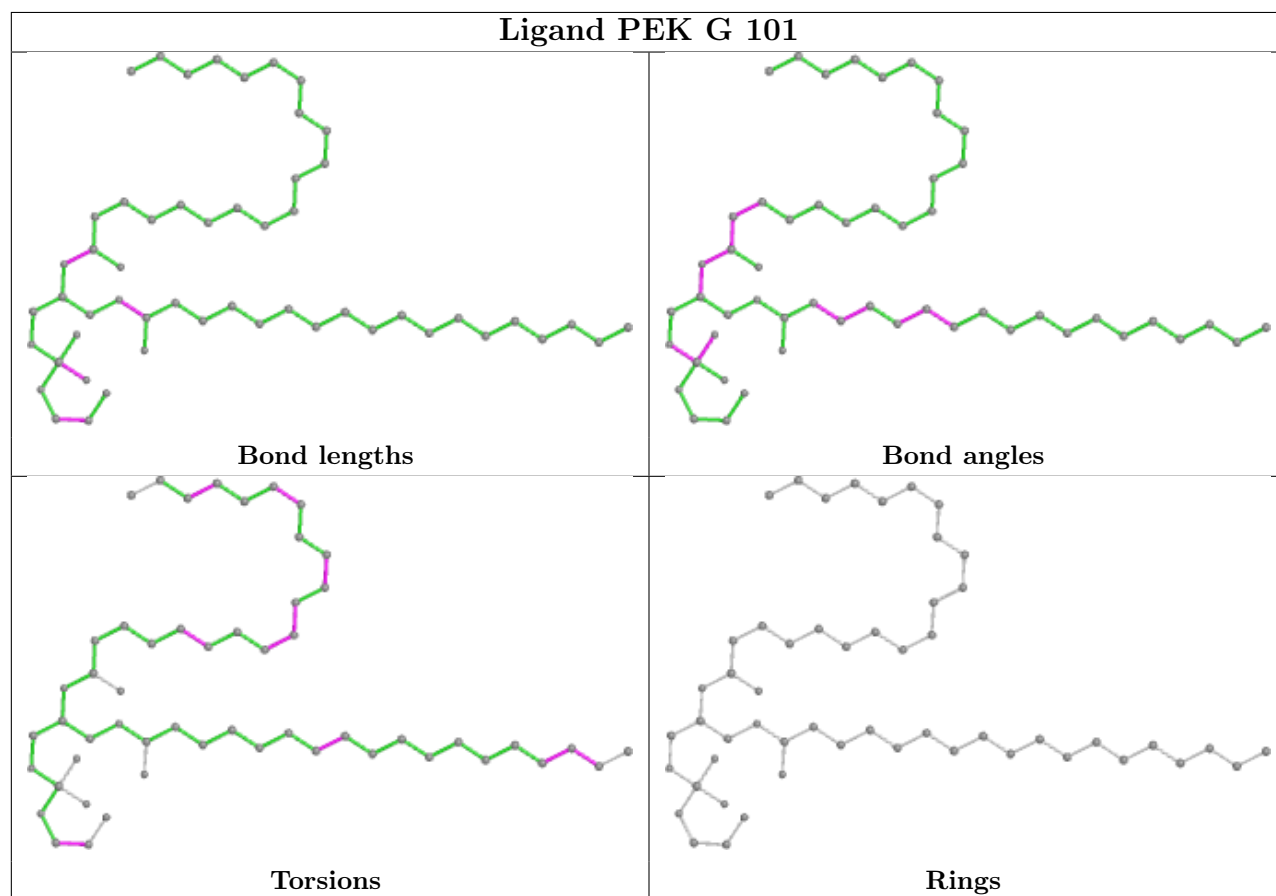
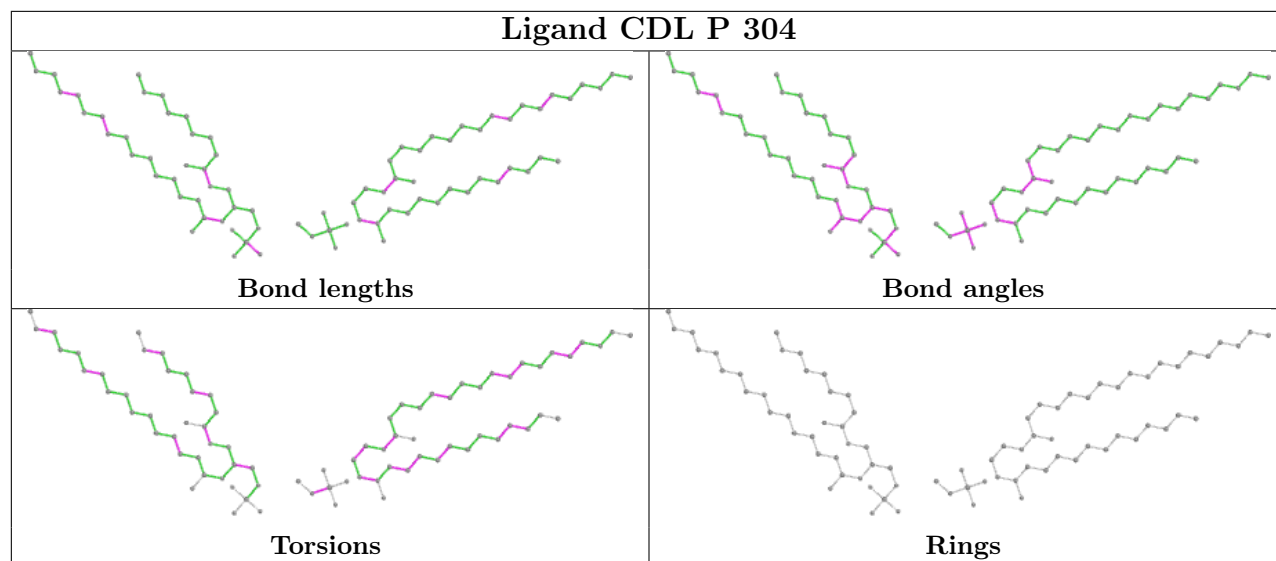
Ligand PGV P 303

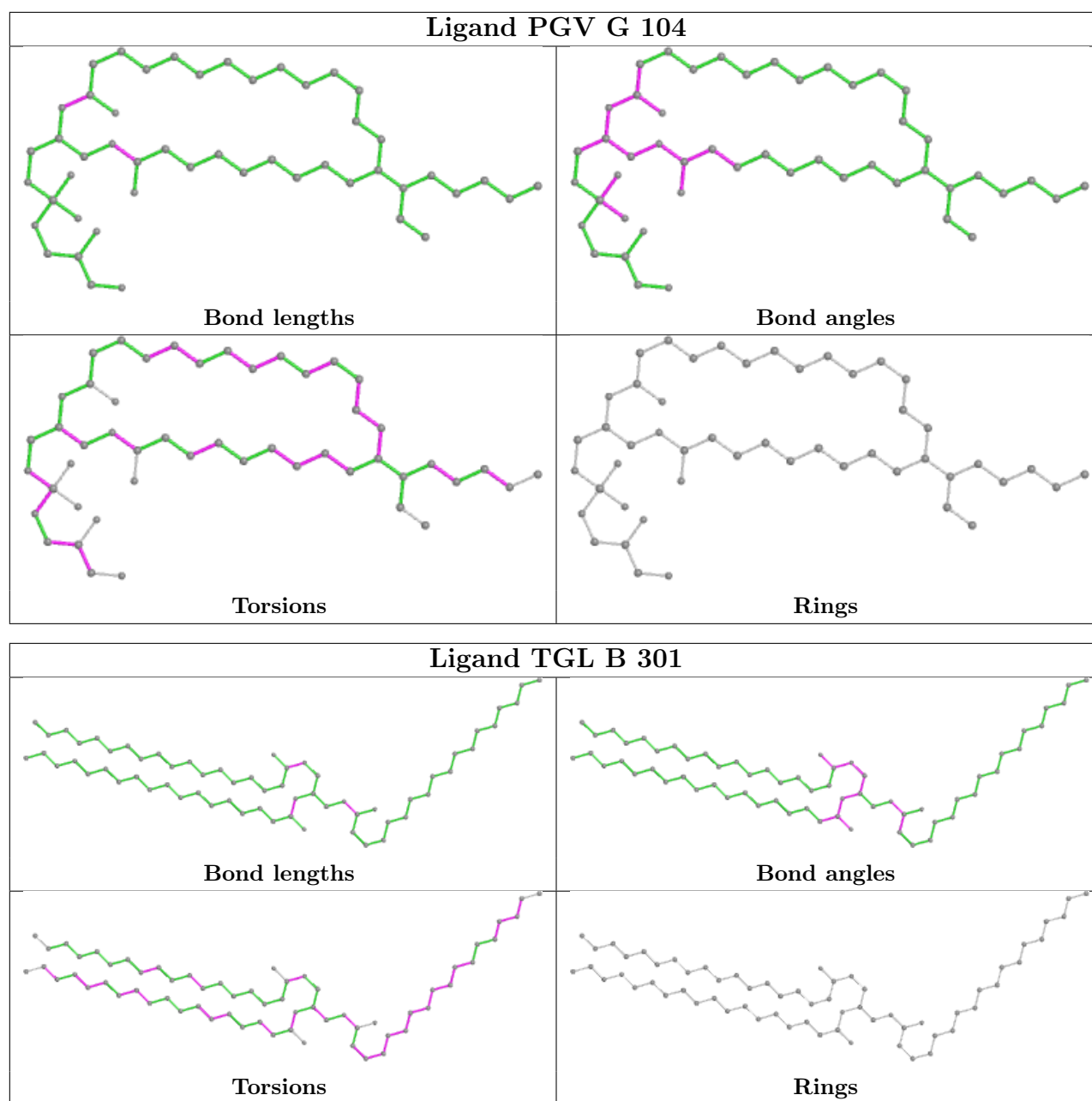


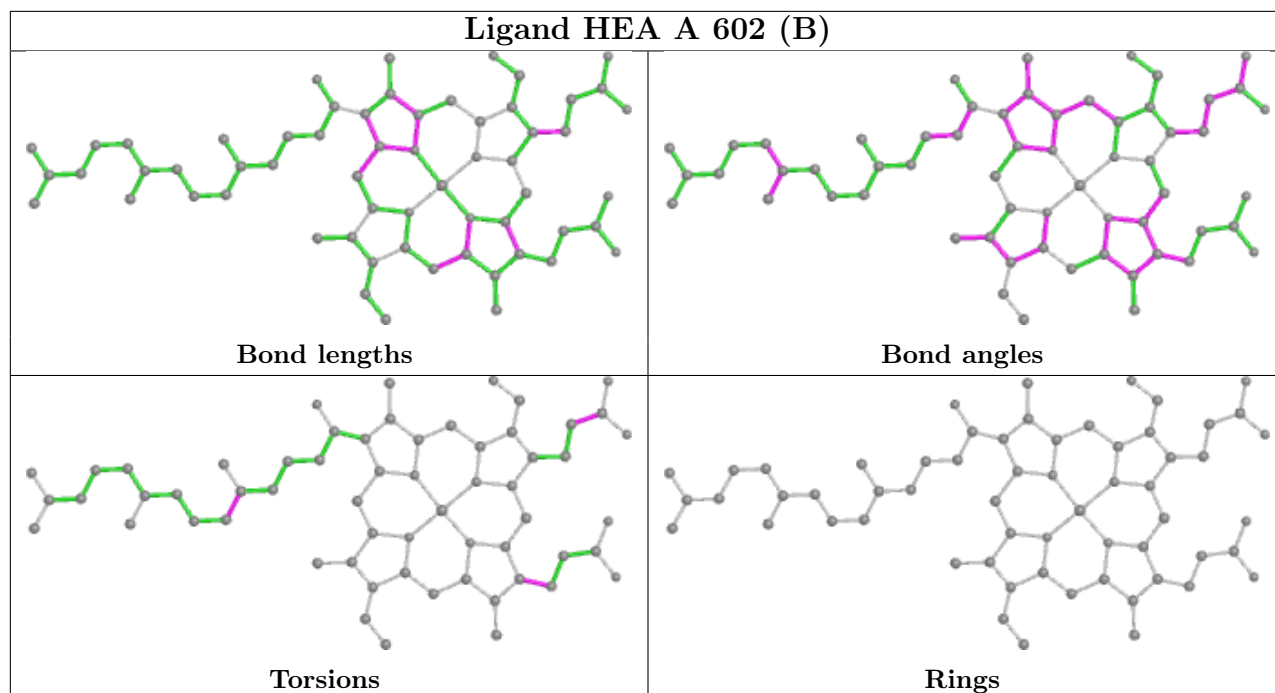
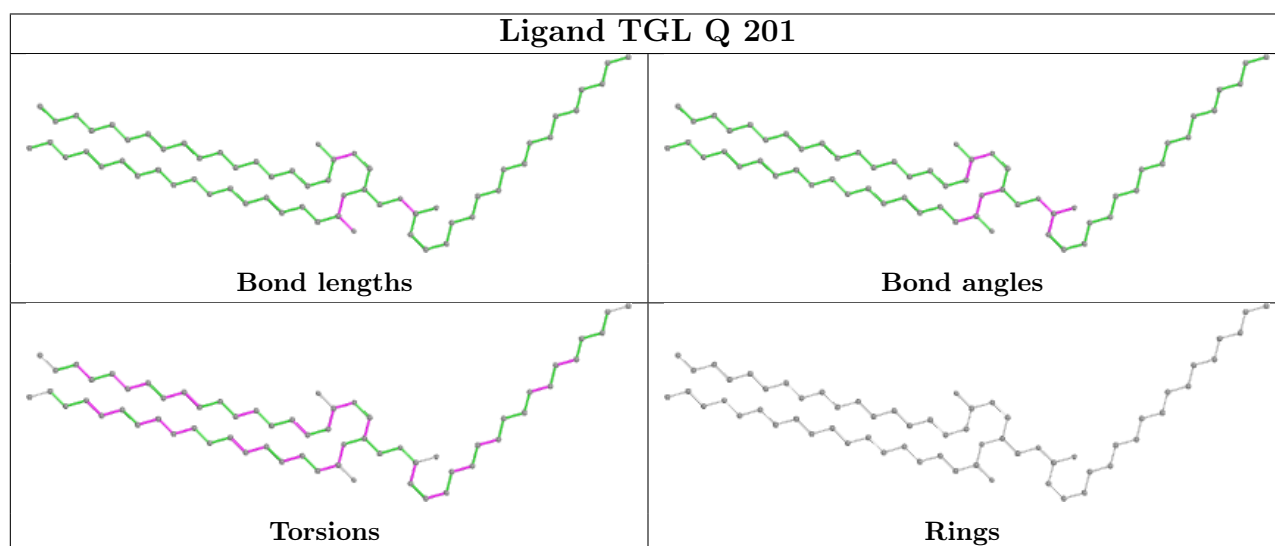
Ligand PSC B 304



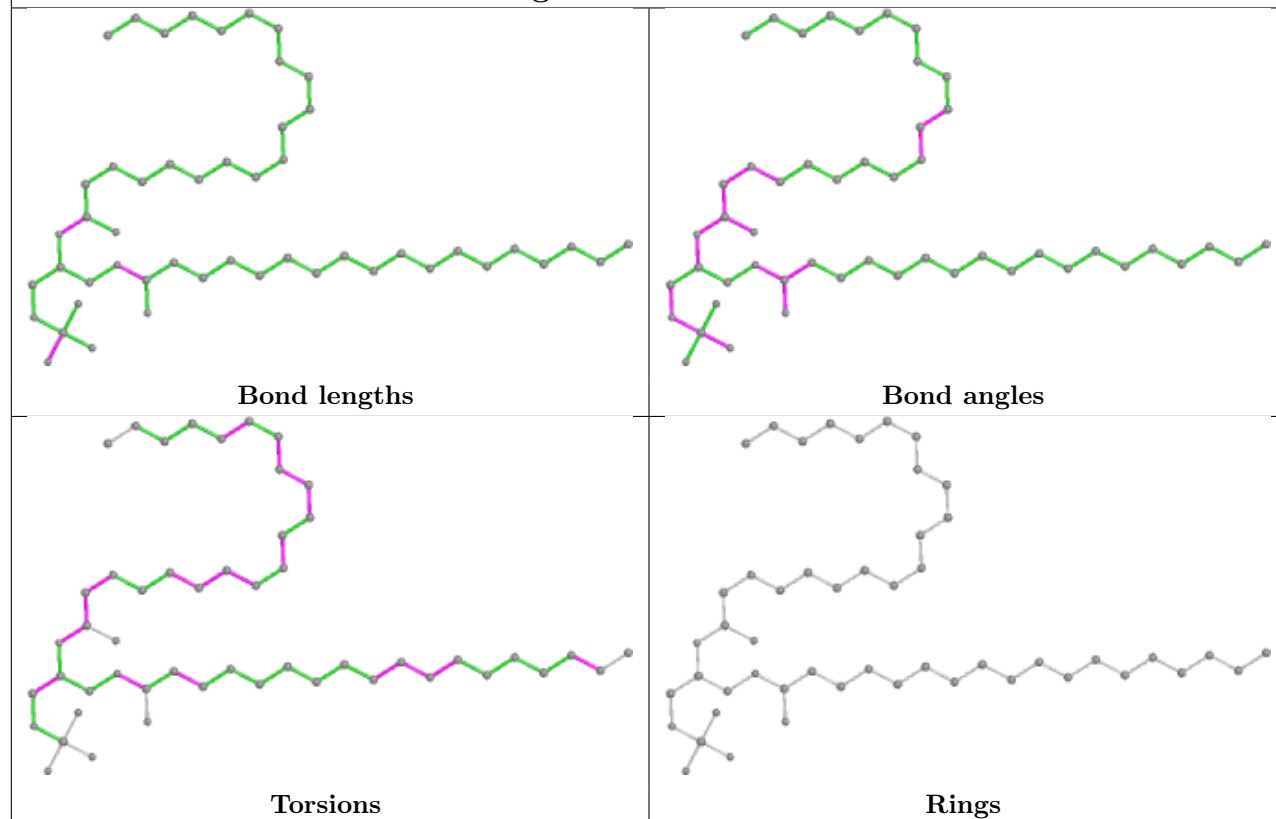




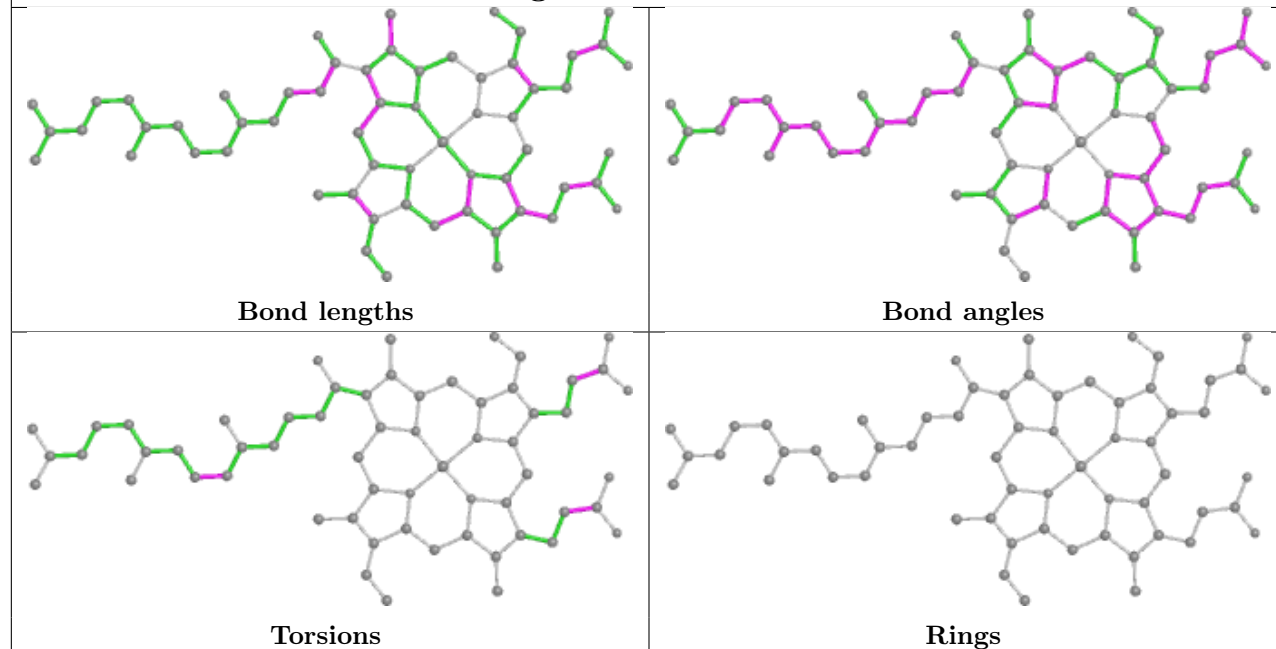


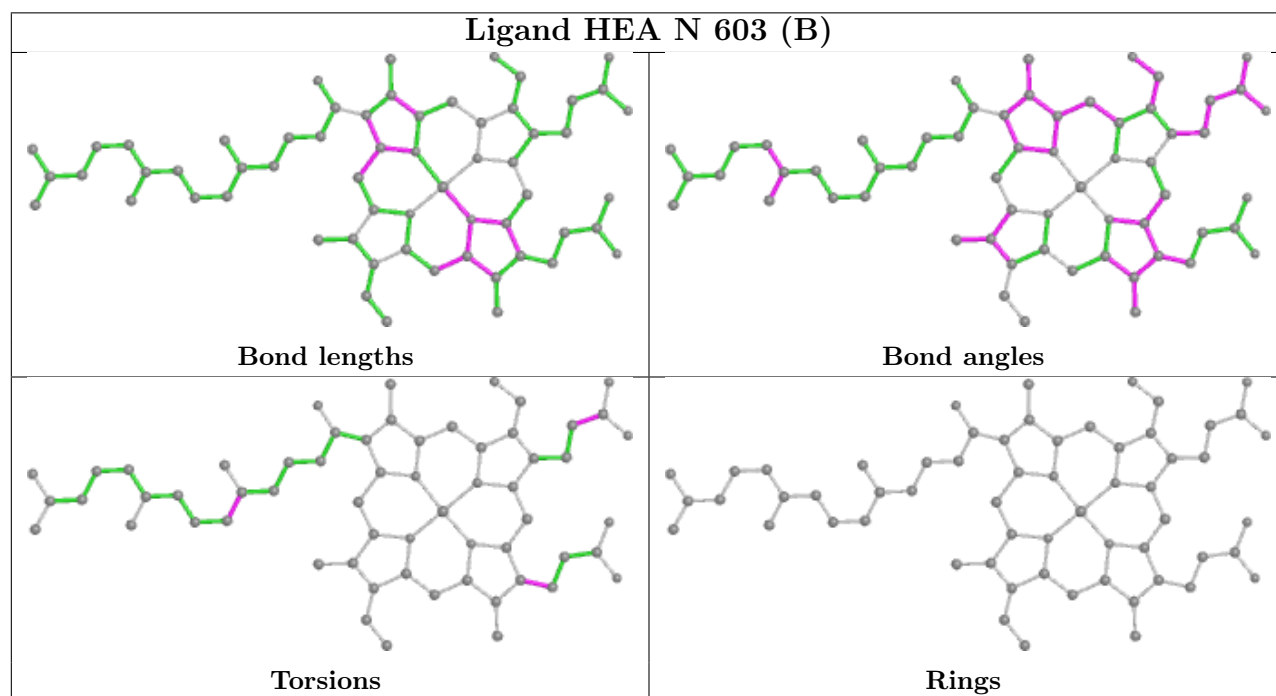
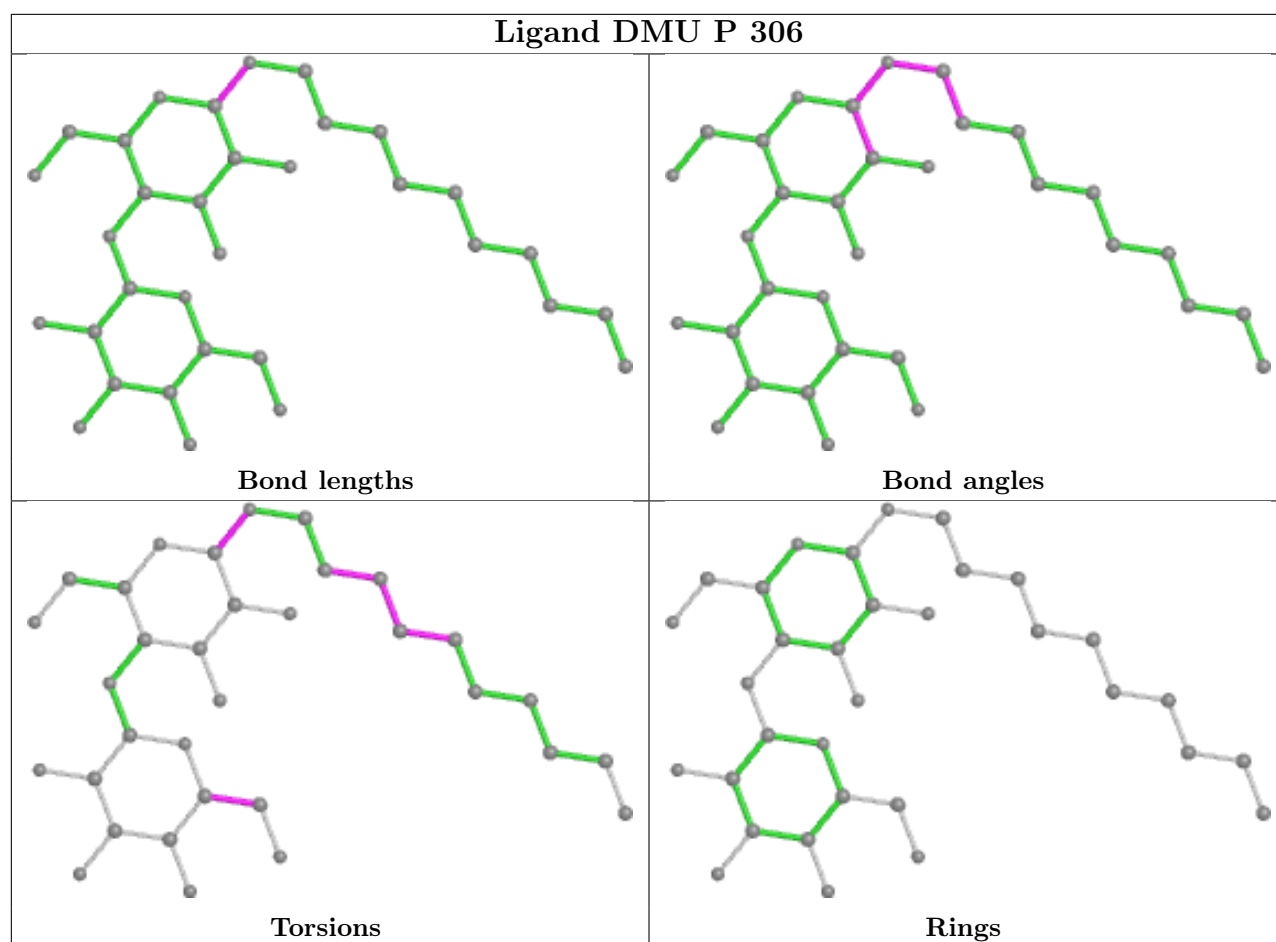
Ligand HEA A 602 (B)**Ligand TGL Q 201**

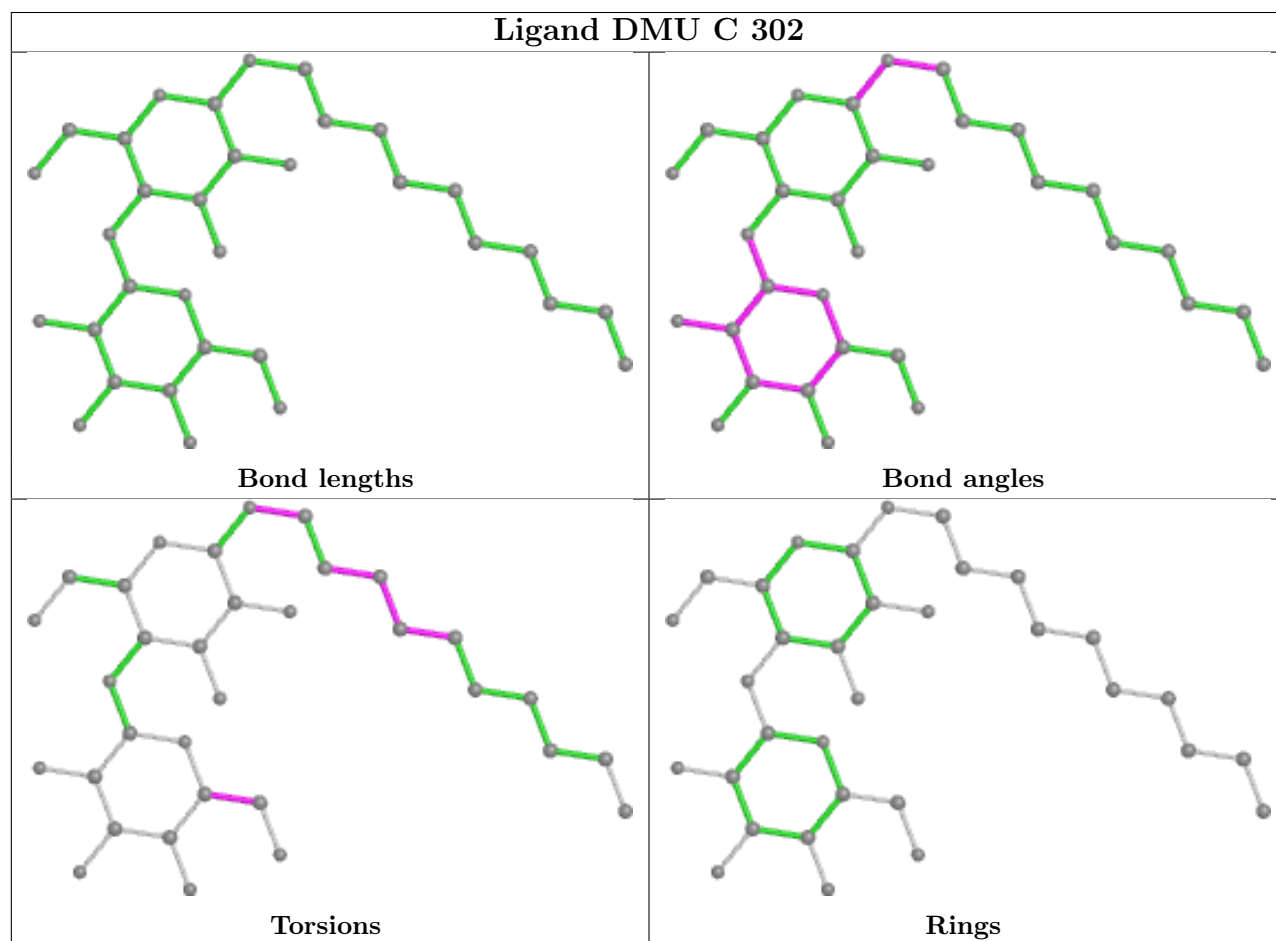
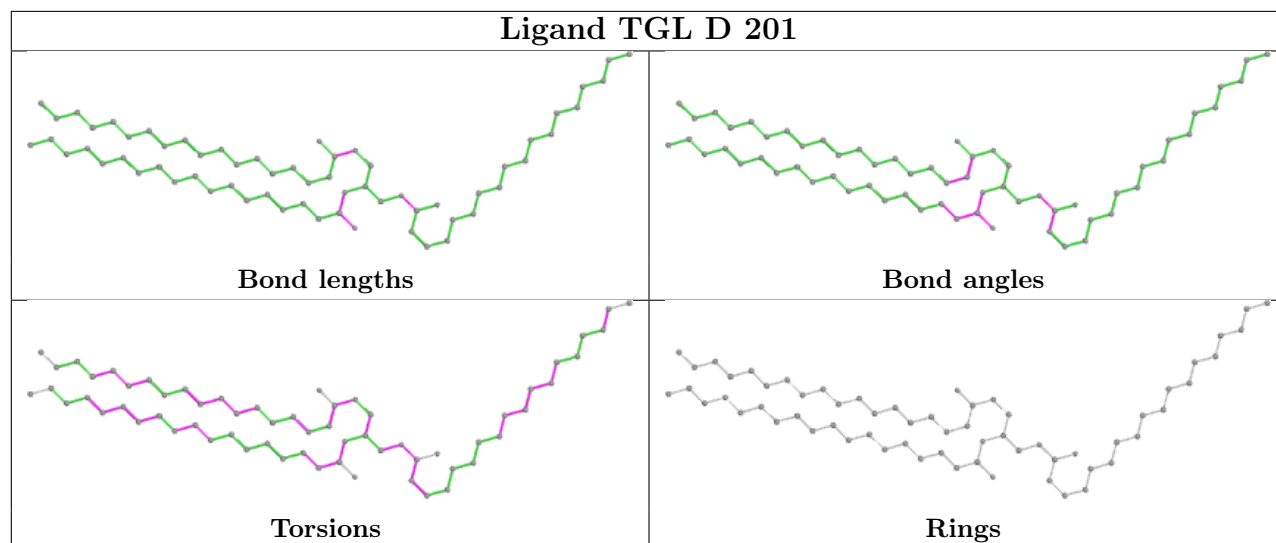
Ligand PEK T 101

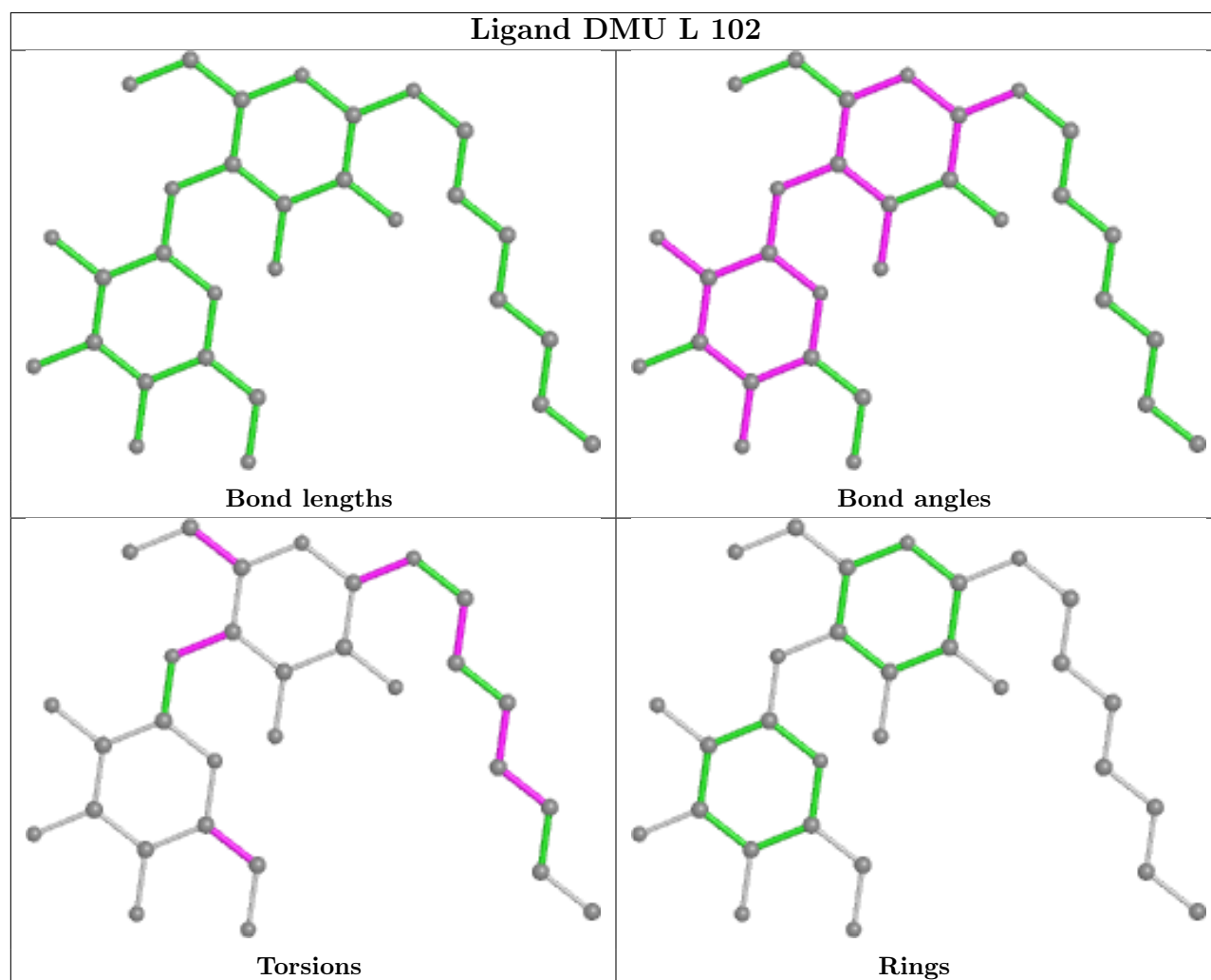
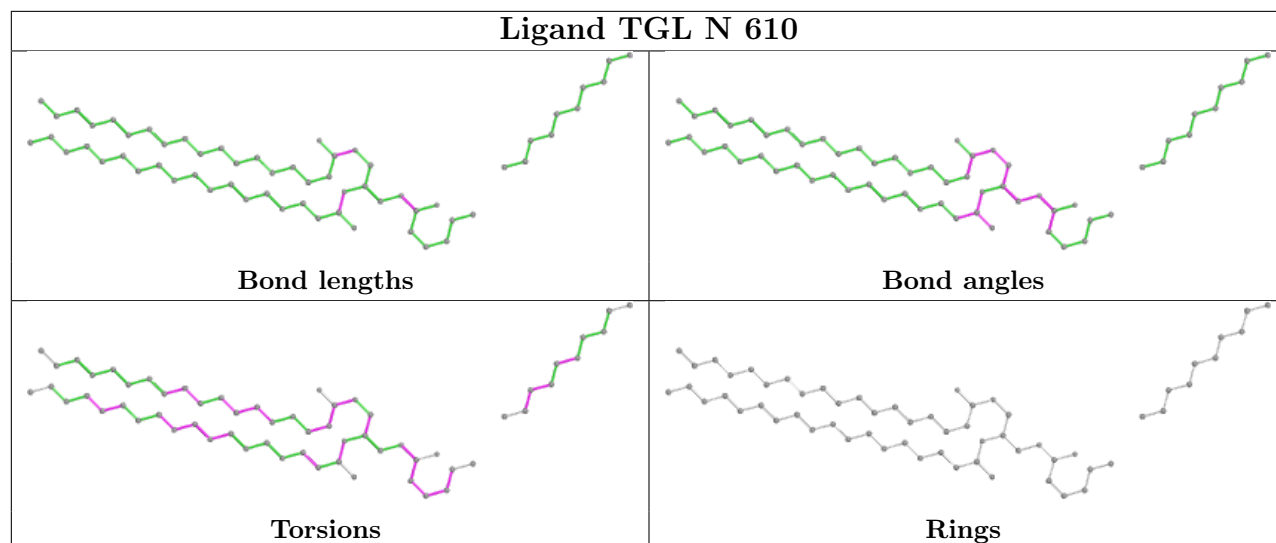


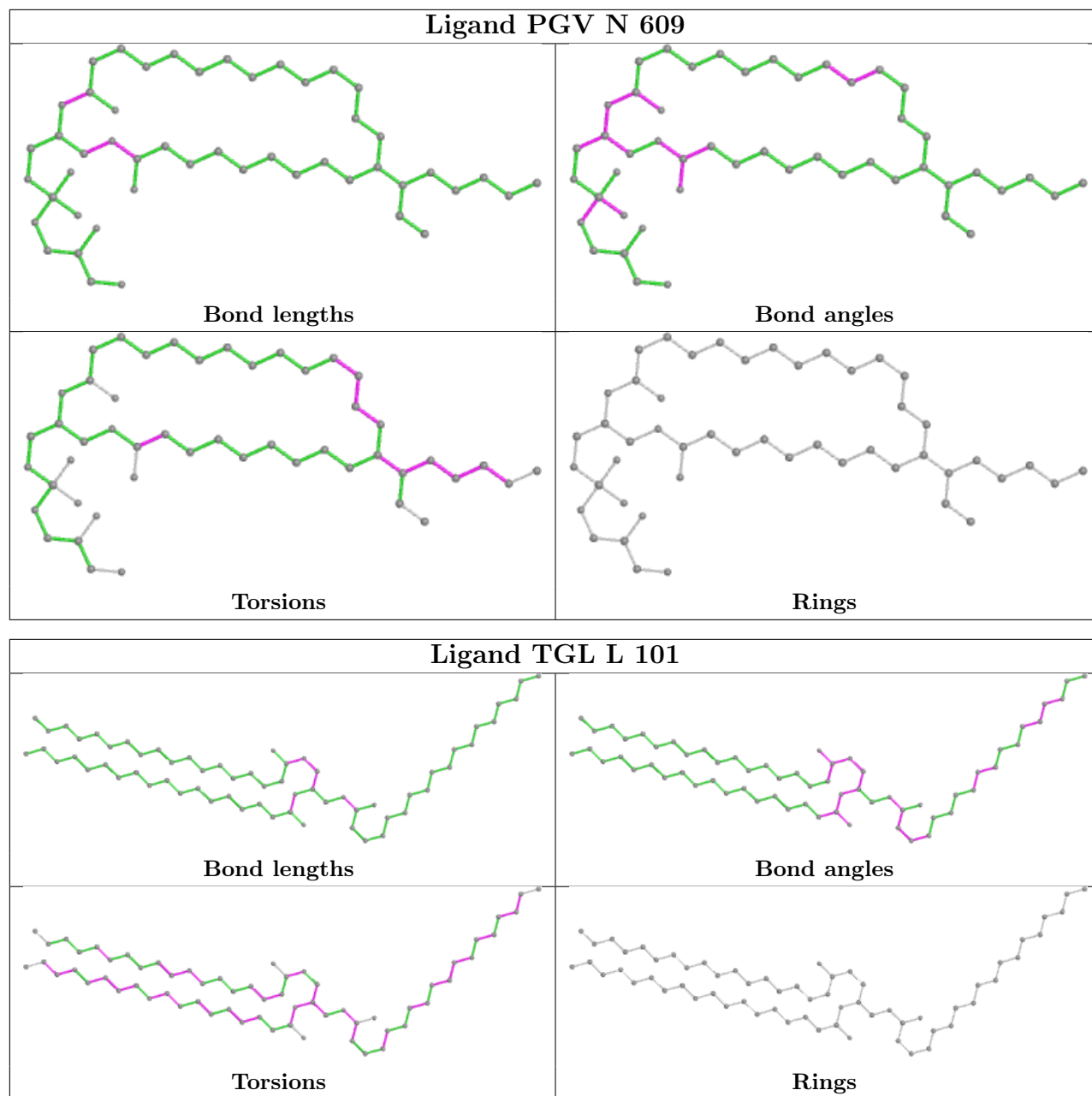
Ligand HEA A 601

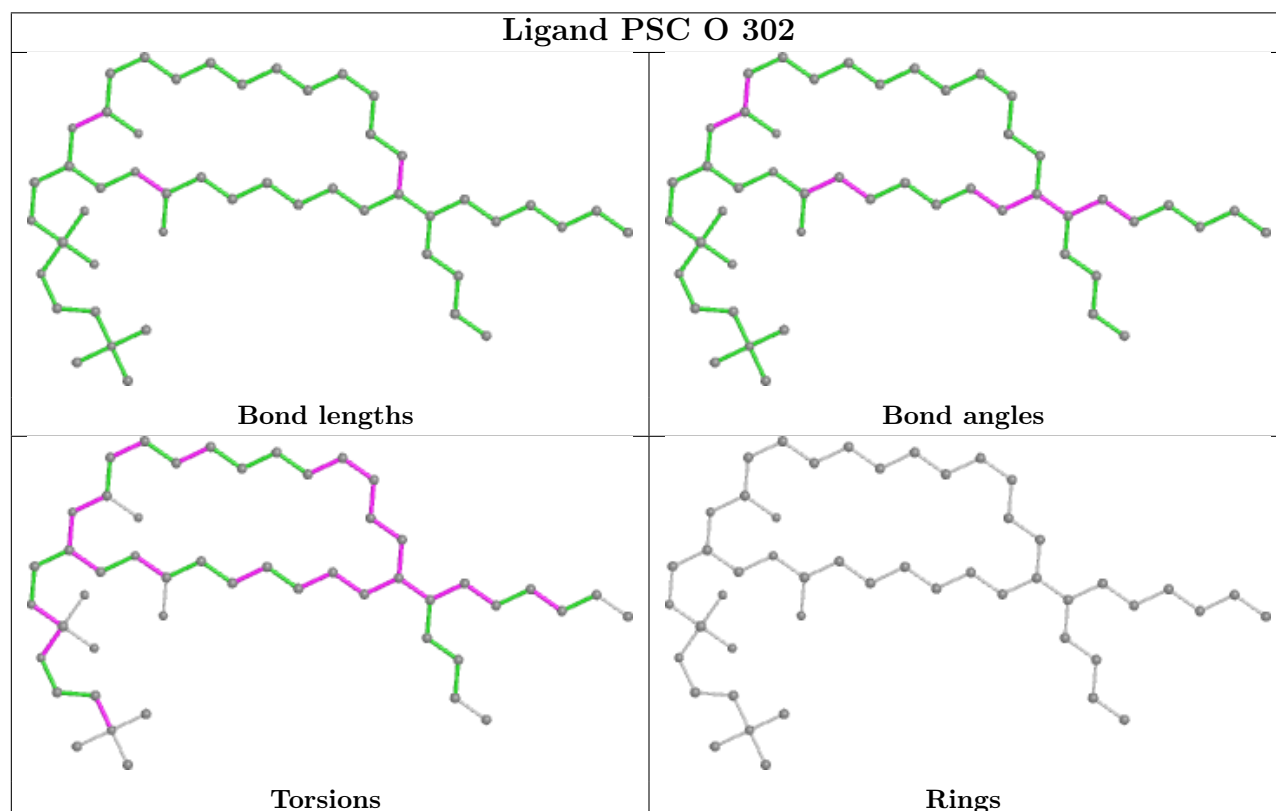
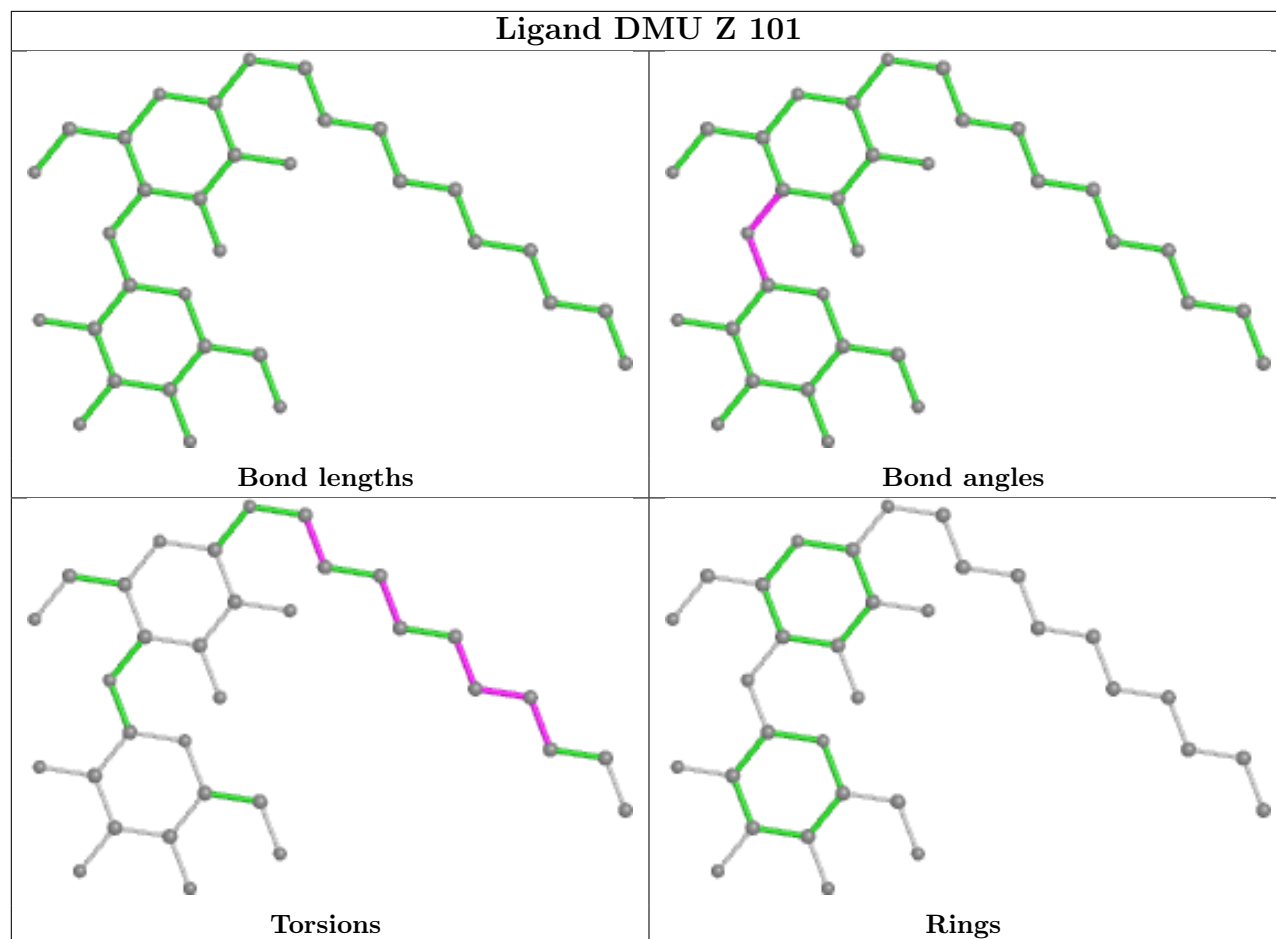


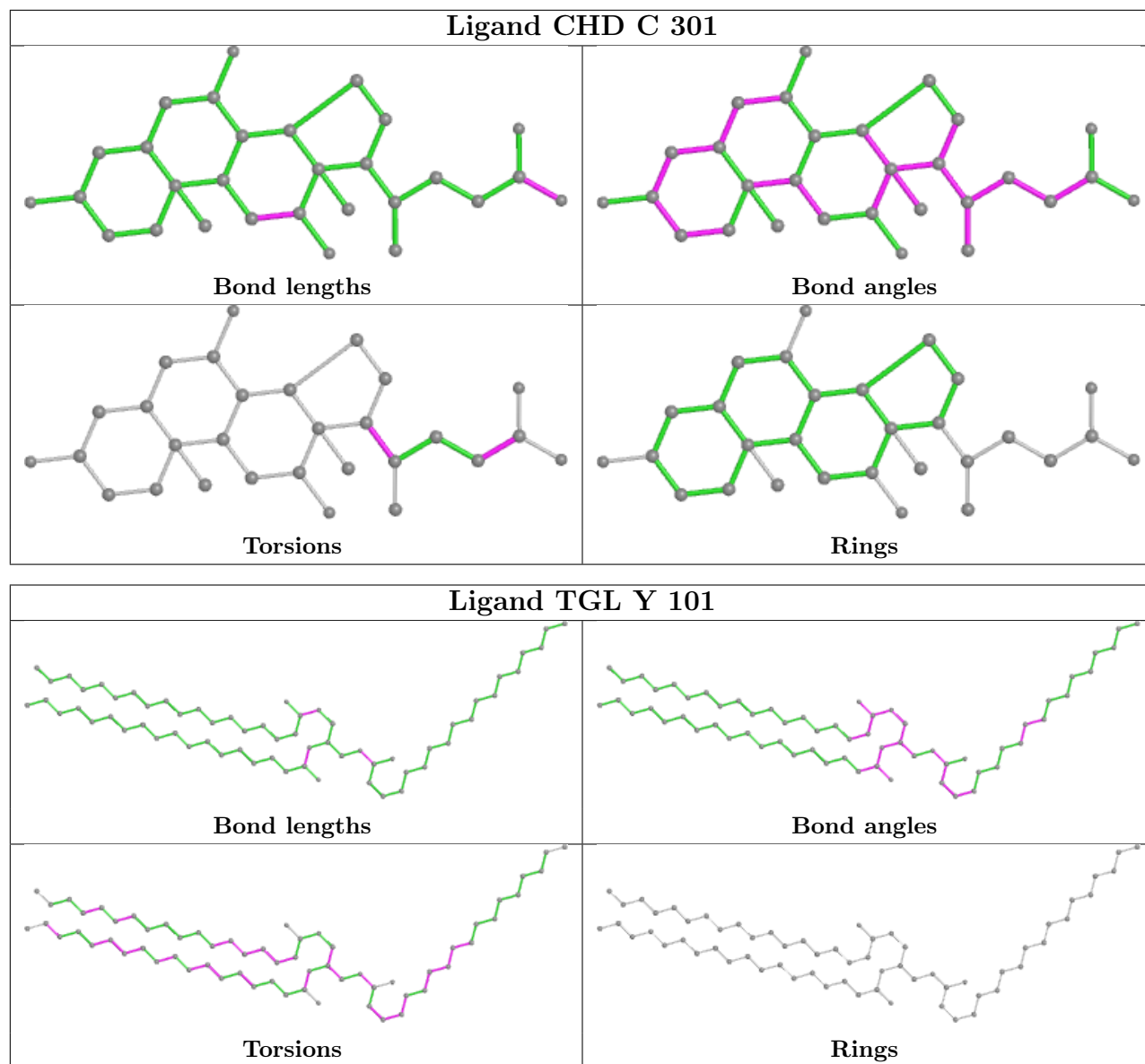


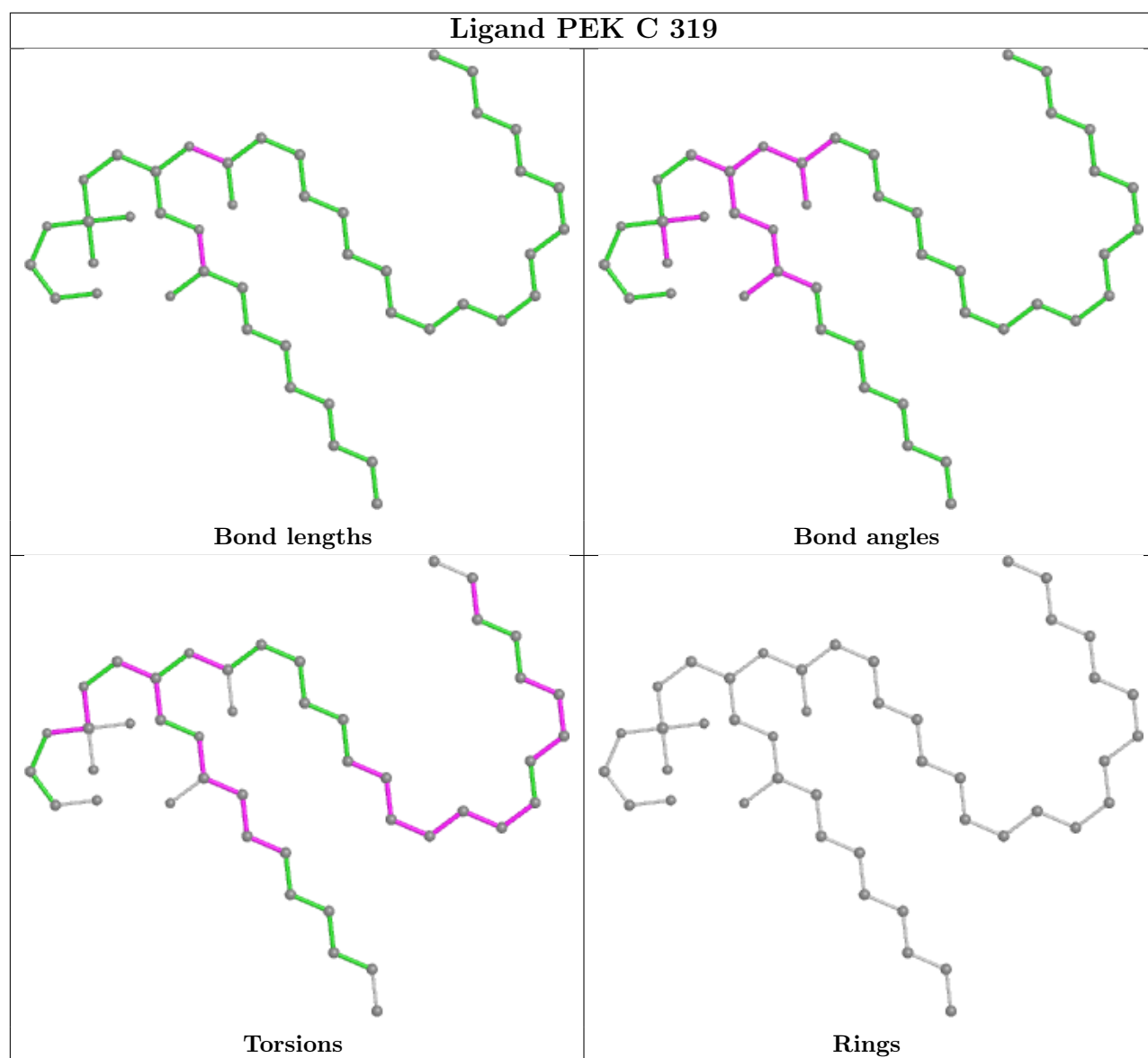


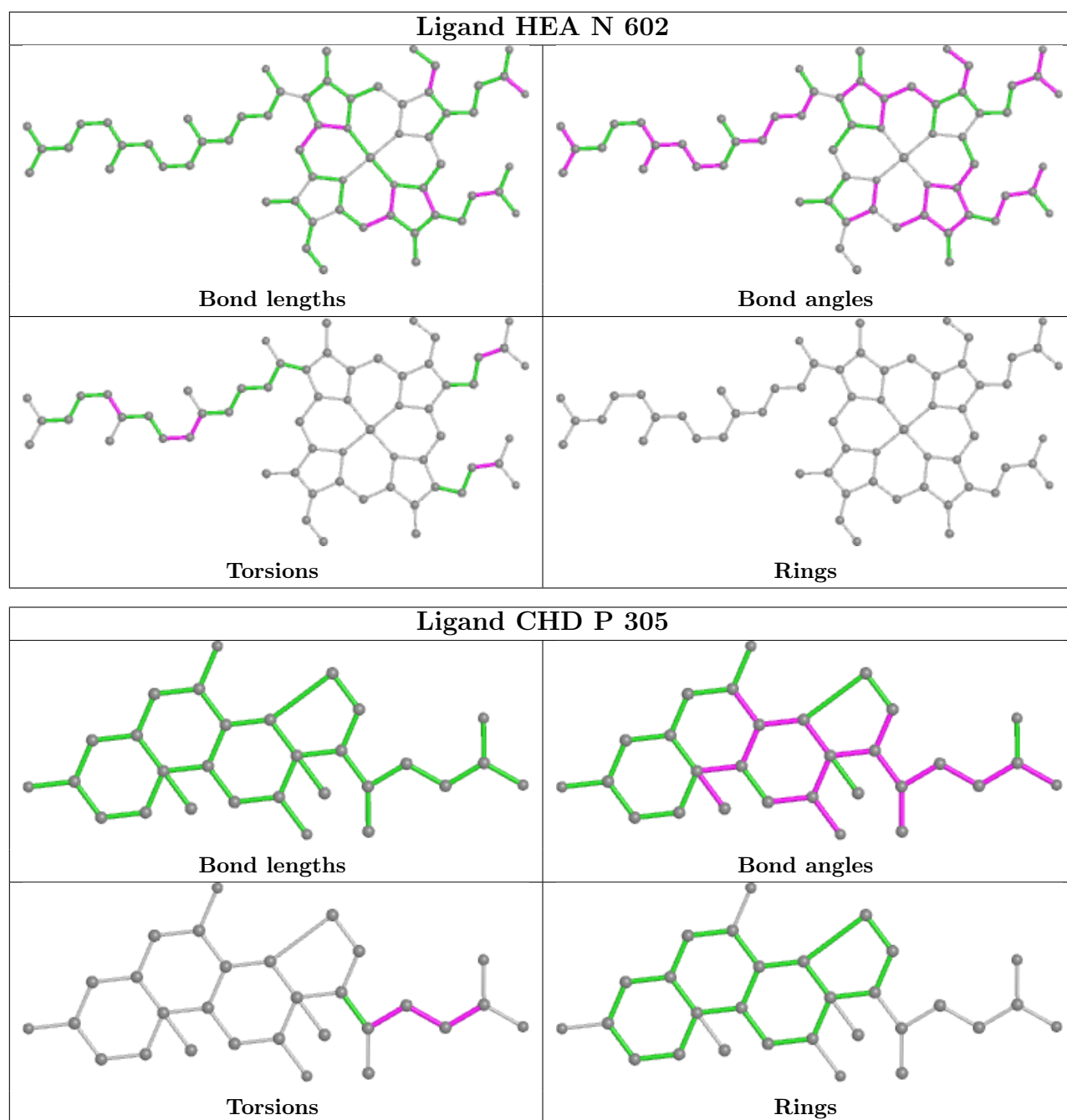


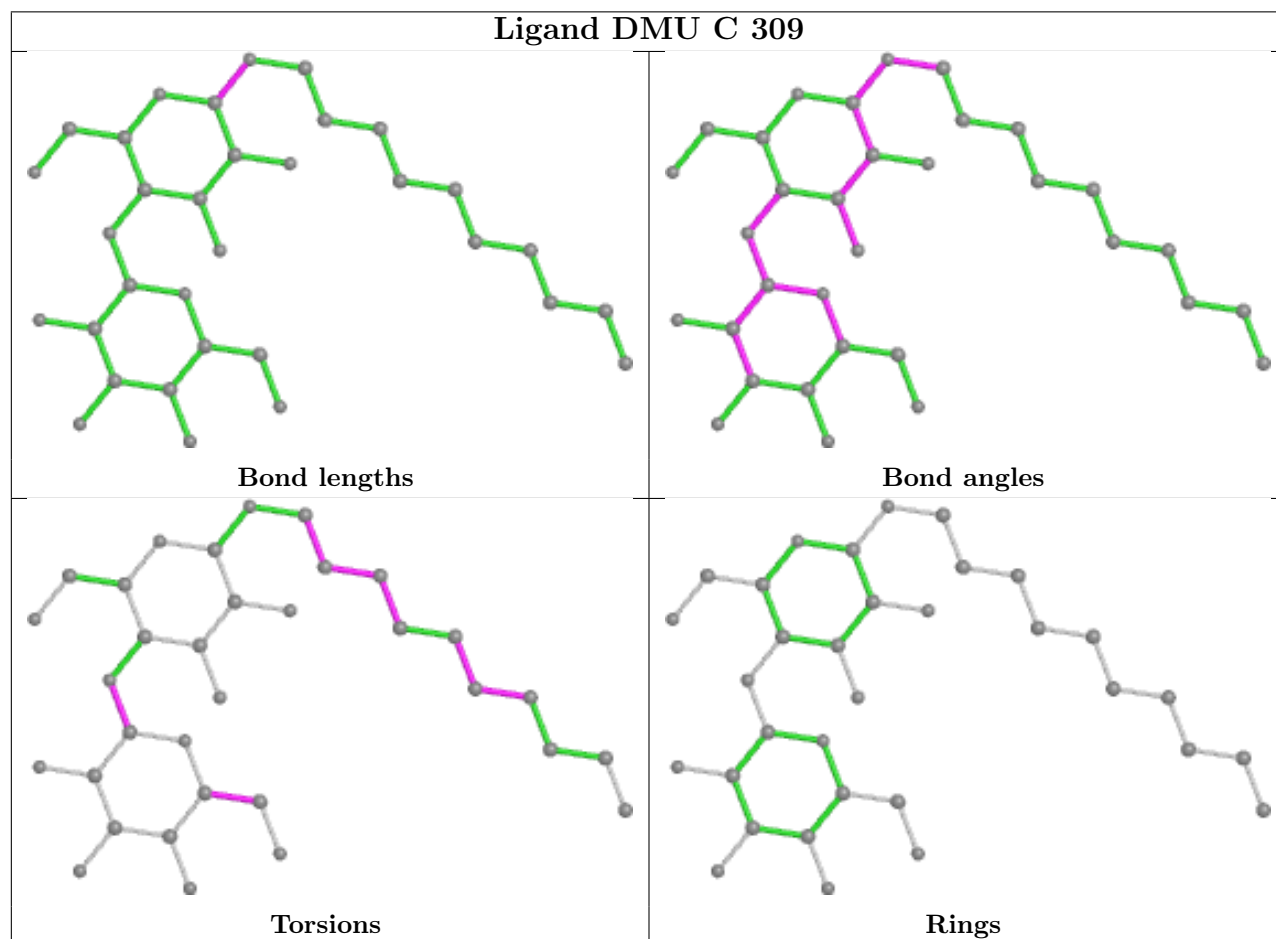
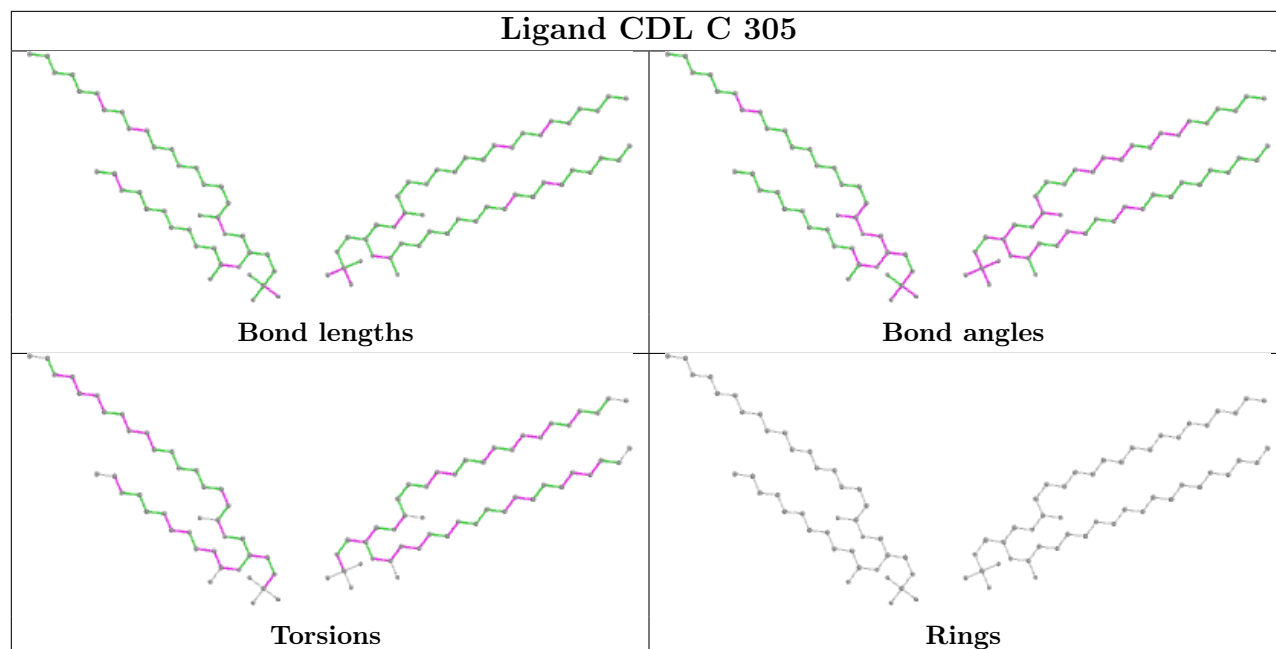


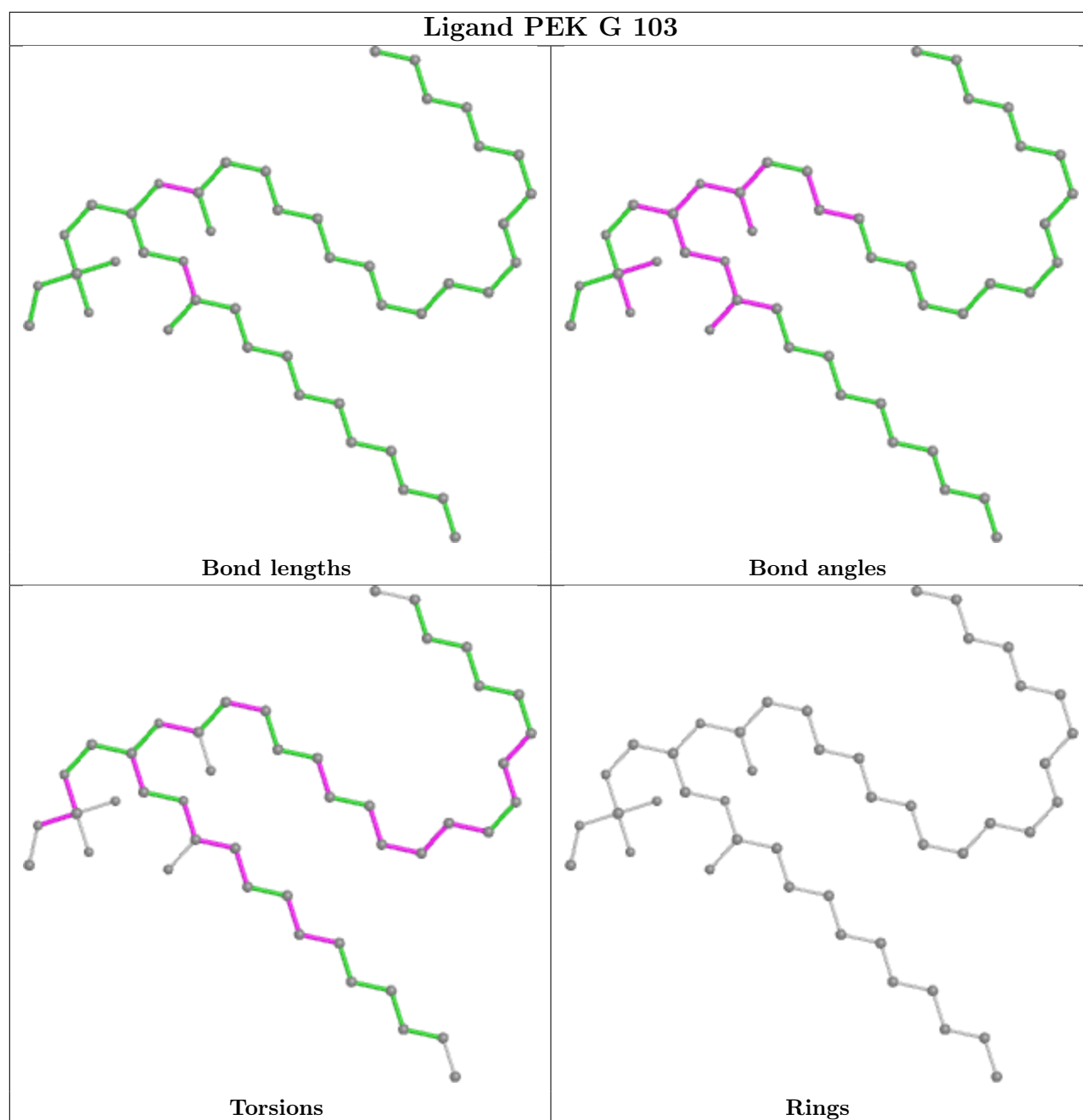


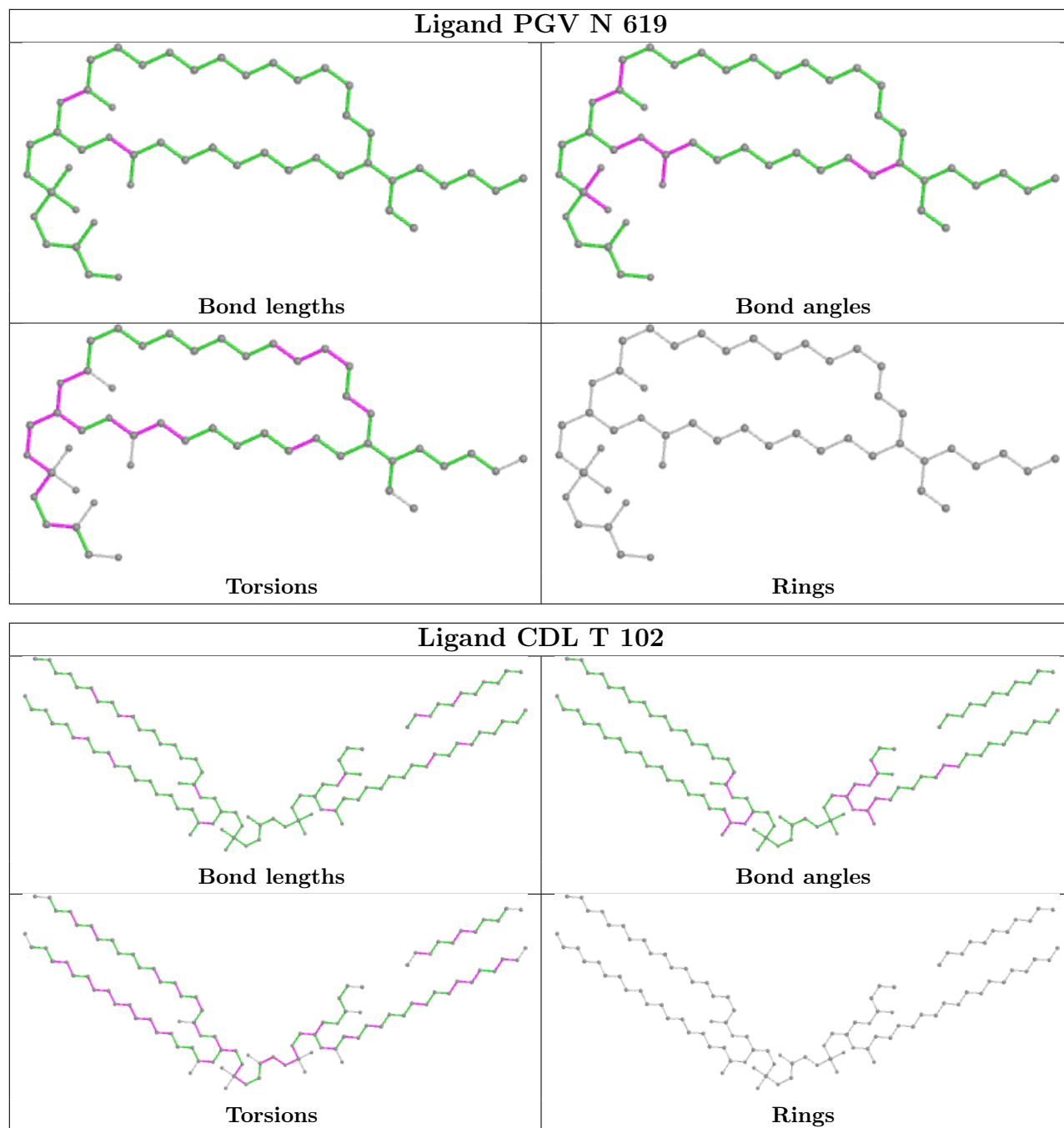


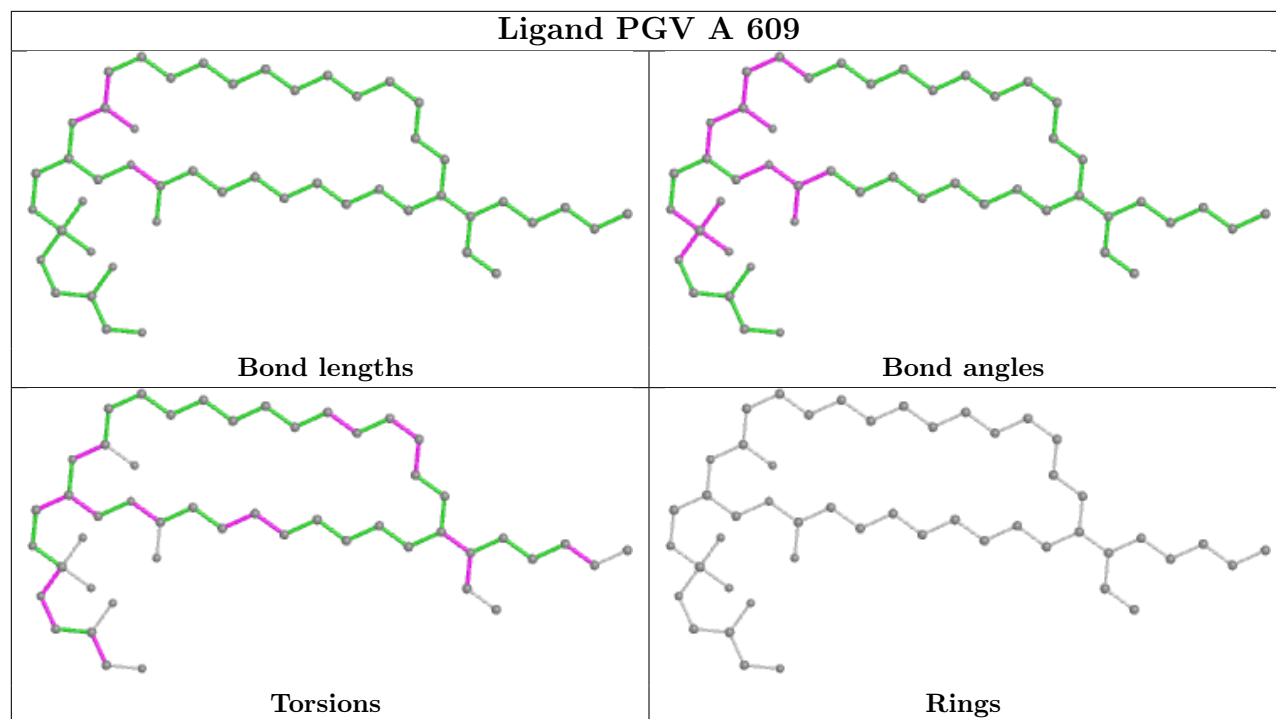












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	0.05	0 100 100	23, 29, 38, 83	0
1	N	513/514 (99%)	-0.01	1 (0%) 95 94	27, 35, 46, 84	0
2	B	226/227 (99%)	0.09	1 (0%) 92 92	27, 38, 59, 83	0
2	O	226/227 (99%)	0.13	4 (1%) 68 68	33, 45, 75, 104	0
3	C	259/261 (99%)	0.06	0 100 100	26, 33, 47, 97	0
3	P	259/261 (99%)	0.01	1 (0%) 92 92	28, 35, 48, 84	0
4	D	144/147 (97%)	-0.07	2 (1%) 75 76	31, 41, 67, 89	0
4	Q	144/147 (97%)	0.51	7 (4%) 29 28	43, 57, 90, 177	0
5	E	105/109 (96%)	-0.02	2 (1%) 66 66	33, 40, 66, 127	0
5	R	105/109 (96%)	-0.01	2 (1%) 66 66	38, 49, 73, 133	0
6	F	98/98 (100%)	0.46	7 (7%) 16 15	30, 41, 114, 163	0
6	S	98/98 (100%)	0.74	8 (8%) 11 11	32, 44, 117, 165	0
7	G	83/85 (97%)	0.92	15 (18%) 1 1	32, 42, 124, 144	0
7	T	83/85 (97%)	0.84	15 (18%) 1 1	30, 44, 113, 143	0
8	H	79/85 (92%)	0.29	7 (8%) 9 9	34, 46, 103, 121	0
8	U	79/85 (92%)	0.30	5 (6%) 20 19	39, 51, 118, 143	0
9	I	72/73 (98%)	0.43	6 (8%) 11 11	35, 51, 88, 99	0
9	V	72/73 (98%)	0.36	4 (5%) 24 23	38, 64, 88, 140	0
10	J	58/59 (98%)	0.31	3 (5%) 27 26	34, 44, 77, 122	0
10	W	58/59 (98%)	0.36	5 (8%) 10 10	37, 51, 80, 148	0
11	K	49/56 (87%)	0.03	1 (2%) 65 64	35, 44, 60, 69	0
11	X	49/56 (87%)	0.31	4 (8%) 11 11	49, 59, 87, 96	0
12	L	46/47 (97%)	0.02	1 (2%) 62 61	30, 35, 59, 93	0
12	Y	46/47 (97%)	0.11	1 (2%) 62 61	39, 47, 78, 132	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.23	4 (9%) 8 8	32, 37, 74, 118	0
13	Z	43/46 (93%)	0.29	3 (6%) 16 15	45, 53, 95, 174	0
All	All	3550/3614 (98%)	0.17	109 (3%) 49 47	23, 39, 78, 177	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	97	ALA	26.1
4	Q	6	VAL	14.2
4	Q	4	SER	13.5
4	Q	5	VAL	12.3
6	F	98	HIS	12.1
6	F	97	ALA	10.7
6	S	98	HIS	10.6
7	G	3	ALA	10.3
10	W	58	LYS	10.0
6	F	96	LEU	9.6
6	S	96	LEU	9.6
6	F	1	ALA	8.8
10	J	58	LYS	8.8
7	T	3	ALA	8.3
7	G	2	SER	8.3
6	S	94	HIS	7.8
13	Z	43	SER	7.7
4	Q	8	SER	6.6
7	G	42	ARG	6.6
9	I	37	PHE	6.4
6	F	2	SER	6.3
6	S	1	ALA	6.0
6	S	2	SER	5.9
7	T	40	GLY	5.8
5	R	5	HIS	5.5
7	T	36	TRP	5.4
5	E	109	VAL	5.2
8	H	46	LYS	4.9
13	M	42	LYS	4.8
7	G	10	GLY	4.6
7	T	8	HIS	4.6
9	I	25	PHE	4.6
7	G	4	ALA	4.5
7	T	7	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
7	T	5	LYS	4.4
7	G	5	LYS	4.4
8	U	7	LYS	4.3
6	S	93	PRO	4.2
6	F	95	GLN	4.2
7	G	6	GLY	4.2
7	T	10	GLY	4.2
7	T	42	ARG	4.1
8	U	8	ILE	4.1
9	I	30	GLY	4.1
7	T	39	SER	3.9
5	R	109	VAL	3.9
6	S	95	GLN	3.9
11	X	6	ALA	3.9
9	V	37	PHE	3.9
7	T	2	SER	3.9
13	Z	42	LYS	3.8
2	O	113	TYR	3.7
9	V	25	PHE	3.7
7	G	40	GLY	3.7
7	G	1	ALA	3.7
3	P	3	HIS	3.6
4	Q	7	LYS	3.6
8	U	44	THR	3.6
9	I	29	LEU	3.6
7	G	36	TRP	3.4
8	H	45	ALA	3.4
12	Y	47	LYS	3.4
8	H	44	THR	3.4
7	G	8	HIS	3.2
7	G	7	ASP	3.1
2	O	91	ASN	3.1
13	M	40	TYR	3.0
7	G	37	LEU	3.0
10	J	1	PHE	2.9
7	T	9	GLY	2.9
10	W	57	HIS	2.9
9	V	34	PHE	2.9
1	N	311[A]	ILE	2.8
4	Q	87[A]	PHE	2.8
4	D	4	SER	2.8
5	E	5	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
7	T	4	ALA	2.7
9	V	29	LEU	2.7
8	U	10	ASN	2.6
9	I	33	THR	2.6
7	T	6	GLY	2.6
11	X	7	PRO	2.6
4	D	5	VAL	2.6
7	T	84	LYS	2.5
4	Q	147	LYS	2.5
7	G	9	GLY	2.5
11	X	13	TYR	2.4
10	J	57	HIS	2.4
10	W	52	TRP	2.4
13	Z	40	TYR	2.3
8	H	43	MET	2.3
6	F	94	HIS	2.3
12	L	2	HIS	2.3
8	H	47	GLY	2.3
8	H	48	GLY	2.2
11	X	52	GLU	2.2
2	O	32[A]	PHE	2.2
8	H	8	ILE	2.2
10	W	55	PHE	2.2
7	G	12	GLY	2.1
11	K	47	ARG	2.1
8	U	46	LYS	2.1
7	T	41	HIS	2.1
2	O	40[A]	TYR	2.1
13	M	43	SER	2.0
9	I	34	PHE	2.0
10	W	56	PRO	2.0
2	B	59	GLN	2.0
13	M	39	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	TPO	G	11	11/12	0.52	0.38	98,137,157,162	0
7	TPO	T	11	11/12	0.62	0.29	115,127,158,161	0
9	SAC	V	1	9/10	0.69	0.19	128,153,165,171	0
9	SAC	I	1	9/10	0.87	0.17	79,99,108,120	0
1	FME	N	1	10/11	0.97	0.12	44,59,81,83	0
1	FME	A	1	10/11	0.98	0.13	40,51,92,92	0
2	FME	O	1	10/11	0.98	0.13	38,44,54,89	0
2	FME	B	1	10/11	0.99	0.12	29,34,46,89	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	Q	203	4/4	0.40	0.20	78,79,90,92	0
20	EDO	C	317	4/4	0.53	0.71	75,93,107,109	0
22	CHD	W	101	29/29	0.55	0.41	54,125,146,153	0
20	EDO	D	205	4/4	0.57	0.16	61,62,70,72	0
26	CDL	T	102	97/100	0.63	0.33	41,86,149,173	0
25	DMU	C	302	33/33	0.65	0.37	32,85,116,134	0
27	PEK	C	319	44/53	0.67	0.35	50,80,155,168	0
20	EDO	A	616	4/4	0.68	0.39	45,53,54,102	0
25	DMU	L	102	30/33	0.68	0.25	45,95,141,147	0
27	PEK	T	101	50/53	0.68	0.28	40,82,132,162	0
24	PSC	B	304	50/52	0.69	0.33	35,80,154,170	0
26	CDL	N	601	96/100	0.70	0.35	50,90,144,168	0
20	EDO	C	316	4/4	0.71	0.36	56,80,96,103	0
22	CHD	J	101	29/29	0.71	0.24	88,129,148,149	0
27	PEK	G	103	44/53	0.73	0.26	45,84,153,164	0
25	DMU	P	306	33/33	0.74	0.30	45,83,118,130	0
21	TGL	Q	201	63/63	0.74	0.22	46,77,102,118	0
26	CDL	P	304	80/100	0.77	0.29	44,84,125,140	0
19	PGV	C	308	49/51	0.77	0.21	42,76,127,157	0
27	PEK	C	307	53/53	0.77	0.25	43,78,143,155	0
20	EDO	O	305	4/4	0.78	0.12	71,75,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	A	617	4/4	0.78	0.23	59,62,68,72	0
21	TGL	Y	101	63/63	0.79	0.29	45,74,117,149	0
20	EDO	C	312	4/4	0.79	0.14	68,81,88,93	0
19	PGV	G	104	51/51	0.80	0.27	47,82,123,155	0
24	PSC	O	302	51/52	0.80	0.34	46,87,162,170	0
21	TGL	N	610	61/63	0.81	0.25	52,82,106,121	0
20	EDO	A	619	4/4	0.81	0.23	52,52,61,67	0
20	EDO	G	105	4/4	0.81	0.26	55,66,73,94	0
25	DMU	C	309	33/33	0.81	0.27	53,79,115,123	0
21	TGL	D	201	63/63	0.81	0.22	36,68,97,114	0
21	TGL	L	101	63/63	0.81	0.21	29,65,102,125	0
26	CDL	C	305	89/100	0.81	0.25	46,79,109,126	0
20	EDO	D	202	4/4	0.82	0.34	66,77,81,95	0
25	DMU	C	310	22/33	0.82	0.17	59,73,96,117	0
20	EDO	R	201	4/4	0.82	0.27	64,66,69,82	0
19	PGV	N	619	51/51	0.82	0.33	45,84,139,154	0
20	EDO	R	205	4/4	0.83	0.42	54,57,60,80	0
22	CHD	P	305	29/29	0.83	0.24	54,67,81,93	0
20	EDO	C	314	4/4	0.83	0.29	58,79,79,82	0
20	EDO	H	101	4/4	0.84	0.19	53,54,73,76	0
25	DMU	P	307	33/33	0.84	0.21	50,76,108,114	0
25	DMU	P	308	33/33	0.85	0.24	57,85,106,118	0
20	EDO	A	615	4/4	0.85	0.31	48,58,59,63	0
20	EDO	L	103	4/4	0.85	0.17	67,72,75,104	0
21	TGL	B	301	63/63	0.86	0.19	35,76,108,120	0
25	DMU	Z	101	33/33	0.87	0.16	51,63,80,84	0
19	PGV	A	609	51/51	0.87	0.25	34,68,120,156	0
20	EDO	N	616	4/4	0.87	0.14	48,50,53,60	0
20	EDO	E	203	4/4	0.88	0.28	46,49,59,75	0
20	EDO	A	614	4/4	0.88	0.17	39,45,47,50	0
20	EDO	C	315	4/4	0.88	0.17	62,74,76,83	0
17	NA	P	302	1/1	0.88	0.14	43,43,43,43	0
20	EDO	B	306	4/4	0.89	0.19	32,40,50,61	0
20	EDO	N	613	4/4	0.89	0.14	54,58,68,70	0
22	CHD	C	306	29/29	0.89	0.24	48,66,79,86	0
20	EDO	U	101	4/4	0.89	0.14	67,68,73,85	0
20	EDO	A	611	4/4	0.89	0.18	51,54,64,72	0
20	EDO	C	313	4/4	0.89	0.12	57,64,65,88	0
20	EDO	P	311	4/4	0.89	0.29	45,61,76,77	0
17	NA	C	303	1/1	0.89	0.11	41,41,41,41	0
20	EDO	R	202	4/4	0.90	0.13	56,67,69,85	0
20	EDO	V	101	4/4	0.90	0.20	56,66,74,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	S	101	4/4	0.90	0.22	44,52,59,64	0
20	EDO	A	612	4/4	0.91	0.12	32,33,35,39	0
20	EDO	H	102	4/4	0.91	0.10	66,67,78,83	0
20	EDO	P	309	4/4	0.91	0.23	34,43,47,60	0
25	DMU	M	101	33/33	0.91	0.12	38,50,65,78	0
20	EDO	E	205	4/4	0.92	0.21	58,58,71,77	0
20	EDO	E	201	4/4	0.92	0.11	43,49,54,66	0
20	EDO	Q	202	4/4	0.92	0.15	62,64,67,73	0
20	EDO	N	612	4/4	0.93	0.22	40,50,54,55	0
20	EDO	D	204	4/4	0.93	0.22	50,62,68,74	0
20	EDO	N	614	4/4	0.93	0.14	36,37,37,46	0
20	EDO	F	103	4/4	0.93	0.14	36,37,41,41	0
20	EDO	N	617	4/4	0.93	0.21	48,49,54,58	0
20	EDO	O	304	4/4	0.93	0.13	55,67,68,82	0
20	EDO	R	206	4/4	0.93	0.25	47,50,60,71	0
20	EDO	F	105	4/4	0.93	0.18	49,57,71,82	0
20	EDO	S	104	4/4	0.93	0.29	42,47,81,88	0
20	EDO	F	106	4/4	0.93	0.14	42,54,65,68	0
16	MG	N	605	1/1	0.94	0.05	29,29,29,29	0
20	EDO	E	204	4/4	0.94	0.07	39,41,41,49	0
27	PEK	P	312	53/53	0.94	0.16	32,52,90,108	0
20	EDO	F	104	4/4	0.94	0.21	45,51,62,72	0
20	EDO	N	611	4/4	0.95	0.20	65,65,72,81	0
20	EDO	N	615	4/4	0.95	0.12	30,36,39,41	0
20	EDO	R	203	4/4	0.95	0.19	48,64,68,73	0
22	CHD	C	301	29/29	0.95	0.10	30,33,39,43	0
20	EDO	C	318	4/4	0.96	0.26	38,40,47,70	0
18	AZI	A	607[B]	3/3	0.96	0.14	21,21,29,42	3
20	EDO	A	618	4/4	0.96	0.24	35,42,67,70	0
18	AZI	N	608[A]	3/3	0.96	0.12	38,38,40,42	0
27	PEK	G	101	53/53	0.96	0.15	31,48,87,113	0
18	AZI	N	608[B]	3/3	0.96	0.12	29,29,38,39	3
22	CHD	P	301	29/29	0.96	0.09	31,37,46,47	0
18	AZI	A	607[A]	3/3	0.96	0.14	30,30,32,34	3
20	EDO	A	610	4/4	0.97	0.26	34,41,45,77	0
20	EDO	P	310	4/4	0.97	0.20	44,44,45,51	0
20	EDO	T	103	4/4	0.97	0.16	39,39,40,42	0
20	EDO	E	202	4/4	0.97	0.14	44,45,46,47	0
20	EDO	C	311	4/4	0.97	0.09	40,42,44,46	0
20	EDO	G	106	4/4	0.97	0.11	33,36,41,45	0
19	PGV	C	304	51/51	0.97	0.13	26,35,94,112	0
19	PGV	N	609	51/51	0.97	0.14	26,38,74,82	0

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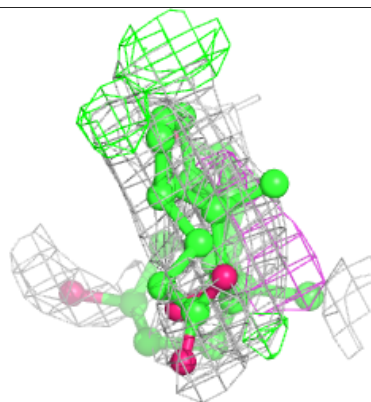
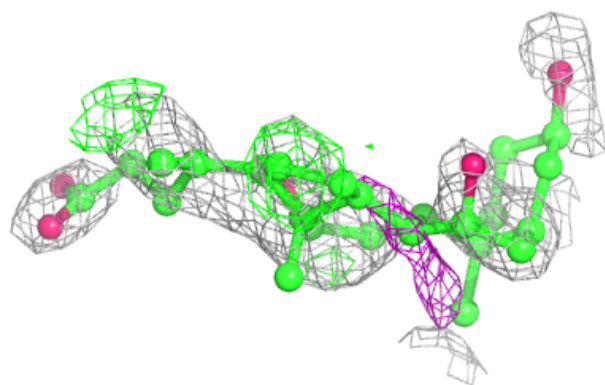
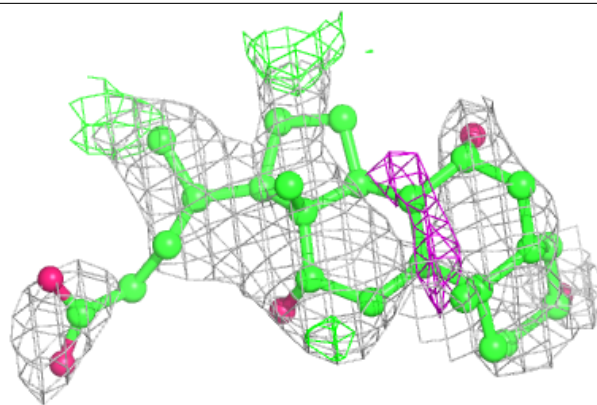
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
20	EDO	O	303	4/4	0.97	0.16	36,39,40,41	0
20	EDO	R	204	4/4	0.97	0.15	41,48,49,52	0
20	EDO	A	613	4/4	0.97	0.11	28,29,32,37	0
22	CHD	B	302	29/29	0.97	0.11	28,33,37,48	0
19	PGV	A	608	51/51	0.97	0.14	25,34,74,81	0
22	CHD	G	102	29/29	0.98	0.11	30,35,41,47	0
20	EDO	D	203	4/4	0.98	0.16	40,43,57,69	0
17	NA	N	606	1/1	0.98	0.07	38,38,38,38	0
19	PGV	P	303	51/51	0.98	0.14	29,39,75,93	0
14	HEA	N	602	60/60	0.98	0.12	27,34,58,61	0
14	HEA	N	603[A]	60/60	0.98	0.14	16,27,36,40	60
20	EDO	N	618	4/4	0.98	0.18	44,57,61,71	0
14	HEA	N	603[B]	60/60	0.98	0.14	19,31,50,59	60
20	EDO	B	305	4/4	0.98	0.15	29,30,34,38	0
14	HEA	A	602[A]	60/60	0.98	0.14	16,26,35,51	60
20	EDO	F	102	4/4	0.98	0.09	27,30,31,32	0
20	EDO	S	103	4/4	0.98	0.14	33,33,35,37	0
14	HEA	A	602[B]	60/60	0.98	0.14	15,26,36,40	60
16	MG	A	604	1/1	0.99	0.07	25,25,25,25	0
14	HEA	A	601	60/60	0.99	0.12	21,27,49,67	0
18	AZI	N	607[A]	3/3	0.99	0.13	34,34,34,39	0
17	NA	A	605	1/1	0.99	0.09	30,30,30,30	0
18	AZI	A	606[A]	3/3	0.99	0.18	27,27,30,33	3
15	CU	A	603	1/1	1.00	0.16	28,28,28,28	0
23	CUA	B	303	2/2	1.00	0.17	28,28,28,29	0
23	CUA	O	301	2/2	1.00	0.14	34,34,34,34	0
15	CU	N	604	1/1	1.00	0.17	31,31,31,31	0
28	ZN	F	101	1/1	1.00	0.13	33,33,33,33	0
28	ZN	S	102	1/1	1.00	0.12	35,35,35,35	0

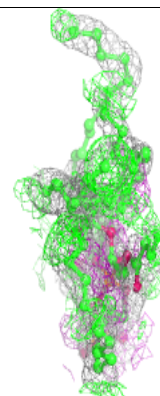
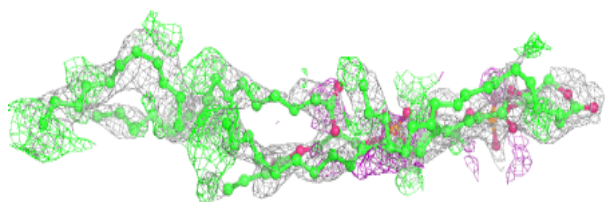
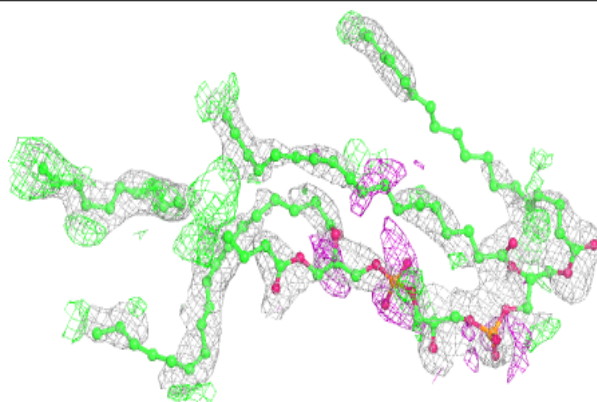
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD W 101:

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

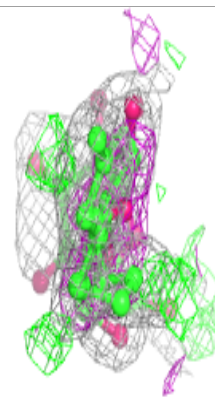
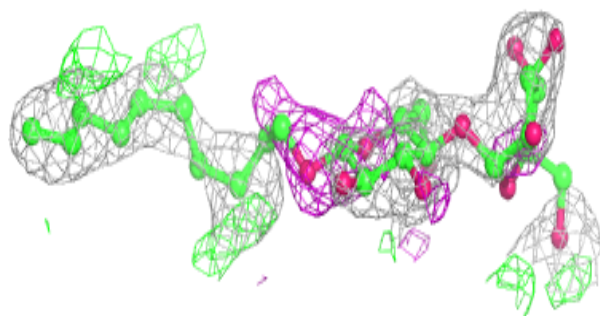
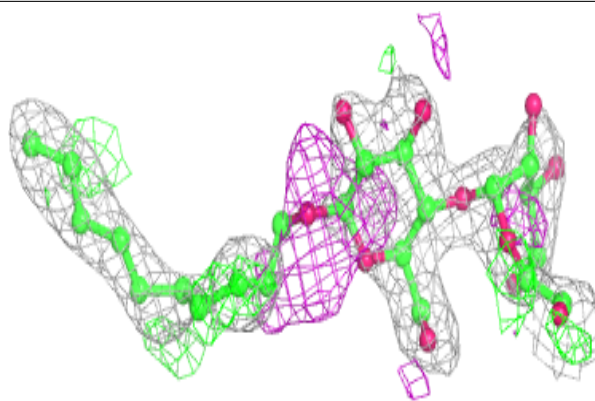
**Electron density around CDL T 102:**

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



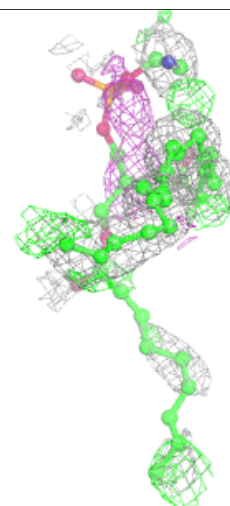
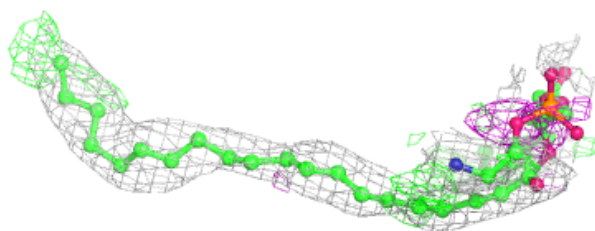
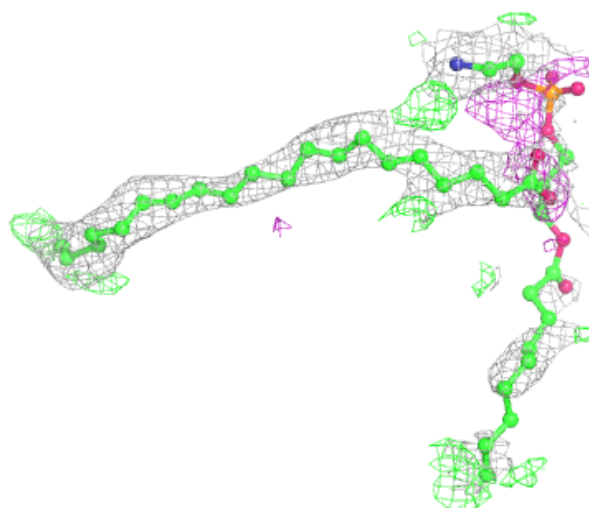
Electron density around DMU C 302:

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



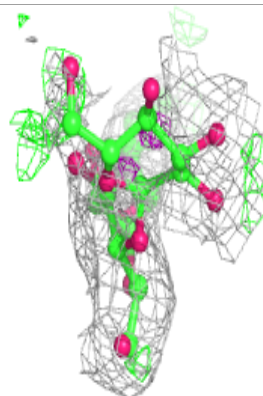
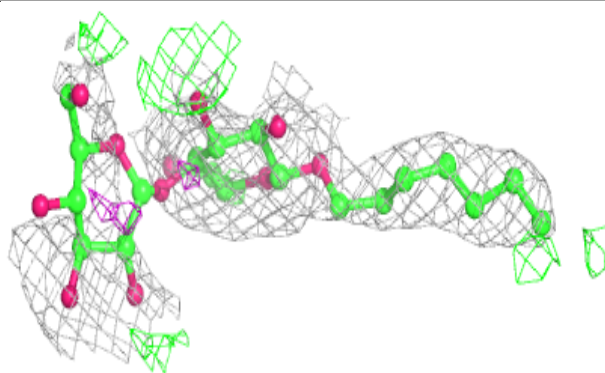
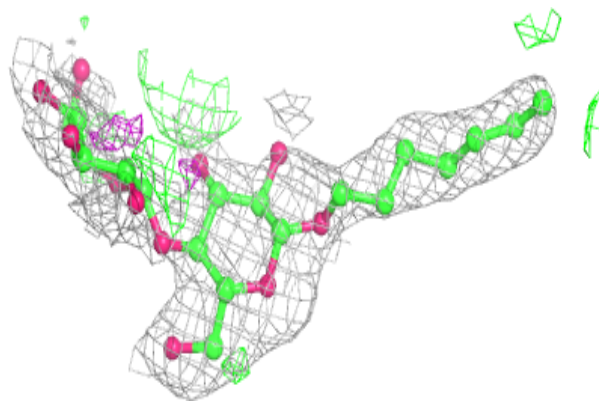
Electron density around PEK C 319:

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

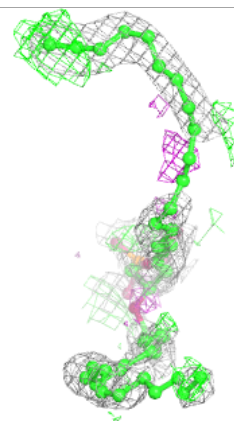
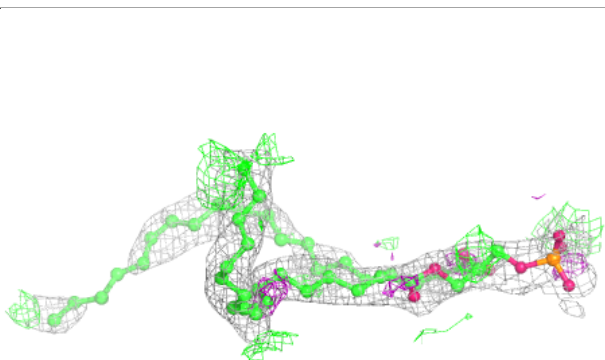
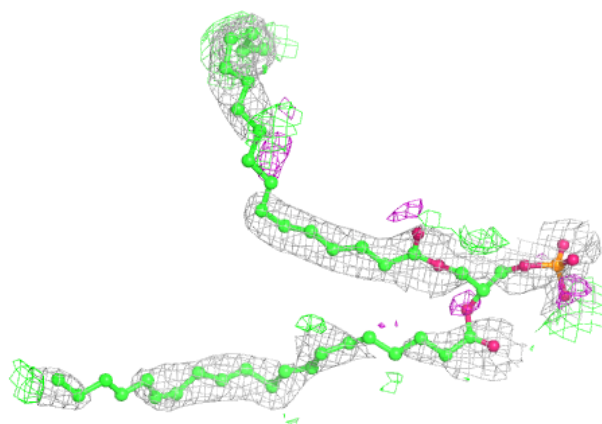


Electron density around DMU L 102:

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

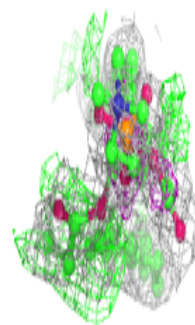
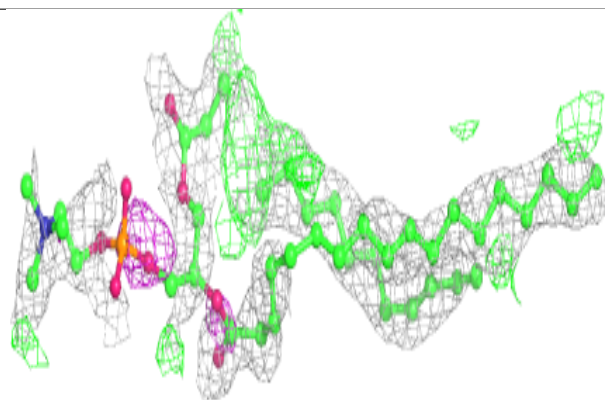
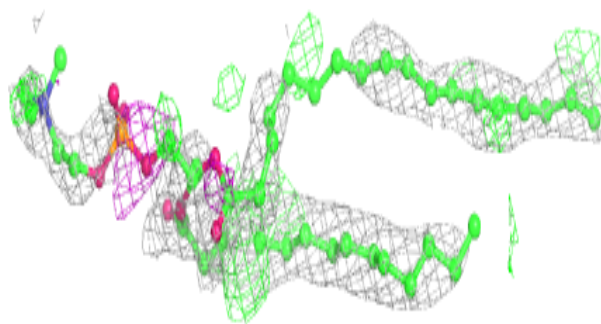
**Electron density around PEK T 101:**

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

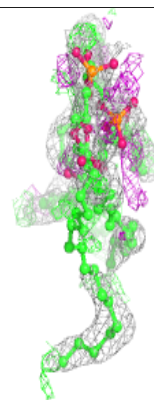
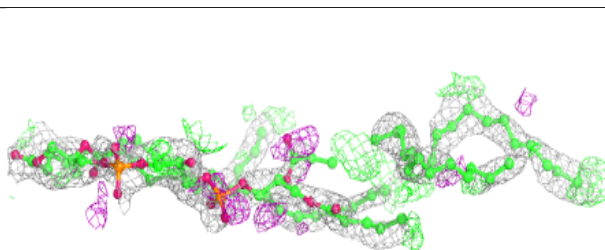
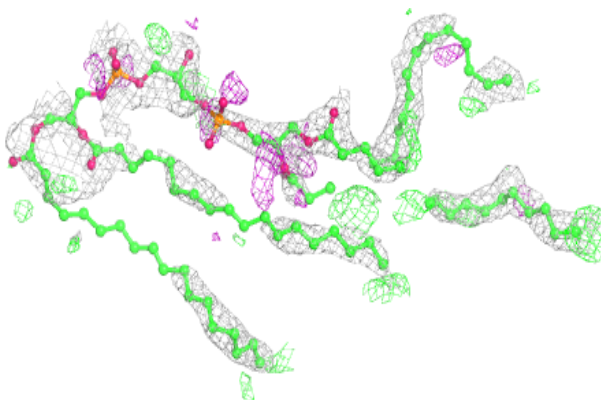


Electron density around PSC B 304:

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

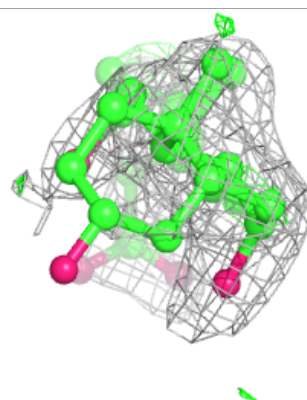
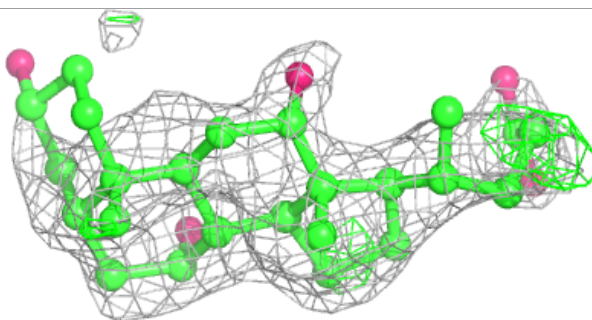
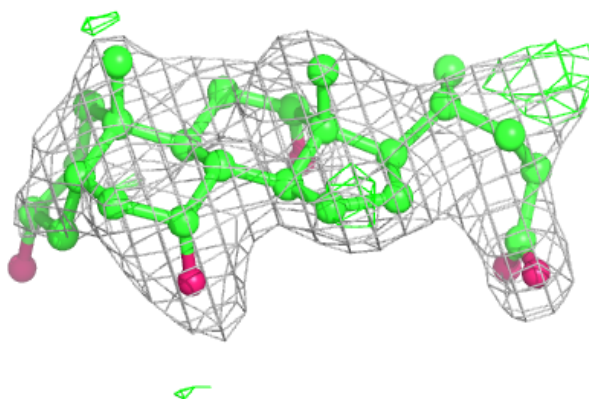
**Electron density around CDL N 601:**

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

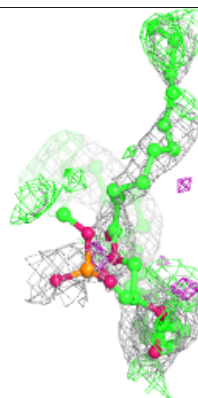
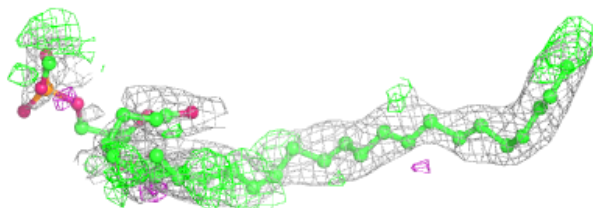
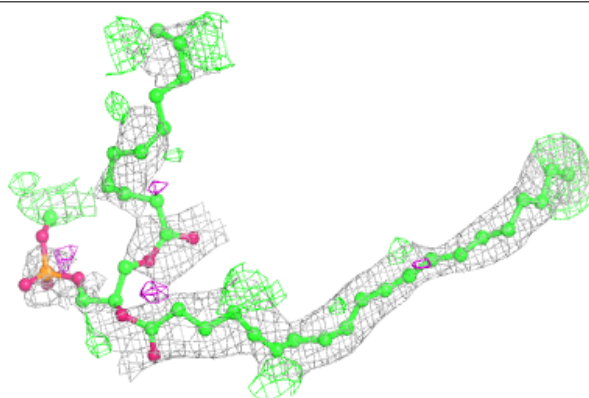


Electron density around CHD J 101:

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

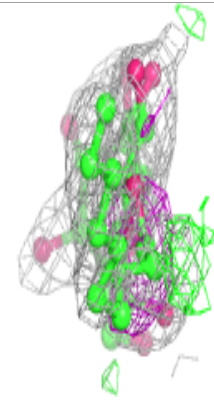
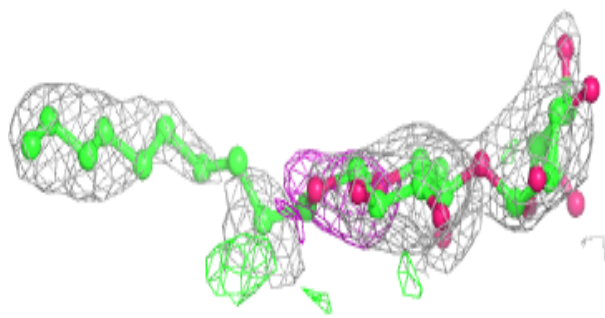
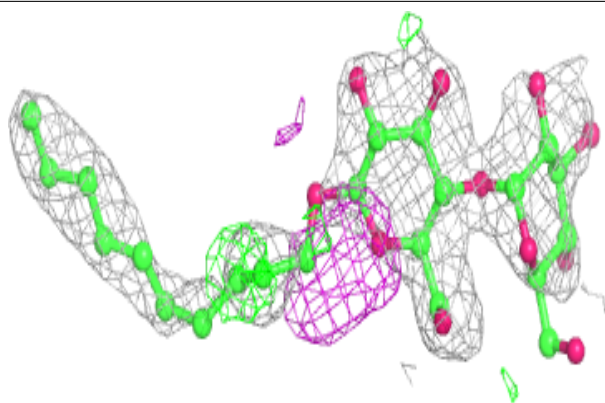
**Electron density around PEK G 103:**

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

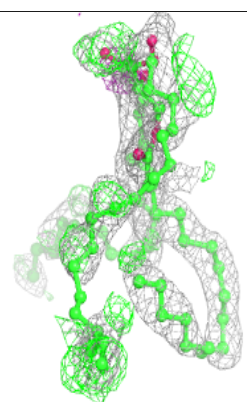
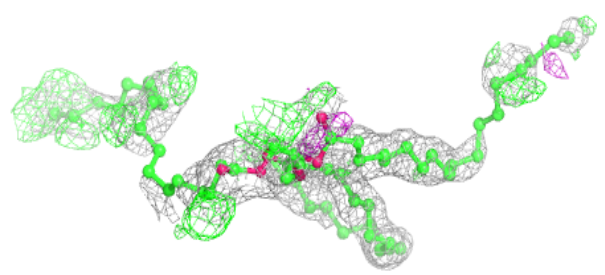
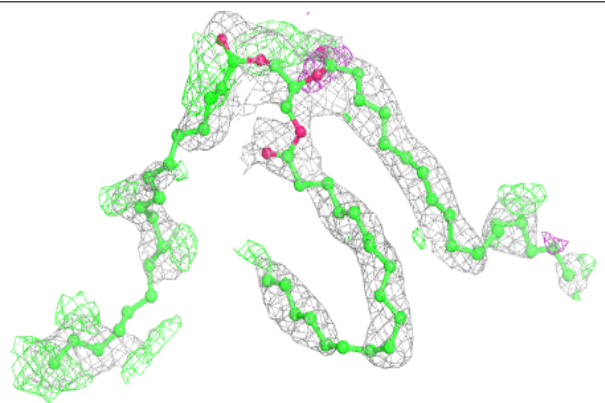


Electron density around DMU P 306:

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

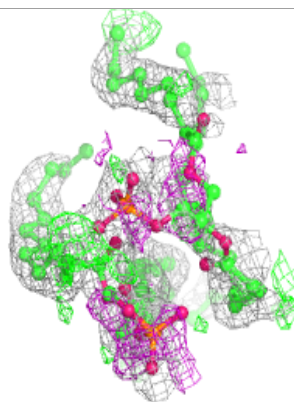
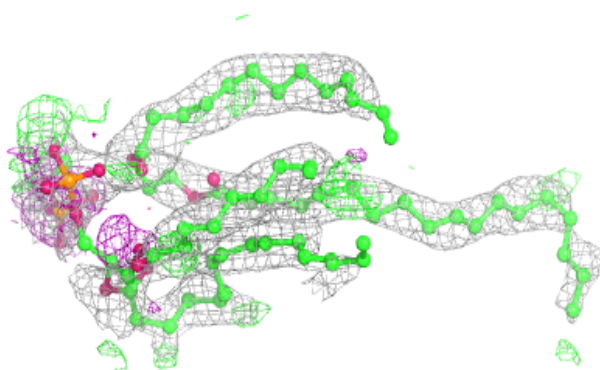
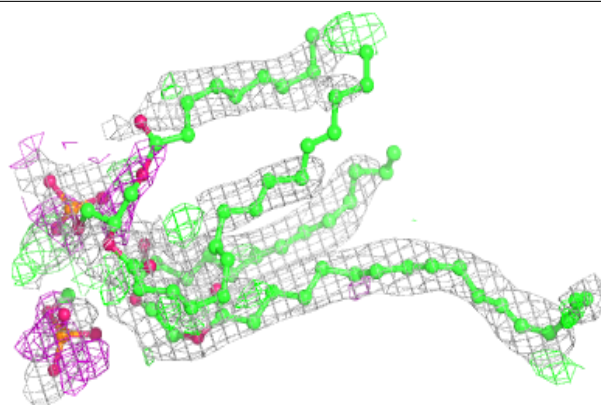
**Electron density around TGL Q 201:**

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

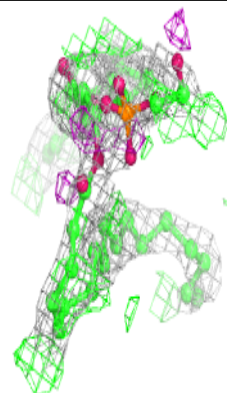
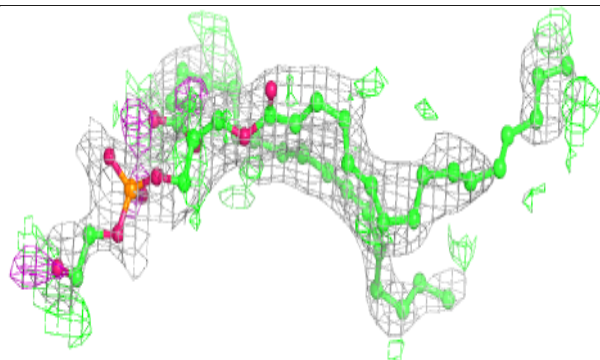
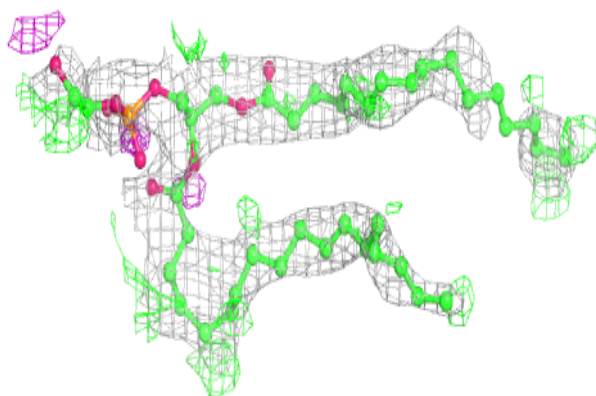


Electron density around CDL P 304:

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

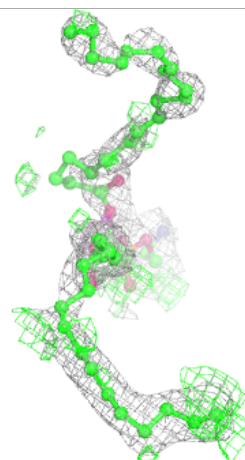
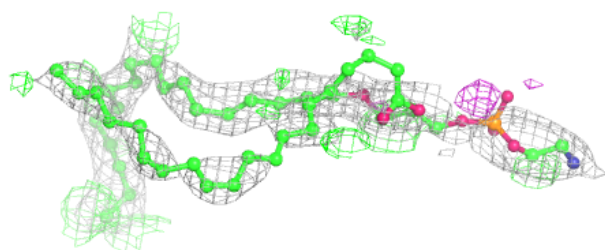
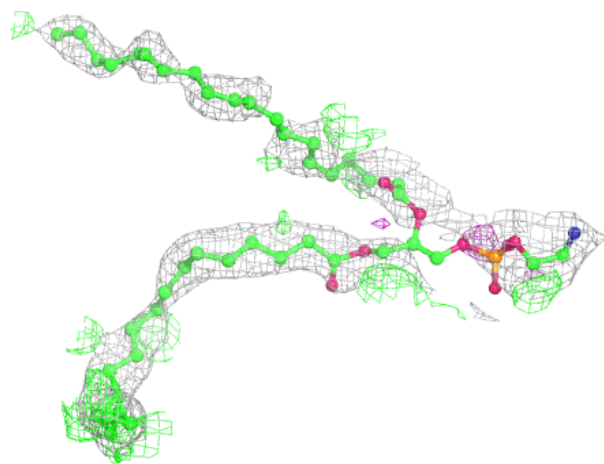
**Electron density around PGV C 308:**

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



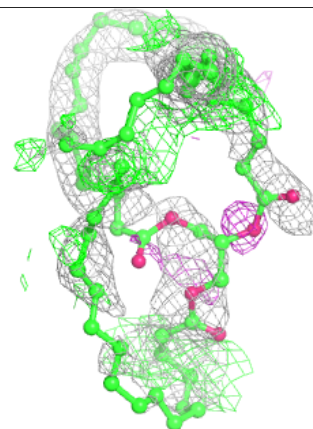
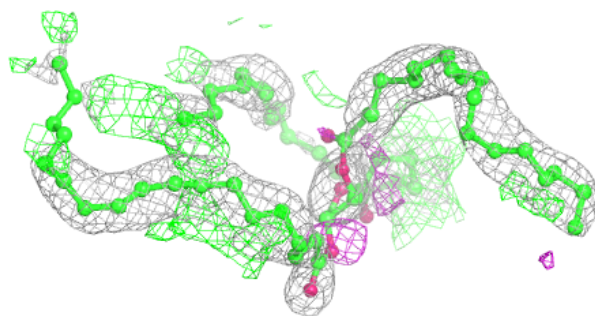
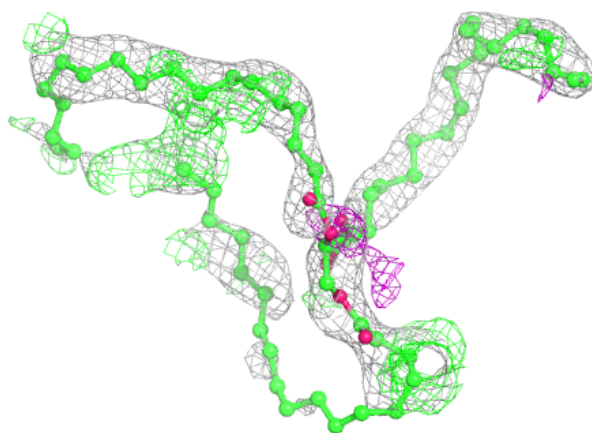
Electron density around PEK C 307:

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

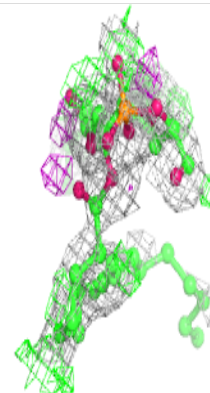
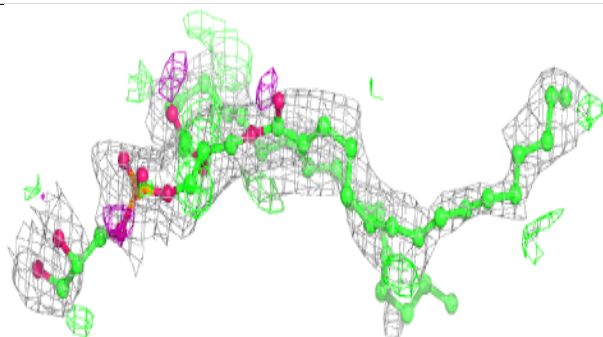
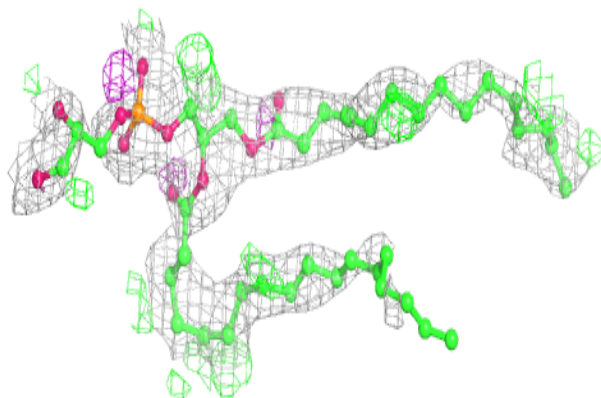


Electron density around TGL Y 101:

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

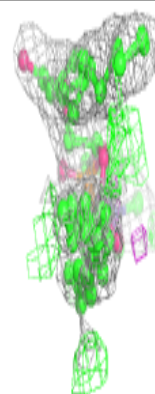
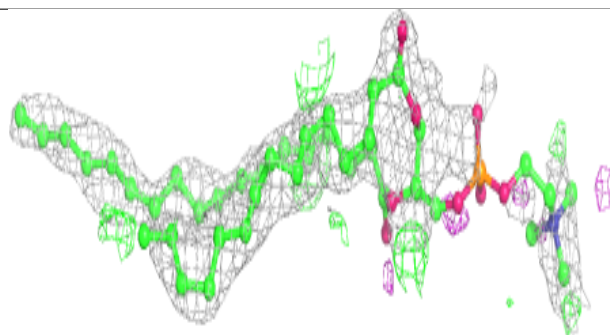
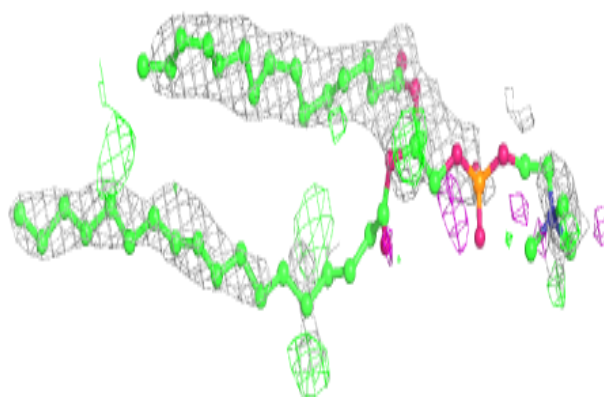
**Electron density around PGV G 104:**

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

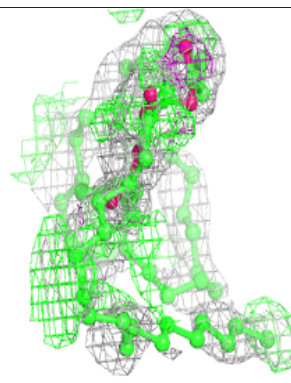
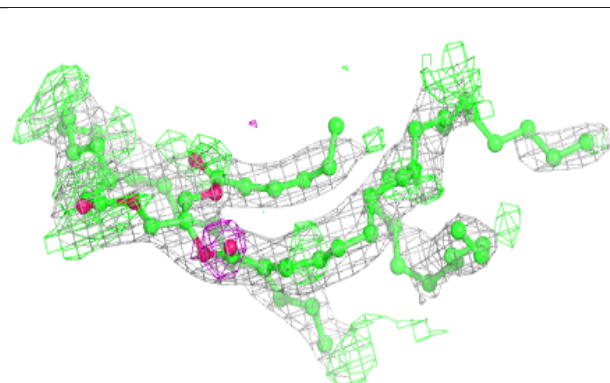
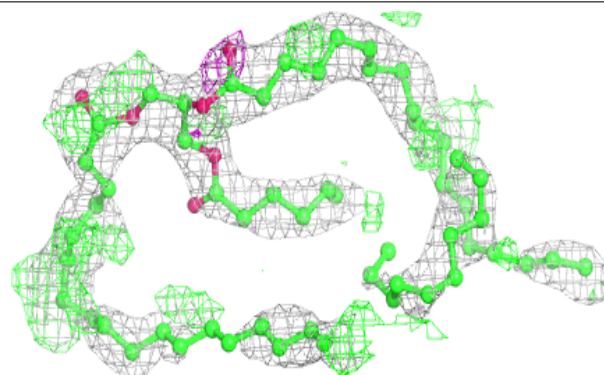


Electron density around PSC O 302:

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

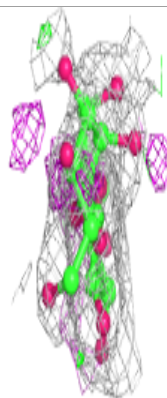
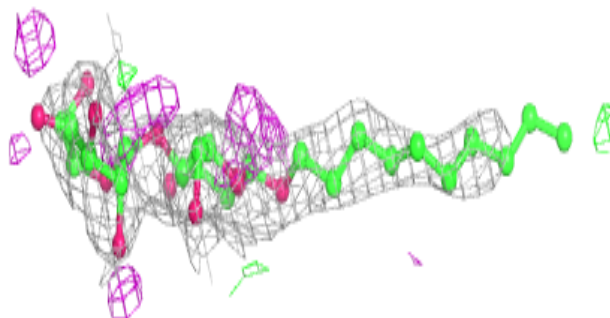
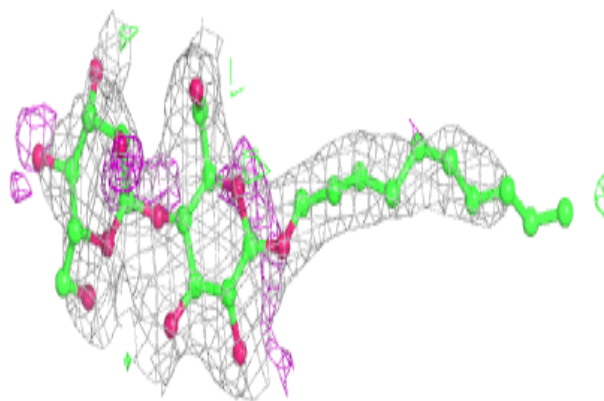
**Electron density around TGL N 610:**

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

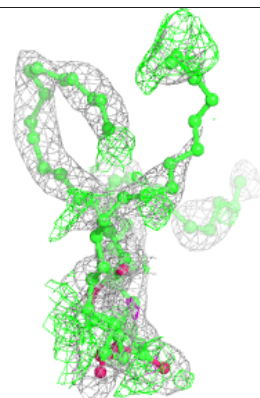
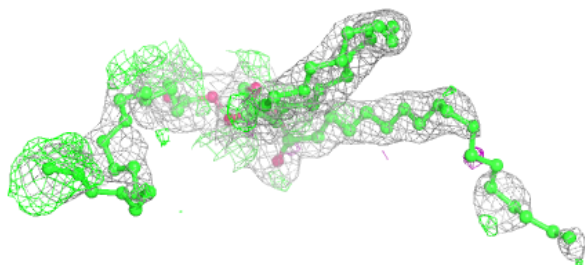
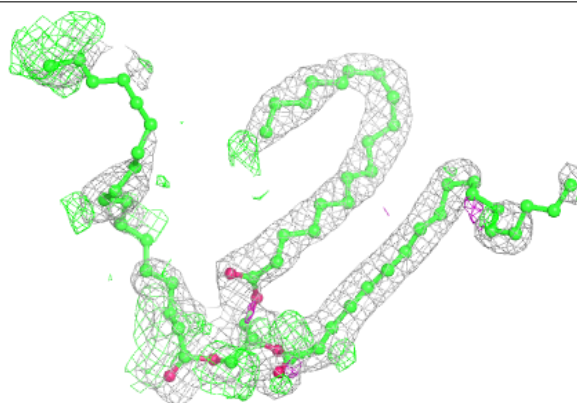


Electron density around DMU C 309:

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

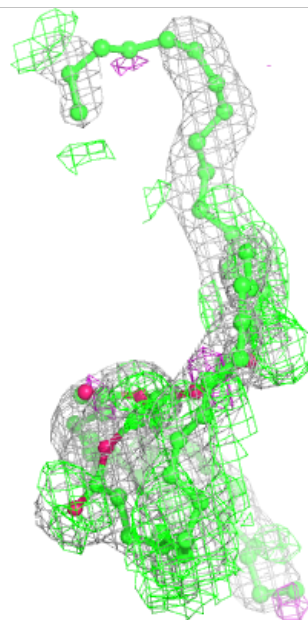
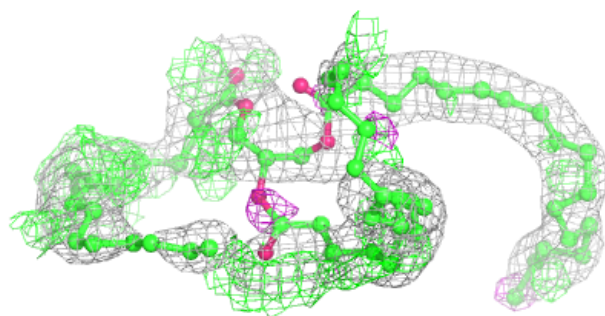
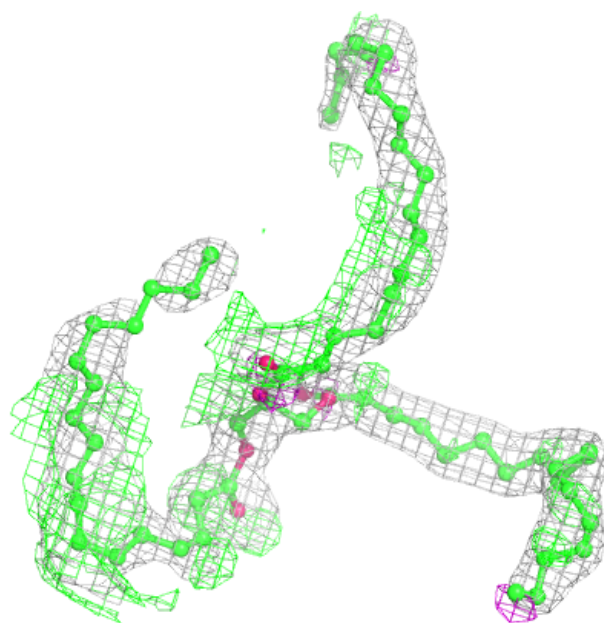
**Electron density around TGL D 201:**

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



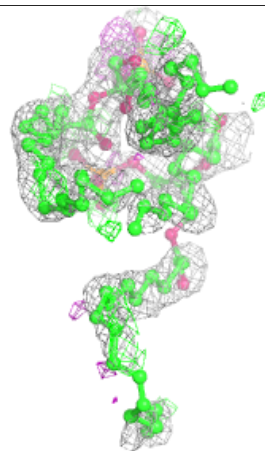
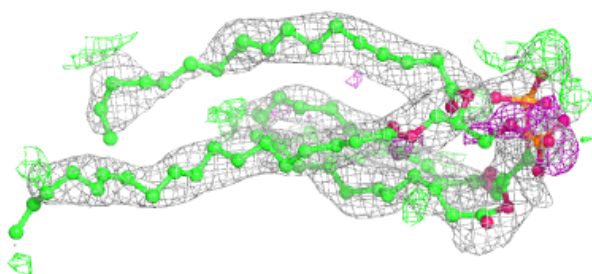
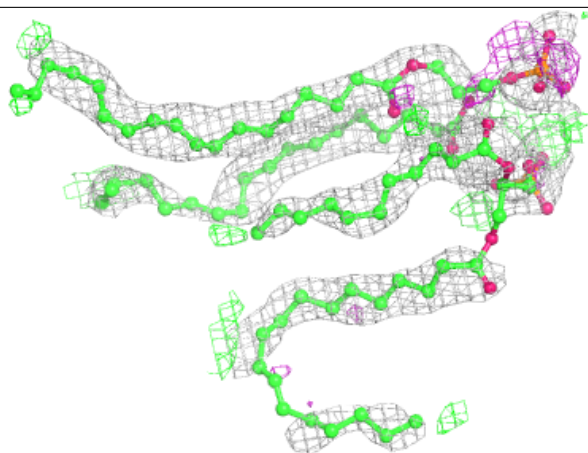
Electron density around TGL L 101:

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

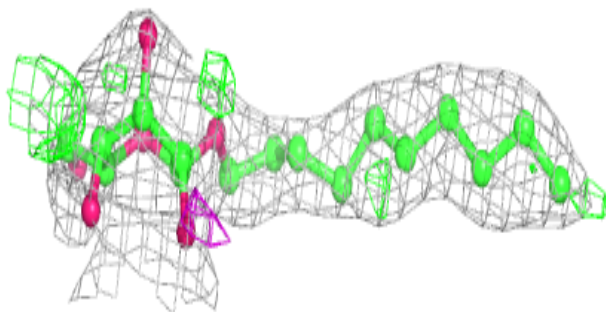
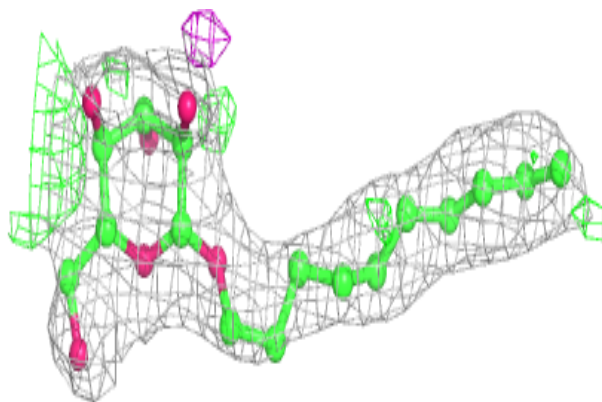


Electron density around CDL C 305:

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

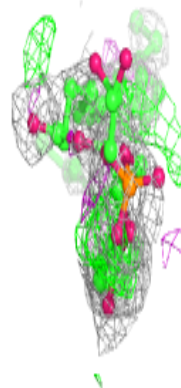
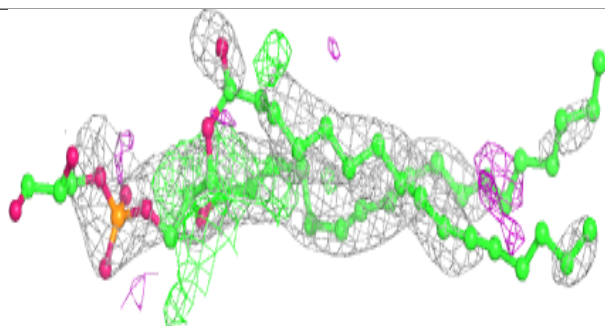
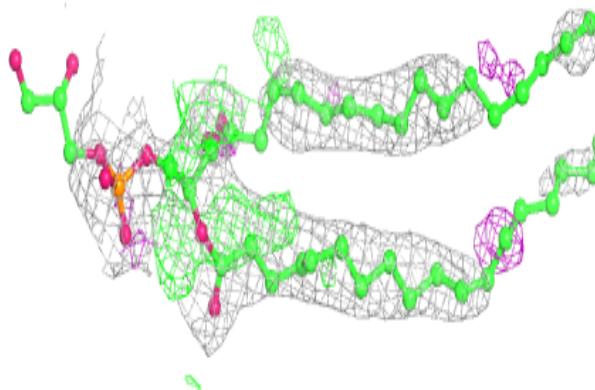
**Electron density around DMU C 310:**

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

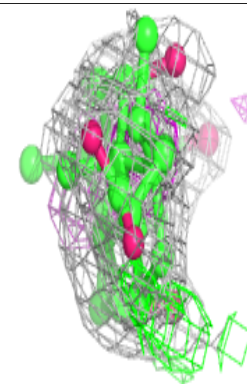
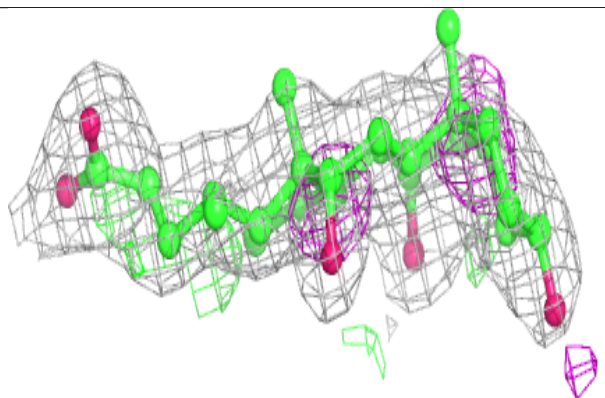
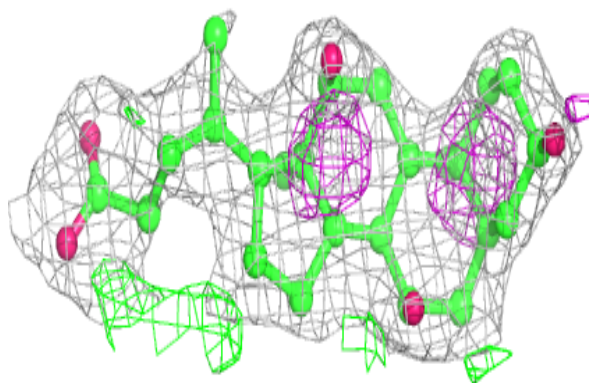


Electron density around PGV N 619:

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

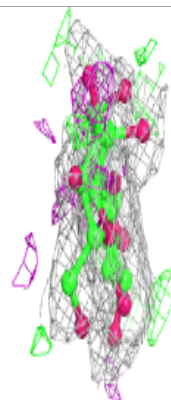
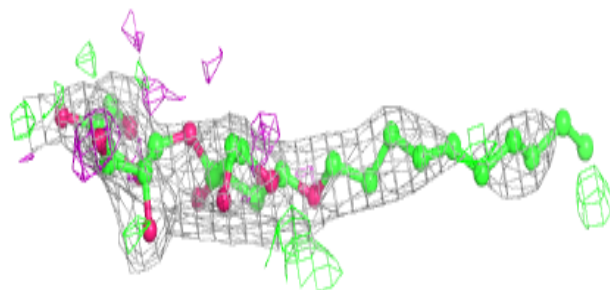
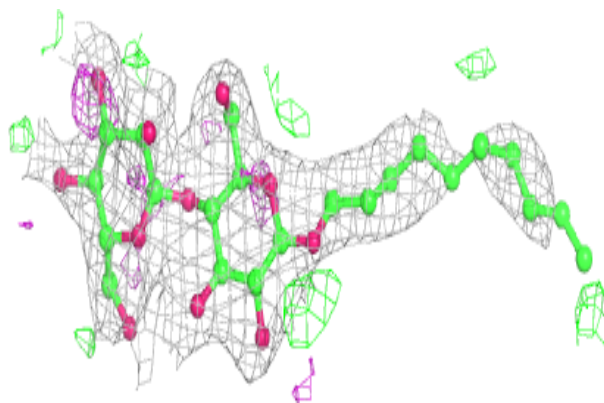
**Electron density around CHD P 305:**

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

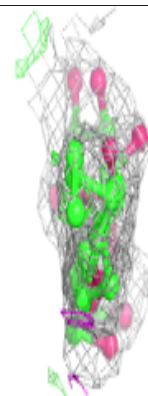
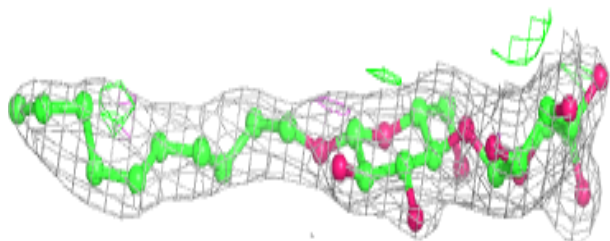
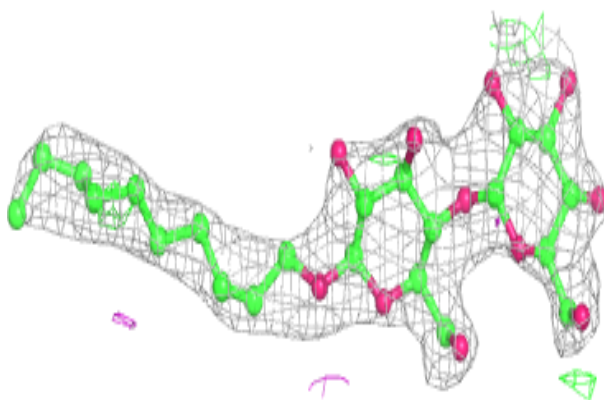


Electron density around DMU P 307:

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

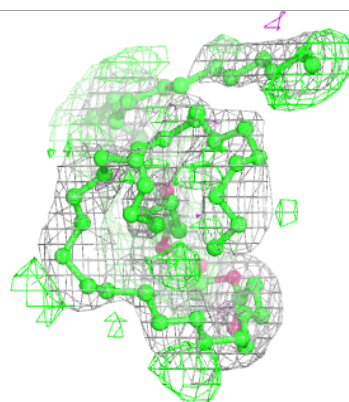
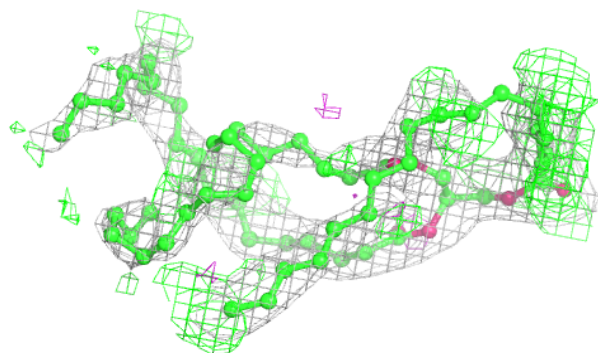
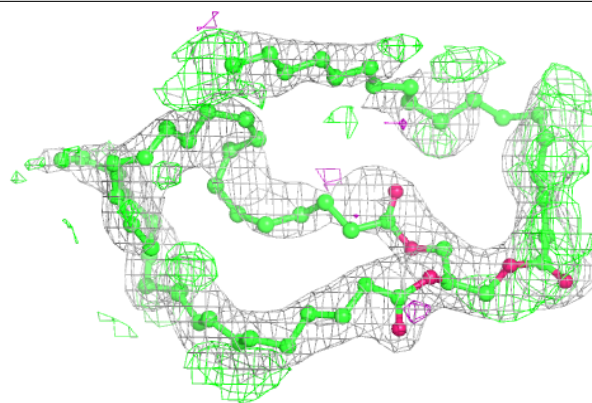
**Electron density around DMU P 308:**

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

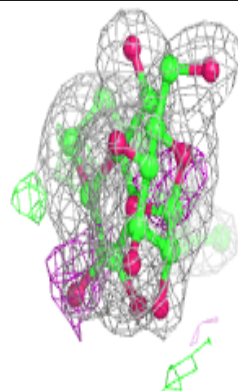
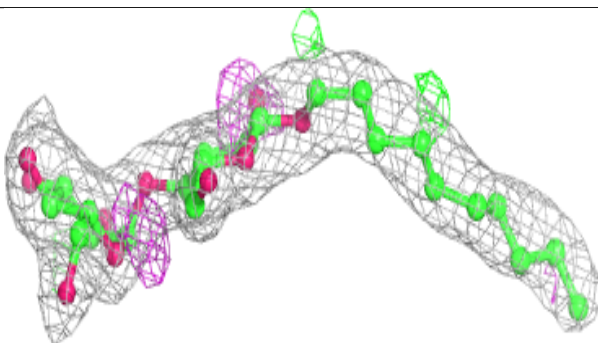
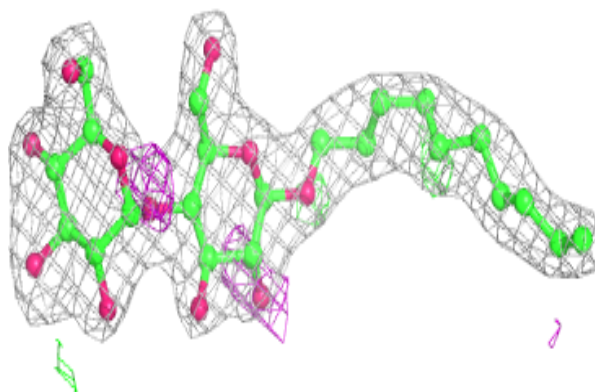


Electron density around TGL B 301:

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

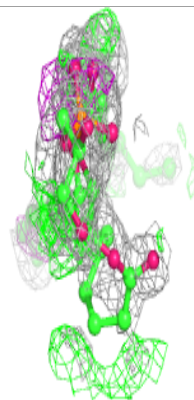
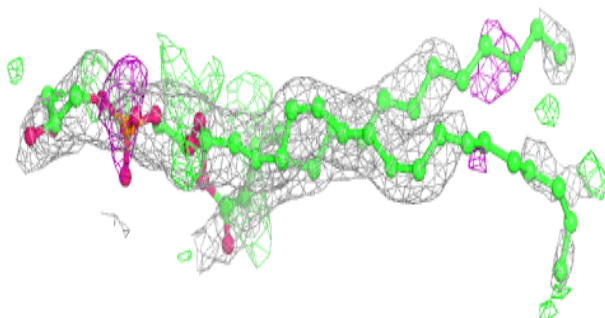
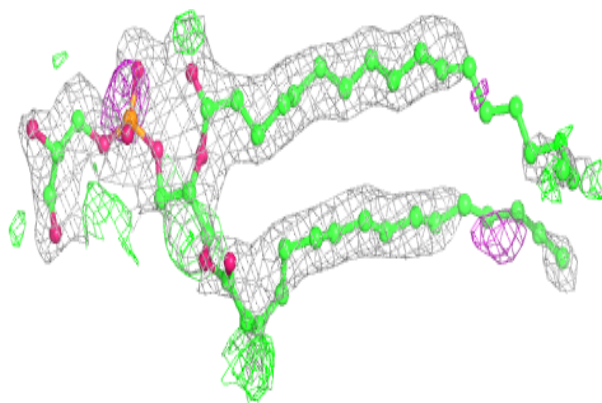
**Electron density around DMU Z 101:**

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

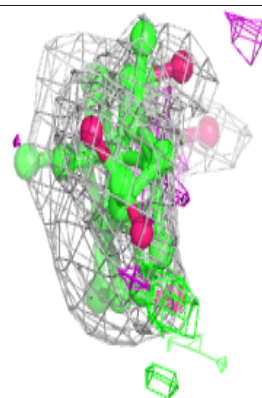
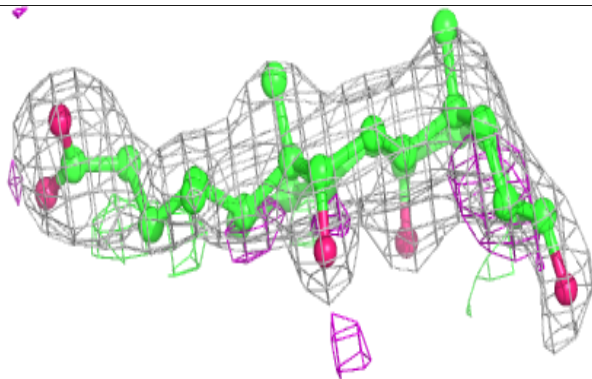
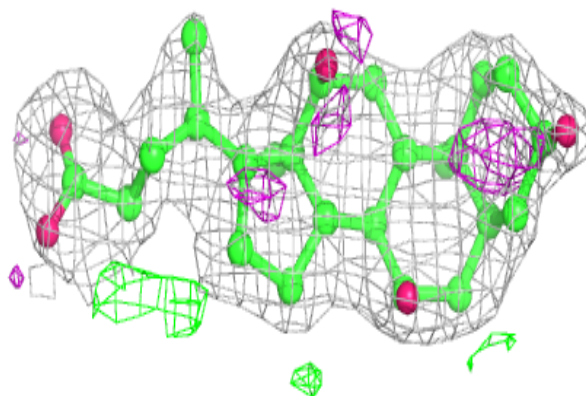


Electron density around PGV A 609:

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

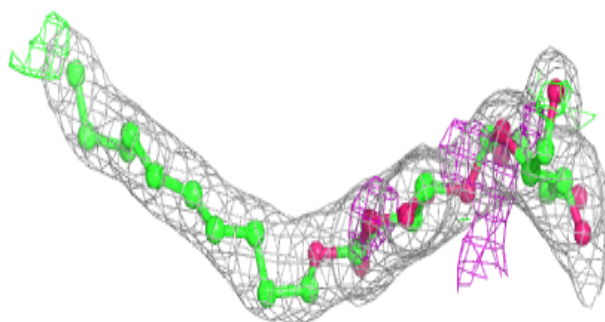
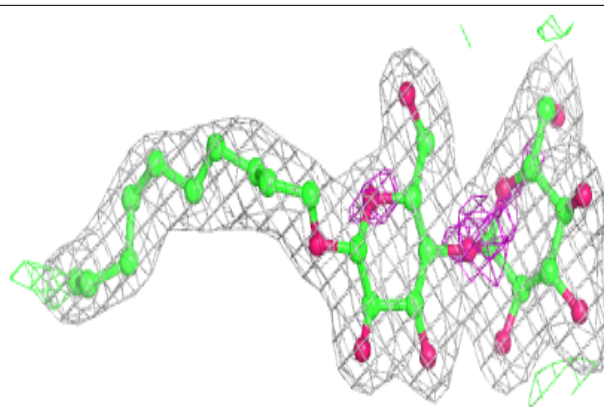
**Electron density around CHD C 306:**

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

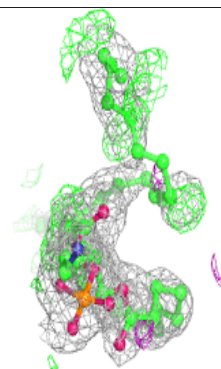
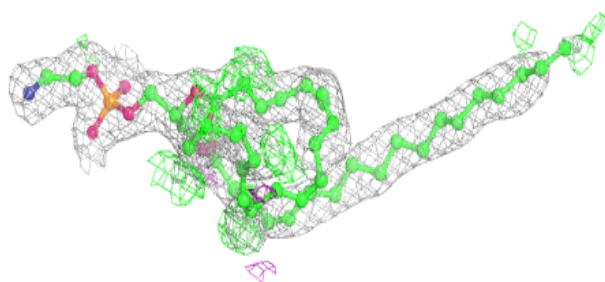
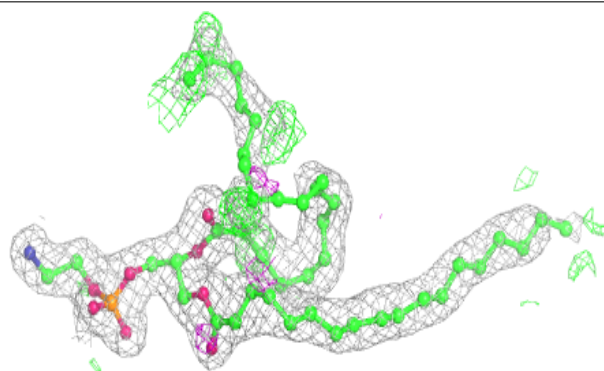


Electron density around DMU M 101:

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

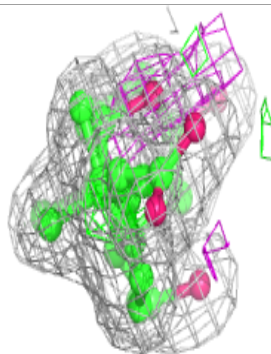
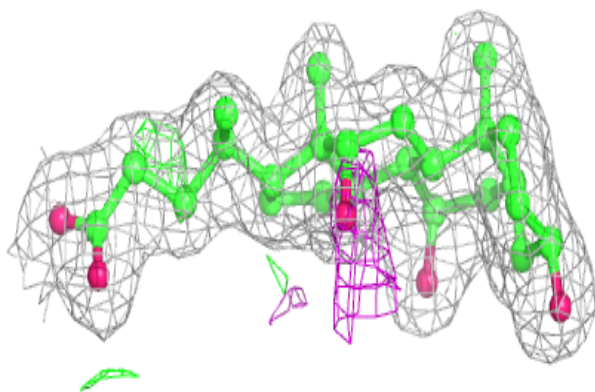
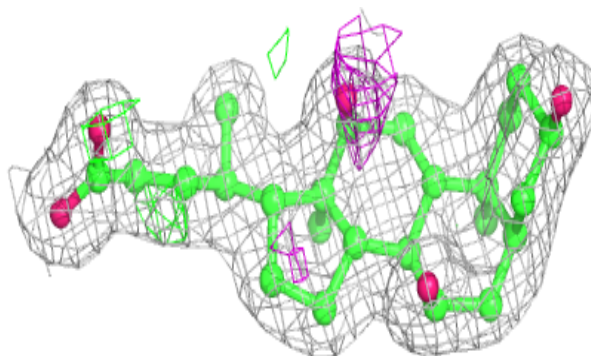
**Electron density around PEK P 312:**

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

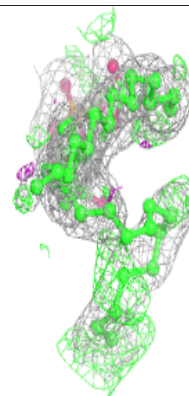
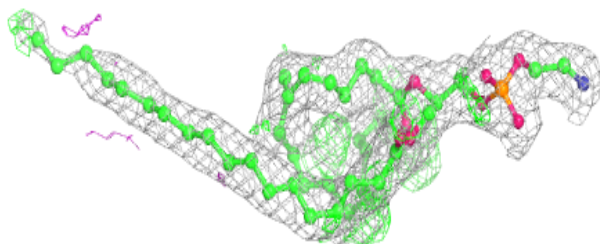
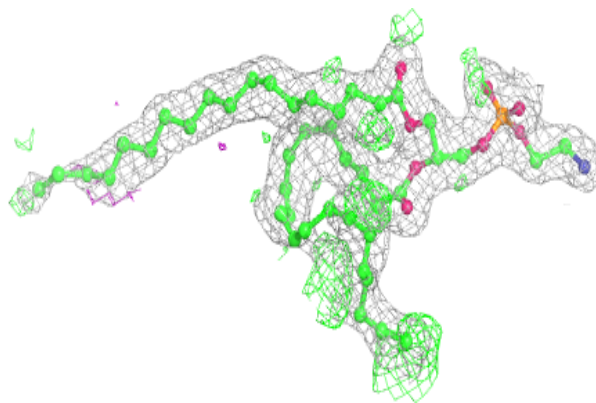


Electron density around CHD C 301:

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

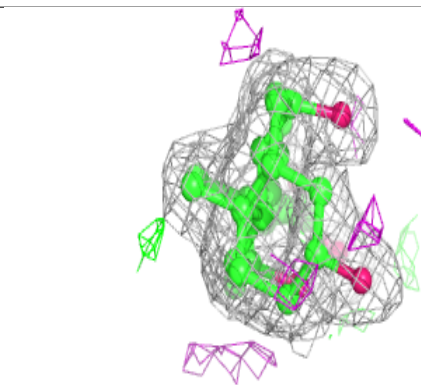
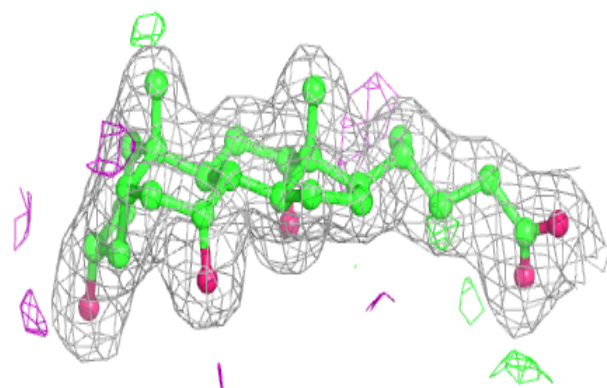
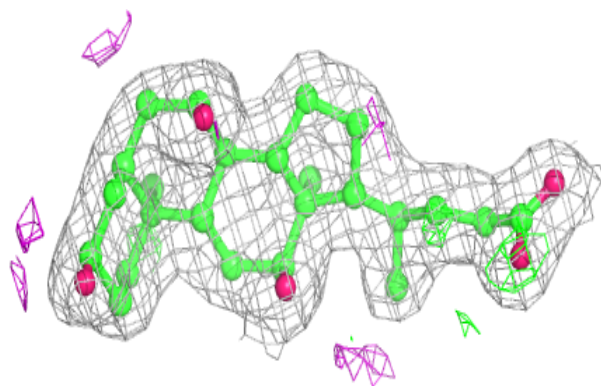
**Electron density around PEK G 101:**

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

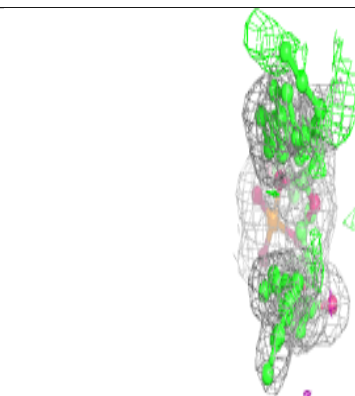
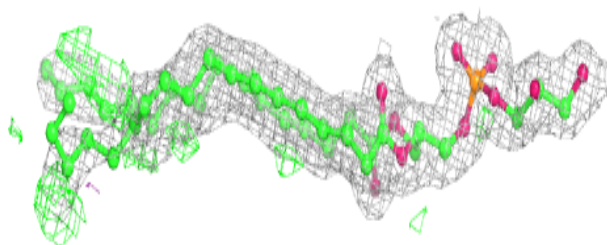
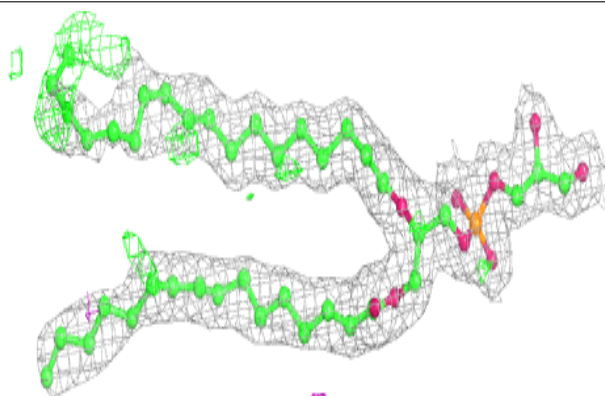


Electron density around CHD P 301:

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

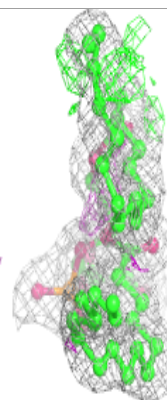
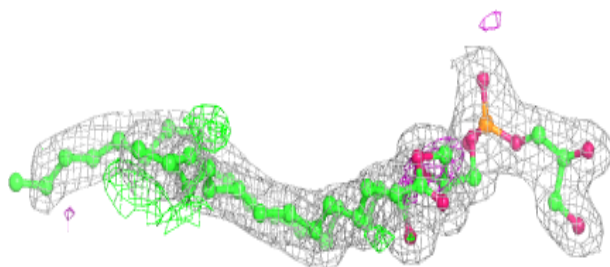
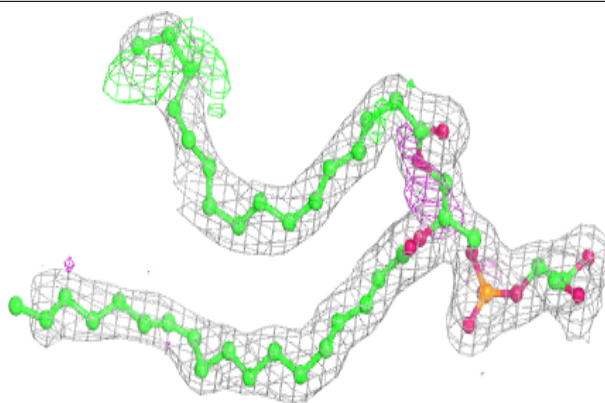
**Electron density around PGV C 304:**

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

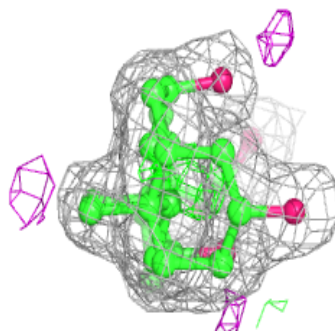
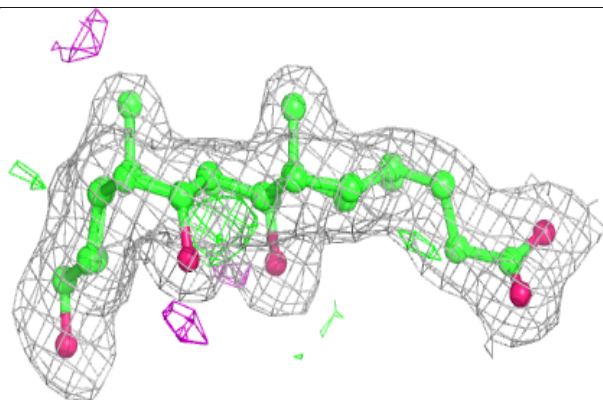
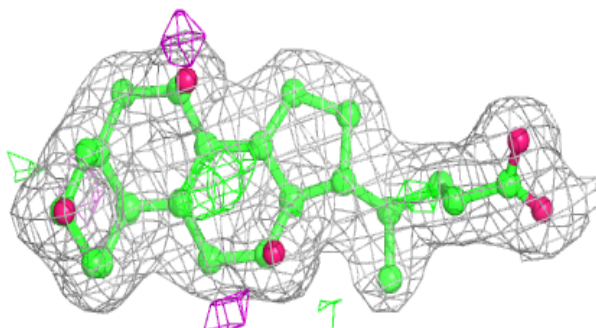


Electron density around PGV N 609:

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

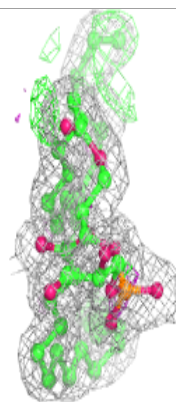
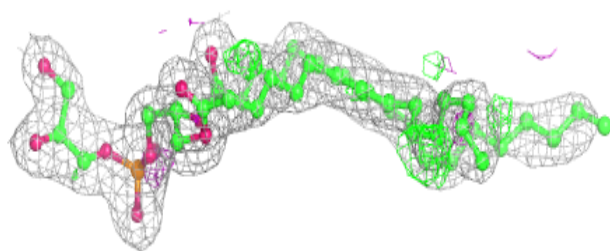
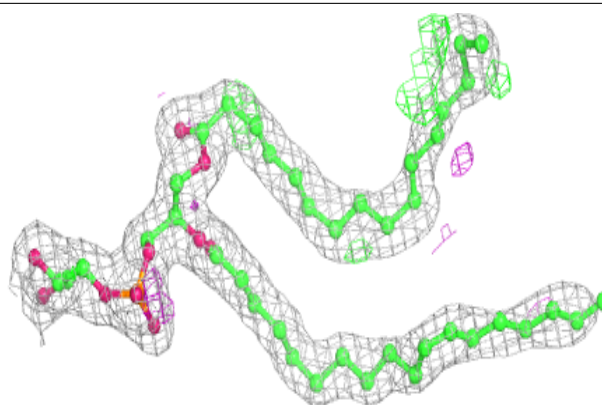
**Electron density around CHD B 302:**

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

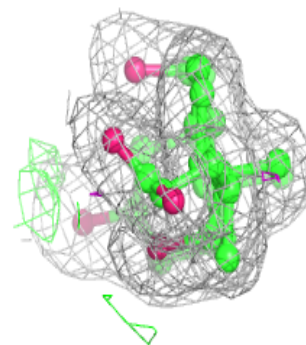
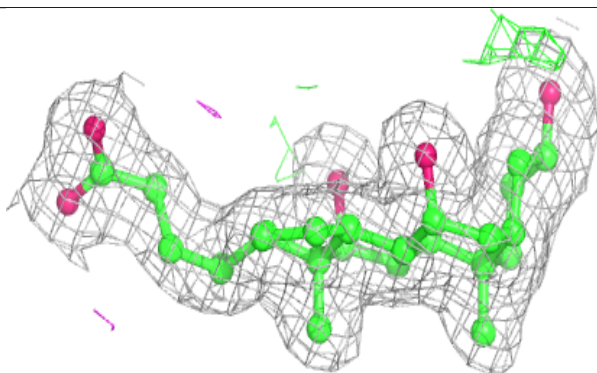
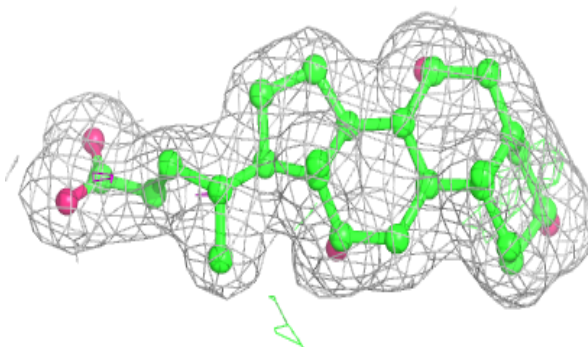


Electron density around PGV A 608:

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

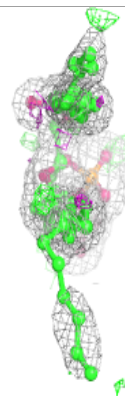
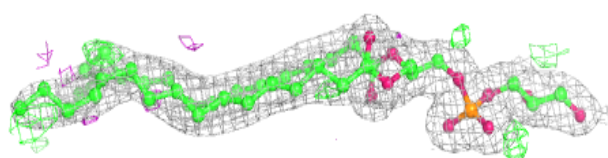
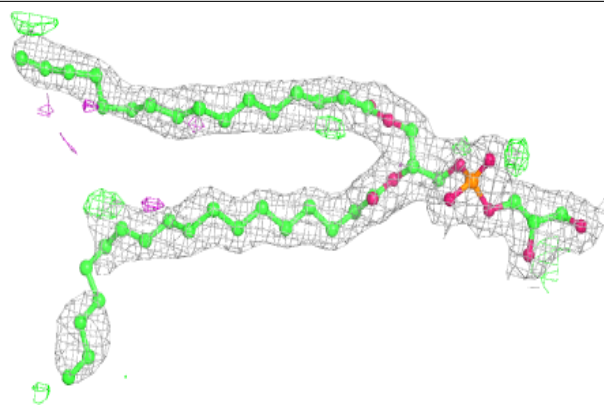
**Electron density around CHD G 102:**

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

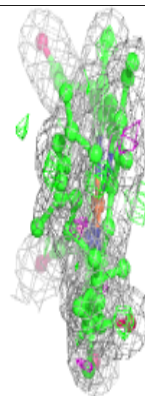
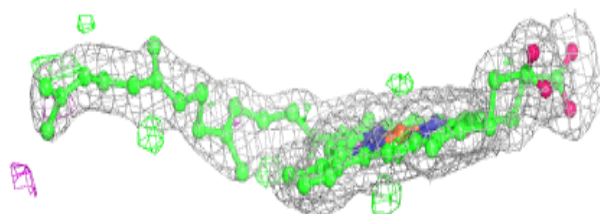
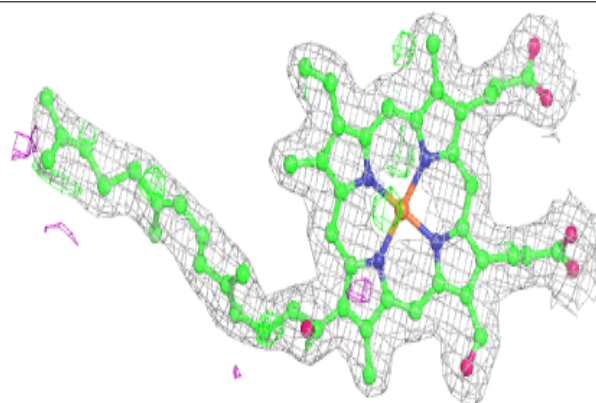


Electron density around PGV P 303:

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

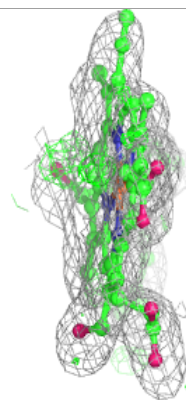
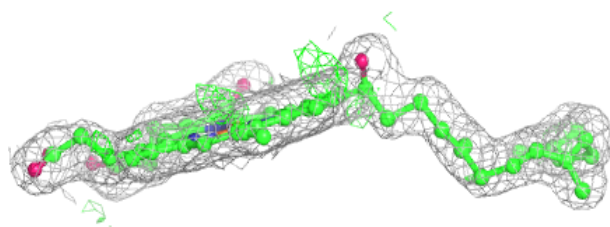
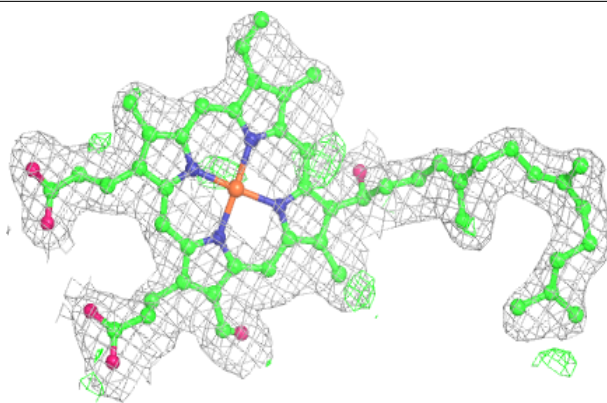
**Electron density around HEA N 602:**

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

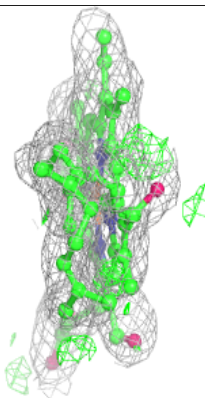
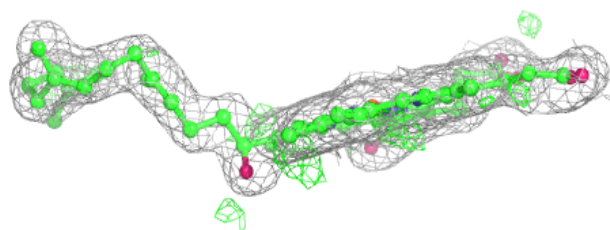
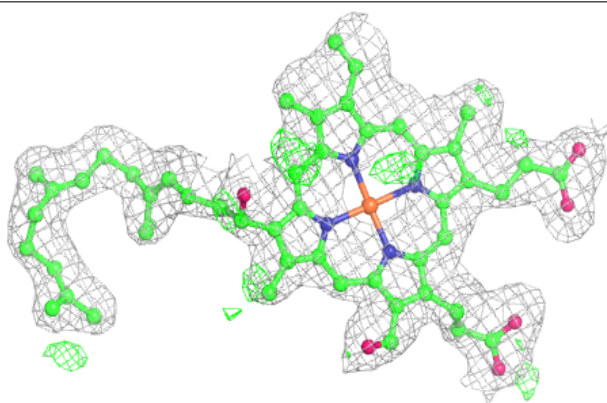


Electron density around HEA N 603 (A):

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

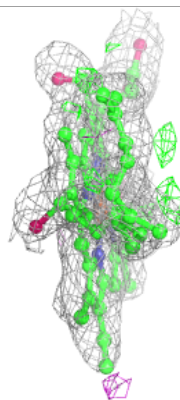
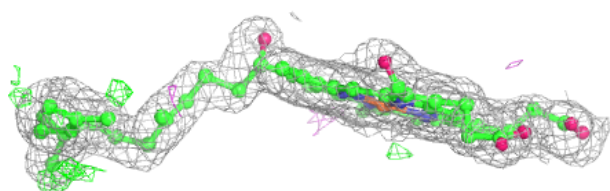
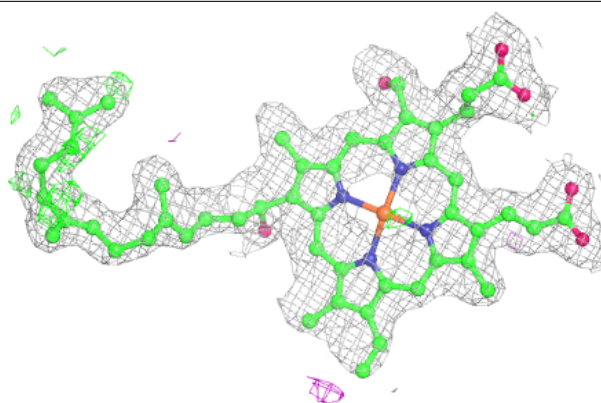
**Electron density around HEA N 603 (B):**

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

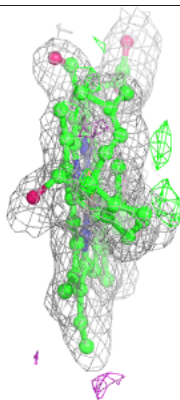
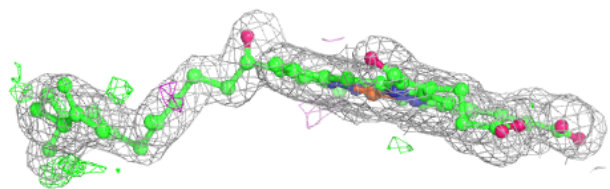
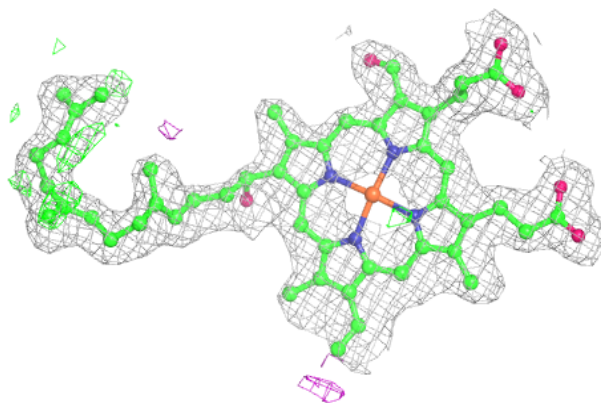


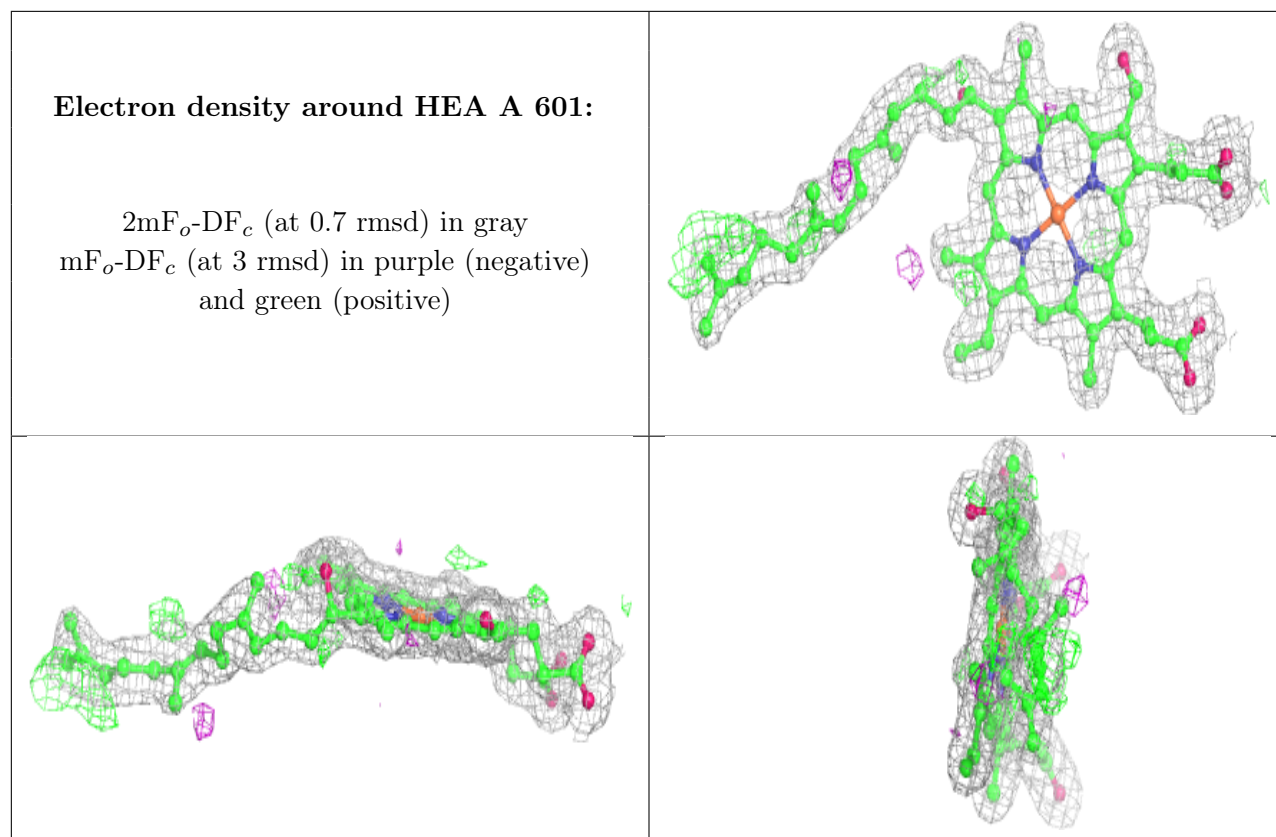
Electron density around HEA A 602 (A):

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

**Electron density around HEA A 602 (B):**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.