



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 04:54 AM JST

PDB ID : 7VVR
Title : Bovine cytochrome c oxidase in CN-bound mixed valence state at 50 K
Authors : Shimada, A.; Tsukihara, T.
Deposited on : 2021-11-08
Resolution : 1.65 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

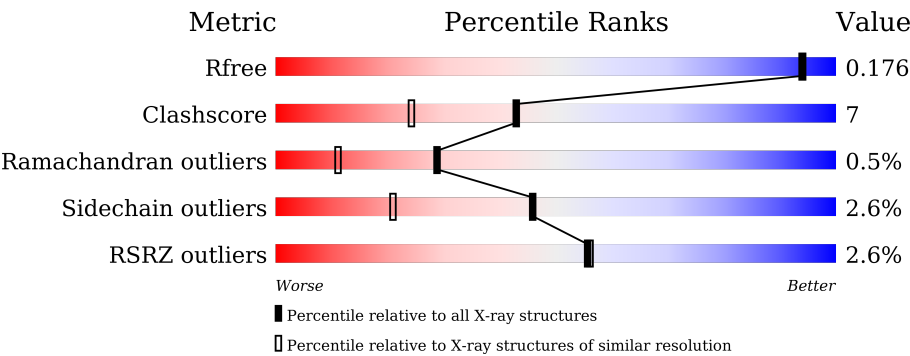
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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.



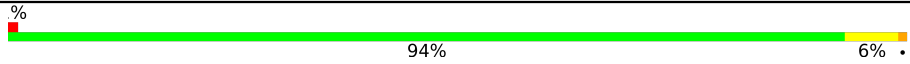

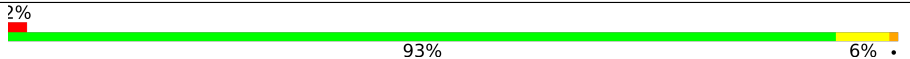

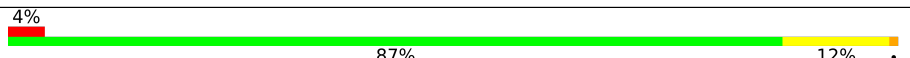
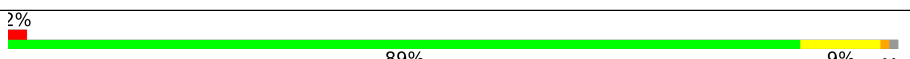
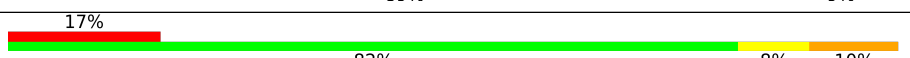
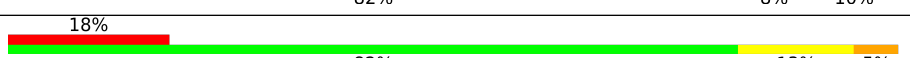
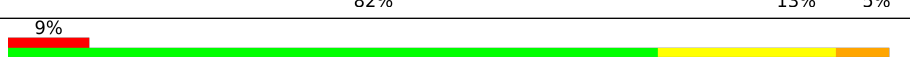

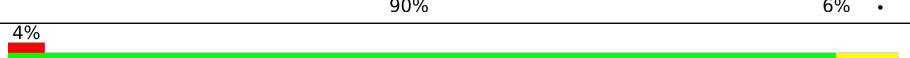
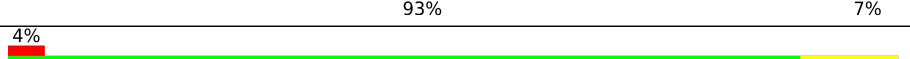


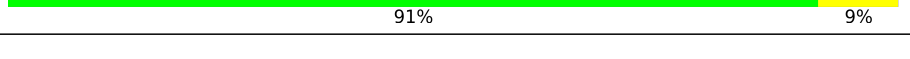
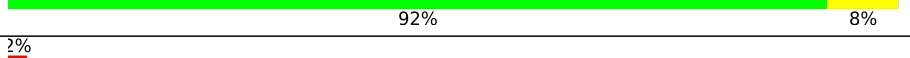
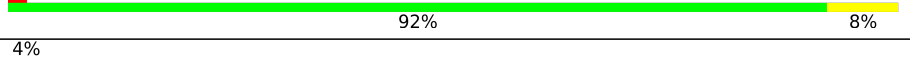

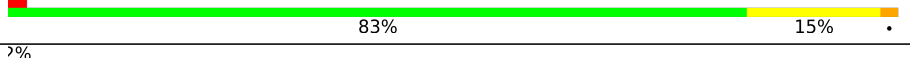
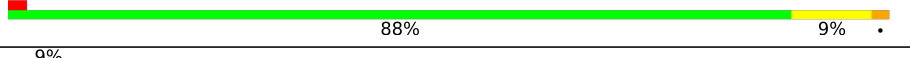
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>89%11%.</div>
1	N	514	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>88%12%</div>
2	B	227	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>2%80%17%.</div>
2	O	227	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%75%24%.</div>
3	C	259	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>91%8%</div>
3	P	259	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>92%8%</div>

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	HEA	A	602	X	-	-	-
14	HEA	N	601[A]	X	-	-	-
14	HEA	N	601[B]	X	-	-	-
14	HEA	N	601[C]	X	-	-	-
14	HEA	N	602	X	-	-	-
21	EDO	A	619	-	-	X	-
21	EDO	A	622	-	-	X	-
21	EDO	B	307	-	-	X	-
21	EDO	D	204	-	-	X	X
24	CHD	Y	104	-	-	-	X
27	DMU	K	103	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34984 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	27	0
			4162	2776	642	700	44			
1	N	514	Total	C	N	O	S	0	28	0
			4133	2755	639	696	43			

- 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	13	0
			1906	1238	294	354	20			
2	O	227	Total	C	N	O	S	0	15	0
			1909	1244	294	351	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
			2157	1438	343	362	14			
3	P	259	Total	C	N	O	S	0	12	0
			2173	1446	348	364	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	5	0
			1232	801	202	225	4			
4	Q	144	Total	C	N	O	S	0	4	0
			1226	798	199	225	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	1	0
			863	550	148	163	2			
5	R	105	Total	C	N	O	S	0	1	0
			858	547	147	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	3	0
			731	452	130	143	6			
6	S	93	Total	C	N	O	S	0	2	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	5	0
			710	456	134	118	1	1			
7	T	84	Total	C	N	O	P	S	0	3	0
			701	449	134	116	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
			661	417	121	118	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	2	0
			621	401	112	104	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	1	0
			392	255	66	69	2			
11	X	49	Total	C	N	O	S	0	1	0
			392	255	66	69	2			

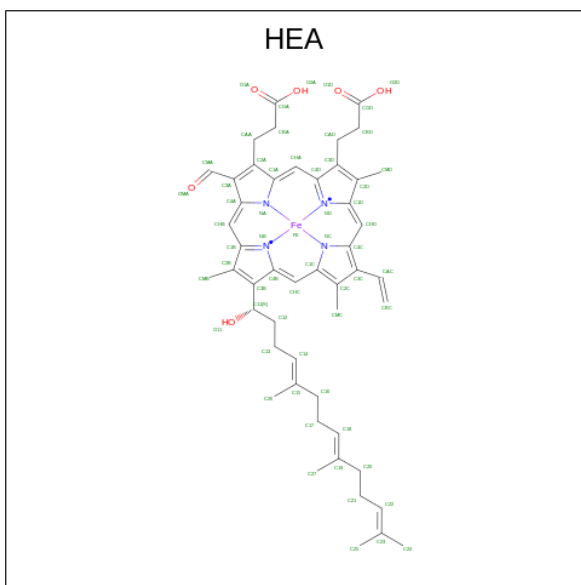
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			384	256	64	62	2			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	1	0
			338	225	53	60			
13	Z	43	Total	C	N	O	0	1	0
			339	224	53	62			

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



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

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

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

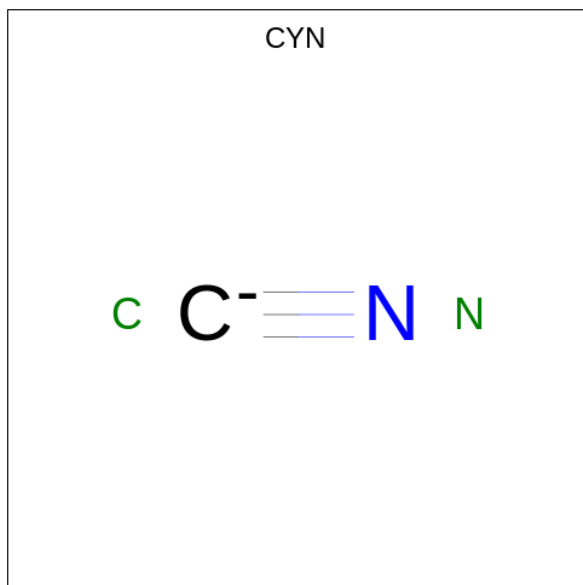
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

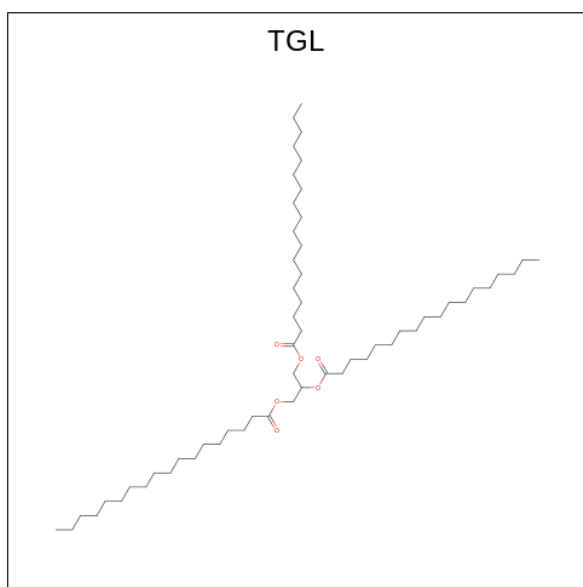
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		

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



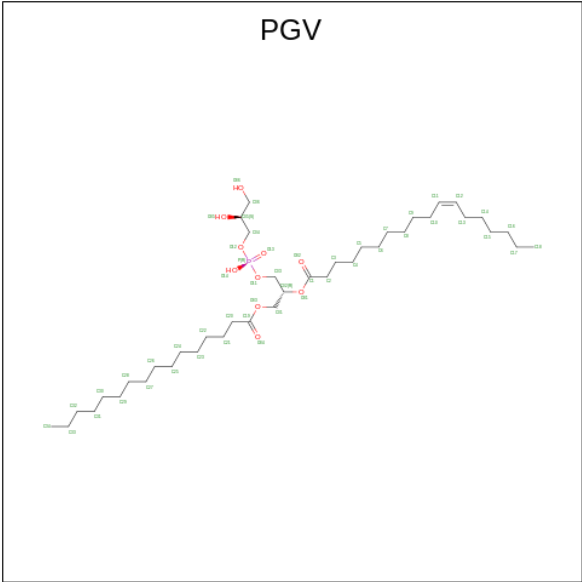
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	N	0	0
			2	1	1		
18	N	1	Total	C	N	0	0
			2	1	1		

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



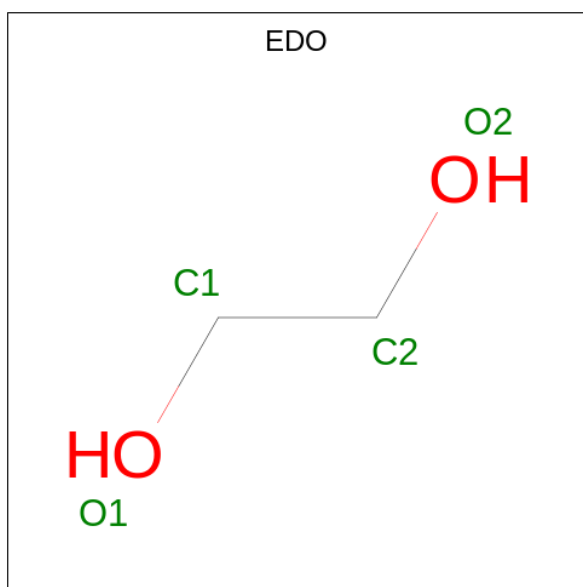
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			60	54	6		
19	B	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			53	47	6		
19	N	1	Total	C	O	0	0
			62	56	6		
19	Q	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			56	50	6		

- Molecule 20 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
20	A	1	Total	C	O	P	0	0
			47	36	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			50	39	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			46	35	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

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

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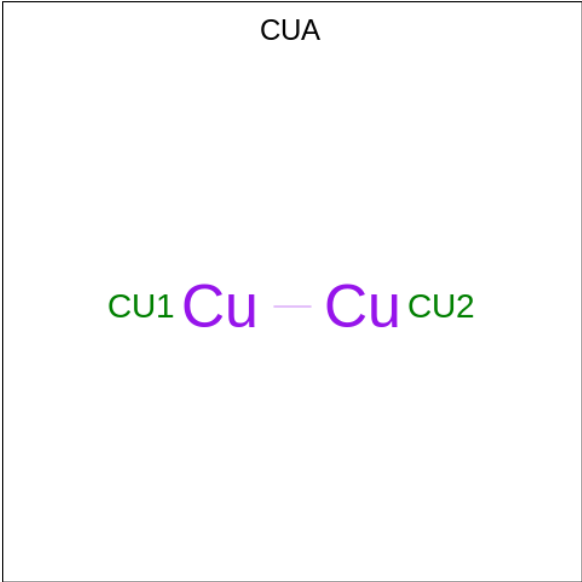
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	N	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4 2 2	0	0
21	O	1	Total C O 4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

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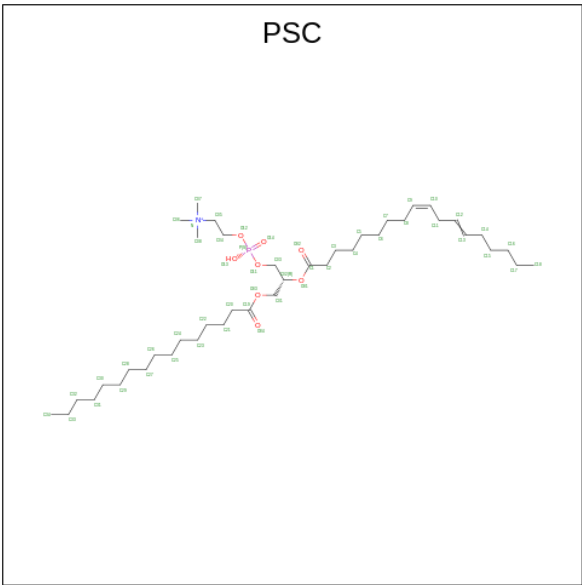
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	U	1	Total 4	C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

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



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

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



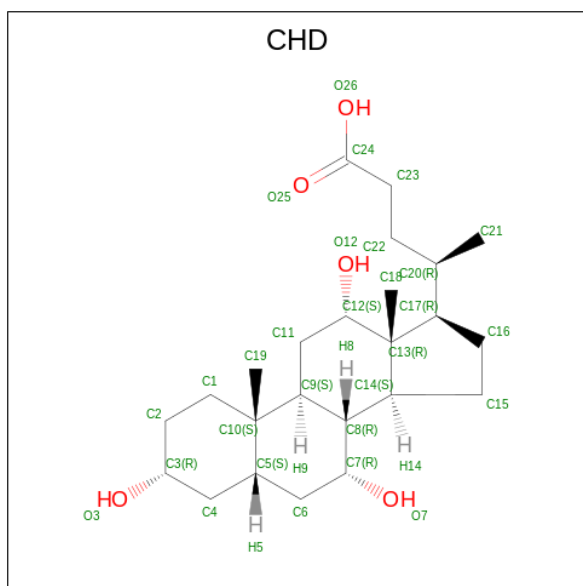
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			48	38	1	8	1		

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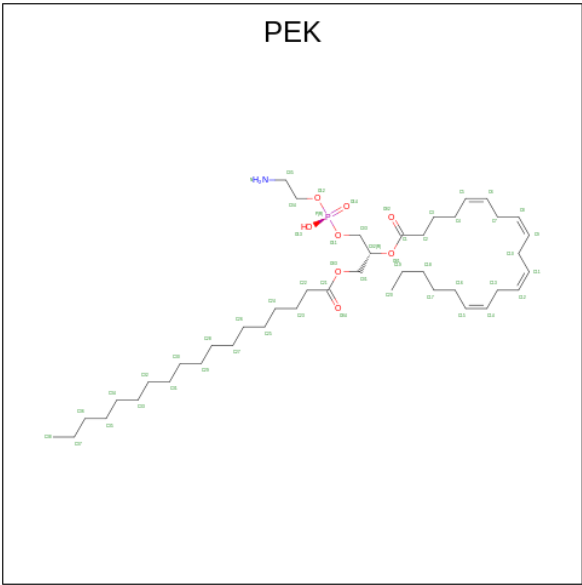
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	R	1	Total	C	N	O	P	
			49	39	1	8	1	
							0	0

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



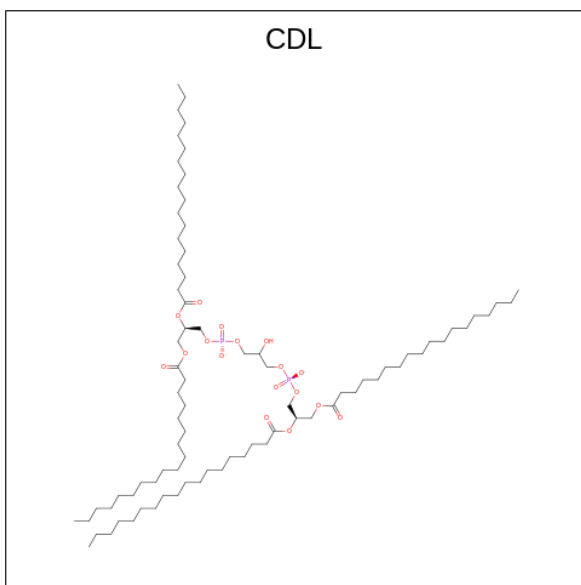
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O		
			29	24	5	0	0
24	C	1	Total	C	O		
			29	24	5	0	0
24	C	1	Total	C	O		
			29	24	5	0	0
24	J	1	Total	C	O		
			29	24	5	0	0
24	L	1	Total	C	O		
			29	24	5	0	0
24	O	1	Total	C	O		
			29	24	5	0	0
24	P	1	Total	C	O		
			29	24	5	0	0
24	P	1	Total	C	O		
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

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



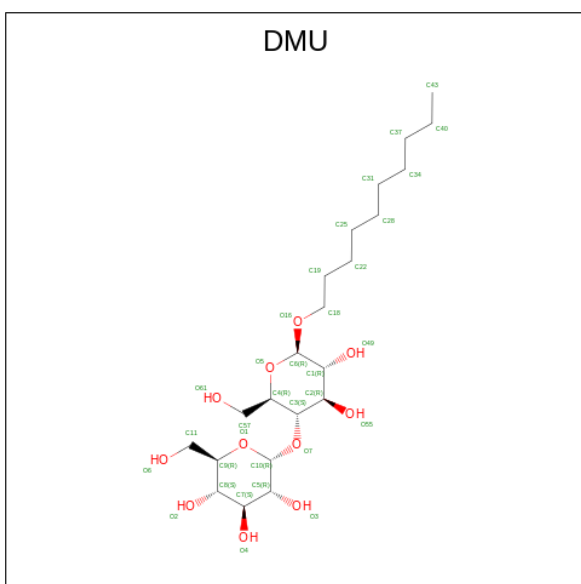
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			37	27	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	O	P		0	0
			50	41	8	1			
25	T	1	Total	C	N	O	P	0	0
			40	32	1	6	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total 91	C 72	O 17	P 2	0	0
26	G	1	Total 84	C 66	O 16	P 2	0	0
26	P	1	Total 84	C 65	O 17	P 2	0	0
26	T	1	Total 90	C 71	O 17	P 2	0	0

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

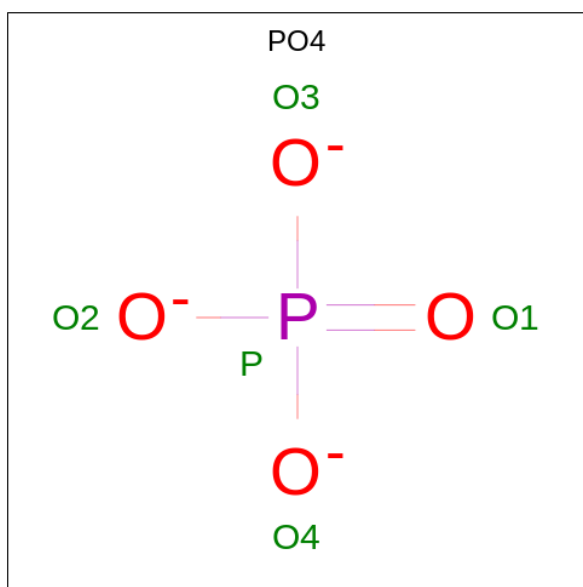


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	J	1	Total C O 33 22 11	0	0
27	K	1	Total C O 22 16 6	0	0
27	K	1	Total C O 22 16 6	0	0
27	K	1	Total C O 33 22 11	0	0
27	L	1	Total C O 22 16 6	0	0
27	M	1	Total C O 33 22 11	0	0
27	O	1	Total C O 22 16 6	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 22 16 6	0	0
27	Z	1	Total C O 33 22 11	0	0

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

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

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



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	266	Total	O	0	0
			266	266		
30	B	231	Total	O	0	1
			232	232		
30	C	162	Total	O	0	0
			162	162		
30	D	207	Total	O	0	0
			207	207		
30	E	145	Total	O	0	0
			145	145		
30	F	156	Total	O	0	0
			156	156		
30	G	84	Total	O	0	0
			84	84		
30	H	97	Total	O	0	0
			97	97		
30	I	68	Total	O	0	0
			68	68		
30	J	48	Total	O	0	0
			48	48		

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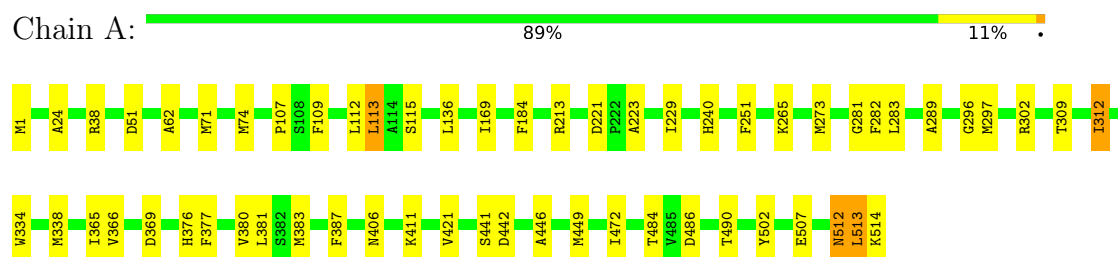
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	45	Total 45	O 45	0	0
30	L	37	Total 37	O 37	0	0
30	M	36	Total 36	O 36	0	0
30	N	278	Total 278	O 278	0	0
30	O	194	Total 195	O 195	0	1
30	P	161	Total 161	O 161	0	1
30	Q	128	Total 128	O 128	0	1
30	R	117	Total 117	O 117	0	0
30	S	141	Total 141	O 141	0	0
30	T	83	Total 83	O 83	0	0
30	U	96	Total 96	O 96	0	0
30	V	68	Total 68	O 68	0	0
30	W	44	Total 44	O 44	0	0
30	X	43	Total 43	O 43	0	0
30	Y	36	Total 36	O 36	0	0
30	Z	27	Total 27	O 27	0	0

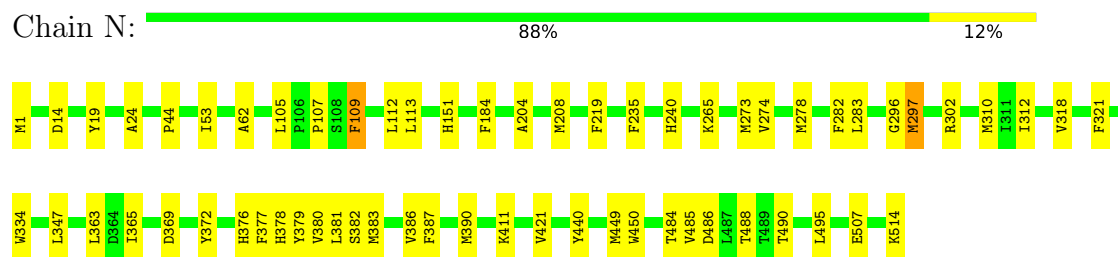
3 Residue-property plots

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.

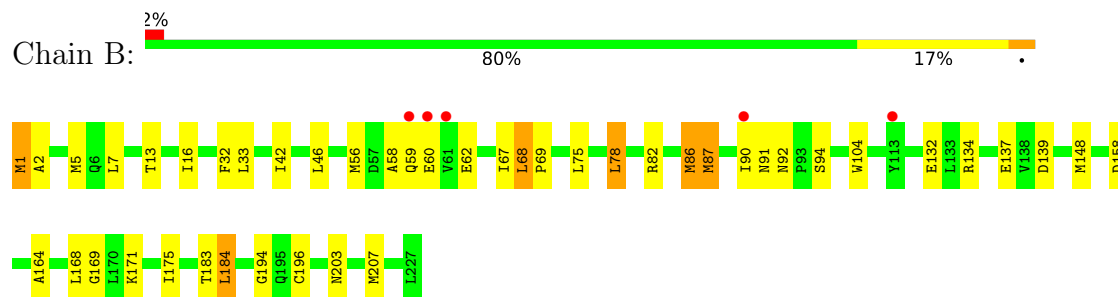
• Molecule 1: Cytochrome c oxidase subunit 1



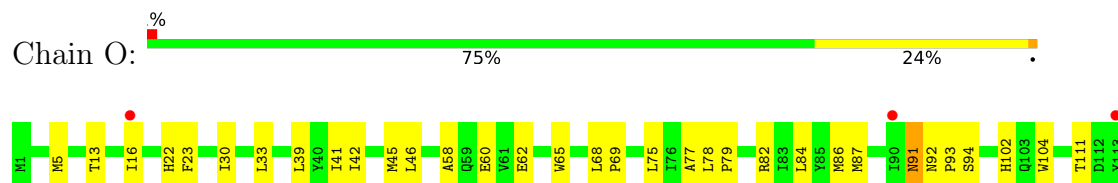
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

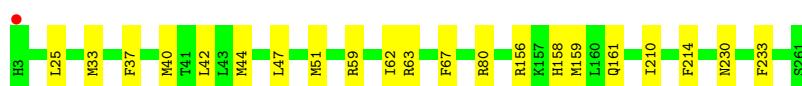




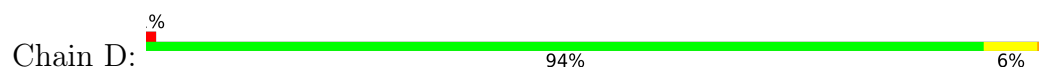
- Molecule 3: Cytochrome c oxidase subunit 3



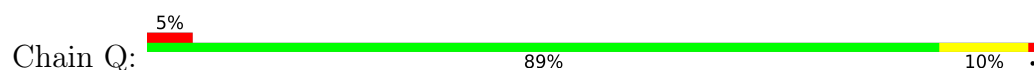
- Molecule 3: Cytochrome c oxidase subunit 3



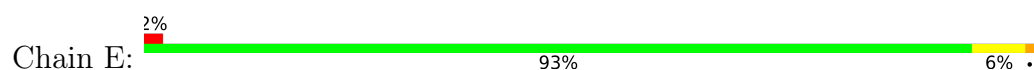
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



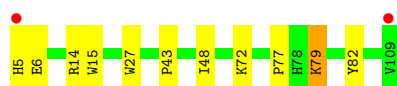
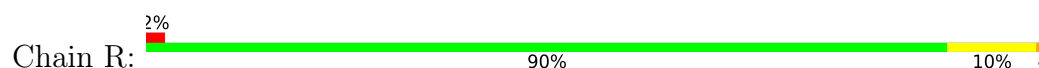
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



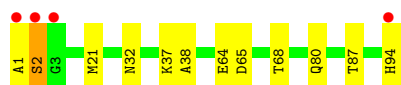
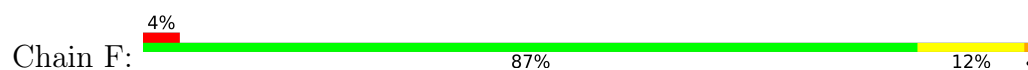
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



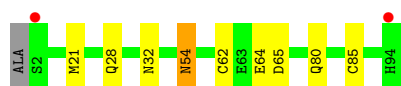
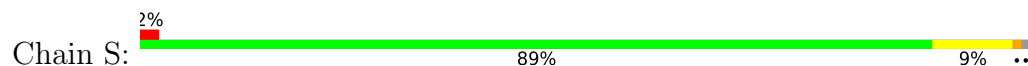
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



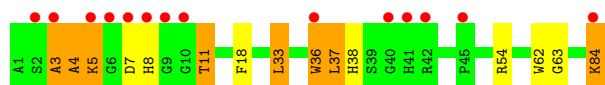
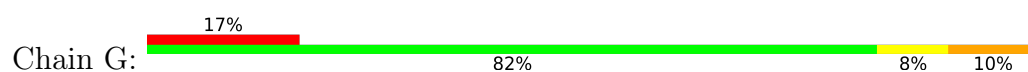
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



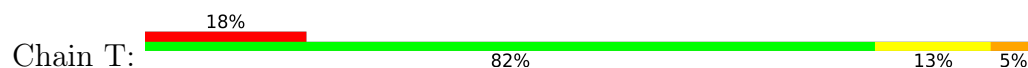
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



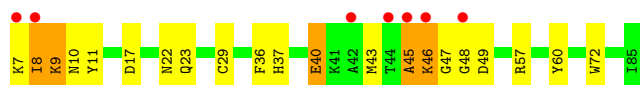
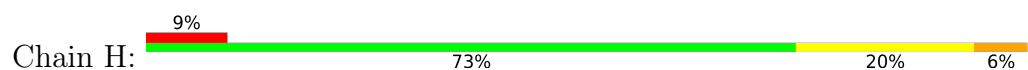
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



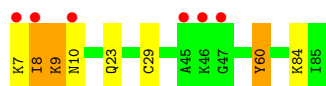
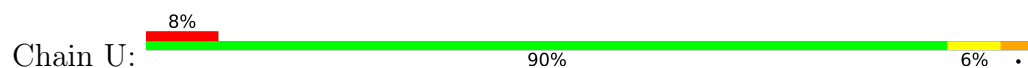
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



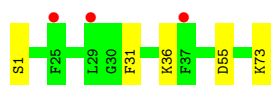
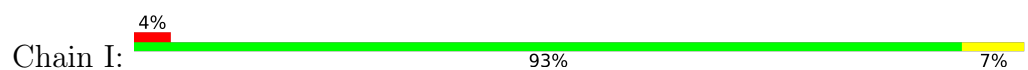
- Molecule 8: Cytochrome c oxidase subunit 6B1



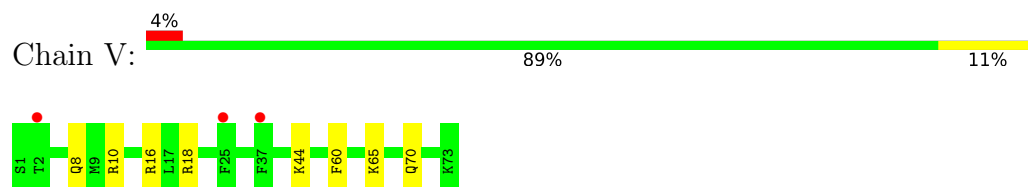
- Molecule 8: Cytochrome c oxidase subunit 6B1



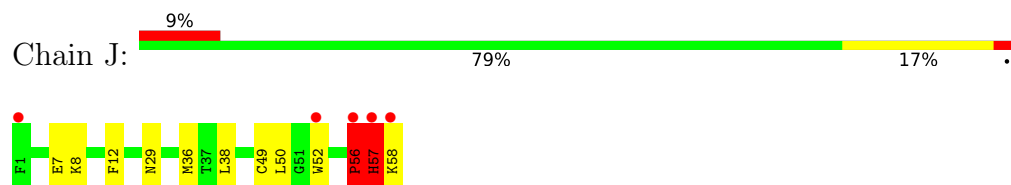
- Molecule 9: Cytochrome c oxidase subunit 6C



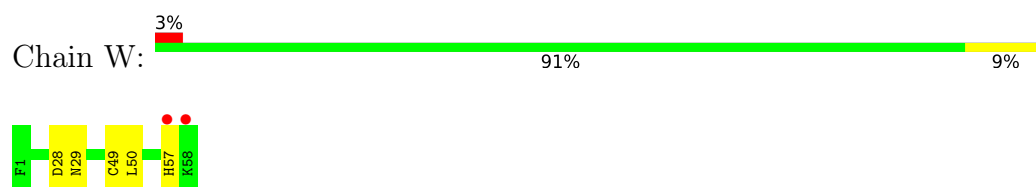
● Molecule 9: Cytochrome c oxidase subunit 6C



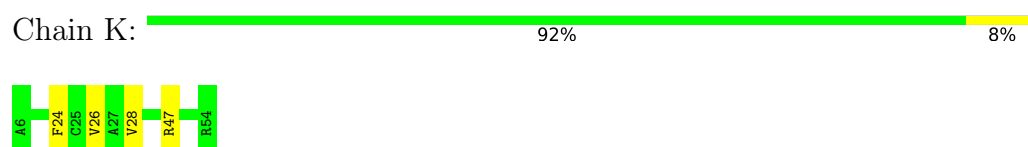
● Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



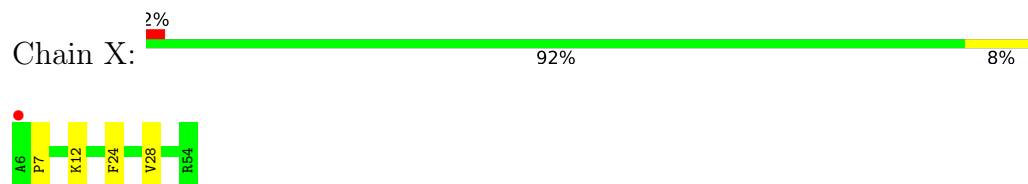
● Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



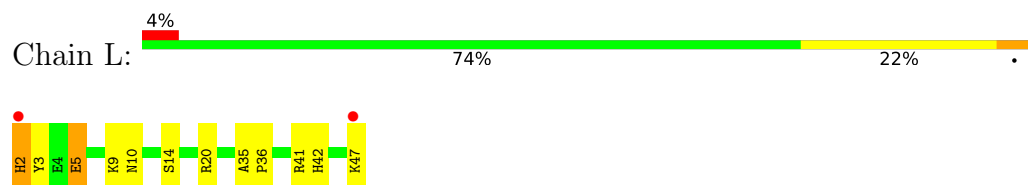
● Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



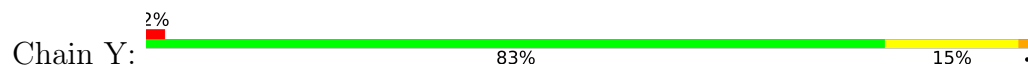
● Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

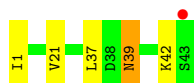
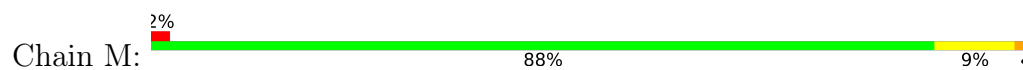


● Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

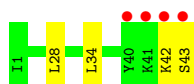




- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.31Å 204.71Å 177.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.95 – 1.65 136.14 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.95-1.65) 100.0 (136.14-1.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.152 , 0.176 0.152 , 0.176	Depositor DCC
R_{free} test set	43326 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34984	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.96	1/4369 (0.0%)	1.01	11/5961 (0.2%)
1	N	0.90	3/4377 (0.1%)	0.86	3/5972 (0.1%)
2	B	0.87	0/1968	0.97	4/2678 (0.1%)
2	O	0.76	1/1994 (0.1%)	0.88	2/2715 (0.1%)
3	C	0.87	1/2261 (0.0%)	0.83	3/3090 (0.1%)
3	P	0.84	1/2295 (0.0%)	0.79	0/3134
4	D	0.87	0/1277	0.83	1/1722 (0.1%)
4	Q	0.62	0/1266	0.77	2/1708 (0.1%)
5	E	0.78	1/882 (0.1%)	0.81	2/1196 (0.2%)
5	R	0.67	0/882	0.75	0/1196
6	F	0.83	1/757 (0.1%)	0.85	0/1026
6	S	0.82	0/744	0.87	0/1008
7	G	0.81	0/742	0.85	0/1005
7	T	0.71	0/722	0.80	0/978
8	H	0.87	2/682 (0.3%)	0.84	1/921 (0.1%)
8	U	0.70	0/681	0.75	0/919
9	I	0.69	0/625	0.74	1/828 (0.1%)
9	V	0.62	0/605	0.74	0/802
10	J	0.64	0/472	0.86	2/636 (0.3%)
10	W	0.63	0/472	0.73	1/636 (0.2%)
11	K	0.69	0/406	0.74	1/556 (0.2%)
11	X	0.61	0/406	0.67	0/556
12	L	0.87	0/402	0.80	0/538
12	Y	0.72	0/401	0.71	0/536
13	M	0.84	0/354	0.81	0/481
13	Z	0.67	0/354	0.71	0/481
All	All	0.83	11/30396 (0.0%)	0.86	34/41279 (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
10	J	0	2
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	102	TYR	CG-CD2	-6.23	1.31	1.39
1	A	184	PHE	CE2-CZ	5.96	1.48	1.37
2	O	167	SER	CA-CB	5.79	1.61	1.52
8	H	11	TYR	CD2-CE2	5.64	1.47	1.39
1	N	184	PHE	CE2-CZ	5.51	1.47	1.37
1	N	235	PHE	CE1-CZ	5.47	1.47	1.37
8	H	72	TRP	CZ3-CH2	5.14	1.48	1.40
3	P	233	PHE	CD1-CE1	5.08	1.49	1.39
5	E	70	VAL	CB-CG2	5.07	1.63	1.52
6	F	87	THR	CB-CG2	-5.07	1.35	1.52
1	N	372	TYR	CD1-CE1	5.05	1.47	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71[A]	MET	CG-SD-CE	-17.99	71.42	100.20
1	A	71[B]	MET	CG-SD-CE	-17.99	71.42	100.20
4	Q	20	ARG	NE-CZ-NH2	-10.84	114.88	120.30
4	Q	20	ARG	NE-CZ-NH1	9.87	125.23	120.30
1	A	213	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	38	ARG	NE-CZ-NH2	-6.88	116.86	120.30
10	J	56	PRO	C-N-CA	-6.87	104.53	121.70
5	E	40	ASP	CB-CG-OD1	6.82	124.44	118.30
9	I	55	ASP	CB-CG-OD1	6.53	124.18	118.30
1	A	513	LEU	CA-CB-CG	-6.27	100.89	115.30
10	J	36	MET	CG-SD-CE	-6.16	90.35	100.20
3	C	51[A]	MET	CG-SD-CE	-6.08	90.46	100.20
3	C	51[B]	MET	CG-SD-CE	-6.08	90.46	100.20
2	B	184	LEU	CA-CB-CG	5.90	128.86	115.30
2	B	134	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	442	ASP	CB-CG-OD2	-5.82	113.06	118.30
2	O	173	ASP	CB-CG-OD2	-5.71	113.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	139	ASP	CB-CG-OD1	5.62	123.36	118.30
1	N	486[A]	ASP	CB-CG-OD1	5.58	123.32	118.30
1	N	486[B]	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	113[A]	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	113[B]	LEU	CB-CG-CD2	5.55	120.44	111.00
5	E	30	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	38	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	251	PHE	CB-CG-CD2	-5.46	116.98	120.80
11	K	47	ARG	NE-CZ-NH2	5.45	123.03	120.30
2	B	87	MET	CA-CB-CG	5.34	122.39	113.30
3	C	233	PHE	CB-CG-CD1	-5.17	117.18	120.80
8	H	17	ASP	CB-CG-OD1	5.16	122.94	118.30
1	N	390	MET	CG-SD-CE	5.14	108.43	100.20
10	W	28	ASP	CB-CG-OD2	-5.12	113.69	118.30
4	D	20	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	A	74	MET	CG-SD-CE	-5.06	92.11	100.20
2	O	141	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
10	J	56	PRO	Peptide
10	J	57	HIS	Sidechain
1	N	240	HIS	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4162	0	4153	61	0
1	N	4133	0	4127	59	0
2	B	1906	0	1920	35	0
2	O	1909	0	1926	39	0
3	C	2157	0	2064	21	0
3	P	2173	0	2087	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1232	0	1215	11	0
4	Q	1226	0	1206	12	0
5	E	863	0	857	3	0
5	R	858	0	854	6	0
6	F	731	0	711	9	0
6	S	716	0	693	8	0
7	G	710	0	675	17	0
7	T	701	0	671	10	0
8	H	662	0	623	12	0
8	U	661	0	621	4	0
9	I	621	0	630	3	0
9	V	601	0	613	8	0
10	J	461	0	459	11	0
10	W	461	0	459	2	0
11	K	392	0	374	2	0
11	X	392	0	374	2	0
12	L	384	0	382	11	0
12	Y	382	0	381	6	0
13	M	338	0	355	7	0
13	Z	339	0	352	2	0
14	A	139	0	112	9	0
14	N	139	0	112	8	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	2	0	0	0	0
18	N	2	0	0	0	0
19	A	60	0	101	5	0
19	B	63	0	110	5	0
19	D	53	0	87	9	0
19	N	62	0	105	2	0
19	Q	63	0	110	5	0
19	Y	56	0	89	4	0
20	A	98	0	141	5	0
20	C	101	0	147	9	0
20	N	97	0	139	4	0
20	P	102	0	152	2	0
21	A	68	0	102	25	0
21	B	24	0	36	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	C	32	0	48	1	0
21	D	12	0	18	8	0
21	E	8	0	12	0	0
21	F	16	0	24	1	0
21	G	8	0	12	1	0
21	H	4	0	6	0	0
21	J	4	0	6	0	0
21	L	8	0	12	0	0
21	M	8	0	12	1	0
21	N	60	0	90	8	0
21	O	20	0	30	1	0
21	P	24	0	36	1	0
21	Q	12	0	18	2	0
21	R	8	0	12	0	0
21	S	16	0	24	0	0
21	T	8	0	12	0	0
21	U	4	0	6	0	0
21	W	4	0	6	0	0
21	Y	8	0	12	0	0
21	Z	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	48	0	66	5	0
23	R	49	0	69	7	0
24	B	29	0	39	0	0
24	C	58	0	78	3	0
24	J	29	0	39	1	0
24	L	29	0	39	2	0
24	O	29	0	39	1	0
24	P	58	0	78	3	0
24	W	29	0	39	0	0
24	Y	29	0	39	2	0
25	C	53	0	77	1	0
25	G	51	0	70	1	0
25	P	140	0	190	7	0
25	T	40	0	51	1	0
26	C	91	0	131	15	0
26	G	84	0	114	4	0
26	P	84	0	114	9	0
26	T	90	0	119	11	0
27	C	33	0	42	2	0
27	G	33	0	42	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	J	33	0	42	4	0
27	K	77	0	104	2	0
27	L	22	0	31	4	0
27	M	33	0	42	0	0
27	O	22	0	31	1	0
27	P	66	0	84	3	0
27	T	22	0	31	1	0
27	Z	33	0	42	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	266	0	0	16	0
30	B	232	0	0	7	0
30	C	162	0	0	3	0
30	D	207	0	0	4	0
30	E	145	0	0	1	0
30	F	156	0	0	4	0
30	G	84	0	0	5	0
30	H	97	0	0	1	0
30	I	68	0	0	4	0
30	J	48	0	0	1	0
30	K	45	0	0	0	0
30	L	37	0	0	3	0
30	M	36	0	0	1	0
30	N	278	0	0	12	0
30	O	195	0	0	2	0
30	P	161	0	0	4	0
30	Q	128	0	0	2	0
30	R	117	0	0	0	0
30	S	141	0	0	3	0
30	T	83	0	0	1	0
30	U	96	0	0	1	0
30	V	68	0	0	5	0
30	W	44	0	0	0	0
30	X	43	0	0	0	0
30	Y	36	0	0	3	0
30	Z	27	0	0	0	0
All	All	34984	0	32609	436	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 7.

All (436) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:105:LEU:HD11	21:N:610:EDO:H22	1.54	0.90
7:G:11:TPO:HA	7:G:11:TPO:O2P	1.77	0.83
19:A:607:TGL:HC32	12:L:20:ARG:HH12	1.42	0.82
1:A:446:ALA:HB2	21:A:617:EDO:H11	1.62	0.81
21:A:618:EDO:H12	21:B:307:EDO:H22	1.62	0.80
19:D:201:TGL:HG31	30:D:413:HOH:O	1.80	0.80
21:A:625:EDO:H21	2:B:203:ASN:OD1	1.82	0.79
21:A:617:EDO:H12	2:B:1:FME:HE3	1.64	0.79
10:J:56:PRO:O	10:J:58:LYS:N	2.16	0.79
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.65	0.78
21:A:615:EDO:H12	30:A:708:HOH:O	1.85	0.77
10:J:49:CYS:HB3	27:J:101:DMU:H11	1.68	0.76
1:A:411:LYS:NZ	21:A:614:EDO:H22	1.99	0.76
26:C:305:CDL:HB21	10:J:8:LYS:HE3	1.67	0.76
7:G:63:GLY:H	27:G:105:DMU:H40	1.52	0.75
1:A:115[A]:SER:OG	21:A:610:EDO:H12	1.86	0.74
21:A:619:EDO:H11	21:B:306:EDO:H12	1.70	0.73
30:A:733:HOH:O	21:M:103:EDO:H12	1.89	0.72
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.70	0.72
4:D:4:SER:HB3	30:D:354:HOH:O	1.90	0.71
21:N:616:EDO:H22	6:S:32:ASN:HD21	1.55	0.71
2:B:67:ILE:HD11	21:B:310:EDO:H11	1.73	0.69
3:C:67:PHE:HE2	26:C:305:CDL:HA21	1.57	0.69
4:D:4:SER:HB3	30:D:319:HOH:O	1.91	0.69
1:A:221:ASP:OD1	21:A:619:EDO:H21	1.92	0.69
21:A:622:EDO:H12	13:M:1:ILE:CA	2.23	0.69
1:N:365:ILE:HD11	30:N:701:HOH:O	1.92	0.68
20:A:608:PGV:H061	30:M:211:HOH:O	1.93	0.67
12:L:42:HIS:HB2	27:L:104:DMU:H6	1.76	0.67
2:B:158:ASP:HB2	21:B:307:EDO:H12	1.77	0.66
21:A:617:EDO:H12	2:B:1:FME:CE	2.25	0.66
1:A:223:ALA:HB2	21:A:619:EDO:H22	1.77	0.65
1:A:365:ILE:HD11	30:A:704:HOH:O	1.95	0.65
1:N:381[B]:LEU:HB2	14:N:602:HEA:CAC	2.27	0.65
1:A:112:LEU:HD13	30:A:775:HOH:O	1.96	0.65
27:G:105:DMU:H30	27:G:105:DMU:O1	1.97	0.64
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.79	0.64
21:N:614:EDO:H22	12:Y:10:ASN:HD22	1.61	0.64
3:C:230[A]:ASN:ND2	30:C:401:HOH:O	2.31	0.63
12:Y:26:THR:HA	30:Y:218:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:HA	7:T:4:ALA:CB	2.28	0.63
1:N:302[A]:ARG:CZ	30:N:701:HOH:O	2.46	0.63
1:N:449:MET:HE2	2:O:5:MET:HG2	1.81	0.62
19:N:607:TGL:HC22	30:V:161:HOH:O	1.97	0.62
19:B:301:TGL:HC22	30:I:159:HOH:O	1.98	0.62
1:A:411:LYS:HZ1	21:A:614:EDO:H22	1.63	0.62
23:R:201:PSC:H61	30:V:168:HOH:O	2.00	0.62
1:N:24:ALA:HB2	14:N:601[A]:HEA:H253	1.82	0.61
24:P:308:CHD:H231	30:P:536:HOH:O	1.99	0.61
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.31	0.61
1:N:302[A]:ARG:NH2	30:N:701:HOH:O	2.32	0.61
7:G:36:TRP:HB3	30:G:258:HOH:O	2.00	0.60
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.83	0.60
2:B:13:THR:HB	2:B:168:LEU:HD23	1.84	0.60
1:N:484[B]:THR:HG22	30:N:717:HOH:O	2.02	0.60
1:N:109:PHE:CE1	19:Y:101:TGL:H312	2.37	0.59
3:P:230[B]:ASN:ND2	30:P:403:HOH:O	2.33	0.59
21:A:619:EDO:H12	30:B:409:HOH:O	2.02	0.59
20:A:608:PGV:H031	30:A:882:HOH:O	2.00	0.59
4:D:78:TRP:HA	19:D:201:TGL:HB22	1.84	0.59
1:A:472:ILE:HG21	19:A:607:TGL:HA92	1.85	0.59
21:P:311:EDO:H21	30:P:529:HOH:O	2.02	0.59
12:L:41:ARG:HH12	27:L:104:DMU:H2	1.67	0.59
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.85	0.58
1:A:273:MET:HE2	30:A:706:HOH:O	2.02	0.58
21:A:615:EDO:H21	30:A:935:HOH:O	2.02	0.58
6:F:94:HIS:HD2	30:F:258:HOH:O	1.86	0.58
20:A:608:PGV:H041	30:A:902:HOH:O	2.02	0.58
26:T:102:CDL:H541	26:T:102:CDL:H241	1.86	0.57
8:H:45:ALA:O	8:H:47:GLY:N	2.38	0.57
26:P:307:CDL:OA5	26:P:307:CDL:H1	2.04	0.57
1:N:112[A]:LEU:HD13	30:N:926:HOH:O	2.05	0.57
6:F:1:ALA:O	6:F:2:SER:HB2	2.05	0.56
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	1.87	0.56
3:C:156:ARG:HE	24:C:306:CHD:C24	2.18	0.56
26:T:102:CDL:H222	26:T:102:CDL:H531	1.86	0.56
1:A:283:LEU:HB3	1:A:312[A]:ILE:HD12	1.87	0.56
27:L:104:DMU:H7	30:L:211:HOH:O	2.05	0.56
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.88	0.56
6:F:68:THR:HB	21:F:104:EDO:H21	1.87	0.56
20:N:609:PGV:H342	25:P:303:PEK:H372	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.88	0.56
2:O:58:ALA:O	2:O:62:GLU:HG3	2.07	0.55
3:P:33:MET:SD	27:P:309:DMU:H8	2.45	0.55
21:B:309:EDO:H21	30:B:580:HOH:O	2.06	0.55
20:C:304:PGV:H031	30:C:507:HOH:O	2.06	0.55
1:N:19:TYR:CE1	21:N:610:EDO:H11	2.42	0.55
21:A:623:EDO:H22	6:F:32:ASN:HD21	1.72	0.55
12:Y:9:LYS:NZ	30:Y:201:HOH:O	2.40	0.55
1:N:151[B]:HIS:CE1	25:P:303:PEK:H361	2.41	0.55
30:P:539:HOH:O	7:T:11:TPO:HG21	2.06	0.55
7:T:31:CYS:SG	26:T:102:CDL:H551	2.47	0.55
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.89	0.54
6:S:80[B]:GLN:NE2	30:S:202:HOH:O	2.39	0.54
1:A:297[B]:MET:HG2	1:A:302[B]:ARG:HG3	1.90	0.54
7:G:3:ALA:O	21:G:104:EDO:O2	2.26	0.54
1:N:53:ILE:HG12	30:N:904:HOH:O	2.06	0.54
1:A:484[B]:THR:HG22	30:A:914:HOH:O	2.07	0.54
21:B:307:EDO:H21	30:B:420:HOH:O	2.07	0.54
1:A:297[A]:MET:HB2	30:A:748:HOH:O	2.07	0.54
7:G:62:TRP:HB3	27:G:105:DMU:H29	1.89	0.54
3:P:67:PHE:CE2	26:P:307:CDL:HB22	2.43	0.54
1:N:273:MET:HE2	30:N:754:HOH:O	2.07	0.54
27:C:315:DMU:O4	27:J:101:DMU:O6	2.25	0.53
6:F:37:LYS:HD3	30:F:313:HOH:O	2.08	0.53
9:I:73:LYS:HE2	30:I:161:HOH:O	2.09	0.53
1:N:514:LYS:NZ	30:N:704:HOH:O	2.40	0.53
1:A:381[B]:LEU:HA	14:A:602:HEA:CBC	2.38	0.53
20:C:304:PGV:H012	30:C:507:HOH:O	2.09	0.53
5:E:90:ARG:HD2	30:E:394:HOH:O	2.08	0.53
1:A:411:LYS:NZ	30:A:703:HOH:O	2.36	0.53
2:B:16[B]:ILE:HG12	2:B:87:MET:HG2	1.91	0.53
2:O:22[B]:HIS:CD2	9:V:44:LYS:HE2	2.43	0.53
9:V:18:ARG:HD3	30:V:147:HOH:O	2.08	0.53
1:A:289:ALA:HB1	1:A:297[B]:MET:HE1	1.89	0.53
1:N:302[A]:ARG:NH1	30:N:706:HOH:O	2.43	0.52
4:Q:81:VAL:HG11	19:Q:201:TGL:HB52	1.91	0.52
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.92	0.52
7:G:63:GLY:N	27:G:105:DMU:H40	2.24	0.52
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.74	0.52
19:Q:201:TGL:H361	9:V:16:ARG:HE	1.74	0.52
2:B:56:MET:HG2	23:B:303:PSC:H211	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.92	0.51
2:B:90:ILE:HG13	30:B:547:HOH:O	2.11	0.51
8:H:45:ALA:C	8:H:47:GLY:H	2.13	0.51
10:J:7:GLU:HG3	30:J:224:HOH:O	2.09	0.51
24:L:103:CHD:H232	13:M:21:VAL:HG11	1.92	0.51
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.92	0.51
30:A:703:HOH:O	19:D:201:TGL:HG11	2.10	0.51
7:G:5:LYS:HG3	30:G:275:HOH:O	2.09	0.51
30:B:566:HOH:O	19:D:201:TGL:HC61	2.11	0.51
12:L:5[B]:GLU:HG3	30:L:221:HOH:O	2.09	0.51
8:U:9:LYS:O	8:U:10:ASN:HB2	2.10	0.51
30:N:881:HOH:O	4:Q:20:ARG:HG2	2.10	0.51
13:Z:28:LEU:HD23	27:Z:101:DMU:H7	1.92	0.51
2:B:68[B]:LEU:HB3	2:B:69:PRO:HD3	1.93	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.51
12:L:9:LYS:HE3	30:L:225:HOH:O	2.11	0.51
4:D:19[B]:ARG:HE	4:D:21:ASP:CG	2.14	0.51
26:P:307:CDL:HA4	26:P:307:CDL:H131	1.92	0.50
21:A:622:EDO:H12	13:M:1:ILE:N	2.25	0.50
26:T:102:CDL:H541	26:T:102:CDL:H231	1.93	0.50
26:C:305:CDL:HA22	10:J:12:PHE:CZ	2.47	0.50
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.12	0.50
12:Y:24[B]:MET:HE2	30:Y:214:HOH:O	2.12	0.50
1:A:502:TYR:CE2	21:A:624:EDO:H12	2.46	0.50
19:A:607:TGL:HC31	12:L:14:SER:H	1.76	0.50
3:C:220:PHE:HB2	26:C:305:CDL:H711	1.93	0.50
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.12	0.50
3:P:62:ILE:HD12	26:P:307:CDL:H511	1.94	0.50
2:B:94:SER:HB2	2:B:148[B]:MET:SD	2.52	0.50
3:C:54:MET:HE1	20:C:303:PGV:H142	1.94	0.50
4:D:78:TRP:CA	19:D:201:TGL:HB22	2.41	0.50
23:R:201:PSC:C07	9:V:10:ARG:HH21	2.25	0.50
4:Q:19:ARG:HG3	4:Q:21:ASP:OD1	2.12	0.49
1:A:512[A]:ASN:C	1:A:512[A]:ASN:HD22	2.15	0.49
2:O:22[B]:HIS:NE2	9:V:44:LYS:HE2	2.27	0.49
1:A:513:LEU:O	1:A:514:LYS:HB2	2.12	0.49
1:N:449:MET:HE3	1:N:450:TRP:CH2	2.48	0.49
26:T:102:CDL:OA7	26:T:102:CDL:H311	2.12	0.49
10:J:52:TRP:CE2	10:J:57:HIS:CE1	3.01	0.49
1:N:514:LYS:HD2	30:S:255:HOH:O	2.12	0.49
26:G:102:CDL:H332	30:O:406:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:305:CDL:H162	26:C:305:CDL:H332	1.95	0.49
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.12	0.49
21:N:617:EDO:H21	19:Q:201:TGL:H321	1.94	0.49
21:Q:203:EDO:H11	5:R:27:TRP:NE1	2.28	0.49
2:O:41:ILE:O	2:O:45:MET:HG2	2.13	0.48
1:A:486:ASP:HA	21:D:204:EDO:H11	1.95	0.48
14:A:602:HEA:HMC1	14:A:602:HEA:CBC	2.44	0.48
8:H:8:ILE:O	8:H:8:ILE:HG22	2.13	0.48
2:B:82[B]:ARG:CZ	2:B:86:MET:HE1	2.44	0.48
27:K:103:DMU:O1	27:K:103:DMU:H29	2.14	0.48
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.48	0.48
1:A:302[B]:ARG:CZ	30:A:704:HOH:O	2.61	0.48
3:C:91:VAL:HG22	25:T:101:PEK:H12	1.95	0.48
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.95	0.47
20:A:608:PGV:H202	20:A:608:PGV:H231	1.62	0.47
7:G:33[B]:LEU:CD1	7:G:37:LEU:HD22	2.44	0.47
7:G:38:HIS:HD2	30:G:207:HOH:O	1.95	0.47
1:N:363[A]:LEU:HG	2:O:23:PHE:HD2	1.79	0.47
2:O:68[B]:LEU:HD23	23:R:201:PSC:H151	1.95	0.47
3:C:55:TYR:CE1	26:C:305:CDL:H521	2.50	0.47
2:B:56:MET:HA	23:B:303:PSC:H202	1.95	0.47
5:R:77:PRO:O	5:R:79:LYS:HD2	2.13	0.47
6:F:64:GLU:O	6:F:65:ASP:HB2	2.13	0.47
7:G:5:LYS:HB3	1:N:278[A]:MET:HE1	1.96	0.47
1:A:334:TRP:HZ3	19:D:201:TGL:HA72	1.80	0.47
1:A:221:ASP:OD1	21:A:619:EDO:C2	2.62	0.47
26:G:102:CDL:H592	26:G:102:CDL:H621	1.29	0.47
10:J:52:TRP:CZ2	27:J:101:DMU:H4	2.50	0.47
1:N:14:ASP:OD1	21:N:614:EDO:H11	2.14	0.47
20:N:608:PGV:H11	4:Q:84:ALA:CB	2.45	0.47
2:O:130:PRO:HA	4:Q:115:TRP:CZ3	2.50	0.47
6:S:64:GLU:O	6:S:65:ASP:HB2	2.13	0.47
3:C:67:PHE:CE2	26:C:305:CDL:HA21	2.45	0.47
2:O:16[B]:ILE:HG12	2:O:87:MET:HG2	1.97	0.47
25:P:303:PEK:H72	25:P:303:PEK:H102	1.47	0.47
3:C:48:THR:HG23	26:C:305:CDL:C41	2.45	0.47
23:R:201:PSC:C10	23:R:201:PSC:H343	2.45	0.47
1:A:383[A]:MET:HG2	1:A:421:VAL:HG21	1.97	0.46
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.96	0.46
20:C:304:PGV:H061	8:H:22:ASN:HB2	1.97	0.46
1:N:204:ALA:O	1:N:208[A]:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ASP:CB	21:B:307:EDO:H12	2.46	0.46
1:N:386:VAL:HG21	14:N:601[A]:HEA:H261	1.98	0.46
1:A:136[B]:LEU:HD23	1:A:136[B]:LEU:HA	1.67	0.46
1:A:366[B]:VAL:CG1	2:B:169:GLY:HA2	2.46	0.46
26:C:305:CDL:OA5	26:C:305:CDL:H1	2.11	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.46
1:A:484[A]:THR:HG22	21:D:204:EDO:O1	2.15	0.46
1:A:507:GLU:OE1	21:A:623:EDO:O2	2.21	0.46
21:A:621:EDO:H11	12:L:10:ASN:HB2	1.97	0.46
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.97	0.46
4:Q:109:HIS:HE1	4:Q:115:TRP:CZ3	2.34	0.46
19:A:607:TGL:H162	19:A:607:TGL:HC82	1.52	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.46
4:D:107:ILE:H	21:D:203:EDO:C2	2.29	0.46
2:O:217[B]:LYS:HG2	30:O:574:HOH:O	2.16	0.46
1:A:449:MET:SD	2:B:5:MET:HG2	2.55	0.46
5:R:5:HIS:HB3	5:R:6:GLU:H	1.59	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.46
2:B:184:LEU:HA	30:B:406:HOH:O	2.15	0.46
27:C:315:DMU:H22	10:J:38:LEU:HD23	1.98	0.46
10:J:52:TRP:CD2	10:J:57:HIS:CE1	3.04	0.46
1:N:411:LYS:NZ	30:N:707:HOH:O	2.46	0.46
27:P:309:DMU:H11	10:W:49:CYS:HB3	1.97	0.46
5:E:86:ILE:O	5:E:90:ARG:HG2	2.15	0.46
21:A:622:EDO:H12	13:M:1:ILE:HA	1.97	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.45
7:G:5:LYS:HB3	1:N:278[A]:MET:CE	2.46	0.45
1:N:113:LEU:HB2	19:Y:101:TGL:H301	1.98	0.45
7:T:12:GLY:HA3	30:T:259:HOH:O	2.17	0.45
2:B:58:ALA:O	2:B:62:GLU:HG3	2.17	0.45
12:Y:47:LYS:HA	12:Y:47:LYS:HE2	1.97	0.45
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.51	0.45
2:O:68[B]:LEU:HB3	2:O:69:PRO:HD3	1.99	0.45
26:P:307:CDL:OB5	26:P:307:CDL:CB4	2.64	0.45
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.98	0.45
1:N:283:LEU:HB3	1:N:312[B]:ILE:HD11	1.99	0.45
1:N:302[A]:ARG:NE	30:N:701:HOH:O	2.50	0.45
23:R:201:PSC:H292	23:R:201:PSC:H321	1.68	0.45
3:C:207:HIS:CE1	20:C:303:PGV:H343	2.52	0.45
2:O:116:LEU:HD22	2:O:117:SER:N	2.31	0.45
26:C:305:CDL:OB5	26:C:305:CDL:CB4	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:363[A]:LEU:HG	2:O:23:PHE:CD2	2.52	0.45
21:A:622:EDO:H12	13:M:1:ILE:H2	1.81	0.45
1:N:321:PHE:HB3	2:O:65[A]:TRP:CE3	2.51	0.45
3:P:210:ILE:HG12	20:P:305:PGV:H132	1.99	0.45
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.99	0.45
1:A:281:GLY:O	7:T:4:ALA:HB1	2.16	0.45
19:A:607:TGL:OC1	19:A:607:TGL:HC42	2.16	0.45
8:H:23:GLN:HG3	30:H:242:HOH:O	2.17	0.45
26:T:102:CDL:H541	26:T:102:CDL:C24	2.46	0.45
19:B:301:TGL:HC61	30:I:167:HOH:O	2.17	0.45
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.99	0.45
3:P:158:HIS:HD2	3:P:161[B]:GLN:OE1	1.98	0.45
1:A:376:HIS:CE1	1:A:380[B]:VAL:HG11	2.53	0.44
26:G:102:CDL:H761	1:N:282:PHE:HZ	1.81	0.44
1:A:51:ASP:OD2	1:A:441:SER:OG	2.31	0.44
14:N:601[B]:HEA:H172	14:N:601[B]:HEA:H261	1.85	0.44
11:X:7:PRO:HB2	11:X:12:LYS:HE3	1.98	0.44
11:K:24:PHE:O	11:K:28[A]:VAL:HG12	2.16	0.44
1:N:274:VAL:O	1:N:278[A]:MET:HG3	2.17	0.44
1:N:347:LEU:HD13	1:N:383[A]:MET:HB3	1.98	0.44
26:T:102:CDL:H541	26:T:102:CDL:C23	2.47	0.44
8:H:37:HIS:HD2	8:H:40:GLU:OE2	2.01	0.44
2:O:30:ILE:HG12	27:O:308:DMU:H14	1.99	0.44
26:P:307:CDL:H181	26:P:307:CDL:H741	2.00	0.44
4:Q:46:ALA:HB3	30:Q:330:HOH:O	2.16	0.44
23:R:201:PSC:H202	23:R:201:PSC:H232	1.59	0.44
2:B:42:ILE:CG2	19:D:201:TGL:H242	2.48	0.44
3:C:67:PHE:CE2	26:C:305:CDL:HB22	2.53	0.44
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.36	0.44
11:K:26:VAL:HG11	27:K:101:DMU:H4	1.99	0.44
3:P:59:ARG:HA	26:P:307:CDL:H512	2.00	0.44
23:R:201:PSC:H02	23:R:201:PSC:H212	1.99	0.44
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.18	0.44
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.18	0.44
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.53	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.99	0.44
1:A:377:PHE:CD2	14:A:602:HEA:HAD1	2.53	0.44
1:A:383[A]:MET:HA	1:A:387:PHE:CD1	2.52	0.44
2:B:1:FME:HE2	2:B:2:ALA:O	2.18	0.44
8:H:43:MET:HE3	8:H:48:GLY:HA3	2.00	0.44
23:B:303:PSC:H61	23:B:303:PSC:H241	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:305:CDL:H312	26:C:305:CDL:H151	1.99	0.43
20:N:608:PGV:H11	4:Q:84:ALA:HB2	2.00	0.43
2:O:79:PRO:HA	2:O:82[A]:ARG:HE	1.83	0.43
19:Y:101:TGL:H202	19:Y:101:TGL:H231	1.47	0.43
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.53	0.43
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.17	0.43
7:G:84:LYS:HD2	7:G:84:LYS:HA	1.82	0.43
14:N:602:HEA:HMC1	14:N:602:HEA:CBC	2.48	0.43
2:O:5:MET:HB3	2:O:5:MET:HE2	1.65	0.43
26:T:102:CDL:H771	26:T:102:CDL:H571	2.00	0.43
1:A:136[A]:LEU:HD23	21:B:307:EDO:H11	2.00	0.43
2:B:56:MET:HB3	23:B:303:PSC:H232	2.00	0.43
25:C:302:PEK:H382	26:G:102:CDL:C20	2.48	0.43
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.78	0.43
3:C:210:ILE:HG12	20:C:303:PGV:H132	2.01	0.43
8:H:46:LYS:HD2	30:U:217:HOH:O	2.18	0.43
21:A:626:EDO:H11	20:C:304:PGV:H132	2.01	0.43
2:B:42:ILE:HG21	19:D:201:TGL:H242	2.00	0.43
4:D:19[A]:ARG:HB3	4:D:21:ASP:OD1	2.19	0.43
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.43
6:S:28:GLN:HG2	30:S:327:HOH:O	2.17	0.43
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.54	0.43
1:A:381[B]:LEU:HD13	14:A:602:HEA:HBC2	2.00	0.43
21:C:308:EDO:O2	21:C:314:EDO:H22	2.18	0.43
1:N:383[A]:MET:HA	1:N:387:PHE:CD1	2.53	0.43
3:P:33:MET:CE	3:P:42:LEU:H	2.32	0.43
8:U:84:LYS:HE2	8:U:84:LYS:HB2	1.34	0.43
11:X:24:PHE:O	11:X:28[A]:VAL:HG12	2.19	0.43
19:B:301:TGL:H252	19:B:301:TGL:H282	1.80	0.43
3:P:156:ARG:HE	24:P:308:CHD:C24	2.31	0.43
2:B:183[A]:THR:HG22	30:B:477:HOH:O	2.19	0.42
3:C:48:THR:HG23	26:C:305:CDL:H412	2.01	0.42
3:C:95:THR:HG21	20:C:304:PGV:H311	2.00	0.42
26:T:102:CDL:H182	26:T:102:CDL:H511	2.00	0.42
19:Y:101:TGL:HC82	19:Y:101:TGL:HC51	1.83	0.42
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.01	0.42
1:N:297[A]:MET:SD	1:N:302[A]:ARG:HG2	2.58	0.42
1:A:169[A]:ILE:HD12	7:T:8:HIS:O	2.19	0.42
2:B:7:LEU:HD11	19:B:301:TGL:H161	1.99	0.42
3:C:44[A]:MET:HE1	3:C:47:LEU:HD12	2.00	0.42
3:C:67:PHE:CZ	26:C:305:CDL:HB22	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:SER:OG	21:D:204:EDO:H21	2.19	0.42
25:G:101:PEK:H102	25:G:101:PEK:H72	1.67	0.42
10:J:52:TRP:O	10:J:57:HIS:CE1	2.72	0.42
24:J:102:CHD:H111	24:J:102:CHD:H193	1.68	0.42
12:L:2:HIS:ND1	12:L:2:HIS:N	2.67	0.42
25:P:304:PEK:H222	7:T:21:PHE:CD1	2.54	0.42
24:C:306:CHD:H112	24:C:306:CHD:H12A	1.81	0.42
27:G:105:DMU:H30	27:G:105:DMU:C10	2.49	0.42
1:N:488:THR:HB	1:N:495:LEU:HD13	2.02	0.42
2:O:82[B]:ARG:CZ	2:O:86:MET:HE1	2.50	0.42
3:P:161[A]:GLN:HE22	25:P:304:PEK:H41	1.85	0.42
9:V:8:GLN:HG2	30:V:130:HOH:O	2.19	0.42
24:Y:104:CHD:H112	24:Y:104:CHD:H12A	1.53	0.42
1:A:302[B]:ARG:NE	30:A:704:HOH:O	2.52	0.42
1:A:514:LYS:HD3	30:F:242:HOH:O	2.19	0.42
19:B:301:TGL:H252	19:B:301:TGL:H222	1.69	0.42
20:C:304:PGV:H272	20:C:304:PGV:H241	1.53	0.42
8:H:9:LYS:O	8:H:10:ASN:HB2	2.19	0.42
1:N:310:MET:HE1	2:O:77:ALA:HB2	2.01	0.42
4:Q:9:GLU:HG3	30:Q:412:HOH:O	2.19	0.42
1:A:309:THR:O	1:A:312[A]:ILE:HG12	2.19	0.42
9:I:1:SAC:HB3	30:I:103:HOH:O	2.20	0.42
1:N:302[A]:ARG:CZ	2:O:84:LEU:HD11	2.49	0.42
2:O:42:ILE:HG21	19:Q:201:TGL:H231	2.01	0.42
8:U:60:TYR:CD1	8:U:60:TYR:C	2.93	0.42
24:C:306:CHD:H183	24:C:306:CHD:H20	1.66	0.42
4:D:107:ILE:HG23	21:D:203:EDO:H21	2.02	0.42
1:N:208[B]:MET:HG2	1:N:219:PHE:CE2	2.55	0.42
19:D:201:TGL:HA91	19:D:201:TGL:H241	2.02	0.42
1:N:383[A]:MET:HG2	1:N:421:VAL:HG21	2.02	0.42
26:T:102:CDL:H241	26:T:102:CDL:C54	2.50	0.42
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.20	0.42
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.55	0.42
1:N:378:HIS:HA	1:N:382[B]:SER:HB2	2.02	0.42
1:N:381[B]:LEU:HA	14:N:602:HEA:CBC	2.50	0.42
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.54	0.42
3:P:63:ARG:NH2	26:P:307:CDL:OA4	2.48	0.42
21:A:624:EDO:H11	12:L:3:TYR:CE2	2.54	0.41
19:N:607:TGL:H241	19:N:607:TGL:H211	1.77	0.41
2:O:22[B]:HIS:HE2	9:V:44:LYS:HE2	1.84	0.41
2:O:93:PRO:HG3	2:O:151:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.41
26:C:305:CDL:H201	26:C:305:CDL:H752	2.02	0.41
4:D:17[A]:VAL:HG12	30:D:314:HOH:O	2.20	0.41
3:P:37:PHE:CE2	27:P:309:DMU:H13	2.55	0.41
26:T:102:CDL:H171	26:T:102:CDL:OB6	2.20	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
1:N:151[B]:HIS:CE1	25:P:303:PEK:H341	2.56	0.41
1:N:318:VAL:HG22	2:O:65[A]:TRP:CD1	2.54	0.41
7:T:84:LYS:NZ	7:T:84:LYS:H	2.18	0.41
30:A:780:HOH:O	21:D:204:EDO:H22	2.19	0.41
6:F:80[B]:GLN:NE2	30:F:203:HOH:O	2.53	0.41
7:G:38:HIS:CD2	30:G:207:HOH:O	2.72	0.41
6:S:54:ASN:HD22	6:S:54:ASN:C	2.23	0.41
2:B:16[B]:ILE:CG2	21:B:309:EDO:H11	2.51	0.41
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.08	0.41
3:C:33:MET:HB2	27:J:101:DMU:C19	2.51	0.41
13:M:39:ASN:OD1	13:M:39:ASN:N	2.53	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.20	0.41
6:S:21[A]:MET:HE2	6:S:21[A]:MET:HB2	1.63	0.41
24:Y:104:CHD:H212	24:Y:104:CHD:H183	2.02	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.48	0.41
10:J:29:ASN:HD22	10:J:29:ASN:H	1.68	0.41
23:B:303:PSC:H231	23:B:303:PSC:H201	1.55	0.41
4:Q:121:LYS:HE2	21:Q:202:EDO:O2	2.21	0.41
1:A:283:LEU:HD13	1:A:312[A]:ILE:HD12	2.02	0.41
1:A:406:ASN:HD21	20:A:608:PGV:H22	1.86	0.41
2:O:104:TRP:HB2	21:O:306:EDO:H11	2.02	0.41
2:O:111:THR:HA	2:O:114:GLU:O	2.21	0.41
10:W:29:ASN:HD22	10:W:29:ASN:H	1.68	0.41
1:A:283:LEU:CB	1:A:312[A]:ILE:HD12	2.51	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.89	0.41
4:D:17[B]:VAL:HG21	21:D:204:EDO:H12	2.02	0.41
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.03	0.41
12:L:41:ARG:NH1	27:L:104:DMU:H2	2.34	0.41
1:N:507:GLU:O	21:N:623:EDO:H12	2.20	0.41
21:N:616:EDO:C2	6:S:32:ASN:HD21	2.30	0.41
24:P:301:CHD:H162	20:P:306:PGV:H231	2.03	0.41
30:A:780:HOH:O	21:D:204:EDO:H11	2.20	0.41
1:N:378:HIS:O	1:N:382[B]:SER:HB2	2.21	0.41
21:B:310:EDO:O2	25:P:304:PEK:H291	2.21	0.40
8:H:43:MET:CE	8:H:49:ASP:H	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.02	0.40
2:O:39:LEU:CD1	19:Q:201:TGL:H232	2.51	0.40
2:O:218:TYR:HB3	30:V:110:HOH:O	2.20	0.40
3:C:191:GLY:HA3	30:G:222:HOH:O	2.20	0.40
24:L:103:CHD:H111	24:L:103:CHD:H193	1.77	0.40
20:N:608:PGV:H142	4:Q:87[A]:PHE:CD2	2.56	0.40
5:R:43:PRO:HB2	5:R:48:ILE:HD11	2.04	0.40
5:R:72:LYS:HB2	5:R:82:TYR:CD1	2.56	0.40
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.57	0.40
3:P:40[B]:MET:HE1	27:T:105:DMU:H9	2.03	0.40
3:P:51[A]:MET:SD	26:P:307:CDL:H612	2.61	0.40
6:F:21[B]:MET:HB2	6:F:21[B]:MET:HE2	1.68	0.40
24:O:301:CHD:H12	24:O:301:CHD:H212	2.04	0.40
5:R:14[B]:ARG:HG3	5:R:15:TRP:N	2.36	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	540/514 (105%)	526 (97%)	14 (3%)	0	100	100
1	N	541/514 (105%)	527 (97%)	14 (3%)	0	100	100
2	B	238/227 (105%)	232 (98%)	5 (2%)	1 (0%)	34	16
2	O	240/227 (106%)	234 (98%)	5 (2%)	1 (0%)	34	16
3	C	265/259 (102%)	259 (98%)	6 (2%)	0	100	100
3	P	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
4	D	147/144 (102%)	143 (97%)	4 (3%)	0	100	100
4	Q	146/144 (101%)	141 (97%)	4 (3%)	1 (1%)	22	6
5	E	104/105 (99%)	104 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	R	104/105 (99%)	104 (100%)	0	0	100	100
6	F	95/94 (101%)	93 (98%)	1 (1%)	1 (1%)	14	2
6	S	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
7	G	86/84 (102%)	79 (92%)	3 (4%)	4 (5%)	2	0
7	T	84/84 (100%)	75 (89%)	3 (4%)	6 (7%)	1	0
8	H	77/79 (98%)	71 (92%)	3 (4%)	3 (4%)	3	0
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	12	1
9	I	73/73 (100%)	72 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
11	X	48/49 (98%)	47 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	43 (96%)	2 (4%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	42/43 (98%)	41 (98%)	1 (2%)	0	100	100
13	Z	42/43 (98%)	42 (100%)	0	0	100	100
All	All	3632/3550 (102%)	3532 (97%)	82 (2%)	18 (0%)	29	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	92	ASN
6	F	2	SER
7	G	4	ALA
7	G	8	HIS
8	H	8	ILE
4	Q	6	VAL
7	T	3	ALA
7	T	4	ALA
7	T	5	LYS
7	T	8	HIS
8	U	8	ILE
7	G	3	ALA
7	G	5	LYS
8	H	46	LYS

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Mol	Chain	Res	Type
2	O	92	ASN
7	T	7	ASP
8	H	45	ALA
7	T	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	453/426 (106%)	444 (98%)	9 (2%)	55	32
1	N	454/426 (107%)	449 (99%)	5 (1%)	73	57
2	B	223/210 (106%)	212 (95%)	11 (5%)	25	5
2	O	225/210 (107%)	216 (96%)	9 (4%)	31	9
3	C	232/224 (104%)	230 (99%)	2 (1%)	78	66
3	P	236/224 (105%)	234 (99%)	2 (1%)	81	70
4	D	133/128 (104%)	130 (98%)	3 (2%)	50	25
4	Q	132/128 (103%)	128 (97%)	4 (3%)	41	15
5	E	93/92 (101%)	92 (99%)	1 (1%)	73	57
5	R	93/92 (101%)	92 (99%)	1 (1%)	73	57
6	F	81/78 (104%)	81 (100%)	0	100	100
6	S	80/78 (103%)	79 (99%)	1 (1%)	69	50
7	G	72/67 (108%)	62 (86%)	10 (14%)	3	0
7	T	70/67 (104%)	66 (94%)	4 (6%)	20	4
8	H	71/71 (100%)	66 (93%)	5 (7%)	15	2
8	U	70/71 (99%)	65 (93%)	5 (7%)	14	2
9	I	59/57 (104%)	58 (98%)	1 (2%)	60	39
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	11
10	J	49/49 (100%)	47 (96%)	2 (4%)	30	8
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	40/39 (103%)	40 (100%)	0	100	100
11	X	40/39 (103%)	40 (100%)	0	100	100
12	L	40/39 (103%)	36 (90%)	4 (10%)	7	1
12	Y	40/39 (103%)	38 (95%)	2 (5%)	24	5
13	M	38/37 (103%)	36 (95%)	2 (5%)	22	4
13	Z	38/37 (103%)	36 (95%)	2 (5%)	22	4
All	All	3168/3034 (104%)	3079 (97%)	89 (3%)	46	18

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	PHE
1	A	113[A]	LEU
1	A	113[B]	LEU
1	A	312[A]	ILE
1	A	312[B]	ILE
1	A	338	MET
1	A	369	ASP
1	A	512[A]	ASN
1	A	512[B]	ASN
2	B	33	LEU
2	B	59[A]	GLN
2	B	59[B]	GLN
2	B	60	GLU
2	B	68[A]	LEU
2	B	68[B]	LEU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	171	LYS
3	C	159	MET
3	C	214	PHE
4	D	4	SER
4	D	58[A]	GLU
4	D	58[B]	GLU
5	E	90	ARG
7	G	7[A]	ASP
7	G	7[B]	ASP
7	G	18[A]	PHE

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Mol	Chain	Res	Type
7	G	18[B]	PHE
7	G	33[A]	LEU
7	G	33[B]	LEU
7	G	36	TRP
7	G	37	LEU
7	G	54	ARG
7	G	84	LYS
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	40	GLU
8	H	60	TYR
9	I	36	LYS
10	J	50	LEU
10	J	57	HIS
12	L	2	HIS
12	L	5[A]	GLU
12	L	5[B]	GLU
12	L	47	LYS
13	M	39	ASN
13	M	42	LYS
1	N	109	PHE
1	N	297[A]	MET
1	N	297[B]	MET
1	N	369	ASP
1	N	485	VAL
2	O	33	LEU
2	O	60	GLU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	116	LEU
2	O	171	LYS
3	P	159	MET
3	P	214	PHE
4	Q	5	VAL
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
5	R	79	LYS

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Mol	Chain	Res	Type
6	S	54	ASN
7	T	7	ASP
7	T	18	PHE
7	T	37	LEU
7	T	54	ARG
8	U	7	LYS
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
9	V	65	LYS
9	V	70	GLN
10	W	50	LEU
10	W	57	HIS
12	Y	46	LYS
12	Y	47	LYS
13	Z	34	LEU
13	Z	43	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
2	B	10	GLN
2	B	91	ASN
2	B	92	ASN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
8	H	12	GLN
8	H	22	ASN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN

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Mol	Chain	Res	Type
2	O	10	GLN
2	O	59	GLN
2	O	91	ASN
2	O	92	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	ASN
3	P	68	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	94	ASN
6	S	32	ASN
6	S	54	ASN
7	T	8	HIS
8	U	37	HIS
10	W	29	ASN
11	X	35	GLN

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	$\# Z > 2$
9	SAC	I	1	9	7,8,9	0.62	0	8,9,11	0.96	0
9	SAC	V	1	9	7,8,9	0.58	0	8,9,11	0.92	0
1	FME	A	1	1	8,9,10	0.63	0	7,9,11	1.22	1 (14%)
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.61	2 (28%)
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	1.03	0

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	1.32	1 (12%)	10,14,16	1.29	2 (20%)
7	TPO	T	11	7	8,10,11	1.47	1 (12%)	10,14,16	0.74	0
2	FME	B	1	2	8,9,10	0.96	0	7,9,11	1.60	1 (14%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	3.20	1.60	1.50
7	G	11	TPO	P-O1P	2.48	1.58	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O-C-CA	-2.93	117.09	124.78
1	N	1	FME	CE-SD-CG	2.72	109.75	100.40
1	A	1	FME	O-C-CA	-2.61	117.94	124.78
7	G	11	TPO	O2P-P-OG1	2.36	116.55	105.99
7	G	11	TPO	CG2-CB-CA	2.25	117.61	113.16
2	B	1	FME	O1-CN-N	-2.08	119.79	125.27

There are no chirality outliers.

All (22) 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
7	G	11	TPO	CB-OG1-P-O3P
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CB-OG1-P-O1P
7	T	11	TPO	CB-OG1-P-O2P
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	N-CA-CB-OG
9	V	1	SAC	C-CA-CB-OG
1	A	1	FME	C-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD

There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 8 are monoatomic - leaving 153 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
27	DMU	C	315	-	34,34,34	0.91	1 (2%)	45,45,45	2.53	18 (40%)
21	EDO	R	203	-	3,3,3	0.73	0	2,2,2	0.13	0
21	EDO	T	104	-	3,3,3	0.67	0	2,2,2	0.86	0
21	EDO	C	313	-	3,3,3	0.43	0	2,2,2	0.41	0
21	EDO	A	617	-	3,3,3	0.46	0	2,2,2	0.17	0
19	TGL	B	301	-	62,62,62	1.19	3 (4%)	65,65,65	1.63	6 (9%)
21	EDO	O	307	-	3,3,3	0.78	0	2,2,2	0.46	0
21	EDO	C	312	-	3,3,3	0.60	0	2,2,2	0.18	0
19	TGL	Q	201	-	62,62,62	1.03	3 (4%)	65,65,65	1.35	8 (12%)
21	EDO	Q	202	-	3,3,3	0.43	0	2,2,2	0.78	0
21	EDO	D	204	-	3,3,3	0.47	0	2,2,2	0.12	0
26	CDL	T	102	-	87,87,99	1.43	11 (12%)	91,97,111	1.50	12 (13%)
21	EDO	P	310	-	3,3,3	0.61	0	2,2,2	0.19	0
21	EDO	T	103	-	3,3,3	0.41	0	2,2,2	0.71	0
25	PEK	C	302	-	52,52,52	1.11	2 (3%)	55,57,57	1.42	5 (9%)
21	EDO	N	615	-	3,3,3	1.03	0	2,2,2	0.64	0
24	CHD	W	101	-	32,32,32	0.82	0	51,51,51	1.99	12 (23%)
25	PEK	P	303	-	52,52,52	0.69	2 (3%)	55,57,57	1.14	5 (9%)
18	CYN	N	606	15	0,1,1	-	-	-	-	-
21	EDO	U	101	-	3,3,3	0.63	0	2,2,2	0.30	0
21	EDO	A	622	-	3,3,3	0.62	0	2,2,2	0.72	0
21	EDO	N	622	-	3,3,3	0.73	0	2,2,2	0.39	0
27	DMU	Z	101	-	34,34,34	0.55	1 (2%)	45,45,45	1.11	2 (4%)
27	DMU	L	104	-	22,22,34	0.81	1 (4%)	27,27,45	1.39	5 (18%)
21	EDO	P	314	-	3,3,3	0.93	0	2,2,2	1.01	0
21	EDO	C	310	-	3,3,3	0.40	0	2,2,2	1.35	0
21	EDO	E	202	-	3,3,3	0.60	0	2,2,2	0.28	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-
27	DMU	J	101	-	34,34,34	0.77	1 (2%)	45,45,45	2.53	16 (35%)
21	EDO	J	103	-	3,3,3	0.67	0	2,2,2	0.50	0
21	EDO	G	103	-	3,3,3	0.75	0	2,2,2	0.83	0
21	EDO	N	624	-	3,3,3	0.52	0	2,2,2	0.20	0
29	PO4	U	102	-	4,4,4	0.77	0	6,6,6	0.45	0
21	EDO	F	103	-	3,3,3	0.78	0	2,2,2	0.57	0
27	DMU	P	316	-	34,34,34	0.59	1 (2%)	45,45,45	1.76	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	K	101	-	22,22,34	1.27	2 (9%)	27,27,45	1.61	7 (25%)
27	DMU	P	309	-	34,34,34	0.88	1 (2%)	45,45,45	1.18	5 (11%)
21	EDO	A	620	-	3,3,3	0.61	0	2,2,2	0.81	0
24	CHD	C	306	-	32,32,32	1.00	2 (6%)	51,51,51	2.80	22 (43%)
19	TGL	A	607	-	59,59,62	1.25	4 (6%)	62,62,65	1.89	15 (24%)
21	EDO	A	618	-	3,3,3	0.58	0	2,2,2	0.33	0
21	EDO	G	104	-	3,3,3	0.52	0	2,2,2	0.34	0
23	PSC	B	303	-	47,47,51	1.31	3 (6%)	50,52,59	1.44	5 (10%)
21	EDO	C	314	-	3,3,3	0.64	0	2,2,2	0.79	0
21	EDO	A	621	-	3,3,3	0.74	0	2,2,2	2.40	1 (50%)
21	EDO	B	307	-	3,3,3	0.37	0	2,2,2	1.69	0
25	PEK	T	101	-	38,38,52	1.06	1 (2%)	39,40,57	1.34	4 (10%)
21	EDO	A	616	-	3,3,3	0.73	0	2,2,2	0.42	0
26	CDL	C	305	-	89,89,99	1.43	13 (14%)	95,99,111	1.97	22 (23%)
21	EDO	N	617	-	3,3,3	0.61	0	2,2,2	0.25	0
19	TGL	D	201	-	52,52,62	1.13	3 (5%)	55,55,65	1.31	6 (10%)
21	EDO	P	313	-	3,3,3	0.53	0	2,2,2	0.72	0
21	EDO	B	310	-	3,3,3	0.66	0	2,2,2	0.25	0
26	CDL	P	307	-	82,82,99	1.44	11 (13%)	88,92,111	2.23	17 (19%)
21	EDO	A	613	-	3,3,3	0.73	0	2,2,2	0.71	0
21	EDO	N	613	-	3,3,3	1.00	0	2,2,2	0.07	0
21	EDO	A	626	-	3,3,3	0.49	0	2,2,2	0.62	0
21	EDO	O	306	-	3,3,3	0.65	0	2,2,2	0.44	0
21	EDO	B	308	-	3,3,3	0.93	0	2,2,2	0.14	0
21	EDO	C	309	-	3,3,3	0.81	0	2,2,2	1.05	0
27	DMU	O	308	-	22,22,34	1.04	1 (4%)	27,27,45	1.49	3 (11%)
29	PO4	H	102	-	4,4,4	0.77	0	6,6,6	0.45	0
21	EDO	N	612	-	3,3,3	0.50	0	2,2,2	0.55	0
20	PGV	N	609	-	50,50,50	1.02	3 (6%)	53,56,56	1.17	3 (5%)
14	HEA	A	602	1	57,67,67	1.62	11 (19%)	61,103,103	2.64	21 (34%)
20	PGV	P	305	-	50,50,50	0.74	2 (4%)	53,56,56	1.11	4 (7%)
25	PEK	P	302	-	36,36,52	1.14	2 (5%)	39,41,57	1.92	9 (23%)
21	EDO	F	105	-	3,3,3	0.64	0	2,2,2	0.63	0
21	EDO	A	614	-	3,3,3	0.62	0	2,2,2	0.08	0
27	DMU	K	102	-	22,22,34	1.30	3 (13%)	27,27,45	1.69	9 (33%)
25	PEK	P	304	-	49,49,52	1.20	3 (6%)	53,54,57	1.71	7 (13%)
21	EDO	O	305	-	3,3,3	0.76	0	2,2,2	0.48	0
24	CHD	P	308	-	32,32,32	0.67	0	51,51,51	1.69	13 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	HEA	A	601[B]	-	57,67,67	1.76	10 (17%)	61,103,103	2.03	18 (29%)
20	PGV	A	608	-	46,46,50	1.19	2 (4%)	49,52,56	1.40	10 (20%)
21	EDO	N	620	-	3,3,3	0.60	0	2,2,2	0.58	0
18	CYN	A	606	15	0,1,1	-	-	-	-	-
21	EDO	B	306	-	3,3,3	0.68	0	2,2,2	0.35	0
21	EDO	C	308	-	3,3,3	0.75	0	2,2,2	0.52	0
21	EDO	D	203	-	3,3,3	0.67	0	2,2,2	0.26	0
21	EDO	P	312	-	3,3,3	0.88	0	2,2,2	0.25	0
21	EDO	N	621	-	3,3,3	0.61	0	2,2,2	0.35	0
20	PGV	A	609	-	50,50,50	0.88	2 (4%)	53,56,56	1.01	1 (1%)
21	EDO	Q	204	-	3,3,3	0.49	0	2,2,2	0.10	0
21	EDO	A	610	-	3,3,3	0.43	0	2,2,2	1.18	0
21	EDO	S	105	-	3,3,3	0.71	0	2,2,2	0.62	0
21	EDO	N	618	-	3,3,3	0.76	0	2,2,2	0.41	0
14	HEA	N	601[B]	-	57,67,67	1.41	7 (12%)	61,103,103	1.87	17 (27%)
21	EDO	C	307	-	3,3,3	0.83	0	2,2,2	0.11	0
21	EDO	R	202	-	3,3,3	0.55	0	2,2,2	0.50	0
27	DMU	K	103	-	34,34,34	1.23	3 (8%)	45,45,45	2.05	16 (35%)
21	EDO	Y	103	-	3,3,3	0.64	0	2,2,2	0.07	0
24	CHD	O	301	-	32,32,32	1.06	0	51,51,51	1.25	4 (7%)
14	HEA	N	602	1	57,67,67	1.59	12 (21%)	61,103,103	2.09	19 (31%)
26	CDL	G	102	-	80,80,99	1.49	11 (13%)	80,86,111	1.59	12 (15%)
27	DMU	M	101	-	34,34,34	0.55	1 (2%)	45,45,45	1.15	3 (6%)
14	HEA	A	601[A]	-	57,67,67	1.69	10 (17%)	61,103,103	2.12	18 (29%)
21	EDO	D	202	-	3,3,3	0.39	0	2,2,2	0.79	0
20	PGV	P	306	-	50,50,50	1.09	2 (4%)	53,56,56	1.39	8 (15%)
21	EDO	H	101	-	3,3,3	0.50	0	2,2,2	0.51	0
21	EDO	L	101	-	3,3,3	0.55	0	2,2,2	0.18	0
21	EDO	A	615	-	3,3,3	0.69	0	2,2,2	1.09	0
25	PEK	G	101	-	50,50,52	0.87	2 (4%)	53,55,57	1.05	3 (5%)
21	EDO	E	201	-	3,3,3	0.61	0	2,2,2	0.46	0
21	EDO	S	103	-	3,3,3	0.81	0	2,2,2	0.63	0
21	EDO	Q	203	-	3,3,3	0.69	0	2,2,2	0.60	0
19	TGL	Y	101	-	54,54,62	1.31	4 (7%)	56,56,65	1.70	12 (21%)
21	EDO	L	102	-	3,3,3	0.52	0	2,2,2	0.12	0
21	EDO	A	612	-	3,3,3	0.87	0	2,2,2	0.42	0
14	HEA	N	601[A]	-	57,67,67	1.35	6 (10%)	61,103,103	1.89	16 (26%)
22	CUA	O	302	2	0,1,1	-	-	-	-	-
24	CHD	B	304	-	32,32,32	0.95	1 (3%)	51,51,51	1.60	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	G	105	-	34,34,34	1.05	1 (2%)	45,45,45	2.49	15 (33%)
21	EDO	N	614	-	3,3,3	0.60	0	2,2,2	0.81	0
21	EDO	S	104	-	3,3,3	0.89	0	2,2,2	0.51	0
21	EDO	N	623	-	3,3,3	1.16	0	2,2,2	0.74	0
21	EDO	Z	102	-	3,3,3	0.51	0	2,2,2	0.20	0
19	TGL	N	607	-	61,61,62	1.17	3 (4%)	64,64,65	1.29	6 (9%)
21	EDO	C	311	-	3,3,3	0.35	0	2,2,2	0.96	0
24	CHD	L	103	-	32,32,32	0.90	0	51,51,51	3.10	28 (54%)
24	CHD	J	102	-	32,32,32	0.83	0	51,51,51	2.14	17 (33%)
20	PGV	N	608	-	45,45,50	1.07	3 (6%)	48,51,56	1.40	6 (12%)
21	EDO	M	102	-	3,3,3	0.49	0	2,2,2	0.14	0
21	EDO	Y	102	-	3,3,3	0.61	0	2,2,2	0.08	0
27	DMU	T	105	-	22,22,34	1.39	3 (13%)	27,27,45	1.85	8 (29%)
21	EDO	A	611	-	3,3,3	0.37	0	2,2,2	0.60	0
21	EDO	N	611	-	3,3,3	0.61	0	2,2,2	0.62	0
23	PSC	R	201	-	47,47,51	1.67	5 (10%)	50,53,59	1.51	6 (12%)
21	EDO	O	304	-	3,3,3	0.61	0	2,2,2	0.31	0
21	EDO	B	309	-	3,3,3	0.59	0	2,2,2	0.59	0
21	EDO	S	102	-	3,3,3	0.71	0	2,2,2	0.08	0
21	EDO	N	610	-	3,3,3	0.75	0	2,2,2	2.43	1 (50%)
21	EDO	N	619	-	3,3,3	0.42	0	2,2,2	0.64	0
21	EDO	F	102	-	3,3,3	1.04	0	2,2,2	0.66	0
24	CHD	P	301	-	32,32,32	1.03	1 (3%)	51,51,51	1.50	10 (19%)
21	EDO	W	102	-	3,3,3	0.80	0	2,2,2	0.54	0
21	EDO	A	625	-	3,3,3	0.57	0	2,2,2	0.26	0
21	EDO	A	619	-	3,3,3	0.25	0	2,2,2	0.18	0
21	EDO	F	104	-	3,3,3	0.66	0	2,2,2	0.64	0
21	EDO	N	616	-	3,3,3	0.31	0	2,2,2	0.39	0
21	EDO	M	103	-	3,3,3	0.53	0	2,2,2	0.23	0
20	PGV	C	304	-	50,50,50	1.13	2 (4%)	53,56,56	1.79	12 (22%)
20	PGV	C	303	-	49,49,50	0.76	1 (2%)	52,55,56	0.98	1 (1%)
21	EDO	O	303	-	3,3,3	0.63	0	2,2,2	0.26	0
24	CHD	Y	104	-	32,32,32	0.82	0	51,51,51	2.49	19 (37%)
21	EDO	B	305	-	3,3,3	0.42	0	2,2,2	0.16	0
24	CHD	C	301	-	32,32,32	1.00	2 (6%)	51,51,51	1.29	9 (17%)
21	EDO	A	624	-	3,3,3	0.47	0	2,2,2	0.99	0
21	EDO	A	623	-	3,3,3	0.38	0	2,2,2	0.56	0
21	EDO	P	315	-	3,3,3	0.42	0	2,2,2	0.57	0
21	EDO	P	311	-	3,3,3	0.69	0	2,2,2	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	C	315	-	-	7/19/59/59	0/2/2/2
21	EDO	R	203	-	-	1/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	C	313	-	-	0/1/1/1	-
21	EDO	A	617	-	-	1/1/1/1	-
19	TGL	B	301	-	-	22/65/65/65	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	C	312	-	-	1/1/1/1	-
19	TGL	Q	201	-	-	35/65/65/65	-
21	EDO	Q	202	-	-	1/1/1/1	-
21	EDO	D	204	-	-	1/1/1/1	-
26	CDL	T	102	-	-	41/94/94/110	-
21	EDO	P	310	-	-	0/1/1/1	-
21	EDO	T	103	-	-	0/1/1/1	-
25	PEK	C	302	-	-	24/56/56/56	-
21	EDO	N	615	-	-	0/1/1/1	-
24	CHD	W	101	-	-	6/9/74/74	0/4/4/4
25	PEK	P	303	-	-	10/56/56/56	-
21	EDO	U	101	-	-	0/1/1/1	-
21	EDO	A	622	-	-	1/1/1/1	-
21	EDO	N	622	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	2/19/59/59	0/2/2/2
27	DMU	L	104	-	-	8/13/33/59	0/1/1/2
21	EDO	P	314	-	-	1/1/1/1	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
27	DMU	J	101	-	-	8/19/59/59	0/2/2/2
21	EDO	J	103	-	-	0/1/1/1	-
21	EDO	G	103	-	-	0/1/1/1	-
21	EDO	N	624	-	-	0/1/1/1	-
21	EDO	F	103	-	-	0/1/1/1	-
27	DMU	P	316	-	-	8/19/59/59	0/2/2/2
27	DMU	K	101	-	-	7/13/33/59	0/1/1/2
27	DMU	P	309	-	-	4/19/59/59	0/2/2/2
21	EDO	A	620	-	-	0/1/1/1	-
24	CHD	C	306	-	-	7/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	A	607	-	-	34/62/62/65	-
21	EDO	A	618	-	-	1/1/1/1	-
21	EDO	G	104	-	-	0/1/1/1	-
23	PSC	B	303	-	-	20/51/51/55	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	A	621	-	-	0/1/1/1	-
21	EDO	B	307	-	-	1/1/1/1	-
25	PEK	T	101	-	-	14/37/37/56	-
21	EDO	A	616	-	-	0/1/1/1	-
26	CDL	C	305	-	-	46/94/94/110	-
21	EDO	N	617	-	-	0/1/1/1	-
19	TGL	D	201	-	-	29/55/55/65	-
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	B	310	-	-	0/1/1/1	-
26	CDL	P	307	-	-	48/87/87/110	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	A	626	-	-	0/1/1/1	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	B	308	-	-	1/1/1/1	-
21	EDO	C	309	-	-	0/1/1/1	-
27	DMU	O	308	-	-	3/13/33/59	0/1/1/2
21	EDO	N	612	-	-	0/1/1/1	-
20	PGV	N	609	-	-	7/55/55/55	-
14	HEA	A	602	1	3/3/7/16	4/32/76/76	-
20	PGV	P	305	-	-	9/55/55/55	-
25	PEK	P	302	-	-	17/39/39/56	-
21	EDO	F	105	-	-	0/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
27	DMU	K	102	-	-	9/13/33/59	0/1/1/2
25	PEK	P	304	-	-	26/51/51/56	-
21	EDO	O	305	-	-	0/1/1/1	-
24	CHD	P	308	-	-	5/9/74/74	0/4/4/4
14	HEA	A	601[B]	-	3/3/7/16	6/32/76/76	-
20	PGV	A	608	-	-	24/51/51/55	-
21	EDO	N	620	-	-	0/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	C	308	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	D	203	-	-	1/1/1/1	-
21	EDO	P	312	-	-	0/1/1/1	-
21	EDO	N	621	-	-	1/1/1/1	-
20	PGV	A	609	-	-	6/55/55/55	-
21	EDO	Q	204	-	-	0/1/1/1	-
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	N	618	-	-	0/1/1/1	-
14	HEA	N	601[B]	-	3/3/7/16	5/32/76/76	-
14	HEA	A	601[C]	-	3/3/3/16	-	-
21	EDO	C	307	-	-	0/1/1/1	-
21	EDO	R	202	-	-	0/1/1/1	-
27	DMU	K	103	-	-	9/19/59/59	0/2/2/2
21	EDO	Y	103	-	-	0/1/1/1	-
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
14	HEA	N	602	1	3/3/7/16	5/32/76/76	-
26	CDL	G	102	-	-	45/80/80/110	-
27	DMU	M	101	-	-	2/19/59/59	0/2/2/2
14	HEA	A	601[A]	-	3/3/7/16	8/32/76/76	-
21	EDO	D	202	-	-	1/1/1/1	-
20	PGV	P	306	-	-	15/55/55/55	-
21	EDO	H	101	-	-	1/1/1/1	-
14	HEA	N	601[C]	-	3/3/3/16	-	-
21	EDO	A	615	-	-	0/1/1/1	-
21	EDO	L	101	-	-	0/1/1/1	-
25	PEK	G	101	-	-	10/54/54/56	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	Q	203	-	-	0/1/1/1	-
19	TGL	Y	101	-	-	33/54/54/65	-
21	EDO	L	102	-	-	0/1/1/1	-
21	EDO	A	612	-	-	0/1/1/1	-
14	HEA	N	601[A]	-	3/3/7/16	4/32/76/76	-
24	CHD	B	304	-	-	2/9/74/74	0/4/4/4
27	DMU	G	105	-	-	9/19/59/59	0/2/2/2
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	N	623	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	Z	102	-	-	1/1/1/1	-
19	TGL	N	607	-	-	33/64/64/65	-
21	EDO	C	311	-	-	0/1/1/1	-
24	CHD	L	103	-	-	5/9/74/74	0/4/4/4
24	CHD	J	102	-	-	5/9/74/74	0/4/4/4
20	PGV	N	608	-	-	18/50/50/55	-
21	EDO	M	102	-	-	0/1/1/1	-
21	EDO	Y	102	-	-	0/1/1/1	-
27	DMU	T	105	-	-	5/13/33/59	0/1/1/2
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	N	611	-	-	0/1/1/1	-
23	PSC	R	201	-	-	24/48/48/55	-
21	EDO	O	304	-	-	0/1/1/1	-
21	EDO	B	309	-	-	1/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	N	619	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
24	CHD	P	301	-	-	2/9/74/74	0/4/4/4
21	EDO	W	102	-	-	0/1/1/1	-
21	EDO	A	625	-	-	1/1/1/1	-
21	EDO	A	619	-	-	1/1/1/1	-
21	EDO	F	104	-	-	1/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
21	EDO	M	103	-	-	1/1/1/1	-
20	PGV	C	304	-	-	21/55/55/55	-
20	PGV	C	303	-	-	12/54/54/55	-
21	EDO	O	303	-	-	0/1/1/1	-
24	CHD	Y	104	-	-	4/9/74/74	0/4/4/4
21	EDO	B	305	-	-	0/1/1/1	-
24	CHD	C	301	-	-	2/9/74/74	0/4/4/4
21	EDO	A	624	-	-	0/1/1/1	-
21	EDO	A	623	-	-	0/1/1/1	-
21	EDO	P	315	-	-	0/1/1/1	-
21	EDO	P	311	-	-	0/1/1/1	-

All (185) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	R	201	PSC	O01-C1	7.13	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	101	TGL	OG2-CB1	6.10	1.51	1.34
23	B	303	PSC	O01-C1	5.82	1.50	1.34
25	T	101	PEK	O01-C1	5.68	1.50	1.33
26	G	102	CDL	OB6-CB5	5.68	1.45	1.33
19	A	607	TGL	OG2-CB1	5.66	1.50	1.34
20	C	304	PGV	O03-C19	5.43	1.49	1.33
19	Y	101	TGL	OG1-CA1	5.20	1.48	1.33
26	T	102	CDL	OB8-CB7	5.15	1.48	1.33
19	N	607	TGL	OG2-CB1	5.15	1.48	1.34
26	P	307	CDL	OA8-CA7	5.14	1.48	1.33
25	P	304	PEK	O01-C1	5.14	1.48	1.34
14	N	601[A]	HEA	CHC-C4B	5.11	1.48	1.35
14	N	601[B]	HEA	CHC-C4B	5.11	1.48	1.35
19	B	301	TGL	OG1-CA1	5.07	1.48	1.33
20	A	608	PGV	O03-C19	5.05	1.48	1.33
26	C	305	CDL	OA8-CA7	5.03	1.48	1.33
19	A	607	TGL	OG3-CC1	4.97	1.47	1.33
26	C	305	CDL	OB8-CB7	4.96	1.47	1.33
26	G	102	CDL	OB8-CB7	4.94	1.47	1.33
19	B	301	TGL	OG3-CC1	4.87	1.47	1.33
26	T	102	CDL	OB6-CB5	4.82	1.47	1.34
26	P	307	CDL	OA6-CA5	4.81	1.47	1.34
25	C	302	PEK	O01-C1	4.80	1.47	1.34
25	P	302	PEK	O01-C1	4.77	1.47	1.34
20	P	306	PGV	O03-C19	4.76	1.47	1.33
19	B	301	TGL	OG2-CB1	4.70	1.47	1.34
25	P	304	PEK	O03-C21	4.70	1.47	1.33
20	N	608	PGV	O03-C19	4.69	1.47	1.33
26	T	102	CDL	OA6-CA5	4.68	1.47	1.34
19	N	607	TGL	OG1-CA1	4.68	1.47	1.33
26	C	305	CDL	OA6-CA5	4.67	1.47	1.34
23	R	201	PSC	C7-C8	-4.62	1.33	1.52
25	C	302	PEK	O03-C21	4.58	1.46	1.33
20	P	306	PGV	O01-C1	4.57	1.47	1.34
14	A	601[A]	HEA	C3C-C2C	-4.56	1.34	1.40
14	A	601[B]	HEA	C3C-C2C	-4.56	1.34	1.40
20	C	304	PGV	O01-C1	4.44	1.46	1.34
20	A	608	PGV	O01-C1	4.44	1.46	1.34
19	N	607	TGL	OG3-CC1	4.43	1.46	1.33
26	G	102	CDL	OA8-CA7	4.41	1.45	1.30
14	A	602	HEA	CHD-C1D	4.41	1.46	1.35
19	D	201	TGL	OG1-CA1	4.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Q	201	TGL	OG3-CC1	4.35	1.46	1.33
26	P	307	CDL	OB8-CB7	4.34	1.46	1.33
26	T	102	CDL	OA8-CA7	4.33	1.46	1.33
19	A	607	TGL	OG1-CA1	4.32	1.46	1.33
19	D	201	TGL	OG3-CC1	4.08	1.45	1.33
23	R	201	PSC	O03-C19	4.07	1.45	1.33
14	A	601[B]	HEA	O11-C11	4.04	1.51	1.42
14	A	601[A]	HEA	CHC-C4B	4.00	1.45	1.35
14	A	601[B]	HEA	CHC-C4B	4.00	1.45	1.35
14	A	601[A]	HEA	CBD-CGD	3.92	1.59	1.50
14	A	601[B]	HEA	CBD-CGD	3.92	1.59	1.50
19	Q	201	TGL	OG1-CA1	3.90	1.44	1.33
23	R	201	PSC	C13-C12	3.84	1.54	1.31
14	A	601[A]	HEA	CHD-C1D	3.81	1.44	1.35
14	A	601[B]	HEA	CHD-C1D	3.81	1.44	1.35
23	B	303	PSC	O03-C19	3.79	1.44	1.33
26	P	307	CDL	OB6-CB5	3.79	1.44	1.33
23	B	303	PSC	C13-C12	3.78	1.53	1.31
26	C	305	CDL	C59-C58	-3.77	1.30	1.51
14	A	601[A]	HEA	C4D-C3D	-3.75	1.38	1.45
14	A	601[B]	HEA	C4D-C3D	-3.75	1.38	1.45
25	G	101	PEK	O03-C21	3.75	1.44	1.33
27	T	105	DMU	O16-C6	3.74	1.46	1.40
19	D	201	TGL	OG2-CB1	3.73	1.44	1.34
26	C	305	CDL	OB6-CB5	3.72	1.44	1.33
19	Q	201	TGL	OG2-CB1	3.67	1.44	1.34
23	R	201	PSC	C10-C9	3.62	1.52	1.31
27	K	101	DMU	O16-C6	3.60	1.46	1.40
26	T	102	CDL	C59-C58	-3.58	1.31	1.51
26	T	102	CDL	C62-C61	-3.55	1.31	1.51
19	Y	101	TGL	OG3-CC1	3.54	1.50	1.33
26	P	307	CDL	C79-C78	-3.49	1.32	1.51
26	G	102	CDL	C56-C55	-3.48	1.32	1.51
20	N	608	PGV	O01-C1	3.48	1.44	1.34
27	G	105	DMU	O16-C6	3.41	1.46	1.40
26	G	102	CDL	C59-C58	-3.37	1.32	1.51
27	P	309	DMU	O16-C6	3.36	1.45	1.40
20	N	609	PGV	O01-C1	3.35	1.43	1.34
14	N	601[B]	HEA	O11-C11	3.31	1.50	1.42
14	A	601[A]	HEA	C1D-ND	-3.27	1.34	1.40
14	A	601[B]	HEA	C1D-ND	-3.27	1.34	1.40
14	N	602	HEA	CHD-C1D	3.27	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	O11-C11	3.27	1.49	1.42
26	P	307	CDL	C59-C58	-3.27	1.33	1.51
26	C	305	CDL	C19-C18	-3.27	1.33	1.51
26	G	102	CDL	C42-C41	-3.26	1.33	1.51
14	N	602	HEA	C1D-ND	-3.22	1.34	1.40
14	N	602	HEA	O11-C11	3.19	1.49	1.42
14	N	602	HEA	C4D-C3D	-3.19	1.39	1.45
27	K	103	DMU	O16-C6	3.16	1.45	1.40
14	A	602	HEA	C4D-C3D	-3.16	1.39	1.45
26	T	102	CDL	C80-C79	-3.14	1.33	1.51
26	C	305	CDL	C79-C78	-3.14	1.33	1.51
26	C	305	CDL	C22-C21	-3.12	1.34	1.51
26	C	305	CDL	C82-C81	-3.12	1.34	1.51
14	A	601[A]	HEA	C1D-C2D	-3.09	1.38	1.44
14	A	601[B]	HEA	C1D-C2D	-3.09	1.38	1.44
26	G	102	CDL	C82-C81	-3.06	1.34	1.51
26	C	305	CDL	C39-C38	-3.06	1.34	1.51
26	P	307	CDL	C82-C81	-3.03	1.34	1.51
26	G	102	CDL	C15-C14	-2.99	1.34	1.51
26	P	307	CDL	C39-C38	-2.99	1.34	1.51
26	G	102	CDL	C79-C78	-2.98	1.34	1.51
26	G	102	CDL	C39-C38	-2.96	1.35	1.51
14	N	601[A]	HEA	C4B-NB	-2.94	1.35	1.40
14	N	601[B]	HEA	C4B-NB	-2.94	1.35	1.40
27	K	102	DMU	O16-C6	2.91	1.45	1.40
14	A	602	HEA	C1D-C2D	-2.89	1.39	1.44
25	P	302	PEK	O03-C21	2.88	1.47	1.33
26	C	305	CDL	C42-C41	-2.87	1.35	1.51
25	P	303	PEK	O03-C21	2.87	1.41	1.33
26	T	102	CDL	C37-C36	-2.81	1.35	1.51
26	P	307	CDL	C42-C41	-2.79	1.35	1.51
27	T	105	DMU	C2-C1	2.77	1.59	1.52
14	A	602	HEA	C3C-C2C	-2.75	1.36	1.40
26	T	102	CDL	C22-C21	-2.74	1.36	1.51
14	A	602	HEA	CHC-C4B	2.74	1.42	1.35
26	T	102	CDL	C19-C18	-2.73	1.36	1.51
20	N	609	PGV	O03-C19	2.67	1.41	1.33
20	N	609	PGV	O03-C01	2.67	1.51	1.45
20	C	303	PGV	O01-C1	2.63	1.41	1.34
27	C	315	DMU	O16-C6	2.63	1.44	1.40
14	A	601[A]	HEA	C1B-NB	-2.62	1.33	1.38
14	A	601[B]	HEA	C1B-NB	-2.62	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	C3A-C2A	-2.61	1.36	1.40
14	N	602	HEA	CHC-C4B	2.58	1.41	1.35
20	A	609	PGV	O01-C1	2.57	1.41	1.34
24	C	306	CHD	C10-C9	-2.55	1.51	1.56
25	P	304	PEK	P-O12	2.47	1.64	1.54
24	P	301	CHD	O12-C12	2.46	1.47	1.43
26	P	307	CDL	C62-C61	-2.44	1.34	1.51
14	N	601[A]	HEA	O2D-CGD	-2.43	1.22	1.30
14	N	601[B]	HEA	O2D-CGD	-2.43	1.22	1.30
20	A	609	PGV	O03-C01	2.43	1.50	1.45
14	A	602	HEA	O2D-CGD	-2.41	1.22	1.30
27	T	105	DMU	O55-C2	2.39	1.48	1.43
27	J	101	DMU	O16-C6	2.37	1.44	1.40
27	K	102	DMU	C3-C4	2.37	1.58	1.53
14	A	602	HEA	C18-C19	2.37	1.38	1.33
20	N	608	PGV	O01-C02	-2.34	1.40	1.46
14	N	601[A]	HEA	O1A-CGA	2.33	1.29	1.22
14	N	601[B]	HEA	O1A-CGA	2.33	1.29	1.22
25	P	303	PEK	C05-C04	2.31	1.59	1.50
14	A	602	HEA	C4B-C3B	-2.30	1.40	1.44
14	N	602	HEA	C3C-C2C	-2.30	1.37	1.40
27	P	316	DMU	O16-C6	2.29	1.44	1.40
14	N	602	HEA	C4B-C3B	-2.29	1.40	1.44
27	O	308	DMU	O16-C6	2.27	1.44	1.40
24	C	301	CHD	O25-C24	2.27	1.29	1.22
27	Z	101	DMU	O16-C6	2.26	1.44	1.40
25	G	101	PEK	O01-C1	2.25	1.40	1.34
26	G	102	CDL	OB6-CB4	-2.23	1.44	1.46
20	P	305	PGV	P-O14	-2.21	1.44	1.55
14	N	601[A]	HEA	CBD-CGD	2.19	1.55	1.50
14	N	601[B]	HEA	CBD-CGD	2.19	1.55	1.50
14	A	602	HEA	C1D-ND	-2.18	1.36	1.40
19	Y	101	TGL	CG3-CG2	2.16	1.57	1.50
14	N	602	HEA	CBD-CGD	2.15	1.55	1.50
26	P	307	CDL	PA1-OA2	2.15	1.68	1.59
27	M	101	DMU	O16-C6	2.15	1.43	1.40
27	K	103	DMU	C2-C1	2.15	1.57	1.52
27	L	104	DMU	O16-C6	2.14	1.43	1.40
26	C	305	CDL	PA1-OA2	2.13	1.67	1.59
20	P	305	PGV	O01-C1	2.13	1.40	1.34
26	T	102	CDL	CB6-CB4	2.11	1.57	1.50
14	N	602	HEA	C1C-NC	2.11	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	K	101	DMU	C3-C4	2.09	1.57	1.53
14	A	601[A]	HEA	CAA-C2A	2.08	1.55	1.52
14	A	601[B]	HEA	CAA-C2A	2.08	1.55	1.52
24	B	304	CHD	C10-C9	-2.08	1.52	1.56
24	C	301	CHD	O12-C12	2.08	1.47	1.43
14	N	601[A]	HEA	CHD-C1D	2.07	1.40	1.35
14	N	601[B]	HEA	CHD-C1D	2.07	1.40	1.35
14	N	602	HEA	CMC-C2C	2.05	1.55	1.51
27	K	102	DMU	O55-C2	2.05	1.47	1.43
14	N	602	HEA	C1D-C2D	-2.05	1.40	1.44
24	C	306	CHD	C13-C17	-2.03	1.52	1.55
14	A	602	HEA	CHB-C1B	2.03	1.46	1.41
27	K	103	DMU	C8-C7	2.02	1.57	1.52
26	C	305	CDL	PB2-OB3	2.02	1.57	1.50
19	A	607	TGL	CG3-CG2	2.01	1.56	1.50
14	A	601[A]	HEA	O11-C11	2.01	1.47	1.42

All (579) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	306	CHD	C23-C22-C20	-10.79	94.81	114.52
26	P	307	CDL	OB5-PB2-OB2	-10.36	79.17	106.73
26	G	102	CDL	OB6-CB5-OB7	-9.01	114.10	125.57
26	C	305	CDL	OB5-PB2-OB2	-8.97	82.87	106.73
19	B	301	TGL	OG2-CB1-CB2	8.79	130.44	111.50
27	J	101	DMU	C8-C7-C5	-8.56	95.88	110.82
24	C	306	CHD	C13-C17-C20	-7.52	110.52	119.50
24	W	101	CHD	C13-C17-C20	7.25	128.15	119.50
26	P	307	CDL	OB2-PB2-OB3	7.23	126.74	106.47
14	A	602	HEA	CHA-C4D-ND	6.96	131.99	124.43
14	A	602	HEA	CHC-C4B-NB	6.94	132.96	124.38
24	J	102	CHD	C17-C13-C14	-6.93	93.11	100.09
14	N	602	HEA	CHA-C4D-ND	6.91	131.94	124.43
27	G	105	DMU	O7-C10-C5	6.65	125.32	108.10
14	A	601[A]	HEA	C13-C12-C11	-6.60	104.44	114.35
14	N	601[A]	HEA	C13-C12-C11	-6.59	104.44	114.35
24	Y	104	CHD	C1-C10-C5	6.57	117.48	107.77
27	K	103	DMU	O16-C6-C1	6.51	118.47	108.30
20	C	304	PGV	O03-C19-C20	6.40	131.98	111.91
24	L	103	CHD	C11-C12-C13	6.33	117.74	111.24
24	L	103	CHD	C5-C6-C7	6.25	121.36	114.46
24	L	103	CHD	C6-C5-C10	6.20	119.24	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	302	PEK	C02-O01-C1	-6.19	102.56	117.79
24	L	103	CHD	C9-C11-C12	6.15	122.43	114.30
14	A	602	HEA	C4A-CHB-C1B	-6.11	114.49	122.56
27	C	315	DMU	O16-C6-C1	6.06	117.76	108.30
25	P	302	PEK	O01-C1-C2	5.99	124.41	111.50
26	P	307	CDL	PB2-OB2-CB2	5.93	134.63	118.30
24	Y	104	CHD	C14-C8-C7	5.93	119.67	111.81
24	Y	104	CHD	C21-C20-C17	5.92	121.98	112.92
19	N	607	TGL	OG2-CB1-CB2	5.87	124.14	111.50
23	B	303	PSC	O01-C1-C2	5.72	123.82	111.50
26	T	102	CDL	OB6-CB5-C51	5.69	123.76	111.50
14	A	602	HEA	CHA-C4D-C3D	-5.68	116.49	124.84
27	C	315	DMU	O4-C7-C5	-5.61	97.39	110.35
19	A	607	TGL	OG2-CB1-CB2	5.46	123.27	111.50
27	O	308	DMU	O16-C6-C1	5.37	116.69	108.30
14	N	601[B]	HEA	C13-C12-C11	-5.34	106.33	114.35
23	R	201	PSC	C03-C02-C01	-5.32	99.20	111.79
24	L	103	CHD	C14-C8-C7	5.32	118.86	111.81
25	P	304	PEK	O03-C21-C22	5.28	128.47	111.91
27	G	105	DMU	C7-C8-C9	5.28	119.65	110.24
27	T	105	DMU	C6-C1-C2	5.23	120.88	110.00
27	C	315	DMU	O1-C9-C11	5.20	119.36	106.44
27	C	315	DMU	O1-C10-C5	5.15	121.24	110.35
26	C	305	CDL	OB2-PB2-OB3	5.09	120.75	106.47
24	Y	104	CHD	C6-C5-C4	-5.07	105.36	111.19
26	P	307	CDL	OB8-CB7-C71	4.96	127.47	111.91
25	P	304	PEK	P-O11-C03	4.93	131.87	118.30
24	W	101	CHD	C17-C13-C14	-4.91	95.14	100.09
25	P	304	PEK	O03-C21-O04	-4.90	111.22	123.59
24	C	306	CHD	C15-C14-C13	4.90	108.36	103.55
19	D	201	TGL	CG3-OG3-CC1	4.88	135.19	117.12
24	C	306	CHD	C21-C20-C17	4.86	120.36	112.92
24	L	103	CHD	C17-C13-C12	-4.85	113.24	117.67
14	A	601[A]	HEA	C2B-C1B-NB	4.84	115.68	109.88
14	A	601[B]	HEA	C2B-C1B-NB	4.84	115.68	109.88
27	G	105	DMU	O7-C3-C4	4.82	122.65	109.45
20	P	306	PGV	O03-C19-C20	4.80	126.98	111.91
14	A	601[A]	HEA	O2D-CGD-O1D	4.76	135.16	123.30
14	A	601[B]	HEA	O2D-CGD-O1D	4.76	135.16	123.30
25	C	302	PEK	O03-C21-C22	4.75	126.80	111.91
24	J	102	CHD	C11-C9-C10	-4.71	108.87	113.73
19	A	607	TGL	OG3-CC1-OC1	-4.69	111.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	P	316	DMU	O1-C9-C8	4.68	118.19	109.69
27	J	101	DMU	O1-C9-C8	4.63	118.10	109.69
24	L	103	CHD	C15-C14-C8	4.60	124.76	118.33
27	C	315	DMU	O7-C3-C4	-4.59	96.87	109.45
26	T	102	CDL	OA6-CA5-C11	4.56	121.32	111.50
27	J	101	DMU	O1-C9-C11	4.55	117.76	106.44
14	A	601[A]	HEA	CMC-C2C-C1C	-4.55	121.47	128.46
14	A	601[B]	HEA	CMC-C2C-C1C	-4.55	121.47	128.46
26	C	305	CDL	OB8-CB7-C71	4.55	126.19	111.91
14	A	602	HEA	C4D-CHA-C1A	-4.54	116.57	122.56
27	G	105	DMU	O61-C57-C4	4.52	126.80	111.29
25	P	304	PEK	O01-C1-C2	4.51	121.22	111.50
24	Y	104	CHD	C19-C10-C1	-4.51	101.00	108.26
27	G	105	DMU	O1-C9-C8	4.49	117.84	109.69
14	N	602	HEA	CHC-C4B-NB	4.46	129.89	124.38
14	N	602	HEA	O2D-CGD-O1D	4.45	134.40	123.30
20	C	304	PGV	C01-O03-C19	4.44	133.57	117.12
24	C	306	CHD	C17-C13-C12	-4.43	113.62	117.67
25	C	302	PEK	O03-C21-O04	-4.42	112.44	123.59
26	C	305	CDL	C52-C51-CB5	-4.38	97.69	113.62
20	N	608	PGV	O03-C19-C20	4.37	125.63	111.91
27	J	101	DMU	O2-C8-C9	-4.36	98.47	109.30
27	G	105	DMU	C10-O1-C9	4.35	122.22	113.69
26	P	307	CDL	CB4-OB6-CB5	-4.31	102.99	116.92
27	K	103	DMU	O7-C10-C5	4.29	119.21	108.10
19	Q	201	TGL	CG2-OG2-CB1	-4.28	107.26	117.79
14	A	602	HEA	CHC-C4B-C3B	-4.27	114.80	125.80
24	L	103	CHD	C6-C7-C8	4.27	116.04	111.48
14	N	601[A]	HEA	C3C-C4C-NC	4.25	114.70	109.21
14	N	601[B]	HEA	C3C-C4C-NC	4.25	114.70	109.21
27	G	105	DMU	C10-O7-C3	-4.24	107.46	117.96
26	P	307	CDL	OA6-CA5-C11	4.23	120.61	111.50
24	J	102	CHD	C18-C13-C17	4.19	117.77	111.21
26	P	307	CDL	OA8-CA7-C31	4.19	125.05	111.91
19	Q	201	TGL	OG2-CB1-CB2	4.18	120.51	111.50
24	L	103	CHD	C14-C13-C12	4.17	111.28	107.40
24	L	103	CHD	C6-C5-C4	-4.16	106.41	111.19
24	L	103	CHD	C21-C20-C17	4.14	119.26	112.92
19	Y	101	TGL	OG2-CB1-CB2	4.09	120.32	111.50
27	J	101	DMU	O7-C10-C5	4.04	118.57	108.10
14	A	602	HEA	CMC-C2C-C1C	-4.04	122.26	128.46
24	J	102	CHD	C13-C17-C20	4.00	124.27	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	305	CDL	CB4-OB6-CB5	-3.99	104.02	116.92
27	G	105	DMU	O2-C8-C9	-3.97	99.43	109.30
24	Y	104	CHD	C11-C9-C10	-3.96	109.65	113.73
25	T	101	PEK	O01-C1-C2	3.96	124.32	111.91
27	K	101	DMU	C2-C3-C4	3.95	117.28	110.24
14	A	602	HEA	CAD-CBD-CGD	-3.95	105.11	113.60
23	B	303	PSC	C03-C02-C01	-3.94	102.46	111.79
20	C	304	PGV	O01-C1-C2	3.93	119.98	111.50
26	C	305	CDL	OA5-PA1-OA3	-3.93	93.72	109.07
26	P	307	CDL	OB8-CB7-OB9	-3.92	113.70	123.59
19	B	301	TGL	OG1-CA1-CA2	3.91	124.18	111.91
14	A	602	HEA	C4B-NB-C1B	-3.90	101.04	105.07
19	A	607	TGL	CG2-OG2-CB1	3.90	127.39	117.79
27	J	101	DMU	C10-O1-C9	3.87	121.28	113.69
26	T	102	CDL	OA8-CA7-C31	3.86	121.51	111.38
14	A	601[B]	HEA	C13-C12-C11	-3.85	108.56	114.35
27	P	316	DMU	C10-O7-C3	-3.85	108.44	117.96
14	N	602	HEA	CHA-C4D-C3D	-3.85	119.18	124.84
20	P	306	PGV	O01-C1-C2	3.84	119.79	111.50
24	P	308	CHD	C15-C14-C13	3.84	107.31	103.55
27	G	105	DMU	O3-C5-C7	3.83	119.20	110.35
24	B	304	CHD	C19-C10-C1	-3.81	102.12	108.26
19	Y	101	TGL	CG2-OG2-CB1	3.81	127.17	117.79
27	C	315	DMU	O61-C57-C4	-3.81	98.23	111.29
26	P	307	CDL	OA5-PA1-OA3	-3.79	94.25	109.07
20	N	609	PGV	O01-C1-O02	-3.79	114.54	123.70
27	J	101	DMU	O3-C5-C10	3.79	119.25	110.05
27	J	101	DMU	C7-C8-C9	3.77	116.97	110.24
27	C	315	DMU	C6-C1-C2	3.77	117.84	110.00
24	P	308	CHD	C19-C10-C9	-3.76	106.00	111.18
24	W	101	CHD	C17-C13-C12	3.75	121.09	117.67
27	C	315	DMU	O5-C6-O16	-3.75	101.10	109.97
24	L	103	CHD	C1-C2-C3	3.75	115.28	110.47
20	A	608	PGV	O03-C19-C20	3.73	123.63	111.91
27	P	316	DMU	C10-O1-C9	3.73	121.01	113.69
25	C	302	PEK	O01-C1-C2	3.72	119.52	111.50
14	N	602	HEA	O1A-CGA-CBA	-3.71	111.15	123.08
27	J	101	DMU	O1-C10-C5	-3.71	102.49	110.35
27	K	103	DMU	C10-O1-C9	3.70	120.94	113.69
14	A	602	HEA	C13-C12-C11	-3.69	108.80	114.35
24	W	101	CHD	C6-C5-C4	-3.67	106.97	111.19
24	W	101	CHD	C18-C13-C14	-3.66	105.49	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	304	PGV	O01-C02-C03	-3.66	95.16	108.40
24	P	301	CHD	C19-C10-C1	-3.63	102.42	108.26
27	P	316	DMU	C7-C8-C9	3.63	116.71	110.24
14	A	602	HEA	C20-C19-C18	-3.63	113.78	121.12
19	D	201	TGL	OG1-CA1-CA2	3.63	123.28	111.91
19	Y	101	TGL	OC1-CC1-CC2	-3.62	111.64	124.81
26	P	307	CDL	OA6-CA4-CA3	3.61	121.49	108.40
19	D	201	TGL	OG1-CA1-OA1	-3.61	114.49	123.59
24	L	103	CHD	C23-C22-C20	-3.60	107.94	114.52
19	A	607	TGL	OG3-CC1-CC2	3.60	123.20	111.91
26	C	305	CDL	OA8-CA6-CA4	3.59	118.87	108.43
24	L	103	CHD	C11-C9-C10	-3.58	110.03	113.73
19	B	301	TGL	OB1-CB1-CB2	-3.58	109.78	123.73
24	P	308	CHD	C5-C4-C3	-3.57	107.52	112.76
27	J	101	DMU	O6-C11-C9	3.57	123.54	111.29
14	N	602	HEA	C4A-CHB-C1B	-3.54	117.88	122.56
24	Y	104	CHD	C15-C14-C8	3.53	123.27	118.33
27	K	102	DMU	O5-C4-C3	3.53	116.10	109.69
14	A	602	HEA	C27-C19-C20	3.53	121.20	115.27
19	Y	101	TGL	OG3-CC1-CC2	3.52	127.75	112.38
24	L	103	CHD	C19-C10-C9	-3.52	106.33	111.18
24	Y	104	CHD	C1-C2-C3	-3.52	105.95	110.47
24	L	103	CHD	C2-C1-C10	3.49	118.76	112.78
14	N	602	HEA	CAD-CBD-CGD	-3.48	106.11	113.60
14	A	602	HEA	C2B-C1B-NB	3.47	114.04	109.88
24	C	306	CHD	C22-C23-C24	-3.46	103.32	112.51
19	Y	101	TGL	OG3-CG3-CG2	3.45	118.47	108.43
24	L	103	CHD	C14-C8-C9	-3.44	104.98	109.71
27	T	105	DMU	O16-C6-C1	3.44	113.68	108.30
24	C	306	CHD	C1-C10-C5	3.44	112.86	107.77
19	N	607	TGL	OG1-CA1-CA2	3.44	122.69	111.91
20	N	608	PGV	O03-C19-O04	-3.43	114.93	123.59
24	L	103	CHD	C13-C17-C20	3.41	123.56	119.50
24	J	102	CHD	C10-C9-C8	-3.41	108.16	111.82
19	B	301	TGL	OG2-CG2-CG3	3.39	120.68	108.40
24	W	101	CHD	C19-C10-C1	-3.38	102.81	108.26
14	A	601[B]	HEA	C17-C18-C19	-3.38	119.53	127.66
27	G	105	DMU	C11-C9-C8	3.38	120.91	113.00
20	C	304	PGV	O03-C19-O04	-3.37	115.09	123.59
27	J	101	DMU	O3-C5-C7	3.36	118.11	110.35
21	A	621	EDO	O1-C1-C2	-3.36	87.77	111.91
25	P	304	PEK	C01-O03-C21	3.35	129.52	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	103	DMU	C6-C1-C2	3.35	116.97	110.00
26	C	305	CDL	PB2-OB2-CB2	3.35	127.51	118.30
26	C	305	CDL	OA8-CA7-C31	3.34	122.41	111.91
24	J	102	CHD	C16-C17-C13	3.34	106.83	103.55
24	C	306	CHD	C16-C17-C20	3.33	117.30	112.15
26	C	305	CDL	OA6-CA5-C11	3.32	118.67	111.50
14	N	602	HEA	C27-C19-C20	3.32	120.85	115.27
19	A	607	TGL	CB9-CB8-CB7	-3.31	97.60	114.42
19	A	607	TGL	OG1-CA1-CA2	3.31	122.30	111.91
14	N	601[A]	HEA	C4A-CHB-C1B	3.31	126.92	122.56
14	N	601[B]	HEA	C4A-CHB-C1B	3.31	126.92	122.56
14	A	602	HEA	O2A-CGA-CBA	3.30	124.64	114.03
24	L	103	CHD	C10-C9-C8	3.30	115.36	111.82
26	G	102	CDL	OA8-CA7-OA9	-3.28	115.13	123.30
20	N	608	PGV	C01-O03-C19	3.26	129.21	117.12
24	Y	104	CHD	C10-C9-C8	3.25	115.30	111.82
26	T	102	CDL	CB6-OB8-CB7	3.23	129.09	117.12
27	J	101	DMU	C22-C19-C18	-3.23	99.18	113.49
20	C	304	PGV	O05-C05-C04	-3.22	98.26	109.56
27	C	315	DMU	C6-O5-C4	-3.22	107.37	113.69
27	C	315	DMU	C10-O1-C9	3.21	119.99	113.69
26	T	102	CDL	OB8-CB6-CB4	3.21	117.77	108.43
26	P	307	CDL	C52-C51-CB5	-3.21	101.96	113.62
24	B	304	CHD	C1-C10-C5	3.20	112.50	107.77
14	A	601[A]	HEA	C4B-NB-C1B	-3.19	101.78	105.07
14	A	601[B]	HEA	C4B-NB-C1B	-3.19	101.78	105.07
19	A	607	TGL	CA8-CA7-CA6	-3.17	98.31	114.42
14	A	601[A]	HEA	C2D-C1D-ND	3.17	113.59	109.84
14	A	601[B]	HEA	C2D-C1D-ND	3.17	113.59	109.84
20	P	305	PGV	O01-C1-O02	-3.17	116.04	123.70
27	T	105	DMU	C18-O16-C6	3.16	119.08	113.84
24	Y	104	CHD	C11-C12-C13	3.16	114.49	111.24
14	A	601[A]	HEA	O1D-CGD-CBD	-3.16	112.94	123.08
14	A	601[B]	HEA	O1D-CGD-CBD	-3.16	112.94	123.08
14	N	601[A]	HEA	C3D-C4D-ND	3.15	113.40	110.36
14	N	601[B]	HEA	C3D-C4D-ND	3.15	113.40	110.36
14	N	601[A]	HEA	O2A-CGA-CBA	3.14	124.10	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	3.14	124.10	114.03
24	J	102	CHD	C1-C10-C5	3.13	112.40	107.77
19	Y	101	TGL	CG3-OG3-CC1	3.12	124.95	117.10
19	A	607	TGL	CC4-CC3-CC2	-3.12	101.96	113.19
27	G	105	DMU	C6-O5-C4	3.12	119.81	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	308	CHD	O25-C24-C23	-3.12	113.07	123.08
27	P	309	DMU	C6-O5-C4	3.11	119.80	113.69
14	A	602	HEA	CHB-C1B-NB	-3.10	121.06	124.43
26	G	102	CDL	CB6-OB8-CB7	3.10	128.60	117.12
27	O	308	DMU	O49-C1-C6	3.10	117.56	110.05
24	C	306	CHD	C5-C4-C3	-3.09	108.22	112.76
24	O	301	CHD	C11-C9-C10	-3.08	110.55	113.73
24	L	103	CHD	O7-C7-C8	3.07	116.29	109.43
27	C	315	DMU	C10-C5-C7	3.06	116.38	110.00
14	A	601[A]	HEA	C1B-C2B-C3B	-3.06	103.14	106.80
14	A	601[B]	HEA	C1B-C2B-C3B	-3.06	103.14	106.80
25	P	304	PEK	O13-P-O11	3.05	114.84	106.73
14	A	602	HEA	CHD-C1D-ND	3.05	128.15	124.38
24	B	304	CHD	C2-C1-C10	-3.05	107.56	112.78
27	K	103	DMU	O4-C7-C8	3.04	117.38	110.35
19	Q	201	TGL	OG1-CA1-OA1	-3.04	115.93	123.59
24	P	301	CHD	C6-C7-C8	-3.03	108.25	111.48
23	R	201	PSC	C21-C20-C19	-3.03	102.60	113.62
24	P	301	CHD	C22-C20-C17	-3.01	104.06	110.28
19	Y	101	TGL	CG3-CG2-CG1	-3.01	104.67	111.79
27	K	103	DMU	C10-O7-C3	-3.00	110.53	117.96
27	P	316	DMU	O4-C7-C5	-3.00	103.41	110.35
25	P	302	PEK	C3-C2-C1	-2.99	102.73	113.62
25	P	302	PEK	C8-C7-C6	-2.99	97.29	112.02
27	K	103	DMU	O7-C3-C4	2.99	117.63	109.45
26	C	305	CDL	OB4-PB2-OB3	2.98	122.36	110.68
14	A	601[A]	HEA	CAA-CBA-CGA	-2.98	105.41	113.76
14	A	601[B]	HEA	CAA-CBA-CGA	-2.98	105.41	113.76
20	C	304	PGV	C21-C20-C19	-2.97	102.80	113.62
24	C	306	CHD	C14-C8-C9	-2.97	105.63	109.71
26	P	307	CDL	OA8-CA7-OA9	-2.97	116.10	123.59
24	B	304	CHD	O12-C12-C13	-2.97	106.01	111.03
14	N	601[A]	HEA	CAA-CBA-CGA	-2.97	105.44	113.76
14	N	601[B]	HEA	CAA-CBA-CGA	-2.97	105.44	113.76
19	Q	201	TGL	OG2-CB1-OB1	-2.96	116.56	123.70
24	C	306	CHD	C14-C8-C7	-2.95	107.89	111.81
21	N	610	EDO	O2-C2-C1	-2.95	90.71	111.91
27	C	315	DMU	O6-C11-C9	2.94	121.38	111.29
14	N	602	HEA	C4D-CHA-C1A	-2.94	118.68	122.56
24	L	103	CHD	C17-C13-C14	2.94	103.05	100.09
25	P	302	PEK	O01-C02-C03	2.93	119.03	108.40
27	K	102	DMU	C2-C3-C4	2.93	115.47	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	201	TGL	OG1-CA1-CA2	2.93	121.10	111.91
26	G	102	CDL	OA8-CA7-C31	2.92	123.43	114.03
27	K	103	DMU	O2-C8-C7	2.91	117.08	110.35
25	P	304	PEK	C24-C23-C22	2.91	123.66	113.19
24	Y	104	CHD	C23-C22-C20	-2.91	109.20	114.52
14	A	601[A]	HEA	O1A-CGA-CBA	-2.90	113.76	123.08
14	A	601[B]	HEA	O1A-CGA-CBA	-2.90	113.76	123.08
14	A	602	HEA	CAA-CBA-CGA	-2.90	105.64	113.76
23	R	201	PSC	C28-C27-C26	-2.90	99.73	114.42
14	A	601[A]	HEA	C21-C22-C23	-2.89	117.87	127.75
26	T	102	CDL	C61-C60-C59	-2.88	99.81	114.42
14	N	601[B]	HEA	C27-C19-C20	2.87	120.09	115.27
20	C	304	PGV	O04-C19-C20	-2.86	112.56	123.73
24	O	301	CHD	C13-C17-C20	-2.86	116.08	119.50
19	Q	201	TGL	CB4-CB3-CB2	-2.86	102.90	113.19
14	A	601[A]	HEA	CHA-C4D-C3D	-2.86	120.63	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-2.86	120.63	124.84
24	B	304	CHD	C5-C4-C3	-2.86	108.56	112.76
27	C	315	DMU	C10-O7-C3	-2.85	110.90	117.96
27	K	102	DMU	O61-C57-C4	2.85	121.07	111.29
19	B	301	TGL	CB3-CB2-CB1	-2.84	103.29	113.62
19	Q	201	TGL	OG3-CC1-CC2	2.84	120.81	111.91
20	N	609	PGV	C9-C10-C11	-2.83	96.20	112.43
24	J	102	CHD	C18-C13-C12	2.83	111.95	109.07
19	Y	101	TGL	C12-C11-C10	-2.81	100.17	114.42
27	C	315	DMU	O2-C8-C9	-2.81	102.33	109.30
24	B	304	CHD	C4-C5-C10	-2.80	109.68	112.66
25	G	101	PEK	O03-C21-C22	2.80	120.71	111.91
24	W	101	CHD	C18-C13-C17	2.80	115.59	111.21
24	C	306	CHD	C11-C9-C10	-2.78	110.86	113.73
27	P	316	DMU	O1-C10-C5	2.78	116.24	110.35
14	A	601[A]	HEA	C26-C15-C16	2.77	119.94	115.27
27	M	101	DMU	C22-C19-C18	-2.77	101.21	113.49
27	P	309	DMU	O16-C6-C1	2.77	112.62	108.30
25	T	101	PEK	O01-C02-C03	2.77	116.79	108.61
14	A	601[A]	HEA	C3D-C4D-ND	2.76	113.03	110.36
14	A	601[B]	HEA	C3D-C4D-ND	2.76	113.03	110.36
26	C	305	CDL	C39-C38-C37	2.76	128.43	114.42
14	N	601[B]	HEA	C17-C18-C19	-2.75	121.04	127.66
27	C	315	DMU	O7-C3-C2	2.75	114.59	107.28
27	G	105	DMU	O16-C6-C1	2.74	112.58	108.30
20	C	304	PGV	O01-C1-O02	-2.74	117.09	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	301	CHD	C1-C2-C3	-2.73	106.96	110.47
24	P	301	CHD	C1-C2-C3	-2.73	106.96	110.47
24	P	301	CHD	O12-C12-C13	-2.73	106.42	111.03
24	J	102	CHD	C11-C9-C8	2.73	114.87	110.88
27	K	101	DMU	C6-O5-C4	2.73	119.04	113.69
24	P	308	CHD	C16-C17-C13	2.72	106.22	103.55
20	A	608	PGV	O03-C01-C02	2.72	116.35	108.43
20	A	608	PGV	O01-C1-O02	2.71	130.26	123.70
27	K	103	DMU	C57-C4-C3	2.71	121.20	113.33
14	N	602	HEA	CAD-C3D-C2D	-2.70	122.84	127.88
14	N	601[A]	HEA	C2B-C1B-NB	2.70	113.12	109.88
14	N	601[B]	HEA	C2B-C1B-NB	2.70	113.12	109.88
24	P	308	CHD	O12-C12-C13	2.70	115.60	111.03
24	J	102	CHD	C6-C5-C10	2.70	115.52	112.66
27	P	316	DMU	C18-O16-C6	2.69	118.30	113.84
25	P	303	PEK	O03-C21-O04	-2.69	116.81	123.59
20	P	306	PGV	O04-C19-C20	-2.69	113.25	123.73
25	T	101	PEK	P-O11-C03	2.68	134.80	121.59
24	P	308	CHD	O7-C7-C8	2.68	115.42	109.43
19	A	607	TGL	C21-C20-CA9	-2.68	100.83	114.42
24	P	308	CHD	C22-C23-C24	-2.67	105.41	112.51
24	C	301	CHD	C18-C13-C12	2.67	111.78	109.07
24	W	101	CHD	C11-C12-C13	2.66	113.97	111.24
26	T	102	CDL	PA1-OA5-CA3	2.65	137.22	121.68
24	Y	104	CHD	O7-C7-C8	2.63	115.31	109.43
19	Y	101	TGL	CG1-OG1-CA1	2.63	126.85	117.12
27	K	102	DMU	C6-O5-C4	2.62	118.84	113.69
24	J	102	CHD	C15-C14-C13	2.62	106.12	103.55
24	P	301	CHD	C5-C6-C7	2.62	117.35	114.46
24	P	308	CHD	C11-C12-C13	-2.62	108.56	111.24
26	T	102	CDL	O1-C1-CA2	-2.61	100.42	109.56
20	C	304	PGV	P-O12-C04	-2.60	106.42	121.68
27	L	104	DMU	O55-C2-C3	-2.60	104.33	110.35
24	C	306	CHD	O26-C24-O25	2.60	129.78	123.30
27	T	105	DMU	O55-C2-C1	2.60	116.36	110.35
27	L	104	DMU	O7-C3-C2	-2.59	104.36	110.35
27	L	104	DMU	O7-C3-C4	2.59	115.73	109.30
23	R	201	PSC	C25-C24-C23	-2.59	101.28	114.42
25	C	302	PEK	C2-C3-C4	-2.59	108.62	113.23
27	K	101	DMU	O16-C6-C1	2.59	112.34	108.30
26	G	102	CDL	C83-C82-C81	2.58	127.54	114.42
24	P	301	CHD	C13-C17-C20	2.58	122.57	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	102	CDL	C40-C39-C38	2.57	127.47	114.42
27	K	101	DMU	O61-C57-C4	2.56	120.09	111.29
27	K	101	DMU	C3-C2-C1	2.56	115.30	110.82
14	N	602	HEA	O2A-CGA-CBA	2.56	122.26	114.03
26	C	305	CDL	OB8-CB7-OB9	-2.55	117.15	123.59
19	B	301	TGL	CG3-OG3-CC1	2.55	126.57	117.12
14	N	601[A]	HEA	CHA-C4D-C3D	-2.54	121.11	124.84
14	N	601[B]	HEA	CHA-C4D-C3D	-2.54	121.11	124.84
19	A	607	TGL	C12-C11-C10	-2.54	101.54	114.42
27	G	105	DMU	O5-C4-C3	-2.54	104.41	109.75
14	N	602	HEA	CAD-C3D-C4D	2.53	129.09	124.66
19	D	201	TGL	OG1-CG1-CG2	2.53	115.81	108.43
19	A	607	TGL	OG2-CB1-OB1	-2.53	117.58	123.70
24	C	306	CHD	C14-C13-C12	2.53	109.76	107.40
24	Y	104	CHD	C21-C20-C22	-2.53	106.40	110.36
14	A	602	HEA	O1D-CGD-CBD	-2.53	114.96	123.08
27	K	103	DMU	C1-C2-C3	2.53	115.45	109.68
24	L	103	CHD	C1-C10-C5	2.52	111.50	107.77
27	G	105	DMU	C18-O16-C6	2.51	118.00	113.84
20	P	306	PGV	C21-C20-C19	-2.50	104.52	113.62
24	Y	104	CHD	O25-C24-C23	-2.50	115.05	123.08
27	K	103	DMU	C11-C9-C8	2.50	118.86	113.00
14	A	601[A]	HEA	O2A-CGA-CBA	2.50	122.05	114.03
14	A	601[B]	HEA	O2A-CGA-CBA	2.50	122.05	114.03
23	B	303	PSC	C02-O01-C1	2.50	123.93	117.79
27	K	102	DMU	O16-C6-C1	2.49	112.20	108.30
27	K	103	DMU	O1-C10-C5	2.49	115.62	110.35
20	P	305	PGV	C03-C02-C01	-2.49	105.90	111.79
27	J	101	DMU	O5-C4-C57	2.49	112.62	106.44
26	T	102	CDL	C56-C55-C54	-2.48	101.83	114.42
24	L	103	CHD	C22-C20-C17	2.48	115.40	110.28
24	J	102	CHD	C6-C5-C4	-2.47	108.35	111.19
24	B	304	CHD	C19-C10-C5	-2.46	106.18	110.36
20	A	609	PGV	O03-C19-C20	2.46	119.64	111.91
20	C	303	PGV	C21-C20-C19	-2.46	104.69	113.62
26	P	307	CDL	OB4-PB2-OB3	2.45	120.28	110.68
24	P	308	CHD	C18-C13-C12	-2.45	106.58	109.07
27	K	102	DMU	O55-C2-C3	2.45	116.00	110.35
24	W	101	CHD	C22-C20-C17	2.44	115.33	110.28
26	G	102	CDL	C32-C31-CA7	-2.44	108.31	114.47
14	N	601[B]	HEA	C20-C21-C22	-2.44	103.85	111.88
26	T	102	CDL	C58-C57-C56	-2.44	102.03	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	304	CHD	C11-C9-C10	-2.44	111.21	113.73
26	C	305	CDL	OA6-CA4-CA3	2.44	117.23	108.40
26	C	305	CDL	C82-C81-C80	2.43	126.78	114.42
19	A	607	TGL	CG3-CG2-CG1	-2.43	106.04	111.79
27	L	104	DMU	O16-C6-C1	2.43	112.10	108.30
14	A	602	HEA	C21-C20-C19	2.43	120.96	112.98
27	G	105	DMU	O55-C2-C1	2.42	115.94	110.35
14	A	602	HEA	O1A-CGA-CBA	-2.41	115.33	123.08
23	R	201	PSC	O01-C1-O02	-2.41	122.50	125.57
25	C	302	PEK	O11-P-O14	-2.41	99.66	109.07
14	N	601[A]	HEA	C13-C14-C15	-2.40	121.88	127.66
14	A	601[B]	HEA	C20-C21-C22	-2.40	104.00	111.88
20	A	608	PGV	C6-C5-C4	-2.40	102.25	114.42
20	N	608	PGV	O14-P-O13	2.40	124.09	112.24
24	C	306	CHD	C19-C10-C9	-2.40	107.88	111.18
14	A	602	HEA	CHD-C1D-C2D	-2.39	120.10	126.72
23	B	303	PSC	O01-C02-C03	2.39	117.06	108.40
20	P	305	PGV	C30-C29-C28	-2.39	102.28	114.42
27	T	105	DMU	C2-C3-C4	2.38	114.49	110.24
25	P	303	PEK	O03-C21-C22	2.38	119.37	111.91
24	C	301	CHD	C22-C20-C17	-2.38	105.38	110.28
24	W	101	CHD	C9-C10-C5	2.37	111.92	108.58
24	Y	104	CHD	C13-C17-C20	2.37	122.33	119.50
14	N	601[A]	HEA	C1D-ND-C4D	-2.37	102.62	105.07
14	N	601[B]	HEA	C1D-ND-C4D	-2.37	102.62	105.07
24	C	301	CHD	C5-C4-C3	-2.37	109.28	112.76
25	G	101	PEK	C02-O01-C1	-2.37	111.96	117.79
24	B	304	CHD	C6-C5-C4	-2.37	108.47	111.19
27	P	316	DMU	C10-C5-C7	2.37	114.92	110.00
14	N	601[B]	HEA	C27-C19-C18	-2.36	117.62	123.68
27	L	104	DMU	O49-C1-C6	2.36	115.78	110.05
24	C	306	CHD	C16-C17-C13	2.36	105.87	103.55
24	J	102	CHD	C16-C17-C20	2.35	115.78	112.15
24	P	308	CHD	C1-C10-C9	2.35	115.04	111.35
14	N	602	HEA	CHD-C1D-ND	2.35	127.28	124.38
24	P	308	CHD	C18-C13-C17	-2.34	107.54	111.21
20	N	609	PGV	C01-O03-C19	-2.34	108.45	117.12
19	D	201	TGL	CG1-OG1-CA1	2.34	125.79	117.12
27	J	101	DMU	C10-O7-C3	-2.34	112.18	117.96
27	T	105	DMU	O5-C4-C3	2.33	113.93	109.69
24	C	301	CHD	C19-C10-C1	-2.33	104.50	108.26
27	Z	101	DMU	O61-C57-C4	-2.33	103.31	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	103	CHD	C18-C13-C14	-2.33	107.57	111.21
24	B	304	CHD	C16-C17-C20	-2.32	108.56	112.15
14	N	602	HEA	CHC-C4B-C3B	-2.32	119.83	125.80
24	P	301	CHD	C17-C13-C12	2.31	119.78	117.67
20	C	304	PGV	O14-P-O13	2.31	123.67	112.24
14	N	601[A]	HEA	CMB-C2B-C1B	-2.31	121.52	125.04
14	N	601[B]	HEA	CMB-C2B-C1B	-2.31	121.52	125.04
24	C	306	CHD	C11-C9-C8	2.30	114.25	110.88
19	Y	101	TGL	OG1-CA1-CA2	2.30	119.13	111.91
26	P	307	CDL	C78-C77-C76	-2.30	102.77	114.42
20	P	306	PGV	C03-C02-C01	-2.29	106.36	111.79
26	C	305	CDL	C79-C78-C77	2.29	126.06	114.42
20	P	306	PGV	O01-C1-O02	-2.29	118.17	123.70
26	C	305	CDL	C78-C77-C76	-2.29	102.80	114.42
24	P	301	CHD	C16-C17-C13	2.28	105.79	103.55
14	A	601[A]	HEA	CHB-C1B-C2B	-2.28	121.42	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-2.28	121.42	124.98
26	C	305	CDL	OA8-CA7-OA9	-2.27	117.85	123.59
24	C	301	CHD	C6-C7-C8	-2.27	109.05	111.48
14	A	601[A]	HEA	CHD-C1D-C2D	-2.27	120.44	126.72
14	A	601[B]	HEA	CHD-C1D-C2D	-2.27	120.44	126.72
27	K	101	DMU	O5-C4-C3	2.27	113.82	109.69
27	M	101	DMU	C34-C31-C28	-2.27	102.90	114.42
14	N	602	HEA	C20-C19-C18	-2.27	116.53	121.12
24	J	102	CHD	C17-C13-C12	-2.27	115.60	117.67
20	N	608	PGV	O01-C1-O02	2.27	129.18	123.70
27	P	316	DMU	O5-C4-C57	2.26	112.06	106.44
26	C	305	CDL	OB6-CB5-C51	2.26	119.00	111.91
19	N	607	TGL	OG1-CA1-OA1	-2.26	117.89	123.59
27	C	315	DMU	C11-C9-C8	-2.26	107.72	113.00
25	T	101	PEK	O02-C1-C2	-2.26	114.93	123.73
14	N	602	HEA	O1D-CGD-CBD	-2.25	115.84	123.08
19	N	607	TGL	CG3-OG3-CC1	2.25	125.45	117.12
24	L	103	CHD	C11-C9-C8	2.25	114.17	110.88
20	A	608	PGV	C03-C02-C01	2.24	117.08	111.79
27	K	103	DMU	C7-C8-C9	-2.24	106.25	110.24
27	T	105	DMU	O49-C1-C6	-2.24	104.61	110.05
26	G	102	CDL	OA4-PA1-OA5	2.24	118.13	107.75
14	A	601[B]	HEA	O11-C11-C12	2.23	115.66	109.42
19	N	607	TGL	OG2-CG2-CG3	2.23	116.48	108.40
19	Y	101	TGL	CA4-CA3-CA2	-2.23	105.19	113.19
20	A	608	PGV	O14-P-O13	2.22	123.22	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	304	CHD	C13-C17-C20	-2.22	116.84	119.50
20	A	608	PGV	C4-C3-C2	-2.22	105.22	113.19
27	K	103	DMU	C10-C5-C7	2.21	114.60	110.00
24	J	102	CHD	C18-C13-C14	-2.21	107.75	111.21
25	P	302	PEK	O03-C01-C02	2.20	114.84	108.43
24	Y	104	CHD	C16-C17-C20	2.20	115.55	112.15
14	N	601[A]	HEA	C2D-C1D-ND	2.20	112.44	109.84
14	N	601[B]	HEA	C2D-C1D-ND	2.20	112.44	109.84
24	P	308	CHD	C17-C13-C12	2.19	119.67	117.67
14	N	601[A]	HEA	C26-C15-C16	2.19	118.96	115.27
27	K	102	DMU	C18-O16-C6	2.19	117.47	113.84
27	K	102	DMU	O5-C4-C57	2.19	111.88	106.44
26	G	102	CDL	OA5-CA3-CA4	-2.19	100.34	109.69
25	P	303	PEK	C02-O01-C1	-2.19	112.41	117.79
26	C	305	CDL	OA4-PA1-OA2	2.19	117.90	107.75
27	O	308	DMU	O5-C4-C57	2.19	111.87	106.44
27	Z	101	DMU	C10-O7-C3	-2.18	112.58	117.96
19	A	607	TGL	CC3-CC2-CC1	2.17	121.52	113.62
26	T	102	CDL	OA8-CA7-OA9	-2.17	118.11	123.59
14	N	601[A]	HEA	O1A-CGA-CBA	-2.17	116.11	123.08
14	N	601[B]	HEA	O1A-CGA-CBA	-2.17	116.11	123.08
25	P	302	PEK	C01-O03-C21	2.17	122.55	117.10
14	N	602	HEA	CAA-CBA-CGA	-2.17	107.68	113.76
26	T	102	CDL	C15-C14-C13	-2.17	103.43	114.42
27	K	103	DMU	O5-C4-C3	-2.16	105.20	109.75
24	C	301	CHD	C22-C23-C24	-2.16	106.78	112.51
25	P	303	PEK	O11-P-O14	-2.15	100.65	109.07
19	A	607	TGL	OG3-CG3-CG2	2.15	114.69	108.43
27	C	315	DMU	C7-C8-C9	2.15	114.07	110.24
27	C	315	DMU	O1-C9-C8	2.15	113.59	109.69
14	N	602	HEA	C16-C15-C14	-2.15	116.78	121.12
24	Y	104	CHD	C9-C11-C12	-2.14	111.47	114.30
14	N	601[A]	HEA	C21-C22-C23	-2.14	120.43	127.75
19	D	201	TGL	OG2-CB1-CB2	2.14	116.11	111.50
24	J	102	CHD	C19-C10-C9	-2.13	108.24	111.18
27	J	101	DMU	O49-C1-C6	2.13	115.22	110.05
26	G	102	CDL	CB2-C1-CA2	-2.13	106.52	112.79
24	C	301	CHD	C23-C22-C20	-2.13	110.63	114.52
14	N	601[A]	HEA	O2D-CGD-CBD	2.13	120.86	114.03
14	N	601[B]	HEA	O2D-CGD-CBD	2.13	120.86	114.03
20	N	608	PGV	C4-C3-C2	-2.13	105.55	113.19
14	N	602	HEA	C21-C20-C19	2.12	119.96	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	K	102	DMU	O49-C1-C6	2.12	115.20	110.05
24	P	301	CHD	C21-C20-C22	-2.12	107.05	110.36
20	P	306	PGV	O03-C01-C02	2.11	114.58	108.43
27	P	316	DMU	C2-C3-C4	2.11	115.76	110.93
27	K	103	DMU	O55-C2-C1	2.11	115.22	110.35
24	W	101	CHD	C10-C9-C8	2.11	114.08	111.82
25	P	303	PEK	O03-C01-C02	-2.10	102.31	108.43
27	P	309	DMU	C11-C9-C8	2.10	117.92	113.00
24	C	306	CHD	O25-C24-C23	-2.10	116.34	123.08
20	P	305	PGV	O14-P-O13	2.10	122.61	112.24
20	C	304	PGV	O03-C01-C02	2.10	114.54	108.43
24	B	304	CHD	O7-C7-C6	2.09	115.13	109.94
19	N	607	TGL	OG3-CC1-CC2	2.09	118.47	111.91
27	M	101	DMU	O5-C6-O16	-2.08	105.04	109.97
27	J	101	DMU	C31-C28-C25	-2.08	103.86	114.42
24	C	306	CHD	C10-C9-C8	-2.08	109.58	111.82
24	O	301	CHD	C16-C17-C20	-2.08	108.93	112.15
26	P	307	CDL	C43-C42-C41	2.07	124.93	114.42
25	P	302	PEK	O02-C1-C2	-2.07	115.66	123.73
20	A	608	PGV	O03-C19-O04	-2.07	118.37	123.59
27	P	309	DMU	C22-C19-C18	-2.07	104.33	113.49
20	A	608	PGV	O14-P-O12	-2.06	98.16	107.75
24	C	306	CHD	C6-C5-C4	-2.06	108.81	111.19
27	T	105	DMU	O5-C4-C57	2.06	111.56	106.44
25	G	101	PEK	O12-C04-C05	-2.06	101.38	109.10
24	Y	104	CHD	O3-C3-C4	2.06	113.95	109.85
25	P	302	PEK	O03-C21-C22	2.06	121.36	112.38
20	A	608	PGV	C24-C23-C22	2.06	124.88	114.42
19	Q	201	TGL	OG3-CC1-OC1	-2.06	118.40	123.59
26	P	307	CDL	OA4-PA1-OA3	2.06	122.40	112.24
20	P	306	PGV	O14-P-O13	2.06	122.40	112.24
24	O	301	CHD	C1-C10-C5	2.05	110.80	107.77
26	P	307	CDL	PA1-OA2-CA2	-2.05	109.65	121.68
24	C	306	CHD	C16-C15-C14	-2.05	101.07	105.13
24	L	103	CHD	C19-C10-C1	-2.05	104.96	108.26
24	J	102	CHD	C22-C20-C17	2.05	114.51	110.28
26	C	305	CDL	C20-C19-C18	2.04	124.80	114.42
26	G	102	CDL	C61-C60-C59	-2.04	104.06	114.42
26	C	305	CDL	OA6-CA4-CA6	2.04	115.77	108.40
14	A	601[A]	HEA	C16-C15-C14	-2.03	117.00	121.12
24	L	103	CHD	O26-C24-O25	-2.03	118.24	123.30
24	Y	104	CHD	C1-C10-C9	-2.03	108.17	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	101	CHD	C4-C5-C10	2.02	114.80	112.66
27	K	101	DMU	C57-C4-C3	2.02	117.73	113.00
27	P	309	DMU	C10-O1-C9	-2.02	109.73	113.69
23	R	201	PSC	C27-C26-C25	-2.02	104.19	114.42
19	Y	101	TGL	C20-CA9-CA8	-2.02	104.19	114.42
24	L	103	CHD	C21-C20-C22	-2.01	107.20	110.36
24	C	301	CHD	C6-C5-C10	-2.01	110.52	112.66
23	B	303	PSC	C23-C22-C21	-2.01	104.22	114.42
26	G	102	CDL	PB2-OB2-CB2	-2.01	109.89	121.68
24	C	306	CHD	C11-C12-C13	-2.01	109.18	111.24
19	A	607	TGL	OG1-CA1-OA1	-2.00	118.54	123.59

All (24) chirality outliers are listed below:

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

All (800) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[B]	HEA	C14-C15-C16-C17
14	A	601[B]	HEA	C26-C15-C16-C17
14	N	601[B]	HEA	C14-C15-C16-C17
14	N	601[B]	HEA	C26-C15-C16-C17
19	A	607	TGL	CB2-CB1-OG2-CG2
19	A	607	TGL	OB1-CB1-OG2-CG2
19	D	201	TGL	CG2-CG1-OG1-CA1
19	Y	101	TGL	OB1-CB1-OG2-CG2
20	A	608	PGV	C03-O11-P-O12
20	A	608	PGV	C03-O11-P-O13
20	A	608	PGV	C03-O11-P-O14
20	A	608	PGV	C03-C02-O01-C1
20	A	608	PGV	C2-C1-O01-C02
20	A	608	PGV	O04-C19-O03-C01
20	A	608	PGV	C20-C19-O03-C01
20	C	304	PGV	C03-O11-P-O13
20	N	608	PGV	C03-O11-P-O14
20	N	608	PGV	C04-O12-P-O11
20	N	608	PGV	C04-O12-P-O13
20	N	608	PGV	C02-C03-O11-P
20	N	608	PGV	O04-C19-O03-C01
20	N	608	PGV	C20-C19-O03-C01
23	B	303	PSC	C03-O11-P-O12
23	B	303	PSC	C03-O11-P-O14
23	B	303	PSC	C04-O12-P-O13
23	B	303	PSC	O02-C1-O01-C02
23	B	303	PSC	C9-C10-C11-C12
23	R	201	PSC	C04-O12-P-O13
23	R	201	PSC	C01-C02-O01-C1
23	R	201	PSC	C03-C02-O01-C1
23	R	201	PSC	O12-C04-C05-N
23	R	201	PSC	O02-C1-O01-C02
24	Y	104	CHD	C13-C17-C20-C21
25	C	302	PEK	C04-O12-P-O11
25	C	302	PEK	O12-C04-C05-N
25	C	302	PEK	C4-C5-C6-C7
25	C	302	PEK	C7-C8-C9-C10
25	P	302	PEK	C2-C1-O01-C02
25	P	302	PEK	C7-C8-C9-C10
25	P	302	PEK	C12-C13-C14-C15
25	P	304	PEK	C10-C11-C12-C13
25	T	101	PEK	O12-C04-C05-N
25	T	101	PEK	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	T	101	PEK	C12-C13-C14-C15
26	C	305	CDL	C1-CA2-OA2-PA1
26	C	305	CDL	CA3-OA5-PA1-OA2
26	C	305	CDL	OA6-CA4-CA6-OA8
26	C	305	CDL	C11-CA5-OA6-CA4
26	C	305	CDL	CB2-OB2-PB2-OB4
26	G	102	CDL	CA2-OA2-PA1-OA3
26	G	102	CDL	CA3-OA5-PA1-OA4
26	G	102	CDL	CB2-OB2-PB2-OB3
26	G	102	CDL	CB2-OB2-PB2-OB4
26	G	102	CDL	CB3-OB5-PB2-OB2
26	G	102	CDL	CB3-OB5-PB2-OB3
26	G	102	CDL	CB3-OB5-PB2-OB4
26	G	102	CDL	OB7-CB5-OB6-CB4
26	P	307	CDL	CA2-C1-CB2-OB2
26	P	307	CDL	C1-CA2-OA2-PA1
26	P	307	CDL	CA3-OA5-PA1-OA4
26	P	307	CDL	C11-CA5-OA6-CA4
26	P	307	CDL	CB2-OB2-PB2-OB3
26	P	307	CDL	CB2-OB2-PB2-OB4
26	P	307	CDL	CB2-OB2-PB2-OB5
26	T	102	CDL	CA2-OA2-PA1-OA4
26	T	102	CDL	CB3-OB5-PB2-OB4
26	T	102	CDL	OB6-CB4-CB6-OB8
27	C	315	DMU	C19-C18-O16-C6
27	G	105	DMU	C1-C6-O16-C18
27	G	105	DMU	O5-C6-O16-C18
27	K	102	DMU	O5-C6-O16-C18
27	L	104	DMU	O5-C6-O16-C18
27	L	104	DMU	C19-C18-O16-C6
27	O	308	DMU	O5-C6-O16-C18
27	T	105	DMU	O5-C6-O16-C18
19	Q	201	TGL	OC1-CC1-OG3-CG3
23	R	201	PSC	O04-C19-O03-C01
19	Q	201	TGL	CA2-CA1-OG1-CG1
19	Q	201	TGL	CC2-CC1-OG3-CG3
20	C	304	PGV	C20-C19-O03-C01
23	R	201	PSC	C20-C19-O03-C01
25	P	304	PEK	C22-C21-O03-C01
19	D	201	TGL	OA1-CA1-OG1-CG1
19	Q	201	TGL	OA1-CA1-OG1-CG1
20	C	304	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
25	C	302	PEK	O04-C21-O03-C01
25	P	304	PEK	O04-C21-O03-C01
26	C	305	CDL	OA9-CA7-OA8-CA6
26	T	102	CDL	OA9-CA7-OA8-CA6
20	A	608	PGV	O02-C1-O01-C02
25	P	302	PEK	O02-C1-O01-C02
26	C	305	CDL	OA7-CA5-OA6-CA4
26	P	307	CDL	OA7-CA5-OA6-CA4
19	D	201	TGL	OC1-CC1-OG3-CG3
19	D	201	TGL	CA2-CA1-OG1-CG1
26	T	102	CDL	C31-CA7-OA8-CA6
19	Y	101	TGL	CB2-CB1-OG2-CG2
23	B	303	PSC	C2-C1-O01-C02
27	C	315	DMU	O6-C11-C9-O1
24	L	103	CHD	C20-C22-C23-C24
19	Y	101	TGL	CA2-CA1-OG1-CG1
25	C	302	PEK	C22-C21-O03-C01
25	G	101	PEK	C10-C11-C12-C13
25	G	101	PEK	C13-C14-C15-C16
25	P	304	PEK	C7-C8-C9-C10
25	P	304	PEK	C13-C14-C15-C16
19	Y	101	TGL	OA1-CA1-OG1-CG1
25	P	302	PEK	O04-C21-O03-C01
27	L	104	DMU	O5-C4-C57-O61
26	P	307	CDL	O1-C1-CB2-OB2
26	T	102	CDL	O1-C1-CA2-OA2
26	C	305	CDL	C31-CA7-OA8-CA6
26	C	305	CDL	C51-CB5-OB6-CB4
26	P	307	CDL	C31-CA7-OA8-CA6
26	P	307	CDL	OA9-CA7-OA8-CA6
27	K	103	DMU	O5-C4-C57-O61
19	Q	201	TGL	C21-C22-C23-C24
27	P	309	DMU	O6-C11-C9-O1
24	L	103	CHD	C13-C17-C20-C21
19	D	201	TGL	CC2-CC1-OG3-CG3
20	P	306	PGV	O04-C19-O03-C01
19	Y	101	TGL	CC5-CC6-CC7-CC8
27	J	101	DMU	O6-C11-C9-C8
19	Y	101	TGL	C20-C21-C22-C23
24	C	306	CHD	C21-C20-C22-C23
27	C	315	DMU	O6-C11-C9-C8
27	K	103	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
23	R	201	PSC	C20-C21-C22-C23
19	N	607	TGL	CC2-CC1-OG3-CG3
20	P	306	PGV	C20-C19-O03-C01
24	Y	104	CHD	C16-C17-C20-C22
26	C	305	CDL	OB7-CB5-OB6-CB4
26	G	102	CDL	CA2-C1-CB2-OB2
19	B	301	TGL	CC2-CC1-OG3-CG3
26	P	307	CDL	C51-CB5-OB6-CB4
19	Q	201	TGL	CB1-CB2-CB3-CB4
20	C	304	PGV	C1-C2-C3-C4
24	C	306	CHD	C17-C20-C22-C23
25	P	302	PEK	C22-C21-O03-C01
20	A	609	PGV	C26-C27-C28-C29
27	K	103	DMU	O6-C11-C9-C8
27	T	105	DMU	C1-C6-O16-C18
26	G	102	CDL	OB6-CB4-CB6-OB8
19	B	301	TGL	OC1-CC1-OG3-CG3
27	G	105	DMU	O6-C11-C9-C8
27	P	309	DMU	O6-C11-C9-C8
24	P	308	CHD	C20-C22-C23-C24
19	Q	201	TGL	CB2-CB1-OG2-CG2
24	W	101	CHD	C13-C17-C20-C22
19	D	201	TGL	CB1-CB2-CB3-CB4
26	T	102	CDL	C60-C61-C62-C63
27	K	102	DMU	O5-C4-C57-O61
27	K	102	DMU	C3-C4-C57-O61
25	C	302	PEK	C10-C11-C12-C13
25	P	303	PEK	C13-C14-C15-C16
25	P	304	PEK	C4-C5-C6-C7
25	T	101	PEK	C4-C5-C6-C7
20	P	306	PGV	C20-C21-C22-C23
27	K	103	DMU	O6-C11-C9-O1
20	N	608	PGV	C19-C20-C21-C22
25	C	302	PEK	C21-C22-C23-C24
24	P	308	CHD	C17-C20-C22-C23
20	A	608	PGV	C20-C21-C22-C23
27	P	316	DMU	O5-C4-C57-O61
23	B	303	PSC	C19-C20-C21-C22
25	C	302	PEK	C1-C2-C3-C4
26	P	307	CDL	CB5-C51-C52-C53
26	P	307	CDL	OB6-CB4-CB6-OB8
27	J	101	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
27	P	309	DMU	O16-C18-C19-C22
24	Y	104	CHD	C16-C17-C20-C21
27	J	101	DMU	O6-C11-C9-O1
24	J	102	CHD	C13-C17-C20-C21
19	N	607	TGL	OC1-CC1-OG3-CG3
26	P	307	CDL	OB7-CB5-OB6-CB4
27	K	102	DMU	O16-C18-C19-C22
24	P	308	CHD	C21-C20-C22-C23
27	C	315	DMU	O5-C6-O16-C18
27	K	103	DMU	O5-C6-O16-C18
26	C	305	CDL	O1-C1-CA2-OA2
19	B	301	TGL	OB1-CB1-OG2-CG2
19	Q	201	TGL	OB1-CB1-OG2-CG2
26	T	102	CDL	OA7-CA5-OA6-CA4
19	A	607	TGL	CA2-CA1-OG1-CG1
24	J	102	CHD	C16-C17-C20-C21
27	T	105	DMU	O16-C18-C19-C22
24	W	101	CHD	C13-C17-C20-C21
24	J	102	CHD	C13-C17-C20-C22
20	C	303	PGV	C10-C11-C12-C13
23	B	303	PSC	C11-C10-C9-C8
25	P	303	PEK	C10-C11-C12-C13
23	R	201	PSC	C22-C23-C24-C25
19	B	301	TGL	CB2-CB1-OG2-CG2
26	T	102	CDL	C11-CA5-OA6-CA4
20	C	304	PGV	C03-O11-P-O12
20	N	608	PGV	C03-O11-P-O12
20	P	306	PGV	C03-O11-P-O12
23	B	303	PSC	C04-O12-P-O11
23	R	201	PSC	C04-O12-P-O11
25	P	302	PEK	C03-O11-P-O12
26	G	102	CDL	CB2-OB2-PB2-OB5
26	P	307	CDL	CA3-OA5-PA1-OA2
26	T	102	CDL	CA2-OA2-PA1-OA5
26	T	102	CDL	CA3-OA5-PA1-OA2
26	T	102	CDL	CB3-OB5-PB2-OB2
26	C	305	CDL	C71-CB7-OB8-CB6
25	P	304	PEK	C33-C34-C35-C36
26	C	305	CDL	CB2-C1-CA2-OA2
27	L	104	DMU	C3-C4-C57-O61
23	B	303	PSC	C20-C21-C22-C23
19	Q	201	TGL	CC4-CC5-CC6-CC7

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C37-C38-C39-C40
26	G	102	CDL	C77-C78-C79-C80
19	A	607	TGL	C21-C20-CA9-CA8
19	A	607	TGL	C11-C10-CB9-CB8
19	B	301	TGL	CC7-CC8-CC9-C15
19	B	301	TGL	C17-C18-C19-C33
19	N	607	TGL	CC4-CC5-CC6-CC7
23	B	303	PSC	C29-C30-C31-C32
25	P	304	PEK	C22-C23-C24-C25
19	A	607	TGL	C11-C12-C13-C14
19	Q	201	TGL	C20-C21-C22-C23
19	Y	101	TGL	CA9-C20-C21-C22
26	T	102	CDL	C57-C58-C59-C60
20	P	306	PGV	O02-C1-O01-C02
26	P	307	CDL	C51-C52-C53-C54
26	C	305	CDL	OB9-CB7-OB8-CB6
20	A	608	PGV	C10-C11-C12-C13
19	Q	201	TGL	CC3-CC4-CC5-CC6
26	C	305	CDL	C20-C21-C22-C23
26	C	305	CDL	O1-C1-CB2-OB2
26	G	102	CDL	O1-C1-CB2-OB2
26	C	305	CDL	C40-C41-C42-C43
27	C	315	DMU	C1-C6-O16-C18
27	K	102	DMU	C1-C6-O16-C18
19	A	607	TGL	C10-C11-C12-C13
19	D	201	TGL	C20-C21-C22-C23
19	Q	201	TGL	CA2-CA3-CA4-CA5
20	C	303	PGV	C7-C8-C9-C10
20	C	303	PGV	C25-C26-C27-C28
26	C	305	CDL	C38-C39-C40-C41
26	G	102	CDL	C37-C38-C39-C40
27	L	104	DMU	C31-C34-C37-C40
27	M	101	DMU	O16-C18-C19-C22
19	A	607	TGL	CA5-CA6-CA7-CA8
19	A	607	TGL	CA9-C20-C21-C22
19	N	607	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	CB3-CB4-CB5-CB6
19	D	201	TGL	CC2-CC3-CC4-CC5
19	Q	201	TGL	CB2-CB3-CB4-CB5
26	C	305	CDL	C78-C79-C80-C81
26	G	102	CDL	C53-C54-C55-C56
27	J	101	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
19	A	607	TGL	OA1-CA1-OG1-CG1
19	B	301	TGL	CB2-CB3-CB4-CB5
19	B	301	TGL	CB9-C10-C11-C12
19	D	201	TGL	C11-C10-CB9-CB8
19	Q	201	TGL	C11-C10-CB9-CB8
26	T	102	CDL	C77-C78-C79-C80
20	C	304	PGV	C04-C05-C06-O06
24	W	101	CHD	C16-C17-C20-C21
20	P	306	PGV	C2-C1-O01-C02
19	A	607	TGL	CC2-CC3-CC4-CC5
19	B	301	TGL	C13-C14-C29-C30
19	D	201	TGL	C21-C20-CA9-CA8
19	Q	201	TGL	C21-C20-CA9-CA8
19	Y	101	TGL	CA3-CA4-CA5-CA6
20	C	303	PGV	C20-C21-C22-C23
25	P	302	PEK	C1-C2-C3-C4
19	A	607	TGL	CB6-CB7-CB8-CB9
19	B	301	TGL	CB5-CB6-CB7-CB8
19	B	301	TGL	C22-C23-C24-C25
19	D	201	TGL	CB5-CB6-CB7-CB8
26	C	305	CDL	C19-C20-C21-C22
26	T	102	CDL	C35-C36-C37-C38
19	B	301	TGL	CA5-CA6-CA7-CA8
19	Y	101	TGL	CB5-CB6-CB7-CB8
26	C	305	CDL	C80-C81-C82-C83
27	P	316	DMU	O16-C18-C19-C22
25	T	101	PEK	C24-C25-C26-C27
26	C	305	CDL	C14-C15-C16-C17
19	N	607	TGL	CB4-CB5-CB6-CB7
19	Q	201	TGL	CA4-CA5-CA6-CA7
19	Y	101	TGL	C10-C11-C12-C13
26	P	307	CDL	C36-C37-C38-C39
27	L	104	DMU	C18-C19-C22-C25
19	Y	101	TGL	CA2-CA3-CA4-CA5
25	G	101	PEK	C16-C17-C18-C19
19	N	607	TGL	C16-C15-CC9-CC8
25	P	304	PEK	C28-C29-C30-C31
25	C	302	PEK	C13-C14-C15-C16
25	T	101	PEK	C10-C11-C12-C13
26	P	307	CDL	C58-C59-C60-C61
19	N	607	TGL	CB1-CB2-CB3-CB4
26	P	307	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C72-C73-C74-C75
26	G	102	CDL	C80-C81-C82-C83
20	C	304	PGV	O05-C05-C06-O06
19	A	607	TGL	CA3-CA4-CA5-CA6
19	B	301	TGL	CA9-C20-C21-C22
19	N	607	TGL	C23-C24-C25-C26
20	N	608	PGV	C7-C8-C9-C10
26	G	102	CDL	C56-C57-C58-C59
26	P	307	CDL	C74-C75-C76-C77
23	R	201	PSC	C6-C7-C8-C9
27	K	102	DMU	C18-C19-C22-C25
19	Y	101	TGL	CA5-CA6-CA7-CA8
26	C	305	CDL	CA2-C1-CB2-OB2
27	P	316	DMU	C31-C34-C37-C40
19	D	201	TGL	C21-C22-C23-C24
26	P	307	CDL	C54-C55-C56-C57
21	A	617	EDO	O1-C1-C2-O2
21	A	619	EDO	O1-C1-C2-O2
21	A	622	EDO	O1-C1-C2-O2
21	B	307	EDO	O1-C1-C2-O2
21	B	309	EDO	O1-C1-C2-O2
20	C	304	PGV	C28-C29-C30-C31
25	P	304	PEK	C24-C25-C26-C27
26	C	305	CDL	C74-C75-C76-C77
25	T	101	PEK	O02-C1-O01-C02
20	A	608	PGV	C19-C20-C21-C22
25	P	303	PEK	C22-C23-C24-C25
26	C	305	CDL	C16-C17-C18-C19
26	C	305	CDL	C82-C83-C84-C85
19	N	607	TGL	OB1-CB1-OG2-CG2
25	T	101	PEK	C2-C1-O01-C02
19	Y	101	TGL	CB6-CB7-CB8-CB9
25	T	101	PEK	C1-C2-C3-C4
19	A	607	TGL	C16-C15-CC9-CC8
23	R	201	PSC	C24-C25-C26-C27
26	P	307	CDL	C73-C74-C75-C76
27	P	316	DMU	O5-C6-O16-C18
24	Y	104	CHD	C13-C17-C20-C22
19	B	301	TGL	C12-C13-C14-C29
26	C	305	CDL	C41-C42-C43-C44
19	N	607	TGL	CB2-CB1-OG2-CG2
20	A	609	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	L	104	DMU	C1-C6-O16-C18
19	A	607	TGL	C16-C17-C18-C19
19	Y	101	TGL	C11-C10-CB9-CB8
23	R	201	PSC	C23-C24-C25-C26
20	P	305	PGV	C11-C10-C9-C8
26	T	102	CDL	C55-C56-C57-C58
25	P	303	PEK	C26-C27-C28-C29
27	K	103	DMU	O16-C18-C19-C22
25	G	101	PEK	C4-C5-C6-C7
26	P	307	CDL	C72-C73-C74-C75
19	N	607	TGL	CB9-C10-C11-C12
26	T	102	CDL	C51-CB5-OB6-CB4
19	N	607	TGL	C13-C14-C29-C30
26	G	102	CDL	CA2-OA2-PA1-OA5
27	J	101	DMU	C22-C25-C28-C31
20	A	608	PGV	C01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-CA6
19	D	201	TGL	CA3-CA4-CA5-CA6
19	Q	201	TGL	C16-C15-CC9-CC8
26	G	102	CDL	C78-C79-C80-C81
26	P	307	CDL	C43-C44-C45-C46
27	C	315	DMU	C31-C34-C37-C40
19	B	301	TGL	CB4-CB5-CB6-CB7
26	P	307	CDL	C78-C79-C80-C81
19	N	607	TGL	CA1-CA2-CA3-CA4
19	A	607	TGL	OG1-CG1-CG2-CG3
25	C	302	PEK	O03-C01-C02-C03
20	N	609	PGV	C10-C11-C12-C13
19	A	607	TGL	CC6-CC7-CC8-CC9
19	B	301	TGL	C29-C30-C31-C32
19	A	607	TGL	CA7-CA8-CA9-C20
19	Q	201	TGL	CA6-CA7-CA8-CA9
26	G	102	CDL	C40-C41-C42-C43
20	A	608	PGV	C11-C10-C9-C8
20	N	608	PGV	C11-C10-C9-C8
20	A	608	PGV	O01-C1-C2-C3
20	C	304	PGV	C3-C4-C5-C6
27	K	101	DMU	O5-C4-C57-O61
20	N	608	PGV	C2-C3-C4-C5
27	T	105	DMU	C31-C34-C37-C40
20	A	608	PGV	C1-C2-C3-C4
19	Y	101	TGL	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	B	303	PSC	C03-C02-O01-C1
27	K	101	DMU	C25-C28-C31-C34
20	P	306	PGV	C02-C03-O11-P
20	N	609	PGV	C29-C30-C31-C32
26	C	305	CDL	C17-C18-C19-C20
26	C	305	CDL	C39-C40-C41-C42
24	L	103	CHD	C16-C17-C20-C21
21	H	101	EDO	O1-C1-C2-O2
26	P	307	CDL	O1-C1-CA2-OA2
26	G	102	CDL	C54-C55-C56-C57
19	A	607	TGL	OG2-CG2-CG3-OG3
27	L	104	DMU	C22-C25-C28-C31
26	T	102	CDL	OB7-CB5-OB6-CB4
20	C	304	PGV	C20-C21-C22-C23
26	P	307	CDL	C44-C45-C46-C47
26	T	102	CDL	C23-C24-C25-C26
19	N	607	TGL	CA2-CA1-OG1-CG1
19	D	201	TGL	CC4-CC5-CC6-CC7
27	P	316	DMU	C34-C37-C40-C43
19	Q	201	TGL	CA5-CA6-CA7-CA8
25	C	302	PEK	C25-C26-C27-C28
26	C	305	CDL	C21-C22-C23-C24
23	B	303	PSC	C01-C02-C03-O11
26	T	102	CDL	OB5-CB3-CB4-CB6
26	P	307	CDL	C80-C81-C82-C83
19	B	301	TGL	C16-C17-C18-C19
25	P	304	PEK	C23-C24-C25-C26
19	Y	101	TGL	C14-C29-C30-C31
27	P	309	DMU	C18-C19-C22-C25
20	C	303	PGV	C14-C15-C16-C17
26	C	305	CDL	C31-C32-C33-C34
27	G	105	DMU	C3-C4-C57-O61
19	B	301	TGL	CC4-CC5-CC6-CC7
26	P	307	CDL	C53-C54-C55-C56
25	P	304	PEK	C32-C33-C34-C35
27	K	101	DMU	C19-C18-O16-C6
26	T	102	CDL	C78-C79-C80-C81
20	C	304	PGV	C12-C13-C14-C15
19	A	607	TGL	CC1-CC2-CC3-CC4
26	P	307	CDL	C57-C58-C59-C60
19	A	607	TGL	C17-C18-C19-C33
25	P	304	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	CA3-CA4-CA6-OA8
26	G	102	CDL	CB3-CB4-CB6-OB8
26	T	102	CDL	CB3-CB4-CB6-OB8
25	P	304	PEK	C35-C36-C37-C38
20	A	609	PGV	C10-C11-C12-C13
25	C	302	PEK	C35-C36-C37-C38
27	J	101	DMU	C18-C19-C22-C25
20	P	306	PGV	C23-C24-C25-C26
19	B	301	TGL	C21-C22-C23-C24
19	Q	201	TGL	CB3-CB4-CB5-CB6
27	K	102	DMU	C28-C31-C34-C37
14	A	601[A]	HEA	C27-C19-C20-C21
19	A	607	TGL	CA6-CA7-CA8-CA9
19	Q	201	TGL	CC7-CC8-CC9-C15
20	C	304	PGV	C5-C6-C7-C8
23	B	303	PSC	C10-C11-C12-C13
23	R	201	PSC	C9-C10-C11-C12
23	R	201	PSC	C10-C11-C12-C13
25	C	302	PEK	C5-C6-C7-C8
25	C	302	PEK	C6-C7-C8-C9
25	C	302	PEK	C11-C10-C9-C8
25	C	302	PEK	C9-C10-C11-C12
25	C	302	PEK	C11-C12-C13-C14
25	C	302	PEK	C12-C13-C14-C15
25	P	302	PEK	C5-C6-C7-C8
25	P	303	PEK	C11-C10-C9-C8
25	P	303	PEK	C11-C12-C13-C14
25	P	304	PEK	C5-C6-C7-C8
25	P	304	PEK	C6-C7-C8-C9
25	P	304	PEK	C11-C10-C9-C8
25	P	304	PEK	C9-C10-C11-C12
25	P	304	PEK	C11-C12-C13-C14
25	T	101	PEK	C5-C6-C7-C8
25	T	101	PEK	C6-C7-C8-C9
25	T	101	PEK	C11-C10-C9-C8
25	T	101	PEK	C9-C10-C11-C12
24	L	103	CHD	C21-C20-C22-C23
19	Y	101	TGL	C22-C23-C24-C25
20	A	608	PGV	O01-C02-C03-O11
23	B	303	PSC	O01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-OA6
26	T	102	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
23	B	303	PSC	C20-C19-O03-C01
27	K	101	DMU	O16-C18-C19-C22
26	P	307	CDL	C16-C17-C18-C19
19	N	607	TGL	C17-C18-C19-C33
25	P	303	PEK	C17-C18-C19-C20
19	D	201	TGL	OG1-CG1-CG2-OG2
19	Q	201	TGL	CC5-CC6-CC7-CC8
26	C	305	CDL	C75-C76-C77-C78
26	P	307	CDL	C38-C39-C40-C41
27	G	105	DMU	O16-C18-C19-C22
27	J	101	DMU	C34-C37-C40-C43
20	P	305	PGV	C02-C03-O11-P
25	P	304	PEK	C30-C31-C32-C33
27	K	103	DMU	C22-C25-C28-C31
26	C	305	CDL	C77-C78-C79-C80
21	D	202	EDO	O1-C1-C2-O2
21	D	204	EDO	O1-C1-C2-O2
21	F	104	EDO	O1-C1-C2-O2
19	A	607	TGL	C12-C13-C14-C29
19	Y	101	TGL	CC4-CC5-CC6-CC7
19	Y	101	TGL	CA1-CA2-CA3-CA4
19	D	201	TGL	C23-C24-C25-C26
26	T	102	CDL	C52-C53-C54-C55
26	T	102	CDL	C56-C57-C58-C59
26	P	307	CDL	OA5-CA3-CA4-CA6
20	P	305	PGV	C24-C25-C26-C27
27	K	102	DMU	C19-C22-C25-C28
19	N	607	TGL	OA1-CA1-OG1-CG1
20	P	305	PGV	C12-C13-C14-C15
19	A	607	TGL	CC5-CC6-CC7-CC8
19	N	607	TGL	C20-C21-C22-C23
27	P	316	DMU	C3-C4-C57-O61
27	Z	101	DMU	C22-C25-C28-C31
27	K	101	DMU	O5-C6-O16-C18
26	T	102	CDL	C82-C83-C84-C85
19	D	201	TGL	OG1-CG1-CG2-CG3
19	D	201	TGL	CG1-CG2-CG3-OG3
19	Y	101	TGL	CG1-CG2-CG3-OG3
20	A	608	PGV	O03-C01-C02-C03
20	A	608	PGV	C02-C03-O11-P
20	N	608	PGV	O03-C01-C02-C03
25	P	302	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	C11-C12-C13-C14
26	P	307	CDL	OA5-CA3-CA4-OA6
19	Y	101	TGL	OG1-CA1-CA2-CA3
19	A	607	TGL	CC3-CC4-CC5-CC6
23	B	303	PSC	O04-C19-O03-C01
19	D	201	TGL	OG2-CG2-CG3-OG3
19	Y	101	TGL	OG1-CG1-CG2-OG2
19	Y	101	TGL	OG2-CG2-CG3-OG3
20	N	608	PGV	O03-C01-C02-O01
25	C	302	PEK	O03-C01-C02-O01
25	P	302	PEK	O03-C01-C02-O01
26	T	102	CDL	OA6-CA4-CA6-OA8
19	N	607	TGL	C10-C11-C12-C13
19	D	201	TGL	CC5-CC6-CC7-CC8
19	Q	201	TGL	CA7-CA8-CA9-C20
19	N	607	TGL	C29-C30-C31-C32
27	G	105	DMU	C22-C25-C28-C31
27	G	105	DMU	C4-C3-O7-C10
19	A	607	TGL	C23-C24-C25-C26
20	P	306	PGV	C24-C25-C26-C27
25	P	303	PEK	C4-C5-C6-C7
26	P	307	CDL	C41-C42-C43-C44
27	K	103	DMU	O1-C10-O7-C3
19	Y	101	TGL	CC9-C15-C16-C17
20	P	306	PGV	C30-C31-C32-C33
26	G	102	CDL	CA3-OA5-PA1-OA2
19	A	607	TGL	OG1-CA1-CA2-CA3
20	C	303	PGV	C02-C03-O11-P
26	G	102	CDL	C1-CB2-OB2-PB2
19	D	201	TGL	C13-C14-C29-C30
19	Q	201	TGL	C18-C19-C33-C34
20	C	304	PGV	C03-O11-P-O14
20	P	306	PGV	C03-O11-P-O13
25	C	302	PEK	C04-O12-P-O14
25	P	302	PEK	C03-O11-P-O14
26	C	305	CDL	CA3-OA5-PA1-OA3
26	G	102	CDL	CA2-OA2-PA1-OA4
26	P	307	CDL	CA3-OA5-PA1-OA3
26	T	102	CDL	CA2-OA2-PA1-OA3
26	T	102	CDL	CA3-OA5-PA1-OA3
26	T	102	CDL	CB2-OB2-PB2-OB4
25	P	304	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
23	R	201	PSC	C01-C02-C03-O11
21	Q	202	EDO	O1-C1-C2-O2
21	R	203	EDO	O1-C1-C2-O2
27	O	308	DMU	C25-C28-C31-C34
19	Q	201	TGL	C16-C17-C18-C19
19	Q	201	TGL	C17-C18-C19-C33
19	N	607	TGL	C18-C19-C33-C34
19	Q	201	TGL	CC1-CC2-CC3-CC4
27	G	105	DMU	C2-C3-O7-C10
26	C	305	CDL	C76-C77-C78-C79
26	G	102	CDL	C79-C80-C81-C82
23	R	201	PSC	O01-C02-C03-O11
19	N	607	TGL	C19-C33-C34-C35
19	A	607	TGL	CG1-CG2-CG3-OG3
20	N	609	PGV	C28-C29-C30-C31
27	P	316	DMU	C1-C6-O16-C18
19	A	607	TGL	OG1-CG1-CG2-OG2
20	A	608	PGV	O03-C01-C02-O01
20	C	304	PGV	O03-C01-C02-O01
25	P	304	PEK	O03-C01-C02-O01
26	T	102	CDL	C1-CA2-OA2-PA1
26	P	307	CDL	C59-C60-C61-C62
24	W	101	CHD	C16-C17-C20-C22
19	N	607	TGL	C16-C17-C18-C19
23	R	201	PSC	C25-C26-C27-C28
19	Y	101	TGL	C21-C22-C23-C24
26	P	307	CDL	C40-C41-C42-C43
26	C	305	CDL	C58-C59-C60-C61
19	A	607	TGL	CC4-CC5-CC6-CC7
20	C	304	PGV	C2-C3-C4-C5
25	G	101	PEK	C7-C8-C9-C10
20	A	609	PGV	C11-C12-C13-C14
25	C	302	PEK	C3-C4-C5-C6
19	N	607	TGL	C15-C16-C17-C18
19	B	301	TGL	CA6-CA7-CA8-CA9
24	C	306	CHD	C13-C17-C20-C22
27	G	105	DMU	O5-C4-C57-O61
20	C	303	PGV	C28-C29-C30-C31
27	J	101	DMU	C28-C31-C34-C37
27	T	105	DMU	C22-C25-C28-C31
20	A	608	PGV	C05-C04-O12-P
20	C	304	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	306	CHD	C16-C17-C20-C22
19	N	607	TGL	CA2-CA3-CA4-CA5
21	C	312	EDO	O1-C1-C2-O2
21	M	103	EDO	O1-C1-C2-O2
21	Z	102	EDO	O1-C1-C2-O2
20	A	608	PGV	C04-O12-P-O11
20	C	304	PGV	C04-O12-P-O11
23	R	201	PSC	C21-C22-C23-C24
14	A	601[A]	HEA	C18-C19-C20-C21
19	A	607	TGL	CA2-CA3-CA4-CA5
25	G	101	PEK	C25-C26-C27-C28
26	C	305	CDL	OB6-CB4-CB6-OB8
26	G	102	CDL	C13-C14-C15-C16
27	K	102	DMU	C22-C25-C28-C31
19	D	201	TGL	OB1-CB1-OG2-CG2
27	P	316	DMU	O6-C11-C9-C8
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
24	J	102	CHD	C22-C23-C24-O26
19	Q	201	TGL	C23-C24-C25-C26
20	C	303	PGV	C1-C2-C3-C4
19	A	607	TGL	CB3-CB4-CB5-CB6
27	C	315	DMU	C34-C37-C40-C43
26	T	102	CDL	OA5-CA3-CA4-CA6
19	A	607	TGL	CB5-CB6-CB7-CB8
26	P	307	CDL	CA5-C11-C12-C13
27	K	101	DMU	C31-C34-C37-C40
20	N	608	PGV	O01-C1-C2-C3
19	Y	101	TGL	C24-C25-C26-C27
24	O	301	CHD	C22-C23-C24-O26
19	Q	201	TGL	C22-C23-C24-C25
20	P	305	PGV	C7-C8-C9-C10
26	G	102	CDL	C58-C59-C60-C61
24	B	304	CHD	C22-C23-C24-O26
27	O	308	DMU	O5-C4-C57-O61
19	Y	101	TGL	C12-C13-C14-C29
24	O	301	CHD	C22-C23-C24-O25
26	G	102	CDL	C32-C31-CA7-OA9
20	C	304	PGV	C24-C25-C26-C27
20	C	304	PGV	O03-C01-C02-C03
24	J	102	CHD	C22-C23-C24-O25
19	D	201	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
26	T	102	CDL	C22-C23-C24-C25
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	N	602	HEA	CAA-CBA-CGA-O2A
26	G	102	CDL	C81-C82-C83-C84
26	P	307	CDL	C12-C13-C14-C15
24	W	101	CHD	C22-C23-C24-O26
20	N	609	PGV	C11-C12-C13-C14
23	R	201	PSC	C7-C8-C9-C10
24	C	306	CHD	C22-C23-C24-O26
20	P	306	PGV	C2-C3-C4-C5
25	G	101	PEK	C26-C27-C28-C29
25	P	302	PEK	C6-C7-C8-C9
25	P	302	PEK	C11-C10-C9-C8
25	P	302	PEK	C9-C10-C11-C12
25	P	302	PEK	C11-C12-C13-C14
25	P	303	PEK	C6-C7-C8-C9
26	T	102	CDL	CB2-OB2-PB2-OB5
14	A	602	HEA	CAD-CBD-CGD-O2D
24	W	101	CHD	C22-C23-C24-O25
26	G	102	CDL	C33-C34-C35-C36
24	C	306	CHD	C22-C23-C24-O25
26	T	102	CDL	C37-C38-C39-C40
24	C	306	CHD	C13-C17-C20-C21
14	A	602	HEA	CAA-CBA-CGA-O2A
24	B	304	CHD	C22-C23-C24-O25
19	B	301	TGL	CB1-CB2-CB3-CB4
26	T	102	CDL	C19-C20-C21-C22
14	A	602	HEA	CAD-CBD-CGD-O1D
19	B	301	TGL	C18-C19-C33-C34
19	Q	201	TGL	C33-C34-C35-C36
19	Y	101	TGL	CB2-CB3-CB4-CB5
26	G	102	CDL	C35-C36-C37-C38
26	G	102	CDL	C72-C73-C74-C75
26	T	102	CDL	CB2-C1-CA2-OA2
19	Q	201	TGL	C15-C16-C17-C18
26	G	102	CDL	C36-C37-C38-C39
20	P	305	PGV	C13-C14-C15-C16
24	P	308	CHD	C22-C23-C24-O26
21	A	625	EDO	O1-C1-C2-O2
21	N	621	EDO	O1-C1-C2-O2
21	N	623	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
21	P	314	EDO	O1-C1-C2-O2
24	L	103	CHD	C16-C17-C20-C22
14	A	602	HEA	CAA-CBA-CGA-O1A
26	G	102	CDL	OB9-CB7-OB8-CB6
23	B	303	PSC	C7-C8-C9-C10
25	P	303	PEK	C14-C15-C16-C17
23	B	303	PSC	C1-C2-C3-C4
27	K	101	DMU	C22-C25-C28-C31
20	P	306	PGV	C13-C14-C15-C16
26	P	307	CDL	C37-C38-C39-C40
19	D	201	TGL	CA4-CA5-CA6-CA7
26	T	102	CDL	C54-C55-C56-C57
26	P	307	CDL	C60-C61-C62-C63
20	P	306	PGV	C3-C4-C5-C6
26	P	307	CDL	CB2-C1-CA2-OA2
26	G	102	CDL	C52-C53-C54-C55
26	G	102	CDL	C57-C58-C59-C60
14	N	602	HEA	CAD-CBD-CGD-O2D
19	N	607	TGL	CA9-C20-C21-C22
14	N	602	HEA	CAD-CBD-CGD-O1D
25	P	304	PEK	C03-O11-P-O13
19	Y	101	TGL	CA6-CA7-CA8-CA9
25	G	101	PEK	C15-C16-C17-C18
26	C	305	CDL	C12-C13-C14-C15
26	G	102	CDL	C14-C15-C16-C17
14	N	602	HEA	CAA-CBA-CGA-O1A
26	G	102	CDL	C32-C31-CA7-OA8
26	T	102	CDL	O1-C1-CB2-OB2
19	Q	201	TGL	OG1-CA1-CA2-CA3
19	Q	201	TGL	OG3-CC1-CC2-CC3
20	C	303	PGV	C9-C10-C11-C12
23	B	303	PSC	C12-C13-C14-C15
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
26	G	102	CDL	C12-C13-C14-C15
24	C	301	CHD	C22-C23-C24-O26
25	C	302	PEK	C29-C30-C31-C32
20	N	608	PGV	C9-C10-C11-C12
20	P	306	PGV	C9-C10-C11-C12
23	R	201	PSC	C12-C13-C14-C15
25	P	304	PEK	C14-C15-C16-C17
14	A	601[A]	HEA	C12-C11-C3B-C2B

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Mol	Chain	Res	Type	Atoms
14	N	601[A]	HEA	C12-C11-C3B-C2B
26	T	102	CDL	CA3-CA4-CA6-OA8
26	G	102	CDL	OB5-CB3-CB4-OB6
19	Y	101	TGL	OA1-CA1-CA2-CA3
24	P	308	CHD	C22-C23-C24-O25
26	C	305	CDL	C51-C52-C53-C54
21	A	614	EDO	O1-C1-C2-O2
21	A	618	EDO	O1-C1-C2-O2
21	B	308	EDO	O1-C1-C2-O2
21	E	202	EDO	O1-C1-C2-O2
21	N	614	EDO	O1-C1-C2-O2
24	C	301	CHD	C22-C23-C24-O25
20	C	303	PGV	C11-C12-C13-C14
19	D	201	TGL	CA7-CA8-CA9-C20
24	P	301	CHD	C22-C23-C24-O25
26	G	102	CDL	C59-C60-C61-C62
19	D	201	TGL	CB2-CB1-OG2-CG2
19	N	607	TGL	OG1-CG1-CG2-OG2
26	C	305	CDL	C81-C82-C83-C84
20	C	304	PGV	C10-C11-C12-C13
25	P	302	PEK	C10-C11-C12-C13
20	N	608	PGV	C22-C23-C24-C25
19	D	201	TGL	OG1-CA1-CA2-CA3
19	N	607	TGL	OG1-CA1-CA2-CA3
20	N	609	PGV	O03-C19-C20-C21
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
26	G	102	CDL	CB4-CB3-OB5-PB2
20	P	305	PGV	C9-C10-C11-C12
25	P	304	PEK	C3-C4-C5-C6
20	A	609	PGV	O03-C19-C20-C21
26	P	307	CDL	C12-C11-CA5-OA6
25	P	304	PEK	C27-C28-C29-C30
26	G	102	CDL	C71-CB7-OB8-CB6
20	A	608	PGV	O03-C19-C20-C21
20	A	609	PGV	C29-C30-C31-C32
26	T	102	CDL	C59-C60-C61-C62
19	Q	201	TGL	OA1-CA1-CA2-CA3
20	C	303	PGV	C24-C25-C26-C27
20	N	609	PGV	O04-C19-C20-C21
27	K	103	DMU	C19-C22-C25-C28
19	Q	201	TGL	OC1-CC1-CC2-CC3

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Mol	Chain	Res	Type	Atoms
24	P	301	CHD	C22-C23-C24-O26
23	R	201	PSC	O03-C01-C02-C03
19	N	607	TGL	OG3-CC1-CC2-CC3
19	N	607	TGL	CC9-C15-C16-C17
23	R	201	PSC	C29-C30-C31-C32
20	C	303	PGV	C27-C28-C29-C30
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A
19	D	201	TGL	OA1-CA1-CA2-CA3
19	N	607	TGL	OA1-CA1-CA2-CA3
20	C	304	PGV	C04-O12-P-O13
25	T	101	PEK	O01-C02-C03-O11
26	G	102	CDL	CA3-OA5-PA1-OA3
27	M	101	DMU	O6-C11-C9-C8
20	N	608	PGV	C01-C02-C03-O11
20	A	608	PGV	C22-C23-C24-C25
19	N	607	TGL	CC5-CC6-CC7-CC8
26	P	307	CDL	C15-C16-C17-C18
25	G	101	PEK	O12-C04-C05-N
21	D	203	EDO	O1-C1-C2-O2
19	A	607	TGL	C22-C23-C24-C25
14	N	602	HEA	C26-C15-C16-C17
23	R	201	PSC	C05-C04-O12-P
26	C	305	CDL	C53-C54-C55-C56
14	A	601[A]	HEA	CAA-CBA-CGA-O1A
14	A	601[B]	HEA	CAA-CBA-CGA-O1A
19	N	607	TGL	OC1-CC1-CC2-CC3
20	N	608	PGV	C21-C22-C23-C24
25	C	302	PEK	O01-C1-C2-C3
27	Z	101	DMU	O16-C18-C19-C22
20	A	608	PGV	O04-C19-C20-C21
19	N	607	TGL	CA4-CA5-CA6-CA7
20	P	305	PGV	C1-C2-C3-C4
14	A	601[A]	HEA	O11-C11-C3B-C2B
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
14	A	601[B]	HEA	CAA-CBA-CGA-O2A
26	P	307	CDL	C32-C31-CA7-OA8
20	N	609	PGV	C27-C28-C29-C30
25	G	101	PEK	O03-C21-C22-C23
19	Y	101	TGL	C21-C20-CA9-CA8
26	P	307	CDL	C76-C77-C78-C79
20	P	305	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OG2-CB1-CB2-CB3

There are no ring outliers.

78 monomers are involved in 213 short contacts:

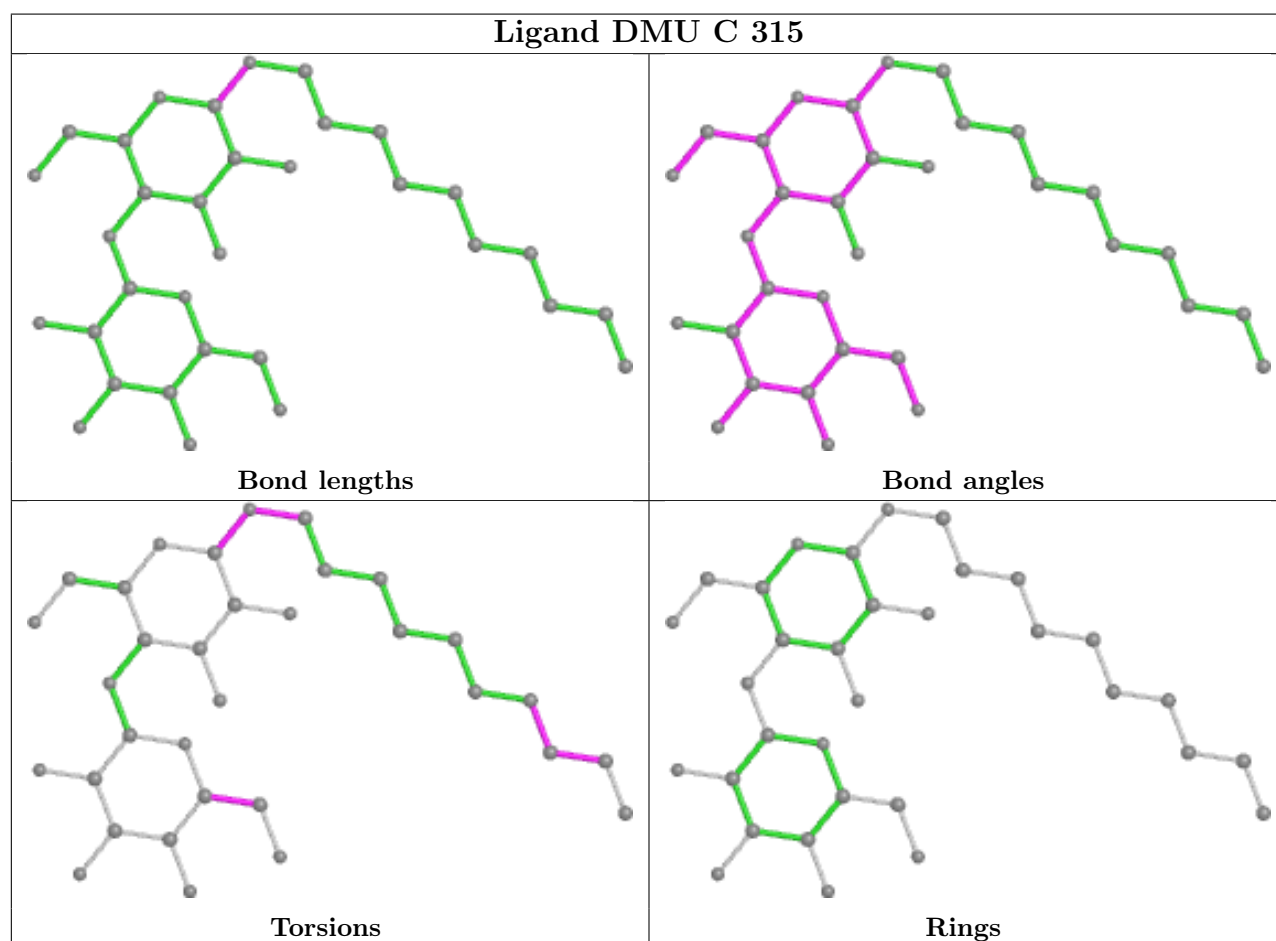
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	315	DMU	2	0
21	A	617	EDO	3	0
19	B	301	TGL	5	0
19	Q	201	TGL	5	0
21	Q	202	EDO	1	0
21	D	204	EDO	6	0
26	T	102	CDL	11	0
25	C	302	PEK	1	0
25	P	303	PEK	4	0
21	A	622	EDO	4	0
27	Z	101	DMU	1	0
27	L	104	DMU	4	0
27	J	101	DMU	4	0
27	K	101	DMU	1	0
27	P	309	DMU	3	0
24	C	306	CHD	3	0
19	A	607	TGL	5	0
21	A	618	EDO	1	0
21	G	104	EDO	1	0
23	B	303	PSC	5	0
21	C	314	EDO	1	0
21	A	621	EDO	1	0
21	B	307	EDO	5	0
25	T	101	PEK	1	0
26	C	305	CDL	15	0
21	N	617	EDO	1	0
19	D	201	TGL	9	0
21	B	310	EDO	2	0
26	P	307	CDL	9	0
21	A	626	EDO	1	0
21	O	306	EDO	1	0
27	O	308	DMU	1	0
20	N	609	PGV	1	0
14	A	602	HEA	7	0
20	P	305	PGV	1	0
21	A	614	EDO	2	0

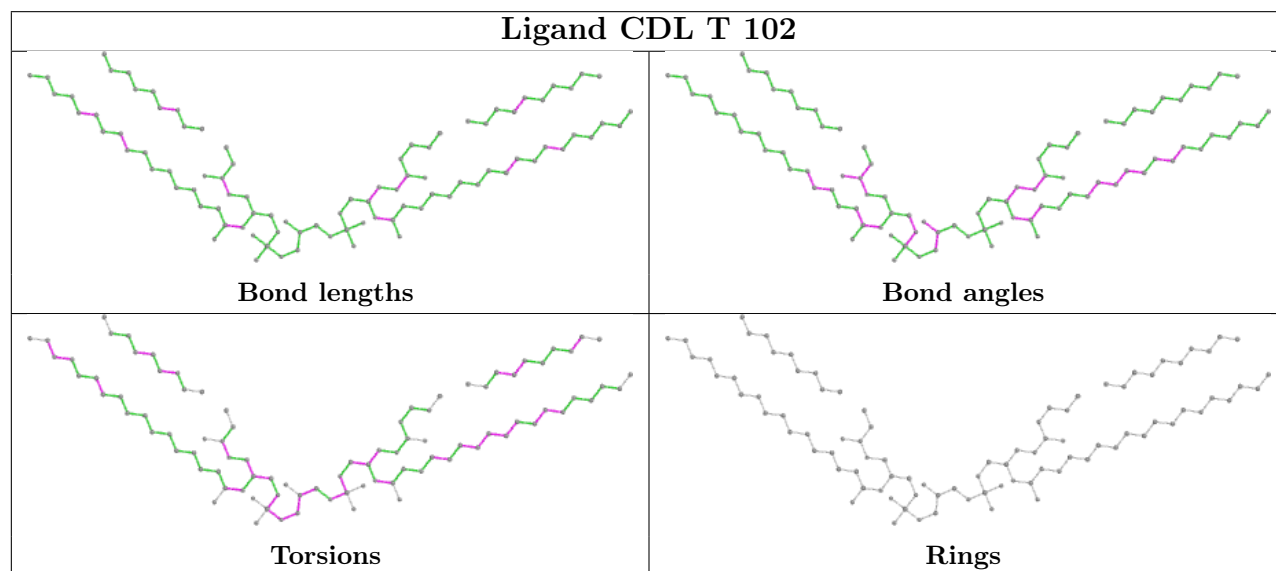
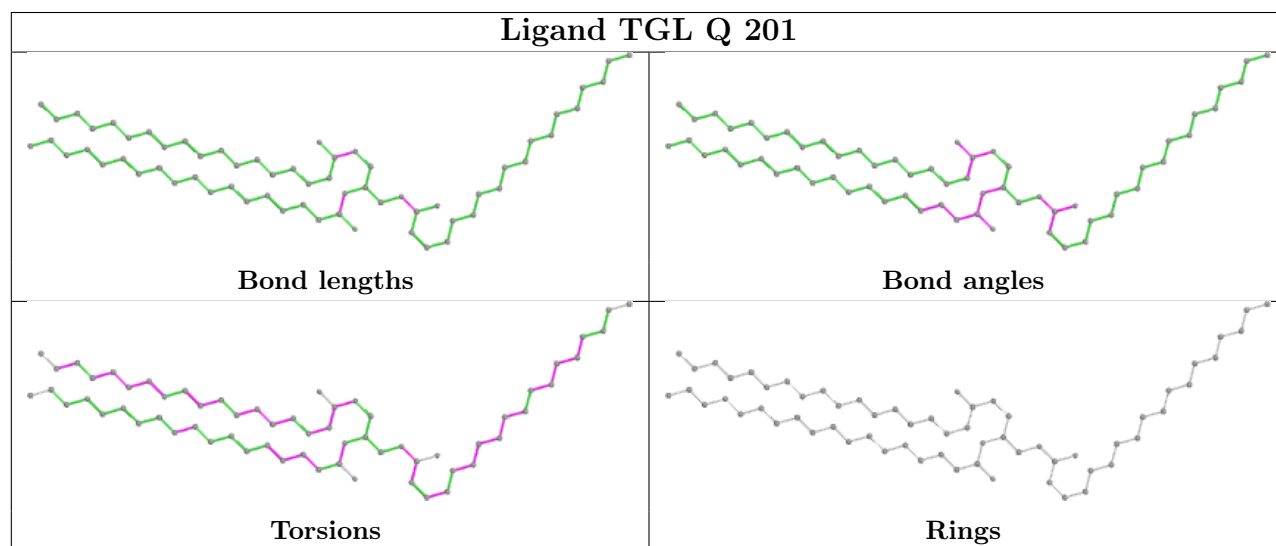
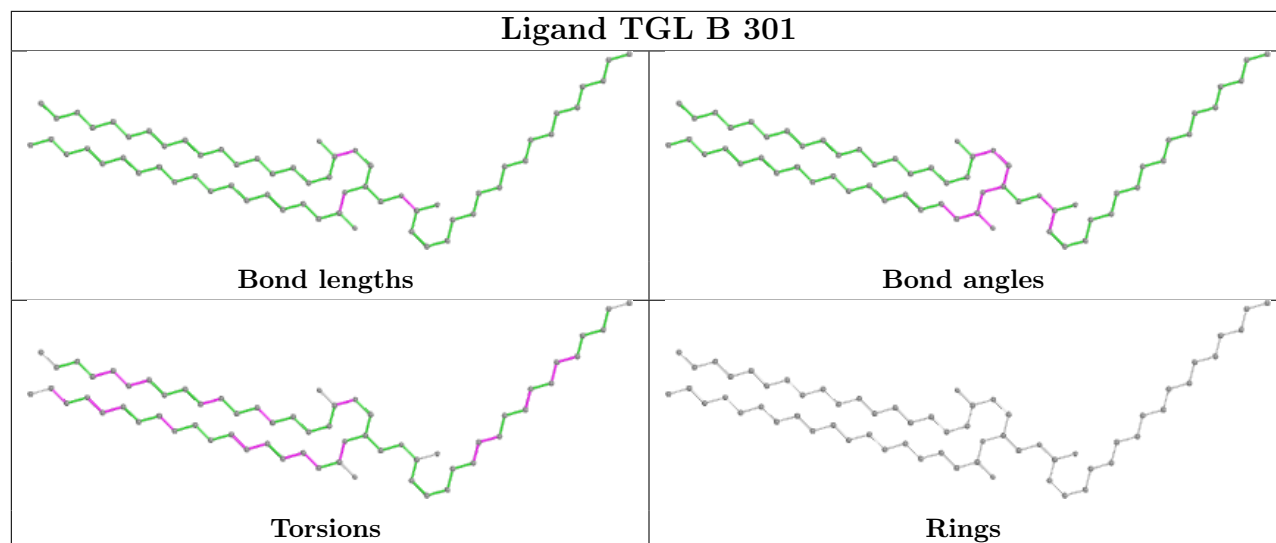
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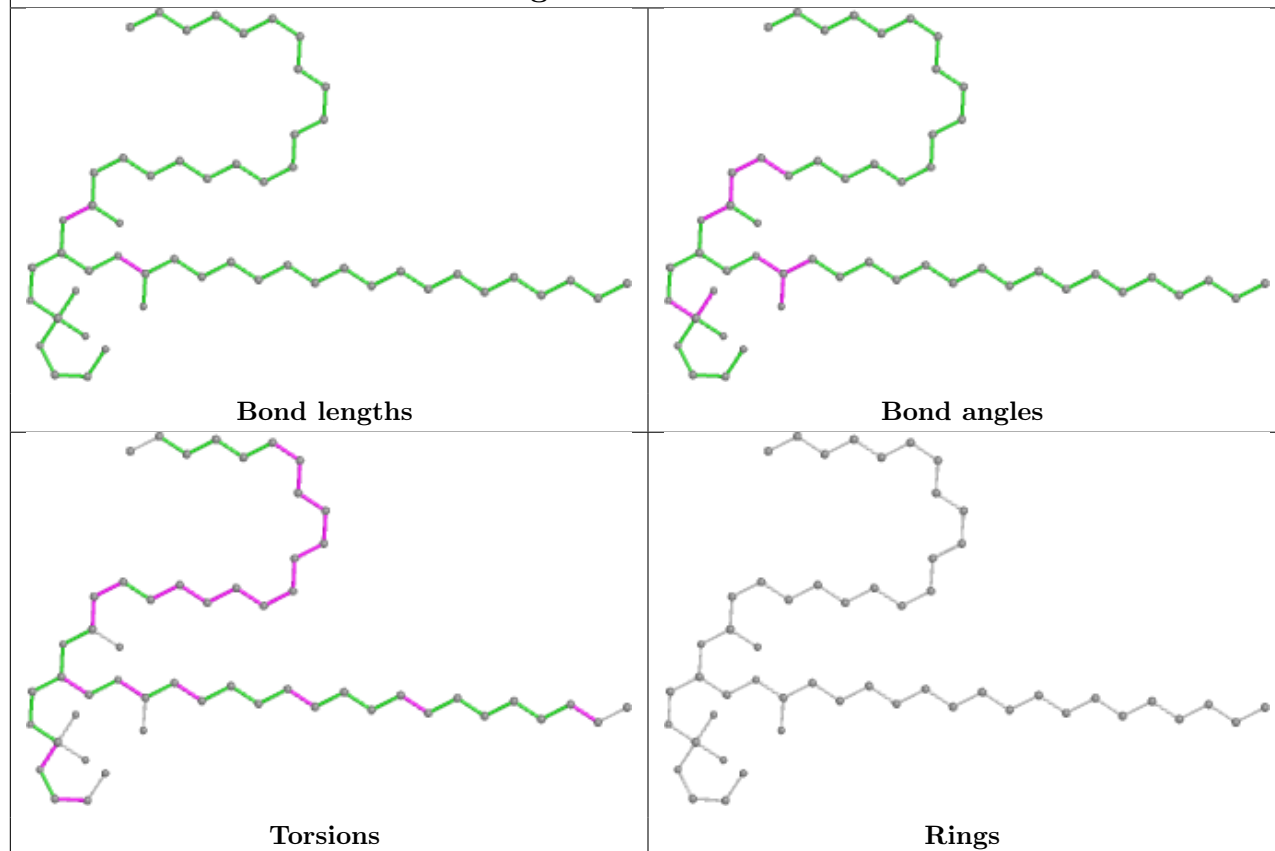
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	304	PEK	3	0
24	P	308	CHD	2	0
20	A	608	PGV	5	0
21	B	306	EDO	1	0
21	C	308	EDO	1	0
21	D	203	EDO	2	0
21	A	610	EDO	1	0
14	N	601[B]	HEA	1	0
27	K	103	DMU	1	0
24	O	301	CHD	1	0
14	N	602	HEA	4	0
26	G	102	CDL	4	0
14	A	601[A]	HEA	2	0
20	P	306	PGV	1	0
21	A	615	EDO	2	0
25	G	101	PEK	1	0
21	Q	203	EDO	1	0
19	Y	101	TGL	4	0
14	N	601[A]	HEA	3	0
27	G	105	DMU	5	0
21	N	614	EDO	2	0
21	N	623	EDO	1	0
19	N	607	TGL	2	0
24	L	103	CHD	2	0
24	J	102	CHD	1	0
20	N	608	PGV	3	0
27	T	105	DMU	1	0
23	R	201	PSC	7	0
21	B	309	EDO	2	0
21	N	610	EDO	2	0
24	P	301	CHD	1	0
21	A	625	EDO	1	0
21	A	619	EDO	5	0
21	F	104	EDO	1	0
21	N	616	EDO	2	0
21	M	103	EDO	1	0
20	C	304	PGV	6	0
20	C	303	PGV	3	0
24	Y	104	CHD	2	0
21	A	624	EDO	2	0
21	A	623	EDO	2	0
21	P	311	EDO	1	0

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

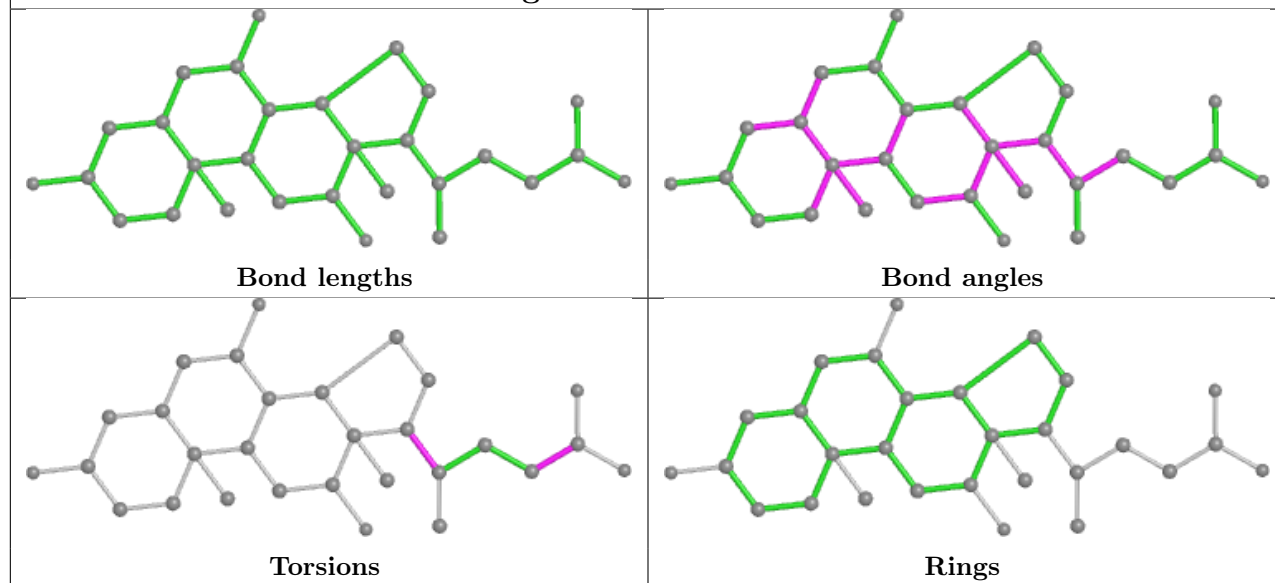


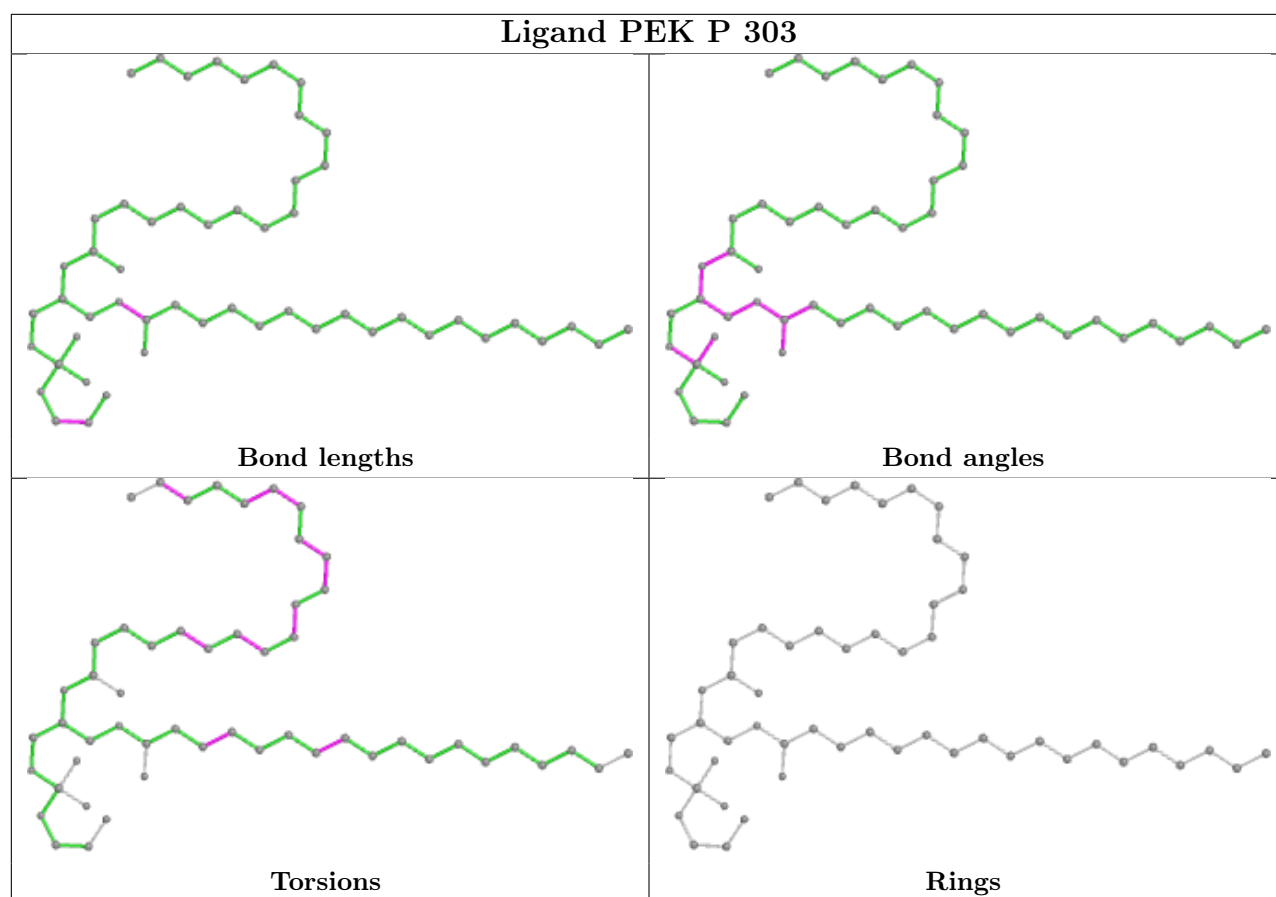


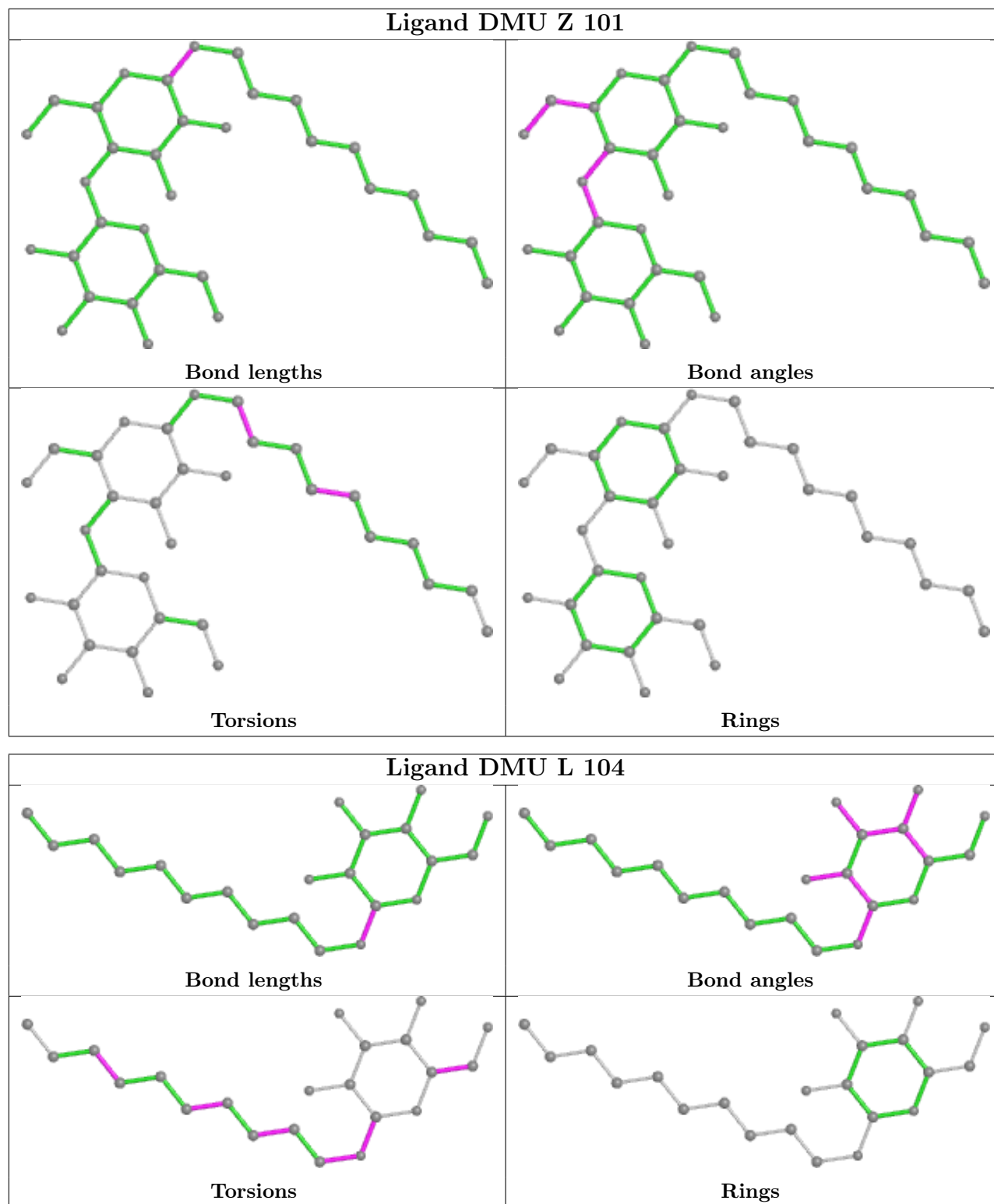
Ligand PEK C 302

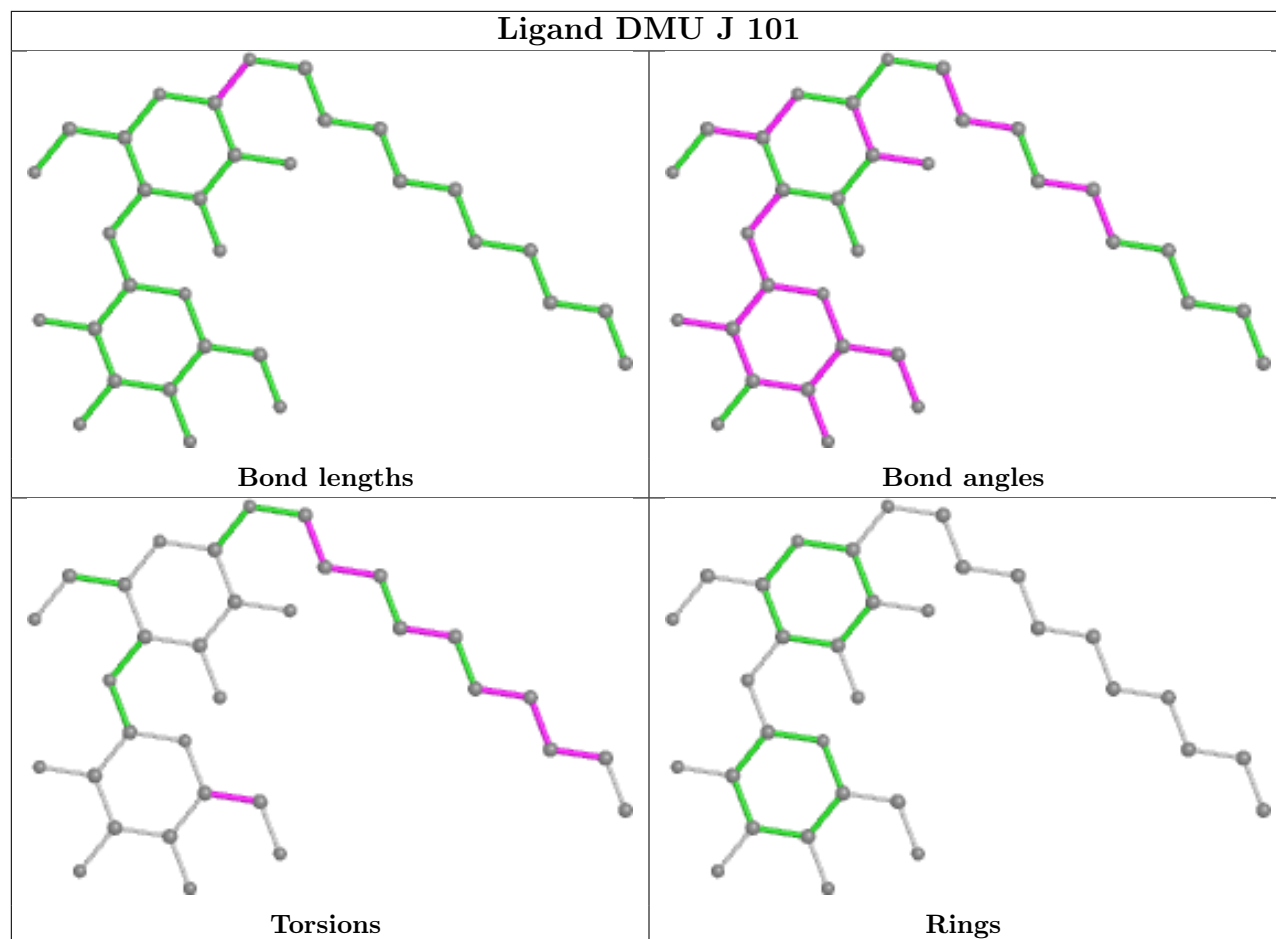


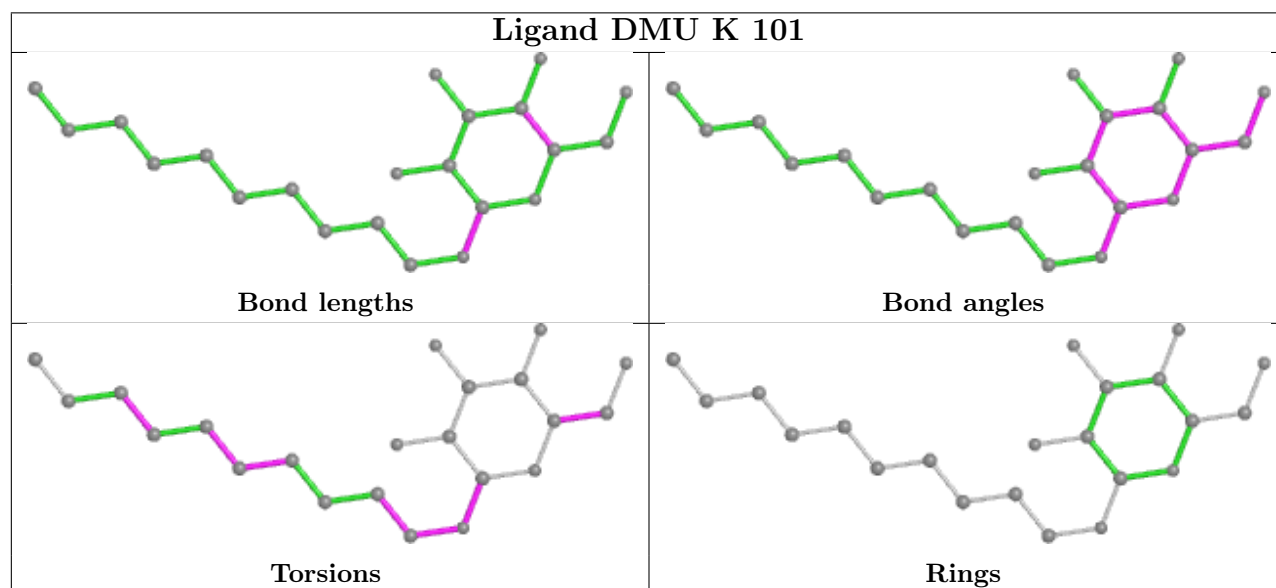
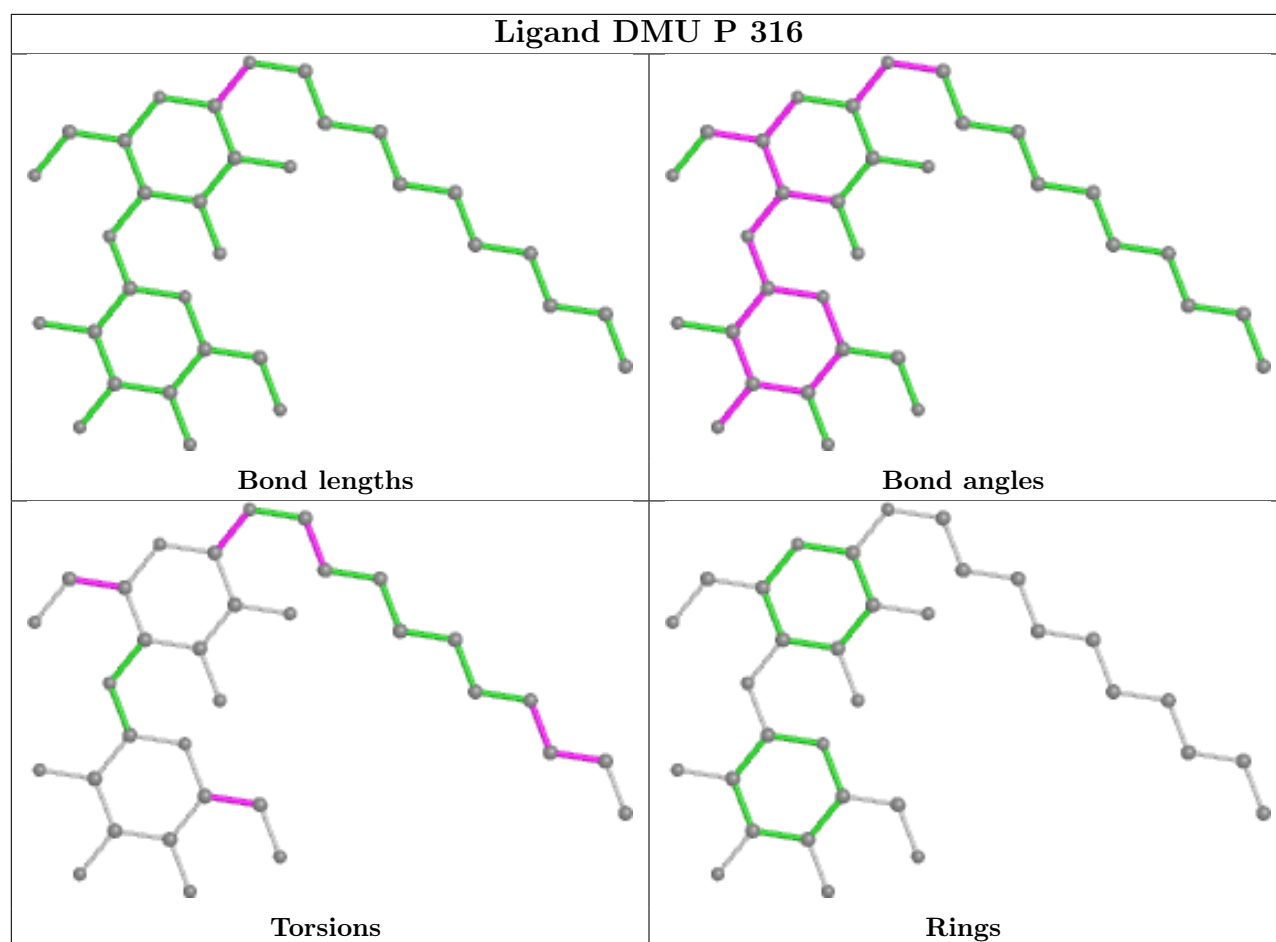
Ligand CHD W 101

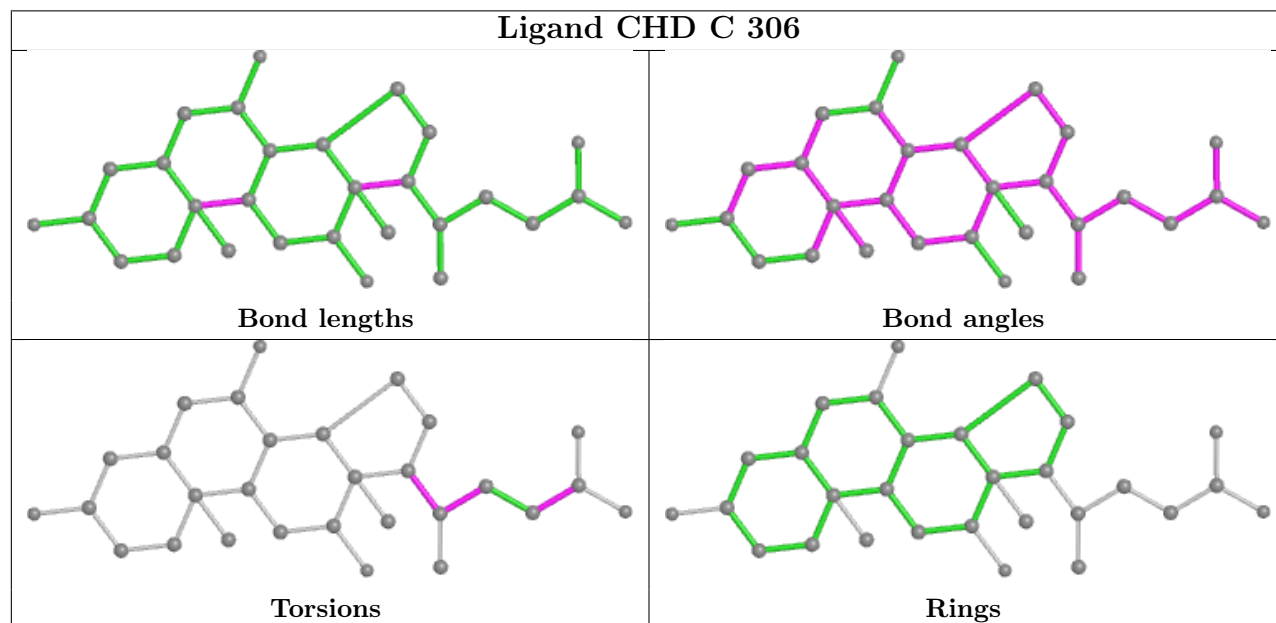
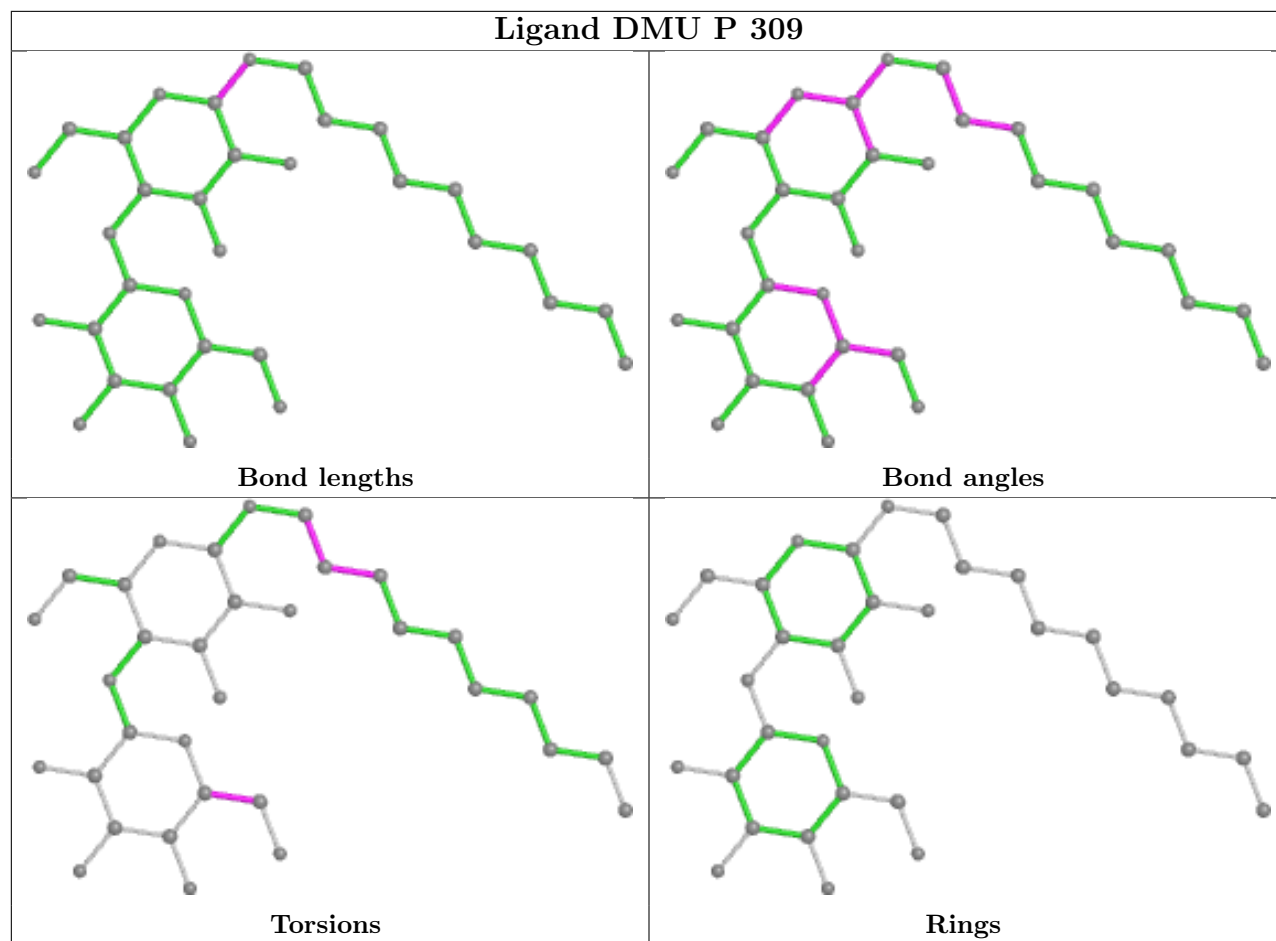


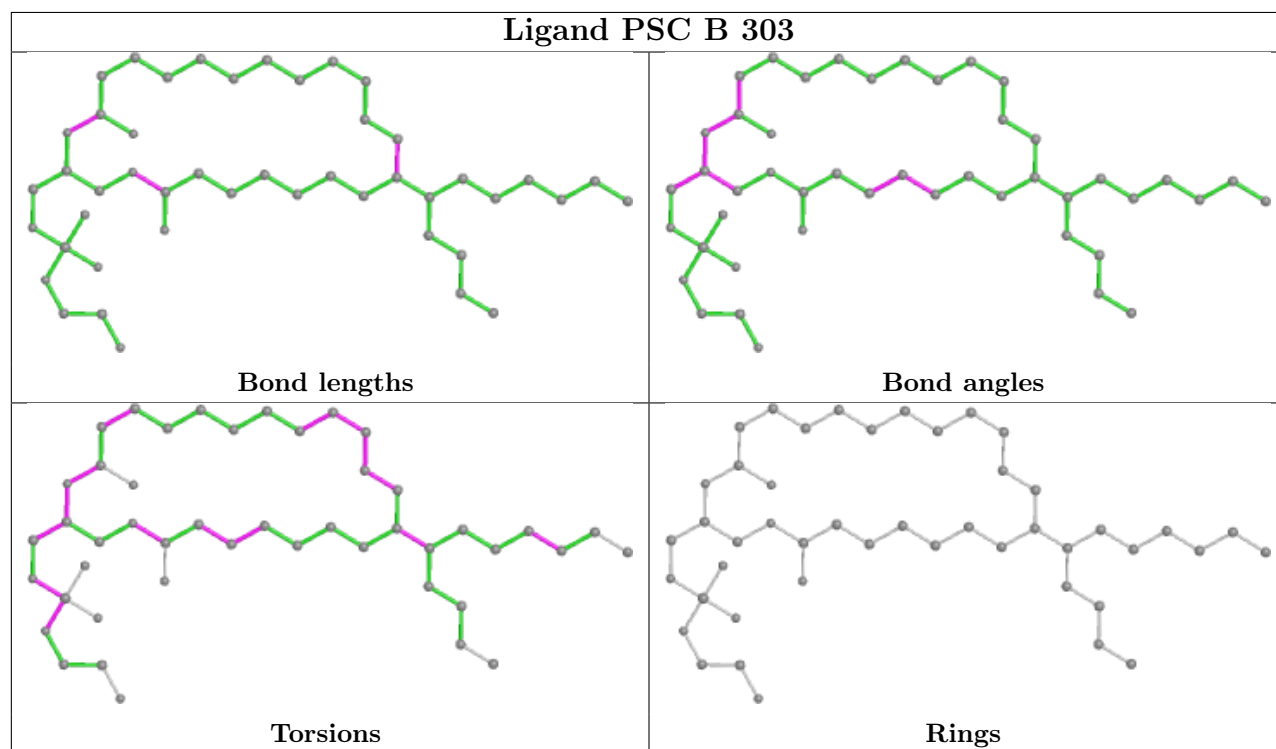
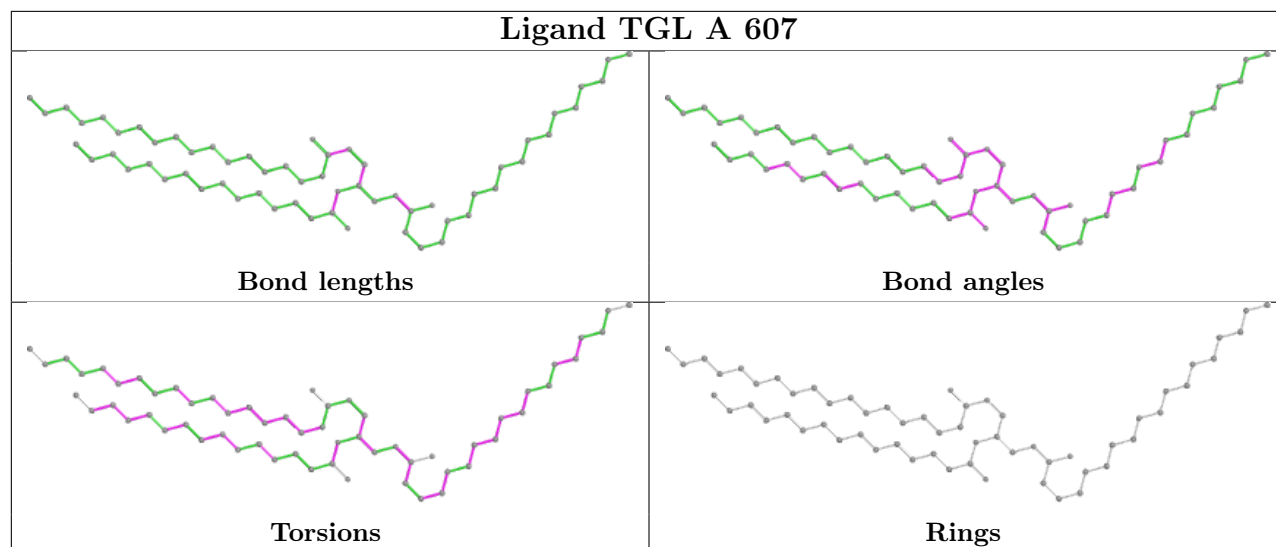


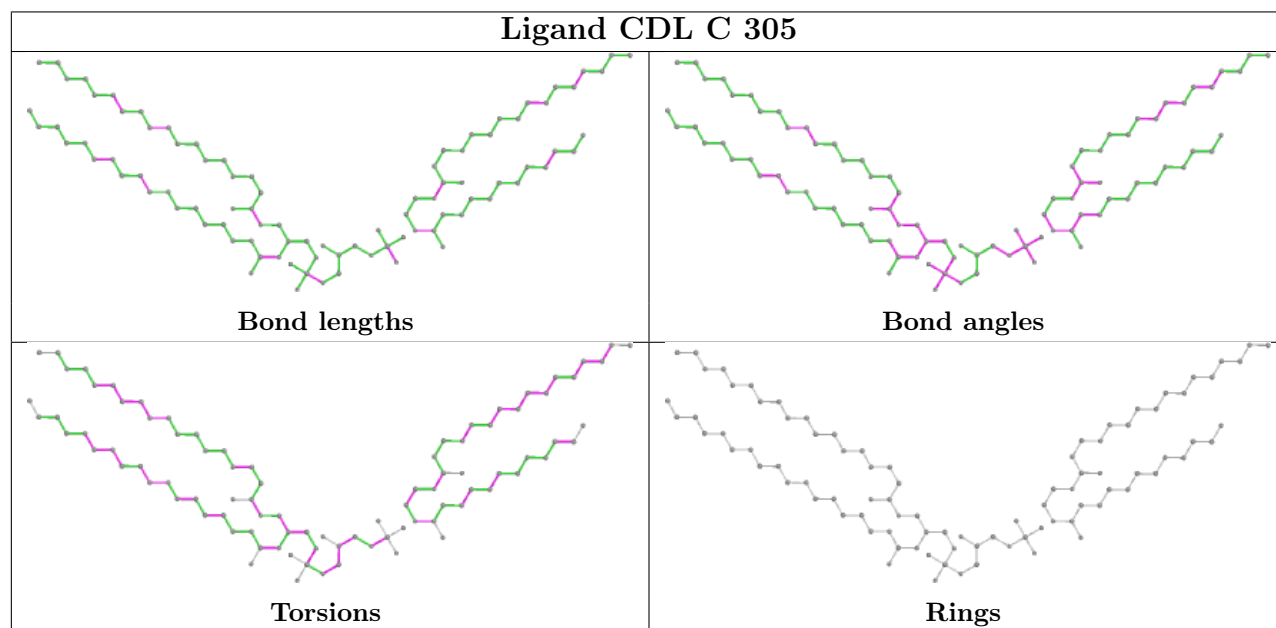
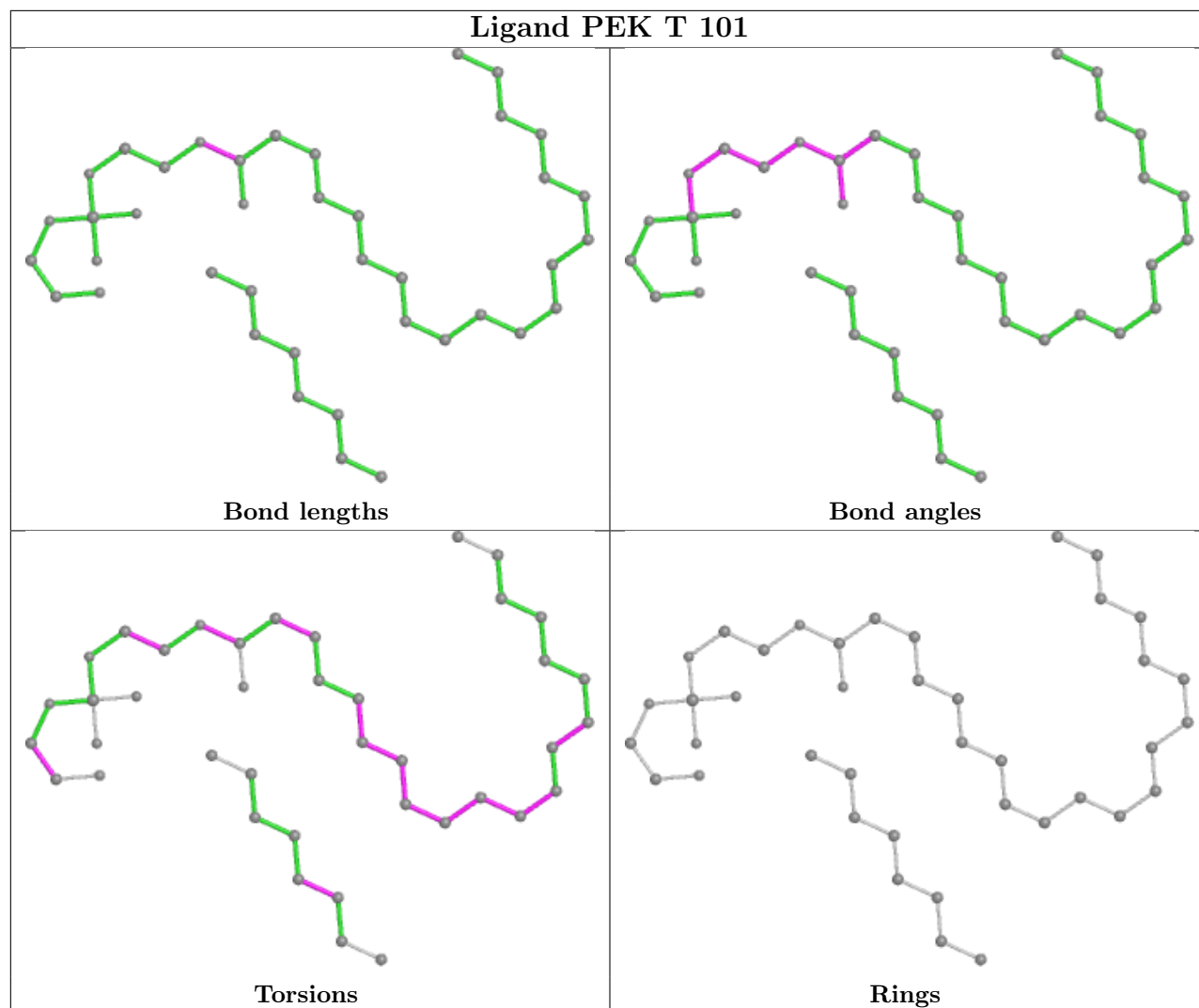


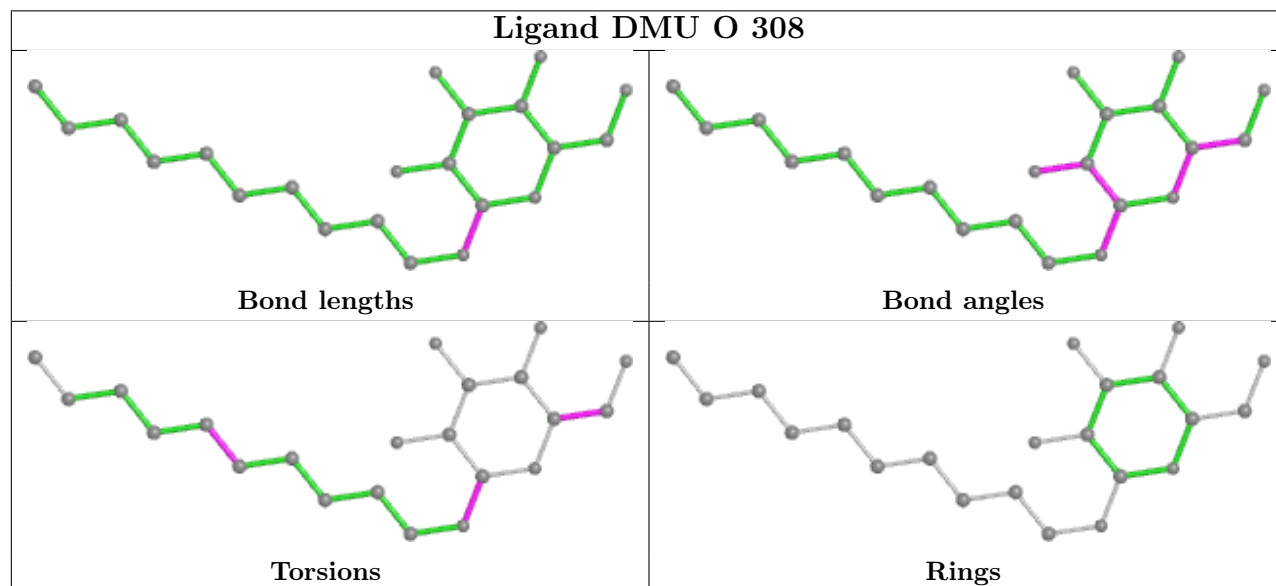
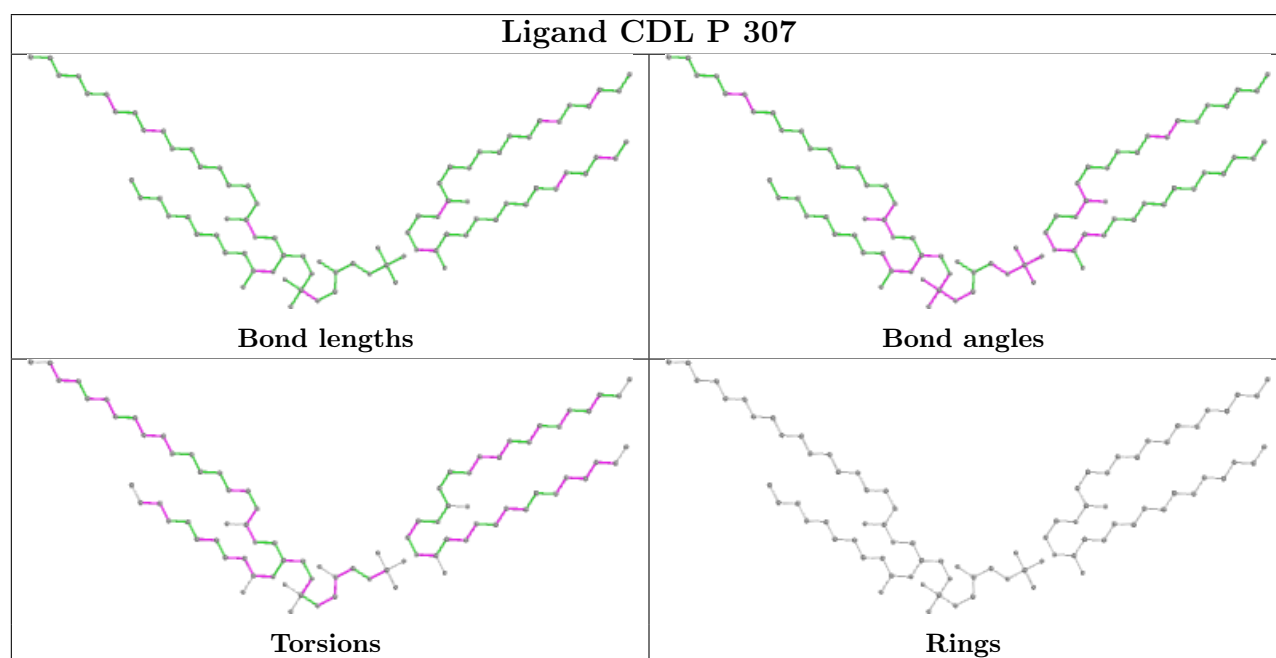
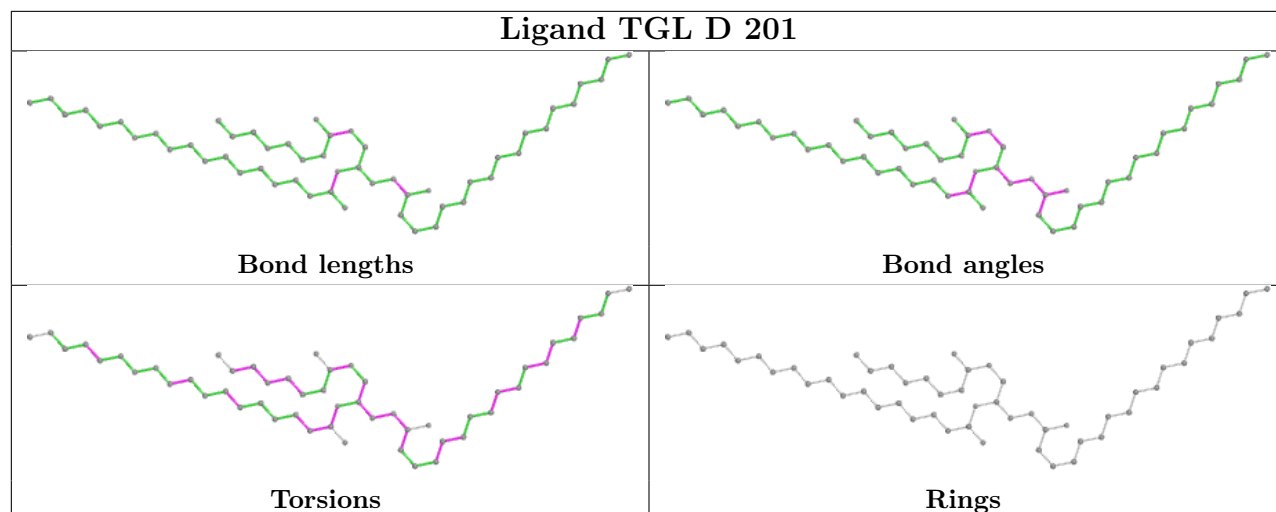


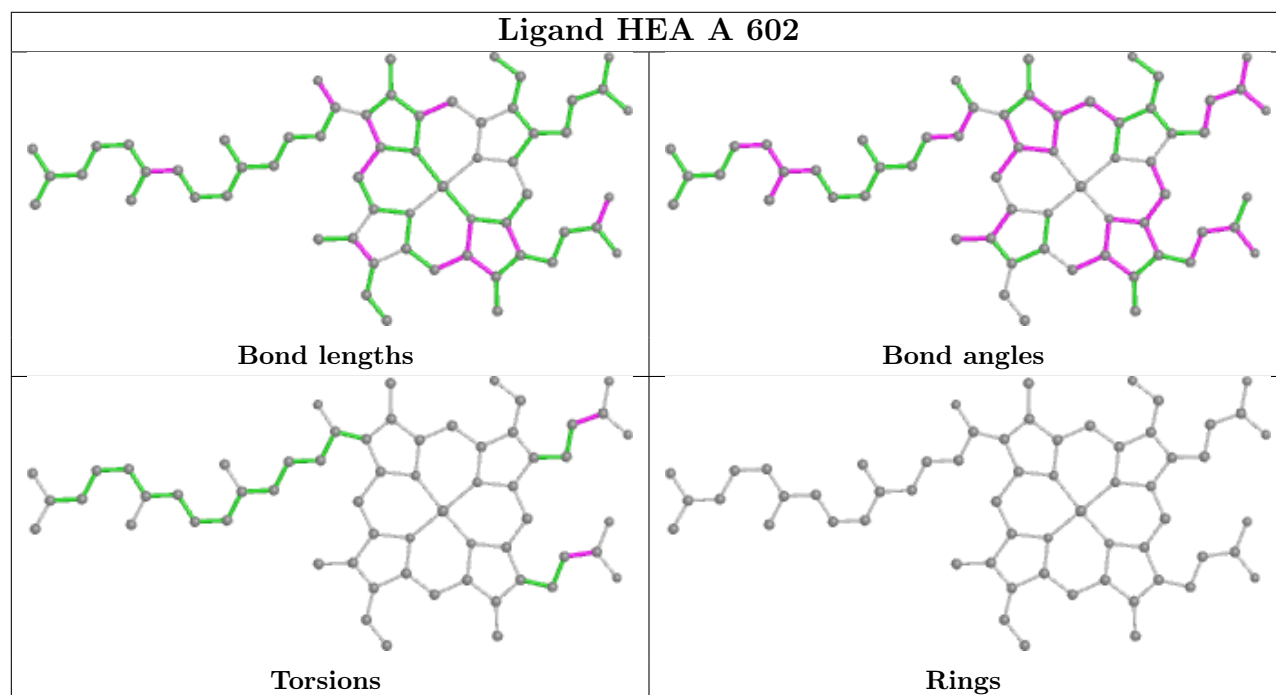
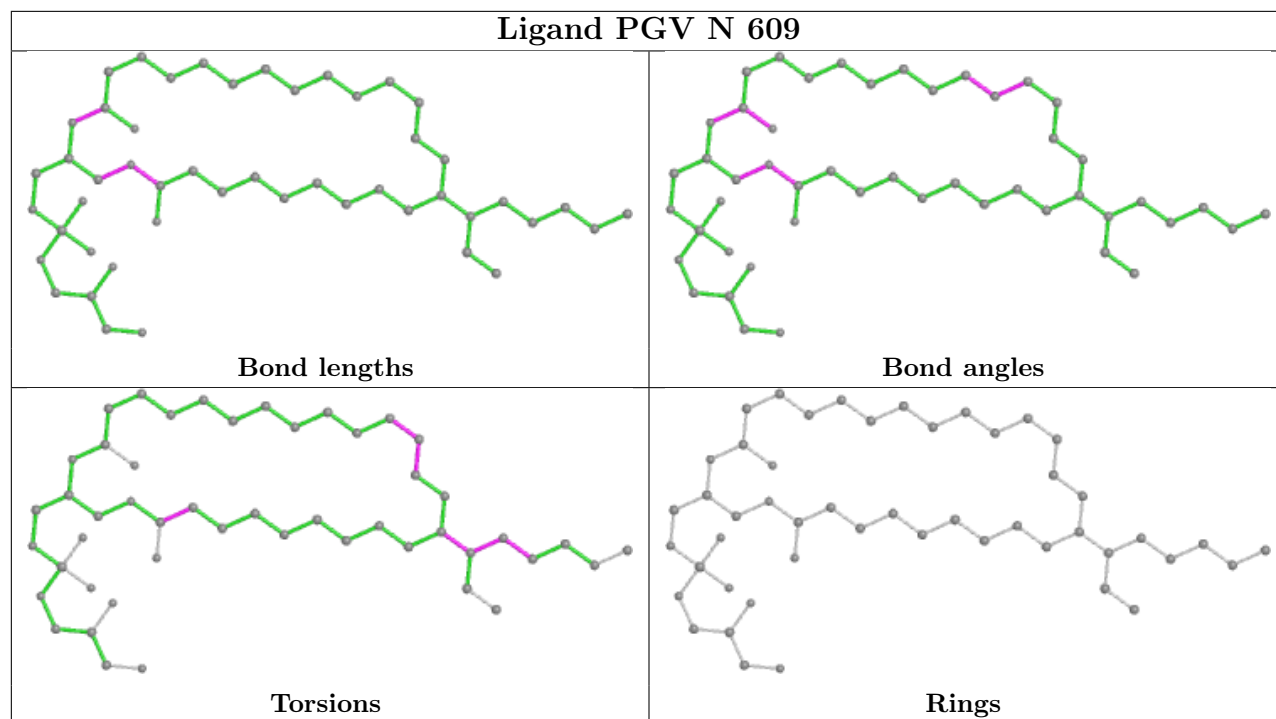


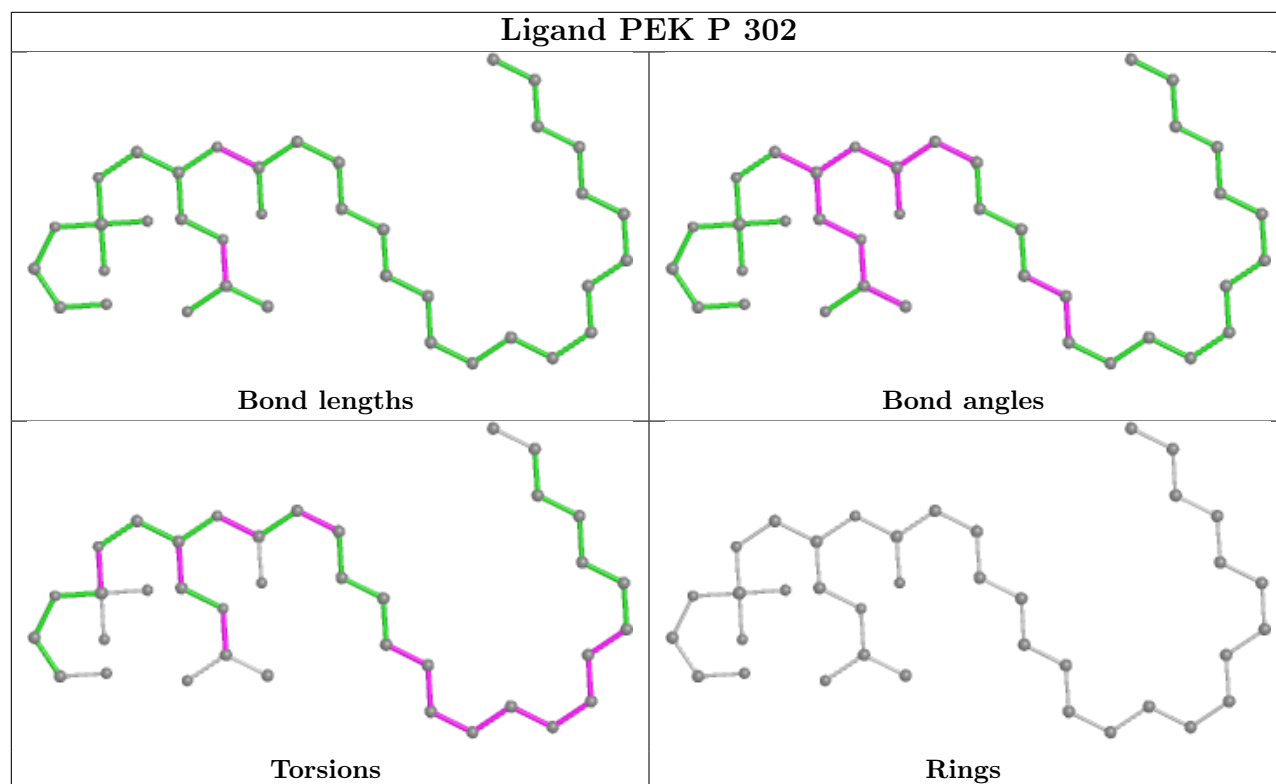
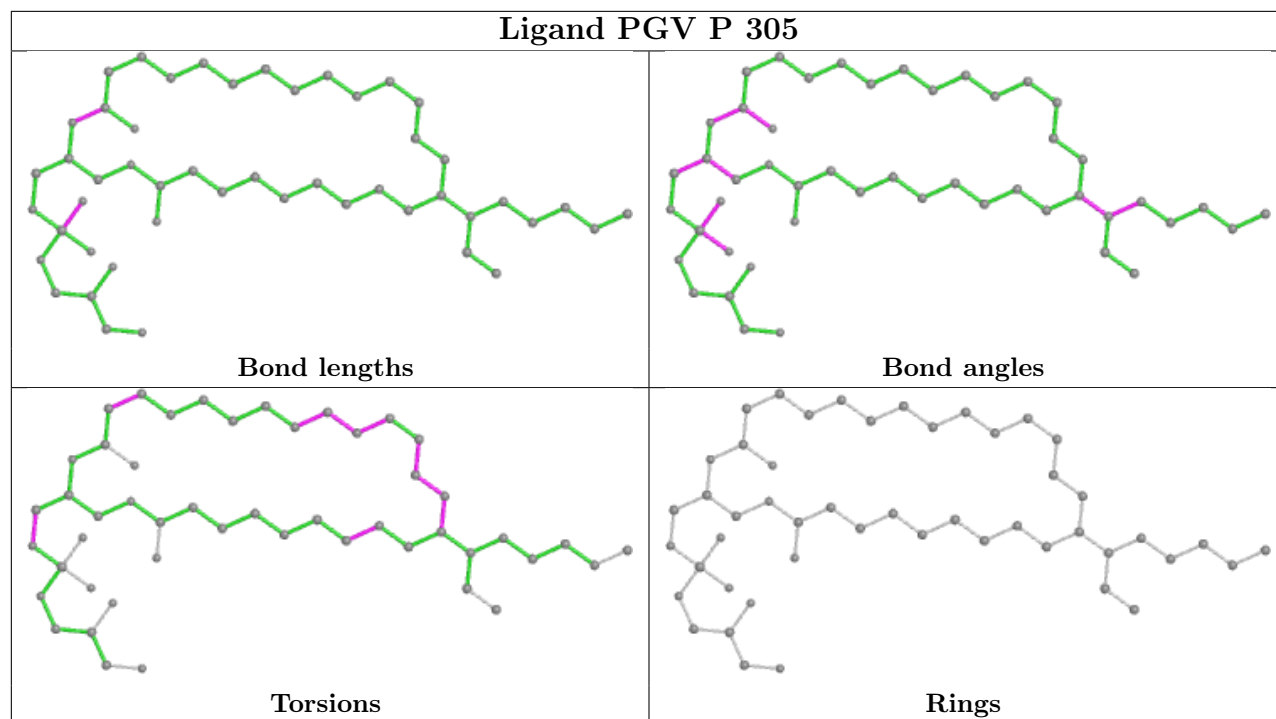


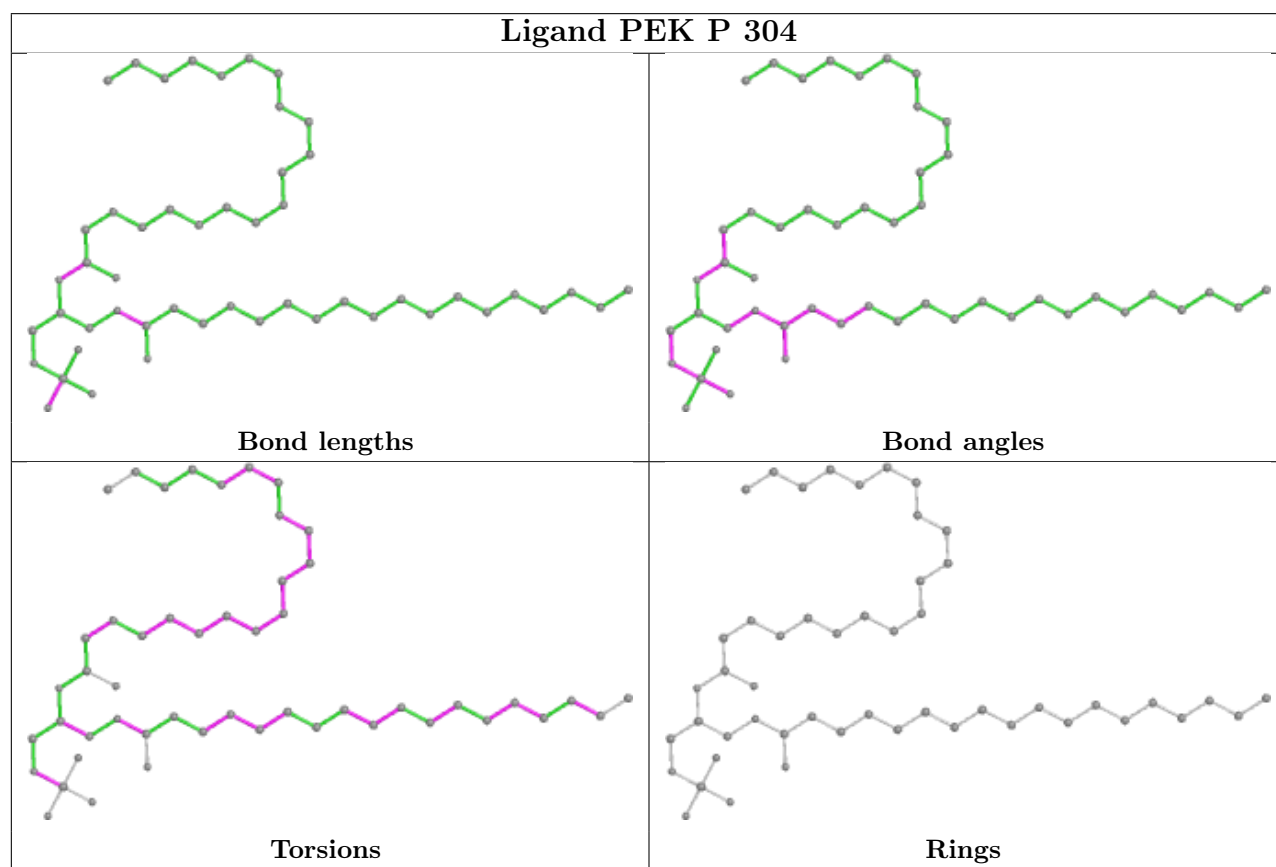
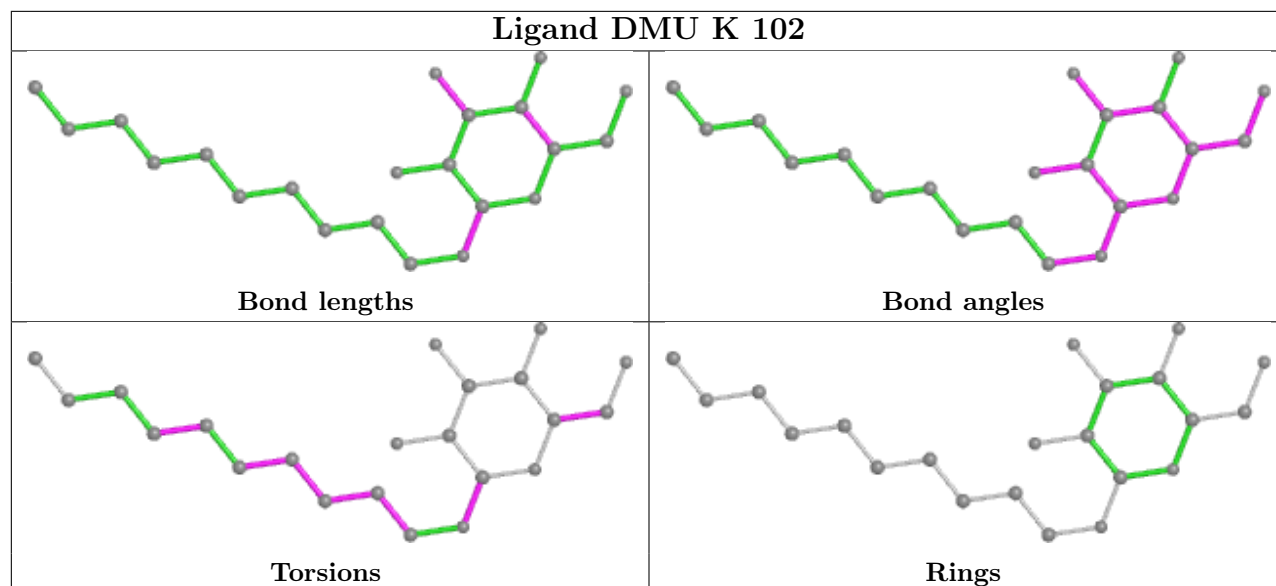


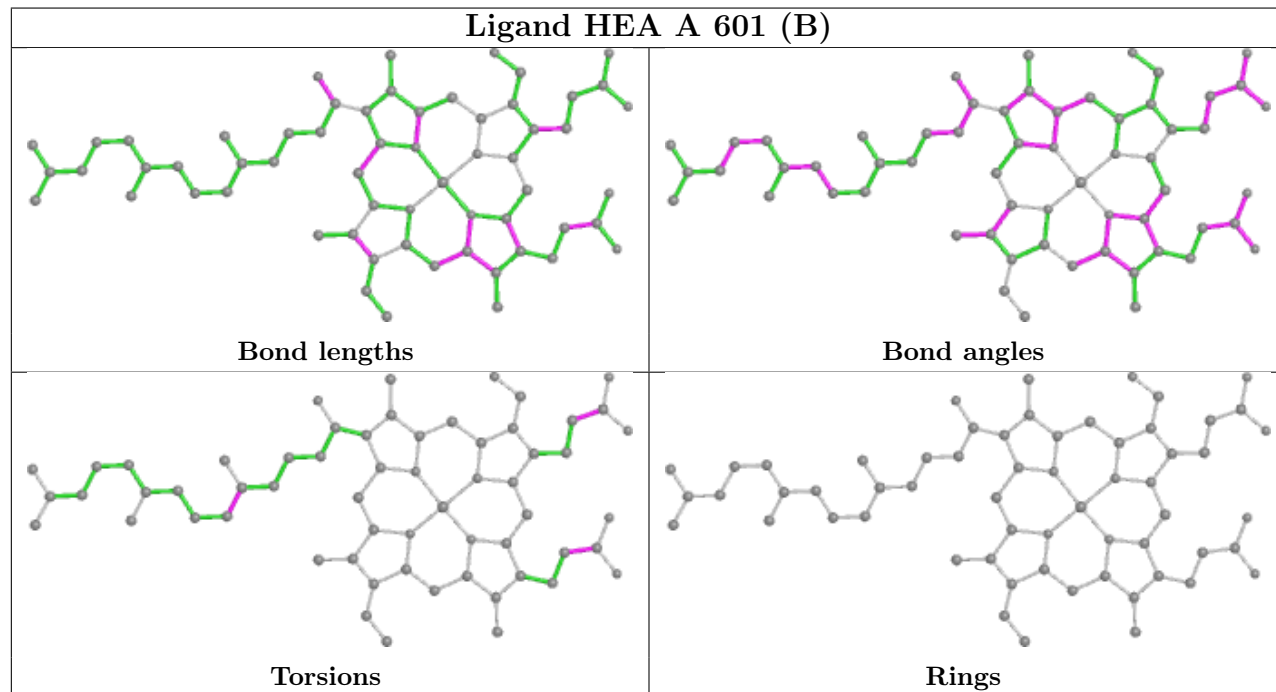
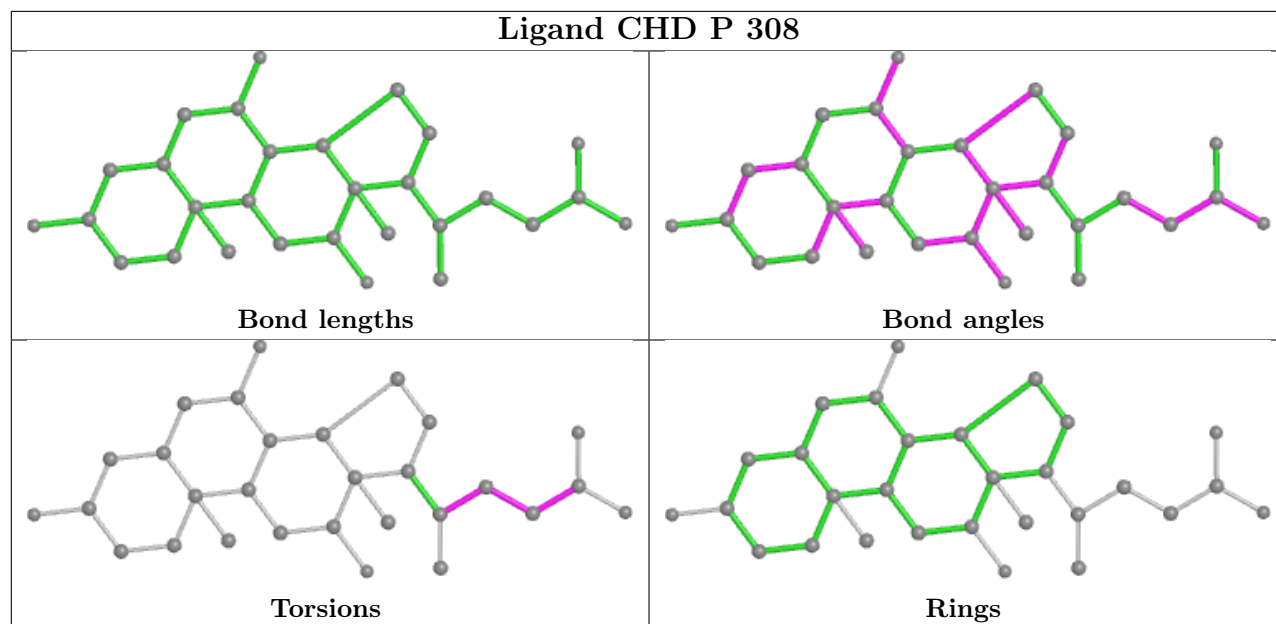


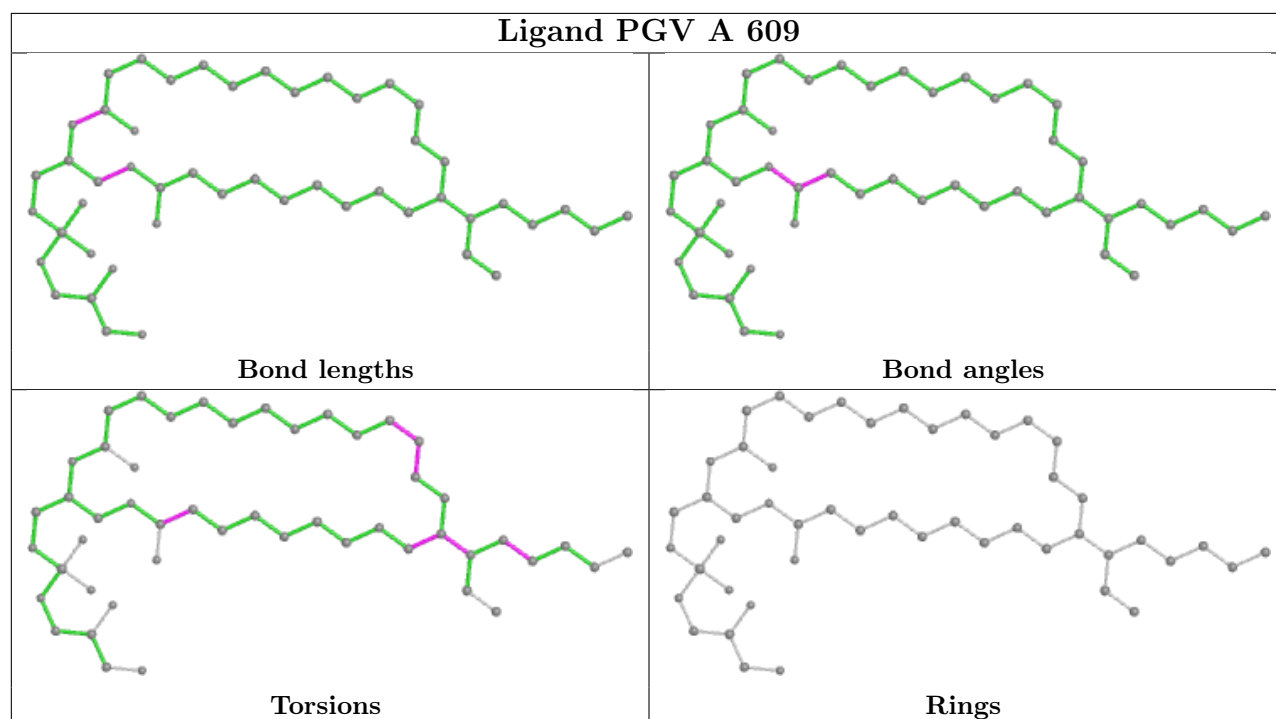
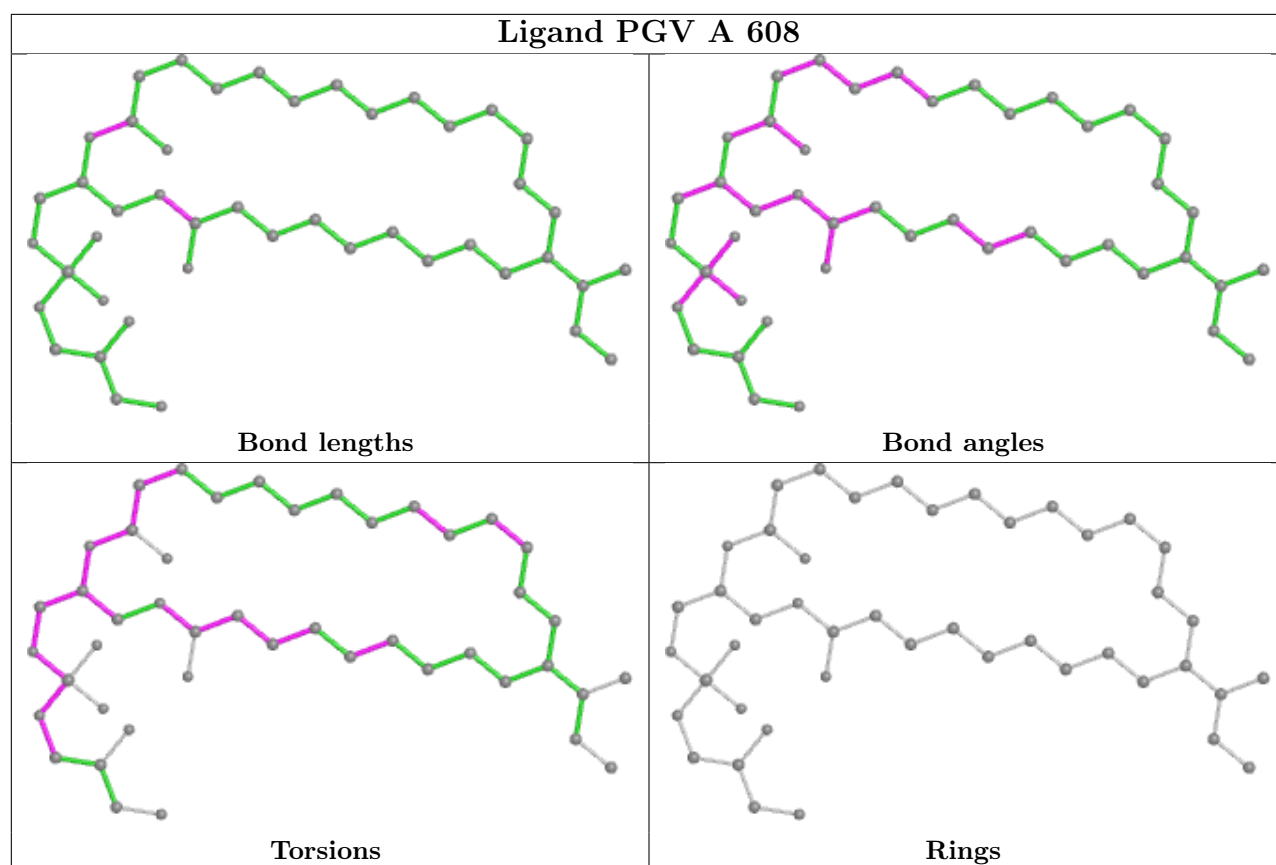




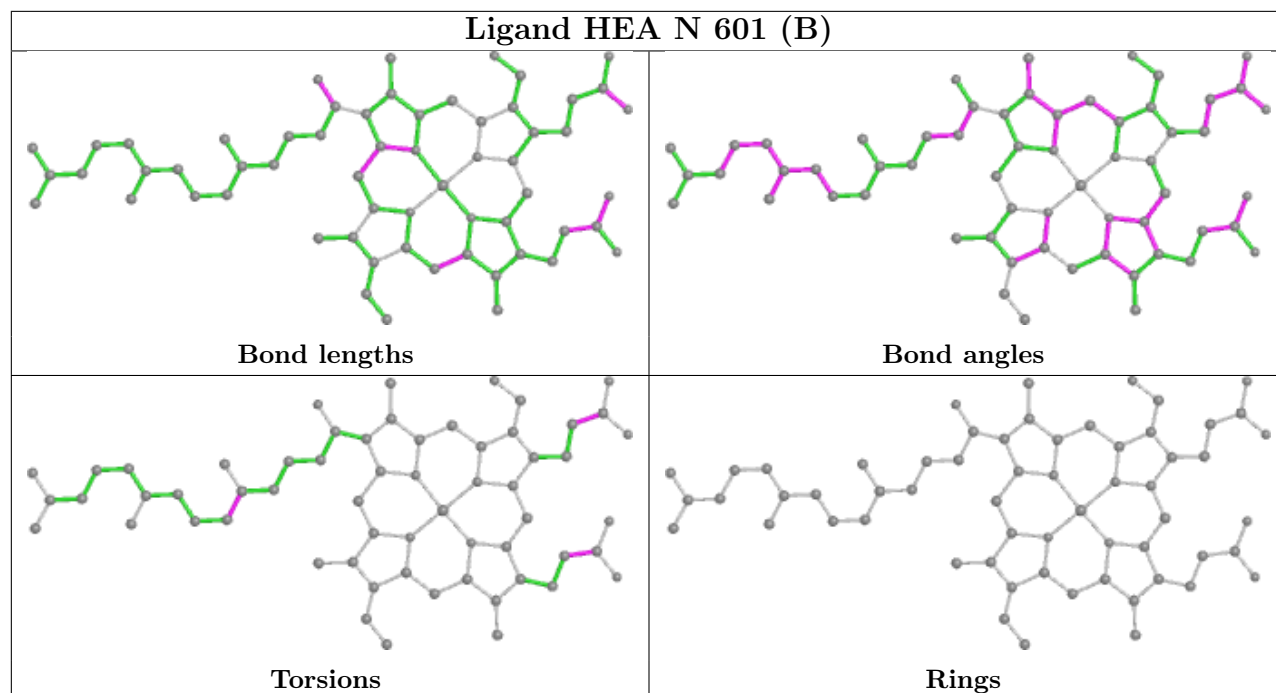




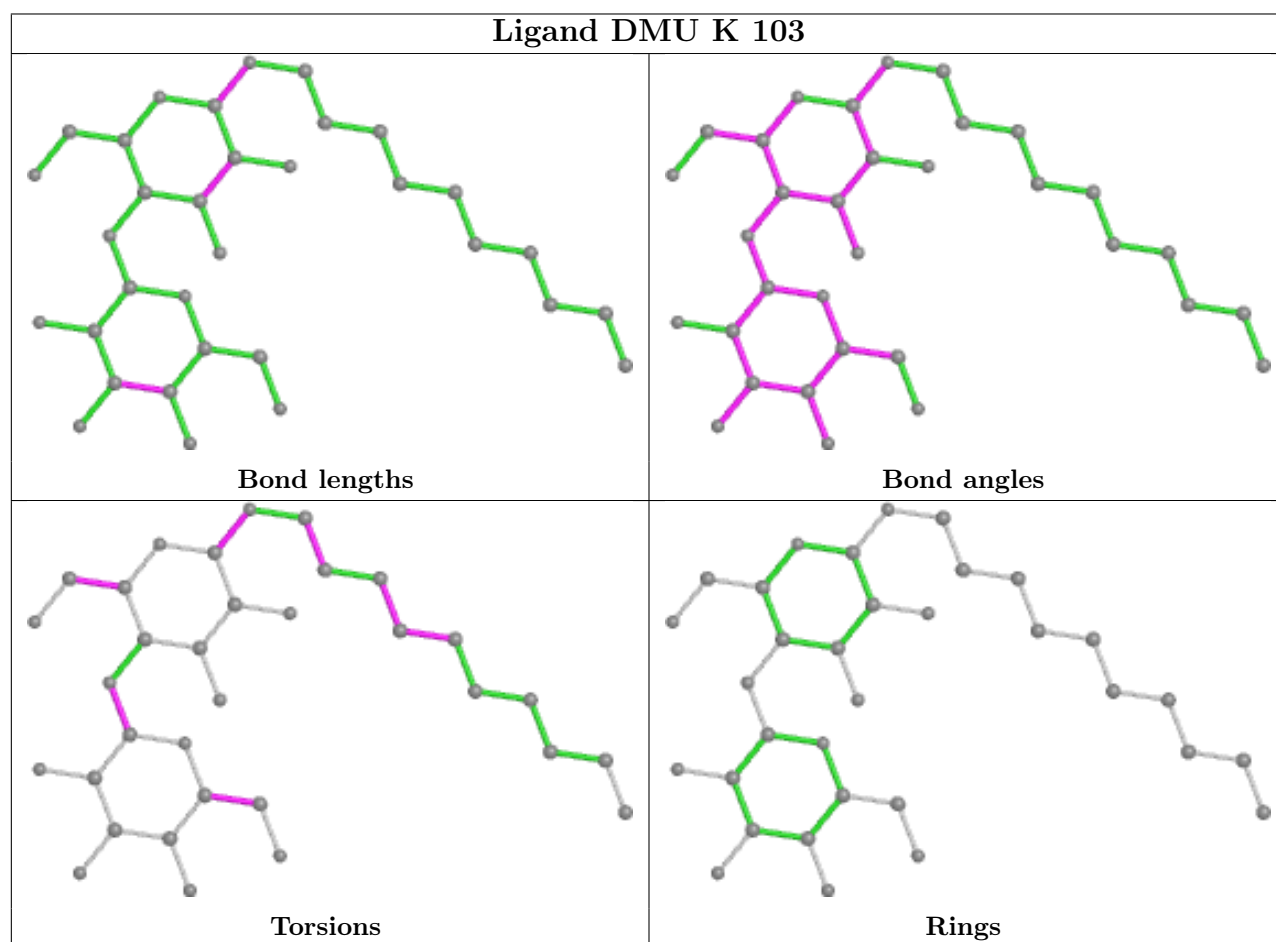


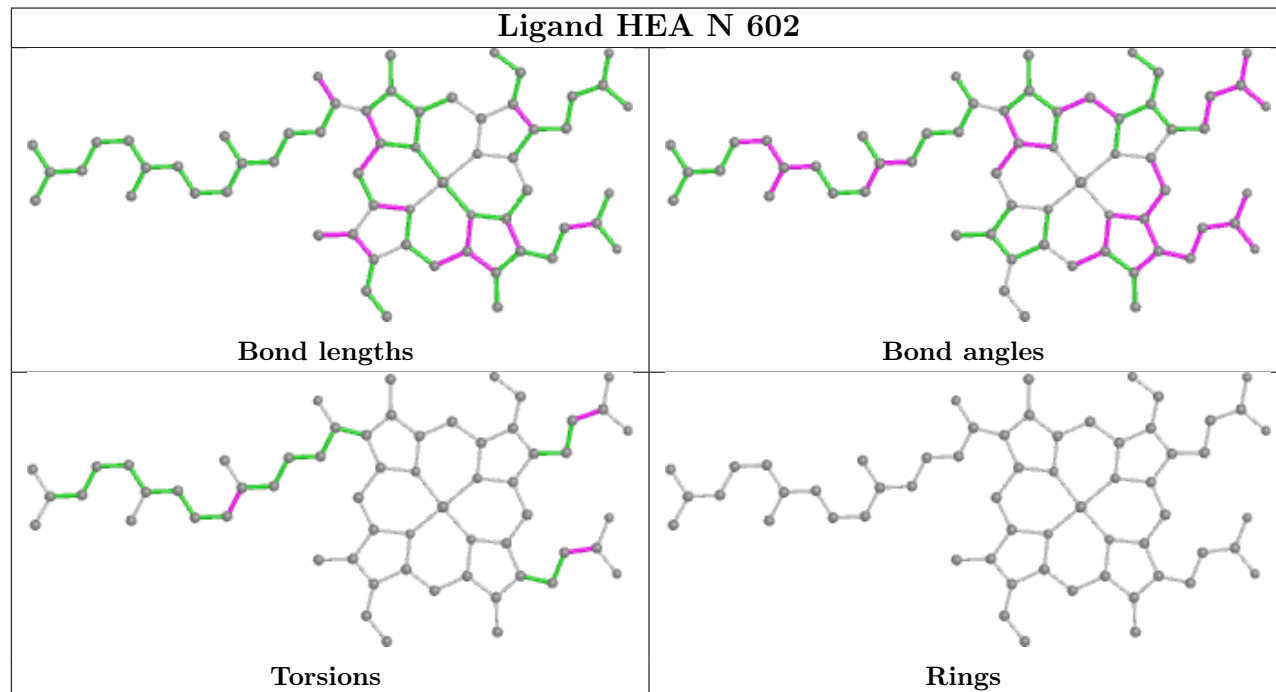
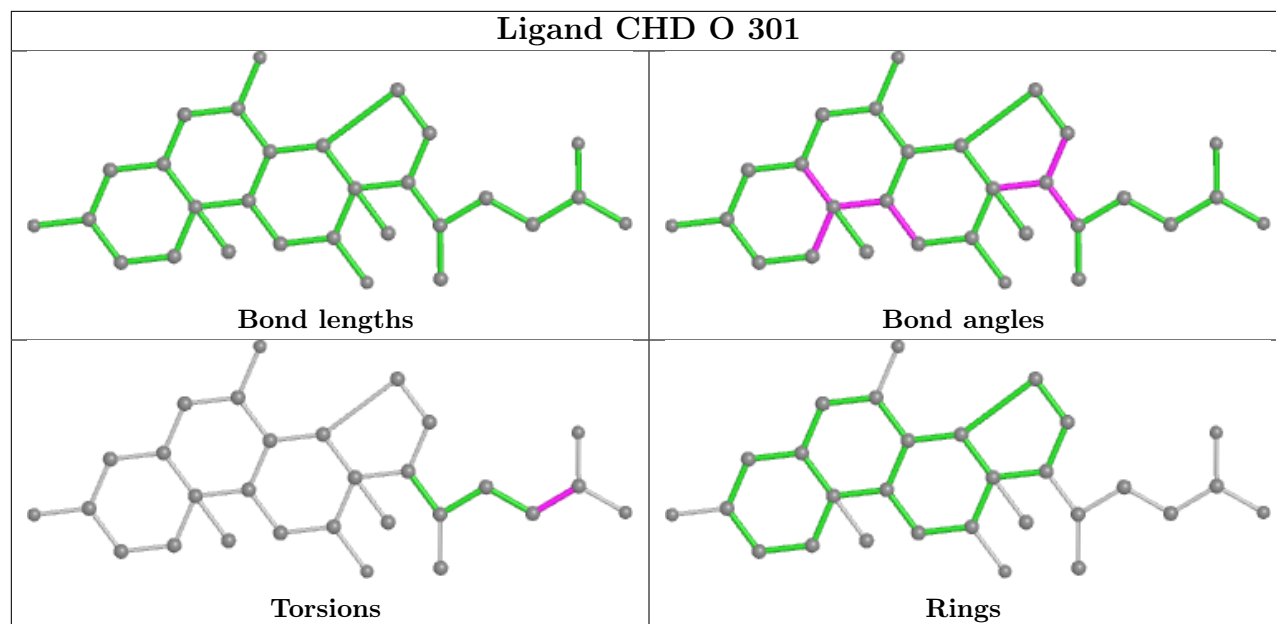


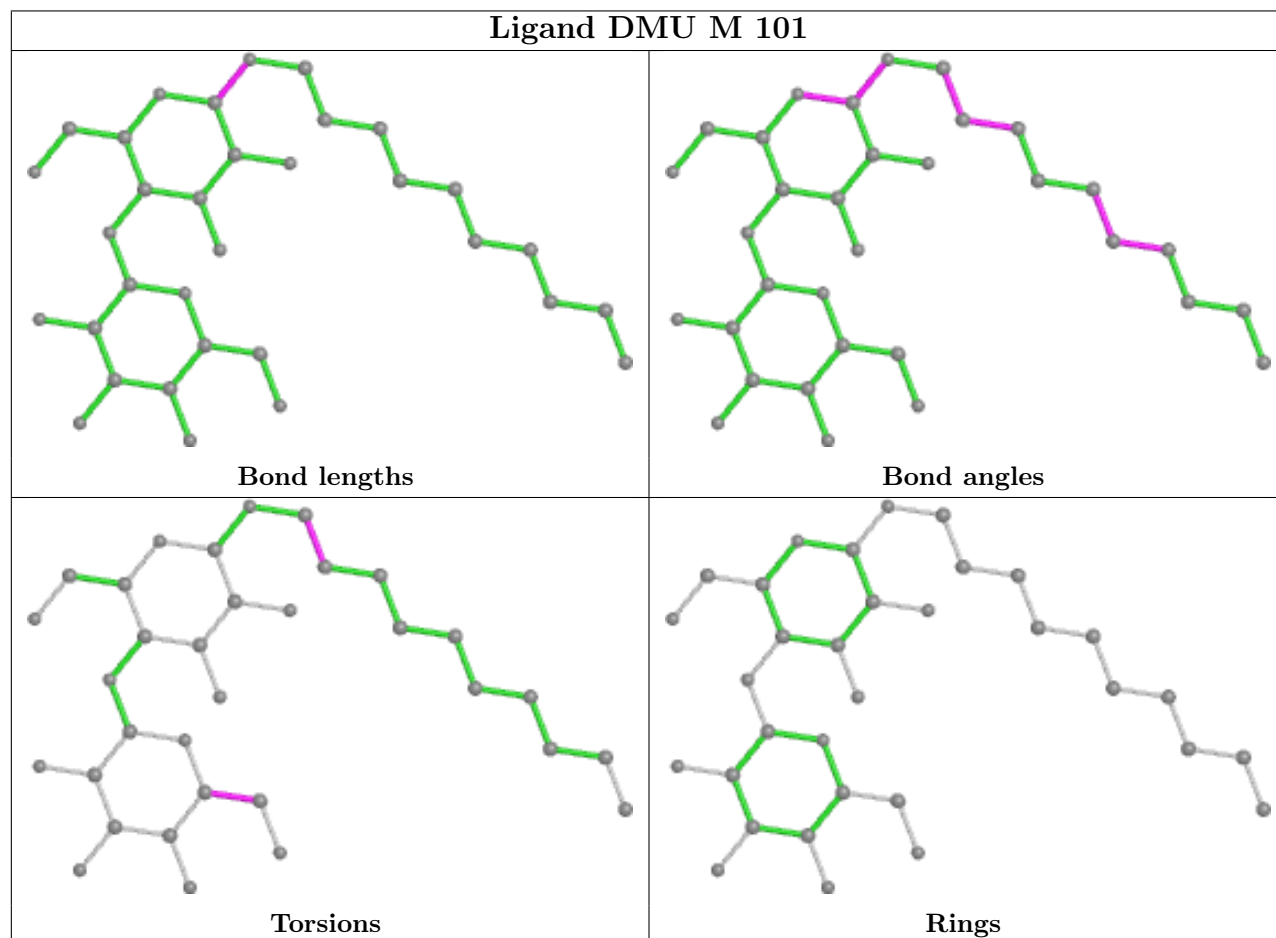
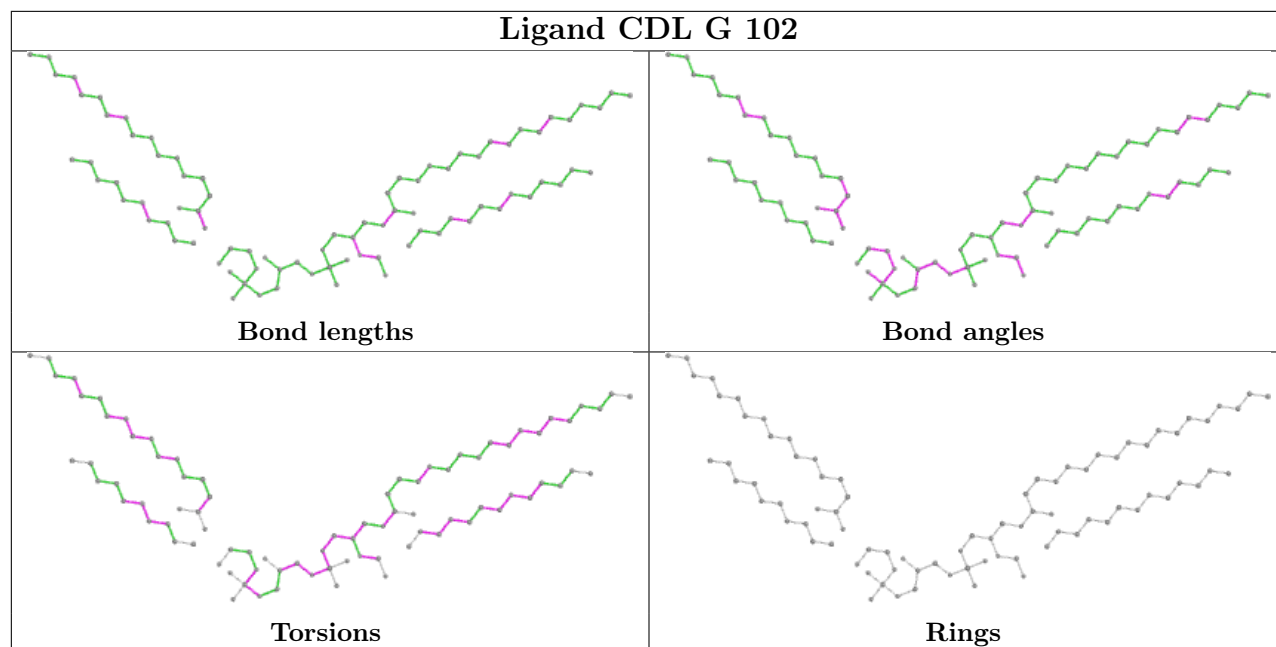
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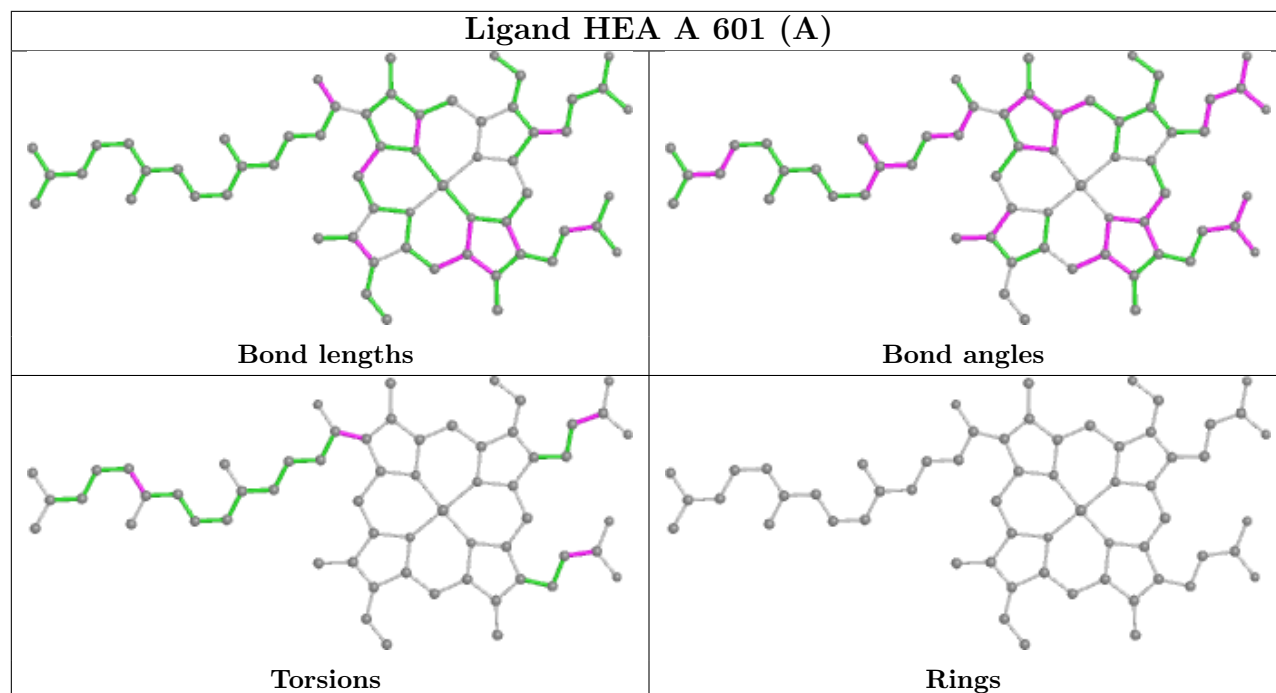
Ligand DMU K 103



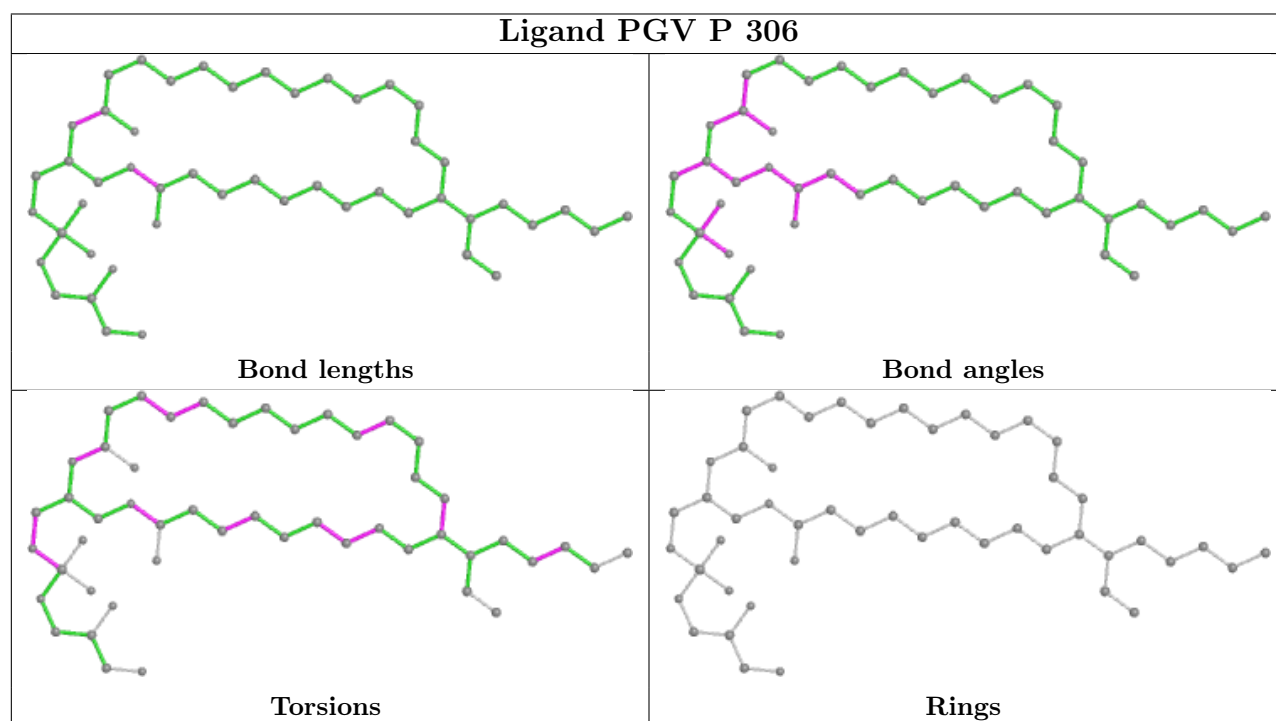




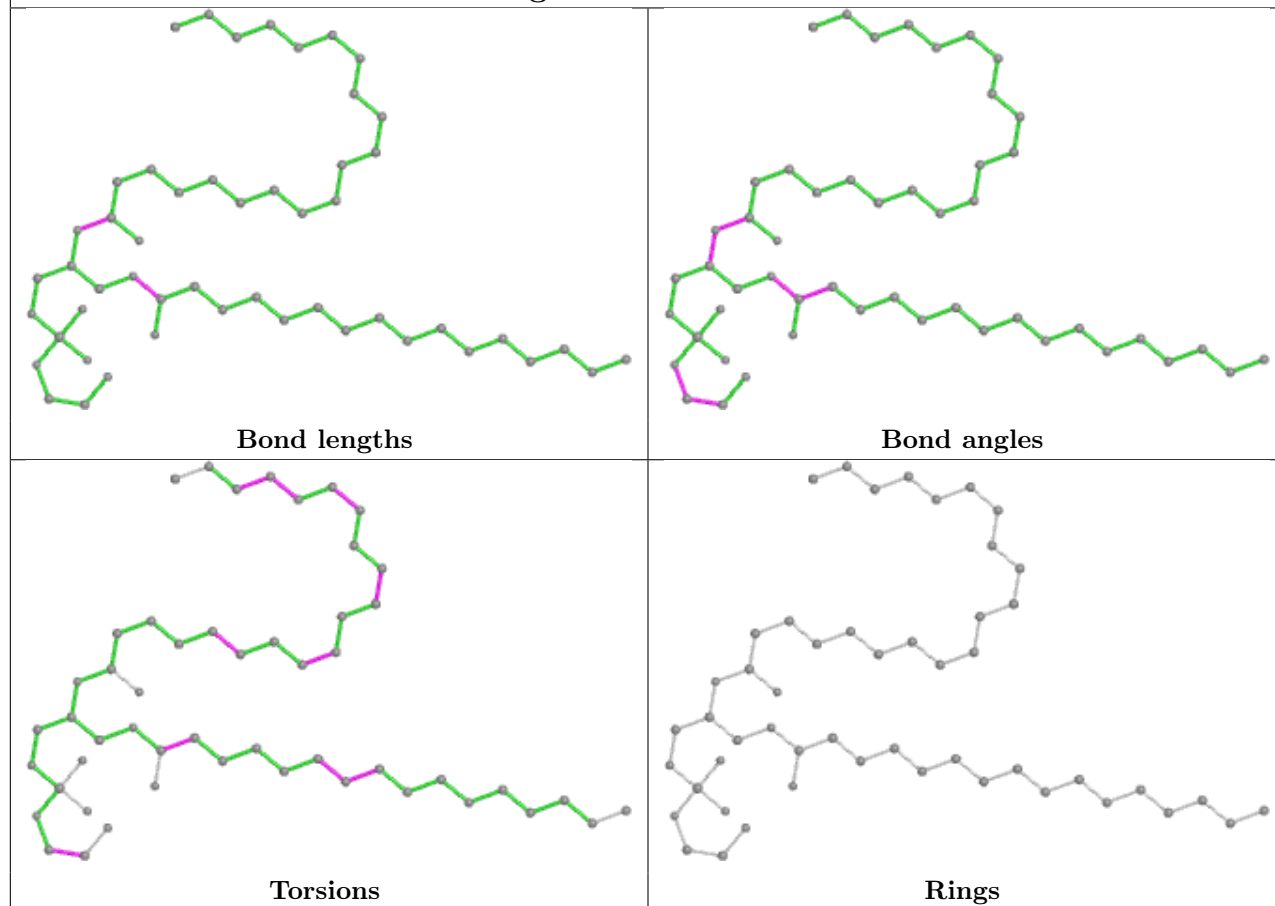
Ligand HEA A 601 (A)



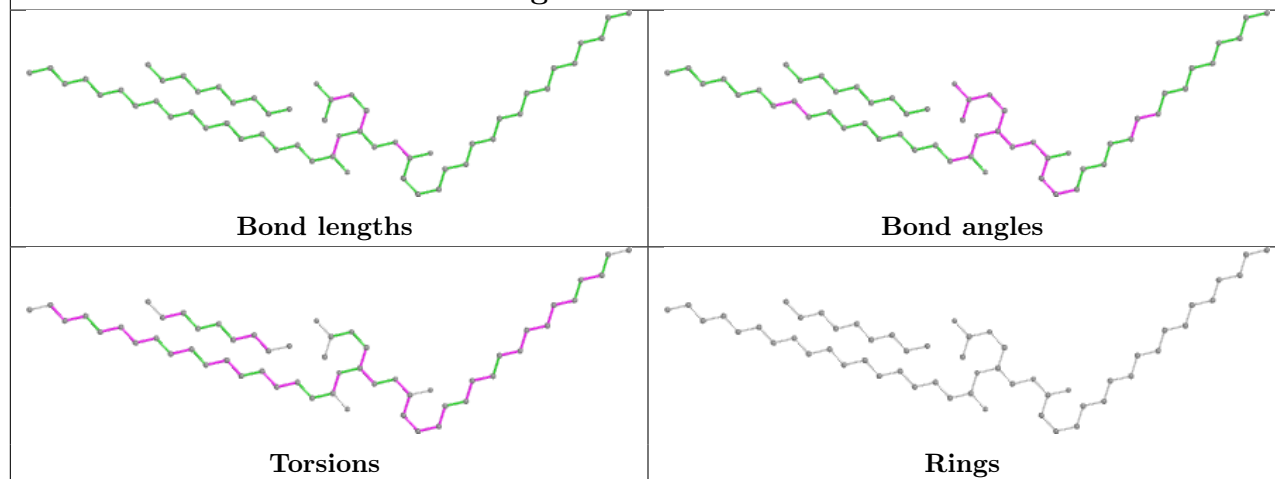
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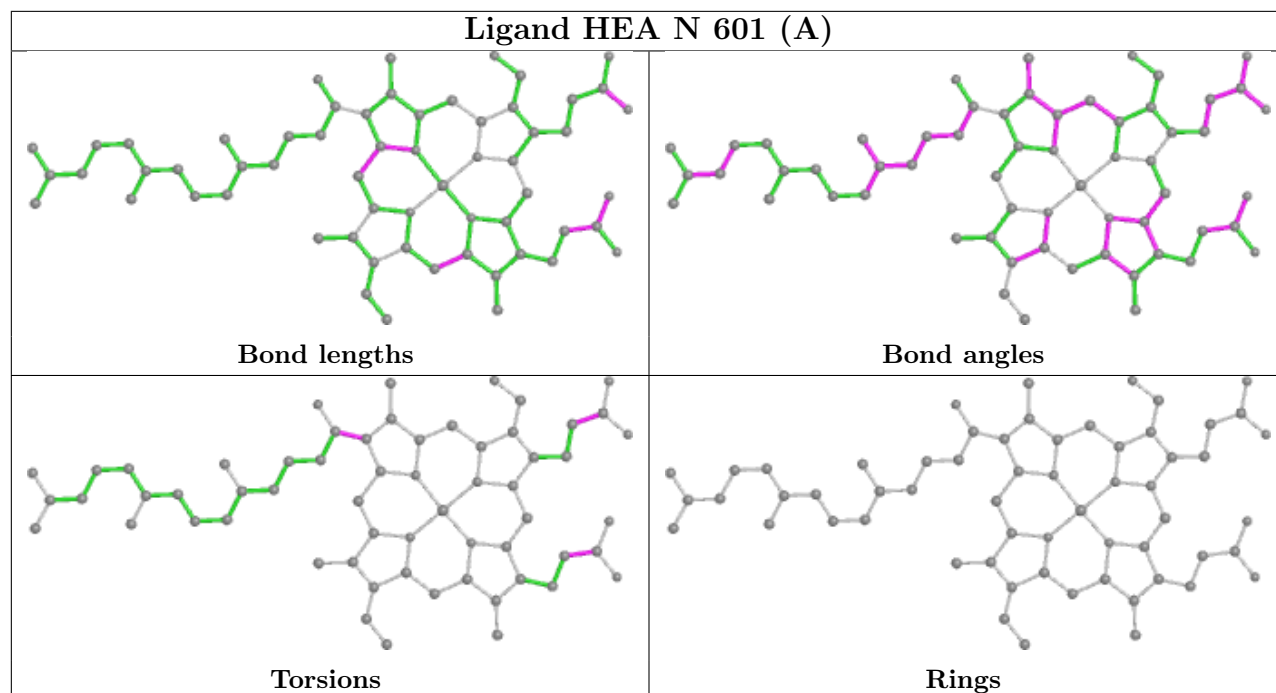
Ligand PEK G 101



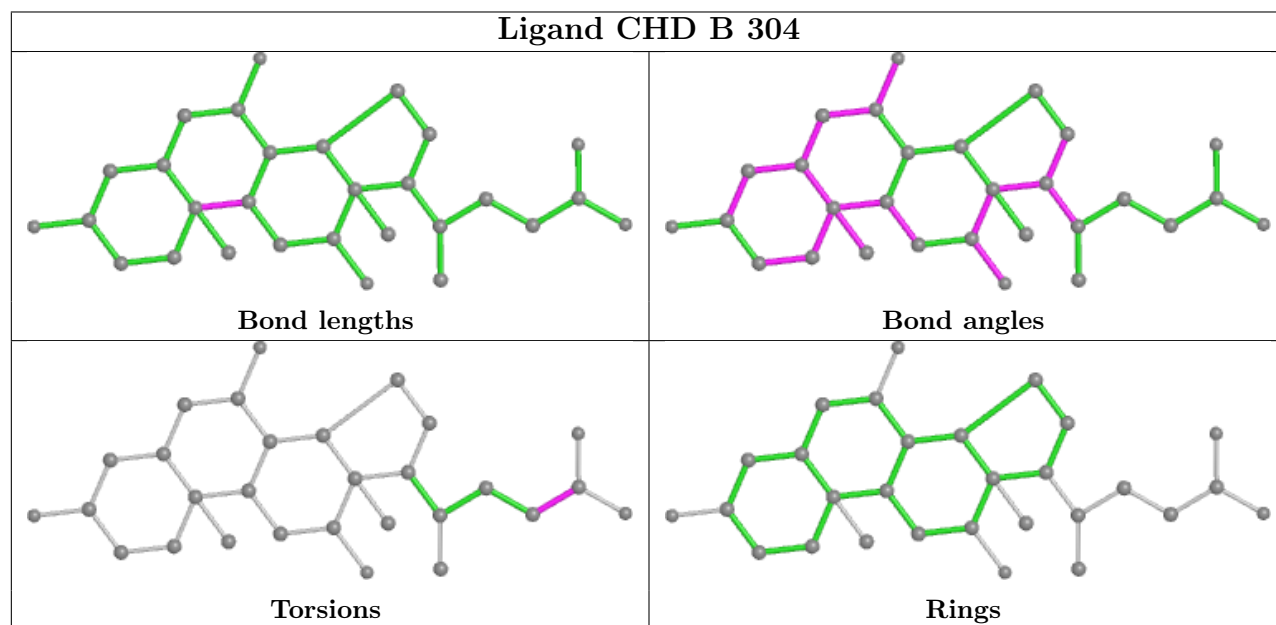
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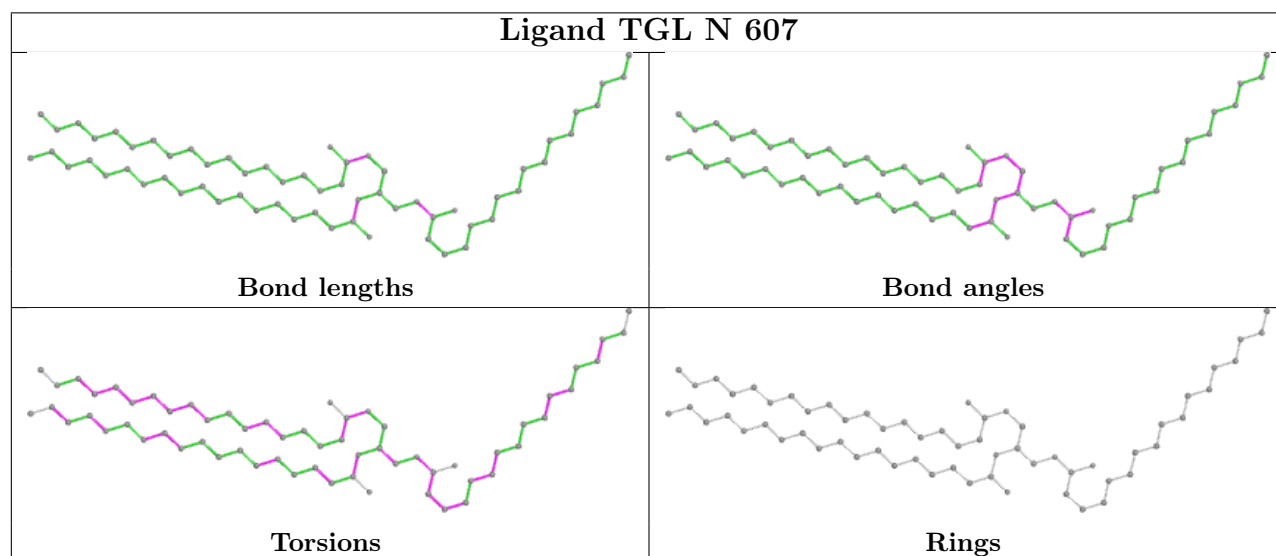
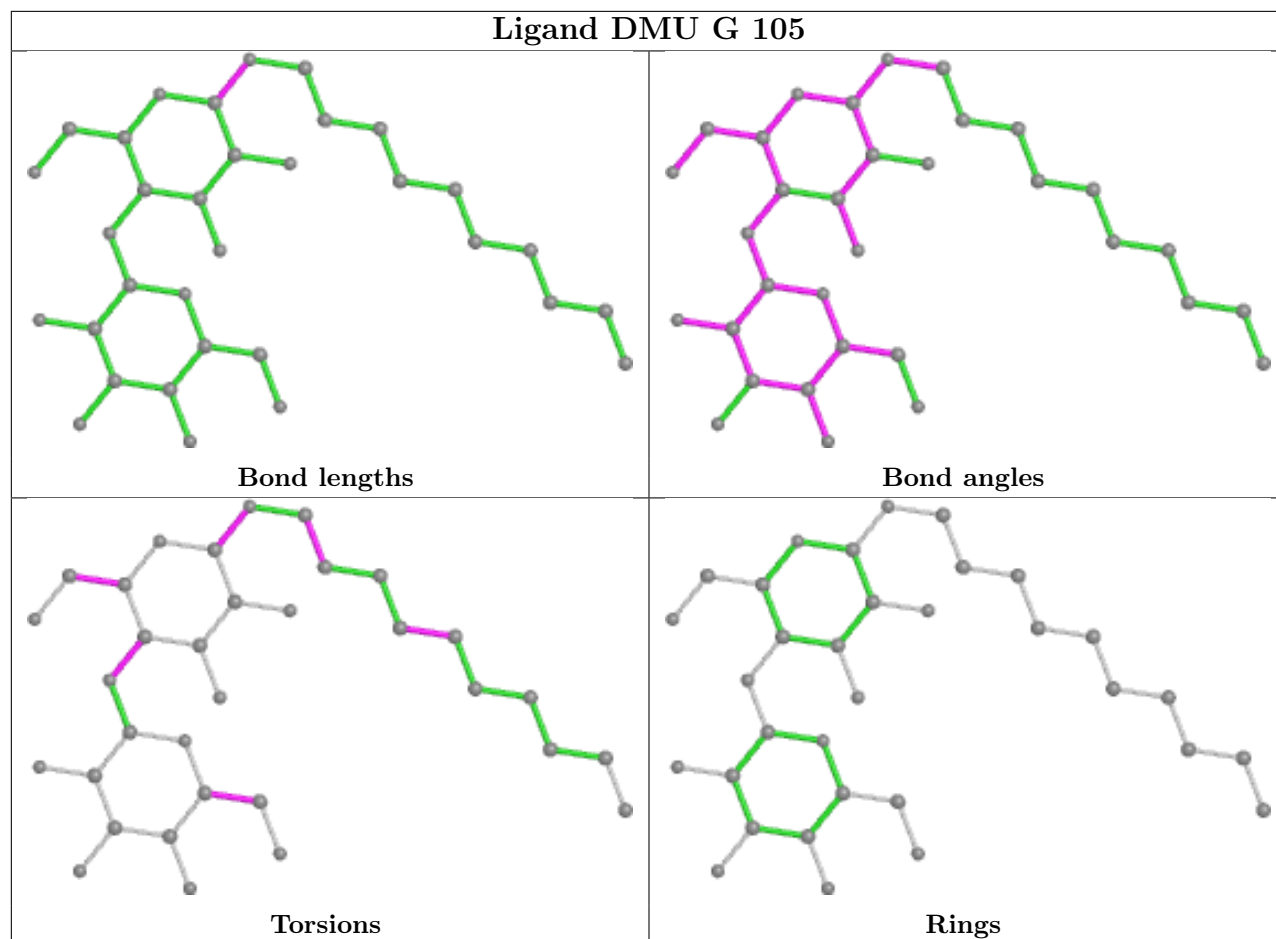


Ligand HEA N 601 (A)

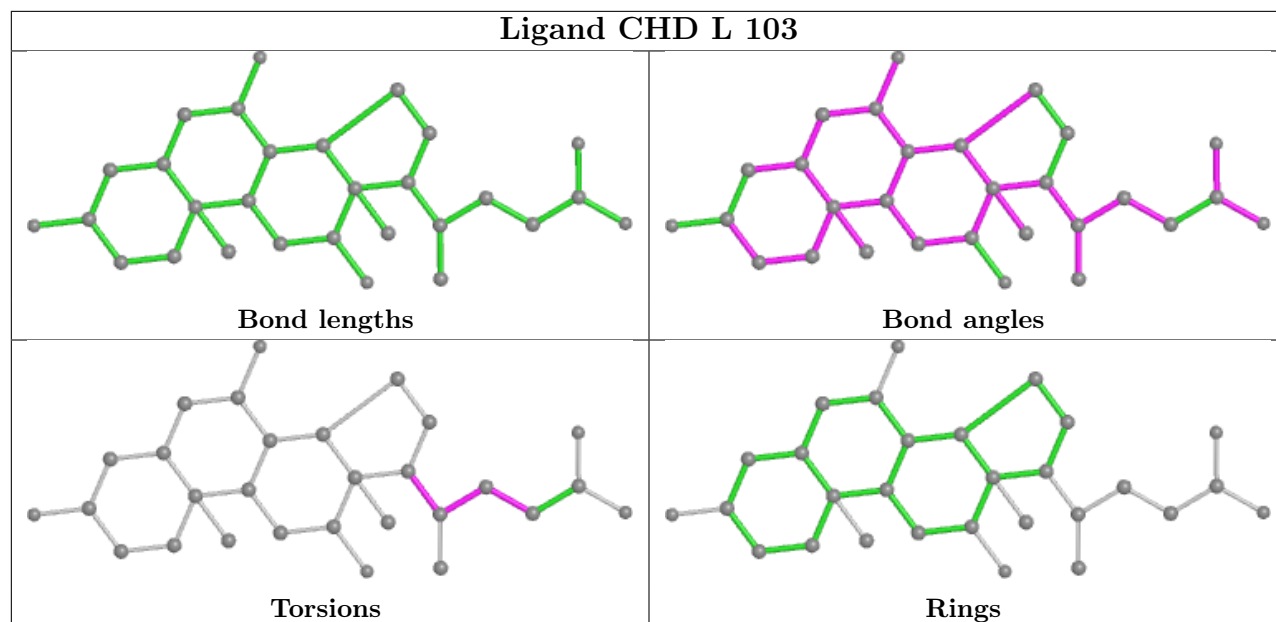


Ligand CHD B 304

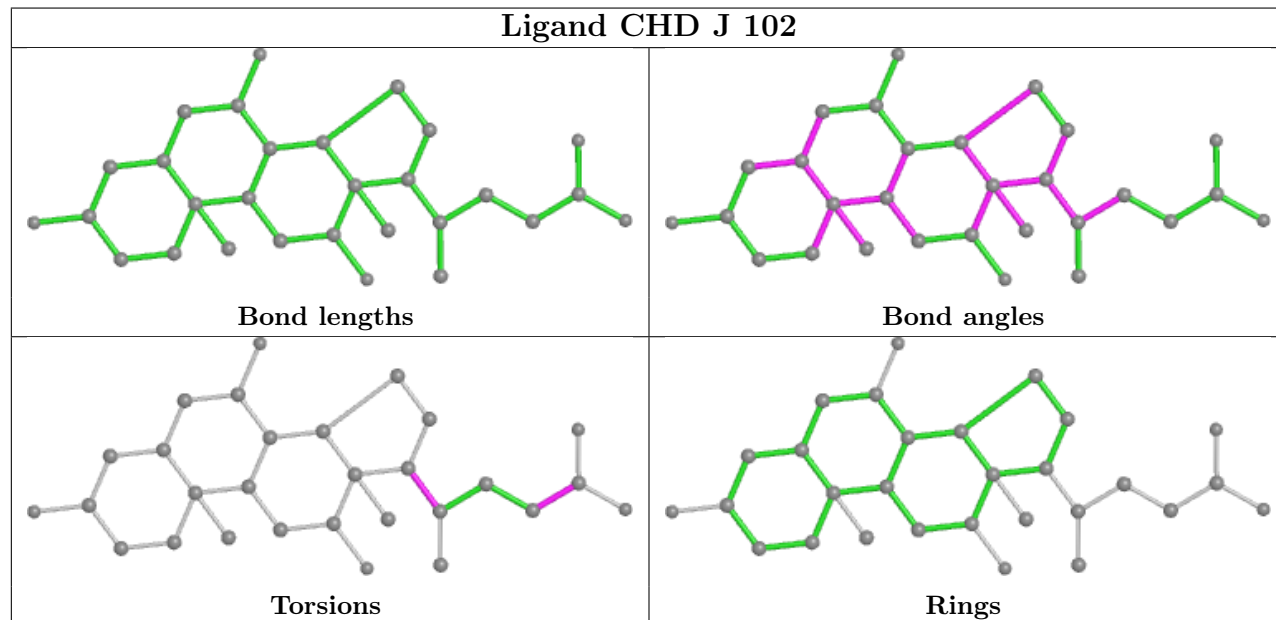


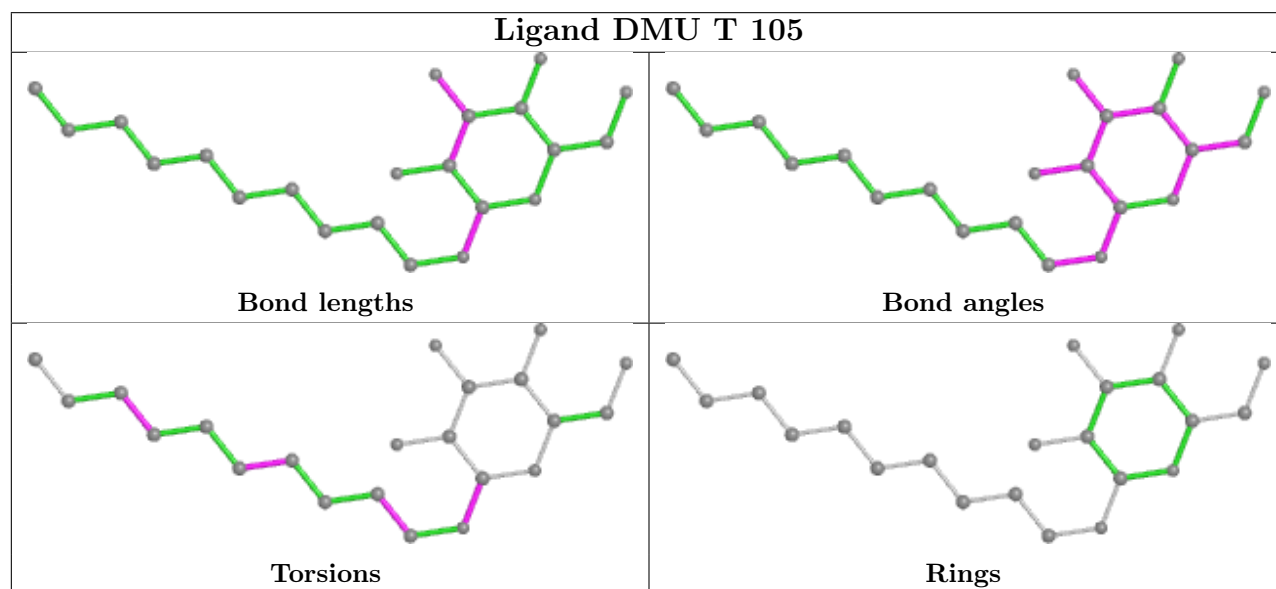
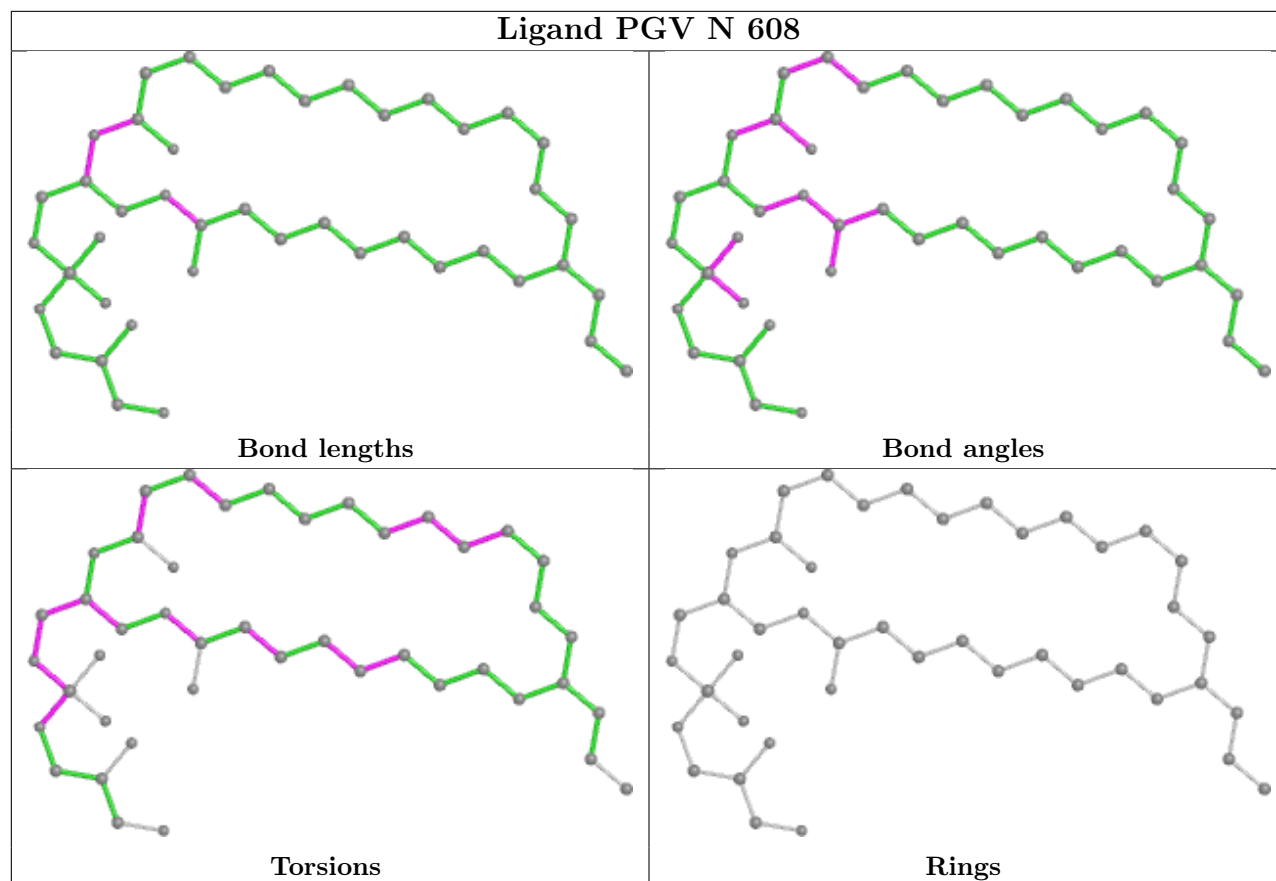


Ligand CHD L 103

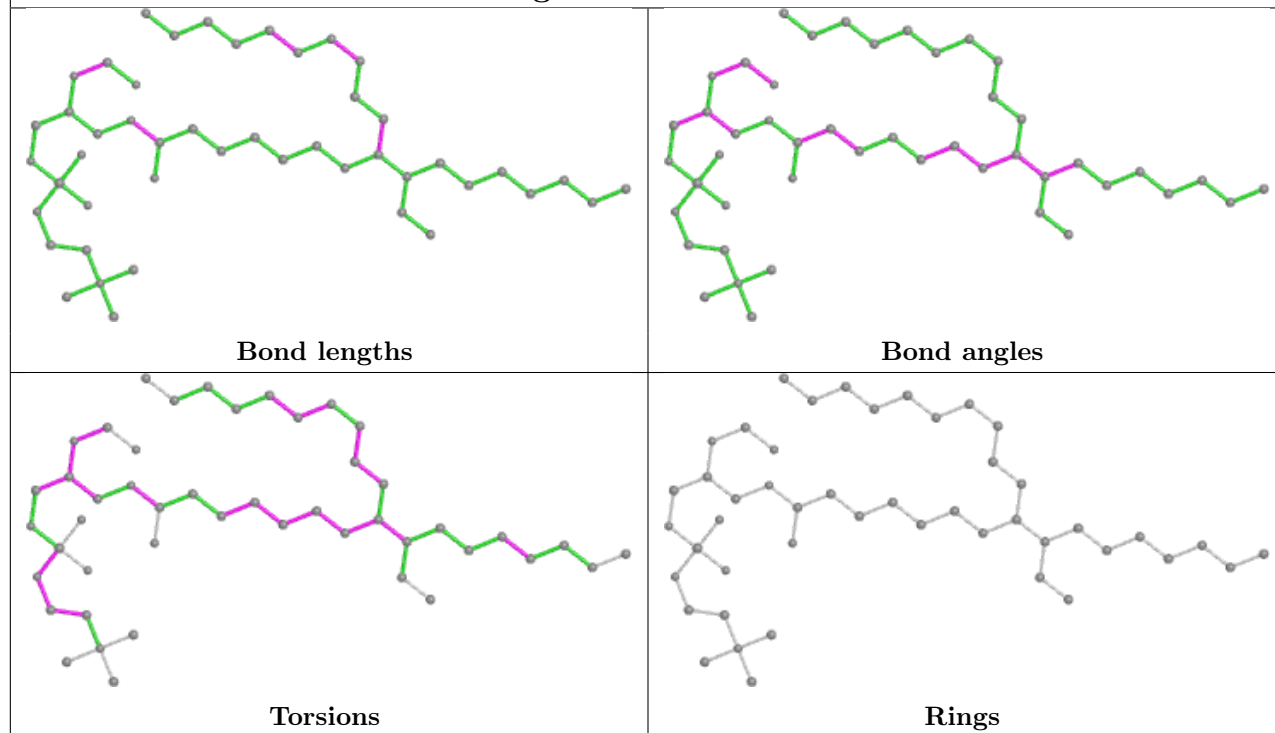


Ligand CHD J 102

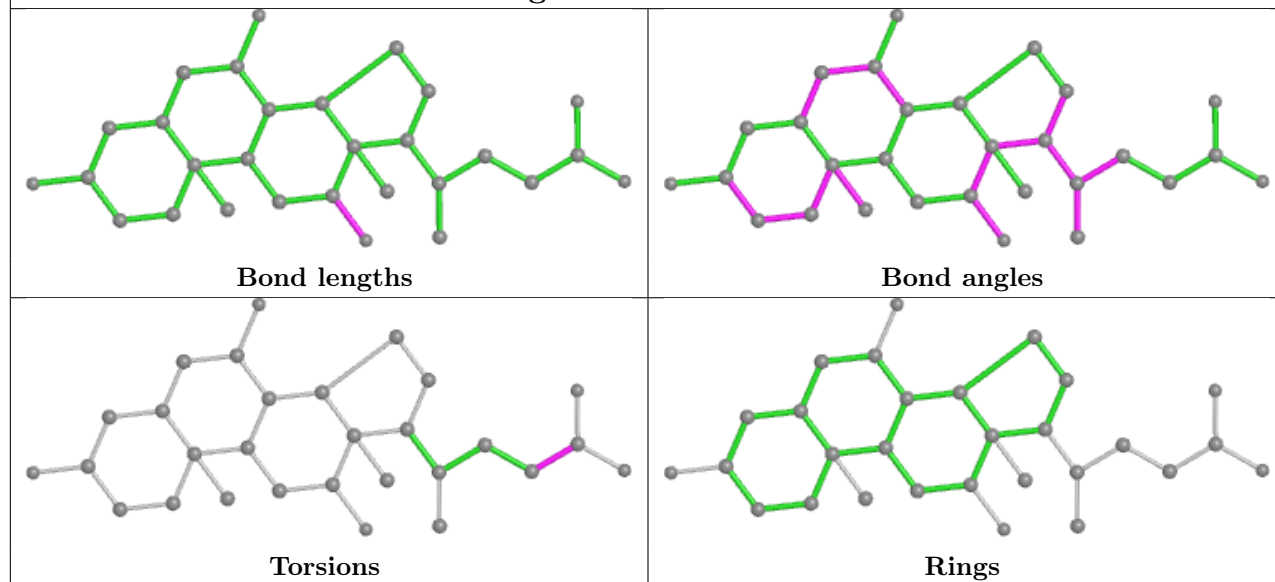


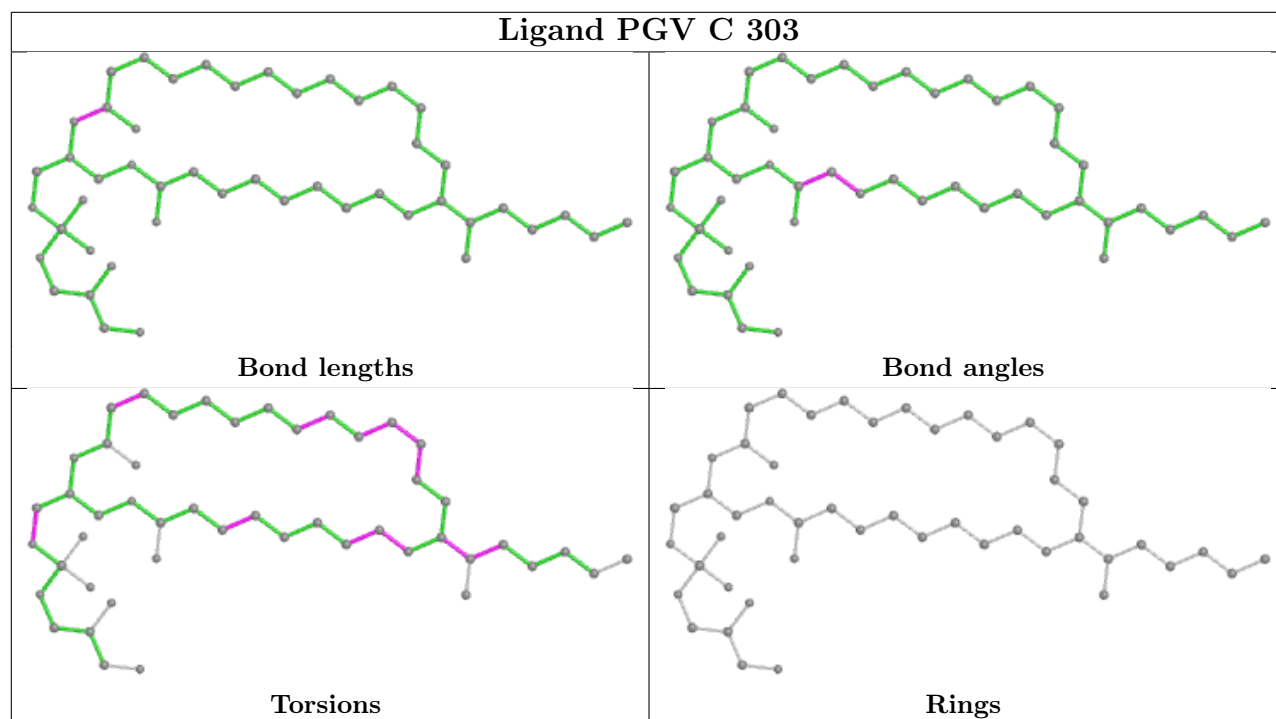
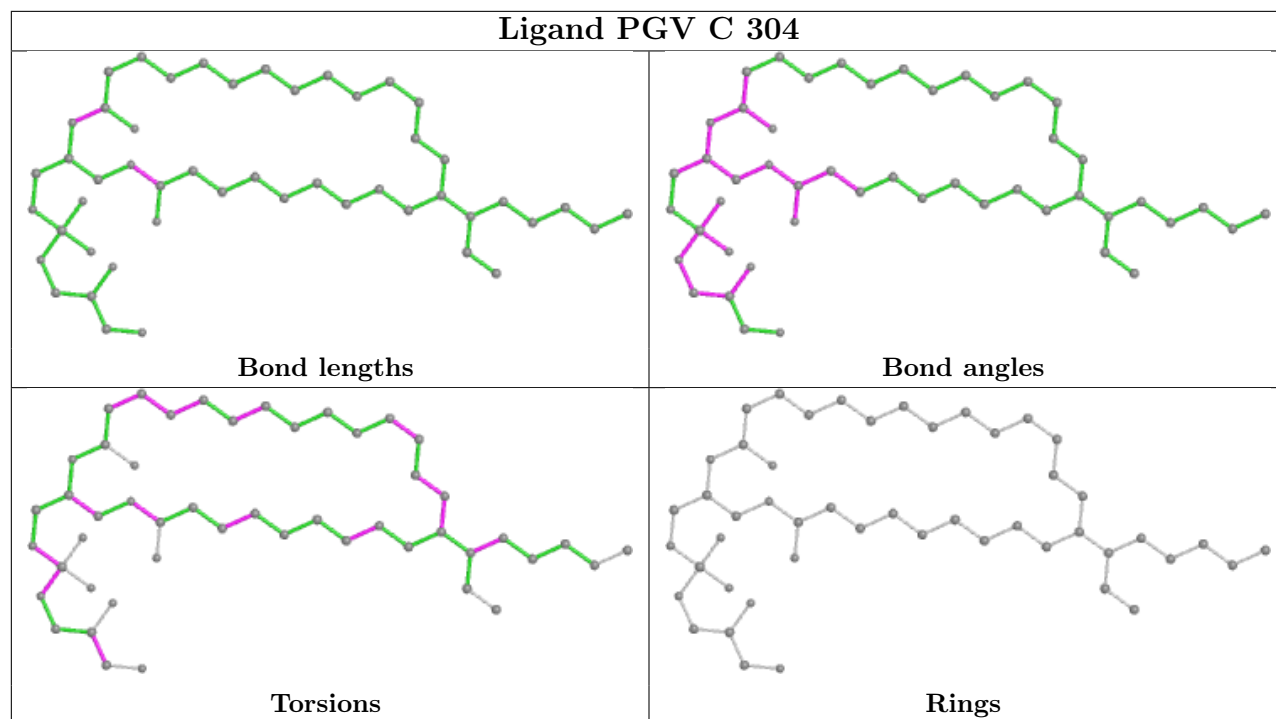


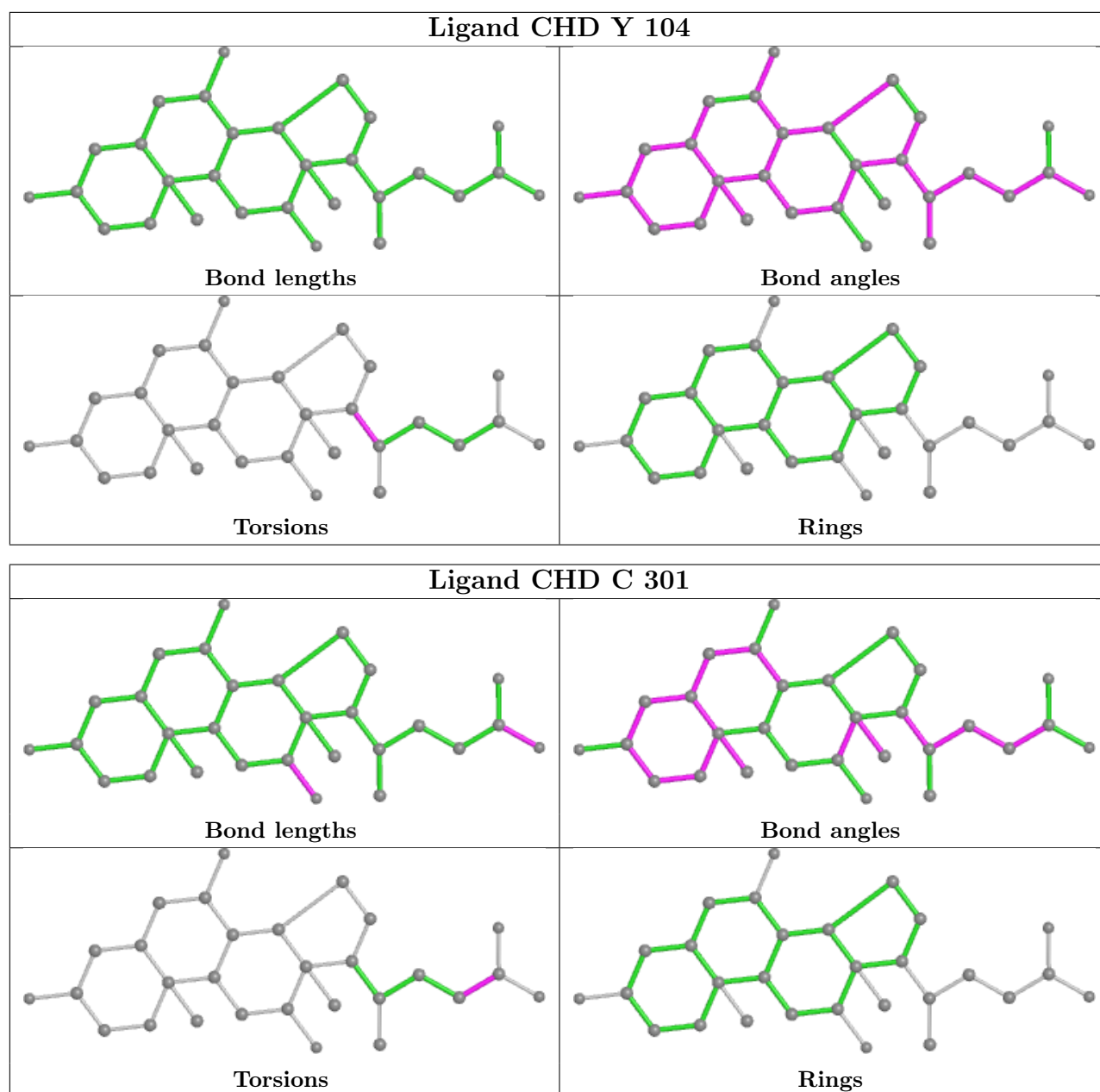
Ligand PSC R 201



Ligand CHD P 301







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%)	-0.36	0 100 100	19, 24, 32, 87	0
1	N	513/514 (99%)	-0.40	0 100 100	20, 27, 36, 84	0
2	B	226/227 (99%)	-0.37	5 (2%) 62 63	23, 31, 49, 116	0
2	O	226/227 (99%)	-0.34	3 (1%) 77 80	26, 36, 64, 130	0
3	C	259/259 (100%)	-0.37	0 100 100	21, 27, 39, 74	0
3	P	259/259 (100%)	-0.37	1 (0%) 92 93	21, 27, 40, 93	0
4	D	144/144 (100%)	-0.49	1 (0%) 87 89	26, 33, 56, 87	0
4	Q	144/144 (100%)	0.38	7 (4%) 29 28	32, 46, 83, 183	0
5	E	105/105 (100%)	-0.51	2 (1%) 66 69	26, 32, 60, 149	0
5	R	105/105 (100%)	-0.45	2 (1%) 66 69	27, 38, 64, 156	0
6	F	94/94 (100%)	-0.32	4 (4%) 35 34	23, 33, 59, 158	0
6	S	93/94 (98%)	-0.30	2 (2%) 62 63	23, 32, 58, 178	0
7	G	83/84 (98%)	0.55	14 (16%) 1 1	25, 36, 123, 171	0
7	T	83/84 (98%)	0.57	15 (18%) 1 1	24, 37, 120, 191	0
8	H	79/79 (100%)	0.02	7 (8%) 9 8	28, 38, 104, 125	0
8	U	79/79 (100%)	-0.00	6 (7%) 13 13	32, 42, 120, 165	0
9	I	72/73 (98%)	-0.05	3 (4%) 36 35	28, 42, 80, 95	0
9	V	72/73 (98%)	-0.01	3 (4%) 36 35	29, 51, 76, 179	0
10	J	58/58 (100%)	-0.14	5 (8%) 10 10	26, 37, 71, 114	0
10	W	58/58 (100%)	-0.23	2 (3%) 45 45	28, 40, 74, 185	0
11	K	49/49 (100%)	-0.48	0 100 100	30, 37, 54, 58	0
11	X	49/49 (100%)	-0.10	1 (2%) 65 67	36, 46, 68, 89	0
12	L	46/46 (100%)	-0.33	2 (4%) 35 34	24, 29, 51, 112	0
12	Y	46/46 (100%)	-0.41	1 (2%) 62 63	29, 36, 61, 126	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	-0.17	1 (2%) 60 61	26, 30, 70, 146	0
13	Z	43/43 (100%)	-0.10	4 (9%) 8 7	33, 39, 91, 169	0
All	All	3541/3550 (99%)	-0.26	91 (2%) 56 56	19, 31, 66, 191	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	23.2
4	Q	6	VAL	20.7
4	Q	4	SER	16.4
4	Q	7	LYS	13.1
7	T	3	ALA	11.3
4	Q	8	SER	11.0
5	R	5	HIS	9.9
6	F	1	ALA	9.3
7	T	8	HIS	9.1
7	G	3	ALA	8.7
7	T	10	GLY	7.6
13	M	43	SER	7.1
7	G	6	GLY	6.6
6	S	2	SER	6.1
7	G	9	GLY	6.1
8	U	7	LYS	5.7
10	J	57	HIS	5.4
7	G	42	ARG	5.3
7	G	10	GLY	5.3
7	G	5	LYS	5.0
8	H	44	THR	4.9
8	H	45	ALA	4.9
5	E	5	HIS	4.7
7	T	42	ARG	4.6
2	O	113	TYR	4.5
7	G	8	HIS	4.5
7	T	2	SER	4.4
8	U	8	ILE	4.4
10	W	58	LYS	4.3
9	I	25	PHE	4.3
8	H	8	ILE	4.2
10	W	57	HIS	4.2
9	V	25	PHE	4.1
7	T	4	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
9	V	37	PHE	4.0
7	G	2	SER	3.9
6	S	94	HIS	3.9
7	G	36	TRP	3.9
9	V	2	THR	3.8
8	U	45	ALA	3.8
2	O	90	ILE	3.7
13	Z	42	LYS	3.6
9	I	29	LEU	3.5
12	L	2	HIS	3.5
7	T	9	GLY	3.4
7	G	7[A]	ASP	3.4
9	I	37	PHE	3.4
7	T	7	ASP	3.3
8	H	46	LYS	3.3
13	Z	43	SER	3.3
3	P	3	HIS	3.2
6	F	2	SER	3.1
10	J	58	LYS	3.1
2	B	59[A]	GLN	3.1
7	T	36	TRP	3.1
7	T	6	GLY	3.1
7	T	40	GLY	3.1
10	J	1	PHE	3.1
7	G	40	GLY	3.0
7	T	5	LYS	2.9
8	H	7	LYS	2.9
8	U	46	LYS	2.7
8	U	47	GLY	2.7
7	T	39	SER	2.6
10	J	56	PRO	2.6
11	X	6	ALA	2.6
4	D	5	VAL	2.5
12	L	47	LYS	2.5
8	U	10	ASN	2.5
7	T	1	ALA	2.5
6	F	3	GLY	2.4
12	Y	47	LYS	2.4
13	Z	41	LYS	2.4
2	B	60	GLU	2.4
7	G	84	LYS	2.3
4	Q	9	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
8	H	48	GLY	2.3
5	R	109	VAL	2.3
2	O	16[A]	ILE	2.3
4	Q	147	LYS	2.2
7	T	33[A]	LEU	2.2
13	Z	40	TYR	2.2
8	H	42	ALA	2.2
2	B	61[A]	VAL	2.2
5	E	109	VAL	2.2
7	G	41	HIS	2.1
7	G	45	PRO	2.1
2	B	113	TYR	2.1
10	J	52	TRP	2.1
6	F	94	HIS	2.1
2	B	90	ILE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.45	0.32	199,206,224,225	0
7	TPO	G	11	11/12	0.52	0.38	98,131,187,273	0
7	TPO	T	11	11/12	0.73	0.23	59,104,147,283	0
9	SAC	I	1	9/10	0.79	0.18	106,117,130,136	0
1	FME	A	1	10/11	0.94	0.08	34,43,78,247	0
1	FME	N	1	10/11	0.97	0.13	34,44,87,91	0
2	FME	B	1	10/11	0.98	0.08	27,30,36,67	0
2	FME	O	1	10/11	0.98	0.08	34,36,40,71	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	DMU	K	103	33/33	0.21	0.49	63,75,85,88	0
27	DMU	K	102	22/33	0.22	0.36	46,74,82,88	0
21	EDO	P	314	4/4	0.28	0.26	52,57,70,76	0
27	DMU	K	101	22/33	0.33	0.32	44,71,84,86	0
27	DMU	T	105	22/33	0.50	0.24	54,68,79,88	0
21	EDO	W	102	4/4	0.55	0.25	48,55,71,72	0
27	DMU	C	315	33/33	0.57	0.22	56,78,92,94	0
27	DMU	O	308	22/33	0.58	0.28	49,70,85,86	0
27	DMU	J	101	33/33	0.59	0.29	47,72,87,95	0
21	EDO	D	204	4/4	0.59	0.77	72,85,85,92	0
21	EDO	U	101	4/4	0.59	0.21	63,69,78,79	0
27	DMU	G	105	33/33	0.60	0.30	56,76,98,99	0
21	EDO	B	310	4/4	0.61	0.22	69,69,79,88	0
24	CHD	W	101	29/29	0.61	0.28	56,73,83,84	0
24	CHD	L	103	29/29	0.63	0.38	59,82,95,106	0
24	CHD	Y	104	29/29	0.63	0.44	68,85,91,98	0
21	EDO	J	103	4/4	0.64	0.19	46,49,68,77	0
23	PSC	B	303	48/52	0.65	0.29	43,71,103,194	0
25	PEK	T	101	40/53	0.66	0.26	48,67,116,204	0
21	EDO	C	314	4/4	0.66	0.14	59,61,65,82	0
25	PEK	P	302	37/53	0.66	0.20	45,69,106,186	0
25	PEK	P	304	50/53	0.67	0.26	36,72,108,183	0
26	CDL	T	102	90/100	0.67	0.27	46,73,102,173	0
21	EDO	Y	102	4/4	0.68	0.15	59,62,65,73	0
25	PEK	C	302	53/53	0.68	0.24	41,68,111,197	0
21	EDO	N	623	4/4	0.69	0.14	34,42,44,60	0
21	EDO	F	104	4/4	0.69	0.18	46,48,57,65	0
26	CDL	G	102	84/100	0.72	0.29	46,74,103,186	0
19	TGL	Y	101	56/63	0.72	0.20	40,62,94,105	0
27	DMU	P	309	33/33	0.73	0.24	45,73,86,92	0
21	EDO	A	622	4/4	0.74	0.20	50,58,63,73	0
20	PGV	N	608	46/51	0.74	0.25	42,71,109,162	0
21	EDO	D	203	4/4	0.75	0.24	48,60,70,71	0
19	TGL	Q	201	63/63	0.77	0.19	45,69,87,103	0
20	PGV	P	306	51/51	0.77	0.26	43,74,99,167	0
20	PGV	C	304	51/51	0.77	0.23	38,68,102,170	0
23	PSC	R	201	49/52	0.77	0.24	36,68,104,175	0
27	DMU	P	316	33/33	0.77	0.22	54,64,77,82	0
26	CDL	P	307	84/100	0.77	0.24	37,71,98,148	0
27	DMU	L	104	22/33	0.78	0.20	46,69,80,82	0
21	EDO	G	104	4/4	0.80	0.12	46,70,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	TGL	D	201	53/63	0.80	0.17	36,60,83,94	0
24	CHD	J	102	29/29	0.80	0.22	49,68,93,104	0
21	EDO	Q	203	4/4	0.80	0.13	52,53,53,56	0
19	TGL	A	607	60/63	0.81	0.17	30,61,95,112	0
24	CHD	P	308	29/29	0.81	0.17	46,56,80,93	0
19	TGL	N	607	62/63	0.82	0.19	45,69,83,90	0
21	EDO	C	309	4/4	0.83	0.12	33,37,39,43	0
21	EDO	P	310	4/4	0.83	0.15	50,58,64,67	0
21	EDO	S	105	4/4	0.83	0.20	43,46,63,66	0
21	EDO	Y	103	4/4	0.83	0.23	58,67,76,85	0
21	EDO	Z	102	4/4	0.83	0.19	63,71,78,78	0
26	CDL	C	305	91/100	0.84	0.23	40,68,97,127	0
21	EDO	N	620	4/4	0.84	0.12	37,64,65,74	0
20	PGV	A	608	47/51	0.84	0.20	36,61,99,182	0
21	EDO	B	309	4/4	0.85	0.24	37,68,75,84	0
21	EDO	C	308	4/4	0.86	0.14	59,59,60,68	0
21	EDO	A	614	4/4	0.86	0.12	49,63,65,67	0
21	EDO	Q	204	4/4	0.86	0.21	44,50,54,55	0
21	EDO	C	312	4/4	0.86	0.11	57,68,76,76	0
21	EDO	A	625	4/4	0.86	0.29	34,43,77,84	0
19	TGL	B	301	63/63	0.87	0.16	31,64,87,93	0
27	DMU	Z	101	33/33	0.87	0.10	37,49,66,74	0
21	EDO	B	308	4/4	0.88	0.15	30,44,53,64	0
21	EDO	A	620	4/4	0.88	0.10	36,40,41,45	0
24	CHD	C	306	29/29	0.88	0.18	48,55,71,75	0
21	EDO	M	102	4/4	0.88	0.13	54,61,72,72	0
21	EDO	L	101	4/4	0.89	0.09	45,50,59,64	0
21	EDO	M	103	4/4	0.89	0.30	47,52,55,60	0
21	EDO	T	103	4/4	0.89	0.09	55,73,79,83	0
21	EDO	N	624	4/4	0.89	0.07	51,53,64,76	0
27	DMU	M	101	33/33	0.90	0.10	35,41,52,73	0
21	EDO	A	624	4/4	0.90	0.22	40,69,78,86	0
21	EDO	P	313	4/4	0.90	0.15	38,55,67,72	0
21	EDO	A	610	4/4	0.90	0.20	25,31,68,79	0
21	EDO	A	619	4/4	0.90	0.32	31,40,56,77	0
21	EDO	A	623	4/4	0.90	0.19	41,50,61,65	0
21	EDO	C	313	4/4	0.91	0.08	55,62,63,79	0
21	EDO	N	617	4/4	0.92	0.07	56,58,59,72	0
21	EDO	Q	202	4/4	0.92	0.12	45,56,64,74	0
21	EDO	O	303	4/4	0.92	0.12	38,43,44,47	0
21	EDO	H	101	4/4	0.92	0.12	52,62,65,74	0
21	EDO	L	102	4/4	0.92	0.15	38,68,75,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
29	PO4	U	102	5/5	0.92	0.31	54,57,73,89	0
21	EDO	N	616	4/4	0.93	0.17	34,52,57,70	0
21	EDO	A	612	4/4	0.93	0.11	37,38,41,46	0
21	EDO	O	304	4/4	0.93	0.15	39,51,53,57	0
21	EDO	O	307	4/4	0.93	0.15	35,43,53,55	0
21	EDO	R	203	4/4	0.93	0.10	39,42,53,54	0
21	EDO	A	615	4/4	0.93	0.09	29,30,31,34	0
21	EDO	A	626	4/4	0.93	0.11	45,58,63,63	0
21	EDO	O	306	4/4	0.94	0.11	34,42,49,60	0
24	CHD	C	301	29/29	0.94	0.07	23,28,33,35	0
21	EDO	D	202	4/4	0.94	0.21	42,50,57,62	0
21	EDO	A	621	4/4	0.94	0.14	29,36,38,65	0
21	EDO	B	306	4/4	0.94	0.16	36,41,48,59	0
21	EDO	F	103	4/4	0.94	0.08	35,38,40,47	0
21	EDO	P	315	4/4	0.94	0.10	31,37,44,54	0
21	EDO	N	610	4/4	0.94	0.22	30,34,48,59	0
21	EDO	N	611	4/4	0.94	0.09	41,42,48,50	0
21	EDO	N	613	4/4	0.94	0.09	37,37,44,47	0
21	EDO	N	614	4/4	0.95	0.17	32,43,49,67	0
21	EDO	A	616	4/4	0.95	0.13	38,41,41,60	0
21	EDO	C	310	4/4	0.95	0.12	30,36,48,50	0
21	EDO	B	307	4/4	0.95	0.30	39,41,61,72	0
21	EDO	N	622	4/4	0.95	0.09	40,40,43,44	0
21	EDO	A	617	4/4	0.95	0.24	27,43,53,68	0
24	CHD	P	301	29/29	0.95	0.07	24,29,34,34	0
29	PO4	H	102	5/5	0.95	0.25	57,68,74,78	0
21	EDO	P	311	4/4	0.95	0.11	36,53,56,62	0
21	EDO	T	104	4/4	0.96	0.07	30,32,39,44	0
21	EDO	R	202	4/4	0.96	0.08	37,40,41,42	0
21	EDO	C	311	4/4	0.96	0.30	45,56,59,62	0
21	EDO	S	102	4/4	0.96	0.07	34,36,37,46	0
21	EDO	B	305	4/4	0.96	0.09	26,26,29,30	0
21	EDO	N	615	4/4	0.96	0.07	28,29,29,34	0
25	PEK	P	303	53/53	0.96	0.11	26,44,80,86	0
21	EDO	S	103	4/4	0.97	0.09	29,30,31,34	0
21	EDO	N	619	4/4	0.97	0.14	30,42,62,74	0
24	CHD	O	301	29/29	0.97	0.08	23,27,31,38	0
21	EDO	E	201	4/4	0.97	0.09	37,37,39,44	0
21	EDO	P	312	4/4	0.97	0.13	35,37,38,42	0
21	EDO	N	621	4/4	0.97	0.17	31,38,42,48	0
21	EDO	N	612	4/4	0.97	0.11	25,28,29,32	0
20	PGV	N	609	51/51	0.97	0.11	22,29,65,72	0

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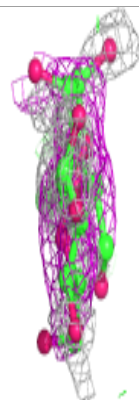
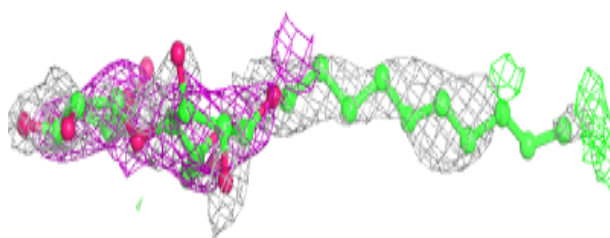
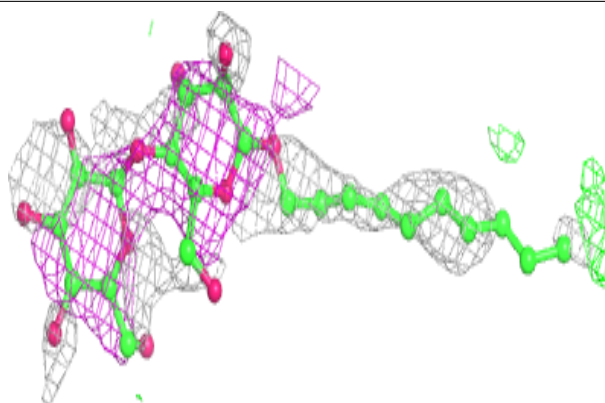
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
25	PEK	G	101	51/53	0.97	0.11	27,42,75,92	0
21	EDO	C	307	4/4	0.97	0.08	32,33,33,35	0
21	EDO	G	103	4/4	0.97	0.06	31,32,37,38	0
21	EDO	A	618	4/4	0.97	0.14	30,36,39,43	0
21	EDO	O	305	4/4	0.97	0.07	29,30,32,32	0
24	CHD	B	304	29/29	0.97	0.07	24,27,34,45	0
20	PGV	P	305	51/51	0.97	0.10	23,30,70,84	0
21	EDO	N	618	4/4	0.97	0.11	36,38,42,42	0
21	EDO	F	105	4/4	0.98	0.08	30,31,33,34	0
14	HEA	N	601[C]	43/60	0.98	0.09	21,24,28,29	1
14	HEA	N	602	60/60	0.98	0.08	21,24,29,35	0
17	NA	N	605	1/1	0.98	0.09	30,30,30,30	0
14	HEA	A	602	60/60	0.98	0.08	20,23,28,31	0
21	EDO	A	611	4/4	0.98	0.12	30,41,61,85	0
21	EDO	S	104	4/4	0.98	0.08	25,25,25,25	0
20	PGV	A	609	51/51	0.98	0.10	21,27,66,71	0
21	EDO	A	613	4/4	0.98	0.09	21,24,24,26	0
20	PGV	C	303	50/51	0.98	0.10	22,29,76,79	0
21	EDO	E	202	4/4	0.98	0.07	37,38,41,44	0
14	HEA	N	601[A]	60/60	0.98	0.09	19,25,32,35	18
14	HEA	N	601[B]	60/60	0.98	0.09	21,25,33,41	18
17	NA	A	605	1/1	0.99	0.07	25,25,25,25	0
14	HEA	A	601[C]	43/60	0.99	0.09	18,21,23,24	1
18	CYN	A	606	2/2	0.99	0.07	21,21,21,21	0
18	CYN	N	606	2/2	0.99	0.07	25,25,25,26	0
14	HEA	A	601[A]	60/60	0.99	0.09	18,21,31,32	18
21	EDO	F	102	4/4	0.99	0.06	24,24,26,26	0
14	HEA	A	601[B]	60/60	0.99	0.09	18,21,30,39	18
16	MG	N	604	1/1	0.99	0.04	23,23,23,23	0
15	CU	A	603	1/1	1.00	0.14	21,21,21,21	0
22	CUA	B	302	2/2	1.00	0.12	23,23,23,24	0
22	CUA	O	302	2/2	1.00	0.12	27,27,27,28	0
28	ZN	F	101	1/1	1.00	0.10	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.12	28,28,28,28	0
15	CU	N	603	1/1	1.00	0.13	23,23,23,23	0
16	MG	A	604	1/1	1.00	0.04	19,19,19,19	0

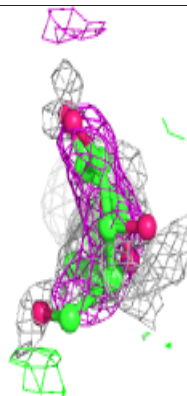
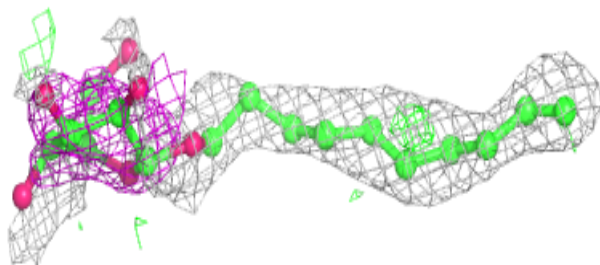
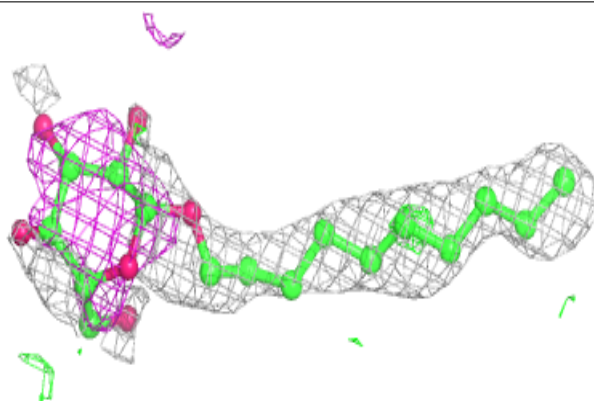
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU K 103:

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

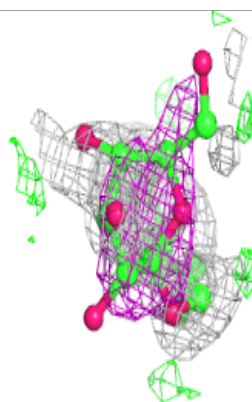
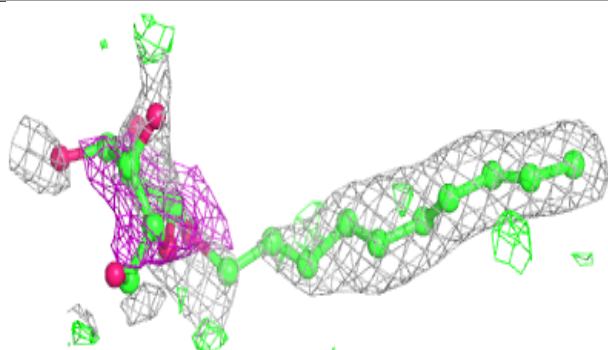
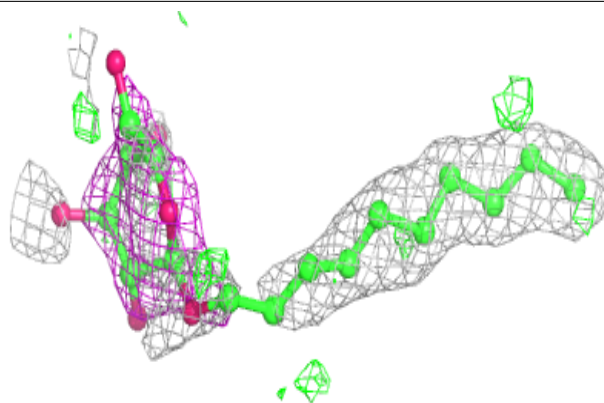
**Electron density around DMU K 102:**

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

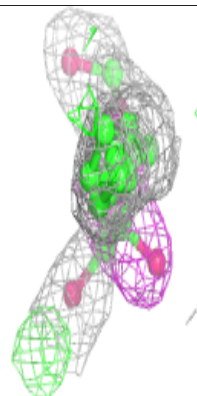
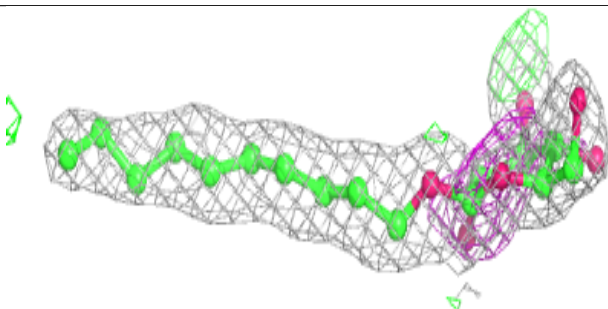
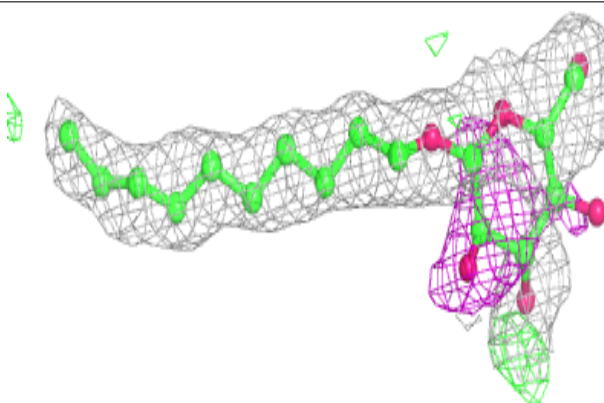


Electron density around DMU K 101:

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

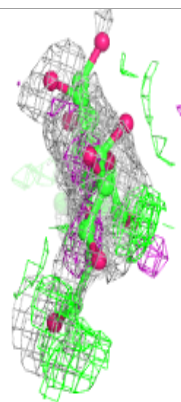
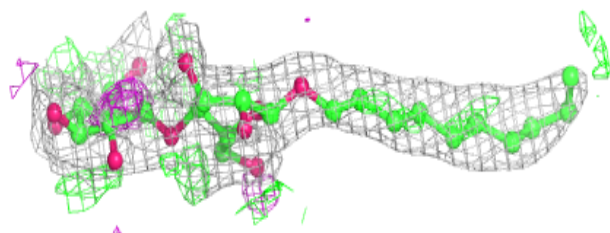
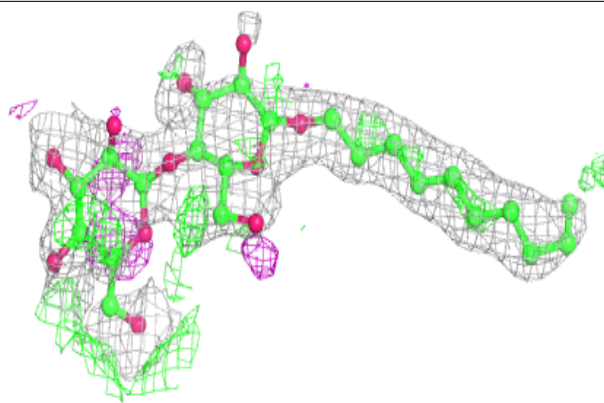
**Electron density around DMU T 105:**

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

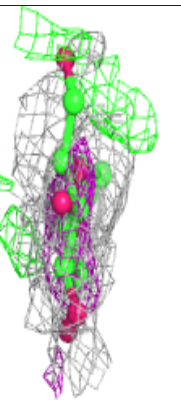
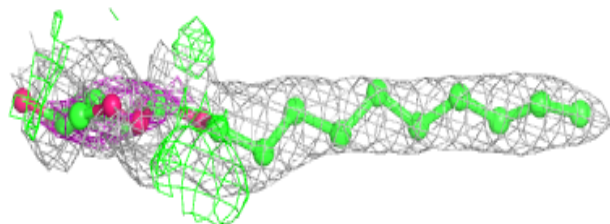
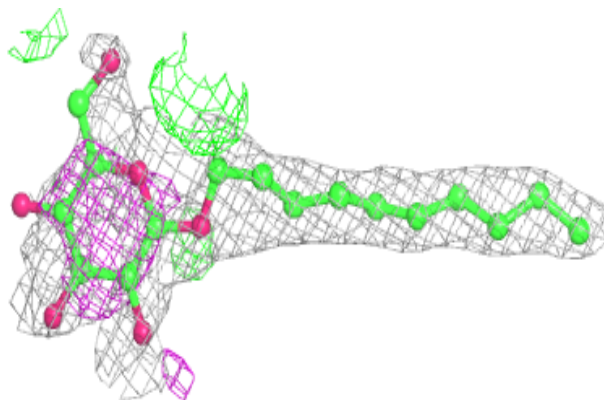


Electron density around DMU C 315:

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

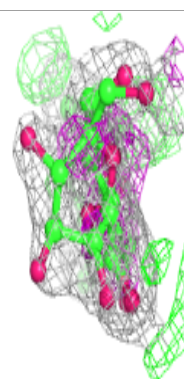
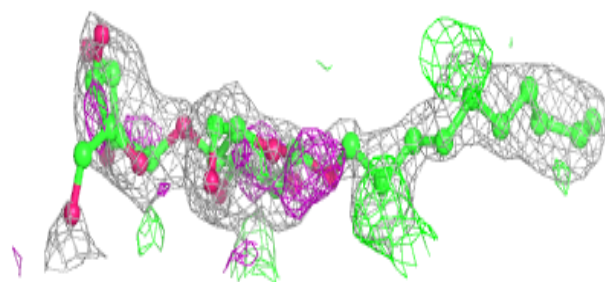
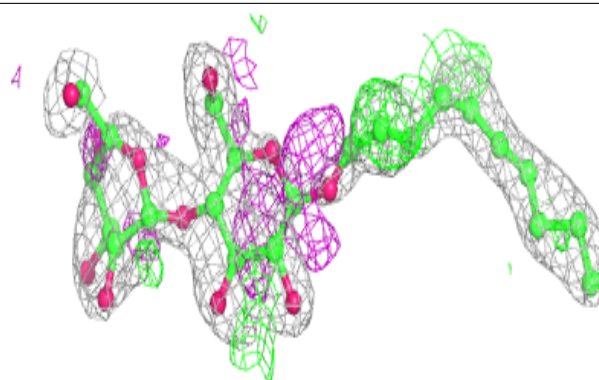
**Electron density around DMU O 308:**

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

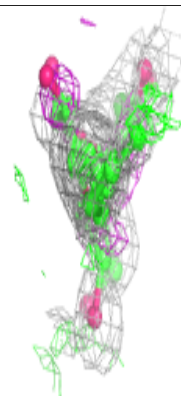
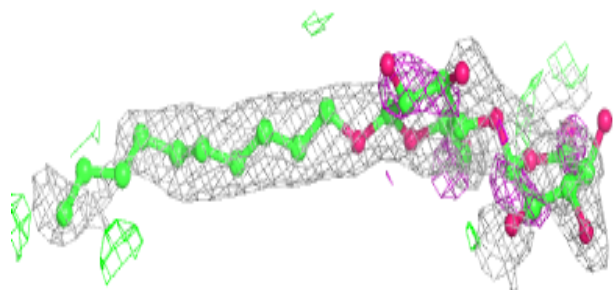
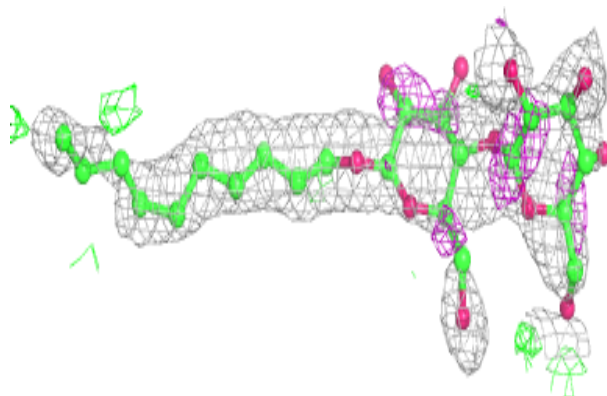


Electron density around DMU J 101:

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

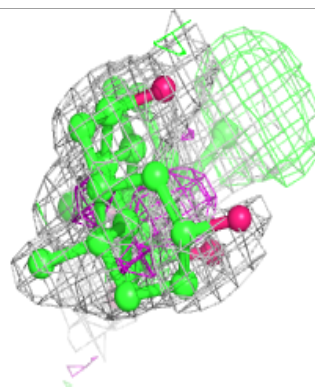
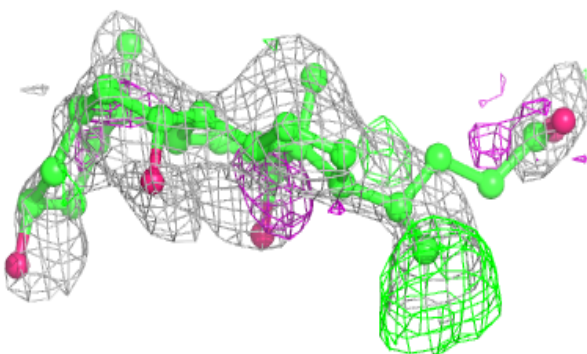
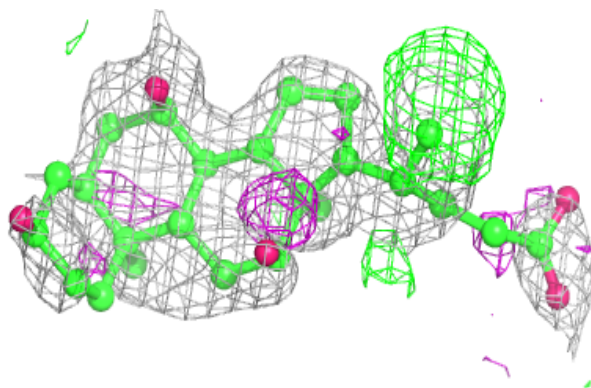
**Electron density around DMU G 105:**

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

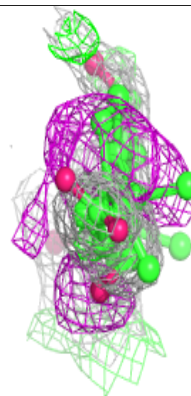
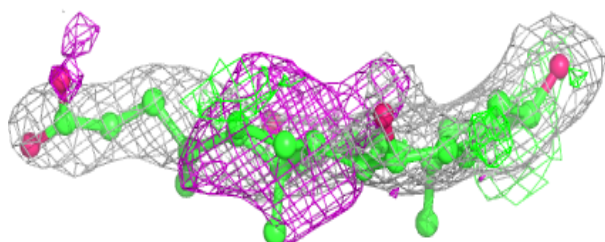
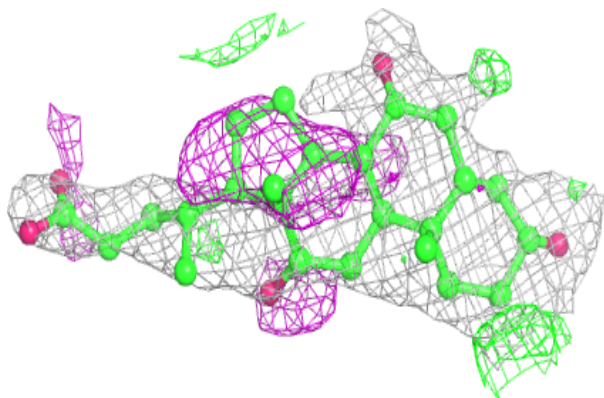


Electron density around CHD W 101:

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

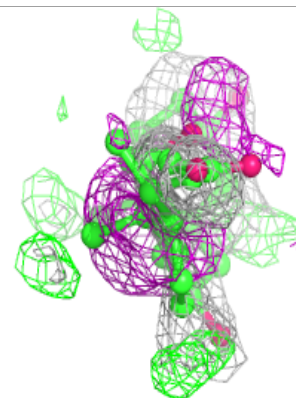
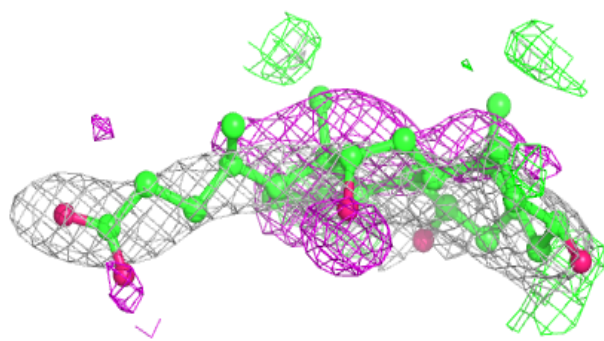
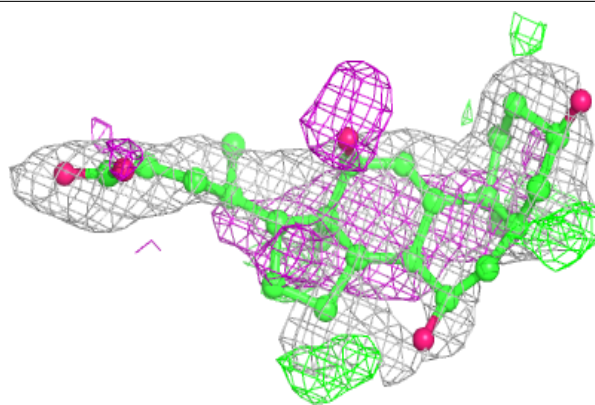
**Electron density around CHD L 103:**

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

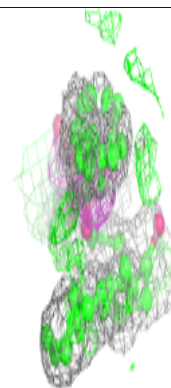
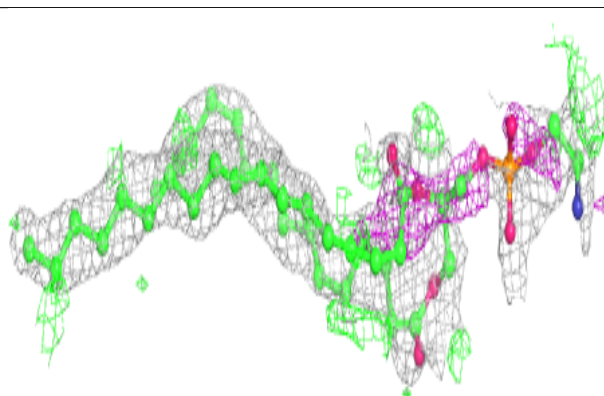
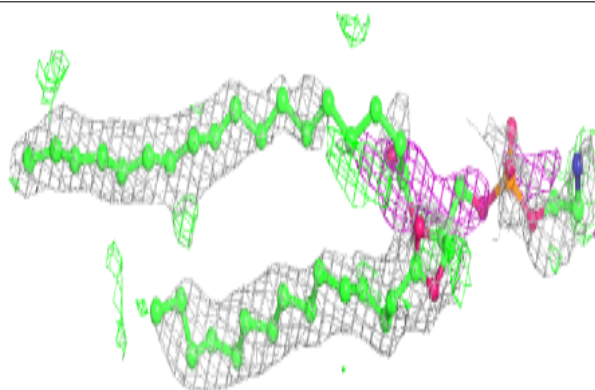


Electron density around CHD Y 104:

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

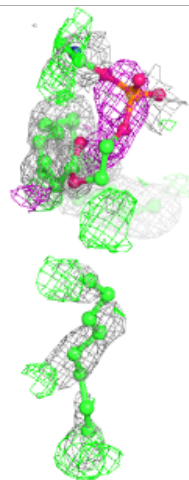
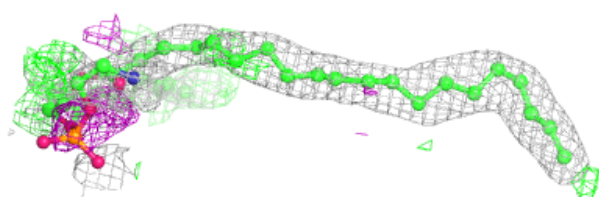
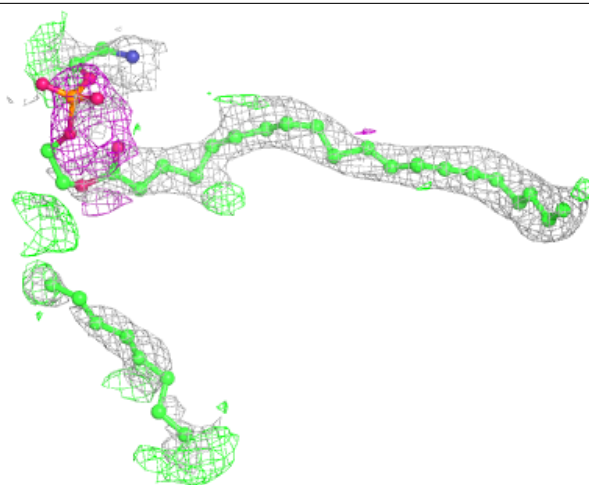
**Electron density around PSC B 303:**

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



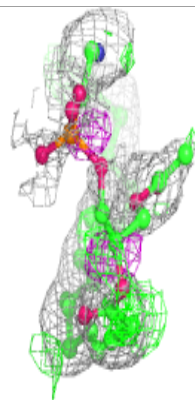
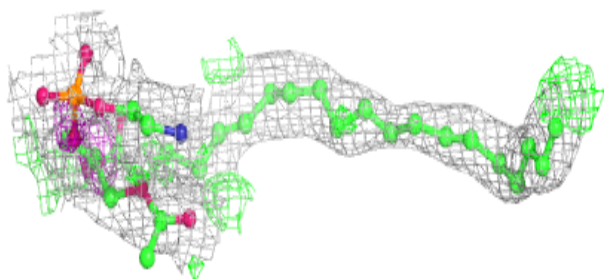
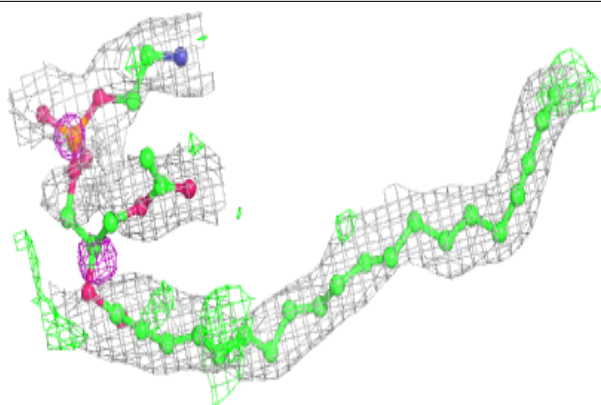
Electron density around PEK T 101:

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

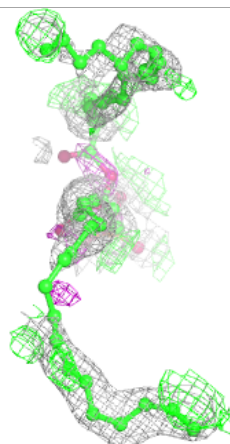
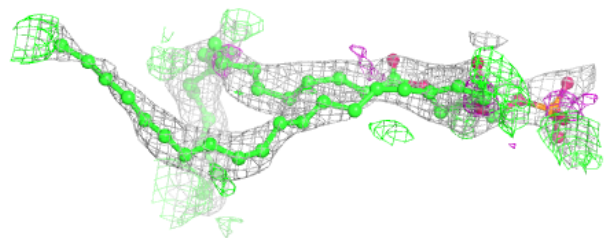
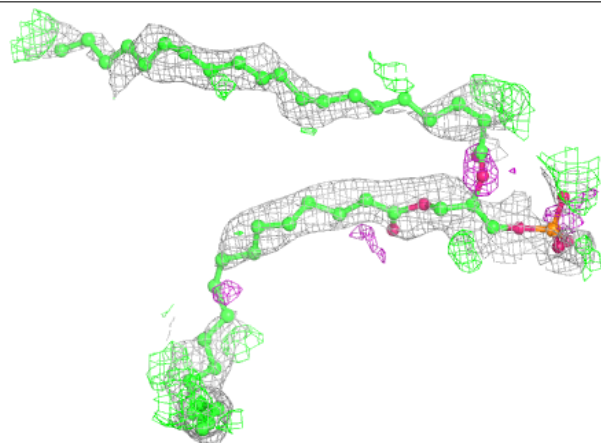


Electron density around PEK P 302:

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

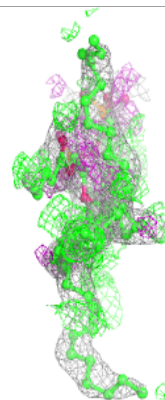
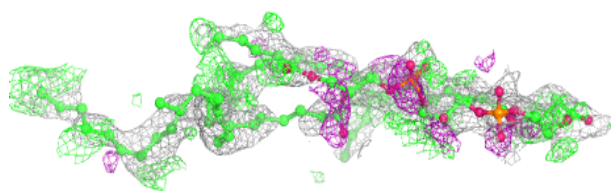
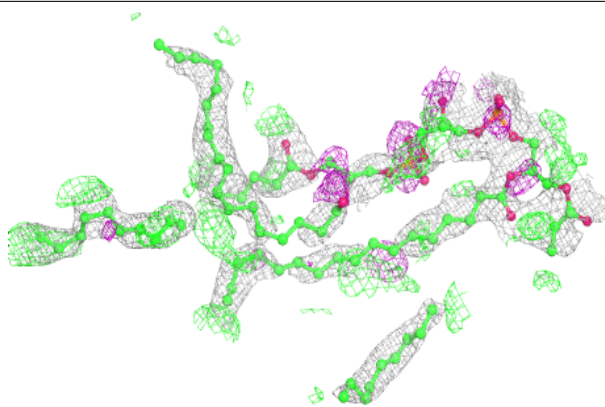
**Electron density around PEK P 304:**

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



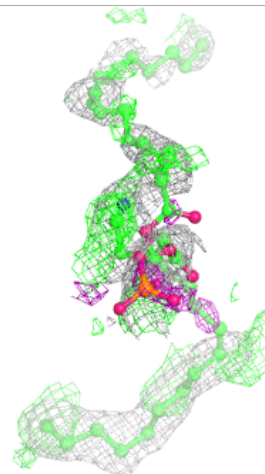
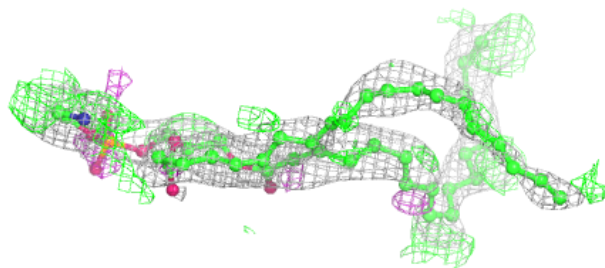
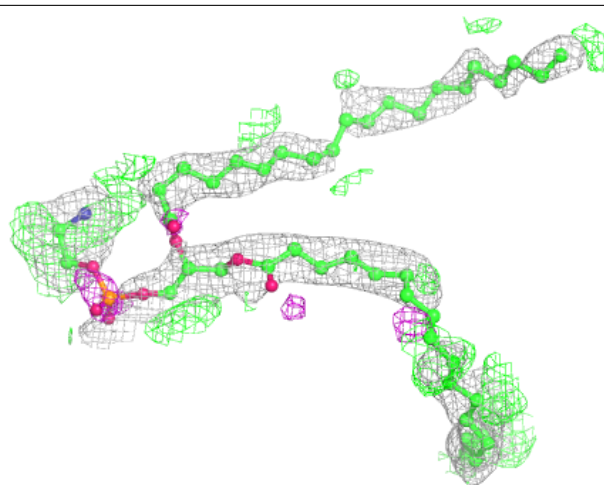
Electron density around CDL T 102:

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



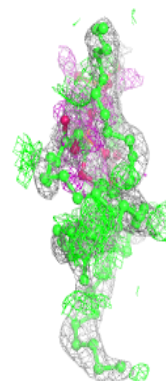
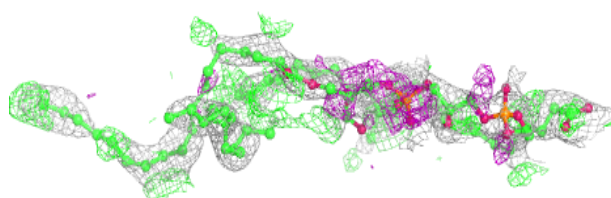
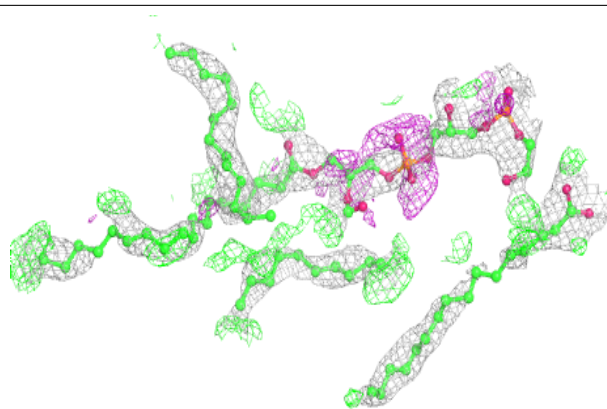
Electron density around PEK C 302:

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

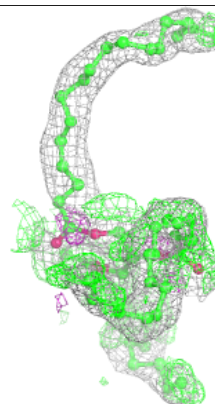
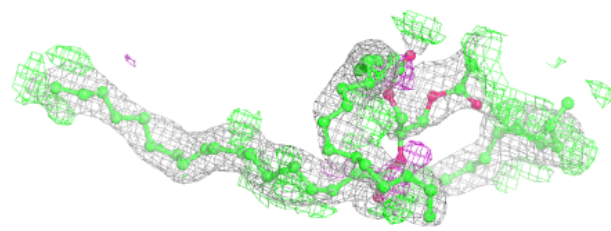
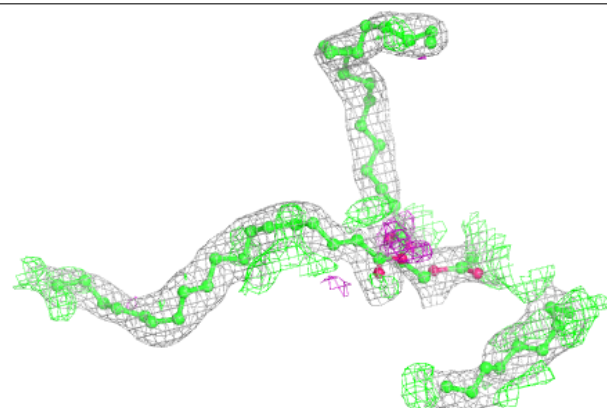


Electron density around CDL G 102:

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

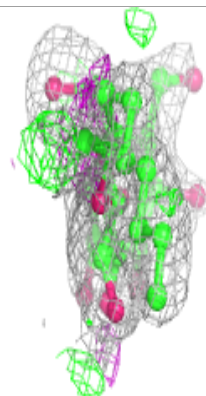
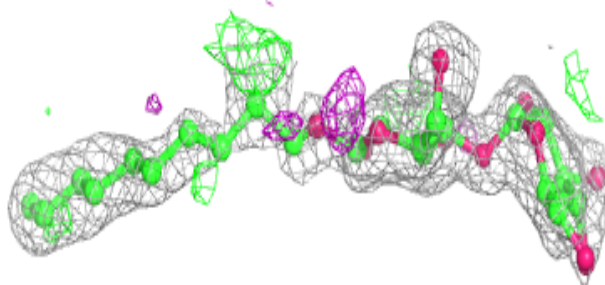
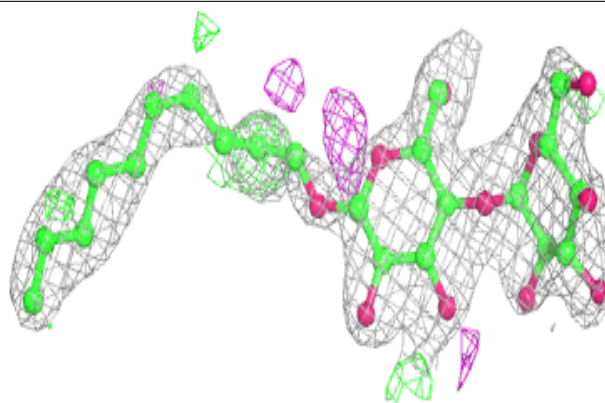
**Electron density around TGL Y 101:**

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

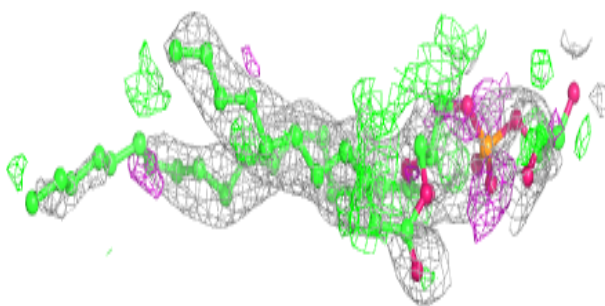
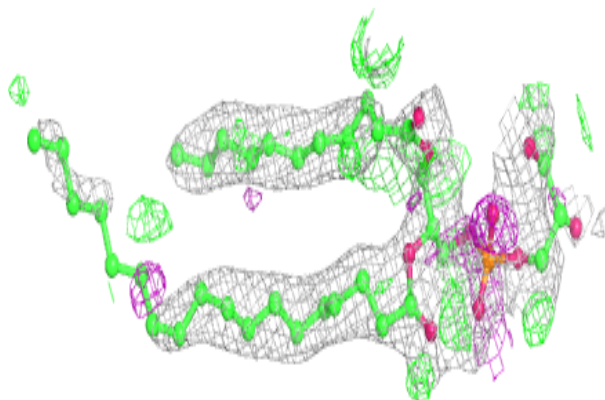


Electron density around DMU P 309:

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

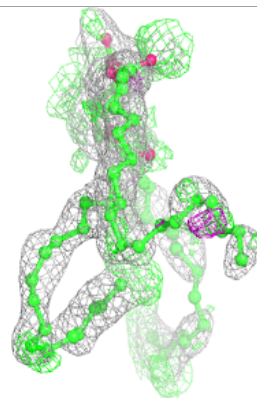
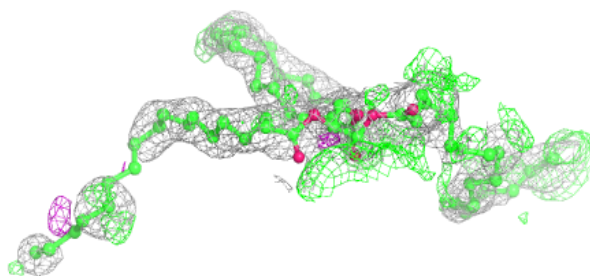
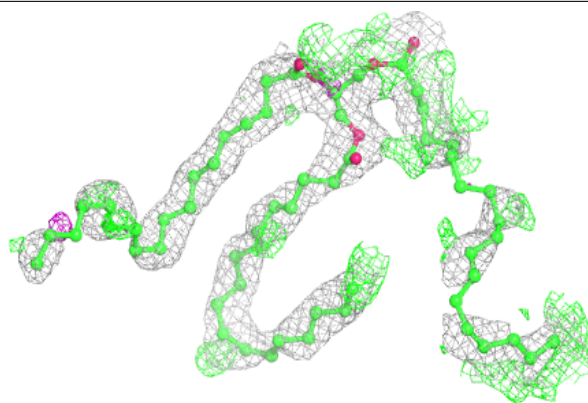
**Electron density around PGV N 608:**

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

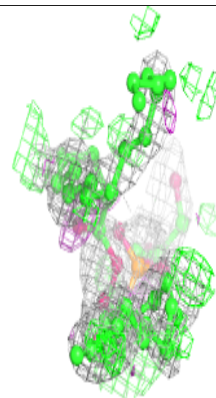
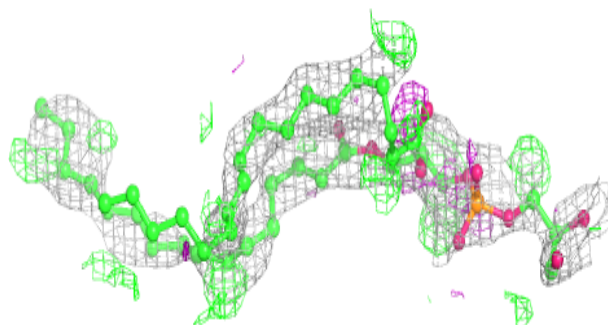
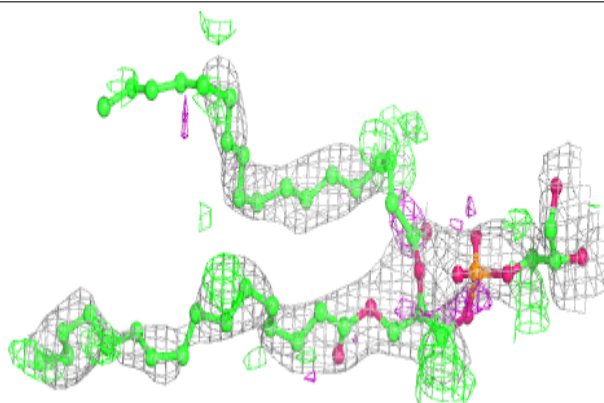


Electron density around TGL Q 201:

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

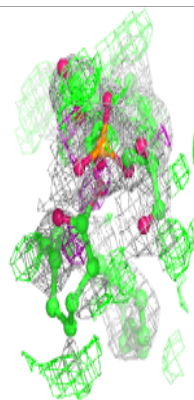
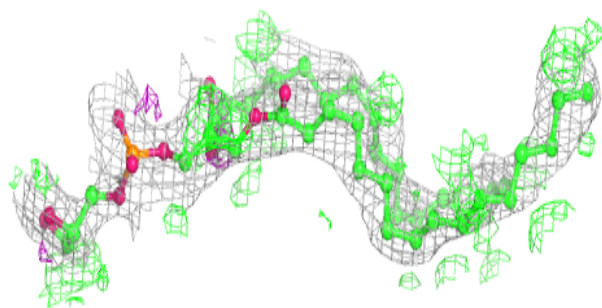
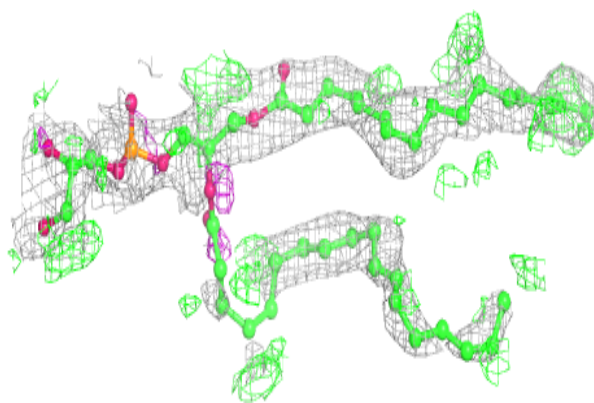
**Electron density around PGV P 306:**

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

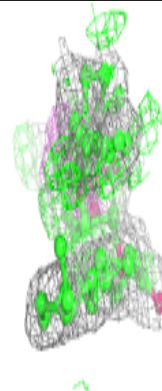
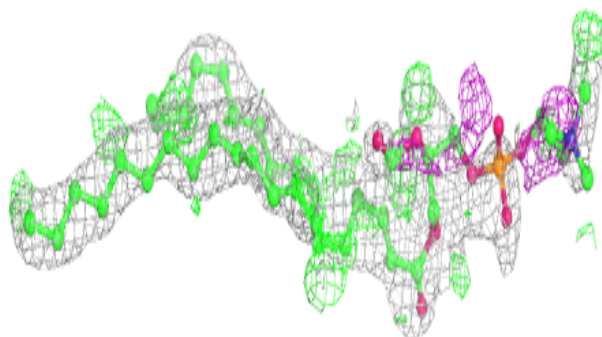
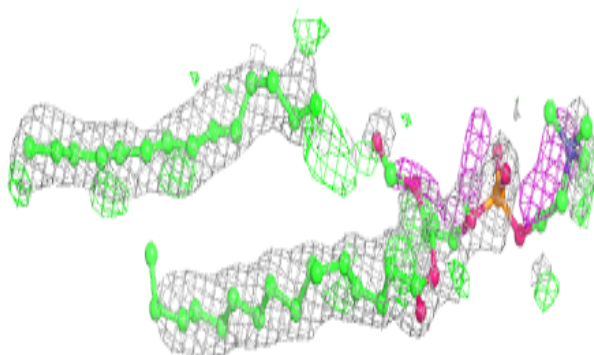


Electron density around PGV C 304:

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

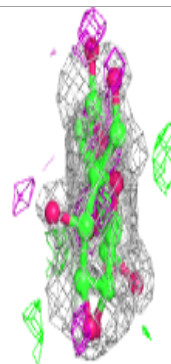
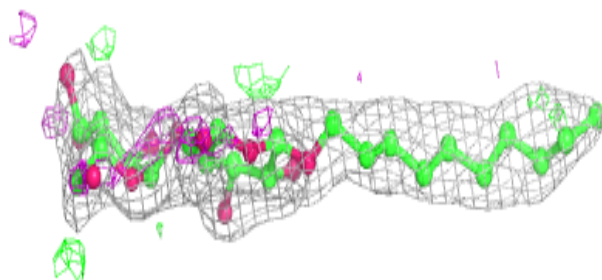
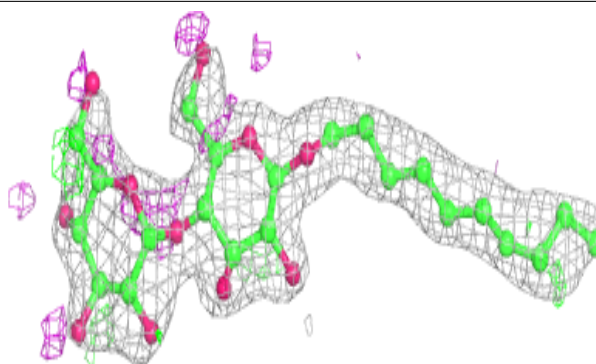
**Electron density around PSC R 201:**

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



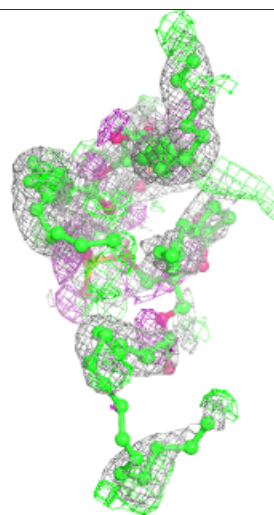
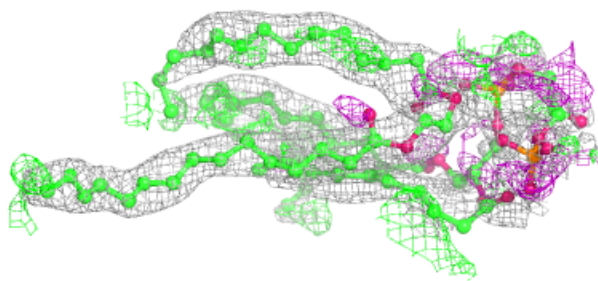
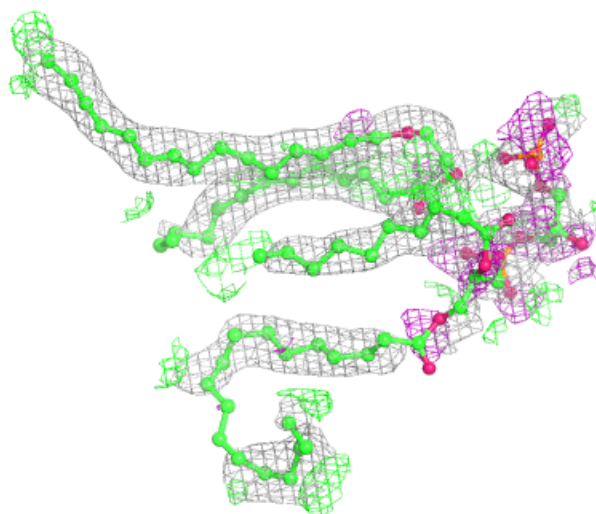
Electron density around DMU P 316:

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



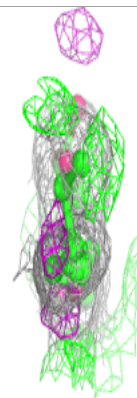
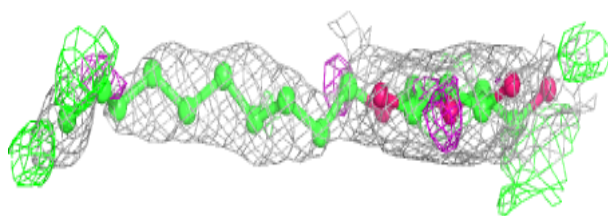
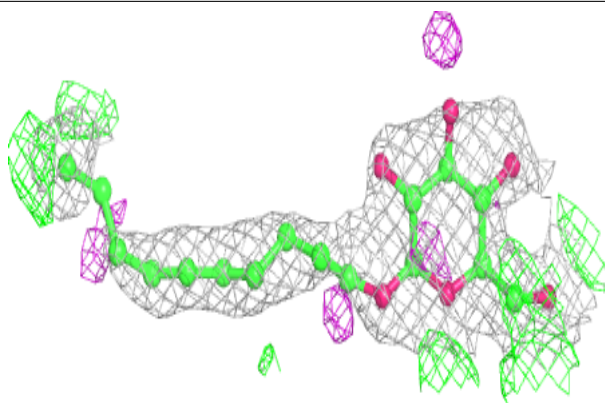
Electron density around CDL P 307:

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

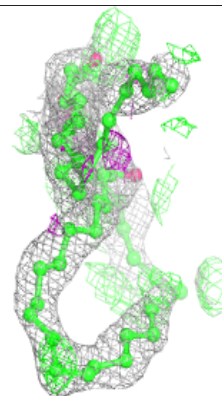
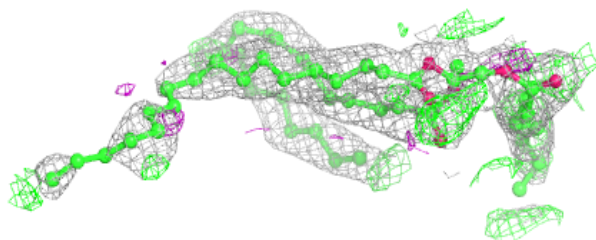
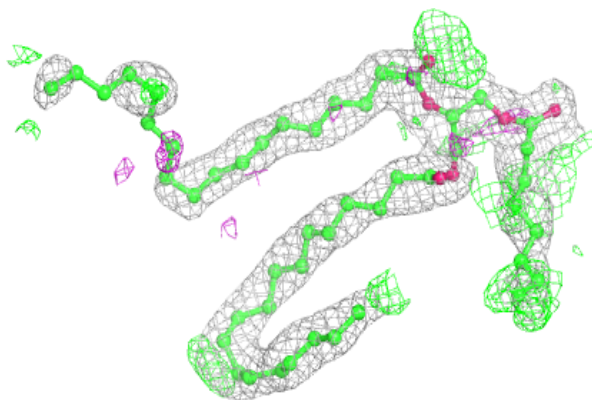


Electron density around DMU L 104:

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

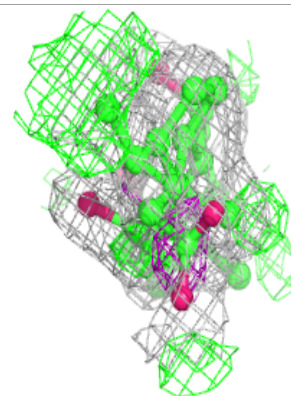
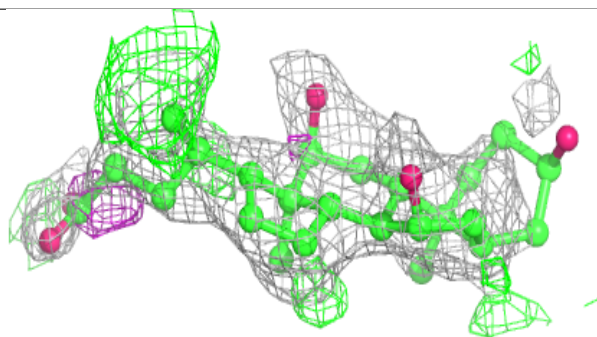
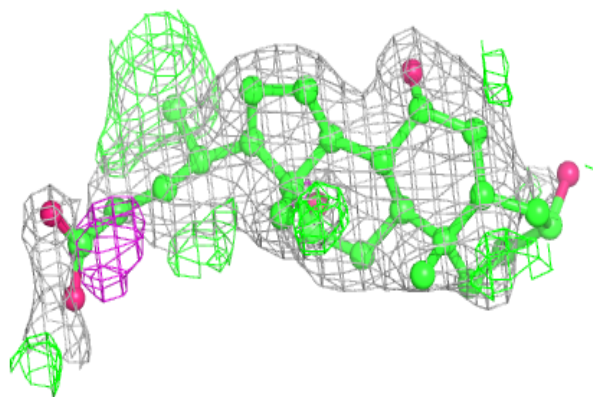
**Electron density around TGL D 201:**

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



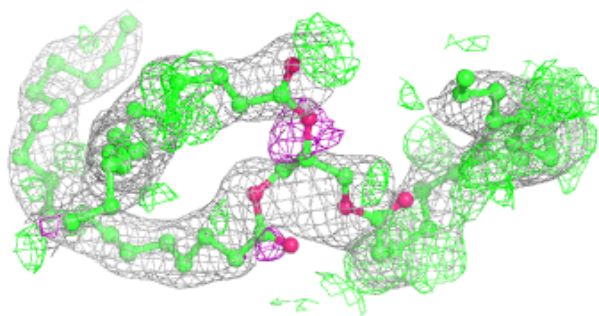
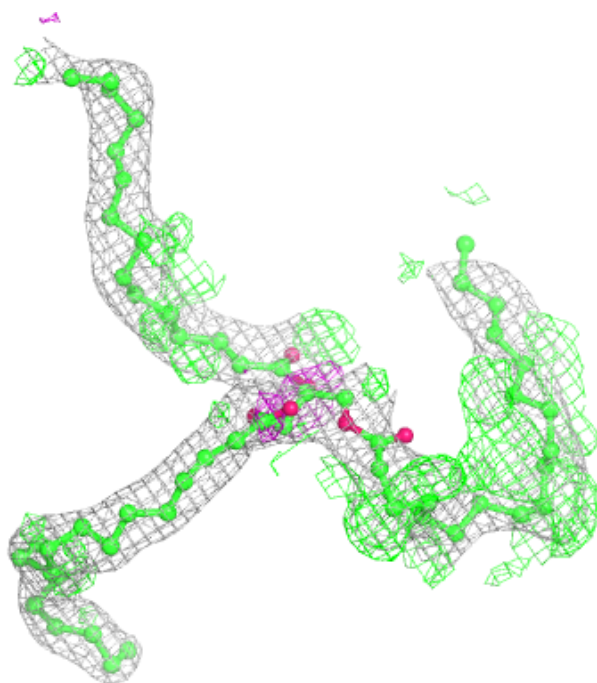
Electron density around CHD J 102:

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



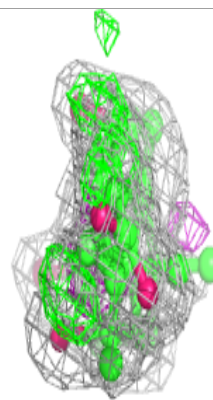
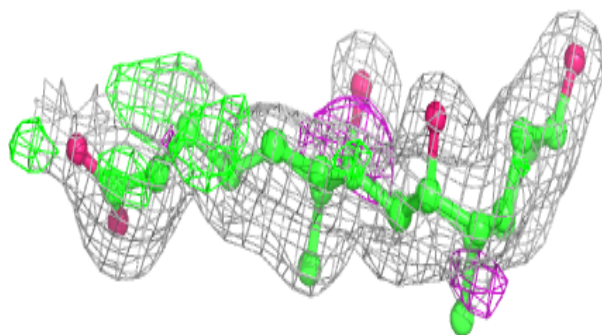
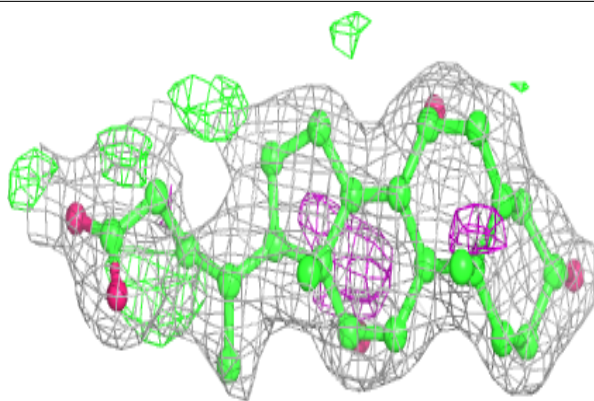
Electron density around TGL A 607:

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

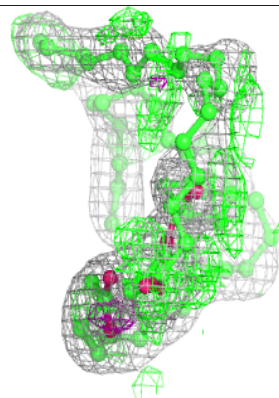
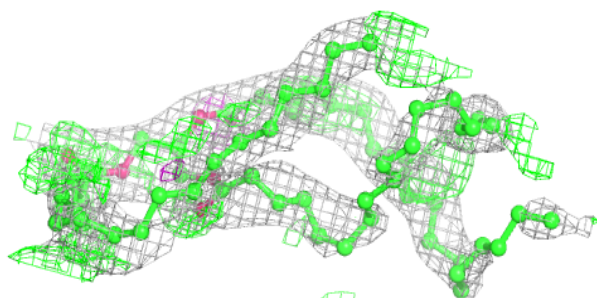
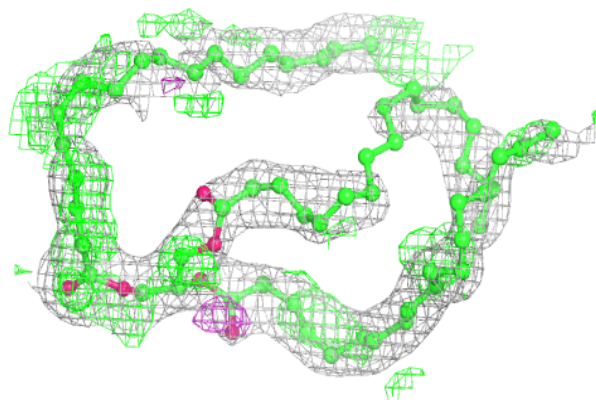


Electron density around CHD P 308:

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

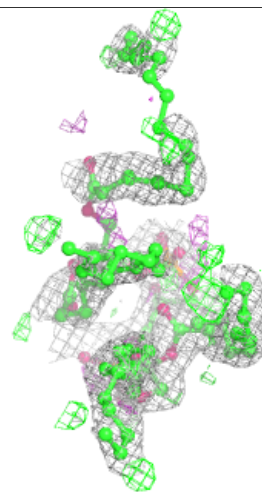
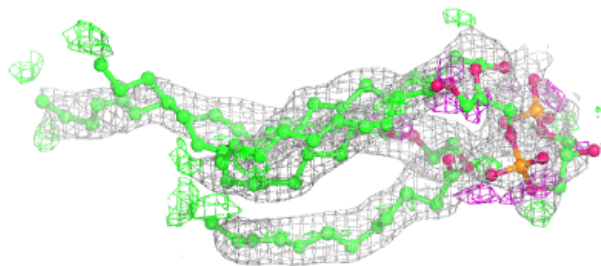
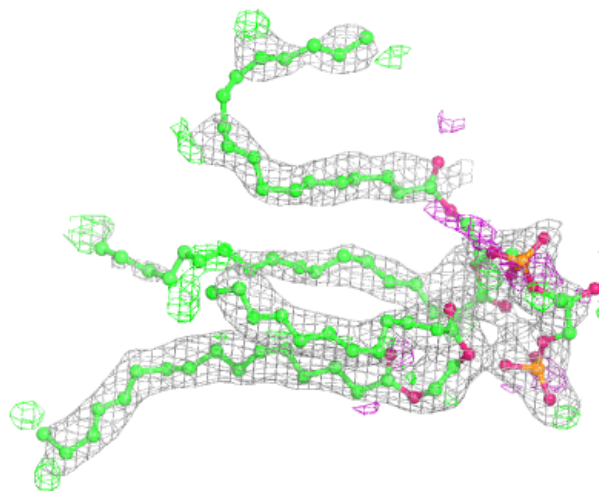
**Electron density around TGL N 607:**

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



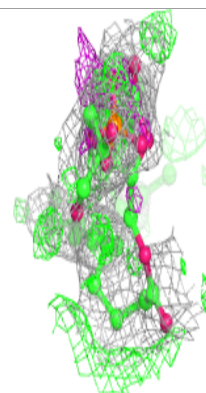
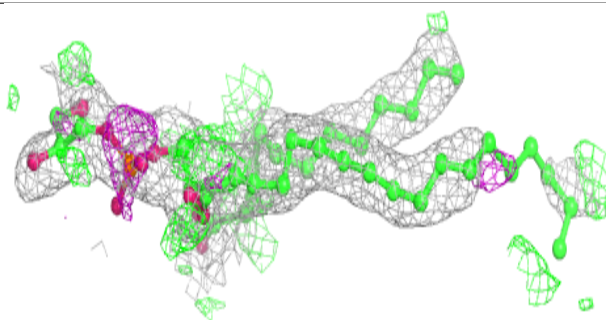
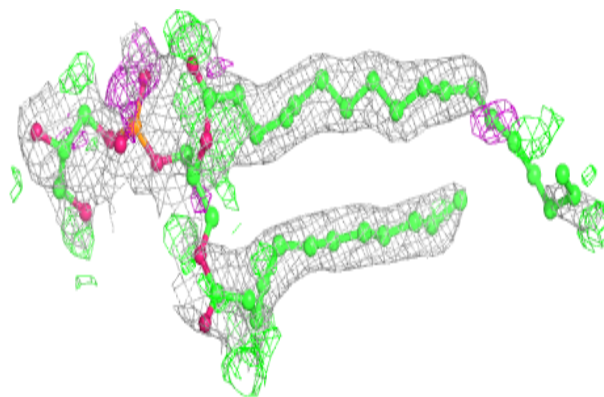
Electron density around CDL C 305:

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

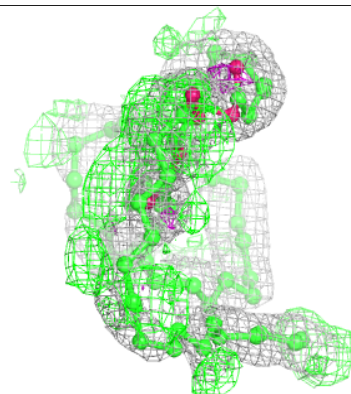
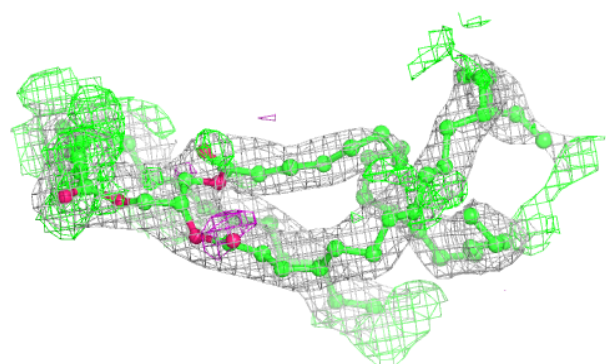
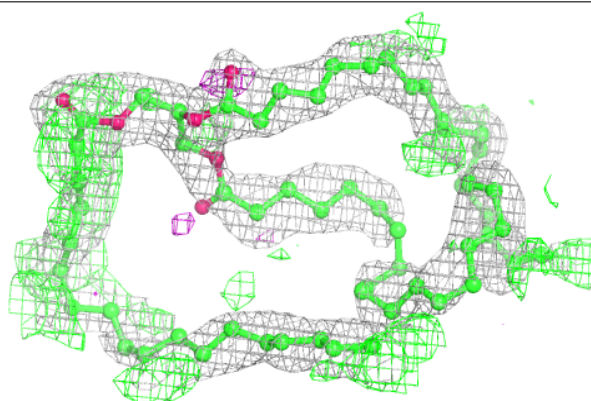


Electron density around PGV A 608:

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

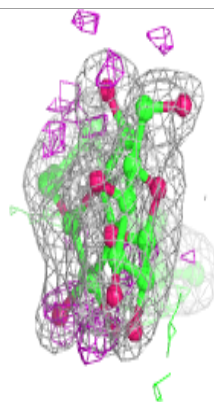
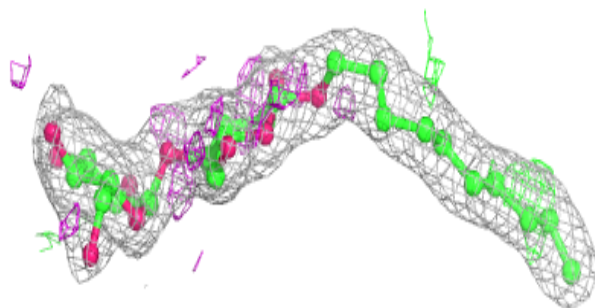
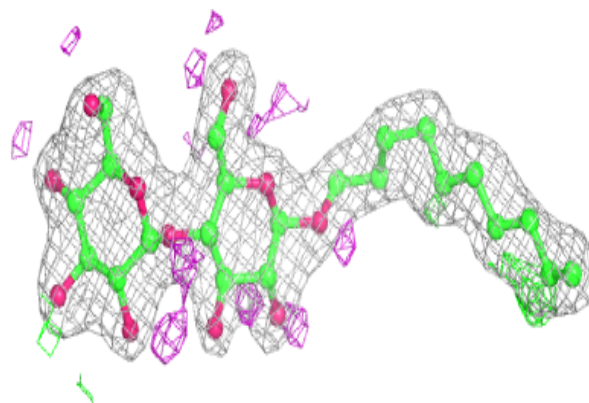
**Electron density around TGL B 301:**

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

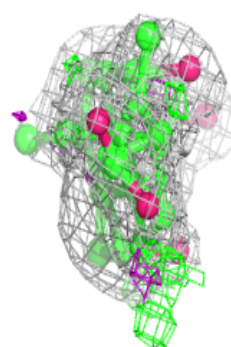
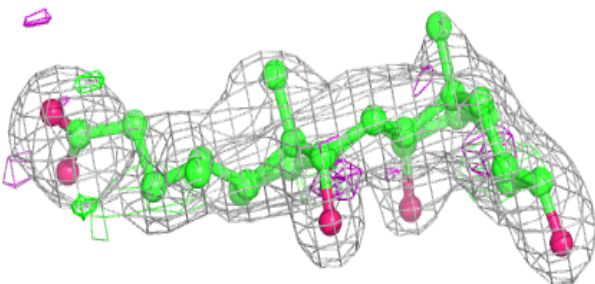
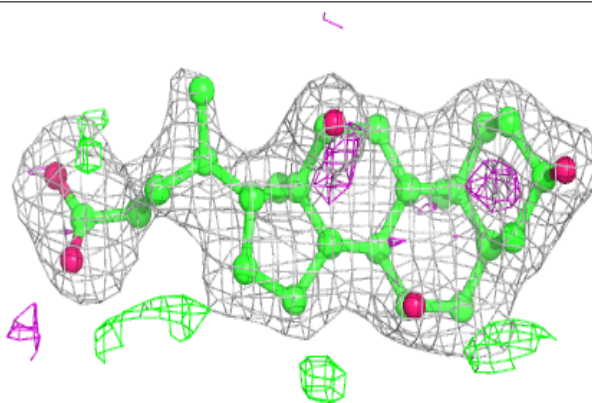


Electron density around DMU Z 101:

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

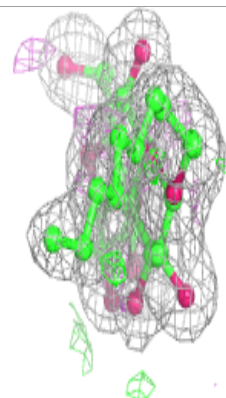
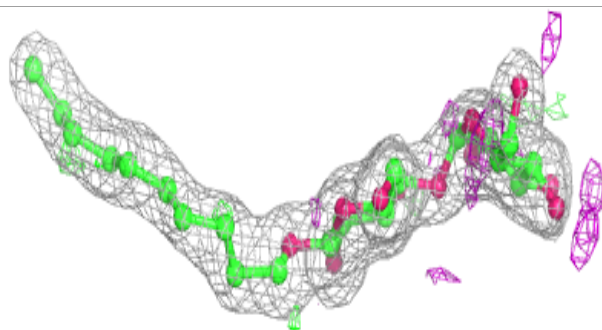
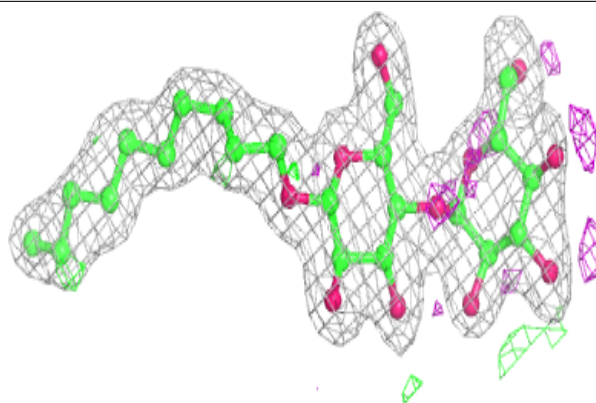
**Electron density around CHD C 306:**

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

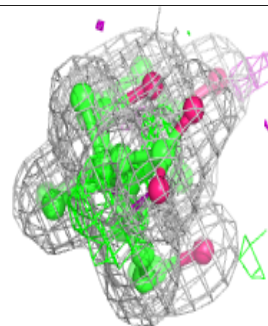
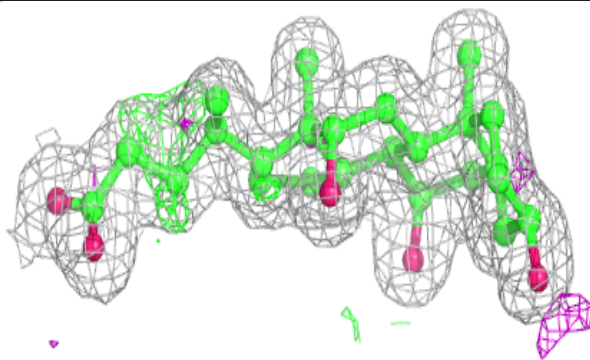
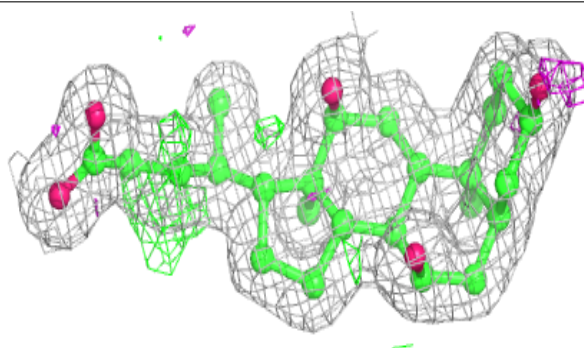


Electron density around DMU M 101:

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

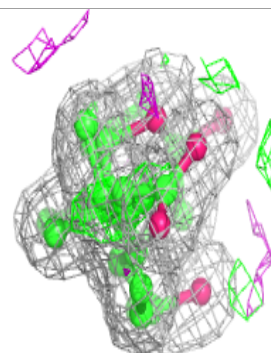
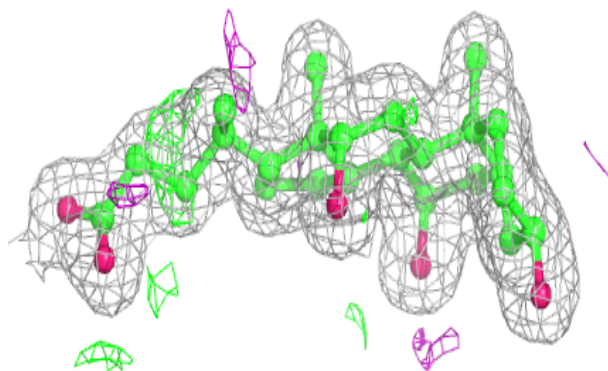
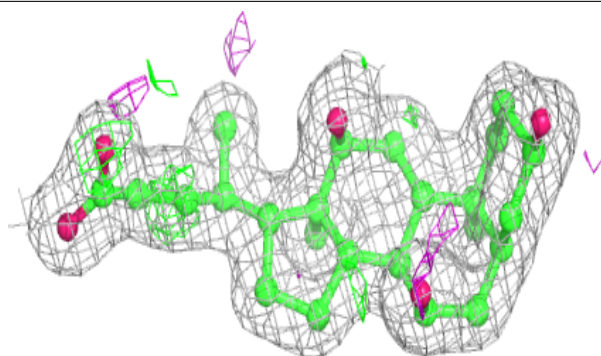
**Electron density around CHD C 301:**

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

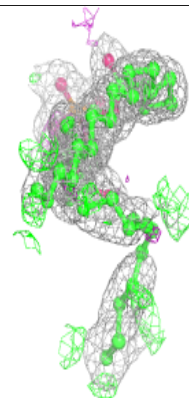
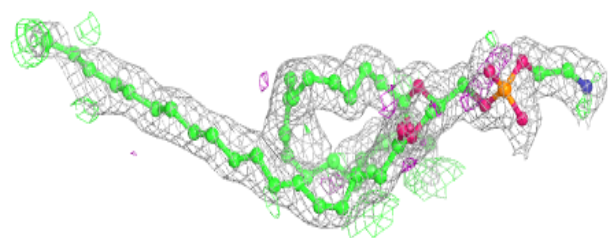
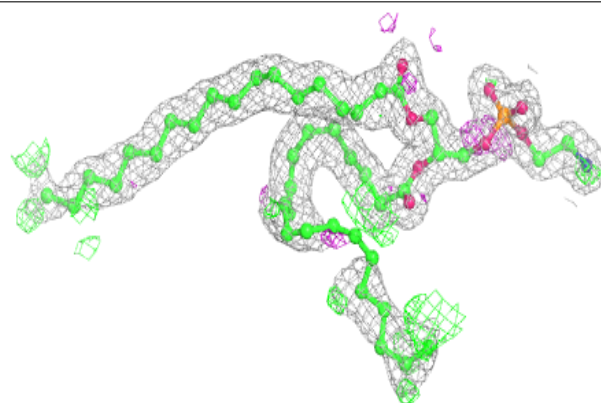


Electron density around CHD P 301:

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

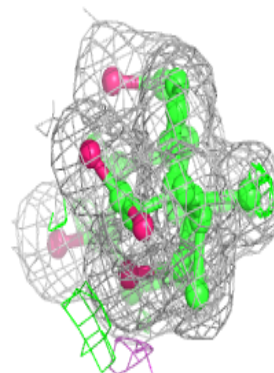
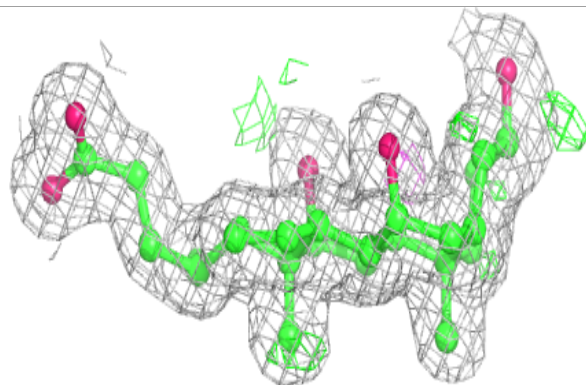
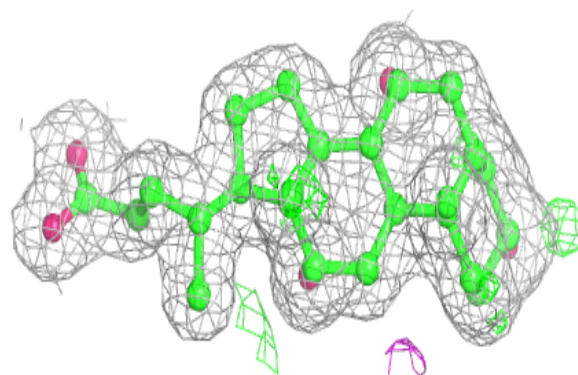
**Electron density around PEK P 303:**

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

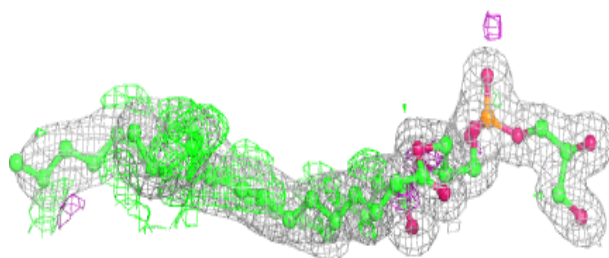
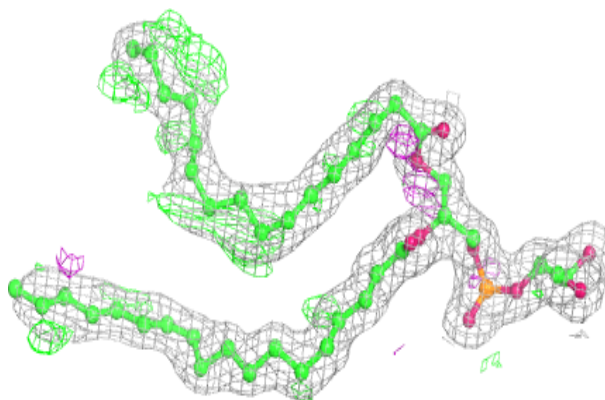


Electron density around CHD O 301:

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

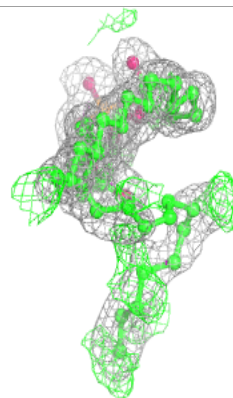
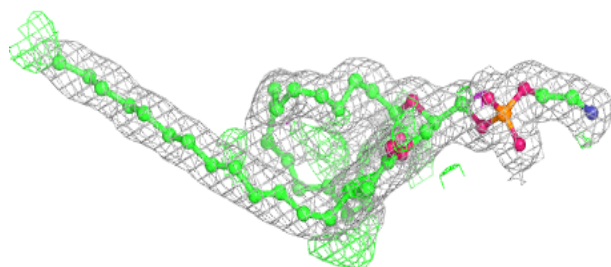
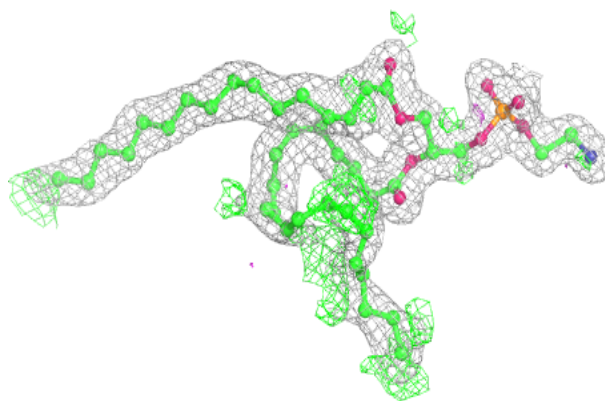
**Electron density around PGV N 609:**

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

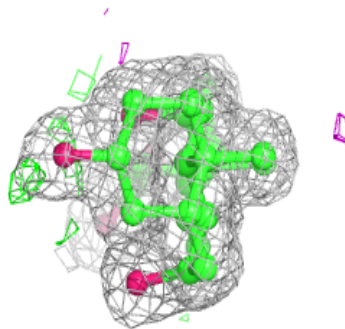
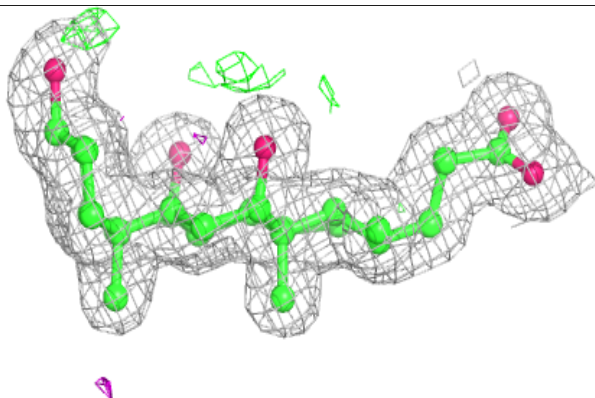
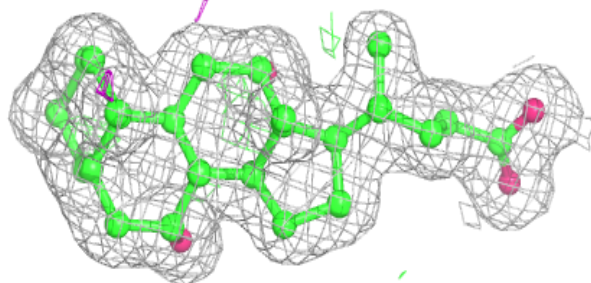


Electron density around PEK G 101:

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

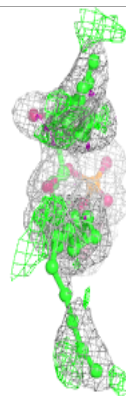
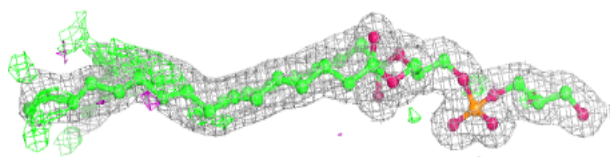
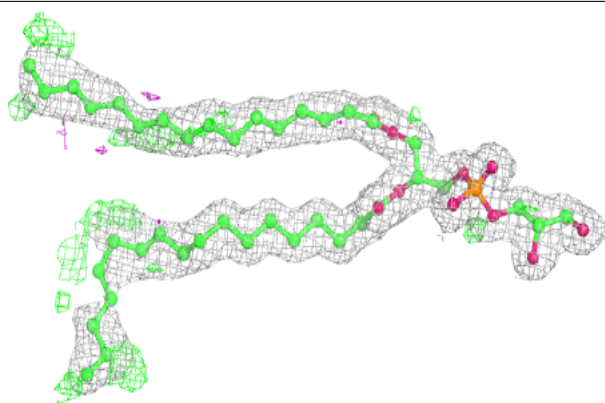
**Electron density around CHD B 304:**

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

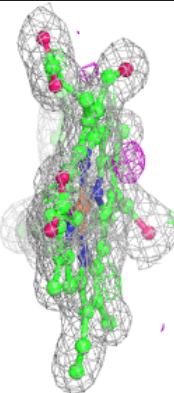
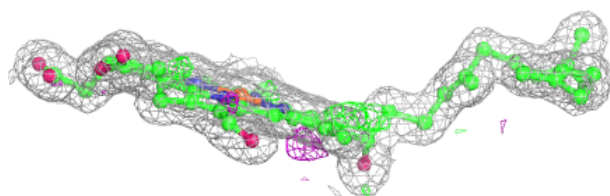
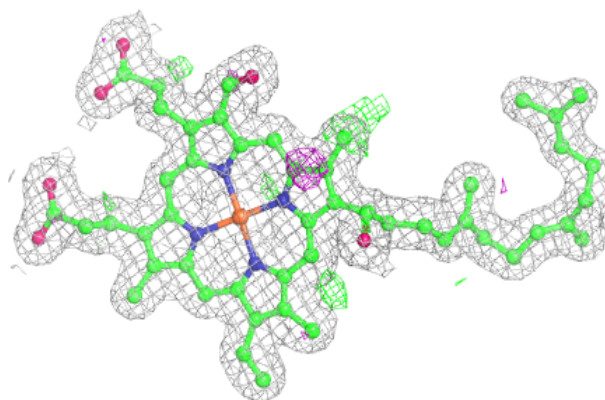


Electron density around PGV P 305:

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

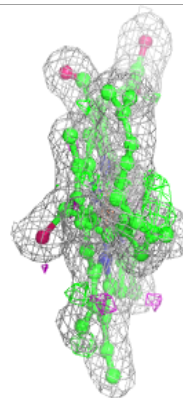
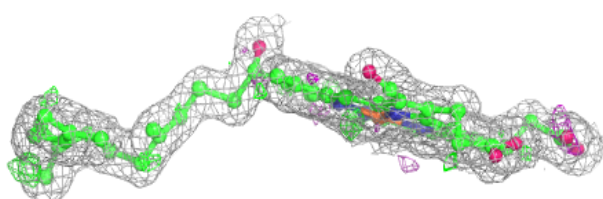
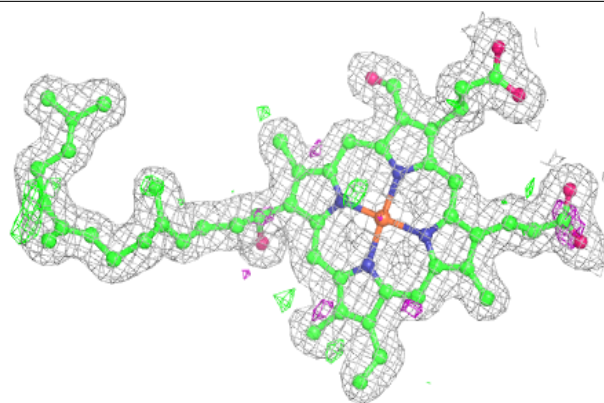
**Electron density around HEA N 602:**

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

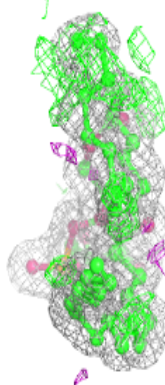
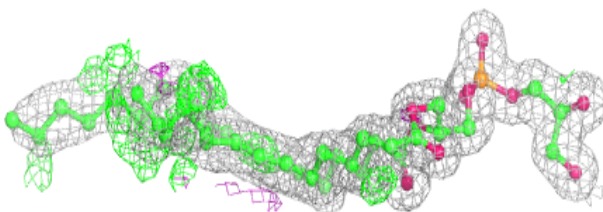
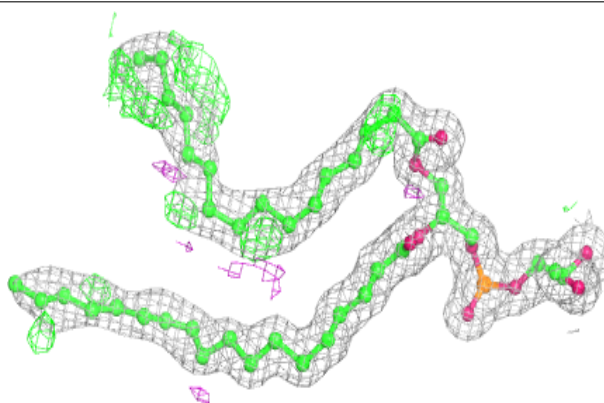


Electron density around HEA A 602:

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

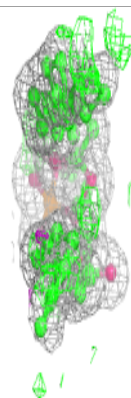
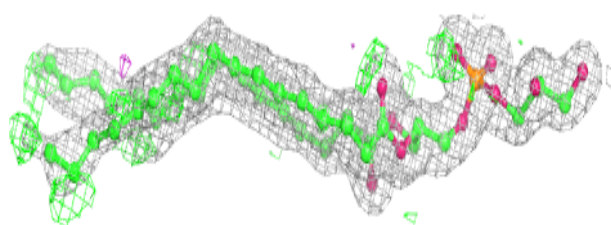
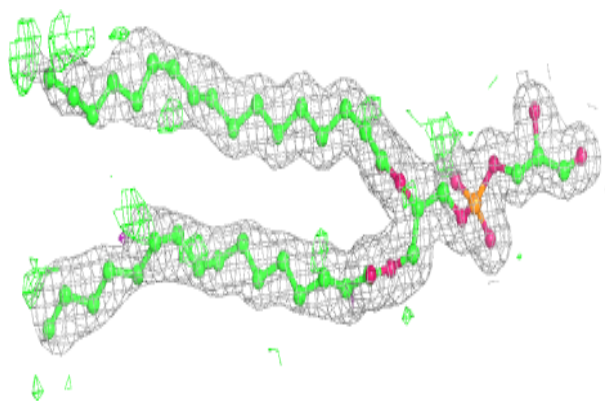
**Electron density around PGV A 609:**

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

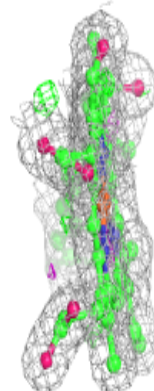
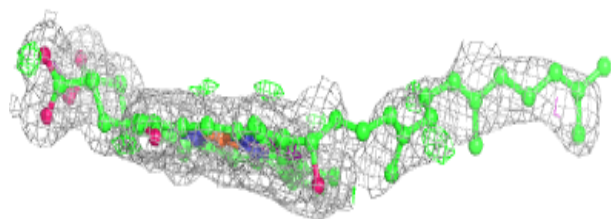
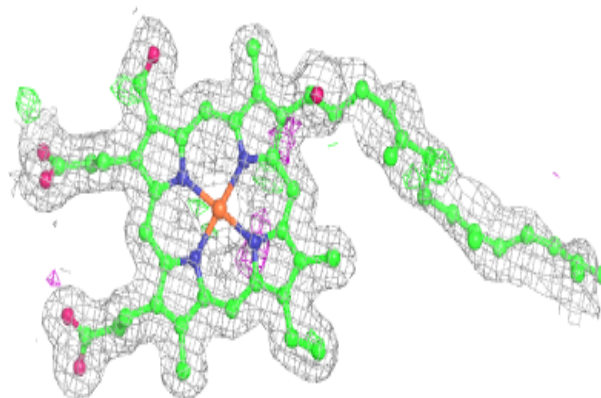


Electron density around PGV C 303:

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

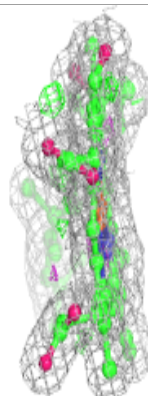
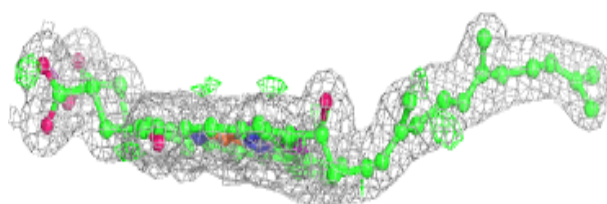
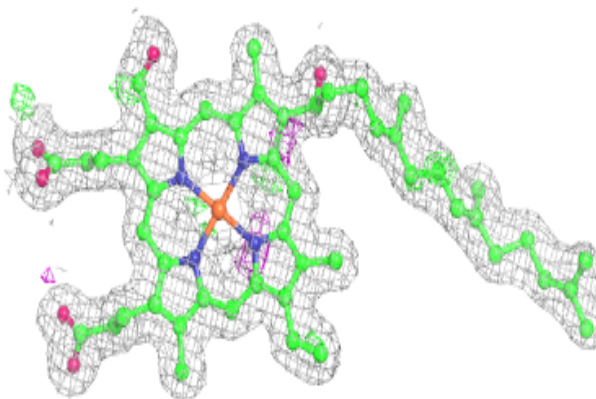
**Electron density around HEA N 601 (A):**

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

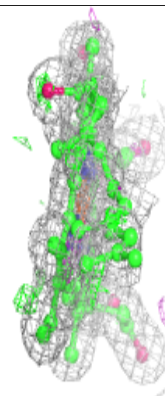
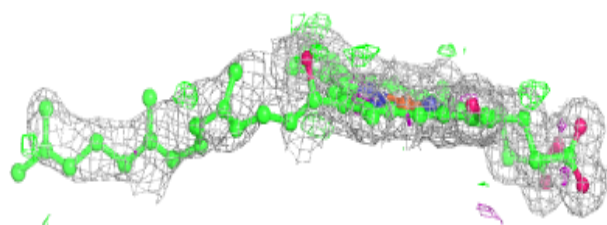
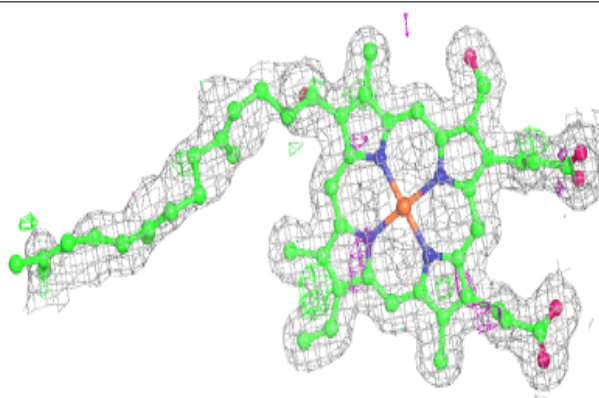


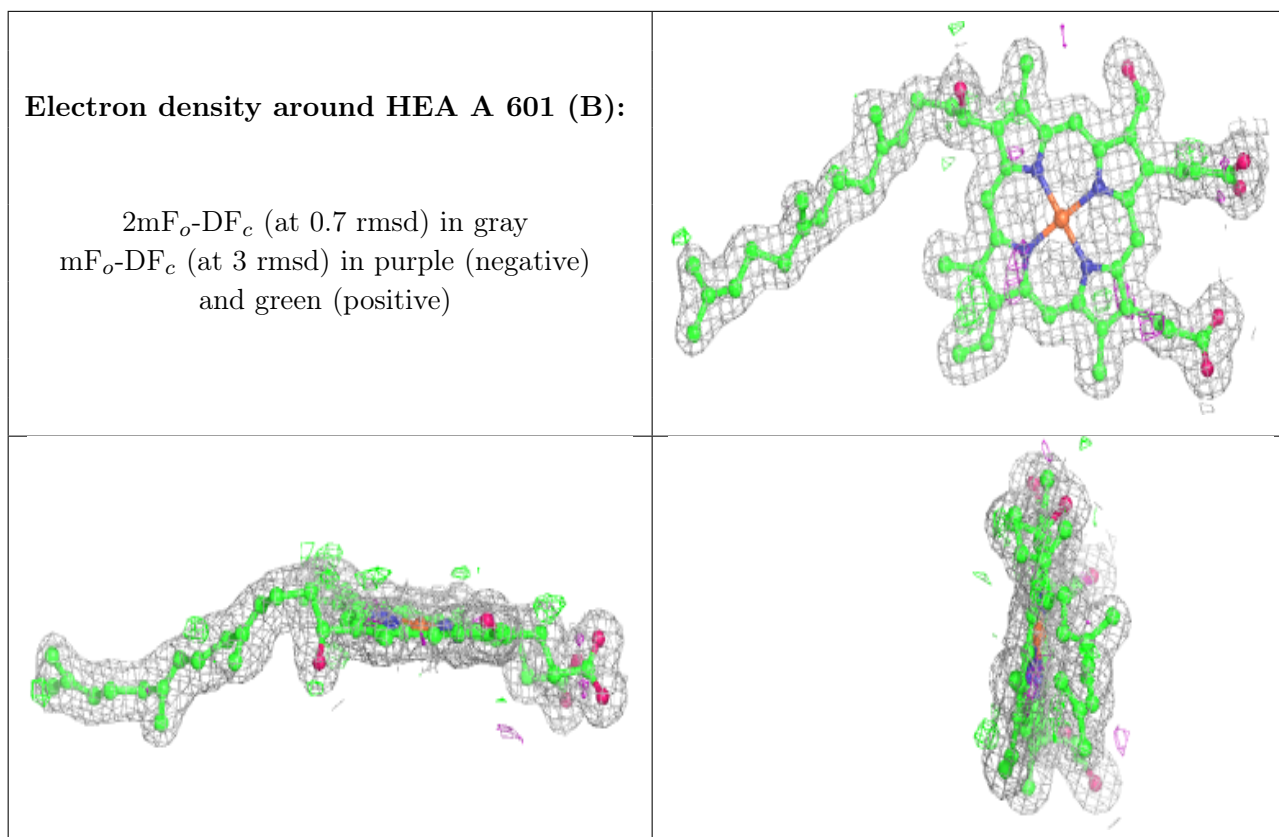
Electron density around HEA N 601 (B):

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

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

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





6.5 Other polymers [i](#)

There are no such residues in this entry.