



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:20 PM UTC

PDB ID : 7THU / pdb_00007thu
Title : Structure of reduced bovine cytochrome c oxidase at 1.93 Angstrom resolution
obtained by synchrotron X-rays
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.
Deposited on : 2022-01-12
Resolution : 1.93 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

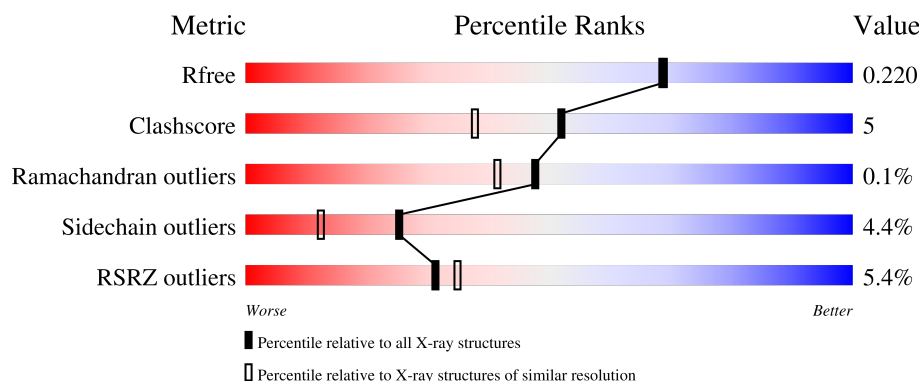
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	88% 11% .
1	N	514	87% 13% .
2	B	227	4% 83% 15% .
2	O	227	4% 81% 18% .
3	C	261	90% 9% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	EDO	N	614	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32695 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	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- 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	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	147	Total	C	N	O	S	0	0	0
			1214	788	201	221	4			
4	Q	147	Total	C	N	O	S	0	0	0
			1214	788	201	221	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			
11	X	52	Total	C	N	O	S	0	0	0
			413	266	72	73	2			

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

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

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

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

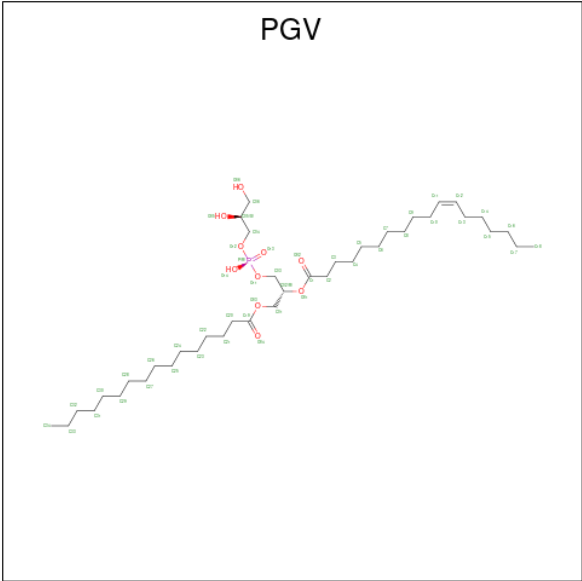
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

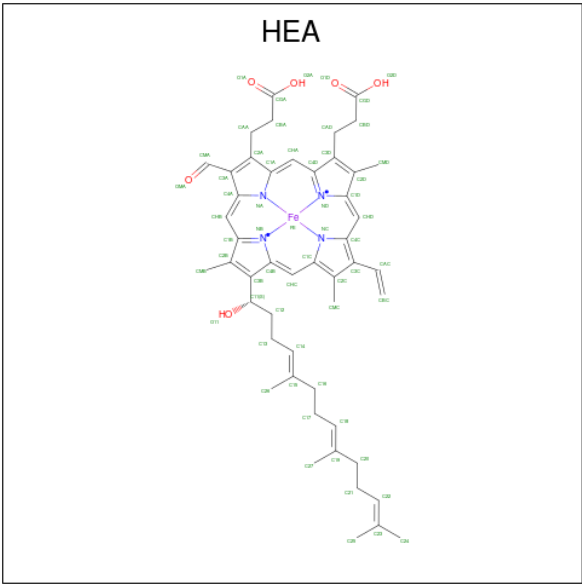
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 19 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total 4	C 2	O 2	0	0
19	F	1	Total 4	C 2	O 2	0	0
19	F	1	Total 4	C 2	O 2	0	0
19	F	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	M	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0

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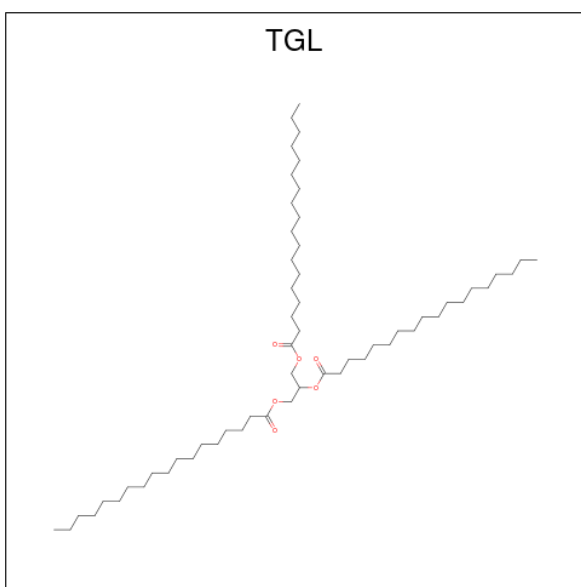
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	O	1	Total 4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

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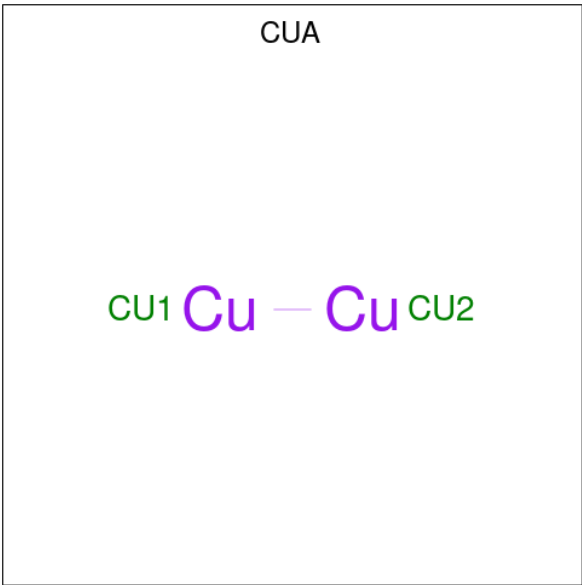
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	S	1	Total 4	C 2	O 2	0	0
19	T	1	Total 4	C 2	O 2	0	0
19	T	1	Total 4	C 2	O 2	0	0
19	U	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	V	1	Total 4	C 2	O 2	0	0
19	W	1	Total 4	C 2	O 2	0	0
19	W	1	Total 4	C 2	O 2	0	0
19	W	1	Total 4	C 2	O 2	0	0
19	Z	1	Total 4	C 2	O 2	0	0

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆) (labeled as "Ligand of Interest" by depositor).



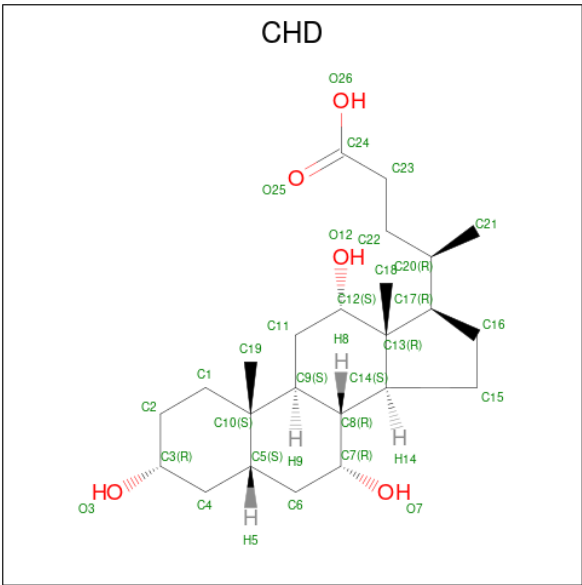
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	Q	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 22 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



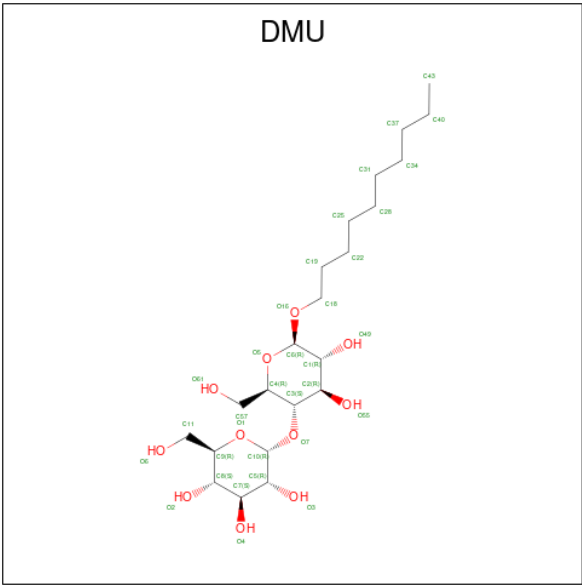
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	C	O	0
			29	24	5	
22	C	1	Total	C	O	0
			29	24	5	

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

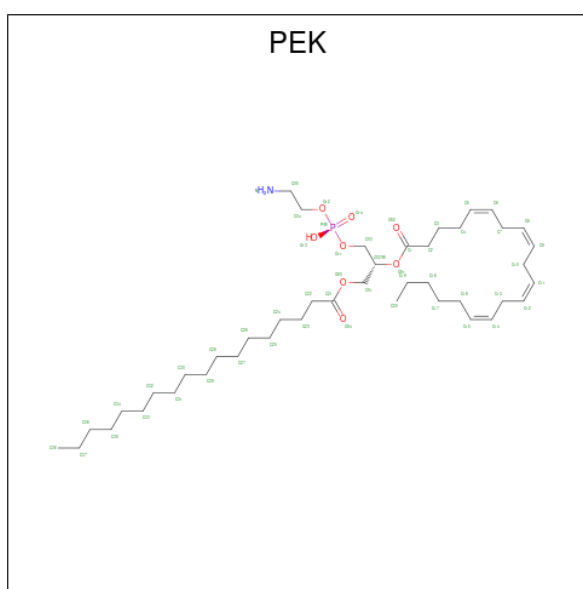
- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



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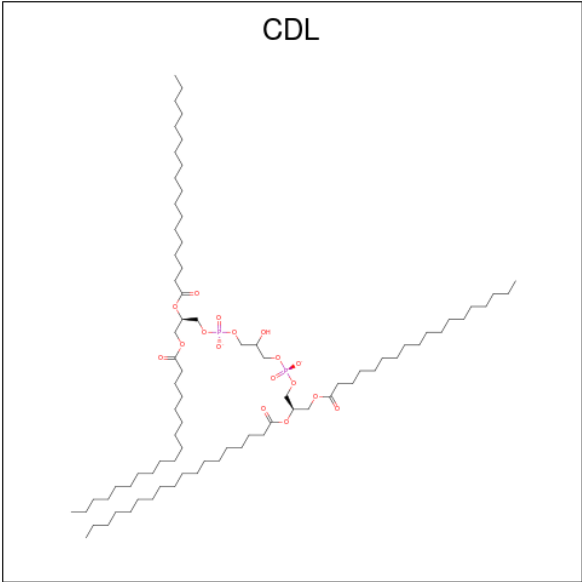
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	M	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



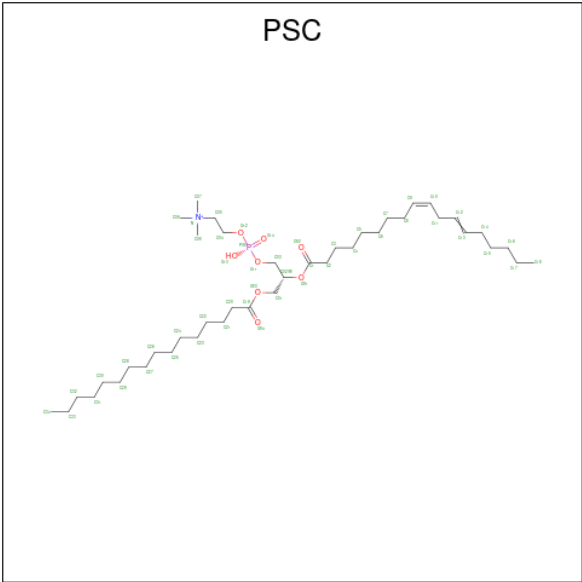
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

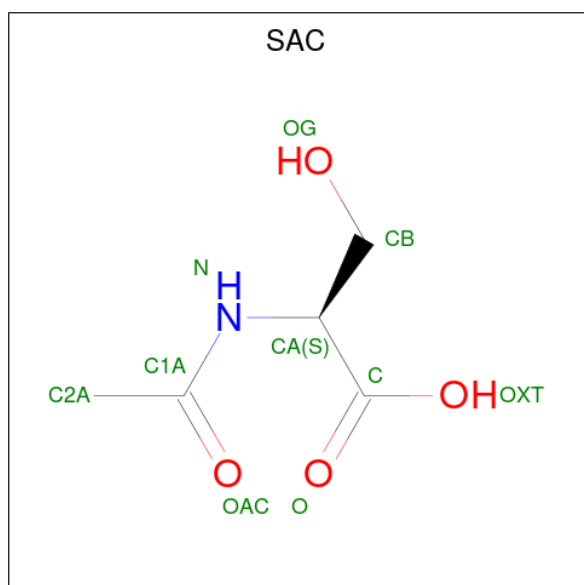


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is N-ACETYL-SERINE (CCD ID: SAC) (formula: C₅H₉NO₄).



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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	190	Total	O	0	0
			190	190		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	B	125	Total 125	O 125	0	0
29	C	96	Total 96	O 96	0	0
29	D	68	Total 68	O 68	0	0
29	E	53	Total 53	O 53	0	0
29	F	70	Total 70	O 70	0	0
29	G	35	Total 35	O 35	0	0
29	H	39	Total 39	O 39	0	0
29	I	24	Total 24	O 24	0	0
29	J	17	Total 17	O 17	0	0
29	K	9	Total 9	O 9	0	0
29	L	21	Total 21	O 21	0	0
29	M	14	Total 14	O 14	0	0
29	N	179	Total 179	O 179	0	0
29	O	85	Total 85	O 85	0	0
29	P	80	Total 80	O 80	0	0
29	Q	46	Total 46	O 46	0	0
29	R	46	Total 46	O 46	0	0
29	S	64	Total 64	O 64	0	0
29	T	23	Total 23	O 23	0	0
29	U	30	Total 30	O 30	0	0
29	V	16	Total 16	O 16	0	0

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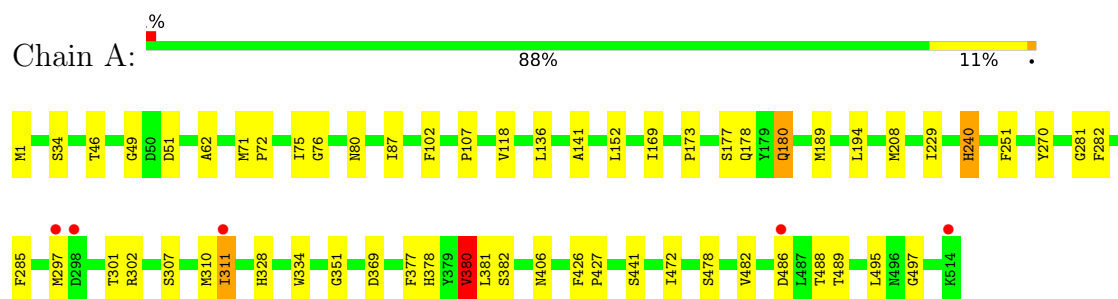
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	W	17	Total 17	O 17	0	0
29	X	11	Total 11	O 11	0	0
29	Y	18	Total 18	O 18	0	0
29	Z	5	Total 5	O 5	0	0

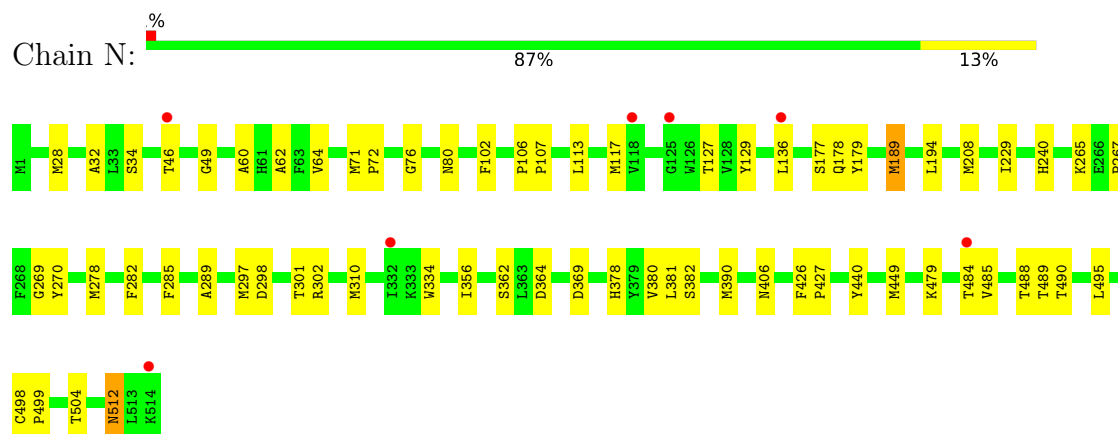
3 Residue-property plots [i](#)

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

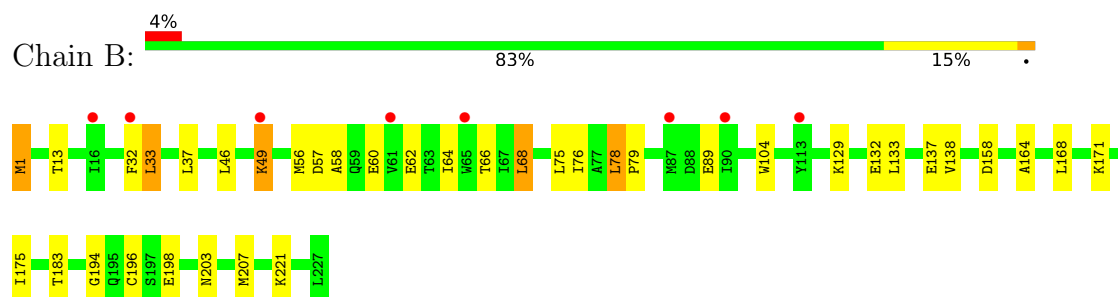
• Molecule 1: Cytochrome c oxidase subunit 1



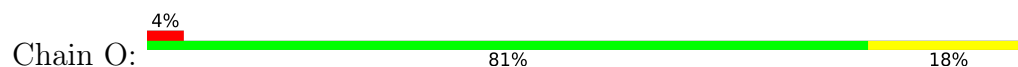
• Molecule 1: Cytochrome c oxidase subunit 1

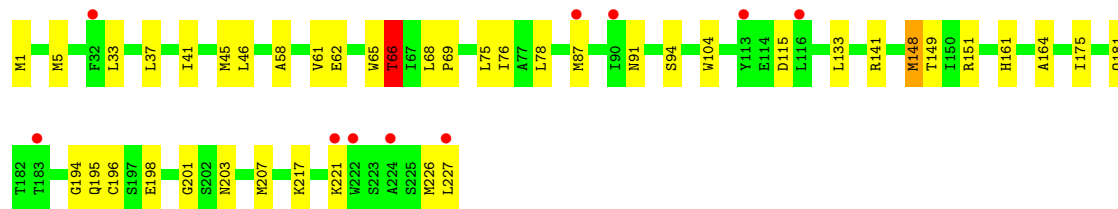


• Molecule 2: Cytochrome c oxidase subunit 2

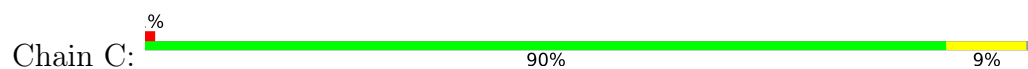


• Molecule 2: Cytochrome c oxidase subunit 2

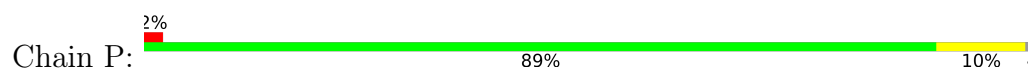




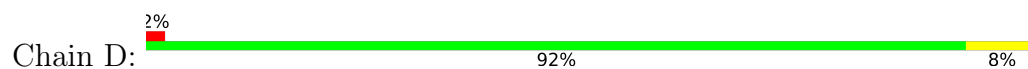
- Molecule 3: Cytochrome c oxidase subunit 3



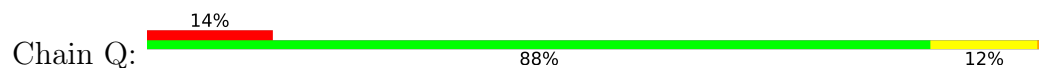
- Molecule 3: Cytochrome c oxidase subunit 3



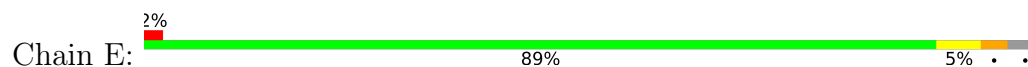
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



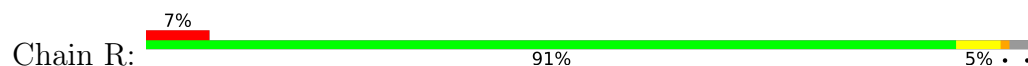
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

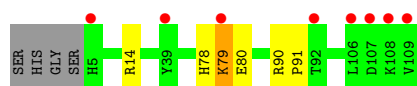


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



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

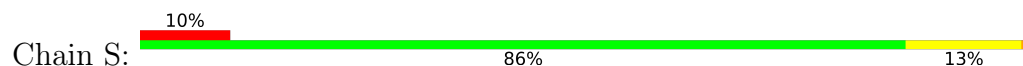




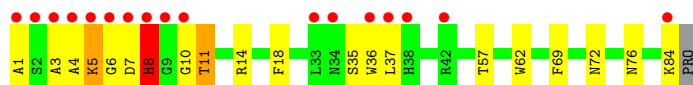
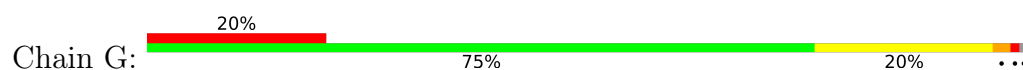
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



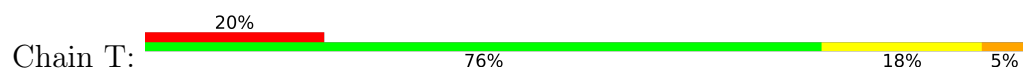
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



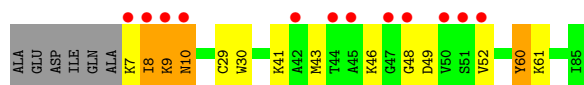
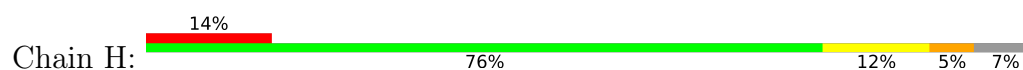
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



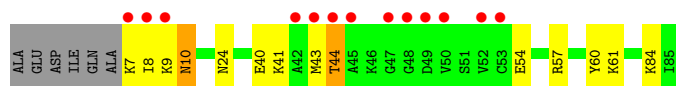
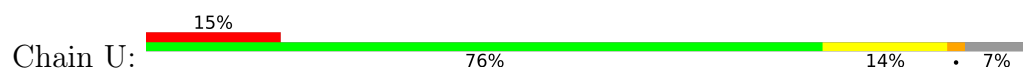
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



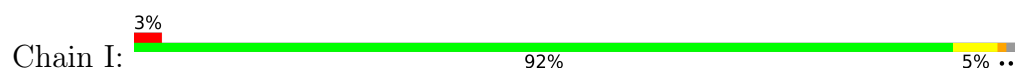
- Molecule 8: Cytochrome c oxidase subunit 6B1



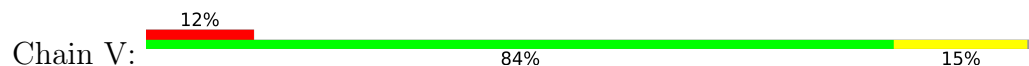
- Molecule 8: Cytochrome c oxidase subunit 6B1



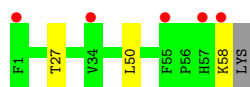
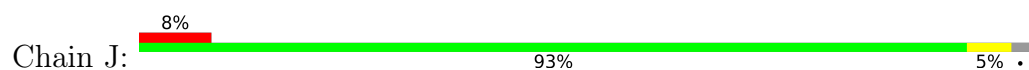
- Molecule 9: Cytochrome c oxidase subunit 6C



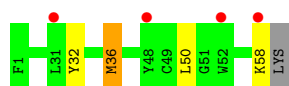
- Molecule 9: Cytochrome c oxidase subunit 6C



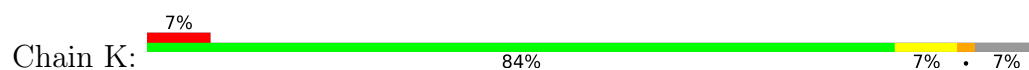
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



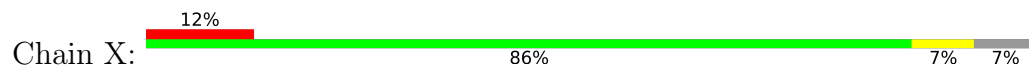
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



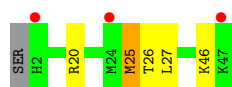
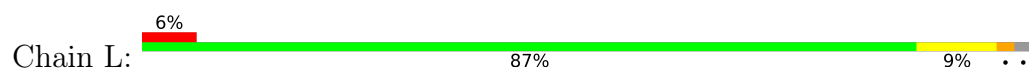
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



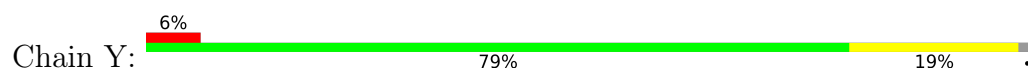
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



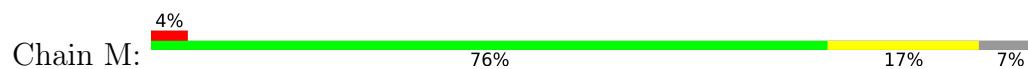
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



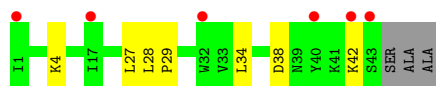
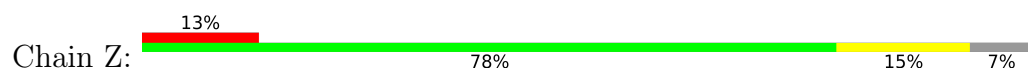
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	178.18Å 182.28Å 208.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.93 40.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.00-1.93) 99.1 (40.00-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.184 , 0.212 0.194 , 0.220	Depositor DCC
R_{free} test set	24681 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32695	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: PGV, DMU, CDL, CUA, PSC, CHD, FME, PEK, CU, MG, TGL, NA, ZN, HEA, SAC, TPO, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	1/4156 (0.0%)	1.35	7/5678 (0.1%)
1	N	1.09	0/4156	1.28	4/5678 (0.1%)
2	B	1.09	2/1860 (0.1%)	1.36	4/2534 (0.2%)
2	O	1.04	2/1860 (0.1%)	1.35	3/2534 (0.1%)
3	C	0.99	0/2197	1.31	1/3005 (0.0%)
3	P	1.07	0/2197	1.23	4/3005 (0.1%)
4	D	1.06	0/1249	1.29	0/1685
4	Q	1.05	0/1249	1.31	0/1685
5	E	1.04	0/871	1.35	0/1182
5	R	1.01	0/871	1.41	2/1182 (0.2%)
6	F	1.08	0/765	1.26	0/1038
6	S	1.05	0/765	1.27	0/1038
7	G	1.05	0/690	1.36	3/937 (0.3%)
7	T	1.04	0/690	1.31	1/937 (0.1%)
8	H	1.03	0/682	1.47	2/921 (0.2%)
8	U	0.99	0/682	1.43	0/921
9	I	0.98	0/605	1.45	0/802
9	V	0.99	0/605	1.40	0/802
10	J	0.95	0/471	1.39	0/636
10	W	1.08	0/471	1.27	0/636
11	K	1.07	0/427	1.37	0/584
11	X	1.08	0/427	1.38	0/584
12	L	0.98	0/393	1.44	2/526 (0.4%)
12	Y	1.07	0/393	1.34	0/526
13	M	1.02	0/345	1.42	0/470
13	Z	1.03	0/345	1.42	0/470
All	All	1.05	5/29422 (0.0%)	1.33	33/39996 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	7.28	1.32	1.23
2	O	198	GLU	C-O	6.75	1.31	1.23
1	A	240	HIS	CE1-NE2	5.67	1.38	1.32
2	B	221	LYS	C-O	5.25	1.30	1.24
2	O	161	HIS	CE1-NE2	5.02	1.37	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-9.95	103.85	113.80
1	A	240	HIS	CA-CB-CG	-9.18	104.62	113.80
1	A	240	HIS	N-CA-CB	7.67	117.68	110.39
2	O	66	THR	CB-CA-C	7.57	122.79	110.83
1	A	102	PHE	CA-CB-CG	-7.23	106.57	113.80
1	N	102	PHE	CA-CB-CG	-7.00	106.80	113.80
2	O	201	GLY	CA-C-N	6.47	129.27	120.54
2	O	201	GLY	C-N-CA	6.47	129.27	120.54
1	N	240	HIS	N-CA-CB	6.29	117.84	110.42
12	L	25	MET	CA-C-N	6.17	128.46	120.44
12	L	25	MET	C-N-CA	6.17	128.46	120.44
7	G	57	THR	N-CA-C	-6.17	105.91	113.50
1	A	251	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	380	VAL	N-CA-CB	5.83	118.04	110.57
8	H	41	LYS	CA-C-N	5.79	128.61	120.28
8	H	41	LYS	C-N-CA	5.79	128.61	120.28
2	B	158	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	75	ILE	N-CA-C	-5.65	106.20	111.45
7	G	8	HIS	CA-CB-CG	5.54	119.34	113.80
5	R	78	HIS	CA-C-N	5.53	128.25	120.28
5	R	78	HIS	C-N-CA	5.53	128.25	120.28
7	T	57	THR	N-CA-C	-5.52	106.71	113.50
1	N	301	THR	CA-CB-OG1	-5.47	101.39	109.60
2	B	138	VAL	CA-C-N	5.43	127.50	120.44
2	B	138	VAL	C-N-CA	5.43	127.50	120.44
1	A	301	THR	CA-CB-OG1	-5.30	101.65	109.60
3	C	233	PHE	CA-CB-CG	-5.26	108.54	113.80
3	P	122	HIS	CB-CA-C	5.19	116.05	110.65
3	P	29	SER	CA-C-N	5.19	125.70	119.94
3	P	29	SER	C-N-CA	5.19	125.70	119.94
7	G	18	PHE	CA-CB-CG	5.14	118.94	113.80
2	B	183	THR	CA-CB-OG1	-5.03	102.06	109.60
3	P	135	SER	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	47	0
1	N	4027	0	4001	62	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	24	0
3	C	2110	0	2027	24	0
3	P	2110	0	2027	17	0
4	D	1214	0	1201	11	0
4	Q	1214	0	1201	11	0
5	E	852	0	845	6	0
5	R	852	0	845	2	0
6	F	748	0	728	2	0
6	S	748	0	728	9	0
7	G	675	0	644	26	0
7	T	675	0	644	19	0
8	H	662	0	623	10	0
8	U	662	0	623	7	0
9	I	592	0	604	6	0
9	V	592	0	604	7	0
10	J	460	0	459	1	0
10	W	460	0	459	2	0
11	K	413	0	393	1	0
11	X	413	0	393	1	0
12	L	380	0	380	2	0
12	Y	380	0	380	4	0
13	M	335	0	352	5	0
13	Z	335	0	352	3	0
14	A	1	0	0	0	0
14	N	1	0	0	0	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	102	0	152	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	51	0	76	0	0
17	N	102	0	152	2	0
17	P	51	0	76	1	0
17	T	51	0	76	1	0
17	Z	51	0	76	2	0
18	A	120	0	108	3	0
18	N	120	0	108	5	0
19	A	48	0	72	6	0
19	B	28	0	42	0	0
19	C	20	0	30	0	0
19	D	28	0	42	0	0
19	E	16	0	24	0	0
19	F	16	0	24	1	0
19	G	16	0	24	2	0
19	I	8	0	12	0	0
19	J	16	0	24	2	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	48	0	72	11	0
19	O	8	0	12	0	0
19	P	12	0	18	0	0
19	Q	12	0	18	0	0
19	R	8	0	12	0	0
19	S	24	0	36	4	0
19	T	8	0	12	0	0
19	U	4	0	6	3	0
19	V	12	0	18	1	0
19	W	12	0	18	0	0
19	Z	4	0	6	0	0
20	A	63	0	110	1	0
20	D	63	0	110	7	0
20	L	63	0	110	2	0
20	N	63	0	110	0	0
20	Q	63	0	110	5	0
20	Y	63	0	110	2	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	39	0	0
22	C	58	0	78	1	0
22	G	29	0	39	1	0
22	J	29	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	P	58	0	78	1	0
22	T	29	0	39	7	0
22	W	29	0	39	0	0
22	Y	29	0	39	4	0
23	C	66	0	84	1	0
23	G	33	0	42	2	0
23	M	33	0	41	0	0
23	P	33	0	42	0	0
23	Z	33	0	42	1	0
24	C	159	0	231	8	0
24	P	159	0	231	6	0
25	C	200	0	312	15	0
25	P	100	0	156	4	0
25	T	100	0	156	3	0
26	E	52	0	80	5	0
26	O	52	0	80	5	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	I	9	0	8	2	0
28	V	9	0	8	1	0
29	A	190	0	0	0	0
29	B	125	0	0	1	0
29	C	96	0	0	7	0
29	D	68	0	0	0	0
29	E	53	0	0	0	0
29	F	70	0	0	0	0
29	G	35	0	0	0	0
29	H	39	0	0	1	0
29	I	24	0	0	0	0
29	J	17	0	0	0	0
29	K	9	0	0	0	0
29	L	21	0	0	2	0
29	M	14	0	0	0	0
29	N	179	0	0	7	0
29	O	85	0	0	3	0
29	P	80	0	0	1	0
29	Q	46	0	0	1	0
29	R	46	0	0	0	0
29	S	64	0	0	2	0
29	T	23	0	0	3	0
29	U	30	0	0	1	0
29	V	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	W	17	0	0	0	0
29	X	11	0	0	0	0
29	Y	18	0	0	1	0
29	Z	5	0	0	1	0
All	All	32695	0	32113	325	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 5.

All (325) 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)
3:C:44:MET:HG3	29:C:496:HOH:O	1.38	1.19
9:I:2:THR:N	28:I:101:SAC:HG	1.47	1.12
1:A:270:TYR:H	19:A:614:EDO:H11	1.21	1.04
24:P:305:PEK:C38	25:T:102:CDL:H271	1.91	1.00
7:T:73:PRO:HG3	7:T:84:LYS:HE2	1.49	0.94
1:N:270:TYR:H	19:N:614:EDO:H21	1.31	0.93
1:N:270:TYR:HB2	19:N:614:EDO:H11	1.51	0.93
7:G:72:ASN:H	7:G:76:ASN:HD22	1.15	0.89
7:G:11:TPO:HA	7:G:11:TPO:O2P	1.69	0.88
7:T:5:LYS:NZ	29:T:201:HOH:O	1.99	0.87
24:P:305:PEK:H383	25:T:102:CDL:H271	1.59	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.28	0.82
25:C:306:CDL:OA5	25:C:306:CDL:H1	1.78	0.81
6:S:94:HIS:HB2	29:S:2301:HOH:O	1.80	0.81
1:N:267:PRO:O	19:N:614:EDO:H12	1.79	0.81
22:T:104:CHD:H22	29:T:203:HOH:O	1.80	0.81
3:P:246:ASP:HB2	29:P:474:HOH:O	1.81	0.80
7:G:11:TPO:HG23	7:G:14:ARG:H	1.46	0.78
24:P:304:PEK:HN2	7:T:76:ASN:HD21	1.32	0.77
8:U:10:ASN:HA	29:U:1603:HOH:O	1.84	0.77
7:G:10:GLY:HA2	1:N:177:SER:HB2	1.66	0.76
6:S:94:HIS:CB	29:S:2301:HOH:O	2.33	0.76
3:C:149:HIS:NE2	23:G:1302:DMU:H5	2.01	0.76
1:N:270:TYR:N	19:N:614:EDO:H21	2.01	0.76
24:C:303:PEK:HN2	7:G:76:ASN:HD21	1.32	0.75
19:N:613:EDO:H11	29:N:793:HOH:O	1.86	0.75
9:V:50:PHE:O	19:V:103:EDO:H21	1.87	0.75
6:S:75:HIS:H	6:S:80:GLN:HE22	1.34	0.75
1:N:297:MET:HG3	1:N:302:ARG:HG3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.03	0.72
7:G:4:ALA:HB1	1:N:194:LEU:CD2	2.20	0.72
1:A:46:THR:HG22	1:A:49:GLY:H	1.55	0.71
8:H:43:MET:SD	8:U:43:MET:HE1	2.30	0.71
1:A:270:TYR:H	19:A:614:EDO:C1	2.00	0.71
1:A:486:ASP:OD1	4:D:19:ARG:HD2	1.90	0.70
1:A:194:LEU:CD2	7:T:4:ALA:HB1	2.21	0.70
8:U:24:ASN:HD21	19:U:1501:EDO:C1	2.04	0.70
1:A:281:GLY:C	7:T:4:ALA:HB3	2.18	0.69
8:U:24:ASN:HD21	19:U:1501:EDO:H11	1.58	0.68
3:C:258:TRP:CD1	25:C:312:CDL:H562	2.28	0.68
1:A:51:ASP:OD1	1:A:441:SER:OG	2.12	0.68
20:Q:201:TGL:HG31	20:Q:201:TGL:HC31	1.75	0.68
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.77	0.66
2:O:141:ARG:H	9:V:70:GLN:NE2	1.94	0.66
17:Z:102:PGV:H031	29:Z:201:HOH:O	1.96	0.66
3:P:54:MET:HE1	17:P:306:PGV:H131	1.77	0.66
7:G:72:ASN:H	7:G:76:ASN:ND2	1.92	0.65
25:C:312:CDL:H371	29:C:488:HOH:O	1.97	0.65
22:P:308:CHD:H183	22:P:308:CHD:H212	1.79	0.64
29:N:743:HOH:O	20:Q:201:TGL:HB32	1.98	0.63
3:C:127:LEU:CD1	25:C:312:CDL:H552	2.29	0.63
1:A:194:LEU:HD21	7:T:4:ALA:HB1	1.81	0.63
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.34	0.63
3:C:258:TRP:CE2	25:C:312:CDL:H542	2.34	0.63
1:N:270:TYR:H	19:N:614:EDO:C2	2.11	0.62
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.80	0.62
1:N:46:THR:HG22	1:N:49:GLY:H	1.64	0.62
7:G:4:ALA:HB1	1:N:194:LEU:HD23	1.82	0.61
12:Y:41:ARG:HH22	22:Y:102:CHD:H191	1.65	0.61
8:H:46:LYS:NZ	29:H:101:HOH:O	2.32	0.61
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.35	0.61
17:A:604:PGV:H11	13:M:15:GLN:HE22	1.66	0.61
1:N:76:GLY:O	1:N:80:ASN:HB2	2.00	0.61
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.30	0.60
7:T:78:LEU:HD22	7:T:84:LYS:HA	1.81	0.60
8:H:9:LYS:CE	8:H:9:LYS:HA	2.31	0.60
2:O:62:GLU:O	2:O:66:THR:HB	2.01	0.60
22:T:104:CHD:H192	29:T:203:HOH:O	2.02	0.59
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.37	0.59
24:C:304:PEK:H052	19:S:2206:EDO:H11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:71:HIS:NE2	7:T:84:LYS:HD2	2.16	0.59
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.38	0.59
4:Q:5:VAL:HG13	4:Q:5:VAL:O	2.03	0.59
1:A:87:ILE:O	1:A:173:PRO:HD3	2.03	0.58
29:L:220:HOH:O	13:M:32:TRP:HH2	1.85	0.58
19:A:616:EDO:H21	2:B:58:ALA:HB3	1.86	0.58
7:G:8:HIS:H	7:G:8:HIS:CD2	2.21	0.58
3:C:127:LEU:HD13	25:C:312:CDL:H552	1.86	0.57
1:N:289:ALA:HB1	1:N:297:MET:HE1	1.86	0.57
24:P:305:PEK:H382	25:T:102:CDL:H271	1.84	0.57
4:D:78:TRP:N	20:D:201:TGL:HB32	2.20	0.57
8:H:9:LYS:HA	8:H:9:LYS:NZ	2.19	0.56
26:O:302:PSC:H081	9:V:10:ARG:HE	1.71	0.56
2:O:141:ARG:H	9:V:70:GLN:HE22	1.52	0.56
1:A:297:MET:SD	1:A:302:ARG:HG2	2.46	0.56
26:E:201:PSC:H32	9:I:14:ALA:CB	2.35	0.56
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.21	0.56
3:C:98:PHE:CD2	24:C:315:PEK:H12	2.41	0.56
8:H:9:LYS:HA	8:H:9:LYS:HZ2	1.71	0.56
1:N:46:THR:HG21	1:N:49:GLY:HA2	1.88	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.55
1:N:62:ALA:HB2	18:N:607:HEA:HBD1	1.89	0.55
1:N:488:THR:HB	1:N:495:LEU:HD13	1.89	0.55
7:T:67:HIS:NE2	7:T:84:LYS:HB2	2.22	0.55
1:N:267:PRO:O	19:N:614:EDO:C1	2.53	0.54
1:A:169:ILE:CD1	1:A:189:MET:HE1	2.38	0.54
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.90	0.54
19:N:619:EDO:H21	6:S:32:ASN:HD21	1.72	0.54
25:C:312:CDL:H351	29:C:488:HOH:O	2.06	0.54
4:D:23:PRO:HG3	5:E:70:VAL:HG21	1.89	0.54
7:T:73:PRO:CG	7:T:84:LYS:HE2	2.32	0.54
18:N:607:HEA:HMC1	18:N:607:HEA:HBC1	1.88	0.54
25:C:312:CDL:H381	29:O:422:HOH:O	2.07	0.53
4:D:78:TRP:H	20:D:201:TGL:HB32	1.74	0.53
1:N:34:SER:HB2	18:N:607:HEA:C2B	2.39	0.53
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.43	0.53
22:G:1305:CHD:H3	2:O:66:THR:HG21	1.90	0.53
29:N:782:HOH:O	19:S:2201:EDO:C1	2.55	0.53
2:B:57:ASP:H	26:E:201:PSC:H222	1.74	0.53
10:W:32:TYR:CE1	10:W:36:MET:HG3	2.44	0.53
1:N:270:TYR:CB	19:N:614:EDO:H11	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.44	0.52
1:A:482:VAL:O	19:A:613:EDO:H21	2.08	0.52
11:K:16:ALA:O	11:K:20:SER:OG	2.26	0.52
1:N:512:ASN:C	1:N:512:ASN:HD22	2.16	0.52
24:C:304:PEK:H011	24:C:304:PEK:H21	1.91	0.52
4:D:78:TRP:HA	20:D:201:TGL:HB52	1.91	0.52
7:T:16:TRP:HE1	22:T:104:CHD:H152	1.74	0.52
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.92	0.52
22:T:104:CHD:H151	22:T:104:CHD:O7	2.10	0.52
10:W:36:MET:HE3	10:W:36:MET:HA	1.92	0.52
7:G:8:HIS:CB	1:N:179:TYR:OH	2.58	0.52
12:L:25:MET:HG2	20:L:101:TGL:HA71	1.91	0.52
25:C:312:CDL:C35	29:C:488:HOH:O	2.58	0.51
8:U:24:ASN:HD21	19:U:1501:EDO:H12	1.75	0.51
7:G:8:HIS:HB3	1:N:179:TYR:OH	2.10	0.51
22:Y:102:CHD:H41	29:Y:218:HOH:O	2.10	0.51
1:A:62:ALA:HB2	18:A:607:HEA:HBD1	1.91	0.51
17:A:604:PGV:H11	13:M:15:GLN:NE2	2.25	0.51
26:E:201:PSC:H32	9:I:14:ALA:HA	1.93	0.51
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.93	0.51
24:C:303:PEK:C12	24:C:303:PEK:H162	2.41	0.51
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.50
1:A:46:THR:HG21	1:A:49:GLY:HA2	1.91	0.50
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.76	0.50
8:H:9:LYS:HD3	8:H:10:ASN:H	1.77	0.50
7:G:5:LYS:HB3	1:N:278:MET:CG	2.42	0.50
3:C:246:ASP:HB2	29:C:479:HOH:O	2.12	0.50
6:F:64:GLU:O	6:F:65:ASP:HB2	2.11	0.50
1:N:406:ASN:HD21	17:Z:102:PGV:H71	1.77	0.50
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.93	0.50
3:C:153:GLU:OE2	7:G:11:TPO:HG22	2.11	0.49
22:C:302:CHD:H183	22:C:302:CHD:H212	1.93	0.49
7:G:69:PHE:O	19:G:1303:EDO:H11	2.12	0.49
2:B:56:MET:HA	26:E:201:PSC:H222	1.94	0.49
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.93	0.49
2:O:227:LEU:HD12	2:O:227:LEU:OXT	2.13	0.49
1:A:281:GLY:C	7:T:4:ALA:CB	2.86	0.49
29:N:782:HOH:O	19:S:2201:EDO:H11	2.12	0.49
18:A:607:HEA:HBC1	18:A:607:HEA:HMC1	1.95	0.49
1:N:113:LEU:HB2	20:Y:101:TGL:H323	1.94	0.49
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:27:LEU:HD22	23:Z:101:DMU:H14	1.94	0.49
1:A:282:PHE:N	7:T:4:ALA:HB3	2.27	0.49
20:D:201:TGL:HB42	20:D:201:TGL:HG11	1.94	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
1:A:169:ILE:HD11	1:A:189:MET:HE1	1.94	0.48
3:C:127:LEU:HD11	25:C:312:CDL:H552	1.95	0.48
9:I:2:THR:N	28:I:101:SAC:OG	2.28	0.48
6:S:92:VAL:O	6:S:92:VAL:HG23	2.13	0.48
1:N:302:ARG:HD3	29:N:728:HOH:O	2.12	0.48
3:P:59:ARG:HA	25:P:307:CDL:H512	1.94	0.48
9:V:25:PHE:CD2	9:V:26:MET:CE	2.97	0.48
22:Y:102:CHD:H192	22:Y:102:CHD:H3	1.95	0.48
1:A:178:GLN:HG3	7:T:7:ASP:HB2	1.93	0.48
3:C:29:SER:HB2	19:J:1104:EDO:H12	1.95	0.48
24:C:303:PEK:C12	24:C:303:PEK:C16	2.91	0.48
2:B:49:LYS:O	4:D:20:ARG:NH2	2.42	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.95	0.48
1:N:298:ASP:OD2	17:N:616:PGV:O06	2.27	0.48
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.96	0.48
1:N:449:MET:SD	2:O:5:MET:HG2	2.54	0.48
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
12:Y:42:HIS:ND1	22:Y:102:CHD:H151	2.29	0.48
10:J:27:THR:HG22	19:J:1101:EDO:H22	1.94	0.48
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	1.96	0.48
7:G:6:GLY:HA3	1:N:189:MET:HG2	1.96	0.48
5:R:79:LYS:HE3	5:R:79:LYS:HA	1.94	0.48
2:B:129:LYS:NZ	29:B:407:HOH:O	2.47	0.47
1:N:297:MET:CG	1:N:302:ARG:HG3	2.40	0.47
7:G:62:TRP:CD1	19:G:1303:EDO:H22	2.49	0.47
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.79	0.47
3:C:258:TRP:CZ2	25:C:312:CDL:H542	2.49	0.47
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.97	0.47
3:C:39:SER:OG	23:C:313:DMU:H30	2.14	0.47
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.95	0.47
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.45	0.47
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.13	0.47
20:Y:101:TGL:HB21	20:Y:101:TGL:HG12	1.95	0.47
1:A:478:SER:O	13:M:6:ALA:HB1	2.14	0.47
1:N:362:SER:HA	2:O:87:MET:HE1	1.97	0.47
2:O:94:SER:OG	2:O:148:MET:HE3	2.14	0.47
7:T:72:ASN:N	7:T:76:ASN:HD22	2.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:ALA:O	2:B:62:GLU:HG3	2.14	0.47
26:O:302:PSC:H262	26:O:302:PSC:H221	1.97	0.47
1:A:76:GLY:O	1:A:80:ASN:HB2	2.15	0.47
1:A:377:PHE:O	1:A:381:LEU:HB3	2.15	0.47
1:A:488:THR:HB	1:A:495:LEU:HD13	1.97	0.47
2:B:49:LYS:HE2	4:D:20:ARG:CZ	2.45	0.46
25:C:312:CDL:C37	29:C:488:HOH:O	2.57	0.46
6:S:96:LEU:HD23	6:S:96:LEU:C	2.40	0.46
7:G:5:LYS:HB3	1:N:278:MET:HG2	1.98	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.98	0.46
1:A:489:THR:HA	6:F:71:TRP:O	2.15	0.46
7:G:1:ALA:CB	3:P:92:LEU:HD21	2.46	0.46
1:N:489:THR:HA	6:S:71:TRP:O	2.15	0.46
25:P:307:CDL:H711	25:P:307:CDL:H131	1.97	0.46
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.96	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.16	0.46
3:C:88:ILE:HG12	24:C:315:PEK:H231	1.98	0.46
25:C:312:CDL:H471	29:O:484:HOH:O	2.16	0.46
20:Q:201:TGL:HC22	20:Q:201:TGL:HG11	1.98	0.46
1:N:479:LYS:NZ	29:N:706:HOH:O	2.49	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.97	0.45
25:P:307:CDL:OA7	25:P:307:CDL:H673	2.16	0.45
2:B:64:ILE:HG23	2:B:68:LEU:HD22	1.98	0.45
1:N:426:PHE:N	1:N:427:PRO:CD	2.79	0.45
1:A:307:SER:O	1:A:311:ILE:HG23	2.15	0.45
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.97	0.45
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.29	0.45
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.98	0.45
4:Q:16:TYR:OH	4:Q:18:ASP:OD2	2.30	0.45
1:A:270:TYR:N	19:A:614:EDO:H11	2.06	0.45
7:G:1:ALA:HB2	3:P:92:LEU:HD21	1.99	0.45
20:D:201:TGL:HC42	20:D:201:TGL:HG31	1.98	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.98	0.45
8:H:8:ILE:O	8:H:8:ILE:HG22	2.17	0.45
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.99	0.44
3:C:208:VAL:HG22	3:C:245:VAL:CG1	2.48	0.44
5:E:52:LEU:O	5:E:55:CYS:HB2	2.17	0.44
4:Q:7:LYS:HE3	13:Z:4:LYS:HG2	1.98	0.44
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.97	0.44
29:C:484:HOH:O	7:G:11:TPO:HG21	2.17	0.44
4:Q:78:TRP:HB3	20:Q:201:TGL:HB42	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:109:HIS:HD2	29:Q:331:HOH:O	2.00	0.44
6:S:85:CYS:SG	6:S:87:THR:HG23	2.57	0.44
8:U:40:GLU:O	8:U:44:THR:HB	2.18	0.44
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.48	0.44
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.17	0.44
3:P:116:TRP:HA	3:P:117:PRO:C	2.43	0.44
4:Q:122:ARG:HG2	4:Q:126:MET:HE2	1.99	0.44
5:E:90:ARG:HD3	5:E:90:ARG:HA	1.83	0.43
12:L:46:LYS:HD2	29:L:217:HOH:O	2.18	0.43
28:V:101:SAC:C	28:V:101:SAC:H2A1	2.48	0.43
1:A:497:GLY:HA2	19:A:608:EDO:H11	2.00	0.43
29:N:782:HOH:O	19:S:2201:EDO:H12	2.17	0.43
1:N:46:THR:CG2	1:N:49:GLY:H	2.31	0.43
2:O:226:MET:HE2	2:O:226:MET:HA	2.01	0.43
22:T:104:CHD:H181	22:T:104:CHD:C22	2.48	0.43
1:A:328:HIS:NE2	26:E:201:PSC:H22	2.33	0.43
4:D:122:ARG:HG2	4:D:126:MET:HE2	2.01	0.43
1:N:310:MET:HE1	2:O:76:ILE:HG21	2.00	0.43
26:O:302:PSC:C08	9:V:10:ARG:HH21	2.32	0.43
3:P:67:PHE:CE1	25:P:307:CDL:HB22	2.53	0.43
17:N:605:PGV:H101	17:N:605:PGV:H132	1.77	0.43
19:N:614:EDO:H22	29:O:431:HOH:O	2.18	0.43
1:A:472:ILE:HG21	20:L:101:TGL:H202	2.01	0.43
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.18	0.43
7:T:67:HIS:NE2	7:T:84:LYS:HG3	2.33	0.43
1:N:364:ASP:OD2	18:N:606:HEA:O2A	2.36	0.43
1:N:390:MET:HA	1:N:390:MET:HE3	2.01	0.43
4:D:29:HIS:HD2	4:D:61:ARG:O	2.02	0.42
4:D:73:ARG:HB3	5:E:109:VAL:HG11	2.00	0.42
26:O:302:PSC:H211	26:O:302:PSC:H252	2.00	0.42
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.01	0.42
1:A:34:SER:HB2	18:A:607:HEA:C2B	2.49	0.42
1:A:378:HIS:HA	1:A:382:SER:OG	2.19	0.42
24:C:303:PEK:H221	24:C:303:PEK:H251	1.90	0.42
3:P:186:PHE:HA	3:P:190:ASP:OD2	2.20	0.42
17:A:604:PGV:H142	13:M:12:PRO:HG3	2.00	0.42
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.50	0.42
25:C:306:CDL:CB2	25:C:306:CDL:CB3	2.96	0.42
4:D:78:TRP:CA	20:D:201:TGL:HB52	2.49	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.54	0.42
22:T:104:CHD:H181	22:T:104:CHD:C23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:28:GLU:OE1	19:F:702:EDO:C1	2.68	0.42
1:N:28:MET:HE3	12:Y:29:PHE:CD2	2.54	0.42
1:N:378:HIS:HA	1:N:382:SER:OG	2.19	0.42
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.68	0.42
1:A:118:VAL:HG11	1:A:141:ALA:HB3	2.02	0.42
24:P:305:PEK:H012	24:P:305:PEK:O14	2.20	0.42
2:B:32:PHE:CD1	9:I:31:PHE:CZ	3.08	0.42
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.55	0.42
3:C:47:LEU:O	3:C:51:MET:HG2	2.19	0.42
2:O:164:ALA:O	2:O:194:GLY:HA3	2.20	0.42
26:O:302:PSC:H222	26:O:302:PSC:C1	2.49	0.42
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.55	0.42
1:A:406:ASN:HD21	17:A:604:PGV:H02	1.84	0.42
1:N:60:ALA:O	1:N:64:VAL:HG23	2.20	0.42
1:A:351:GLY:C	1:A:380:VAL:HG13	2.45	0.41
7:G:4:ALA:CB	1:N:285:PHE:CE2	3.02	0.41
7:G:3:ALA:HA	1:N:282:PHE:CD1	2.55	0.41
3:C:103:HIS:HA	17:T:101:PGV:H012	2.02	0.41
22:T:104:CHD:O7	22:T:104:CHD:C15	2.68	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.97	0.41
18:N:607:HEA:HBC1	18:N:607:HEA:CMC	2.50	0.41
1:A:240:HIS:CD2	1:A:240:HIS:C	2.97	0.41
20:A:615:TGL:H283	20:A:615:TGL:H121	2.02	0.41
2:O:65:TRP:O	2:O:69:PRO:HG2	2.21	0.41
3:P:161:GLN:HE22	24:P:305:PEK:H31	1.85	0.41
8:U:54:GLU:OE2	8:U:57:ARG:NH2	2.44	0.41
1:A:46:THR:CG2	1:A:49:GLY:H	2.29	0.41
1:A:426:PHE:N	1:A:427:PRO:CD	2.82	0.41
3:C:149:HIS:CE1	23:G:1302:DMU:H5	2.55	0.41
3:C:186:PHE:HA	3:C:190:ASP:OD2	2.21	0.41
7:G:1:ALA:HB1	3:P:92:LEU:HD11	2.02	0.41
7:G:4:ALA:CB	1:N:285:PHE:HE2	2.34	0.41
8:H:60:TYR:CD1	8:H:60:TYR:C	2.98	0.41
1:N:269:GLY:N	19:N:614:EDO:H21	2.35	0.41
3:P:29:SER:HB2	3:P:42:LEU:HD13	2.03	0.41
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.56	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.94	0.41
7:G:4:ALA:CB	1:N:194:LEU:CD2	2.95	0.40
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.56	0.40
2:B:13:THR:HB	2:B:168:LEU:HD23	2.02	0.40
3:C:258:TRP:NE1	25:C:312:CDL:C56	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.40
4:Q:2:HIS:O	4:Q:2:HIS:CG	2.72	0.40
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.56	0.40
3:P:129:VAL:N	3:P:130:PRO:CD	2.84	0.40
20:D:201:TGL:CC3	20:D:201:TGL:CG3	3.00	0.40
20:Q:201:TGL:H352	9:V:16:ARG:HE	1.86	0.40
8:H:49:ASP:O	8:H:52:VAL:HG22	2.21	0.40
1:N:127:THR:HB	1:N:129:TYR:CE2	2.57	0.40
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	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	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
2	O	225/227 (99%)	219 (97%)	6 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	145/147 (99%)	142 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
7	G	81/85 (95%)	77 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	3
8	H	77/85 (91%)	71 (92%)	5 (6%)	1 (1%)	9	3
8	U	77/85 (91%)	71 (92%)	6 (8%)	0	100	100
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	68 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
11	X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3514/3614 (97%)	3412 (97%)	100 (3%)	2 (0%)	48	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	48	GLY
7	T	4	ALA

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	426/426 (100%)	420 (99%)	6 (1%)	59	52
1	N	426/426 (100%)	415 (97%)	11 (3%)	40	28
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	10
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	8
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	35
4	D	129/129 (100%)	126 (98%)	3 (2%)	44	33
4	Q	129/129 (100%)	124 (96%)	5 (4%)	28	15
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	20
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	20
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	16
6	S	81/81 (100%)	76 (94%)	5 (6%)	16	5
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	1
7	T	67/68 (98%)	59 (88%)	8 (12%)	5	0
8	H	71/75 (95%)	64 (90%)	7 (10%)	7	1
8	U	71/75 (95%)	62 (87%)	9 (13%)	4	0
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	7
9	V	57/57 (100%)	52 (91%)	5 (9%)	9	2
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	14
10	W	49/50 (98%)	46 (94%)	3 (6%)	17	5
11	K	42/46 (91%)	38 (90%)	4 (10%)	8	1
11	X	42/46 (91%)	39 (93%)	3 (7%)	13	3
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	3
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	0
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	1
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	2
All	All	3048/3082 (99%)	2914 (96%)	134 (4%)	25	12

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	152	LEU
1	A	180	GLN
1	A	311	ILE
1	A	369	ASP
1	A	380	VAL
2	B	33	LEU
2	B	37	LEU
2	B	49	LYS

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Mol	Chain	Res	Type
2	B	60	GLU
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	89	GLU
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	230	ASN
4	D	31	LYS
4	D	51	LEU
4	D	147	LYS
5	E	70	VAL
5	E	90	ARG
5	E	109	VAL
6	F	43	LYS
6	F	48	LEU
6	F	96	LEU
7	G	5	LYS
7	G	7	ASP
7	G	8	HIS
7	G	35	SER
7	G	36	TRP
7	G	37	LEU
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	10	ASN
8	H	29	CYS
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	18	ARG
9	I	29	LEU
10	J	50	LEU
10	J	58	LYS
11	K	12	LYS
11	K	20	SER
11	K	51	LYS
11	K	54	ARG

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Mol	Chain	Res	Type
12	L	20	ARG
12	L	26	THR
12	L	27	LEU
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	117	MET
1	N	136	LEU
1	N	178	GLN
1	N	189	MET
1	N	369	ASP
1	N	380	VAL
1	N	381	LEU
1	N	484	THR
1	N	485	VAL
1	N	504	THR
1	N	512	ASN
2	O	33	LEU
2	O	37	LEU
2	O	61	VAL
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	115	ASP
2	O	148	MET
2	O	217	LYS
2	O	221	LYS
3	P	3	HIS
3	P	127	LEU
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
4	Q	2	HIS
4	Q	6	VAL
4	Q	33	LEU
4	Q	53	ILE
4	Q	58	GLU
5	R	14	ARG
5	R	79	LYS
5	R	80	GLU

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Mol	Chain	Res	Type
6	S	19	GLU
6	S	48	LEU
6	S	54	ASN
6	S	80	GLN
6	S	91	LEU
7	T	2	SER
7	T	5	LYS
7	T	7	ASP
7	T	30	LEU
7	T	33	LEU
7	T	37	LEU
7	T	83	GLU
7	T	84	LYS
8	U	7	LYS
8	U	8	ILE
8	U	9	LYS
8	U	10	ASN
8	U	41	LYS
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	29	LEU
9	V	44	LYS
9	V	45	LYS
9	V	61	GLU
9	V	65	LYS
10	W	36	MET
10	W	50	LEU
10	W	58	LYS
11	X	5	ARG
11	X	12	LYS
11	X	56	GLN
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
12	Y	27	LEU
12	Y	47	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	180	GLN
1	A	422	ASN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
3	C	50	ASN
3	C	68	GLN
3	C	230	ASN
4	D	29	HIS
4	D	32	ASN
4	D	119	GLN
5	E	78	HIS
5	E	94	ASN
6	F	54	ASN
7	G	8	HIS
7	G	71	HIS
7	G	76	ASN
8	H	23	GLN
8	H	31	GLN
10	J	29	ASN
11	K	35	GLN
1	N	178	GLN
1	N	232	GLN
1	N	422	ASN
1	N	512	ASN
2	O	59	GLN
2	O	91	ASN
2	O	181	GLN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	32	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN

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Mol	Chain	Res	Type
8	U	28	ASN
8	U	32	ASN
9	V	8	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	0.77	0	8,9,11	1.15	1 (12%)
1	FME	N	1	1	8,9,10	0.56	0	8,9,11	1.11	0
7	TPO	G	11	7	8,10,11	1.37	1 (12%)	10,14,16	1.33	1 (10%)
7	TPO	T	11	7	8,10,11	0.97	1 (12%)	10,14,16	0.95	0
2	FME	O	1	2	8,9,10	0.39	0	8,9,11	0.87	0
1	FME	A	1	1	8,9,10	0.31	0	8,9,11	0.83	1 (12%)

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
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	6/9/11/13	-
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	1/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	3.23	1.65	1.59
7	T	11	TPO	P-OG1	2.14	1.63	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	11	TPO	P-OG1-CB	3.31	132.33	123.33
2	B	1	FME	O-C-CA	-2.04	119.51	124.77
1	A	1	FME	O-C-CA	-2.02	119.57	124.77

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0
7	G	11	TPO	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 149 ligands modelled in this entry, 8 are monoatomic - leaving 141 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
19	EDO	G	1304	-	3,3,3	0.16	0	2,2,2	0.31	0
22	CHD	Y	102	-	32,32,32	0.59	0	51,51,51	0.95	3 (5%)
19	EDO	B	306	-	3,3,3	0.22	0	2,2,2	0.22	0
19	EDO	N	610	-	3,3,3	0.39	0	2,2,2	0.67	0
19	EDO	V	103	-	3,3,3	0.16	0	2,2,2	0.29	0
25	CDL	P	307	-	99,99,99	0.34	0	105,111,111	0.52	1 (0%)
19	EDO	I	102	-	3,3,3	0.10	0	2,2,2	0.17	0
19	EDO	P	309	-	3,3,3	0.16	0	2,2,2	0.25	0
19	EDO	K	102	-	3,3,3	0.12	0	2,2,2	0.24	0
19	EDO	N	608	-	3,3,3	0.25	0	2,2,2	0.38	0
18	HEA	N	607	1	67,67,67	2.34	24 (35%)	81,103,103	2.79	35 (43%)
21	CUA	B	301	2	0,1,1	-	-	-	-	-
19	EDO	N	618	-	3,3,3	0.17	0	2,2,2	0.07	0
19	EDO	B	308	-	3,3,3	0.08	0	2,2,2	0.04	0
19	EDO	L	102	-	3,3,3	0.25	0	2,2,2	0.33	0
19	EDO	Q	202	-	3,3,3	0.18	0	2,2,2	0.29	0
22	CHD	C	307	-	32,32,32	0.62	0	51,51,51	0.78	0
19	EDO	D	203	-	3,3,3	0.09	0	2,2,2	0.06	0
19	EDO	J	1103	-	3,3,3	0.09	0	2,2,2	0.09	0
24	PEK	P	301	-	52,52,52	0.32	0	55,57,57	0.47	0
19	EDO	N	617	-	3,3,3	0.04	0	2,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	U	1501	-	3,3,3	0.26	0	2,2,2	0.45	0
19	EDO	M	102	-	3,3,3	0.12	0	2,2,2	0.12	0
17	PGV	N	616	-	50,50,50	1.04	2 (4%)	53,56,56	1.06	4 (7%)
24	PEK	C	304	-	52,52,52	0.36	0	55,57,57	0.52	0
22	CHD	P	303	-	32,32,32	0.69	1 (3%)	51,51,51	0.73	0
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.27	0
19	EDO	A	610	-	3,3,3	0.25	0	2,2,2	0.21	0
19	EDO	C	309	-	3,3,3	0.02	0	2,2,2	0.15	0
19	EDO	N	611	-	3,3,3	0.19	0	2,2,2	0.07	0
28	SAC	V	101	-	7,8,9	0.50	0	7,9,11	1.17	1 (14%)
22	CHD	T	104	-	32,32,32	0.72	0	51,51,51	1.26	6 (11%)
19	EDO	Z	103	-	3,3,3	0.23	0	2,2,2	0.26	0
19	EDO	A	619	-	3,3,3	0.36	0	2,2,2	0.48	0
19	EDO	E	204	-	3,3,3	0.11	0	2,2,2	0.28	0
19	EDO	O	303	-	3,3,3	0.46	0	2,2,2	0.65	0
24	PEK	P	304	-	52,52,52	0.43	0	55,57,57	0.72	1 (1%)
19	EDO	C	310	-	3,3,3	0.08	0	2,2,2	0.09	0
23	DMU	P	302	-	34,34,34	1.11	2 (5%)	45,45,45	1.96	9 (20%)
19	EDO	A	613	-	3,3,3	0.38	0	2,2,2	0.35	0
19	EDO	S	2201	-	3,3,3	0.40	0	2,2,2	0.50	0
20	TGL	N	604	-	62,62,62	0.27	0	65,65,65	0.46	1 (1%)
19	EDO	A	618	-	3,3,3	0.16	0	2,2,2	0.49	0
19	EDO	S	2203	-	3,3,3	0.35	0	2,2,2	0.23	0
19	EDO	C	308	-	3,3,3	0.37	0	2,2,2	0.11	0
19	EDO	D	208	-	3,3,3	0.16	0	2,2,2	0.10	0
19	EDO	E	202	-	3,3,3	0.13	0	2,2,2	0.21	0
20	TGL	A	615	-	62,62,62	0.36	0	65,65,65	0.48	1 (1%)
20	TGL	L	101	-	62,62,62	0.35	0	65,65,65	0.27	0
19	EDO	K	101	-	3,3,3	0.08	0	2,2,2	0.15	0
19	EDO	D	205	-	3,3,3	0.30	0	2,2,2	0.25	0
19	EDO	A	609	-	3,3,3	0.19	0	2,2,2	0.09	0
19	EDO	D	202	-	3,3,3	0.12	0	2,2,2	0.17	0
21	CUA	O	301	2	0,1,1	-	-	-	-	-
19	EDO	F	704	-	3,3,3	0.15	0	2,2,2	0.34	0
19	EDO	D	204	-	3,3,3	0.09	0	2,2,2	0.08	0
19	EDO	I	103	-	3,3,3	0.17	0	2,2,2	0.36	0
19	EDO	A	611	-	3,3,3	0.15	0	2,2,2	0.03	0
19	EDO	R	202	-	3,3,3	0.13	0	2,2,2	0.22	0
19	EDO	G	1301	-	3,3,3	0.21	0	2,2,2	0.42	0
19	EDO	B	303	-	3,3,3	0.39	0	2,2,2	0.23	0
19	EDO	E	205	-	3,3,3	0.07	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	TGL	Y	101	-	62,62,62	0.33	0	65,65,65	0.52	1 (1%)
17	PGV	Z	102	-	50,50,50	1.09	2 (4%)	53,56,56	1.18	5 (9%)
18	HEA	N	606	1	67,67,67	2.06	21 (31%)	81,103,103	2.71	38 (46%)
19	EDO	A	608	-	3,3,3	0.31	0	2,2,2	0.26	0
19	EDO	N	609	-	3,3,3	0.17	0	2,2,2	0.09	0
24	PEK	P	305	-	52,52,52	0.34	0	55,57,57	0.40	0
19	EDO	F	705	-	3,3,3	0.32	0	2,2,2	0.33	0
19	EDO	T	103	-	3,3,3	0.37	0	2,2,2	0.12	0
19	EDO	V	104	-	3,3,3	0.37	0	2,2,2	0.41	0
24	PEK	C	303	-	52,52,52	0.49	0	55,57,57	0.80	1 (1%)
19	EDO	N	613	-	3,3,3	0.57	0	2,2,2	0.71	0
25	CDL	C	312	-	99,99,99	0.37	0	105,111,111	0.46	0
19	EDO	D	206	-	3,3,3	0.19	0	2,2,2	0.25	0
19	EDO	E	203	-	3,3,3	0.22	0	2,2,2	0.33	0
19	EDO	A	614	-	3,3,3	0.47	0	2,2,2	0.42	0
17	PGV	N	605	-	50,50,50	0.83	2 (4%)	53,56,56	1.31	4 (7%)
17	PGV	P	306	-	50,50,50	0.77	2 (4%)	53,56,56	0.99	4 (7%)
19	EDO	P	311	-	3,3,3	0.37	0	2,2,2	0.40	0
19	EDO	F	701	-	3,3,3	0.13	0	2,2,2	0.37	0
19	EDO	A	617	-	3,3,3	0.15	0	2,2,2	0.13	0
22	CHD	W	302	-	32,32,32	0.56	0	51,51,51	0.74	0
18	HEA	A	607	1	67,67,67	2.15	23 (34%)	81,103,103	2.79	28 (34%)
24	PEK	C	315	-	52,52,52	0.43	0	55,57,57	0.57	0
26	PSC	O	302	-	51,51,51	0.42	0	57,59,59	0.42	0
19	EDO	T	105	-	3,3,3	0.04	0	2,2,2	0.28	0
18	HEA	A	606	1	67,67,67	1.99	24 (35%)	81,103,103	2.74	34 (41%)
19	EDO	G	1303	-	3,3,3	0.07	0	2,2,2	0.27	0
19	EDO	Q	204	-	3,3,3	0.22	0	2,2,2	0.03	0
19	EDO	S	2205	-	3,3,3	0.11	0	2,2,2	0.14	0
19	EDO	A	616	-	3,3,3	0.08	0	2,2,2	0.21	0
19	EDO	D	207	-	3,3,3	0.23	0	2,2,2	0.17	0
19	EDO	J	1101	-	3,3,3	0.47	0	2,2,2	0.32	0
19	EDO	B	309	-	3,3,3	0.11	0	2,2,2	0.22	0
28	SAC	I	101	-	7,8,9	0.54	0	7,9,11	1.14	1 (14%)
19	EDO	C	311	-	3,3,3	0.12	0	2,2,2	0.18	0
23	DMU	M	101	-	34,34,34	1.10	3 (8%)	45,45,45	1.27	5 (11%)
23	DMU	C	301	-	34,34,34	1.54	5 (14%)	45,45,45	1.86	9 (20%)
23	DMU	C	313	-	34,34,34	1.81	7 (20%)	45,45,45	1.95	10 (22%)
19	EDO	W	303	-	3,3,3	0.39	0	2,2,2	0.40	0
25	CDL	T	102	-	99,99,99	0.36	0	105,111,111	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PGV	C	305	-	50,50,50	0.74	3 (6%)	53,56,56	0.82	1 (1%)
17	PGV	A	605	-	50,50,50	0.85	3 (6%)	53,56,56	1.24	2 (3%)
22	CHD	C	302	-	32,32,32	0.66	1 (3%)	51,51,51	0.78	1 (1%)
19	EDO	N	612	-	3,3,3	0.19	0	2,2,2	0.25	0
19	EDO	N	620	-	3,3,3	0.33	0	2,2,2	0.46	0
19	EDO	J	1104	-	3,3,3	0.50	0	2,2,2	0.63	0
22	CHD	J	1102	-	32,32,32	0.65	1 (3%)	51,51,51	0.78	0
19	EDO	R	201	-	3,3,3	0.11	0	2,2,2	0.12	0
19	EDO	O	304	-	3,3,3	0.25	0	2,2,2	0.30	0
19	EDO	S	2207	-	3,3,3	0.12	0	2,2,2	0.33	0
19	EDO	B	305	-	3,3,3	0.13	0	2,2,2	0.23	0
19	EDO	A	612	-	3,3,3	0.19	0	2,2,2	0.13	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.56	2 (3%)
19	EDO	S	2206	-	3,3,3	0.18	0	2,2,2	0.09	0
19	EDO	F	702	-	3,3,3	0.17	0	2,2,2	0.13	0
22	CHD	G	1305	-	32,32,32	0.57	0	51,51,51	0.81	0
23	DMU	G	1302	-	34,34,34	1.86	10 (29%)	45,45,45	1.45	7 (15%)
19	EDO	W	301	-	3,3,3	0.18	0	2,2,2	0.46	0
17	PGV	T	101	-	50,50,50	1.15	2 (4%)	53,56,56	1.21	4 (7%)
20	TGL	Q	201	-	62,62,62	0.29	0	65,65,65	0.31	0
19	EDO	S	2204	-	3,3,3	0.32	0	2,2,2	0.40	0
19	EDO	Q	203	-	3,3,3	0.21	0	2,2,2	0.09	0
19	EDO	B	304	-	3,3,3	0.22	0	2,2,2	0.20	0
22	CHD	B	302	-	32,32,32	0.62	0	51,51,51	0.86	1 (1%)
22	CHD	P	308	-	32,32,32	0.61	0	51,51,51	1.08	2 (3%)
25	CDL	C	306	-	99,99,99	0.39	0	105,111,111	0.60	2 (1%)
19	EDO	N	614	-	3,3,3	0.54	0	2,2,2	0.70	0
23	DMU	Z	101	-	34,34,34	1.19	4 (11%)	45,45,45	1.56	7 (15%)
19	EDO	A	620	-	3,3,3	0.28	0	2,2,2	0.06	0
19	EDO	N	619	-	3,3,3	0.10	0	2,2,2	0.13	0
19	EDO	P	310	-	3,3,3	0.31	0	2,2,2	0.23	0
26	PSC	E	201	-	51,51,51	0.45	0	57,59,59	0.52	0
19	EDO	C	314	-	3,3,3	0.11	0	2,2,2	0.11	0
19	EDO	N	615	-	3,3,3	0.11	0	2,2,2	0.24	0
19	EDO	W	304	-	3,3,3	0.18	0	2,2,2	0.17	0
17	PGV	A	604	-	50,50,50	1.19	2 (4%)	53,56,56	1.62	5 (9%)
19	EDO	J	1105	-	3,3,3	0.22	0	2,2,2	0.35	0
19	EDO	G	1306	-	3,3,3	0.12	0	2,2,2	0.18	0
19	EDO	B	307	-	3,3,3	0.16	0	2,2,2	0.16	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
19	EDO	G	1304	-	-	1/1/1/1	-
22	CHD	Y	102	-	-	8/9/74/74	0/4/4/4
19	EDO	B	306	-	-	1/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	V	103	-	-	0/1/1/1	-
25	CDL	P	307	-	-	49/110/110/110	-
19	EDO	I	102	-	-	1/1/1/1	-
19	EDO	P	309	-	-	1/1/1/1	-
19	EDO	K	102	-	-	1/1/1/1	-
19	EDO	N	608	-	-	1/1/1/1	-
18	HEA	N	607	1	-	4/36/76/76	-
19	EDO	N	618	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	L	102	-	-	0/1/1/1	-
19	EDO	Q	202	-	-	1/1/1/1	-
22	CHD	C	307	-	-	2/9/74/74	0/4/4/4
19	EDO	D	203	-	-	1/1/1/1	-
19	EDO	J	1103	-	-	0/1/1/1	-
24	PEK	P	301	-	-	29/56/56/56	-
19	EDO	N	617	-	-	0/1/1/1	-
19	EDO	U	1501	-	-	0/1/1/1	-
19	EDO	M	102	-	-	0/1/1/1	-
17	PGV	N	616	-	-	24/55/55/55	-
24	PEK	C	304	-	-	28/56/56/56	-
22	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	A	610	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-
28	SAC	V	101	-	-	3/7/8/10	-
22	CHD	T	104	-	-	6/9/74/74	0/4/4/4
19	EDO	Z	103	-	-	0/1/1/1	-
19	EDO	A	619	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
19	EDO	O	303	-	-	1/1/1/1	-
24	PEK	P	304	-	-	20/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	C	310	-	-	1/1/1/1	-
23	DMU	P	302	-	-	6/19/59/59	0/2/2/2
19	EDO	A	613	-	-	0/1/1/1	-
19	EDO	S	2201	-	-	1/1/1/1	-
20	TGL	N	604	-	-	33/65/65/65	-
19	EDO	A	618	-	-	0/1/1/1	-
19	EDO	S	2203	-	-	0/1/1/1	-
19	EDO	C	308	-	-	0/1/1/1	-
19	EDO	D	208	-	-	0/1/1/1	-
19	EDO	E	202	-	-	1/1/1/1	-
20	TGL	A	615	-	-	42/65/65/65	-
20	TGL	L	101	-	-	36/65/65/65	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	D	205	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
19	EDO	D	202	-	-	0/1/1/1	-
19	EDO	F	704	-	-	1/1/1/1	-
19	EDO	D	204	-	-	1/1/1/1	-
19	EDO	I	103	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
19	EDO	R	202	-	-	1/1/1/1	-
19	EDO	G	1301	-	-	0/1/1/1	-
19	EDO	B	303	-	-	0/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
20	TGL	Y	101	-	-	28/65/65/65	-
17	PGV	Z	102	-	-	24/55/55/55	-
18	HEA	N	606	1	-	4/36/76/76	-
19	EDO	A	608	-	-	0/1/1/1	-
19	EDO	N	609	-	-	1/1/1/1	-
24	PEK	P	305	-	-	31/56/56/56	-
19	EDO	F	705	-	-	0/1/1/1	-
19	EDO	T	103	-	-	1/1/1/1	-
19	EDO	V	104	-	-	0/1/1/1	-
24	PEK	C	303	-	-	22/56/56/56	-
19	EDO	N	613	-	-	0/1/1/1	-
25	CDL	C	312	-	-	60/110/110/110	-
19	EDO	D	206	-	-	1/1/1/1	-
19	EDO	E	203	-	-	0/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
17	PGV	N	605	-	-	14/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	P	306	-	-	8/55/55/55	-
19	EDO	P	311	-	-	1/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-
19	EDO	A	617	-	-	1/1/1/1	-
22	CHD	W	302	-	-	2/9/74/74	0/4/4/4
18	HEA	A	607	1	-	8/36/76/76	-
24	PEK	C	315	-	-	26/56/56/56	-
26	PSC	O	302	-	-	37/55/55/55	-
19	EDO	T	105	-	-	1/1/1/1	-
18	HEA	A	606	1	-	7/36/76/76	-
19	EDO	G	1303	-	-	1/1/1/1	-
19	EDO	Q	204	-	-	0/1/1/1	-
19	EDO	S	2205	-	-	0/1/1/1	-
19	EDO	A	616	-	-	0/1/1/1	-
19	EDO	D	207	-	-	1/1/1/1	-
19	EDO	J	1101	-	-	0/1/1/1	-
19	EDO	B	309	-	-	1/1/1/1	-
28	SAC	I	101	-	-	7/7/8/10	-
19	EDO	C	311	-	-	0/1/1/1	-
23	DMU	M	101	-	-	6/19/59/59	0/2/2/2
23	DMU	C	301	-	-	11/19/59/59	0/2/2/2
23	DMU	C	313	-	-	6/19/59/59	0/2/2/2
19	EDO	W	303	-	-	1/1/1/1	-
25	CDL	T	102	-	-	62/110/110/110	-
17	PGV	C	305	-	-	13/55/55/55	-
17	PGV	A	605	-	-	15/55/55/55	-
22	CHD	C	302	-	-	1/9/74/74	0/4/4/4
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	N	620	-	-	1/1/1/1	-
19	EDO	J	1104	-	-	0/1/1/1	-
22	CHD	J	1102	-	-	2/9/74/74	0/4/4/4
19	EDO	R	201	-	-	1/1/1/1	-
19	EDO	O	304	-	-	0/1/1/1	-
19	EDO	S	2207	-	-	1/1/1/1	-
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	A	612	-	-	0/1/1/1	-
20	TGL	D	201	-	-	36/65/65/65	-
19	EDO	S	2206	-	-	1/1/1/1	-
19	EDO	F	702	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	G	1305	-	-	2/9/74/74	0/4/4/4
23	DMU	G	1302	-	-	11/19/59/59	0/2/2/2
19	EDO	W	301	-	-	1/1/1/1	-
17	PGV	T	101	-	-	25/55/55/55	-
20	TGL	Q	201	-	-	32/65/65/65	-
19	EDO	S	2204	-	-	1/1/1/1	-
19	EDO	Q	203	-	-	1/1/1/1	-
19	EDO	B	304	-	-	1/1/1/1	-
22	CHD	B	302	-	-	2/9/74/74	0/4/4/4
22	CHD	P	308	-	-	4/9/74/74	0/4/4/4
25	CDL	C	306	-	-	59/110/110/110	-
19	EDO	N	614	-	-	1/1/1/1	-
23	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
19	EDO	A	620	-	-	0/1/1/1	-
19	EDO	N	619	-	-	1/1/1/1	-
19	EDO	P	310	-	-	0/1/1/1	-
26	PSC	E	201	-	-	26/55/55/55	-
19	EDO	C	314	-	-	1/1/1/1	-
19	EDO	N	615	-	-	1/1/1/1	-
19	EDO	W	304	-	-	1/1/1/1	-
17	PGV	A	604	-	-	30/55/55/55	-
19	EDO	J	1105	-	-	1/1/1/1	-
19	EDO	G	1306	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	FE-ND	6.21	2.14	1.94
23	G	1302	DMU	O16-C6	5.88	1.50	1.40
18	N	607	HEA	C1D-ND	-5.82	1.30	1.40
23	C	313	DMU	O16-C6	5.70	1.49	1.40
18	N	607	HEA	FE-NB	5.50	2.11	1.94
18	A	607	HEA	C1D-ND	-5.48	1.30	1.40
23	C	301	DMU	O16-C6	5.29	1.49	1.40
18	N	607	HEA	C4B-NB	-5.28	1.31	1.40
17	A	604	PGV	O01-C1	5.23	1.49	1.34
17	Z	102	PGV	O03-C19	5.20	1.48	1.33
17	T	101	PGV	O03-C19	5.14	1.48	1.33
17	A	604	PGV	O03-C19	4.99	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	101	PGV	O01-C1	4.94	1.48	1.34
18	N	606	HEA	CHA-C1A	4.93	1.48	1.38
18	N	606	HEA	FE-ND	4.93	2.10	1.94
17	N	616	PGV	O01-C1	4.87	1.48	1.34
18	A	607	HEA	FE-NC	4.84	2.11	1.95
18	A	606	HEA	FE-NC	4.75	2.10	1.95
18	N	606	HEA	FE-NB	4.69	2.09	1.94
23	C	313	DMU	O1-C9	4.66	1.55	1.44
17	Z	102	PGV	O01-C1	4.50	1.47	1.34
18	A	607	HEA	C4A-NA	-4.44	1.31	1.39
18	N	607	HEA	C3B-C2B	4.43	1.44	1.34
18	A	607	HEA	C4C-NC	-4.38	1.31	1.39
18	N	607	HEA	C11-C3B	-4.32	1.46	1.51
17	N	616	PGV	O03-C19	4.31	1.45	1.33
18	N	606	HEA	C1D-ND	-4.31	1.32	1.40
18	A	606	HEA	C4A-NA	-4.19	1.31	1.39
18	N	607	HEA	C3A-C2A	4.19	1.46	1.37
18	A	607	HEA	C4B-NB	-4.15	1.33	1.40
23	Z	101	DMU	O16-C6	4.09	1.47	1.40
18	A	606	HEA	FE-NA	4.03	2.08	1.95
18	N	607	HEA	CHB-C1B	4.02	1.48	1.39
23	G	1302	DMU	O7-C3	3.85	1.53	1.43
18	N	606	HEA	C11-C3B	-3.81	1.46	1.51
18	A	607	HEA	FE-ND	3.77	2.06	1.94
23	C	313	DMU	O1-C10	3.73	1.51	1.41
18	A	606	HEA	C3B-C2B	3.73	1.43	1.34
18	N	606	HEA	C3A-C2A	3.72	1.45	1.37
18	N	606	HEA	CHB-C1B	3.71	1.47	1.39
18	A	607	HEA	FE-NA	3.64	2.07	1.95
18	A	607	HEA	C1C-NC	-3.64	1.32	1.39
18	A	607	HEA	C3D-C2D	3.63	1.44	1.36
18	N	607	HEA	CHA-C1A	3.63	1.45	1.38
18	A	606	HEA	C3D-C2D	3.55	1.44	1.36
18	N	606	HEA	CHA-C4D	3.54	1.47	1.39
18	N	607	HEA	C1C-NC	-3.46	1.33	1.39
18	A	607	HEA	C3A-C2A	3.43	1.45	1.37
18	N	606	HEA	C4B-NB	-3.40	1.34	1.40
18	A	606	HEA	FE-NB	3.38	2.05	1.94
17	N	605	PGV	O03-C19	3.37	1.43	1.33
18	A	607	HEA	FE-NB	3.36	2.05	1.94
18	N	606	HEA	CHB-C4A	3.36	1.45	1.38
18	A	606	HEA	CHD-C1D	3.35	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	606	HEA	CHB-C1B	3.35	1.46	1.39
18	N	606	HEA	C3B-C2B	3.33	1.42	1.34
23	G	1302	DMU	O7-C10	3.33	1.51	1.41
18	N	606	HEA	FE-NA	3.26	2.05	1.95
18	A	606	HEA	FE-ND	3.19	2.04	1.94
23	M	101	DMU	O16-C6	3.19	1.45	1.40
23	P	302	DMU	O16-C6	3.17	1.45	1.40
18	A	606	HEA	CHA-C4D	3.17	1.46	1.39
18	A	607	HEA	C3B-C2B	3.14	1.41	1.34
17	A	605	PGV	O03-C19	3.14	1.42	1.33
18	N	607	HEA	C3D-C2D	3.10	1.43	1.36
18	A	606	HEA	C1D-ND	-3.08	1.34	1.40
23	C	301	DMU	O5-C4	3.08	1.51	1.44
18	N	607	HEA	CHD-C4C	3.04	1.46	1.39
18	N	607	HEA	CHA-C4D	3.03	1.46	1.39
23	M	101	DMU	O1-C9	3.01	1.51	1.44
18	A	606	HEA	C3A-C2A	2.97	1.43	1.37
18	A	606	HEA	C1A-NA	-2.97	1.34	1.39
23	Z	101	DMU	O1-C9	2.96	1.51	1.44
18	A	607	HEA	CHB-C4A	2.93	1.44	1.38
18	A	607	HEA	C1B-NB	2.90	1.44	1.38
18	N	606	HEA	CHD-C4C	2.90	1.45	1.39
18	N	606	HEA	C4C-NC	-2.88	1.34	1.39
18	A	606	HEA	CHA-C1A	2.87	1.44	1.38
18	N	606	HEA	CHC-C1C	2.85	1.45	1.39
18	A	606	HEA	C4B-C3B	2.80	1.49	1.44
17	A	605	PGV	O01-C1	2.79	1.42	1.34
18	A	606	HEA	CHB-C4A	2.74	1.43	1.38
23	C	301	DMU	C7-C5	2.70	1.59	1.52
18	A	606	HEA	C4C-NC	-2.70	1.34	1.39
18	A	607	HEA	CHB-C1B	2.69	1.45	1.39
23	C	301	DMU	O5-C6	2.67	1.48	1.41
17	P	306	PGV	O01-C1	2.67	1.41	1.34
17	P	306	PGV	O03-C19	2.66	1.41	1.33
17	C	305	PGV	O03-C19	2.63	1.41	1.33
17	N	605	PGV	O01-C1	2.62	1.41	1.34
18	N	606	HEA	CHD-C1D	2.60	1.43	1.38
18	N	607	HEA	C4A-NA	-2.59	1.34	1.39
18	A	606	HEA	C4B-NB	-2.57	1.35	1.40
17	C	305	PGV	O01-C1	2.57	1.41	1.34
23	M	101	DMU	O49-C1	-2.55	1.36	1.43
18	N	607	HEA	FE-NC	2.54	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	607	HEA	CHA-C1A	2.50	1.43	1.38
18	A	607	HEA	CHC-C1C	2.49	1.45	1.39
18	A	606	HEA	C1C-C2C	2.48	1.49	1.43
18	N	607	HEA	CMC-C2C	-2.47	1.45	1.50
18	N	607	HEA	FE-NA	2.46	2.03	1.95
23	C	313	DMU	C8-C7	2.42	1.58	1.52
23	C	313	DMU	O5-C4	2.42	1.50	1.44
18	N	607	HEA	CHC-C1C	2.42	1.44	1.39
23	G	1302	DMU	O5-C4	2.41	1.50	1.44
18	A	607	HEA	C1A-NA	-2.41	1.35	1.39
18	A	606	HEA	C1C-NC	-2.41	1.35	1.39
23	G	1302	DMU	C7-C5	2.37	1.58	1.52
18	N	607	HEA	C1C-C2C	2.37	1.48	1.43
18	A	607	HEA	CHA-C4D	2.35	1.44	1.39
23	C	301	DMU	O3-C5	2.34	1.48	1.43
23	G	1302	DMU	O1-C10	2.30	1.47	1.41
18	A	607	HEA	CHD-C1D	2.29	1.43	1.38
22	P	303	CHD	O26-C24	-2.29	1.23	1.30
18	N	607	HEA	CHB-C4A	2.28	1.42	1.38
18	N	606	HEA	O2A-CGA	-2.26	1.23	1.30
18	A	607	HEA	C1C-C2C	2.25	1.48	1.43
23	G	1302	DMU	O1-C9	2.24	1.49	1.44
18	A	606	HEA	C3C-C4C	2.24	1.49	1.42
23	C	313	DMU	O7-C10	2.24	1.48	1.41
18	N	607	HEA	C4D-C3D	2.23	1.48	1.45
18	A	607	HEA	C4D-ND	2.23	1.43	1.38
23	G	1302	DMU	C10-C5	2.20	1.59	1.52
23	Z	101	DMU	O7-C10	2.19	1.47	1.41
18	A	606	HEA	C1B-NB	2.18	1.43	1.38
23	G	1302	DMU	C2-C1	2.18	1.58	1.52
23	C	313	DMU	C11-C9	2.16	1.59	1.51
18	N	606	HEA	CHC-C4B	2.13	1.42	1.38
18	N	606	HEA	FE-NC	2.12	2.02	1.95
22	C	302	CHD	O26-C24	-2.12	1.23	1.30
18	A	606	HEA	OMA-CMA	-2.11	1.17	1.22
18	A	607	HEA	C11-C3B	-2.09	1.48	1.51
22	J	1102	CHD	O26-C24	-2.09	1.23	1.30
23	Z	101	DMU	O1-C10	2.07	1.47	1.41
18	N	607	HEA	C1D-C2D	2.07	1.48	1.44
17	C	305	PGV	O01-C02	-2.05	1.41	1.46
18	N	606	HEA	C1B-NB	2.02	1.42	1.38
17	A	605	PGV	O01-C02	-2.02	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	606	HEA	CHC-C4B	2.02	1.42	1.38
23	P	302	DMU	O5-C4	2.01	1.49	1.44
18	N	606	HEA	C1D-C2D	2.00	1.48	1.44
18	N	607	HEA	C12-C11	-2.00	1.49	1.53
18	N	607	HEA	CMD-C2D	-2.00	1.46	1.50
23	G	1302	DMU	C3-C4	2.00	1.58	1.52

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	607	HEA	C26-C15-C14	-8.35	102.19	123.63
18	A	607	HEA	C16-C15-C14	8.27	139.74	121.17
23	P	302	DMU	C18-O16-C6	7.82	127.05	113.68
18	A	607	HEA	C3A-C2A-C1A	-7.19	100.25	107.05
23	C	313	DMU	O1-C9-C11	7.16	124.19	106.44
18	N	607	HEA	C3C-C4C-NC	7.16	115.83	109.80
18	A	606	HEA	C1D-C2D-C3D	-7.14	99.47	106.98
18	N	606	HEA	C1D-C2D-C3D	-7.05	99.57	106.98
18	A	606	HEA	C3C-C4C-NC	6.89	115.60	109.80
18	N	606	HEA	C3C-C4C-NC	6.77	115.50	109.80
18	A	606	HEA	C3A-C2A-C1A	-6.64	100.76	107.05
23	C	301	DMU	C18-O16-C6	6.61	124.97	113.68
18	A	607	HEA	C3C-C4C-NC	6.26	115.07	109.80
18	N	607	HEA	C3A-C2A-C1A	-6.22	101.16	107.05
17	A	604	PGV	O01-C1-C2	6.19	124.87	111.48
18	A	607	HEA	C1D-C2D-C3D	-6.13	100.53	106.98
18	N	607	HEA	C2A-C1A-NA	6.04	116.15	110.32
18	N	607	HEA	C3D-C4D-ND	-6.02	104.53	110.35
18	N	606	HEA	C2D-C1D-ND	6.00	116.73	109.84
18	N	606	HEA	CHB-C1B-NB	5.96	130.84	124.42
17	A	604	PGV	C02-O01-C1	5.88	131.86	117.80
18	N	606	HEA	C3C-C2C-C1C	-5.86	100.26	107.17
18	N	607	HEA	CMB-C2B-C1B	-5.75	116.05	125.03
18	A	607	HEA	C2A-C1A-NA	5.59	115.72	110.32
18	A	606	HEA	C2D-C1D-ND	5.49	116.15	109.84
18	A	606	HEA	C2A-C1A-NA	5.46	115.59	110.32
18	N	607	HEA	C2B-C1B-NB	-5.41	103.64	109.90
18	N	607	HEA	C1D-C2D-C3D	-5.30	101.41	106.98
18	N	607	HEA	C13-C12-C11	-5.27	105.97	114.39
18	A	607	HEA	C3C-C2C-C1C	-5.25	100.98	107.17
17	A	605	PGV	O03-C19-O04	-5.22	110.56	123.63
18	A	606	HEA	CHB-C1B-NB	5.17	129.99	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	605	PGV	O03-C19-C20	5.11	127.42	111.83
18	A	606	HEA	C3C-C2C-C1C	-5.10	101.16	107.17
18	N	606	HEA	C2C-C1C-NC	4.88	117.97	110.14
17	A	605	PGV	O03-C19-C20	4.87	126.67	111.83
18	A	606	HEA	CHA-C1A-C2A	-4.86	117.20	124.86
18	A	606	HEA	CMD-C2D-C1D	4.79	132.53	125.03
17	T	101	PGV	O01-C1-C2	4.73	121.72	111.48
17	N	605	PGV	O03-C19-O04	-4.71	111.84	123.63
18	A	606	HEA	C4B-C3B-C2B	-4.60	99.71	107.44
23	C	301	DMU	C6-O5-C4	4.60	122.69	113.72
18	A	606	HEA	C2C-C1C-NC	4.56	117.46	110.14
18	A	606	HEA	C1B-C2B-C3B	4.55	112.06	106.80
17	A	604	PGV	O03-C19-C20	4.54	125.67	111.83
18	N	607	HEA	C3C-C2C-C1C	-4.53	101.83	107.17
18	A	607	HEA	C3D-C4D-ND	-4.52	105.98	110.35
18	N	606	HEA	C2B-C1B-NB	-4.52	104.68	109.90
18	N	607	HEA	C4B-C3B-C2B	-4.47	99.92	107.44
17	T	101	PGV	O03-C19-C20	4.47	125.45	111.83
18	N	606	HEA	C1B-C2B-C3B	4.43	111.93	106.80
23	C	313	DMU	C6-O5-C4	4.41	122.34	113.72
18	N	606	HEA	C2A-C1A-NA	4.41	114.58	110.32
17	N	616	PGV	O03-C19-C20	4.41	125.28	111.83
23	C	301	DMU	O5-C4-C57	4.40	117.34	106.44
18	A	606	HEA	C3D-C4D-ND	-4.36	106.14	110.35
18	A	607	HEA	C2D-C1D-ND	4.32	114.81	109.84
18	N	606	HEA	C3A-C2A-C1A	-4.31	102.96	107.05
18	A	607	HEA	C13-C14-C15	4.29	137.44	127.62
18	N	607	HEA	C3B-C4B-NB	4.29	114.77	109.84
23	P	302	DMU	O5-C6-O16	4.14	119.82	110.04
17	Z	102	PGV	O01-C1-C2	4.13	120.41	111.48
18	N	607	HEA	CHA-C1A-C2A	-4.13	118.35	124.86
18	N	607	HEA	C2C-C1C-NC	4.10	116.71	110.14
18	N	607	HEA	CAA-CBA-CGA	-4.09	102.82	113.67
18	A	606	HEA	C3B-C4B-NB	4.09	114.54	109.84
18	N	606	HEA	CMB-C2B-C1B	-4.07	118.67	125.03
18	N	607	HEA	O11-C11-C3B	-4.05	103.83	111.26
18	N	607	HEA	C26-C15-C16	4.01	122.18	115.23
18	N	606	HEA	CHC-C1C-C2C	-4.00	115.81	127.43
22	P	308	CHD	C1-C2-C3	3.98	115.75	110.48
18	A	607	HEA	C2C-C1C-NC	3.96	116.49	110.14
18	N	606	HEA	C4B-C3B-C2B	-3.96	100.78	107.44
18	A	607	HEA	C2B-C1B-NB	-3.93	105.36	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Z	101	DMU	O16-C6-C1	3.84	114.10	108.27
23	C	301	DMU	C8-C7-C5	3.78	117.47	110.83
17	Z	102	PGV	O03-C19-C20	3.78	123.36	111.83
18	N	607	HEA	CHA-C4D-ND	3.77	128.48	124.42
18	A	607	HEA	C3B-C4B-NB	3.75	114.15	109.84
18	A	607	HEA	CHA-C1A-C2A	-3.73	118.97	124.86
18	N	606	HEA	CMC-C2C-C1C	3.69	131.03	125.42
18	A	606	HEA	O11-C11-C3B	-3.65	104.56	111.26
18	N	607	HEA	C1D-ND-C4D	3.62	109.49	105.21
18	N	606	HEA	CMD-C2D-C1D	3.61	130.68	125.03
23	P	302	DMU	C6-C1-C2	-3.57	102.50	110.01
22	Y	102	CHD	C5-C6-C7	-3.52	110.22	114.40
17	A	604	PGV	O01-C1-O02	-3.51	115.49	123.70
18	N	606	HEA	C4C-NC-C1C	-3.51	100.10	105.82
18	A	607	HEA	C4B-C3B-C2B	-3.47	101.61	107.44
23	C	313	DMU	O5-C4-C3	3.45	116.85	109.72
18	N	606	HEA	CHA-C1A-C2A	-3.44	119.43	124.86
23	M	101	DMU	O1-C9-C11	3.44	114.97	106.44
18	A	607	HEA	O11-C11-C3B	-3.36	105.09	111.26
18	N	606	HEA	C3B-C4B-NB	3.35	113.69	109.84
18	N	607	HEA	CHB-C1B-NB	3.34	128.01	124.42
18	N	607	HEA	C2D-C1D-ND	3.32	113.66	109.84
23	Z	101	DMU	C11-C9-C8	-3.30	104.91	113.02
25	C	306	CDL	OA6-CA5-C11	3.30	118.61	111.48
18	A	606	HEA	C4A-CHB-C1B	-3.27	119.08	126.02
18	N	606	HEA	CAD-CBD-CGD	-3.27	105.00	113.67
23	M	101	DMU	C22-C19-C18	-3.26	99.28	113.47
18	A	606	HEA	C4D-C3D-C2D	3.25	111.63	106.89
23	Z	101	DMU	O1-C9-C11	3.25	114.50	106.44
17	N	616	PGV	O01-C1-C2	3.25	118.50	111.48
18	N	606	HEA	C13-C12-C11	-3.22	109.26	114.39
20	Y	101	TGL	OG2-CB1-CB2	3.20	118.40	111.48
22	T	104	CHD	C17-C13-C14	3.18	103.31	100.11
18	N	607	HEA	CHB-C4A-C3A	-3.17	119.86	125.21
18	A	606	HEA	CHC-C1C-C2C	-3.16	118.25	127.43
18	A	606	HEA	C26-C15-C16	3.15	120.69	115.23
18	A	607	HEA	CHA-C4D-ND	3.14	127.80	124.42
18	A	607	HEA	C17-C18-C19	-3.13	120.45	127.62
18	N	607	HEA	C4B-NB-C1B	3.12	108.90	105.21
18	A	606	HEA	CMB-C2B-C1B	-3.12	120.17	125.03
18	N	606	HEA	O11-C11-C3B	-3.11	105.56	111.26
22	C	302	CHD	C6-C7-C8	3.08	114.87	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	G	1302	DMU	C18-O16-C6	3.07	118.92	113.68
18	N	607	HEA	C4C-C3C-C2C	-3.07	103.49	107.30
17	N	605	PGV	O01-C1-O02	-3.05	116.58	123.70
18	A	607	HEA	C1B-C2B-C3B	3.03	110.30	106.80
18	A	607	HEA	CMD-C2D-C1D	3.03	129.77	125.03
23	C	313	DMU	O7-C10-O1	3.02	118.65	110.69
23	M	101	DMU	C34-C31-C28	-3.02	99.12	114.37
23	P	302	DMU	O16-C18-C19	-3.00	99.19	109.37
18	N	607	HEA	CMC-C2C-C1C	2.97	129.94	125.42
18	A	606	HEA	C12-C11-C3B	-2.97	107.48	112.12
18	N	606	HEA	C27-C19-C20	2.96	120.37	115.23
20	N	604	TGL	OG2-CB1-CB2	2.96	117.89	111.48
17	P	306	PGV	O14-P-O13	2.96	126.22	112.44
18	N	606	HEA	C4B-NB-C1B	2.94	108.68	105.21
18	A	607	HEA	CAA-CBA-CGA	-2.91	105.94	113.67
23	G	1302	DMU	O16-C6-C1	2.90	112.68	108.27
17	P	306	PGV	O01-C1-C2	2.90	117.76	111.48
18	A	607	HEA	O11-C11-C12	2.90	116.83	109.14
18	A	607	HEA	CMB-C2B-C1B	-2.89	120.52	125.03
20	D	201	TGL	OG2-CB1-CB2	2.89	117.73	111.48
23	G	1302	DMU	O7-C3-C2	2.89	114.56	107.23
17	P	306	PGV	O01-C1-O02	-2.87	116.99	123.70
18	N	606	HEA	C4D-C3D-C2D	2.86	111.05	106.89
17	A	604	PGV	O04-C19-C20	-2.85	112.62	123.78
18	N	606	HEA	CHD-C1D-C2D	-2.85	118.86	126.95
18	N	607	HEA	C1B-C2B-C3B	2.84	110.08	106.80
23	P	302	DMU	C10-O7-C3	-2.83	111.27	117.98
23	G	1302	DMU	C10-O1-C9	2.82	119.23	113.72
23	C	313	DMU	C25-C22-C19	-2.82	100.14	114.37
23	Z	101	DMU	O1-C9-C8	2.81	114.76	109.70
18	A	606	HEA	C4C-C3C-C2C	-2.81	103.81	107.30
18	A	606	HEA	CHD-C1D-C2D	-2.80	118.98	126.95
20	A	615	TGL	OG2-CB1-CB2	2.80	117.54	111.48
18	A	606	HEA	C2B-C1B-NB	-2.80	106.67	109.90
28	I	101	SAC	O-C-CA	-2.77	117.64	124.77
18	N	607	HEA	CHC-C1C-C2C	-2.74	119.48	127.43
18	A	607	HEA	C4C-C3C-C2C	-2.71	103.93	107.30
22	T	104	CHD	C14-C8-C7	2.70	115.44	111.85
22	P	308	CHD	C2-C1-C10	2.70	117.30	112.74
18	N	606	HEA	CAA-C2A-C1A	2.69	130.33	124.85
18	N	607	HEA	CAA-C2A-C1A	2.69	130.32	124.85
23	C	313	DMU	C34-C31-C28	-2.68	100.82	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	607	HEA	CMC-C2C-C3C	2.67	132.83	126.55
23	G	1302	DMU	O5-C4-C3	2.67	115.23	109.72
28	V	101	SAC	O-C-CA	-2.64	117.98	124.77
24	P	304	PEK	O01-C1-O02	-2.64	117.54	123.70
18	A	606	HEA	CHB-C4A-C3A	-2.62	120.78	125.21
18	N	606	HEA	C3D-C4D-ND	-2.61	107.83	110.35
18	N	606	HEA	O2D-CGD-CBD	2.60	122.23	114.00
17	N	616	PGV	O03-C19-O04	-2.57	117.20	123.63
23	P	302	DMU	C37-C34-C31	-2.55	101.47	114.37
18	A	606	HEA	CBD-CAD-C3D	2.54	119.57	112.53
18	N	607	HEA	C17-C18-C19	-2.54	121.80	127.62
18	A	606	HEA	CHA-C1A-NA	2.52	127.20	124.45
18	A	606	HEA	CAD-C3D-C4D	-2.51	120.32	124.70
18	N	606	HEA	C25-C23-C24	2.49	120.33	114.59
23	C	301	DMU	C7-C8-C9	2.47	114.72	110.23
18	N	607	HEA	C13-C14-C15	-2.47	121.97	127.62
18	A	606	HEA	C4C-NC-C1C	-2.46	101.81	105.82
23	C	313	DMU	C7-C8-C9	-2.46	105.77	110.23
18	A	607	HEA	CHB-C4A-C3A	-2.45	121.07	125.21
18	N	606	HEA	C12-C11-C3B	-2.45	108.30	112.12
18	N	606	HEA	C4A-C3A-C2A	-2.44	104.70	106.81
23	M	101	DMU	O49-C1-C6	-2.43	104.28	110.08
23	C	301	DMU	C57-C4-C3	-2.43	106.54	113.38
17	C	305	PGV	O14-P-O13	2.42	123.72	112.44
17	Z	102	PGV	C7-C6-C5	-2.42	102.13	114.37
25	P	307	CDL	OB6-CB5-OB7	-2.42	118.06	123.70
20	D	201	TGL	OG2-CB1-OB1	-2.40	118.10	123.70
18	N	606	HEA	C26-C15-C16	2.39	119.37	115.23
17	T	101	PGV	O03-C01-C02	2.38	115.27	108.40
18	N	606	HEA	OMA-CMA-C3A	-2.38	120.25	125.62
23	Z	101	DMU	C10-C5-C7	-2.37	105.02	110.01
18	N	607	HEA	CMD-C2D-C1D	2.35	128.71	125.03
22	T	104	CHD	C15-C14-C8	2.34	121.56	118.36
18	N	607	HEA	CAD-C3D-C4D	-2.33	120.64	124.70
18	N	606	HEA	O1D-CGD-CBD	-2.32	115.74	123.09
18	N	606	HEA	CHB-C4A-C3A	-2.32	121.30	125.21
25	C	306	CDL	OB2-PB2-OB3	2.30	118.06	108.94
18	A	607	HEA	CAA-C2A-C1A	2.30	129.53	124.85
23	C	313	DMU	O2-C8-C7	2.30	115.79	110.38
22	Y	102	CHD	C16-C17-C13	-2.29	101.32	103.54
22	T	104	CHD	C22-C23-C24	2.29	118.59	112.49
23	C	301	DMU	C10-C5-C7	2.28	114.80	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	607	HEA	C4C-NC-C1C	-2.27	102.12	105.82
17	T	101	PGV	O04-C19-C20	-2.27	114.92	123.78
17	Z	102	PGV	O03-C01-C02	2.26	114.92	108.40
23	C	313	DMU	C10-O7-C3	-2.26	112.63	117.98
23	C	313	DMU	C10-O1-C9	2.23	118.07	113.72
18	N	606	HEA	CAD-C3D-C4D	-2.22	120.83	124.70
18	A	606	HEA	C27-C19-C20	2.21	119.06	115.23
23	Z	101	DMU	C10-O1-C9	2.21	118.03	113.72
18	A	607	HEA	CHC-C1C-C2C	-2.20	121.03	127.43
23	G	1302	DMU	O1-C9-C11	2.20	111.89	106.44
18	A	606	HEA	OMA-CMA-C3A	-2.20	120.67	125.62
18	A	606	HEA	CMC-C2C-C3C	2.19	131.70	126.55
18	A	606	HEA	CAA-C2A-C1A	2.18	129.28	124.85
23	C	301	DMU	C1-C2-C3	2.17	114.61	109.68
23	C	301	DMU	O7-C10-C5	2.17	113.43	108.09
18	N	607	HEA	C1A-CHA-C4D	-2.16	121.42	126.02
23	P	302	DMU	O7-C10-C5	2.16	113.41	108.09
23	G	1302	DMU	C6-O5-C4	2.13	117.89	113.72
23	P	302	DMU	C6-O5-C4	2.13	117.88	113.72
18	N	607	HEA	CAD-CBD-CGD	-2.12	108.04	113.67
22	T	104	CHD	C2-C1-C10	2.12	116.32	112.74
18	N	606	HEA	C4C-CHD-C1D	-2.12	121.27	126.25
23	Z	101	DMU	C34-C31-C28	-2.11	103.68	114.37
22	Y	102	CHD	C9-C11-C12	2.10	117.05	114.29
22	B	302	CHD	C17-C13-C14	2.09	102.21	100.11
18	N	606	HEA	CHD-C4C-C3C	-2.09	118.31	127.37
17	N	605	PGV	O12-P-O13	2.07	117.15	108.94
23	M	101	DMU	C37-C34-C31	-2.06	103.93	114.37
23	P	302	DMU	C31-C28-C25	-2.06	103.93	114.37
17	Z	102	PGV	C01-O03-C19	2.05	124.61	117.12
17	P	306	PGV	C22-C21-C20	-2.04	105.61	113.13
18	N	607	HEA	C4A-C3A-C2A	-2.04	105.05	106.81
22	T	104	CHD	C18-C13-C12	-2.03	107.02	109.06
18	A	606	HEA	CHA-C4D-ND	2.01	126.59	124.42
17	N	616	PGV	O01-C1-O02	-2.01	119.00	123.70
24	C	303	PEK	O13-P-O12	-2.01	98.48	107.57

There are no chirality outliers.

All (971) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O12

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Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C03-O11-P-O14
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	C04-O12-P-O14
17	A	604	PGV	C04-C05-C06-O06
17	A	604	PGV	O02-C1-O01-C02
17	A	604	PGV	C2-C1-O01-C02
17	N	616	PGV	C03-O11-P-O12
17	N	616	PGV	C03-O11-P-O13
17	N	616	PGV	C04-O12-P-O11
17	N	616	PGV	C04-O12-P-O13
17	N	616	PGV	O12-C04-C05-O05
17	N	616	PGV	O02-C1-O01-C02
17	T	101	PGV	C04-O12-P-O11
17	T	101	PGV	O12-C04-C05-C06
17	Z	102	PGV	O02-C1-O01-C02
18	A	607	HEA	C11-C12-C13-C14
20	D	201	TGL	CB2-CB1-OG2-CG2
20	L	101	TGL	OB1-CB1-OG2-CG2
20	Y	101	TGL	CB2-CB1-OG2-CG2
20	Y	101	TGL	OB1-CB1-OG2-CG2
23	C	301	DMU	C19-C18-O16-C6
23	C	313	DMU	O5-C6-O16-C18
23	C	313	DMU	C19-C18-O16-C6
24	C	303	PEK	O12-C04-C05-N
24	C	303	PEK	C6-C7-C8-C9
24	C	304	PEK	C04-O12-P-O11
24	C	304	PEK	C04-O12-P-O14
24	C	304	PEK	O12-C04-C05-N
24	C	304	PEK	C2-C1-O01-C02
24	C	304	PEK	C9-C10-C11-C12
24	C	315	PEK	C03-O11-P-O12
24	C	315	PEK	C03-O11-P-O13
24	C	315	PEK	C03-O11-P-O14
24	C	315	PEK	C11-C12-C13-C14
24	P	301	PEK	C03-O11-P-O14
24	P	301	PEK	C2-C1-O01-C02
24	P	305	PEK	C03-O11-P-O12
24	P	305	PEK	C03-O11-P-O14
24	P	305	PEK	C04-O12-P-O11
24	P	305	PEK	C04-O12-P-O14
24	P	305	PEK	O12-C04-C05-N

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Mol	Chain	Res	Type	Atoms
24	P	305	PEK	O02-C1-O01-C02
25	C	306	CDL	O1-C1-CB2-OB2
25	C	306	CDL	C1-CA2-OA2-PA1
25	C	306	CDL	CA3-OA5-PA1-OA2
25	C	306	CDL	OA7-CA5-OA6-CA4
25	C	306	CDL	C11-CA5-OA6-CA4
25	C	306	CDL	CB2-OB2-PB2-OB3
25	C	306	CDL	CB2-OB2-PB2-OB5
25	C	312	CDL	CA2-OA2-PA1-OA4
25	C	312	CDL	CA2-OA2-PA1-OA5
25	C	312	CDL	CA3-OA5-PA1-OA2
25	C	312	CDL	CB2-OB2-PB2-OB3
25	C	312	CDL	CB2-OB2-PB2-OB4
25	C	312	CDL	CB2-OB2-PB2-OB5
25	C	312	CDL	C51-CB5-OB6-CB4
25	P	307	CDL	CB2-C1-CA2-OA2
25	P	307	CDL	C1-CA2-OA2-PA1
25	P	307	CDL	CA3-OA5-PA1-OA2
25	P	307	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CA3-OA5-PA1-OA3
25	T	102	CDL	CB2-OB2-PB2-OB5
26	E	201	PSC	C03-O11-P-O13
26	E	201	PSC	C04-O12-P-O11
26	E	201	PSC	C04-O12-P-O14
26	O	302	PSC	C03-O11-P-O12
26	O	302	PSC	C03-O11-P-O13
26	O	302	PSC	C04-O12-P-O11
26	O	302	PSC	C04-O12-P-O14
26	O	302	PSC	O12-C04-C05-N
28	I	101	SAC	C2A-C1A-N-CA
28	I	101	SAC	OAC-C1A-N-CA
28	I	101	SAC	C-CA-N-C1A
28	I	101	SAC	CB-CA-N-C1A
28	I	101	SAC	O-C-CA-CB
28	V	101	SAC	C2A-C1A-N-CA
28	V	101	SAC	OAC-C1A-N-CA
28	V	101	SAC	C-CA-CB-OG
23	G	1302	DMU	O1-C10-O7-C3
20	Q	201	TGL	OC1-CC1-OG3-CG3
23	P	302	DMU	C3-C4-C57-O61
17	A	604	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	OC1-CC1-OG3-CG3
24	C	304	PEK	O04-C21-O03-C01
25	C	312	CDL	OB9-CB7-OB8-CB6
25	P	307	CDL	OA9-CA7-OA8-CA6
26	O	302	PSC	O04-C19-O03-C01
20	D	201	TGL	OB1-CB1-OG2-CG2
24	C	304	PEK	O02-C1-O01-C02
24	P	301	PEK	O02-C1-O01-C02
25	C	312	CDL	OB7-CB5-OB6-CB4
20	D	201	TGL	CC2-CC1-OG3-CG3
24	C	304	PEK	C22-C21-O03-C01
25	C	312	CDL	C71-CB7-OB8-CB6
25	P	307	CDL	C31-CA7-OA8-CA6
17	N	616	PGV	C2-C1-O01-C02
17	Z	102	PGV	C2-C1-O01-C02
20	L	101	TGL	CB2-CB1-OG2-CG2
24	P	305	PEK	C2-C1-O01-C02
18	A	607	HEA	C26-C15-C16-C17
22	P	308	CHD	C20-C22-C23-C24
17	A	604	PGV	C20-C19-O03-C01
20	Q	201	TGL	CC2-CC1-OG3-CG3
25	T	102	CDL	C31-CA7-OA8-CA6
26	O	302	PSC	C20-C19-O03-C01
17	Z	102	PGV	O04-C19-O03-C01
20	Y	101	TGL	OA1-CA1-OG1-CG1
17	T	101	PGV	O12-C04-C05-O05
17	Z	102	PGV	O12-C04-C05-O05
25	C	312	CDL	O1-C1-CB2-OB2
26	E	201	PSC	C20-C19-O03-C01
25	C	306	CDL	C51-CB5-OB6-CB4
26	E	201	PSC	O04-C19-O03-C01
17	Z	102	PGV	C20-C19-O03-C01
20	Y	101	TGL	CA2-CA1-OG1-CG1
25	T	102	CDL	OA9-CA7-OA8-CA6
23	G	1302	DMU	O5-C4-C57-O61
23	P	302	DMU	O5-C4-C57-O61
23	C	301	DMU	O5-C6-O16-C18
24	C	315	PEK	C26-C27-C28-C29
22	Y	102	CHD	C13-C17-C20-C22
23	C	301	DMU	C5-C10-O7-C3
23	C	301	DMU	O6-C11-C9-O1
24	C	303	PEK	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	L	101	TGL	CA3-CA4-CA5-CA6
17	N	616	PGV	O12-C04-C05-C06
25	C	306	CDL	CA2-C1-CB2-OB2
17	N	616	PGV	C20-C19-O03-C01
25	T	102	CDL	C71-CB7-OB8-CB6
23	G	1302	DMU	O6-C11-C9-C8
20	D	201	TGL	C14-C29-C30-C31
25	T	102	CDL	C79-C80-C81-C82
25	T	102	CDL	C42-C43-C44-C45
23	C	301	DMU	O6-C11-C9-C8
23	C	301	DMU	C1-C6-O16-C18
20	Q	201	TGL	CA1-CA2-CA3-CA4
24	P	305	PEK	C1-C2-C3-C4
25	T	102	CDL	CB7-C71-C72-C73
25	P	307	CDL	O1-C1-CA2-OA2
26	E	201	PSC	C30-C31-C32-C33
23	M	101	DMU	O6-C11-C9-C8
17	N	616	PGV	O04-C19-O03-C01
25	T	102	CDL	OB9-CB7-OB8-CB6
23	G	1302	DMU	O6-C11-C9-O1
22	T	104	CHD	C17-C20-C22-C23
23	G	1302	DMU	C3-C4-C57-O61
25	C	306	CDL	OB7-CB5-OB6-CB4
23	M	101	DMU	O6-C11-C9-O1
17	C	305	PGV	C12-C13-C14-C15
22	Y	102	CHD	C17-C20-C22-C23
24	C	304	PEK	C24-C25-C26-C27
17	A	604	PGV	C19-C20-C21-C22
23	C	301	DMU	O1-C10-O7-C3
26	E	201	PSC	C04-C05-N-C07
17	Z	102	PGV	C1-C2-C3-C4
20	N	604	TGL	CA1-CA2-CA3-CA4
24	C	303	PEK	C1-C2-C3-C4
24	C	315	PEK	C1-C2-C3-C4
24	C	315	PEK	C21-C22-C23-C24
24	P	301	PEK	C21-C22-C23-C24
25	C	312	CDL	CB7-C71-C72-C73
25	T	102	CDL	CA5-C11-C12-C13
25	T	102	CDL	CA7-C31-C32-C33
26	O	302	PSC	C1-C2-C3-C4
25	C	312	CDL	C11-CA5-OA6-CA4
22	J	1102	CHD	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	T	104	CHD	C20-C22-C23-C24
22	T	104	CHD	C21-C20-C22-C23
20	Q	201	TGL	CB1-CB2-CB3-CB4
25	C	306	CDL	CB7-C71-C72-C73
25	C	306	CDL	O1-C1-CA2-OA2
25	T	102	CDL	O1-C1-CB2-OB2
22	T	104	CHD	C16-C17-C20-C21
17	Z	102	PGV	C19-C20-C21-C22
25	C	312	CDL	OA7-CA5-OA6-CA4
23	P	302	DMU	O16-C18-C19-C22
22	Y	102	CHD	C21-C20-C22-C23
20	D	201	TGL	CC1-CC2-CC3-CC4
17	A	605	PGV	C26-C27-C28-C29
20	N	604	TGL	CB1-CB2-CB3-CB4
25	C	306	CDL	CB2-C1-CA2-OA2
25	T	102	CDL	CA2-C1-CB2-OB2
20	N	604	TGL	CA2-CA1-OG1-CG1
26	O	302	PSC	C20-C21-C22-C23
20	D	201	TGL	C21-C22-C23-C24
22	T	104	CHD	C13-C17-C20-C21
22	Y	102	CHD	C13-C17-C20-C21
26	E	201	PSC	C04-C05-N-C08
26	O	302	PSC	C19-C20-C21-C22
26	O	302	PSC	C2-C1-O01-C02
26	O	302	PSC	O02-C1-O01-C02
23	C	313	DMU	C1-C6-O16-C18
23	P	302	DMU	C1-C6-O16-C18
24	C	315	PEK	C10-C11-C12-C13
24	C	315	PEK	C13-C14-C15-C16
22	T	104	CHD	C13-C17-C20-C22
17	A	604	PGV	O12-C04-C05-O05
24	P	301	PEK	C22-C21-O03-C01
24	P	304	PEK	C1-C2-C3-C4
26	O	302	PSC	C02-C03-O11-P
17	Z	102	PGV	C04-C05-C06-O06
20	N	604	TGL	CC1-CC2-CC3-CC4
23	M	101	DMU	O16-C18-C19-C22
20	N	604	TGL	OA1-CA1-OG1-CG1
25	C	306	CDL	C52-C53-C54-C55
25	T	102	CDL	C63-C64-C65-C66
17	P	306	PGV	C7-C8-C9-C10
17	T	101	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	A	615	TGL	CA3-CA4-CA5-CA6
20	A	615	TGL	CB7-CB8-CB9-C10
20	A	615	TGL	CB9-C10-C11-C12
20	D	201	TGL	CA3-CA4-CA5-CA6
20	N	604	TGL	C10-C11-C12-C13
24	C	303	PEK	C31-C32-C33-C34
25	C	312	CDL	C37-C38-C39-C40
25	C	312	CDL	C59-C60-C61-C62
25	P	307	CDL	C36-C37-C38-C39
26	O	302	PSC	C25-C26-C27-C28
17	A	604	PGV	C7-C8-C9-C10
17	N	616	PGV	C28-C29-C30-C31
24	P	301	PEK	C25-C26-C27-C28
25	C	312	CDL	C20-C21-C22-C23
25	P	307	CDL	C12-C13-C14-C15
17	A	604	PGV	C6-C7-C8-C9
17	A	605	PGV	C4-C5-C6-C7
17	T	101	PGV	C23-C24-C25-C26
20	L	101	TGL	CB6-CB7-CB8-CB9
20	L	101	TGL	CC9-C15-C16-C17
24	C	303	PEK	C24-C25-C26-C27
25	C	312	CDL	C57-C58-C59-C60
25	P	307	CDL	C19-C20-C21-C22
17	A	604	PGV	O05-C05-C06-O06
23	G	1302	DMU	C19-C18-O16-C6
20	L	101	TGL	CB7-CB8-CB9-C10
20	N	604	TGL	CB5-CB6-CB7-CB8
24	P	305	PEK	C32-C33-C34-C35
20	Q	201	TGL	CA5-CA6-CA7-CA8
20	Q	201	TGL	CB4-CB5-CB6-CB7
20	Y	101	TGL	CC2-CC3-CC4-CC5
24	P	301	PEK	C26-C27-C28-C29
25	P	307	CDL	C43-C44-C45-C46
23	G	1302	DMU	C2-C3-O7-C10
25	C	306	CDL	C14-C15-C16-C17
25	P	307	CDL	C78-C79-C80-C81
20	A	615	TGL	CB2-CB1-OG2-CG2
25	T	102	CDL	C11-CA5-OA6-CA4
23	Z	101	DMU	C28-C31-C34-C37
25	P	307	CDL	C81-C82-C83-C84
17	N	605	PGV	C4-C5-C6-C7
25	P	307	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
25	C	312	CDL	CB5-C51-C52-C53
17	C	305	PGV	C24-C25-C26-C27
17	N	616	PGV	C3-C4-C5-C6
25	C	306	CDL	C56-C57-C58-C59
20	N	604	TGL	CC7-CC8-CC9-C15
26	E	201	PSC	C4-C5-C6-C7
18	A	607	HEA	C14-C15-C16-C17
20	Q	201	TGL	C16-C17-C18-C19
20	A	615	TGL	C11-C10-CB9-CB8
20	L	101	TGL	C16-C17-C18-C19
24	P	301	PEK	O04-C21-O03-C01
17	T	101	PGV	C28-C29-C30-C31
20	Y	101	TGL	C23-C24-C25-C26
25	C	312	CDL	C56-C57-C58-C59
25	P	307	CDL	C22-C23-C24-C25
25	T	102	CDL	C36-C37-C38-C39
25	C	312	CDL	CA2-C1-CB2-OB2
20	L	101	TGL	C18-C19-C33-C34
23	G	1302	DMU	C31-C34-C37-C40
24	C	304	PEK	C21-C22-C23-C24
26	E	201	PSC	C19-C20-C21-C22
17	N	605	PGV	C5-C6-C7-C8
17	Z	102	PGV	C21-C22-C23-C24
20	N	604	TGL	C22-C23-C24-C25
20	Q	201	TGL	C10-C11-C12-C13
20	Y	101	TGL	CA9-C20-C21-C22
24	C	304	PEK	C26-C27-C28-C29
25	C	306	CDL	C43-C44-C45-C46
25	T	102	CDL	C56-C57-C58-C59
17	A	605	PGV	C6-C7-C8-C9
19	A	614	EDO	O1-C1-C2-O2
19	A	619	EDO	O1-C1-C2-O2
19	B	307	EDO	O1-C1-C2-O2
19	C	310	EDO	O1-C1-C2-O2
19	D	205	EDO	O1-C1-C2-O2
19	N	619	EDO	O1-C1-C2-O2
19	S	2207	EDO	O1-C1-C2-O2
19	W	304	EDO	O1-C1-C2-O2
20	D	201	TGL	CC7-CC8-CC9-C15
20	D	201	TGL	C16-C17-C18-C19
20	L	101	TGL	CC6-CC7-CC8-CC9
20	N	604	TGL	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
25	C	306	CDL	C39-C40-C41-C42
26	O	302	PSC	C22-C23-C24-C25
22	Y	102	CHD	C16-C17-C20-C21
26	E	201	PSC	C04-C05-N-C06
17	A	605	PGV	C5-C6-C7-C8
20	A	615	TGL	CC6-CC7-CC8-CC9
20	D	201	TGL	C16-C15-CC9-CC8
20	N	604	TGL	CA7-CA8-CA9-C20
20	Q	201	TGL	CB2-CB3-CB4-CB5
20	A	615	TGL	CA9-C20-C21-C22
25	C	312	CDL	C31-C32-C33-C34
25	C	312	CDL	C75-C76-C77-C78
25	P	307	CDL	C51-CB5-OB6-CB4
25	T	102	CDL	C51-CB5-OB6-CB4
24	C	315	PEK	C28-C29-C30-C31
24	C	315	PEK	C33-C34-C35-C36
25	C	306	CDL	C36-C37-C38-C39
26	O	302	PSC	C14-C15-C16-C17
20	Q	201	TGL	C21-C20-CA9-CA8
23	C	301	DMU	C19-C22-C25-C28
24	C	315	PEK	C29-C30-C31-C32
25	T	102	CDL	C32-C33-C34-C35
17	A	604	PGV	C5-C6-C7-C8
17	N	605	PGV	C30-C31-C32-C33
20	D	201	TGL	C21-C20-CA9-CA8
20	Q	201	TGL	C16-C15-CC9-CC8
25	T	102	CDL	OA7-CA5-OA6-CA4
25	C	306	CDL	C81-C82-C83-C84
18	N	607	HEA	C14-C15-C16-C17
17	T	101	PGV	C14-C15-C16-C17
20	N	604	TGL	CA9-C20-C21-C22
24	P	305	PEK	C22-C21-O03-C01
17	A	605	PGV	C29-C30-C31-C32
24	P	305	PEK	C27-C28-C29-C30
25	T	102	CDL	C12-C13-C14-C15
25	T	102	CDL	C51-C52-C53-C54
17	Z	102	PGV	C6-C7-C8-C9
25	P	307	CDL	C55-C56-C57-C58
17	N	616	PGV	C29-C30-C31-C32
17	P	306	PGV	C6-C7-C8-C9
24	C	304	PEK	C33-C34-C35-C36
17	N	605	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	C24-C25-C26-C27
20	L	101	TGL	CA9-C20-C21-C22
25	T	102	CDL	C18-C19-C20-C21
20	A	615	TGL	C17-C18-C19-C33
20	D	201	TGL	CB4-CB5-CB6-CB7
20	Y	101	TGL	C13-C14-C29-C30
17	T	101	PGV	C2-C1-O01-C02
20	N	604	TGL	CB2-CB1-OG2-CG2
20	Q	201	TGL	CB2-CB1-OG2-CG2
25	P	307	CDL	C11-CA5-OA6-CA4
17	N	605	PGV	C6-C7-C8-C9
17	Z	102	PGV	C26-C27-C28-C29
20	N	604	TGL	CA5-CA6-CA7-CA8
20	N	604	TGL	OB1-CB1-OG2-CG2
24	P	304	PEK	C28-C29-C30-C31
26	E	201	PSC	C5-C6-C7-C8
17	A	604	PGV	C11-C10-C9-C8
20	Y	101	TGL	C11-C12-C13-C14
25	C	312	CDL	C73-C74-C75-C76
17	A	604	PGV	C4-C5-C6-C7
20	N	604	TGL	C11-C10-CB9-CB8
25	P	307	CDL	C58-C59-C60-C61
20	A	615	TGL	CB6-CB7-CB8-CB9
24	C	315	PEK	C16-C17-C18-C19
25	C	306	CDL	C77-C78-C79-C80
25	C	312	CDL	C15-C16-C17-C18
24	C	303	PEK	C16-C17-C18-C19
25	C	306	CDL	C73-C74-C75-C76
22	Y	102	CHD	C16-C17-C20-C22
20	D	201	TGL	CA6-CA7-CA8-CA9
25	C	306	CDL	C76-C77-C78-C79
20	L	101	TGL	C21-C22-C23-C24
25	T	102	CDL	C34-C35-C36-C37
20	A	615	TGL	OB1-CB1-OG2-CG2
17	N	616	PGV	C24-C25-C26-C27
20	A	615	TGL	CB3-CB4-CB5-CB6
17	A	604	PGV	C26-C27-C28-C29
25	P	307	CDL	C37-C38-C39-C40
20	D	201	TGL	CC5-CC6-CC7-CC8
17	P	306	PGV	C1-C2-C3-C4
20	A	615	TGL	CB1-CB2-CB3-CB4
23	G	1302	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
17	T	101	PGV	C12-C13-C14-C15
24	P	304	PEK	C15-C16-C17-C18
26	O	302	PSC	C13-C14-C15-C16
20	Q	201	TGL	C12-C13-C14-C29
20	Y	101	TGL	C19-C33-C34-C35
25	C	312	CDL	C80-C81-C82-C83
23	G	1302	DMU	C4-C3-O7-C10
20	N	604	TGL	C20-C21-C22-C23
24	P	304	PEK	C23-C24-C25-C26
17	T	101	PGV	C25-C26-C27-C28
20	A	615	TGL	CC4-CC5-CC6-CC7
20	N	604	TGL	C15-C16-C17-C18
24	C	304	PEK	C29-C30-C31-C32
18	N	607	HEA	C26-C15-C16-C17
17	T	101	PGV	O02-C1-O01-C02
20	Q	201	TGL	OB1-CB1-OG2-CG2
25	P	307	CDL	OB7-CB5-OB6-CB4
20	N	604	TGL	CC3-CC4-CC5-CC6
24	P	304	PEK	C34-C35-C36-C37
20	A	615	TGL	CA5-CA6-CA7-CA8
20	N	604	TGL	C21-C22-C23-C24
17	Z	102	PGV	O05-C05-C06-O06
25	C	312	CDL	C52-C53-C54-C55
20	D	201	TGL	C19-C33-C34-C35
17	T	101	PGV	C22-C23-C24-C25
25	C	306	CDL	C78-C79-C80-C81
24	C	304	PEK	C15-C16-C17-C18
24	P	305	PEK	C15-C16-C17-C18
24	P	305	PEK	O04-C21-O03-C01
20	N	604	TGL	C16-C15-CC9-CC8
25	T	102	CDL	OB7-CB5-OB6-CB4
20	Q	201	TGL	C18-C19-C33-C34
17	Z	102	PGV	C13-C14-C15-C16
25	C	306	CDL	C11-C12-C13-C14
24	C	303	PEK	C2-C1-O01-C02
25	C	312	CDL	C60-C61-C62-C63
20	Y	101	TGL	C20-C21-C22-C23
17	Z	102	PGV	C15-C16-C17-C18
25	T	102	CDL	C20-C21-C22-C23
25	P	307	CDL	OA7-CA5-OA6-CA4
20	A	615	TGL	C25-C26-C27-C28
20	D	201	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
24	P	301	PEK	O03-C01-C02-C03
24	P	305	PEK	O03-C01-C02-C03
25	T	102	CDL	CB3-CB4-CB6-OB8
26	E	201	PSC	O03-C01-C02-C03
17	Z	102	PGV	C11-C10-C9-C8
26	E	201	PSC	C13-C14-C15-C16
17	N	605	PGV	C7-C8-C9-C10
20	N	604	TGL	CA2-CA3-CA4-CA5
20	Q	201	TGL	CC3-CC4-CC5-CC6
20	A	615	TGL	CA2-CA1-OG1-CG1
20	L	101	TGL	C12-C13-C14-C29
23	Z	101	DMU	C22-C25-C28-C31
25	T	102	CDL	C37-C38-C39-C40
19	A	611	EDO	O1-C1-C2-O2
19	B	306	EDO	O1-C1-C2-O2
19	B	308	EDO	O1-C1-C2-O2
19	D	206	EDO	O1-C1-C2-O2
19	O	303	EDO	O1-C1-C2-O2
19	Q	203	EDO	O1-C1-C2-O2
19	T	103	EDO	O1-C1-C2-O2
19	V	102	EDO	O1-C1-C2-O2
20	A	615	TGL	CA6-CA7-CA8-CA9
17	Z	102	PGV	C2-C3-C4-C5
20	Q	201	TGL	CA3-CA4-CA5-CA6
24	P	305	PEK	C33-C34-C35-C36
25	T	102	CDL	C35-C36-C37-C38
20	L	101	TGL	C22-C23-C24-C25
20	L	101	TGL	CC3-CC4-CC5-CC6
25	T	102	CDL	C38-C39-C40-C41
24	P	305	PEK	C17-C18-C19-C20
24	C	303	PEK	C33-C34-C35-C36
17	T	101	PGV	C4-C5-C6-C7
20	N	604	TGL	CB4-CB5-CB6-CB7
17	N	616	PGV	C25-C26-C27-C28
17	T	101	PGV	C30-C31-C32-C33
20	Y	101	TGL	C10-C11-C12-C13
25	P	307	CDL	C75-C76-C77-C78
24	P	304	PEK	C2-C3-C4-C5
20	Y	101	TGL	CB2-CB3-CB4-CB5
24	C	304	PEK	C30-C31-C32-C33
25	C	306	CDL	C21-C22-C23-C24
26	O	302	PSC	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
17	C	305	PGV	C7-C8-C9-C10
18	A	606	HEA	C4D-C3D-CAD-CBD
24	P	304	PEK	C30-C31-C32-C33
24	P	301	PEK	O01-C02-C03-O11
20	A	615	TGL	CC2-CC1-OG3-CG3
20	A	615	TGL	CC9-C15-C16-C17
20	D	201	TGL	C12-C13-C14-C29
23	C	301	DMU	C22-C25-C28-C31
18	A	607	HEA	O11-C11-C12-C13
25	T	102	CDL	C82-C83-C84-C85
24	P	301	PEK	C17-C18-C19-C20
20	N	604	TGL	CC4-CC5-CC6-CC7
20	A	615	TGL	C11-C12-C13-C14
25	T	102	CDL	C55-C56-C57-C58
17	P	306	PGV	C15-C16-C17-C18
20	A	615	TGL	CC2-CC3-CC4-CC5
25	C	306	CDL	C62-C63-C64-C65
20	D	201	TGL	OG2-CG2-CG3-OG3
20	L	101	TGL	OG2-CG2-CG3-OG3
20	Q	201	TGL	OG2-CG2-CG3-OG3
24	C	304	PEK	O03-C01-C02-O01
25	T	102	CDL	OB6-CB4-CB6-OB8
23	C	313	DMU	C34-C37-C40-C43
17	C	305	PGV	C22-C23-C24-C25
20	Y	101	TGL	CB5-CB6-CB7-CB8
20	D	201	TGL	CG2-CG1-OG1-CA1
26	O	302	PSC	C15-C16-C17-C18
18	A	606	HEA	C2D-C3D-CAD-CBD
17	C	305	PGV	C27-C28-C29-C30
20	L	101	TGL	CC4-CC5-CC6-CC7
25	T	102	CDL	C72-C73-C74-C75
25	C	312	CDL	C13-C14-C15-C16
25	C	306	CDL	C34-C35-C36-C37
18	A	607	HEA	C3B-C11-C12-C13
17	C	305	PGV	C31-C32-C33-C34
24	P	301	PEK	C35-C36-C37-C38
17	A	605	PGV	C7-C8-C9-C10
17	A	605	PGV	C31-C32-C33-C34
24	P	305	PEK	C35-C36-C37-C38
25	C	312	CDL	C44-C45-C46-C47
25	C	312	CDL	C35-C36-C37-C38
20	L	101	TGL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
24	C	315	PEK	C34-C35-C36-C37
25	C	306	CDL	C37-C38-C39-C40
25	P	307	CDL	C11-C12-C13-C14
17	N	605	PGV	C29-C30-C31-C32
17	T	101	PGV	C15-C16-C17-C18
20	Y	101	TGL	CA3-CA4-CA5-CA6
20	L	101	TGL	CC7-CC8-CC9-C15
24	P	301	PEK	C31-C32-C33-C34
25	T	102	CDL	C40-C41-C42-C43
24	P	301	PEK	C14-C15-C16-C17
25	T	102	CDL	C75-C76-C77-C78
24	P	301	PEK	C02-C03-O11-P
25	T	102	CDL	CA4-CA3-OA5-PA1
20	Q	201	TGL	CB5-CB6-CB7-CB8
26	O	302	PSC	C26-C27-C28-C29
17	P	306	PGV	C20-C21-C22-C23
17	T	101	PGV	C29-C30-C31-C32
20	Y	101	TGL	CC4-CC5-CC6-CC7
24	C	303	PEK	C17-C18-C19-C20
25	C	306	CDL	OA5-CA3-CA4-CA6
25	C	312	CDL	OB5-CB3-CB4-CB6
17	Z	102	PGV	C30-C31-C32-C33
25	C	312	CDL	C74-C75-C76-C77
25	P	307	CDL	C52-C53-C54-C55
20	A	615	TGL	CB4-CB5-CB6-CB7
25	C	312	CDL	C71-C72-C73-C74
25	P	307	CDL	C57-C58-C59-C60
28	I	101	SAC	C-CA-CB-OG
25	T	102	CDL	C22-C23-C24-C25
20	A	615	TGL	OA1-CA1-OG1-CG1
20	L	101	TGL	C29-C30-C31-C32
23	C	301	DMU	O16-C18-C19-C22
20	A	615	TGL	OC1-CC1-OG3-CG3
24	C	303	PEK	C4-C5-C6-C7
23	M	101	DMU	C34-C37-C40-C43
20	D	201	TGL	CB2-CB3-CB4-CB5
25	T	102	CDL	C73-C74-C75-C76
20	A	615	TGL	CA2-CA3-CA4-CA5
20	L	101	TGL	CG1-CG2-CG3-OG3
24	C	304	PEK	O03-C01-C02-C03
25	C	306	CDL	CA3-CA4-CA6-OA8
25	C	306	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
25	P	307	CDL	CB3-CB4-CB6-OB8
20	A	615	TGL	C15-C16-C17-C18
17	N	616	PGV	C22-C23-C24-C25
17	N	616	PGV	C20-C21-C22-C23
25	C	312	CDL	C72-C73-C74-C75
17	A	604	PGV	C29-C30-C31-C32
19	G	1304	EDO	O1-C1-C2-O2
19	G	1306	EDO	O1-C1-C2-O2
19	I	103	EDO	O1-C1-C2-O2
25	C	306	CDL	OB5-CB3-CB4-OB6
25	T	102	CDL	OA5-CA3-CA4-OA6
20	A	615	TGL	CB5-CB6-CB7-CB8
20	A	615	TGL	C16-C17-C18-C19
25	P	307	CDL	C72-C73-C74-C75
24	P	304	PEK	C2-C1-O01-C02
23	Z	101	DMU	C34-C37-C40-C43
25	C	306	CDL	C15-C16-C17-C18
25	C	306	CDL	C79-C80-C81-C82
24	C	303	PEK	C35-C36-C37-C38
20	N	604	TGL	CA3-CA4-CA5-CA6
20	N	604	TGL	C23-C24-C25-C26
20	D	201	TGL	OG1-CG1-CG2-OG2
25	C	306	CDL	OA6-CA4-CA6-OA8
25	C	306	CDL	OB6-CB4-CB6-OB8
25	C	312	CDL	OA6-CA4-CA6-OA8
25	P	307	CDL	OB6-CB4-CB6-OB8
26	E	201	PSC	O03-C01-C02-O01
24	P	301	PEK	C5-C6-C7-C8
24	P	301	PEK	C9-C10-C11-C12
24	P	301	PEK	C11-C12-C13-C14
24	P	304	PEK	C9-C10-C11-C12
24	P	305	PEK	C5-C6-C7-C8
24	P	305	PEK	C9-C10-C11-C12
26	E	201	PSC	C9-C10-C11-C12
26	E	201	PSC	C10-C11-C12-C13
26	O	302	PSC	C10-C11-C12-C13
25	C	306	CDL	C44-C45-C46-C47
24	P	301	PEK	C30-C31-C32-C33
25	C	312	CDL	C76-C77-C78-C79
20	Y	101	TGL	C17-C18-C19-C33
24	C	303	PEK	C28-C29-C30-C31
24	C	315	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	Q	201	TGL	C33-C34-C35-C36
25	C	306	CDL	C31-CA7-OA8-CA6
17	N	616	PGV	C31-C32-C33-C34
24	P	305	PEK	C26-C27-C28-C29
17	C	305	PGV	C1-C2-C3-C4
24	P	305	PEK	C34-C35-C36-C37
25	C	306	CDL	C23-C24-C25-C26
17	A	604	PGV	O12-C04-C05-C06
17	Z	102	PGV	O12-C04-C05-C06
25	P	307	CDL	CA2-C1-CB2-OB2
20	Q	201	TGL	CA4-CA5-CA6-CA7
20	D	201	TGL	C17-C18-C19-C33
25	C	312	CDL	C34-C35-C36-C37
20	D	201	TGL	C13-C14-C29-C30
24	C	315	PEK	O02-C1-O01-C02
24	P	305	PEK	C23-C24-C25-C26
26	E	201	PSC	C3-C4-C5-C6
25	P	307	CDL	C84-C85-C86-C87
20	L	101	TGL	CA1-CA2-CA3-CA4
17	A	604	PGV	C03-C02-O01-C1
25	T	102	CDL	CA3-CA4-OA6-CA5
25	C	312	CDL	C43-C44-C45-C46
24	C	303	PEK	C3-C4-C5-C6
25	C	306	CDL	OA5-CA3-CA4-OA6
20	A	615	TGL	CG1-CG2-CG3-OG3
20	Q	201	TGL	CG1-CG2-CG3-OG3
24	P	301	PEK	C13-C14-C15-C16
24	P	305	PEK	C7-C8-C9-C10
20	N	604	TGL	CC5-CC6-CC7-CC8
25	C	306	CDL	C60-C61-C62-C63
20	L	101	TGL	CA6-CA7-CA8-CA9
20	Y	101	TGL	OG1-CG1-CG2-OG2
24	P	305	PEK	O03-C01-C02-O01
20	A	615	TGL	CC3-CC4-CC5-CC6
26	O	302	PSC	C04-C05-N-C08
25	C	312	CDL	C54-C55-C56-C57
25	P	307	CDL	C74-C75-C76-C77
25	T	102	CDL	C57-C58-C59-C60
20	N	604	TGL	C25-C26-C27-C28
20	A	615	TGL	C13-C14-C29-C30
20	A	615	TGL	C14-C29-C30-C31
17	A	604	PGV	C05-C04-O12-P

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Mol	Chain	Res	Type	Atoms
17	A	605	PGV	C30-C31-C32-C33
25	T	102	CDL	C77-C78-C79-C80
26	E	201	PSC	O12-C04-C05-N
20	D	201	TGL	CC4-CC5-CC6-CC7
20	D	201	TGL	C33-C34-C35-C36
25	C	306	CDL	OA9-CA7-OA8-CA6
20	L	101	TGL	C11-C10-CB9-CB8
24	C	315	PEK	C2-C1-O01-C02
25	C	306	CDL	C35-C36-C37-C38
26	O	302	PSC	C04-C05-N-C07
24	P	304	PEK	C3-C4-C5-C6
24	P	301	PEK	C01-C02-C03-O11
25	C	306	CDL	OB5-CB3-CB4-CB6
25	P	307	CDL	OB5-CB3-CB4-CB6
25	T	102	CDL	OA5-CA3-CA4-CA6
25	T	102	CDL	OB5-CB3-CB4-CB6
20	Y	101	TGL	C16-C17-C18-C19
25	C	312	CDL	C23-C24-C25-C26
24	C	304	PEK	C35-C36-C37-C38
26	O	302	PSC	C3-C4-C5-C6
17	Z	102	PGV	C3-C4-C5-C6
23	G	1302	DMU	C34-C37-C40-C43
20	Q	201	TGL	C23-C24-C25-C26
17	A	604	PGV	C9-C10-C11-C12
17	T	101	PGV	C11-C12-C13-C14
20	Y	101	TGL	CB3-CB4-CB5-CB6
17	T	101	PGV	O04-C19-O03-C01
24	P	304	PEK	C29-C30-C31-C32
24	C	303	PEK	O02-C1-O01-C02
25	P	307	CDL	OB5-CB3-CB4-OB6
26	O	302	PSC	O01-C02-C03-O11
17	N	605	PGV	C12-C13-C14-C15
20	A	615	TGL	C29-C30-C31-C32
25	C	312	CDL	C51-C52-C53-C54
20	Y	101	TGL	C18-C19-C33-C34
25	C	306	CDL	C40-C41-C42-C43
17	C	305	PGV	C25-C26-C27-C28
20	A	615	TGL	OG2-CG2-CG3-OG3
24	P	301	PEK	O03-C01-C02-O01
20	L	101	TGL	CB4-CB5-CB6-CB7
20	D	201	TGL	OG1-CG1-CG2-CG3
20	Q	201	TGL	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
22	J	1102	CHD	C17-C20-C22-C23
25	C	306	CDL	C74-C75-C76-C77
24	P	305	PEK	C2-C3-C4-C5
19	K	102	EDO	O1-C1-C2-O2
19	N	612	EDO	O1-C1-C2-O2
19	P	311	EDO	O1-C1-C2-O2
20	L	101	TGL	C16-C15-CC9-CC8
26	O	302	PSC	C2-C3-C4-C5
23	P	302	DMU	C34-C37-C40-C43
24	P	305	PEK	C28-C29-C30-C31
25	C	306	CDL	C82-C83-C84-C85
17	N	616	PGV	C03-O11-P-O14
17	N	616	PGV	C04-O12-P-O14
17	T	101	PGV	C04-O12-P-O13
24	C	304	PEK	C04-O12-P-O13
24	C	315	PEK	C04-O12-P-O14
24	P	301	PEK	C03-O11-P-O12
24	P	301	PEK	C03-O11-P-O13
24	P	304	PEK	O12-C04-C05-N
24	P	305	PEK	C04-O12-P-O13
25	C	306	CDL	CA3-OA5-PA1-OA3
25	C	306	CDL	CB2-OB2-PB2-OB4
25	C	312	CDL	CA3-OA5-PA1-OA3
25	P	307	CDL	CB2-OB2-PB2-OB3
25	P	307	CDL	CB2-OB2-PB2-OB4
25	P	307	CDL	CB2-OB2-PB2-OB5
25	T	102	CDL	CA2-OA2-PA1-OA3
25	T	102	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	CB2-OB2-PB2-OB3
25	T	102	CDL	CB3-OB5-PB2-OB3
26	E	201	PSC	C03-O11-P-O12
26	E	201	PSC	C03-O11-P-O14
26	E	201	PSC	C04-O12-P-O13
26	O	302	PSC	C04-C05-N-C06
17	T	101	PGV	C7-C8-C9-C10
20	N	604	TGL	C14-C29-C30-C31
20	Q	201	TGL	CA9-C20-C21-C22
26	O	302	PSC	C30-C31-C32-C33
17	C	305	PGV	C02-C03-O11-P
17	P	306	PGV	C02-C03-O11-P
24	C	315	PEK	C02-C03-O11-P
25	C	306	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
24	C	304	PEK	C23-C24-C25-C26
25	C	312	CDL	C63-C64-C65-C66
25	C	312	CDL	C81-C82-C83-C84
24	P	305	PEK	C03-C02-O01-C1
25	C	312	CDL	CB3-CB4-OB6-CB5
17	Z	102	PGV	C31-C32-C33-C34
17	P	306	PGV	C28-C29-C30-C31
20	D	201	TGL	CA4-CA5-CA6-CA7
26	O	302	PSC	C01-C02-C03-O11
20	A	615	TGL	CC5-CC6-CC7-CC8
25	C	312	CDL	OB5-CB3-CB4-OB6
17	A	604	PGV	C13-C14-C15-C16
20	N	604	TGL	OG1-CA1-CA2-CA3
25	C	312	CDL	C18-C19-C20-C21
20	Y	101	TGL	CC6-CC7-CC8-CC9
28	I	101	SAC	N-CA-CB-OG
25	C	312	CDL	C1-CA2-OA2-PA1
17	A	604	PGV	C24-C25-C26-C27
17	T	101	PGV	C20-C19-O03-C01
25	T	102	CDL	C61-C62-C63-C64
20	N	604	TGL	C16-C17-C18-C19
17	A	604	PGV	C28-C29-C30-C31
25	C	306	CDL	C22-C23-C24-C25
20	L	101	TGL	C20-C21-C22-C23
20	D	201	TGL	OG3-CC1-CC2-CC3
25	T	102	CDL	C52-C51-CB5-OB6
19	B	304	EDO	O1-C1-C2-O2
19	C	314	EDO	O1-C1-C2-O2
19	D	207	EDO	O1-C1-C2-O2
19	E	205	EDO	O1-C1-C2-O2
19	I	102	EDO	O1-C1-C2-O2
19	W	301	EDO	O1-C1-C2-O2
19	W	303	EDO	O1-C1-C2-O2
17	T	101	PGV	C27-C28-C29-C30
24	P	305	PEK	C30-C31-C32-C33
25	C	312	CDL	C79-C80-C81-C82
25	C	306	CDL	C51-C52-C53-C54
26	E	201	PSC	C24-C25-C26-C27
17	A	604	PGV	C20-C21-C22-C23
26	E	201	PSC	C15-C16-C17-C18
23	M	101	DMU	C19-C22-C25-C28
20	Y	101	TGL	CB6-CB7-CB8-CB9

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Mol	Chain	Res	Type	Atoms
20	L	101	TGL	C14-C29-C30-C31
17	N	605	PGV	C25-C26-C27-C28
20	Q	201	TGL	C24-C25-C26-C27
24	P	304	PEK	C14-C15-C16-C17
20	A	615	TGL	C21-C20-CA9-CA8
20	A	615	TGL	OG1-CG1-CG2-OG2
24	C	315	PEK	O03-C01-C02-O01
23	P	302	DMU	O5-C6-O16-C18
20	D	201	TGL	CA2-CA3-CA4-CA5
25	T	102	CDL	C60-C61-C62-C63
24	P	305	PEK	C02-C03-O11-P
25	P	307	CDL	C1-CB2-OB2-PB2
23	C	313	DMU	O6-C11-C9-C8
25	C	312	CDL	C58-C59-C60-C61
20	A	615	TGL	CA4-CA5-CA6-CA7
25	P	307	CDL	C56-C57-C58-C59
17	A	604	PGV	C11-C12-C13-C14
17	C	305	PGV	C11-C12-C13-C14
24	C	315	PEK	C22-C23-C24-C25
22	P	308	CHD	C13-C17-C20-C21
22	G	1305	CHD	C22-C23-C24-O25
25	T	102	CDL	CB5-C51-C52-C53
24	P	301	PEK	C33-C34-C35-C36
17	Z	102	PGV	C03-C02-O01-C1
25	C	312	CDL	CB6-CB4-OB6-CB5
24	P	301	PEK	C29-C30-C31-C32
19	A	617	EDO	O1-C1-C2-O2
19	C	309	EDO	O1-C1-C2-O2
19	E	204	EDO	O1-C1-C2-O2
19	N	615	EDO	O1-C1-C2-O2
19	N	620	EDO	O1-C1-C2-O2
19	R	202	EDO	O1-C1-C2-O2
19	S	2201	EDO	O1-C1-C2-O2
19	S	2204	EDO	O1-C1-C2-O2
22	G	1305	CHD	C22-C23-C24-O26
17	T	101	PGV	C24-C25-C26-C27
20	D	201	TGL	CC6-CC7-CC8-CC9
26	O	302	PSC	C4-C5-C6-C7
22	Y	102	CHD	C22-C23-C24-O25
22	B	302	CHD	C22-C23-C24-O26
22	P	308	CHD	C22-C23-C24-O25
17	N	605	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
17	N	616	PGV	C4-C5-C6-C7
25	T	102	CDL	C1-CA2-OA2-PA1
26	O	302	PSC	C31-C32-C33-C34
24	C	304	PEK	C31-C32-C33-C34
22	Y	102	CHD	C22-C23-C24-O26
25	T	102	CDL	C81-C82-C83-C84
18	A	606	HEA	CAA-CBA-CGA-O1A
18	N	606	HEA	CAD-CBD-CGD-O2D
22	C	302	CHD	C16-C17-C20-C22
20	L	101	TGL	C11-C12-C13-C14
25	P	307	CDL	C51-C52-C53-C54
23	Z	101	DMU	O6-C11-C9-O1
17	N	605	PGV	C26-C27-C28-C29
17	N	616	PGV	C9-C10-C11-C12
26	E	201	PSC	C7-C8-C9-C10
24	C	315	PEK	C5-C6-C7-C8
24	C	315	PEK	C11-C10-C9-C8
24	C	315	PEK	C12-C13-C14-C15
24	P	304	PEK	C5-C6-C7-C8
24	P	304	PEK	C11-C10-C9-C8
24	P	304	PEK	C11-C12-C13-C14
26	O	302	PSC	C9-C10-C11-C12
20	L	101	TGL	C13-C14-C29-C30
18	A	606	HEA	CAD-CBD-CGD-O1D
17	A	605	PGV	C11-C10-C9-C8
18	A	606	HEA	CAA-CBA-CGA-O2A
22	B	302	CHD	C22-C23-C24-O25
22	C	307	CHD	C22-C23-C24-O25
18	A	606	HEA	CAD-CBD-CGD-O2D
18	N	606	HEA	CAD-CBD-CGD-O1D
25	C	312	CDL	C62-C63-C64-C65
26	E	201	PSC	C22-C23-C24-C25
17	C	305	PGV	C05-C04-O12-P
17	T	101	PGV	C1-C2-C3-C4
20	L	101	TGL	CC2-CC1-OG3-CG3
18	N	606	HEA	CAA-CBA-CGA-O2A
17	N	616	PGV	C23-C24-C25-C26
24	P	301	PEK	C32-C33-C34-C35
17	A	605	PGV	C23-C24-C25-C26
24	C	304	PEK	C16-C17-C18-C19
22	C	307	CHD	C22-C23-C24-O26
22	P	303	CHD	C22-C23-C24-O26

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Mol	Chain	Res	Type	Atoms
25	T	102	CDL	OB5-CB3-CB4-OB6
22	P	308	CHD	C22-C23-C24-O26
25	P	307	CDL	CA7-C31-C32-C33
19	D	203	EDO	O1-C1-C2-O2
19	G	1303	EDO	O1-C1-C2-O2
19	J	1105	EDO	O1-C1-C2-O2
19	K	101	EDO	O1-C1-C2-O2
19	N	614	EDO	O1-C1-C2-O2
19	S	2206	EDO	O1-C1-C2-O2
25	C	312	CDL	C53-C54-C55-C56
25	T	102	CDL	C13-C14-C15-C16
17	Z	102	PGV	C9-C10-C11-C12
24	P	301	PEK	C3-C4-C5-C6
17	A	605	PGV	O03-C19-C20-C21
17	N	605	PGV	O03-C19-C20-C21
24	C	303	PEK	O03-C21-C22-C23
20	N	604	TGL	OC1-CC1-OG3-CG3
17	C	305	PGV	C14-C15-C16-C17
24	C	303	PEK	C10-C11-C12-C13
20	L	101	TGL	CB2-CB3-CB4-CB5
25	P	307	CDL	OA5-CA3-CA4-CA6
20	L	101	TGL	OG1-CG1-CG2-OG2
24	C	304	PEK	C1-C2-C3-C4
20	L	101	TGL	CB3-CB4-CB5-CB6
17	N	616	PGV	C11-C12-C13-C14
24	C	304	PEK	C3-C4-C5-C6
24	C	304	PEK	C17-C18-C19-C20
20	D	201	TGL	CA9-C20-C21-C22
25	C	306	CDL	C72-C73-C74-C75
25	P	307	CDL	C39-C40-C41-C42
20	A	615	TGL	C10-C11-C12-C13
20	Y	101	TGL	C21-C22-C23-C24
22	W	302	CHD	C22-C23-C24-O26
17	A	605	PGV	C11-C12-C13-C14
25	T	102	CDL	C62-C63-C64-C65
20	D	201	TGL	OG2-CB1-CB2-CB3
24	C	303	PEK	C14-C15-C16-C17
22	P	303	CHD	C22-C23-C24-O25
20	Q	201	TGL	C21-C22-C23-C24
18	A	607	HEA	C2A-C3A-CMA-OMA
26	O	302	PSC	C21-C22-C23-C24
20	L	101	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
25	C	306	CDL	CB4-CB3-OB5-PB2
20	Y	101	TGL	OG1-CG1-CG2-CG3
23	C	301	DMU	C18-C19-C22-C25
17	C	305	PGV	C26-C27-C28-C29
24	C	304	PEK	C22-C23-C24-C25
26	O	302	PSC	C12-C13-C14-C15
24	C	303	PEK	C32-C33-C34-C35
25	P	307	CDL	C16-C17-C18-C19
18	N	606	HEA	CAA-CBA-CGA-O1A
19	B	309	EDO	O1-C1-C2-O2
19	F	701	EDO	O1-C1-C2-O2
19	F	704	EDO	O1-C1-C2-O2
19	Q	202	EDO	O1-C1-C2-O2
19	R	201	EDO	O1-C1-C2-O2
19	T	105	EDO	O1-C1-C2-O2
24	C	304	PEK	O03-C21-C22-C23
20	Q	201	TGL	OG3-CC1-CC2-CC3
18	A	607	HEA	CAD-CBD-CGD-O2D
22	W	302	CHD	C22-C23-C24-O25
25	C	306	CDL	C58-C59-C60-C61
26	O	302	PSC	C23-C24-C25-C26
24	P	304	PEK	O01-C1-C2-C3
17	A	605	PGV	C9-C10-C11-C12
17	N	605	PGV	C9-C10-C11-C12
20	D	201	TGL	CC9-C15-C16-C17
25	P	307	CDL	C31-C32-C33-C34
20	D	201	TGL	C29-C30-C31-C32
24	P	304	PEK	O02-C1-O01-C02
20	N	604	TGL	C24-C25-C26-C27
24	C	303	PEK	O01-C1-C2-C3
25	P	307	CDL	C21-C22-C23-C24
17	T	101	PGV	O01-C02-C03-O11
17	Z	102	PGV	O01-C1-C2-C3
25	C	306	CDL	C57-C58-C59-C60
25	T	102	CDL	O1-C1-CA2-OA2
24	C	303	PEK	C23-C24-C25-C26
18	N	607	HEA	CAD-CBD-CGD-O1D
20	Q	201	TGL	CA6-CA7-CA8-CA9
20	A	615	TGL	OG3-CC1-CC2-CC3
20	Y	101	TGL	OG2-CB1-CB2-CB3
20	Q	201	TGL	C11-C10-CB9-CB8
25	P	307	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
18	N	607	HEA	CAD-CBD-CGD-O2D
26	O	302	PSC	O03-C19-C20-C21
24	P	304	PEK	C35-C36-C37-C38
19	D	204	EDO	O1-C1-C2-O2
19	N	609	EDO	O1-C1-C2-O2
19	P	309	EDO	O1-C1-C2-O2
17	A	605	PGV	C22-C23-C24-C25
23	C	313	DMU	C3-C4-C57-O61
25	C	312	CDL	CA3-CA4-OA6-CA5
25	C	312	CDL	CA6-CA4-OA6-CA5
23	M	101	DMU	C22-C25-C28-C31
25	P	307	CDL	C61-C62-C63-C64
17	A	604	PGV	C27-C28-C29-C30
18	A	607	HEA	CAD-CBD-CGD-O1D
25	T	102	CDL	C16-C17-C18-C19
20	L	101	TGL	C23-C24-C25-C26
20	Y	101	TGL	CC5-CC6-CC7-CC8
25	C	312	CDL	C21-C22-C23-C24
25	C	306	CDL	C72-C71-CB7-OB8
18	A	606	HEA	O11-C11-C12-C13
24	P	301	PEK	C24-C25-C26-C27
24	P	304	PEK	O02-C1-C2-C3
17	P	306	PGV	C27-C28-C29-C30
24	C	315	PEK	O01-C1-C2-C3
24	C	304	PEK	O04-C21-C22-C23
17	N	605	PGV	C15-C16-C17-C18
20	Q	201	TGL	OC1-CC1-CC2-CC3
24	P	305	PEK	C22-C23-C24-C25
25	P	307	CDL	C63-C64-C65-C66
24	C	303	PEK	O02-C1-C2-C3
20	L	101	TGL	OG1-CG1-CG2-CG3
25	C	312	CDL	CB3-CB4-CB6-OB8
24	C	315	PEK	O02-C1-C2-C3
25	T	102	CDL	C58-C59-C60-C61
17	Z	102	PGV	O02-C1-C2-C3
20	Q	201	TGL	CB7-CB8-CB9-C10
25	C	306	CDL	C19-C20-C21-C22
19	E	202	EDO	O1-C1-C2-O2
19	N	608	EDO	O1-C1-C2-O2
25	C	312	CDL	C40-C41-C42-C43
20	A	615	TGL	OG1-CA1-CA2-CA3
20	A	615	TGL	OC1-CC1-CC2-CC3

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Mol	Chain	Res	Type	Atoms
25	C	312	CDL	C12-C11-CA5-OA6
17	A	605	PGV	C19-C20-C21-C22
20	Y	101	TGL	OB1-CB1-CB2-CB3
26	O	302	PSC	O04-C19-C20-C21

There are no ring outliers.

50 monomers are involved in 128 short contacts:

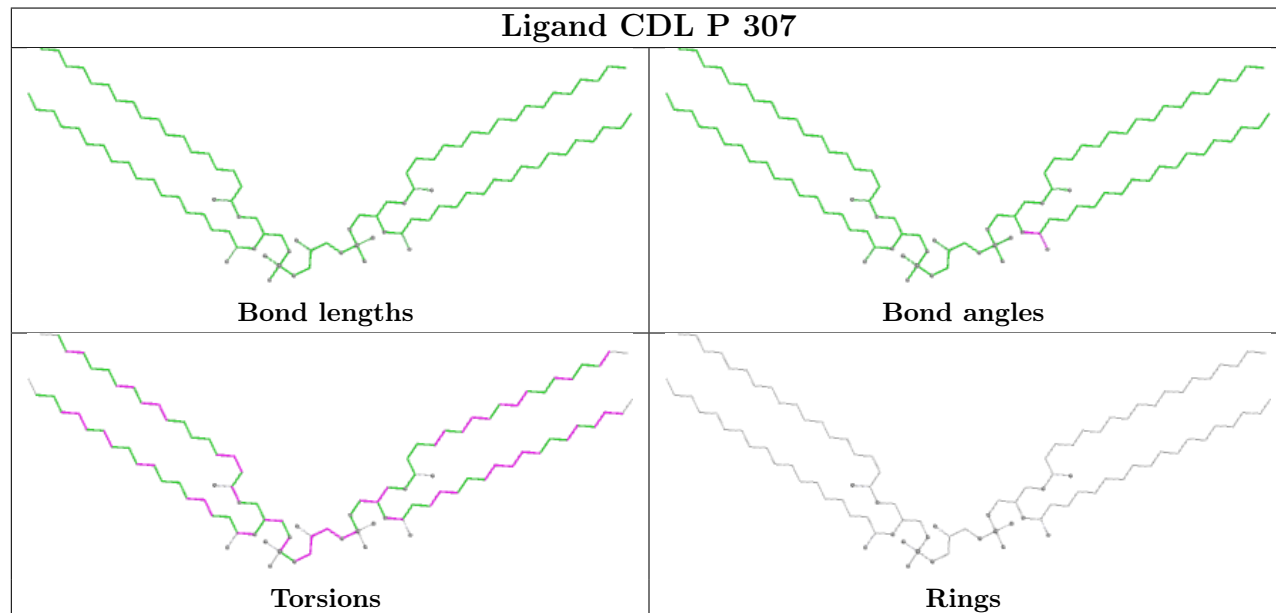
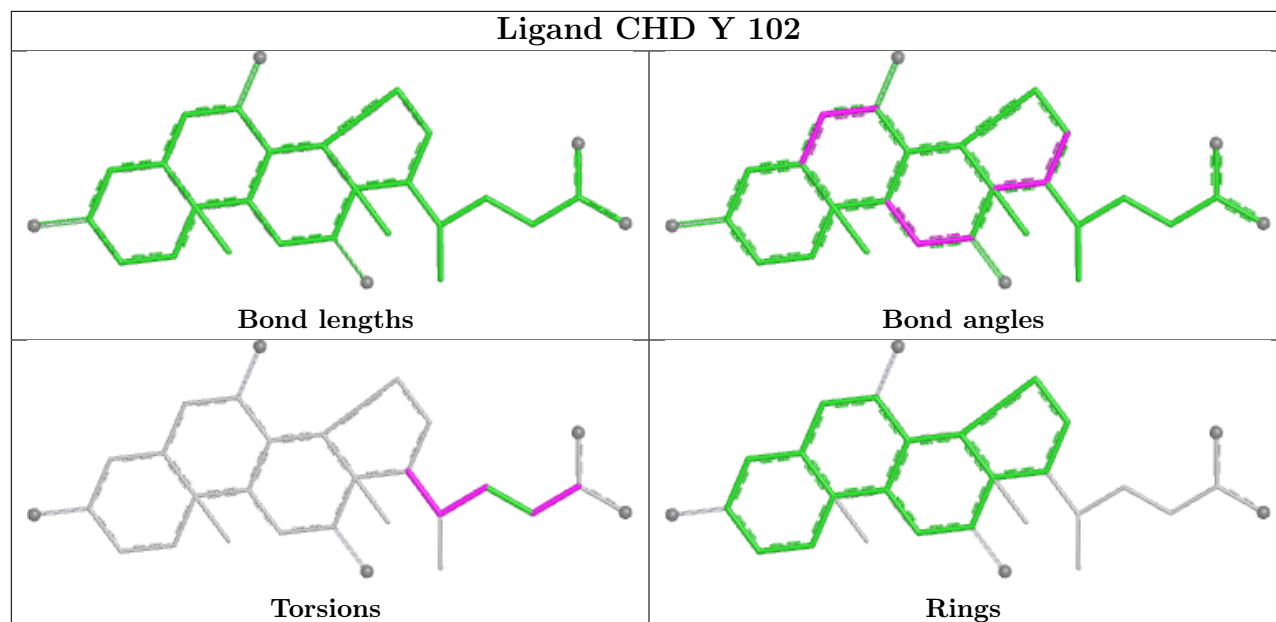
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Y	102	CHD	4	0
19	V	103	EDO	1	0
25	P	307	CDL	4	0
18	N	607	HEA	4	0
19	U	1501	EDO	3	0
17	N	616	PGV	1	0
24	C	304	PEK	2	0
28	V	101	SAC	1	0
22	T	104	CHD	7	0
24	P	304	PEK	1	0
19	A	613	EDO	1	0
19	S	2201	EDO	3	0
20	A	615	TGL	1	0
20	L	101	TGL	2	0
20	Y	101	TGL	2	0
17	Z	102	PGV	2	0
18	N	606	HEA	1	0
19	A	608	EDO	1	0
24	P	305	PEK	5	0
24	C	303	PEK	4	0
19	N	613	EDO	1	0
25	C	312	CDL	13	0
19	A	614	EDO	3	0
17	N	605	PGV	1	0
17	P	306	PGV	1	0
18	A	607	HEA	3	0
24	C	315	PEK	2	0
26	O	302	PSC	5	0
19	G	1303	EDO	2	0
19	A	616	EDO	1	0
19	J	1101	EDO	1	0
28	I	101	SAC	2	0
23	C	313	DMU	1	0

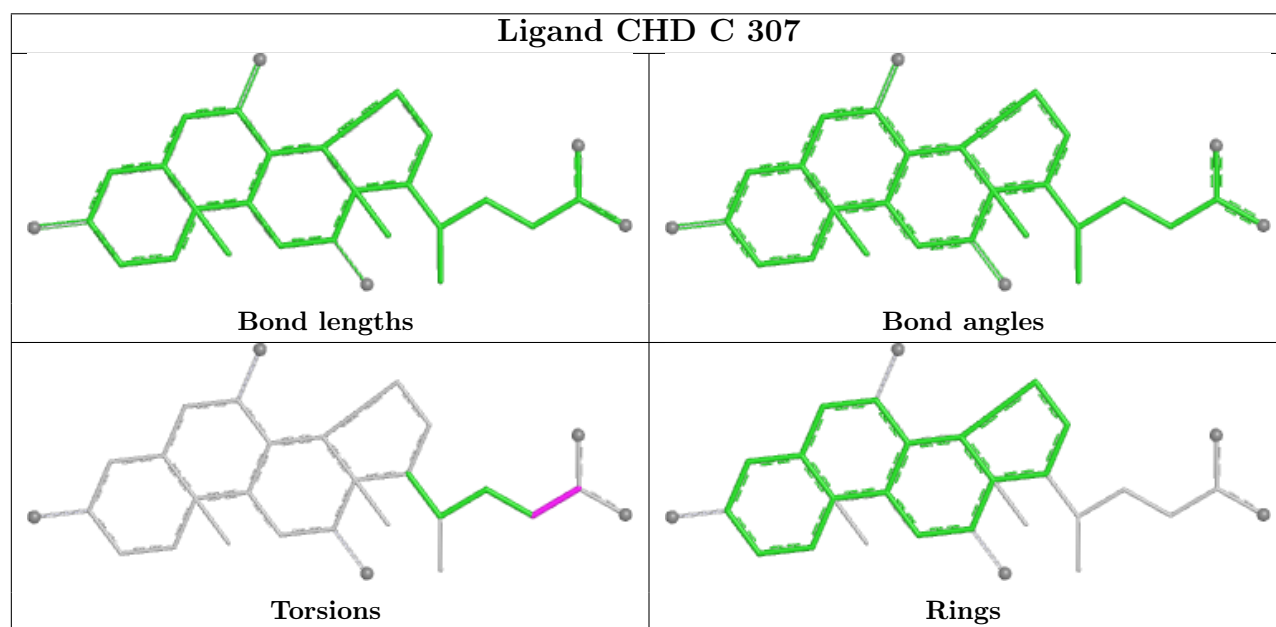
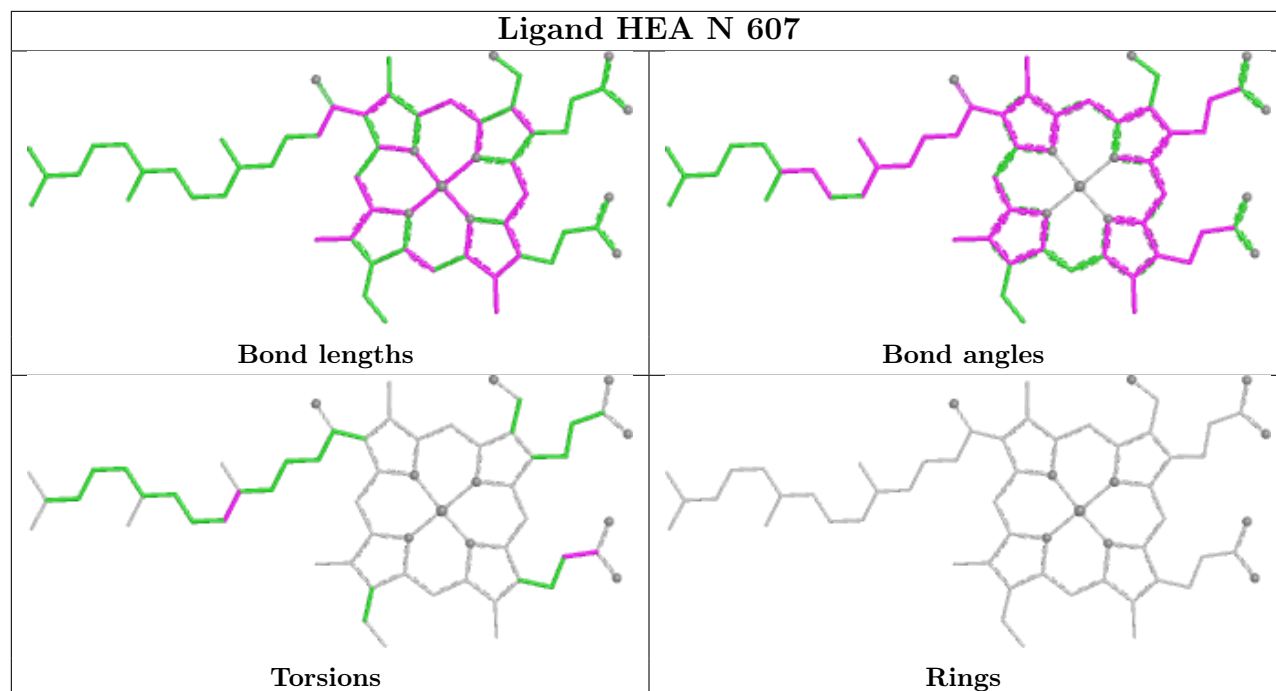
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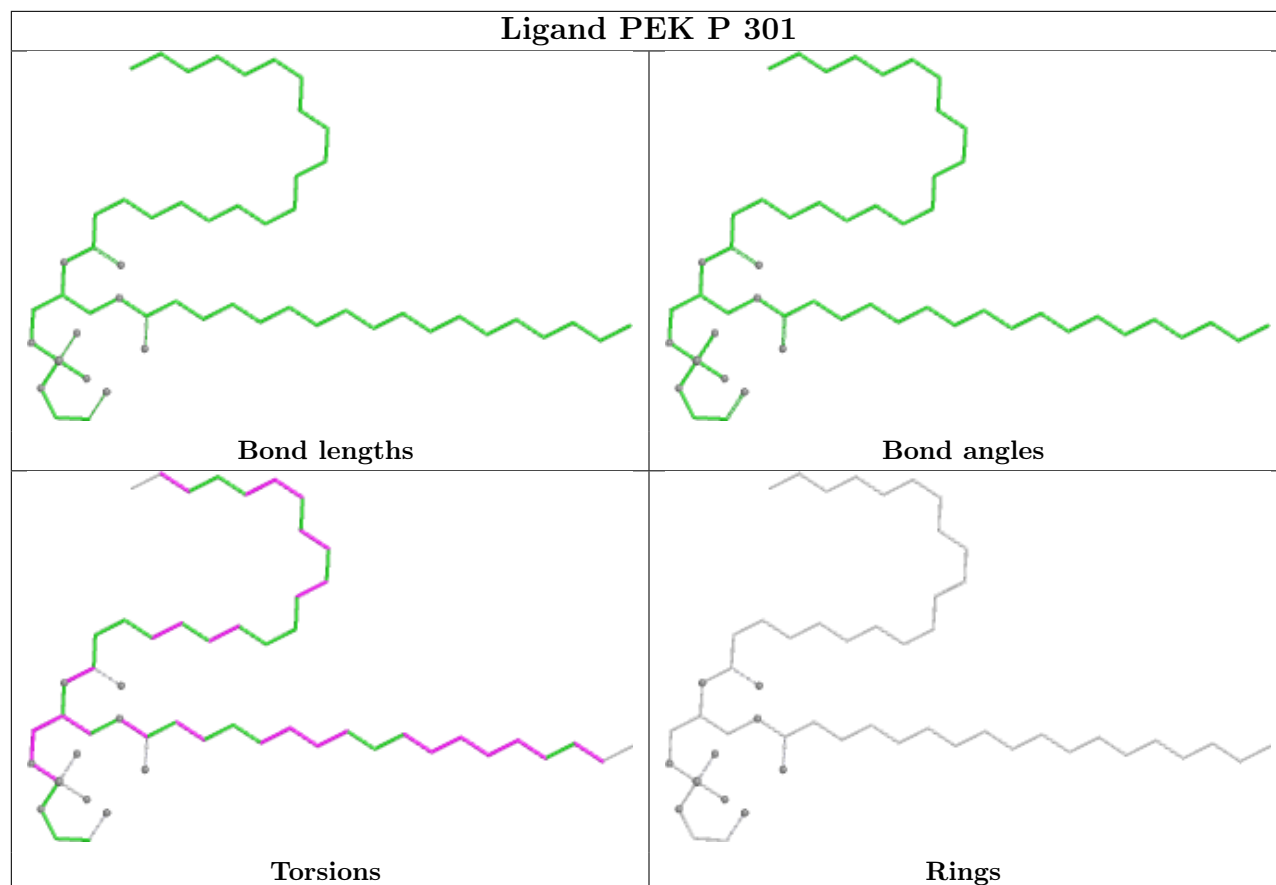
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	T	102	CDL	3	0
22	C	302	CHD	1	0
19	J	1104	EDO	1	0
20	D	201	TGL	7	0
19	S	2206	EDO	1	0
19	F	702	EDO	1	0
22	G	1305	CHD	1	0
23	G	1302	DMU	2	0
17	T	101	PGV	1	0
20	Q	201	TGL	5	0
22	P	308	CHD	1	0
25	C	306	CDL	2	0
19	N	614	EDO	9	0
23	Z	101	DMU	1	0
19	N	619	EDO	1	0
26	E	201	PSC	5	0
17	A	604	PGV	4	0

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

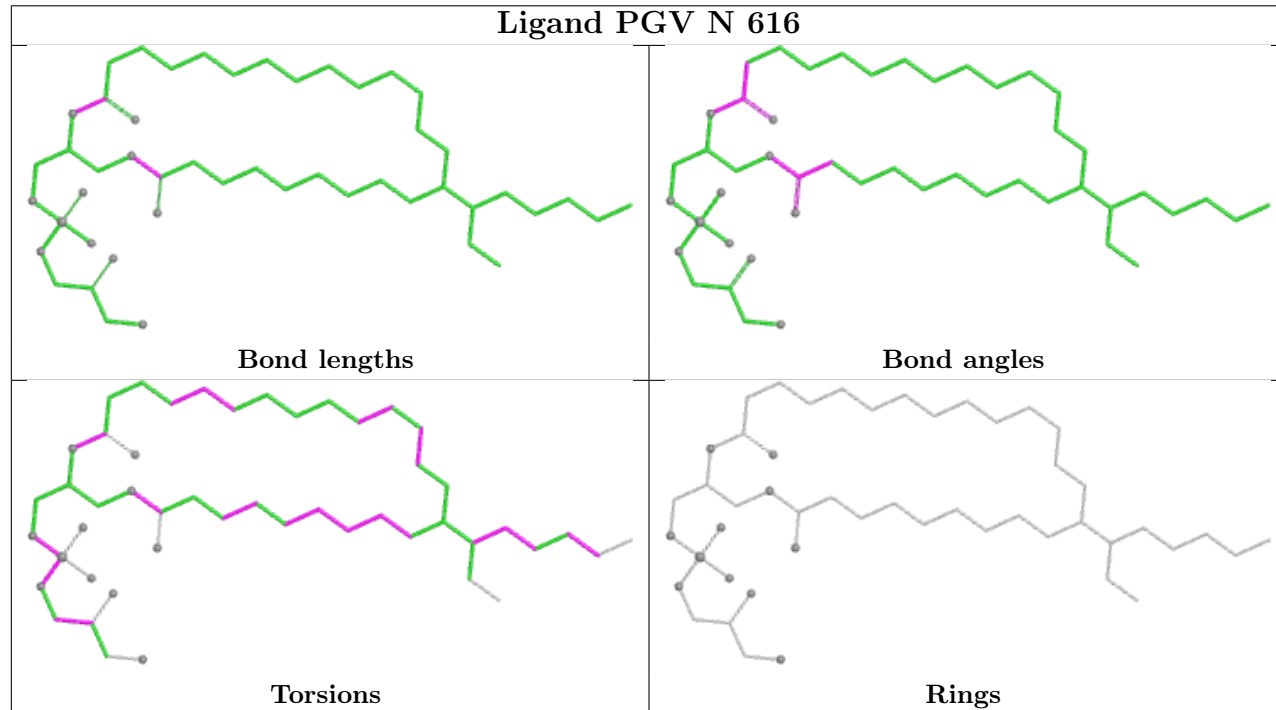




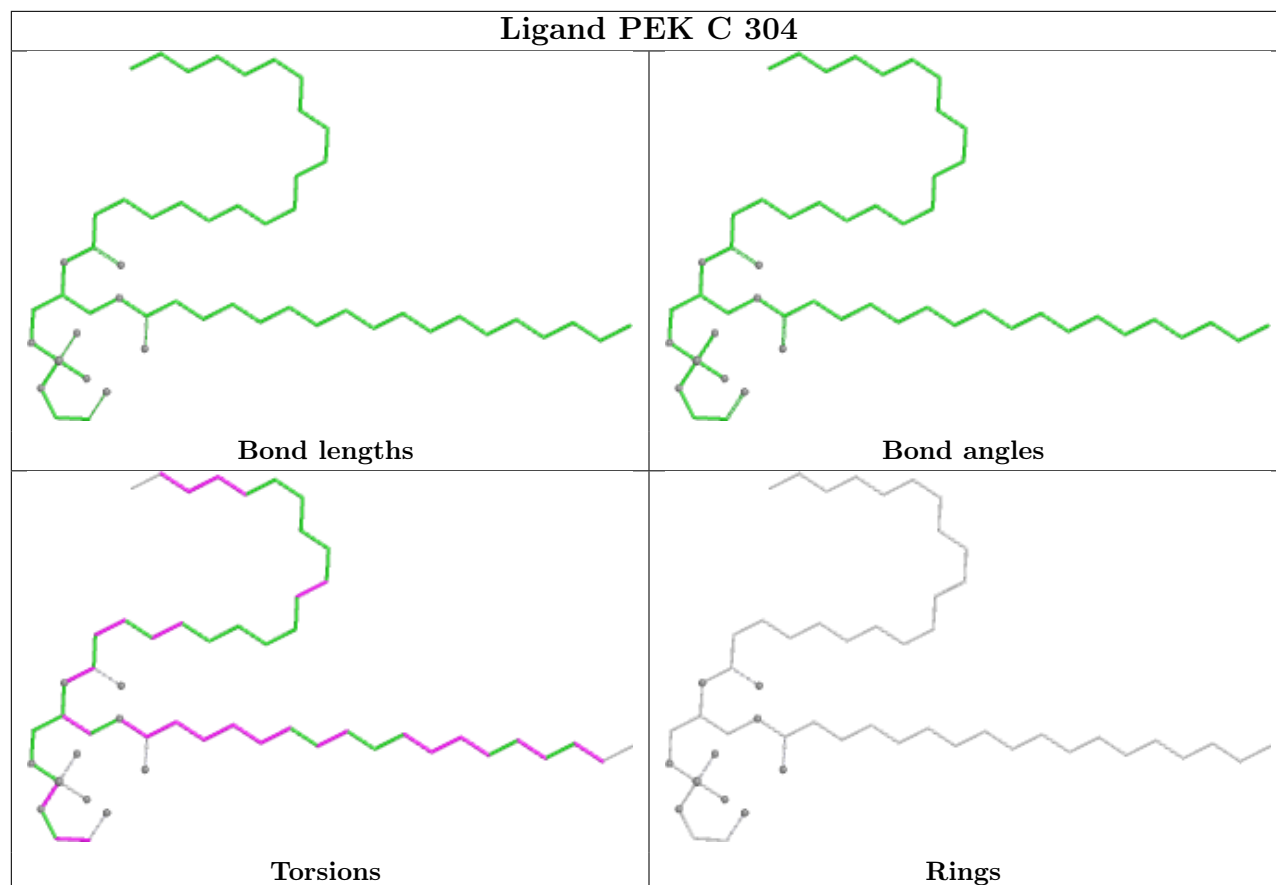
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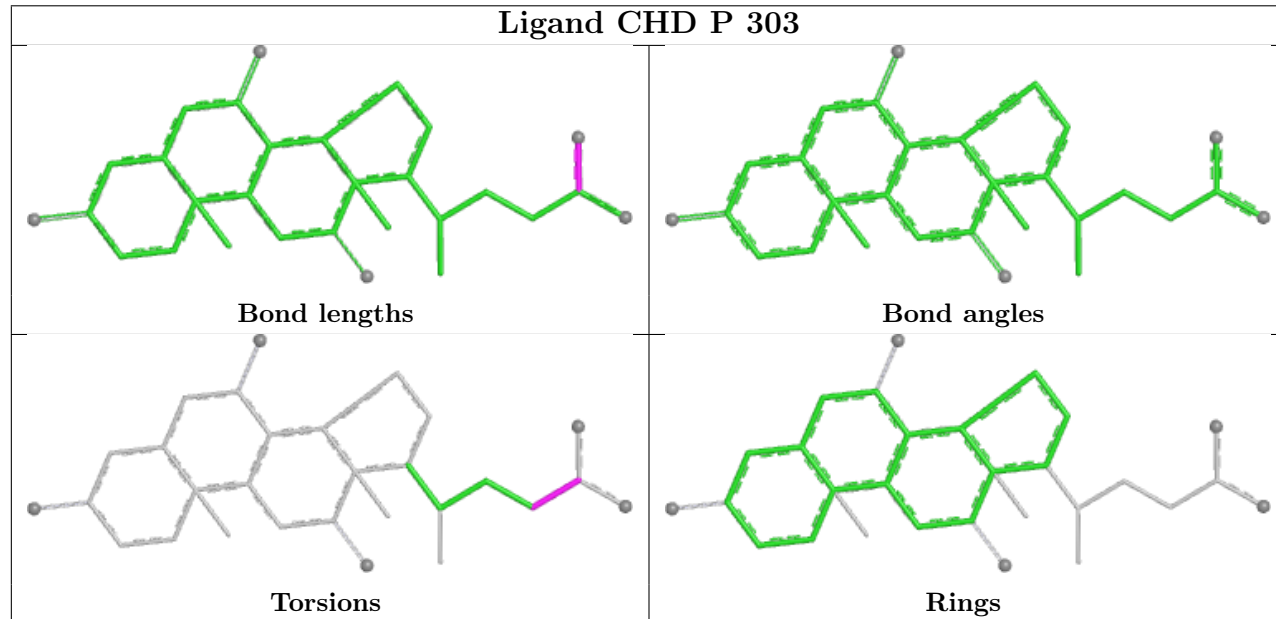
Ligand PGV N 616

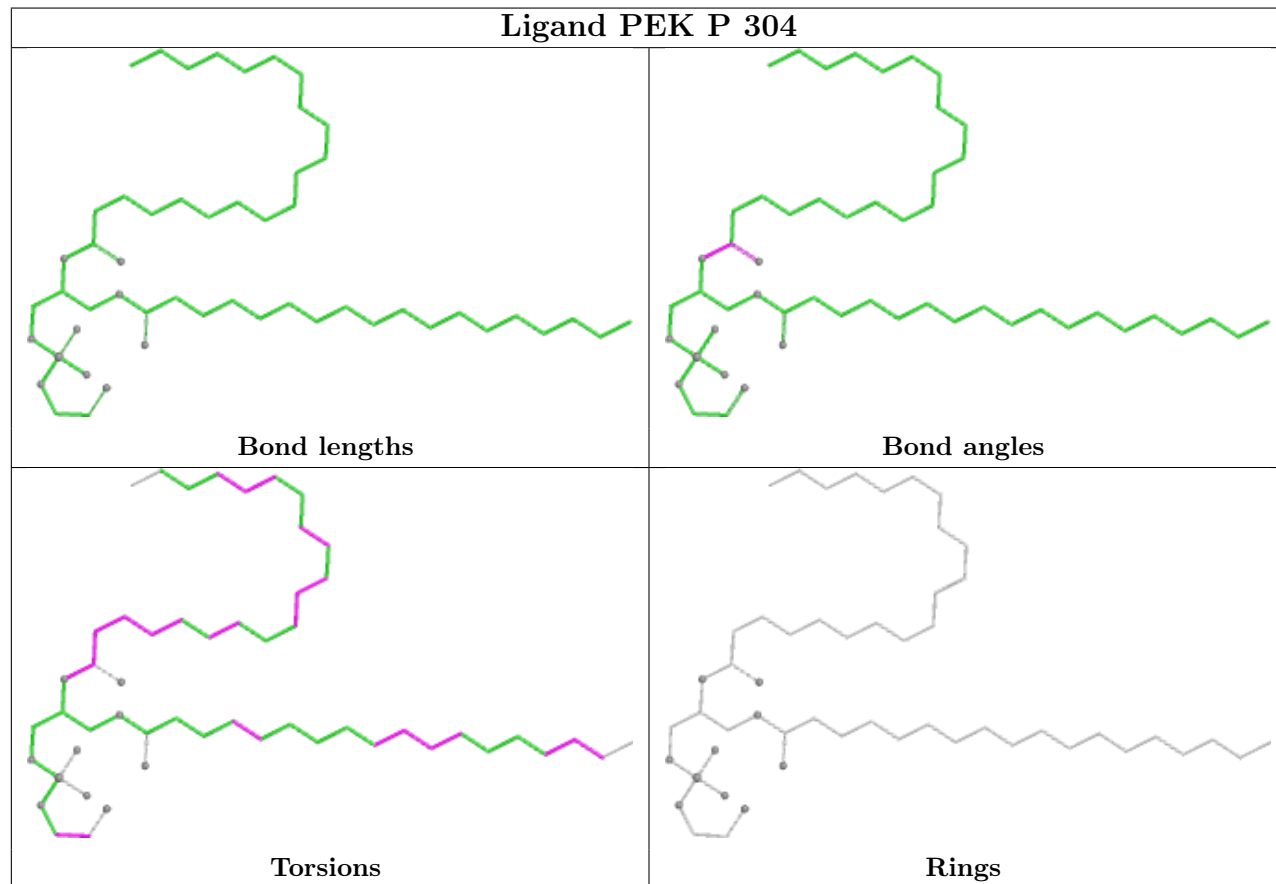
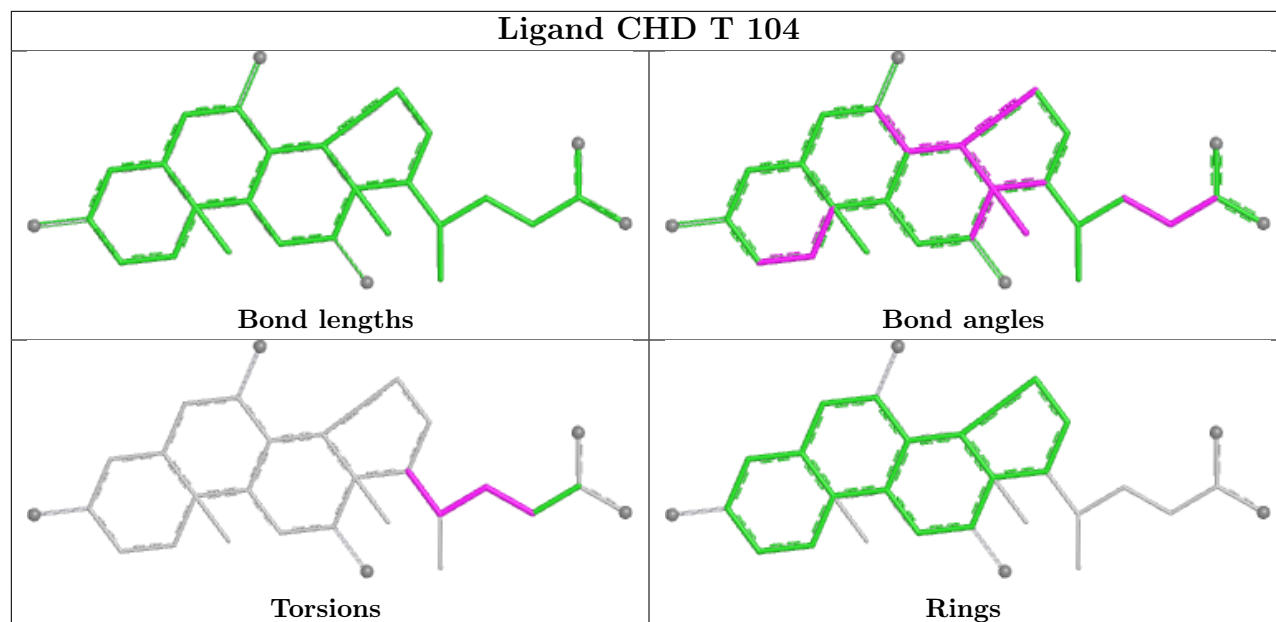


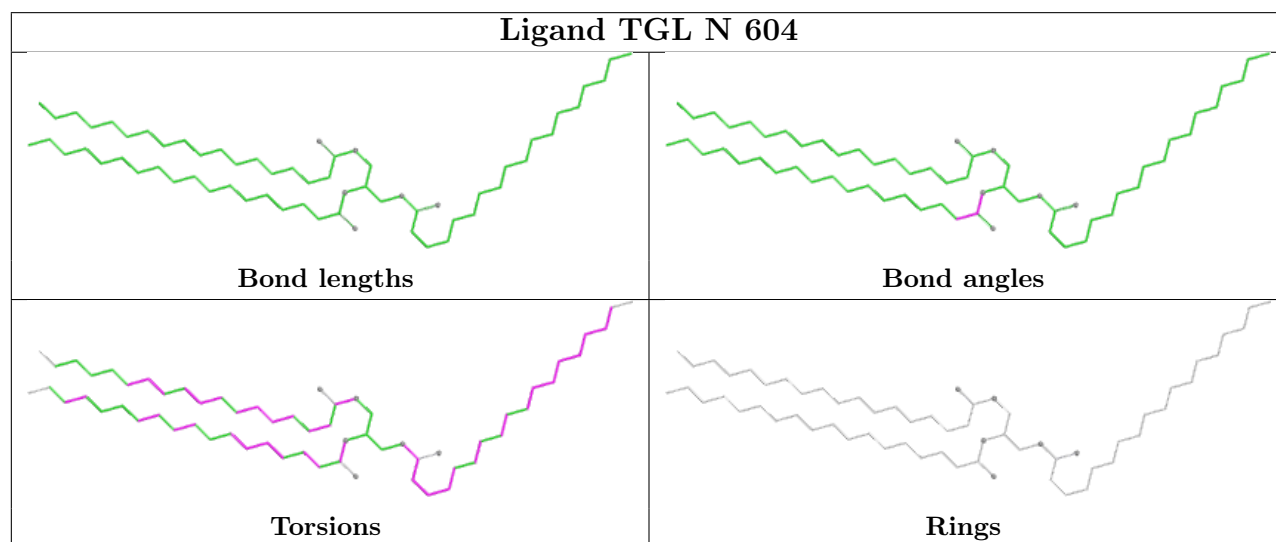
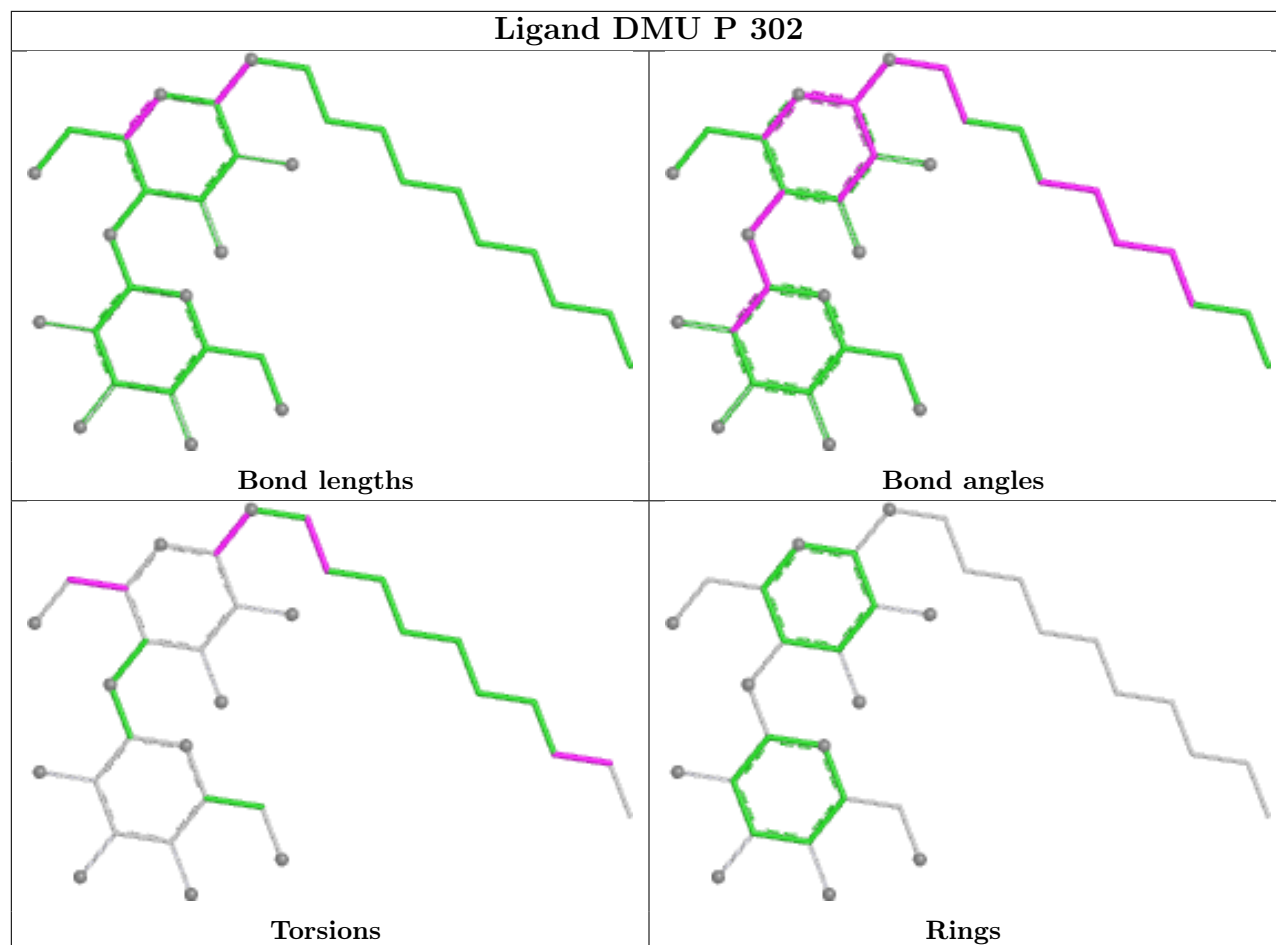
Ligand PEK C 304

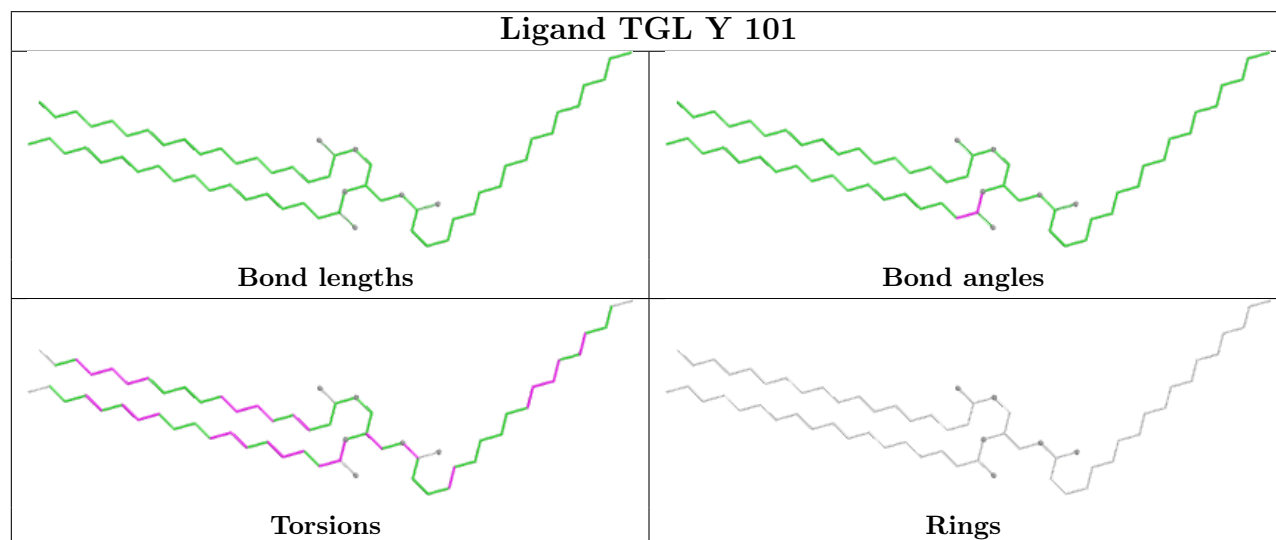
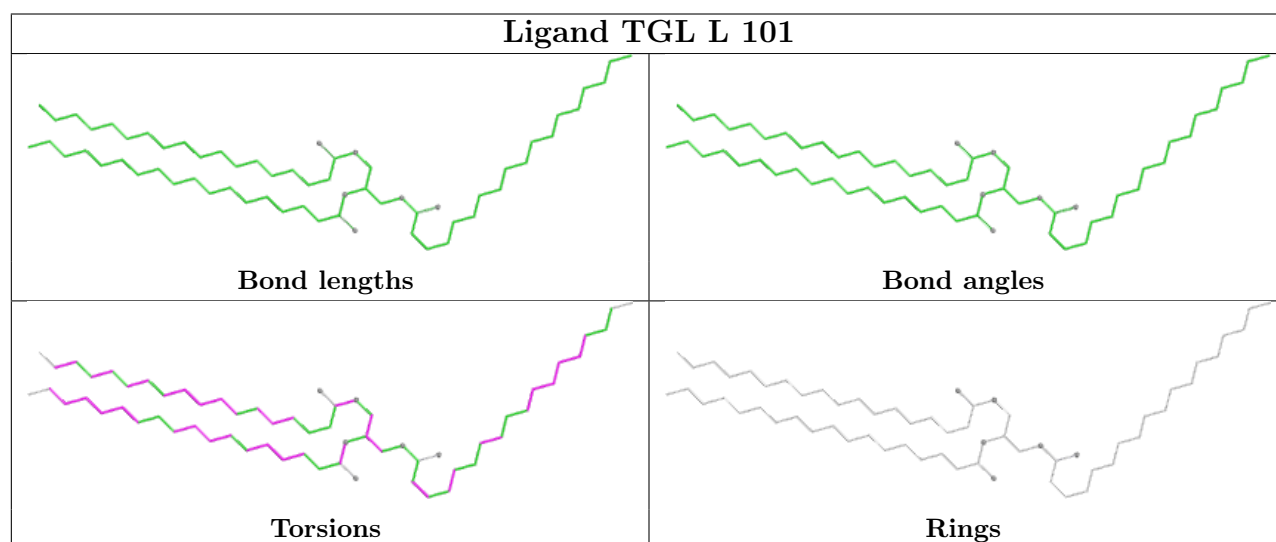
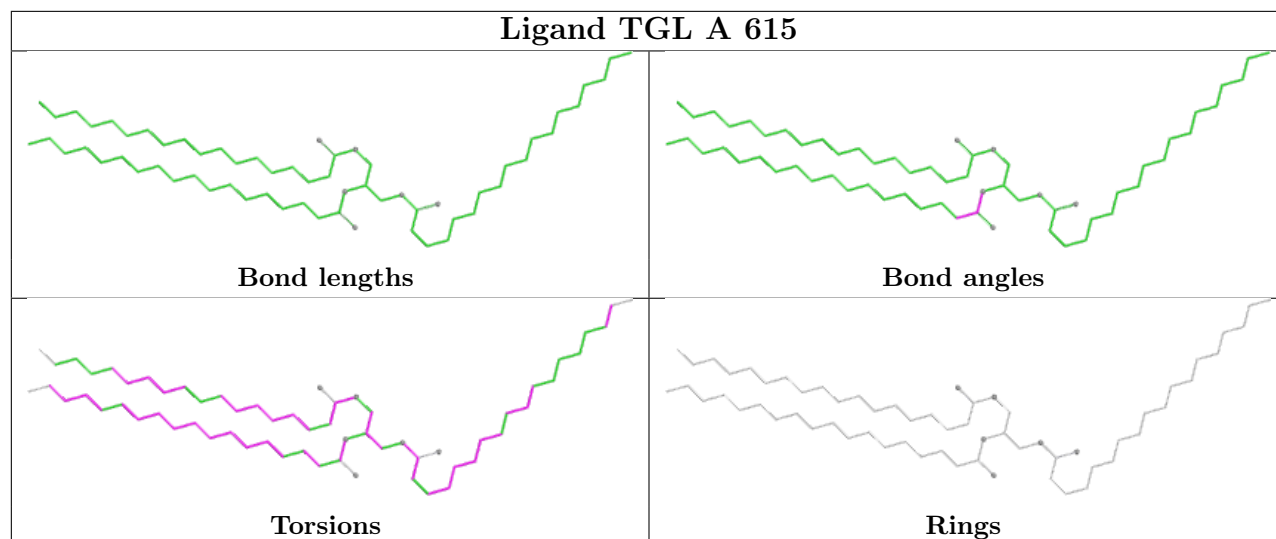


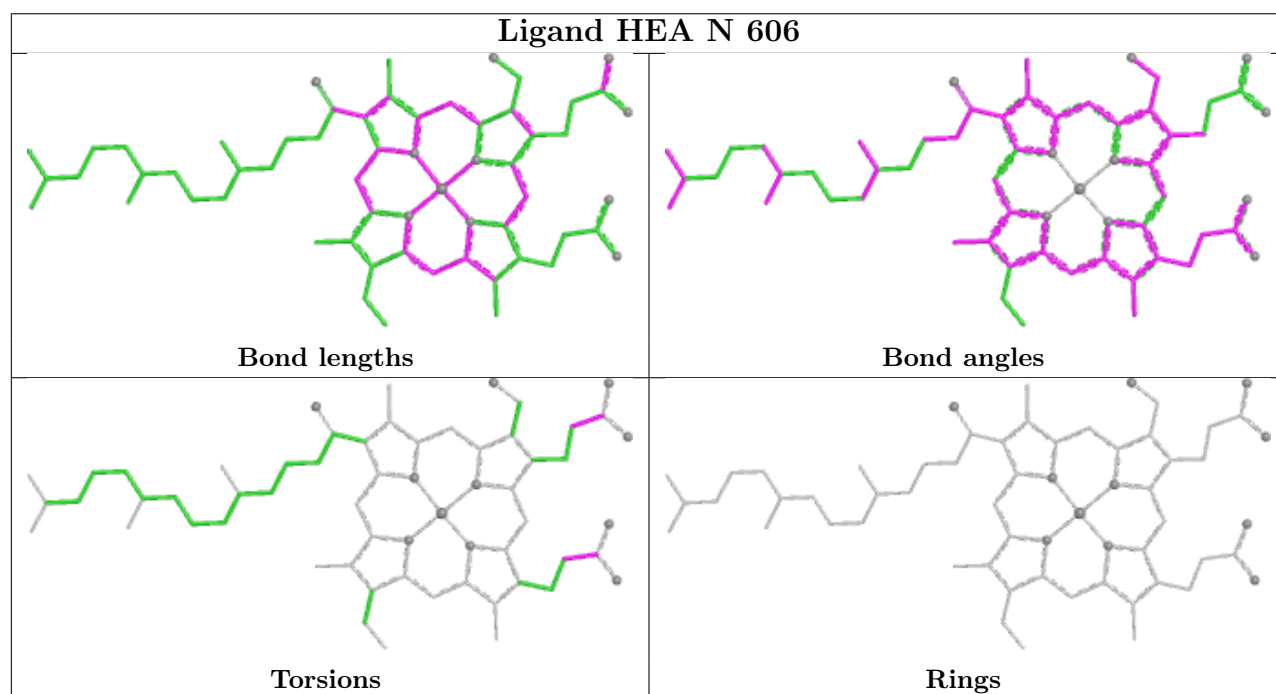
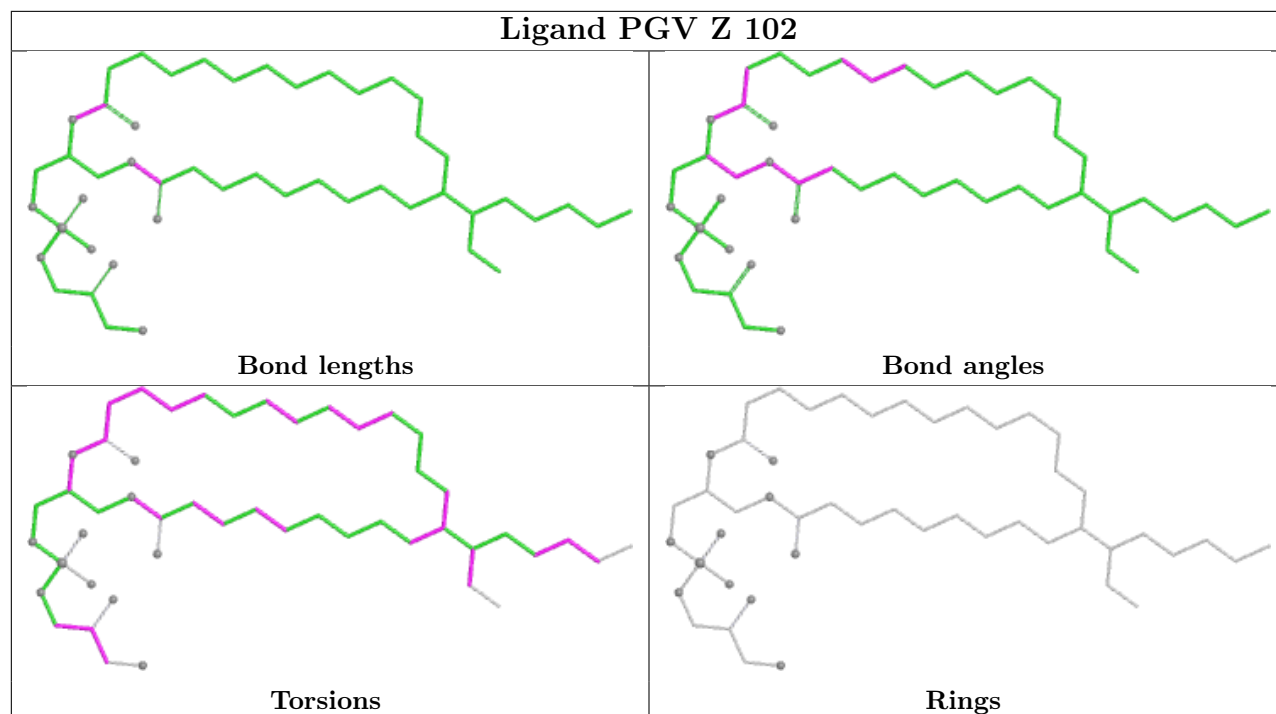
Ligand CHD P 303



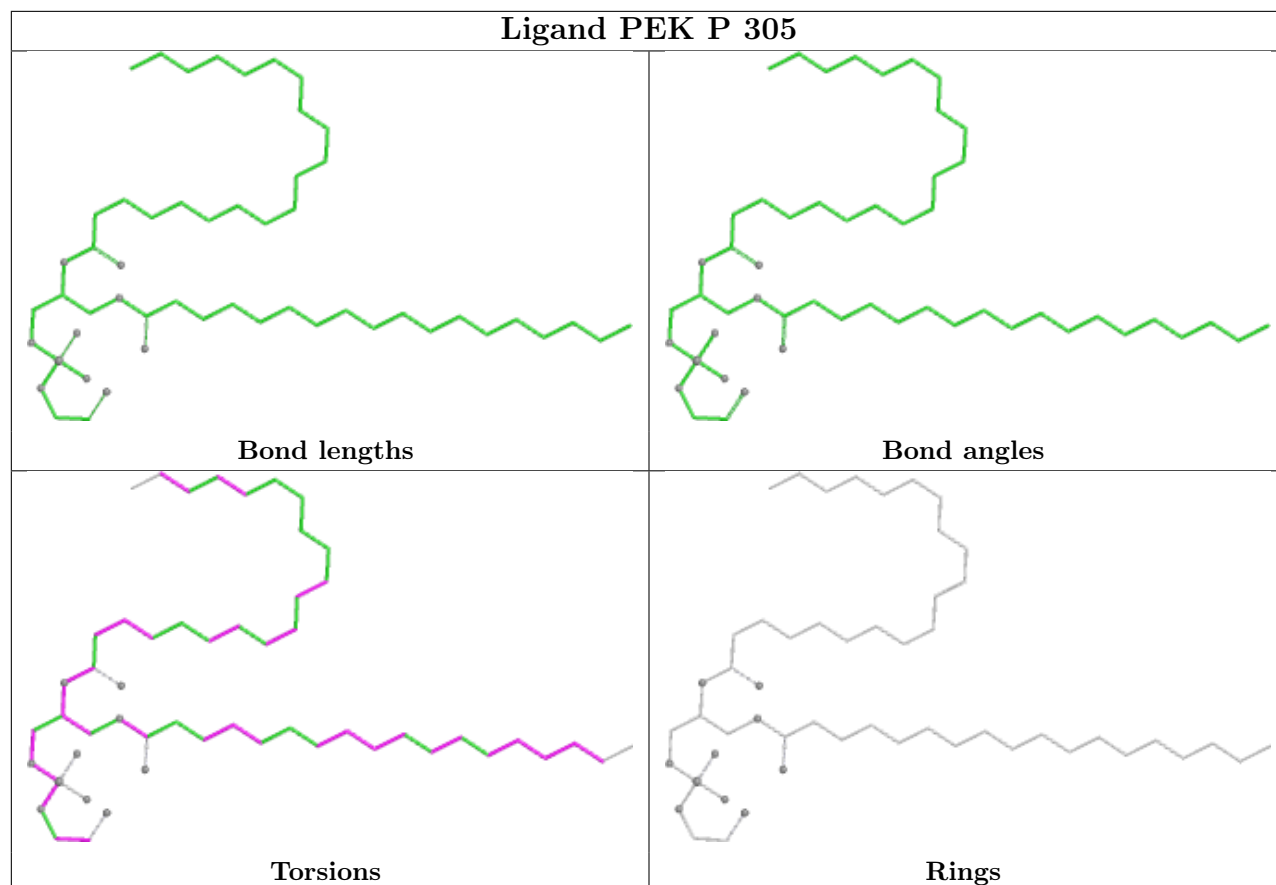




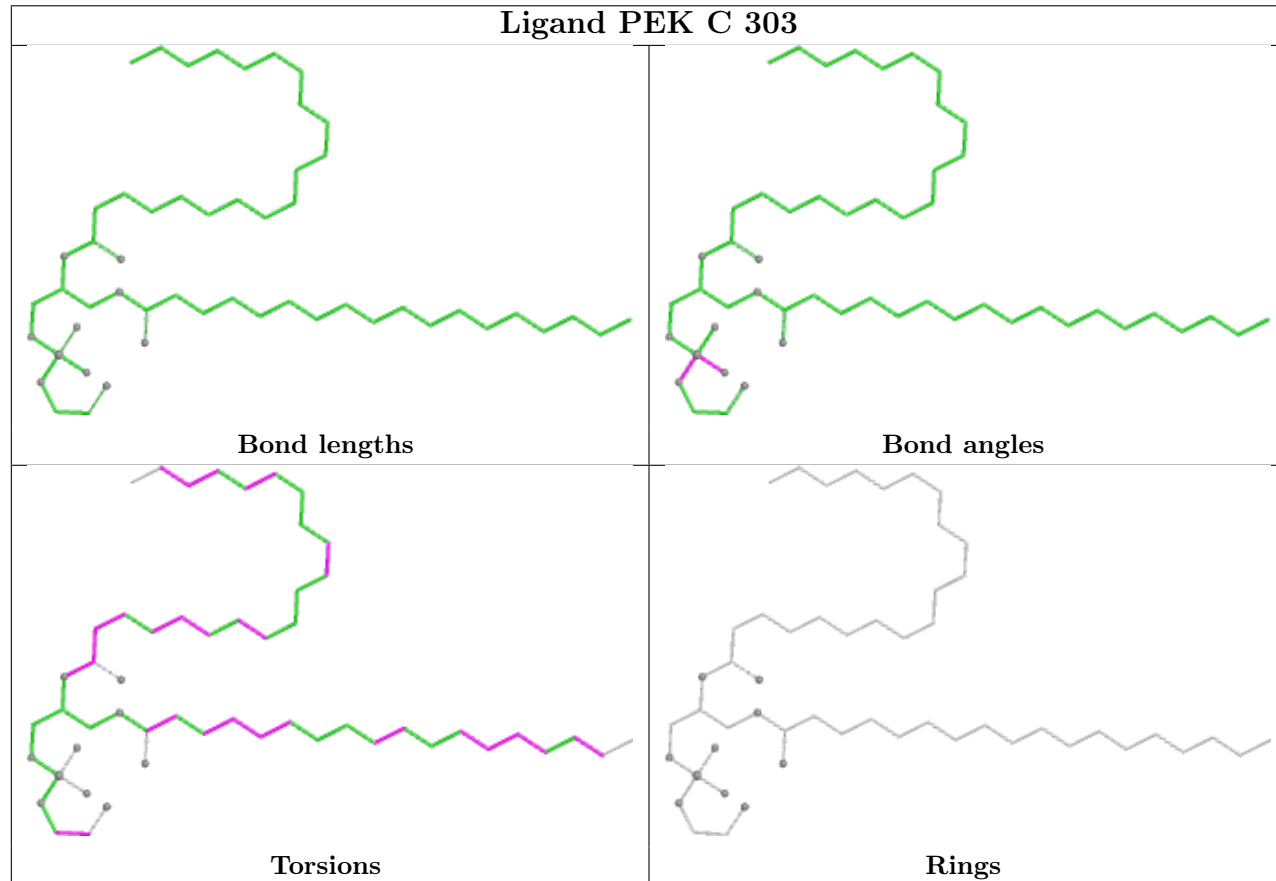


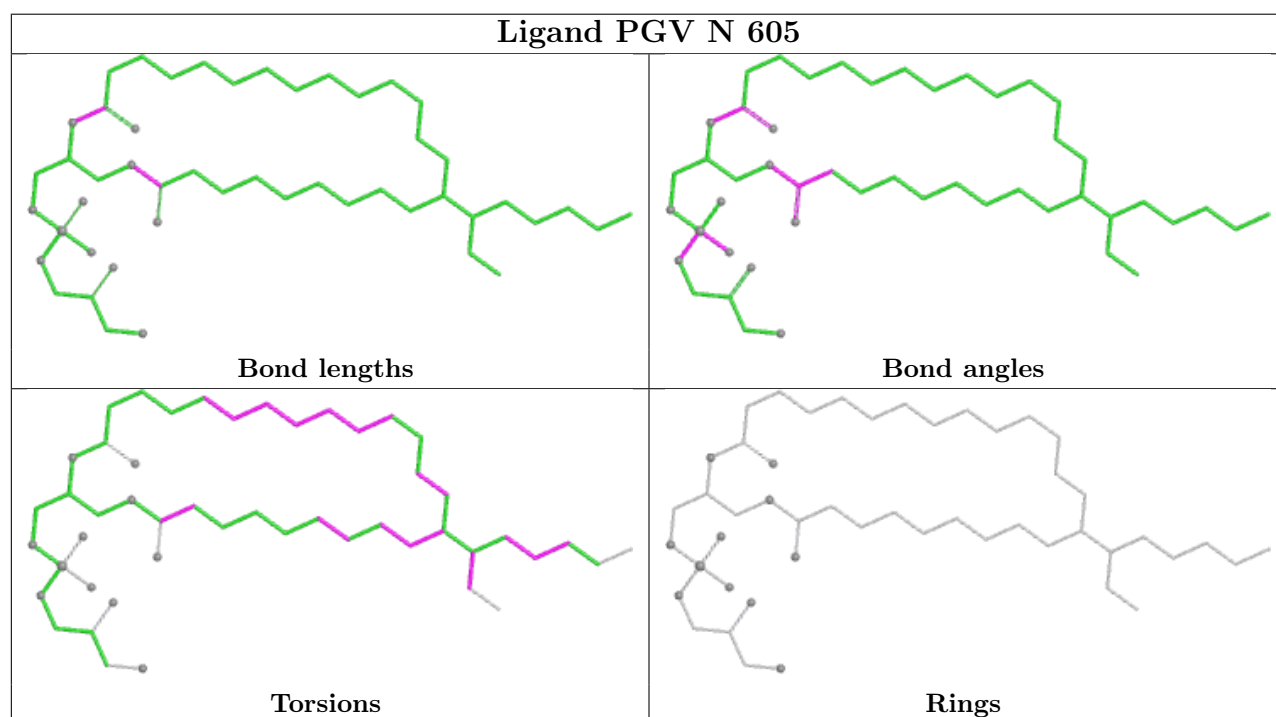
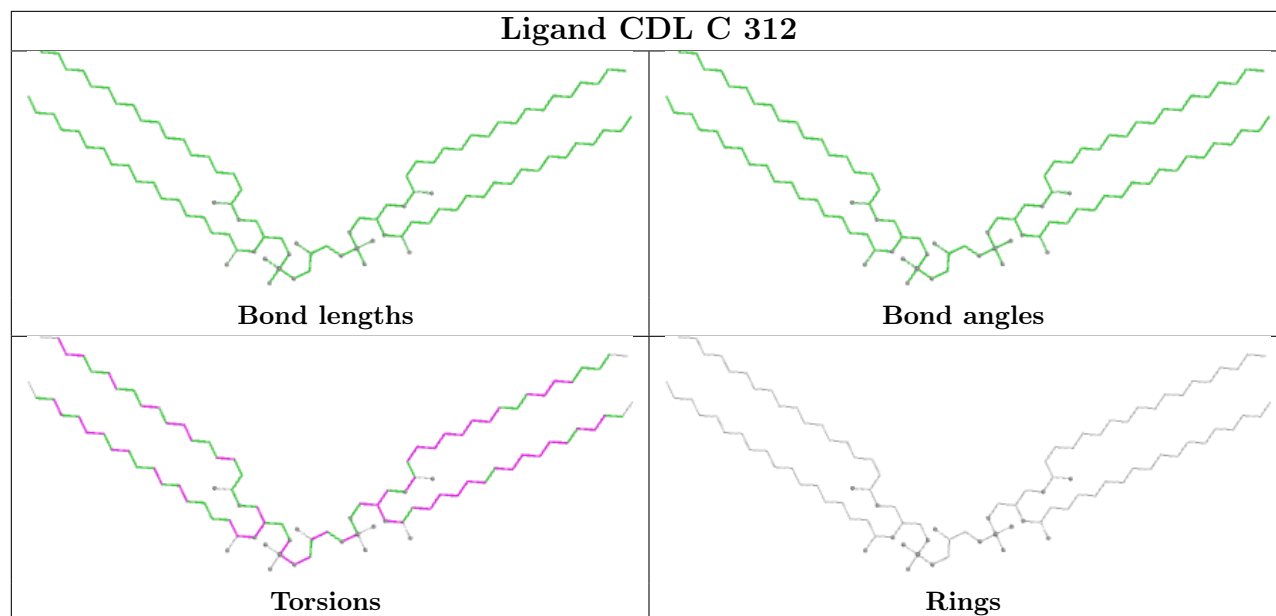


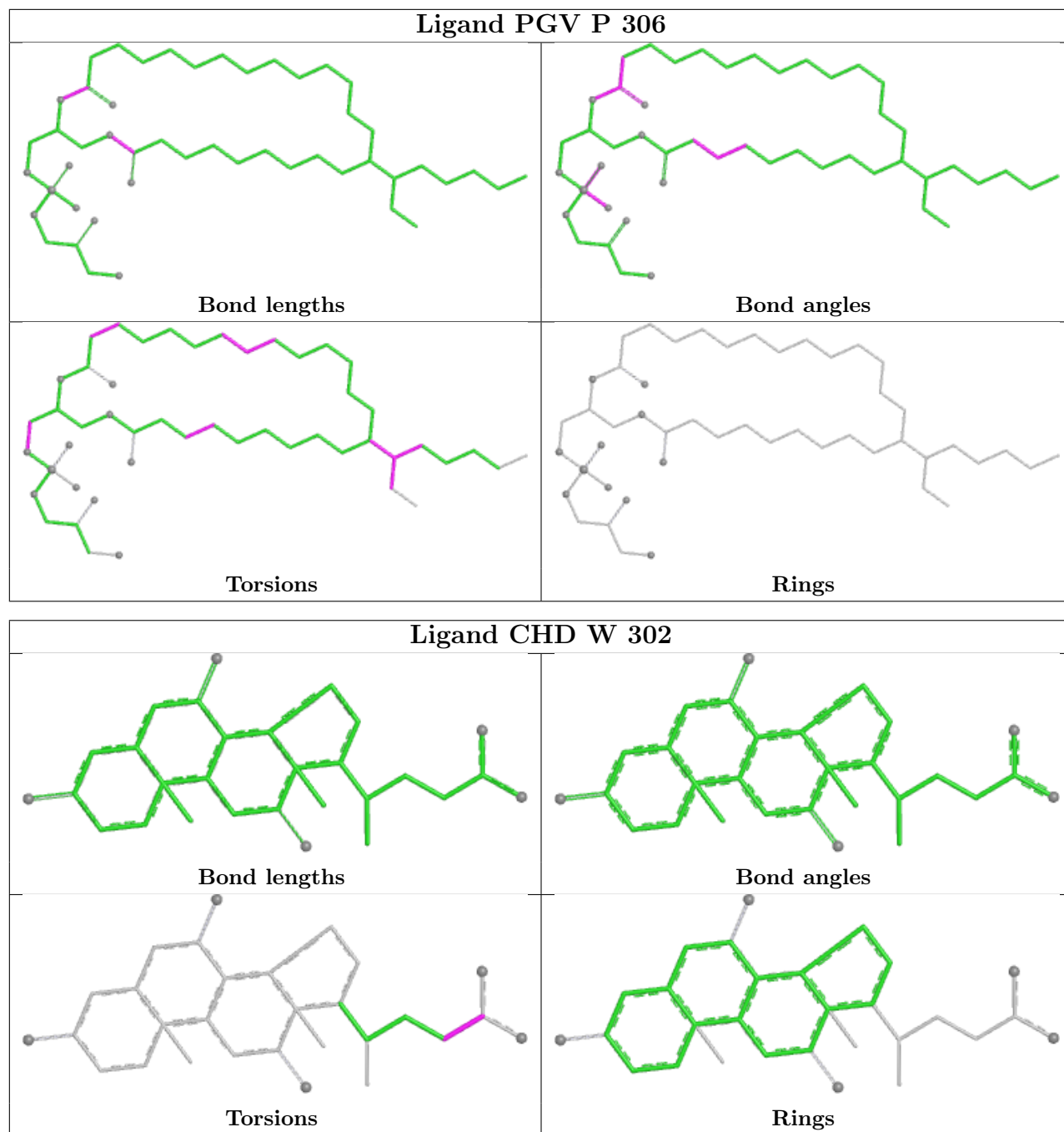
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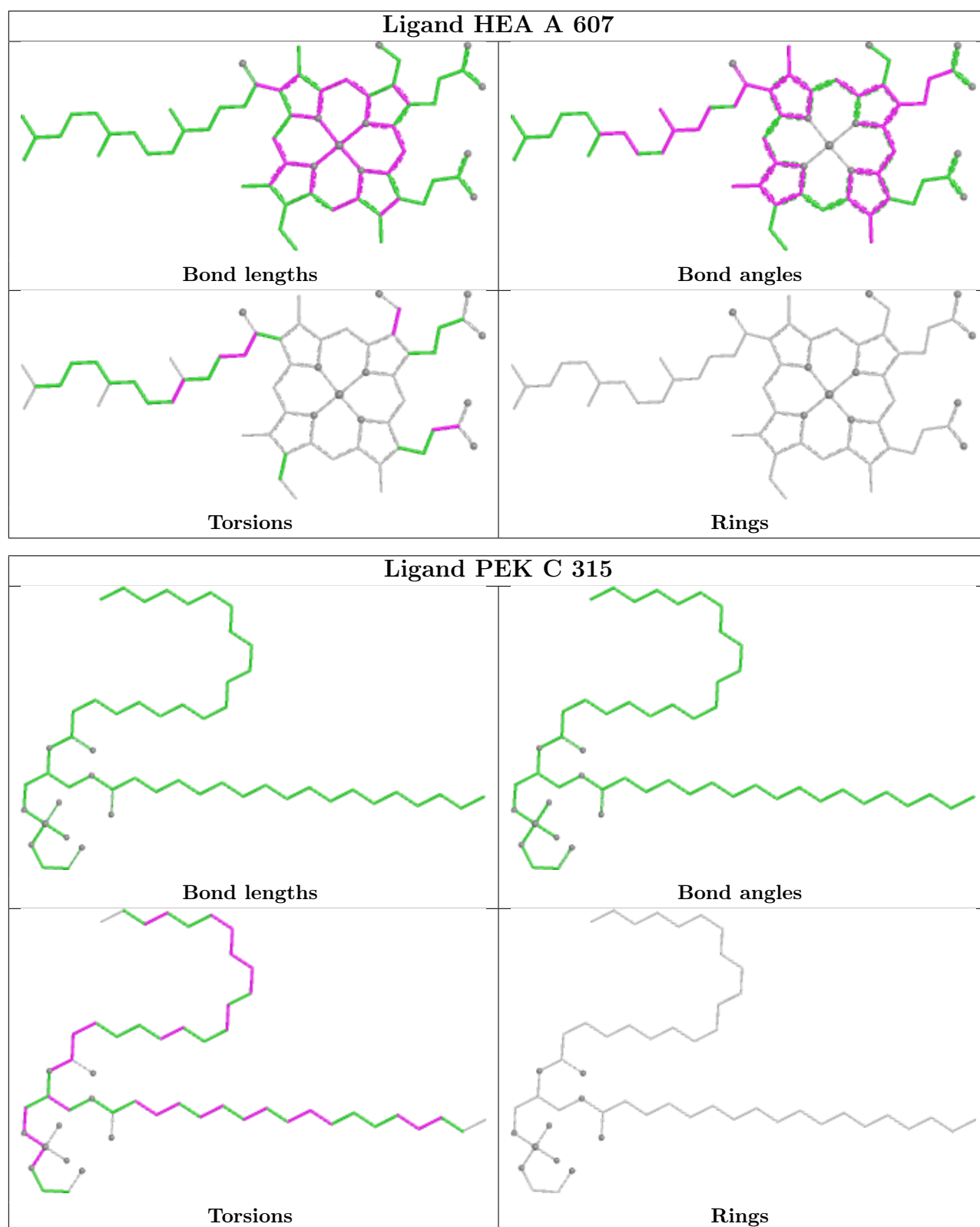


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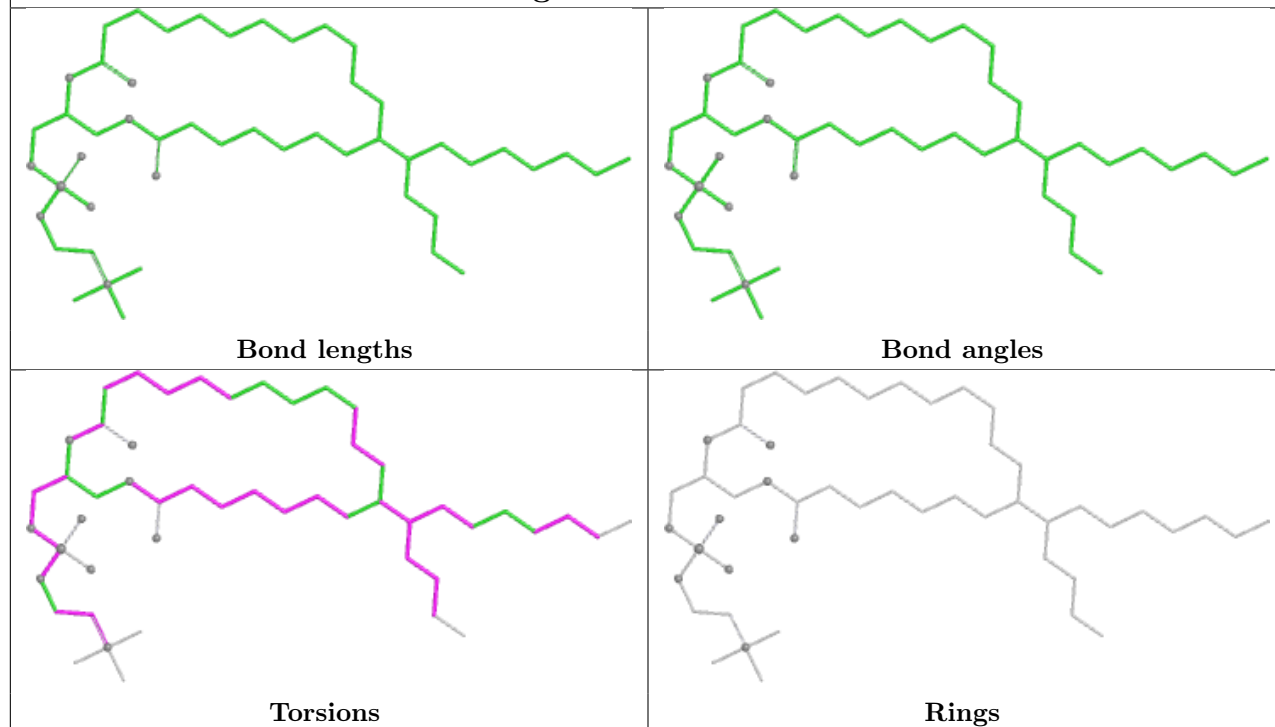




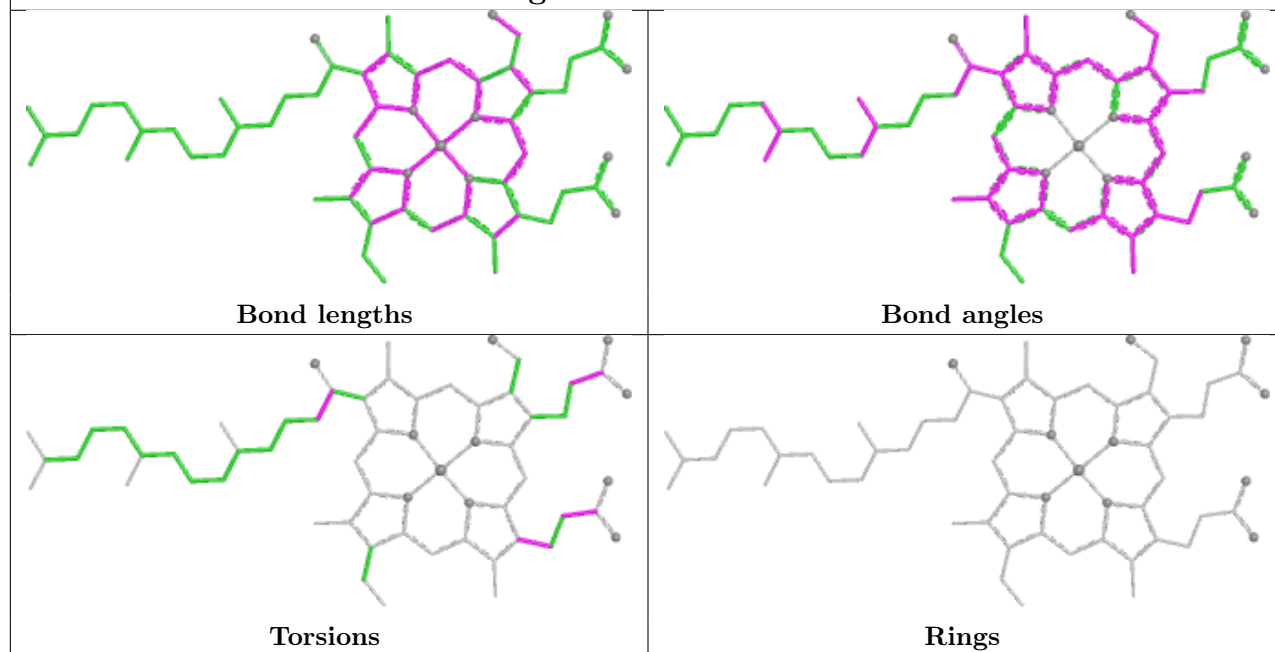


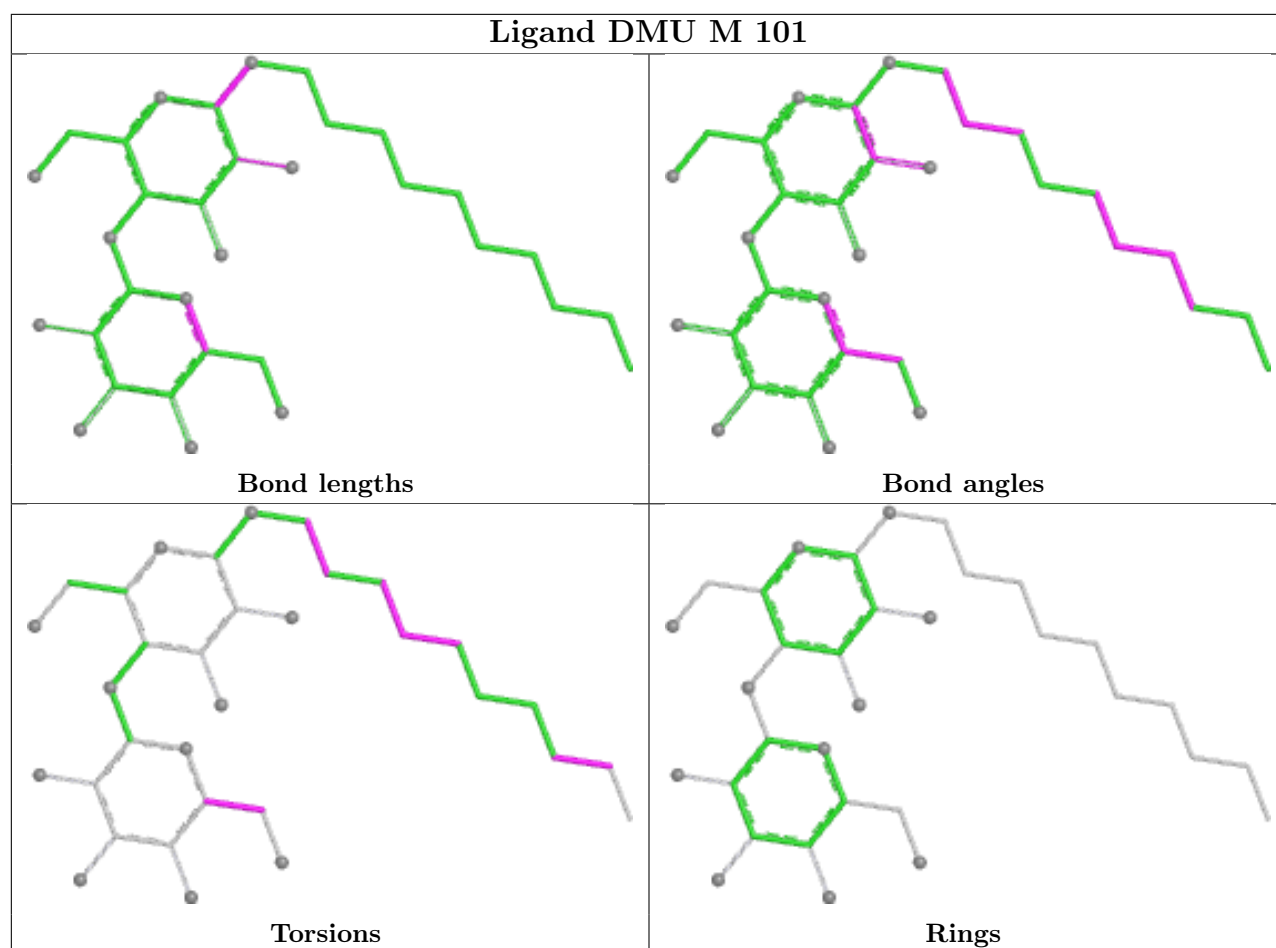


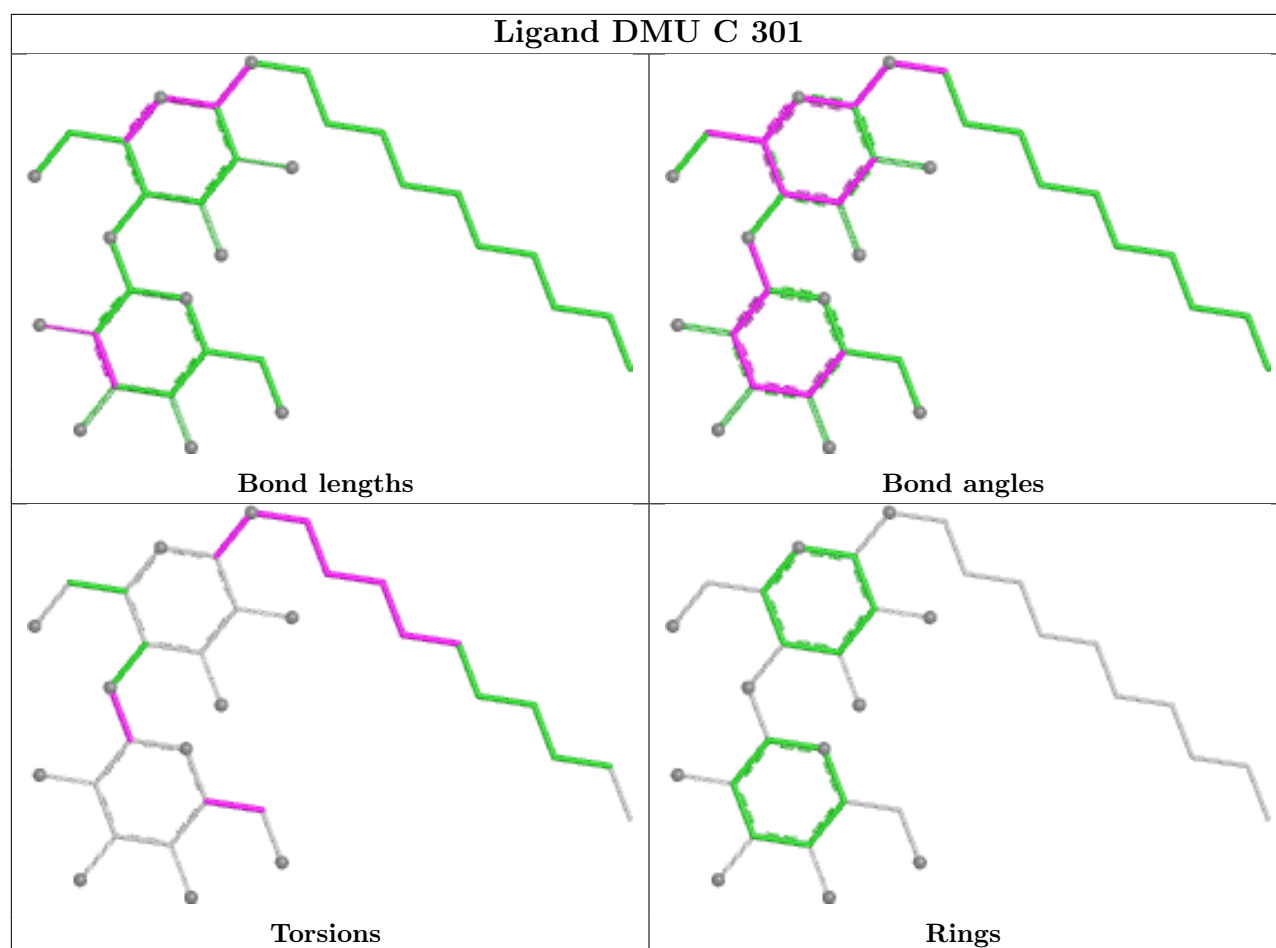
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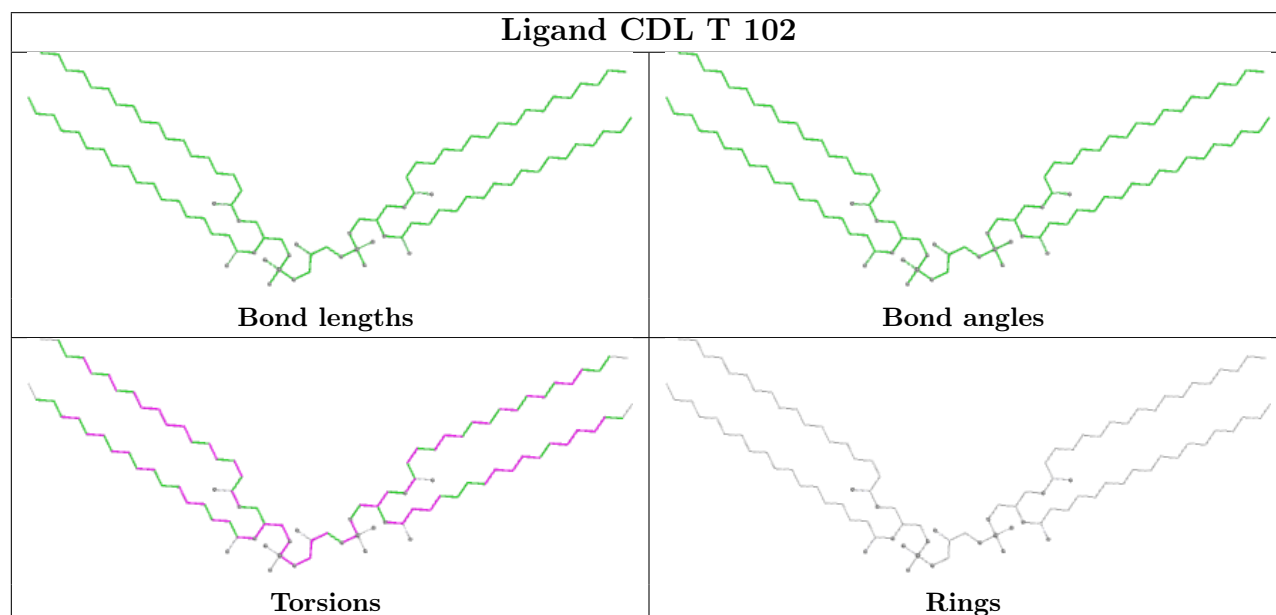
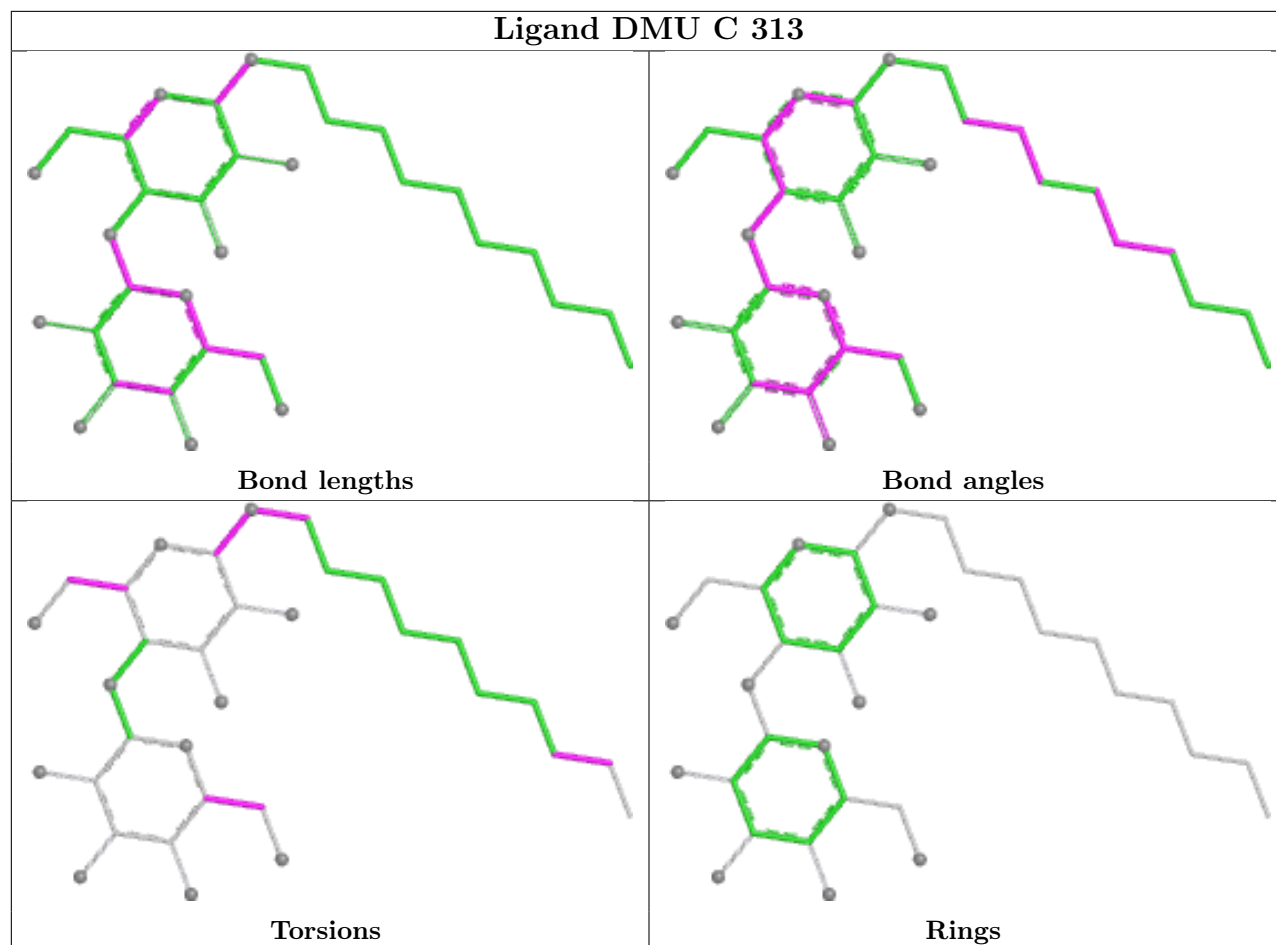


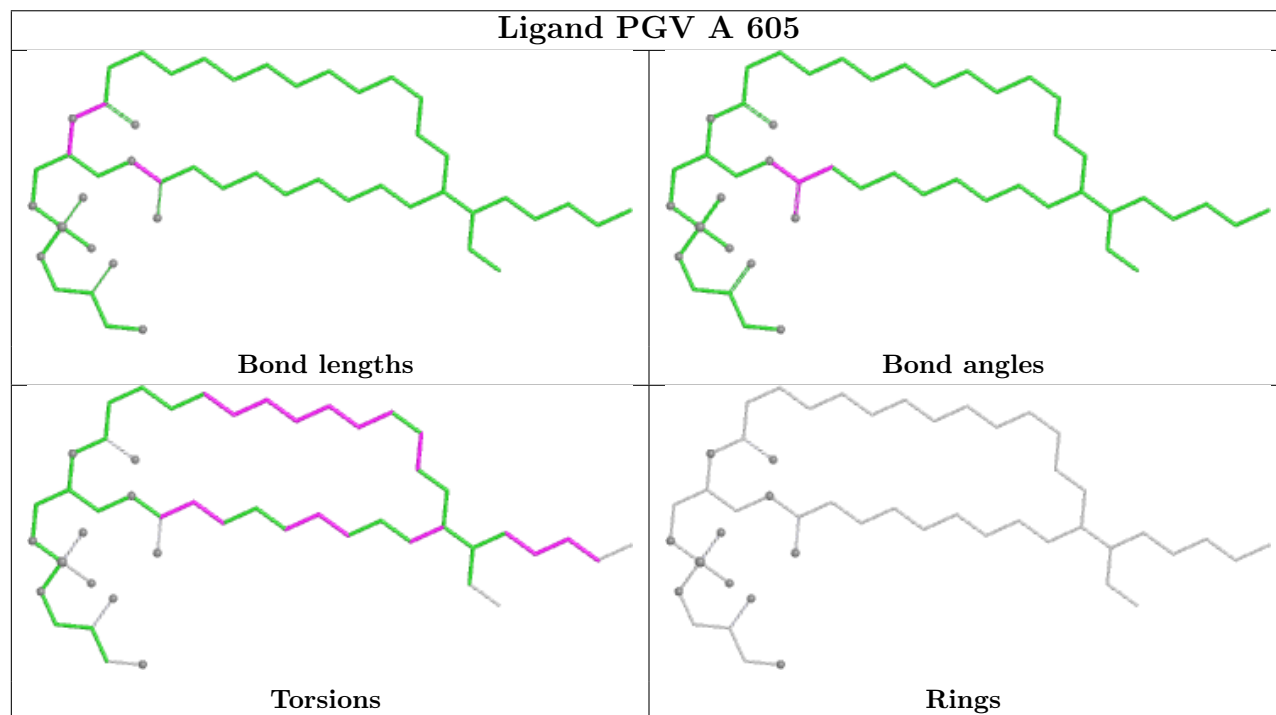
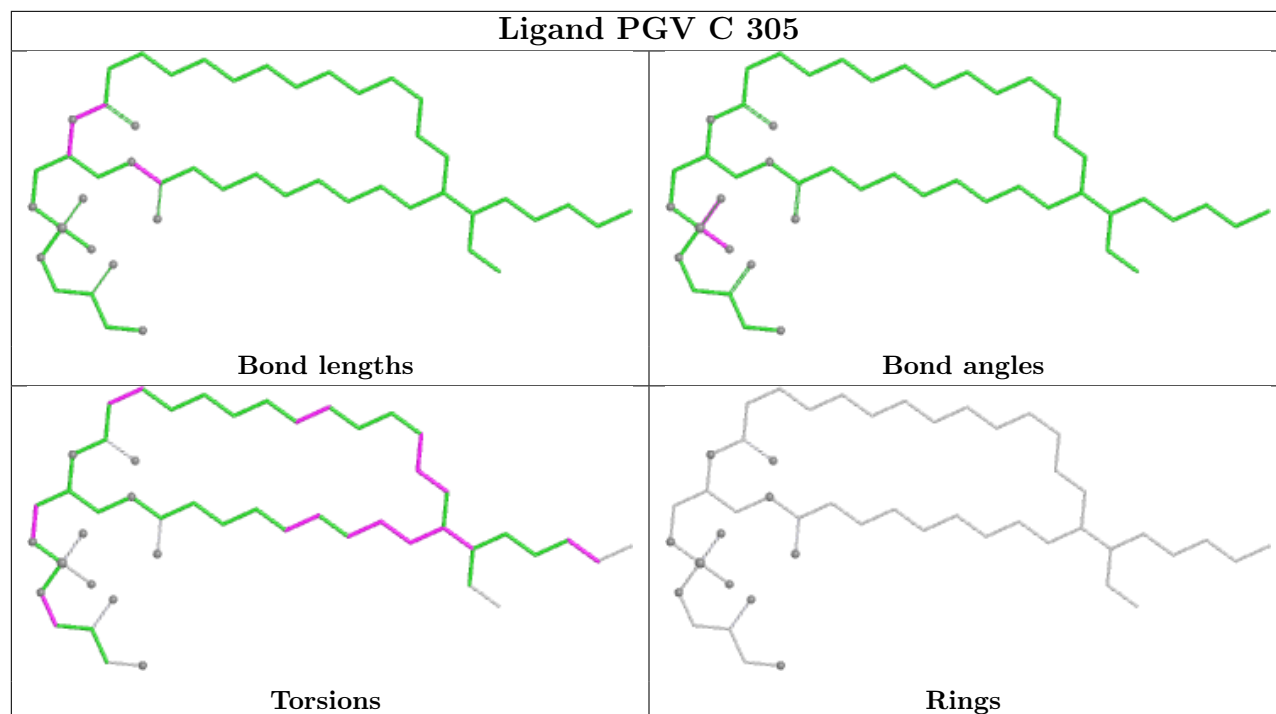
Ligand HEA A 606

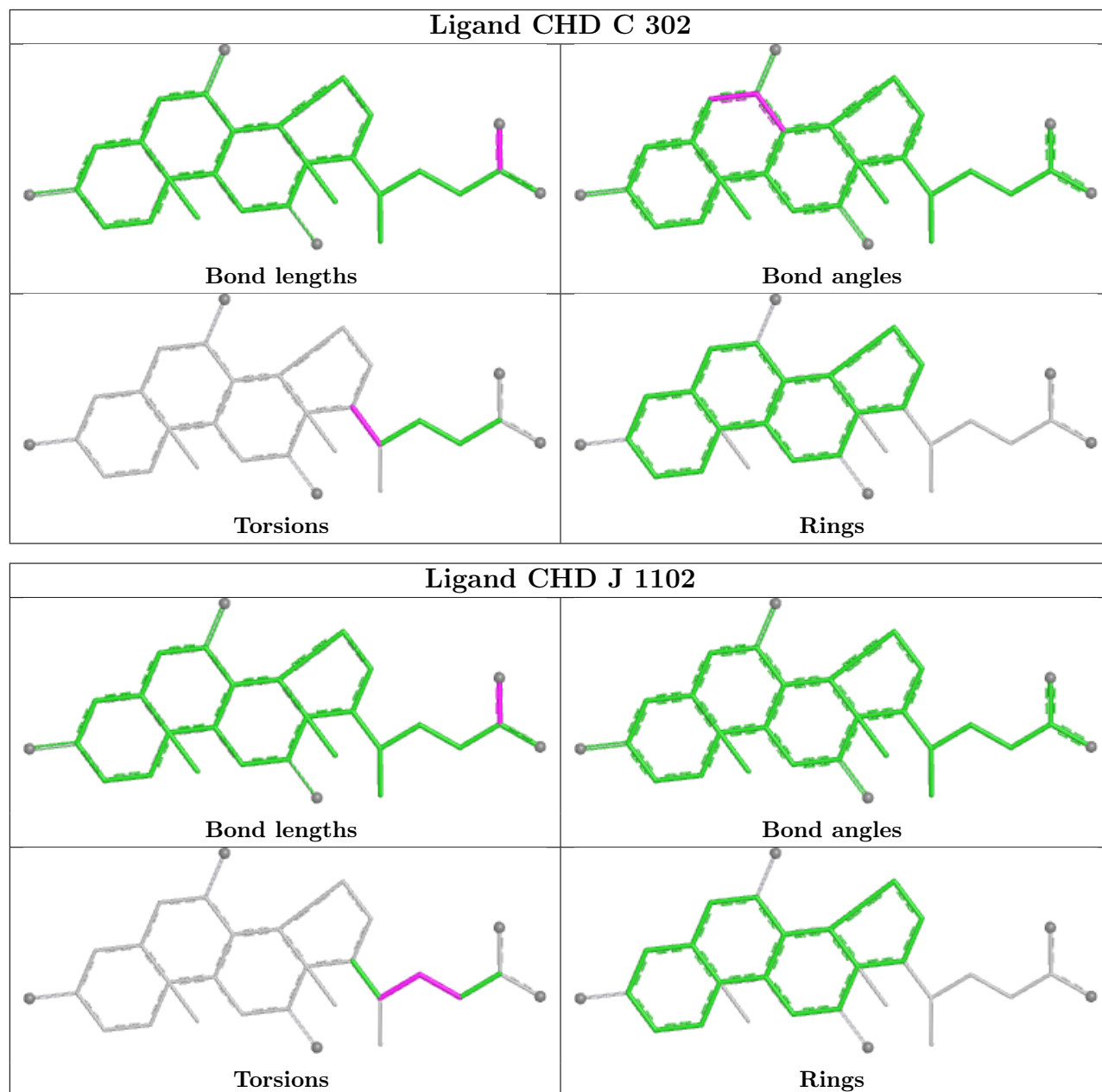


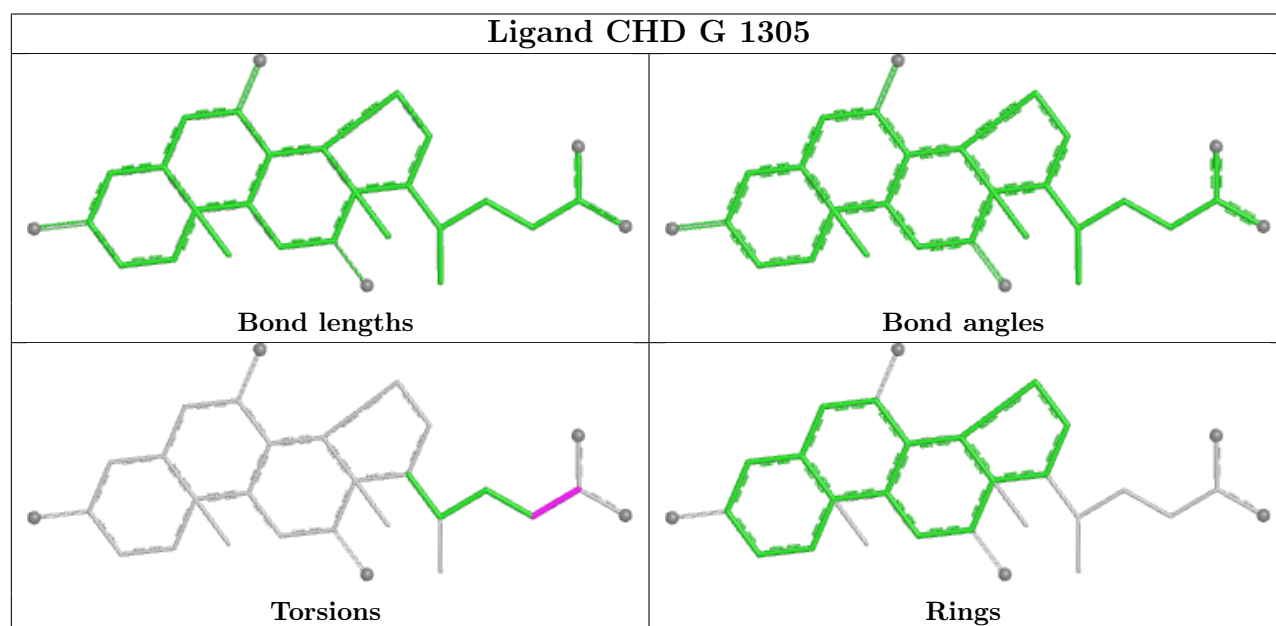
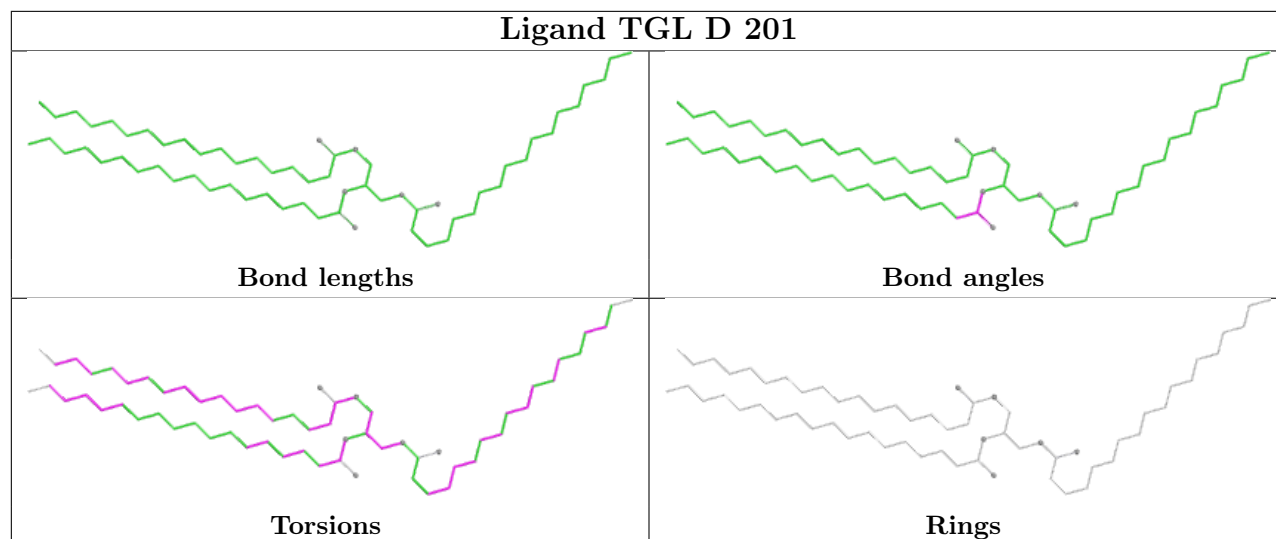




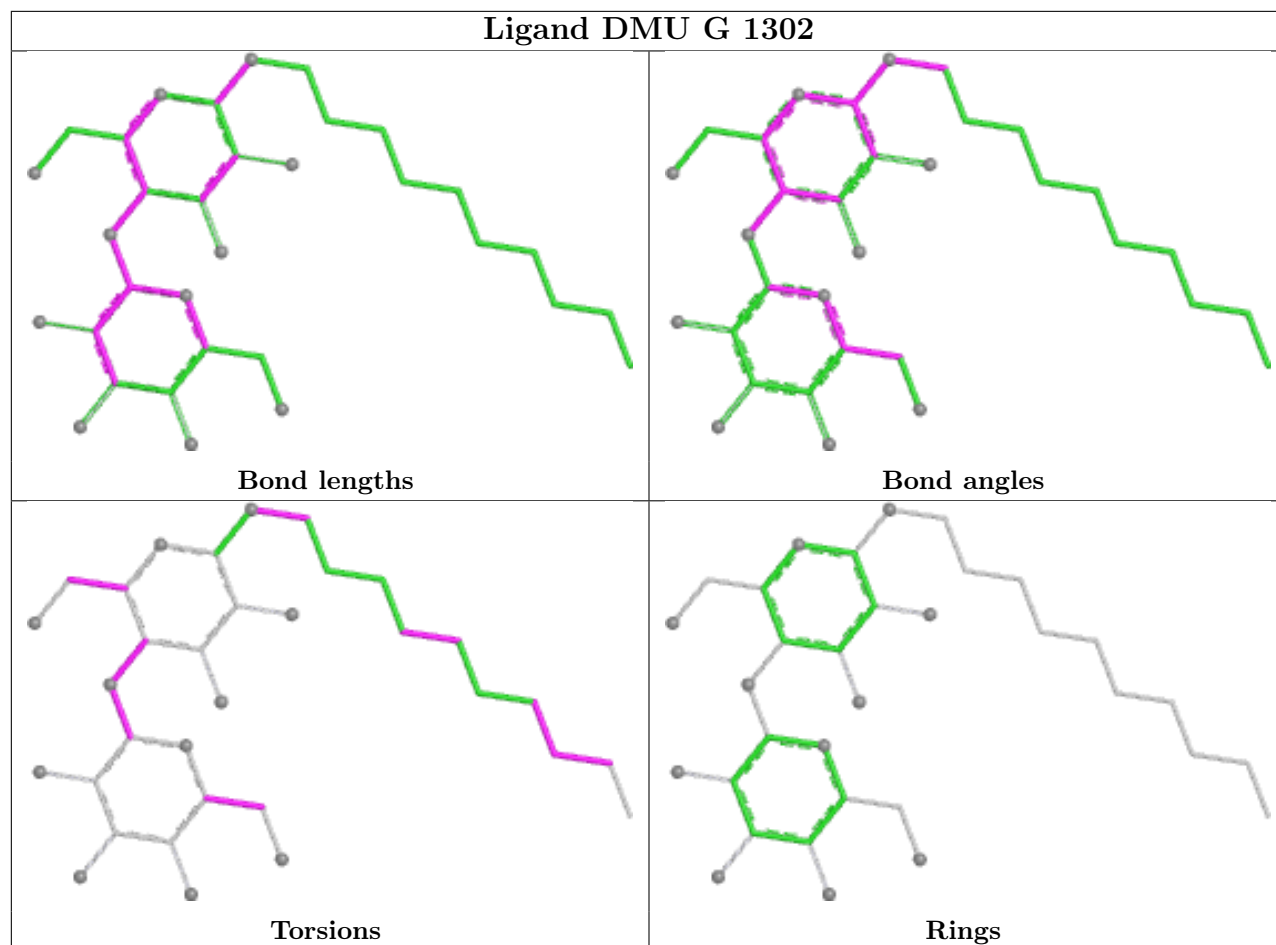




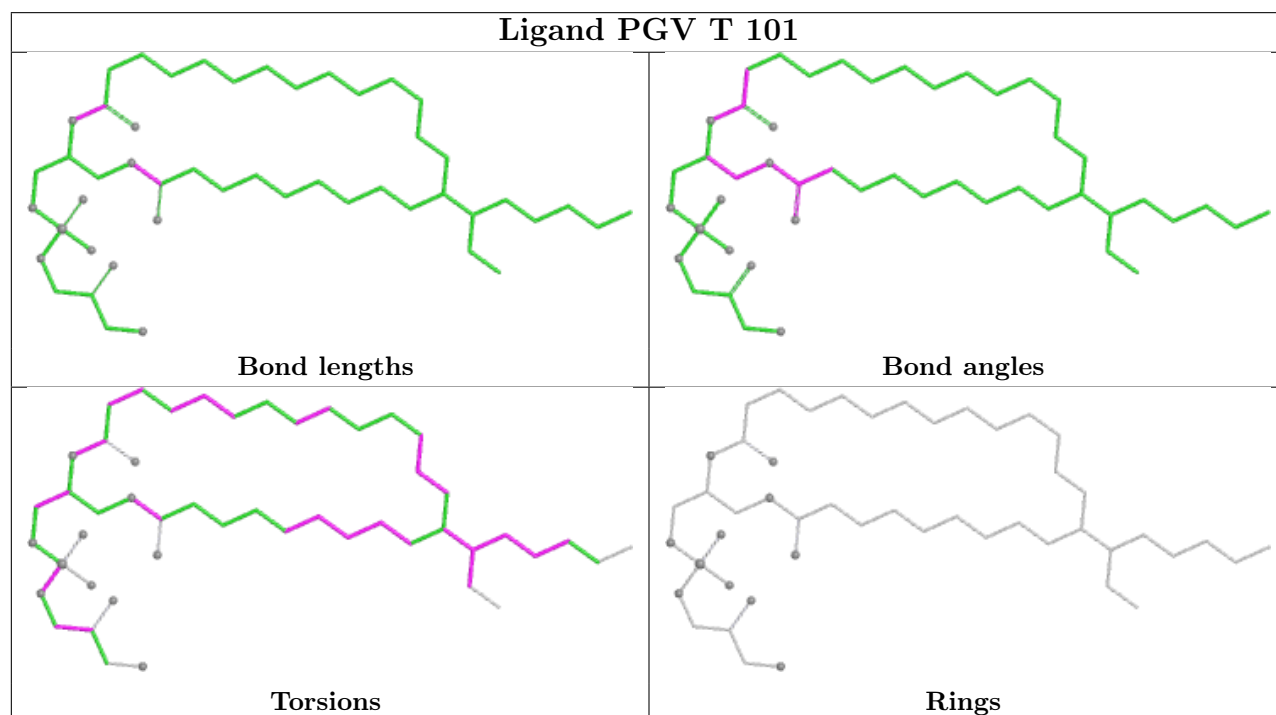


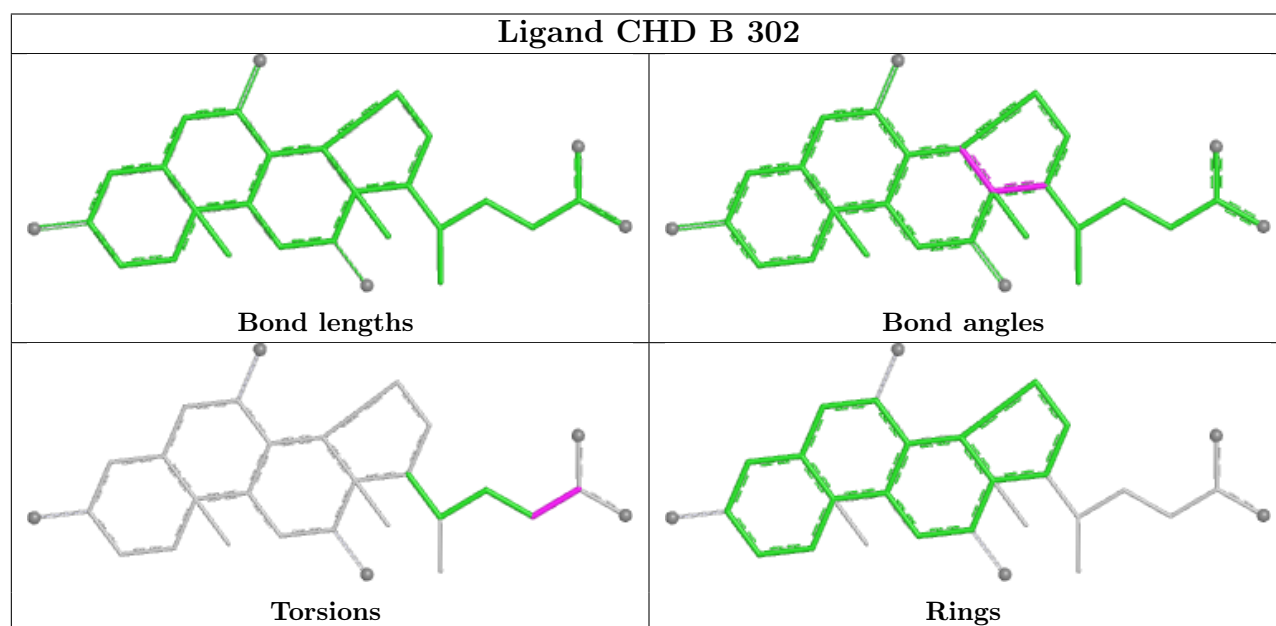
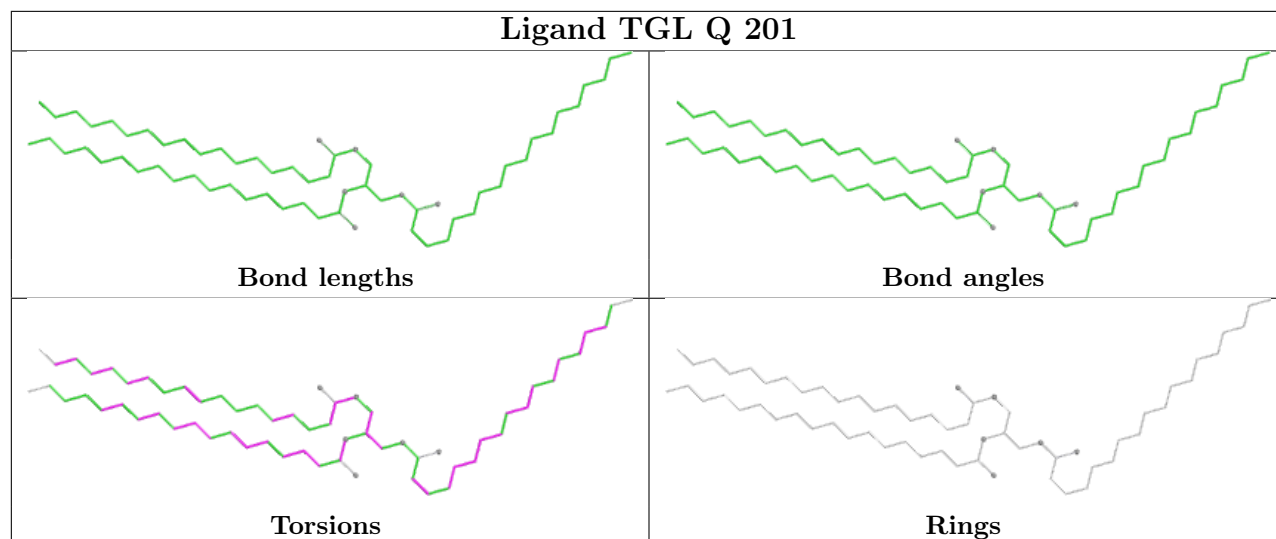


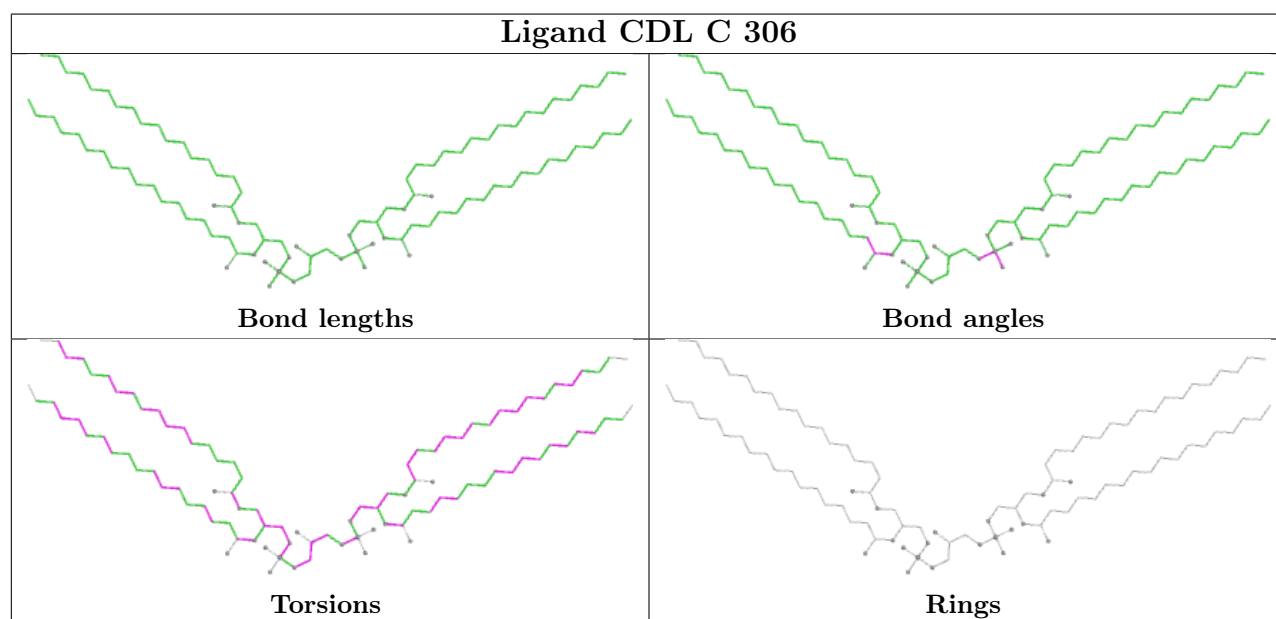
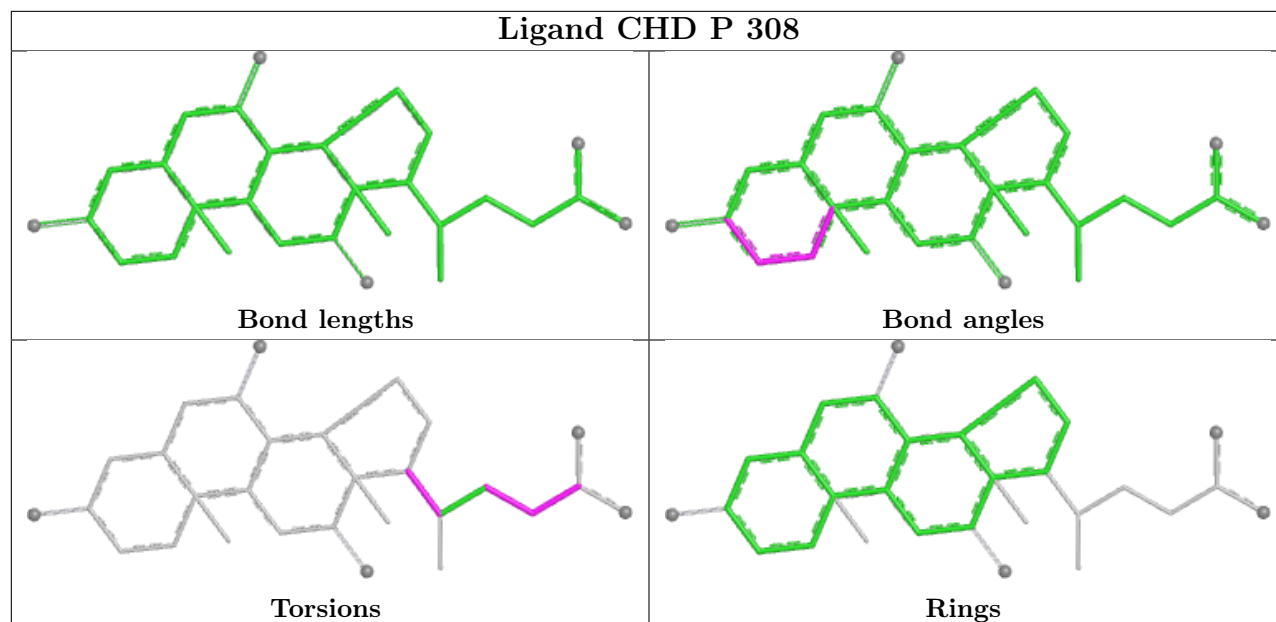
Ligand DMU G 1302

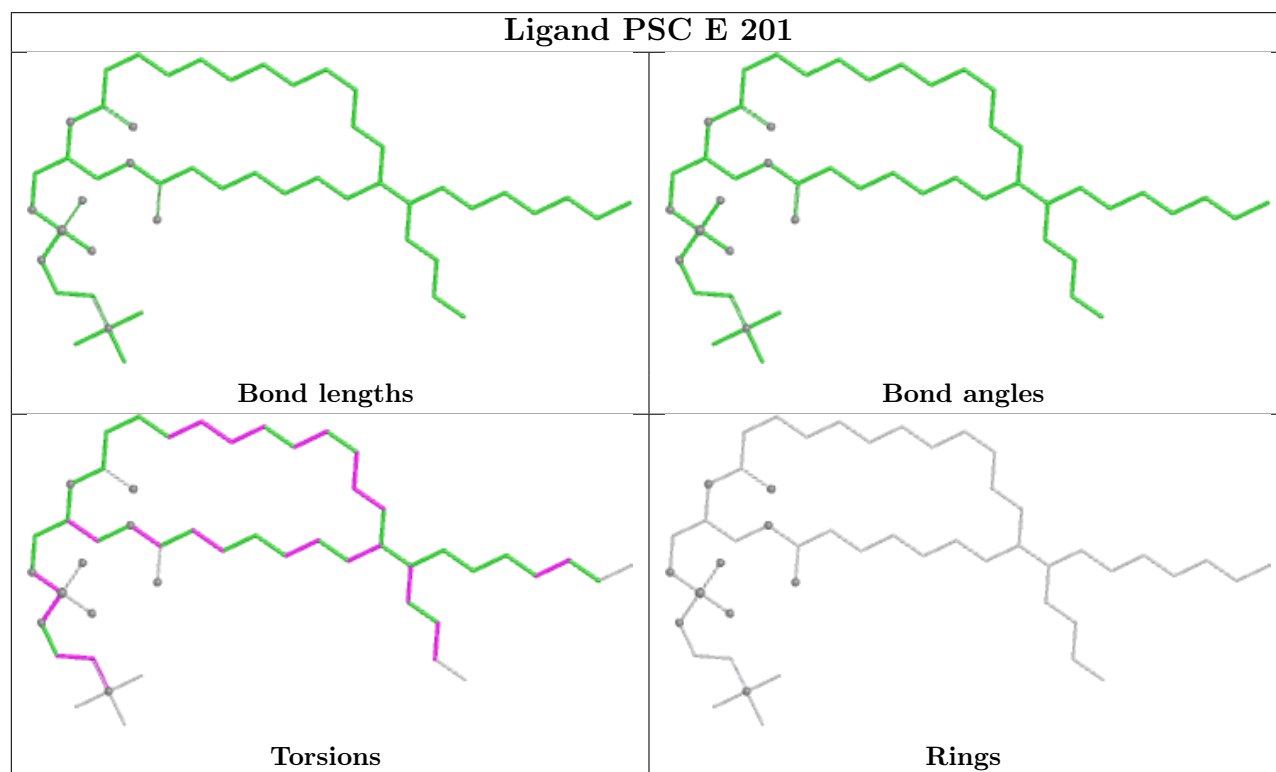
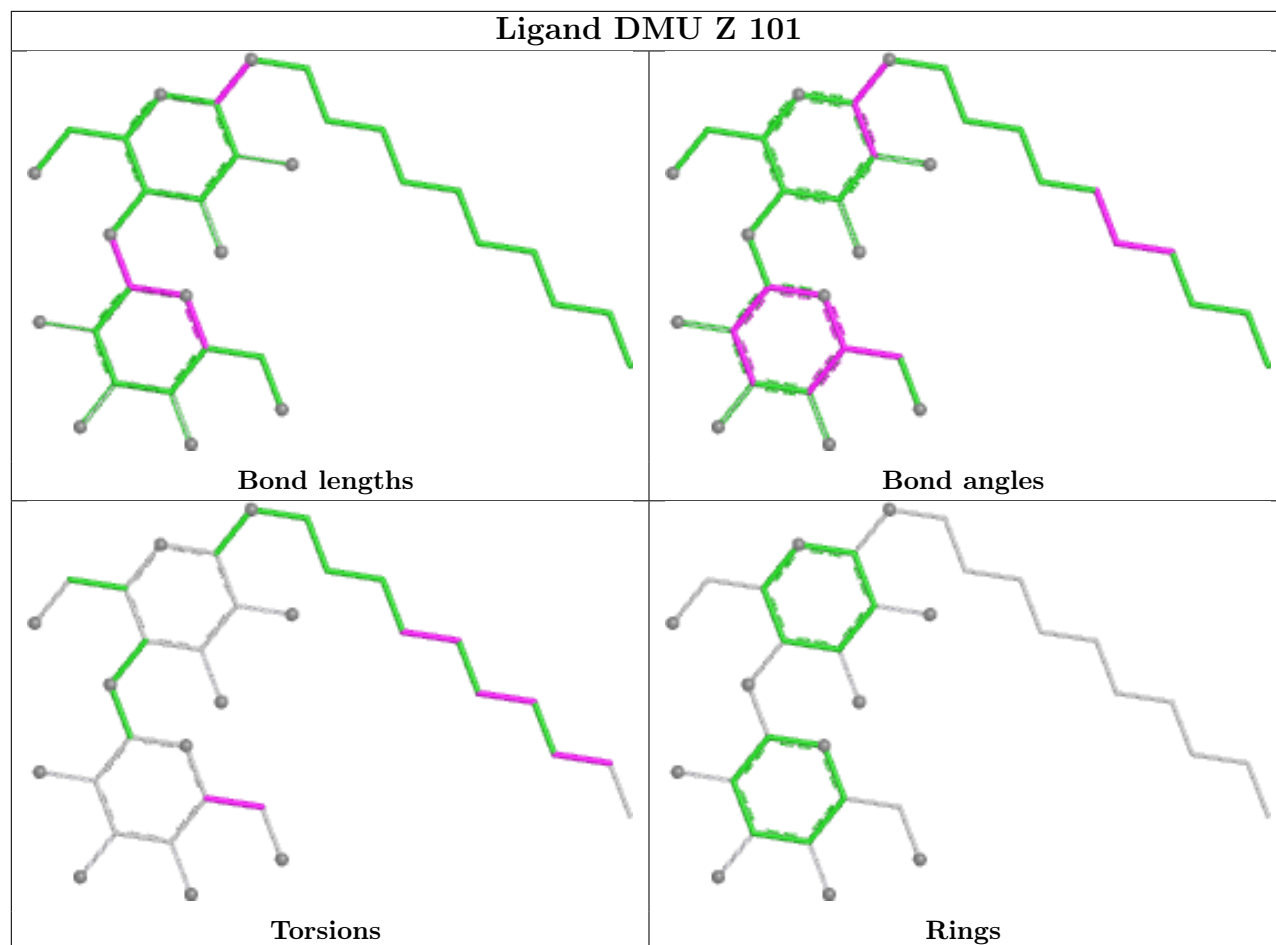


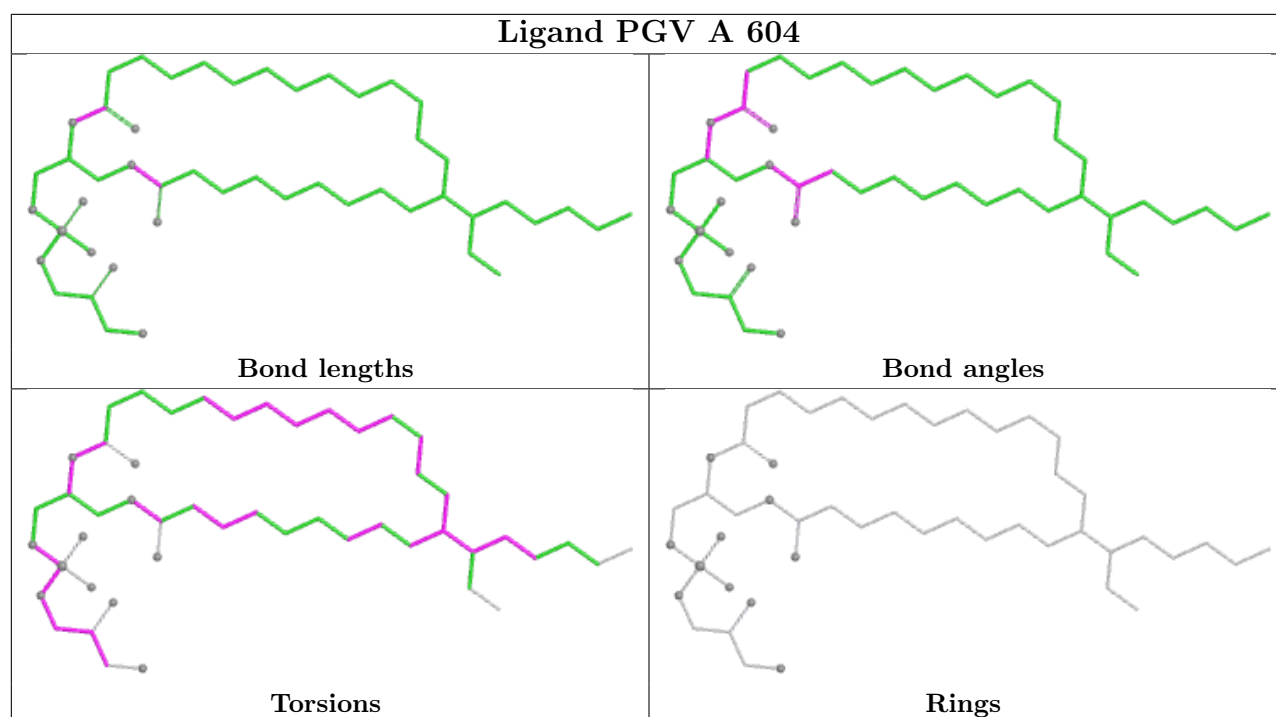
Ligand PGV T 101











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%)	-0.21	5 (0%) 79 84	27, 33, 42, 79	0
1	N	513/514 (99%)	0.19	7 (1%) 73 79	32, 39, 51, 84	0
2	B	226/227 (99%)	0.22	8 (3%) 47 53	28, 38, 61, 99	0
2	O	226/227 (99%)	0.52	10 (4%) 39 43	36, 46, 73, 103	0
3	C	259/261 (99%)	-0.03	2 (0%) 82 87	30, 37, 49, 83	0
3	P	259/261 (99%)	0.21	5 (1%) 66 72	32, 41, 55, 87	0
4	D	147/147 (100%)	0.27	3 (2%) 65 72	35, 43, 59, 90	0
4	Q	147/147 (100%)	1.20	21 (14%) 6 7	41, 57, 98, 154	0
5	E	105/109 (96%)	0.34	2 (1%) 66 72	37, 45, 69, 123	0
5	R	105/109 (96%)	0.80	8 (7%) 20 22	42, 53, 75, 124	0
6	F	98/98 (100%)	0.45	8 (8%) 17 19	32, 43, 85, 138	0
6	S	98/98 (100%)	0.68	10 (10%) 12 13	37, 48, 82, 117	0
7	G	83/85 (97%)	1.23	17 (20%) 2 2	34, 44, 108, 122	0
7	T	83/85 (97%)	1.28	17 (20%) 2 2	36, 50, 104, 130	0
8	H	79/85 (92%)	0.87	12 (15%) 5 6	35, 48, 97, 110	0
8	U	79/85 (92%)	1.07	13 (16%) 4 4	42, 53, 114, 127	0
9	I	72/73 (98%)	0.56	2 (2%) 55 62	36, 51, 67, 86	0
9	V	72/73 (98%)	0.95	9 (12%) 8 9	40, 57, 80, 99	0
10	J	58/59 (98%)	0.58	5 (8%) 16 18	36, 47, 72, 122	0
10	W	58/59 (98%)	0.98	4 (6%) 23 26	41, 53, 84, 123	0
11	K	52/56 (92%)	0.83	4 (7%) 19 22	37, 46, 65, 111	0
11	X	52/56 (92%)	1.06	7 (13%) 7 7	50, 59, 104, 120	0
12	L	46/47 (97%)	0.23	3 (6%) 25 28	33, 39, 62, 93	0
12	Y	46/47 (97%)	0.80	3 (6%) 25 28	42, 49, 73, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.45	2 (4%) 36 41	36, 40, 71, 105	0
13	Z	43/46 (93%)	1.10	6 (13%) 6 7	45, 53, 84, 143	0
All	All	3562/3614 (98%)	0.40	193 (5%) 31 35	27, 42, 76, 154	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	10.2
4	Q	6	VAL	8.7
4	Q	5	VAL	7.5
7	T	9	GLY	7.5
7	T	10	GLY	7.0
5	R	109	VAL	7.0
7	G	6	GLY	6.9
8	H	45	ALA	6.8
6	S	1	ALA	6.7
7	G	1	ALA	6.7
8	H	8	ILE	6.6
7	T	5	LYS	6.5
7	G	5	LYS	6.5
7	G	4	ALA	6.5
8	U	8	ILE	6.5
2	O	90	ILE	6.4
6	F	1	ALA	6.1
7	G	2	SER	5.9
7	T	1	ALA	5.8
7	T	4	ALA	5.8
7	G	36	TRP	5.3
7	G	9	GLY	5.3
4	Q	1	ALA	5.2
7	T	36	TRP	5.2
9	I	37	PHE	5.2
6	F	96	LEU	5.1
12	L	2	HIS	5.1
7	T	3	ALA	5.0
7	T	37	LEU	5.0
1	A	298	ASP	5.0
8	U	45	ALA	4.9
10	W	48	TYR	4.9
8	U	47	GLY	4.9
6	S	96	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
10	J	1	PHE	4.6
8	U	52	VAL	4.6
7	G	37	LEU	4.6
7	G	10	GLY	4.5
9	V	37	PHE	4.5
7	G	8	HIS	4.4
7	G	7	ASP	4.3
7	T	6	GLY	4.2
4	Q	7	LYS	4.1
13	Z	43	SER	4.1
8	H	48	GLY	4.1
11	X	55	GLU	4.0
4	Q	72	ASN	4.0
8	U	43	MET	3.9
9	V	2	THR	3.9
9	V	3	ALA	3.8
2	B	87	MET	3.8
5	E	109	VAL	3.8
1	A	514	LYS	3.8
7	T	2	SER	3.8
7	G	84	LYS	3.7
8	H	9	LYS	3.6
3	P	3	HIS	3.6
8	H	47	GLY	3.5
4	Q	2	HIS	3.5
2	B	90	ILE	3.5
6	F	97	ALA	3.5
7	T	8	HIS	3.5
3	C	3	HIS	3.4
12	Y	47	LYS	3.4
8	U	48	GLY	3.4
2	B	113	TYR	3.4
6	S	98	HIS	3.4
7	T	33	LEU	3.4
7	T	38	HIS	3.3
4	D	1	ALA	3.3
11	X	7	PRO	3.3
13	M	43	SER	3.3
7	T	84	LYS	3.3
2	O	227	LEU	3.3
11	K	7	PRO	3.3
8	H	7	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	N	514	LYS	3.2
5	R	107	ASP	3.2
6	S	97	ALA	3.2
6	F	2	SER	3.2
5	R	39	TYR	3.1
3	P	37	PHE	3.1
4	Q	53	ILE	3.1
12	Y	2	HIS	3.1
4	Q	33	LEU	3.1
5	E	94	ASN	3.1
2	O	224	ALA	3.1
11	X	6	ALA	3.1
4	Q	102	TYR	3.1
4	Q	4	SER	3.1
4	Q	8	SER	3.1
6	F	98	HIS	3.1
1	N	125	GLY	3.1
7	T	7	ASP	3.0
2	O	113	TYR	3.0
8	U	50	VAL	3.0
10	W	52	TRP	3.0
11	K	47	ARG	3.0
10	W	58	LYS	2.9
11	K	6	ALA	2.9
11	X	56	GLN	2.9
4	Q	3	GLY	2.9
6	S	94	HIS	2.9
5	R	5	HIS	2.8
7	G	38	HIS	2.8
5	R	106	LEU	2.8
1	N	484	THR	2.8
8	U	9	LYS	2.7
9	V	73	LYS	2.7
3	P	122	HIS	2.7
2	B	32	PHE	2.7
7	G	33	LEU	2.7
4	Q	46	ALA	2.7
6	F	3	GLY	2.7
8	H	44	THR	2.7
9	V	33	THR	2.7
6	S	2	SER	2.7
1	A	311	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
11	X	51	LYS	2.7
11	K	26	VAL	2.7
1	A	486	ASP	2.6
8	U	53	CYS	2.6
12	Y	24	MET	2.6
8	U	42	ALA	2.6
9	V	72	ALA	2.6
2	O	87	MET	2.6
1	N	332	ILE	2.6
13	Z	42	LYS	2.6
7	G	34	ASN	2.5
7	G	42	ARG	2.5
12	L	24	MET	2.5
2	B	65	TRP	2.5
8	H	42	ALA	2.5
9	I	2	THR	2.5
13	Z	40	TYR	2.4
3	P	44	MET	2.4
8	H	10	ASN	2.4
4	D	51	LEU	2.4
8	U	7	LYS	2.4
12	L	47	LYS	2.4
10	J	58	LYS	2.4
4	Q	51	LEU	2.3
6	F	94	HIS	2.3
6	S	43	LYS	2.3
4	Q	27	VAL	2.3
11	X	54	ARG	2.3
8	H	52	VAL	2.3
6	S	95	GLN	2.3
13	Z	32	TRP	2.3
13	M	40	TYR	2.3
1	N	136	LEU	2.3
2	O	222	TRP	2.2
2	O	221	LYS	2.2
4	Q	147	LYS	2.2
8	U	44	THR	2.2
2	O	116	LEU	2.2
6	S	93	PRO	2.2
8	H	51	SER	2.2
10	J	55	PHE	2.2
4	D	2	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	P	38	ASN	2.2
9	V	65	LYS	2.2
7	T	83	GLU	2.1
3	C	258	TRP	2.1
6	S	37	LYS	2.1
9	V	26	MET	2.1
10	J	57	HIS	2.1
2	B	16	ILE	2.1
13	Z	17	ILE	2.1
5	R	92	THR	2.1
1	N	118	VAL	2.1
5	R	79	LYS	2.1
5	R	108	LYS	2.1
4	Q	39	ALA	2.1
4	Q	69	ALA	2.1
9	V	25	PHE	2.1
8	U	49	ASP	2.1
4	Q	9	GLU	2.1
8	H	50	VAL	2.1
10	W	31	LEU	2.1
2	B	49	LYS	2.0
4	Q	87	PHE	2.0
2	O	183	THR	2.0
4	Q	30	VAL	2.0
10	J	34	VAL	2.0
1	A	297	MET	2.0
2	O	32	PHE	2.0
13	Z	1	ILE	2.0
1	N	46	THR	2.0
6	F	95	GLN	2.0
11	X	13	TYR	2.0
2	B	61	VAL	2.0
7	T	42	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TPO	G	11	11/12	0.70	0.21	47,87,130,139	0
7	TPO	T	11	11/12	0.71	0.17	54,119,161,165	0
1	FME	N	1	10/11	0.94	0.12	51,59,89,92	0
1	FME	A	1	10/11	0.94	0.11	45,53,79,101	0
2	FME	O	1	10/11	0.96	0.12	40,48,59,62	0
2	FME	B	1	10/11	0.97	0.08	36,41,50,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
28	SAC	V	101	9/10	0.31	0.19	129,139,152,154	0
22	CHD	T	104	29/29	0.68	0.27	81,147,172,175	0
28	SAC	I	101	9/10	0.69	0.22	83,101,110,116	0
24	PEK	C	315	53/53	0.70	0.29	60,85,124,172	0
19	EDO	R	202	4/4	0.73	0.20	78,85,89,96	0
19	EDO	P	310	4/4	0.73	0.32	61,83,84,90	0
23	DMU	C	301	33/33	0.73	0.21	87,130,143,153	0
22	CHD	Y	102	29/29	0.74	0.25	96,138,156,166	0
17	PGV	Z	102	51/51	0.75	0.27	50,90,154,168	0
25	CDL	C	312	100/100	0.75	0.34	68,105,138,150	0
24	PEK	P	301	53/53	0.76	0.23	64,88,161,171	0
26	PSC	O	302	52/52	0.77	0.26	47,95,173,185	0
17	PGV	A	604	51/51	0.78	0.27	51,83,114,126	0
19	EDO	C	310	4/4	0.78	0.19	80,89,92,100	0
26	PSC	E	201	52/52	0.78	0.29	46,92,184,199	0
23	DMU	C	313	33/33	0.78	0.14	57,89,100,105	0
24	PEK	C	304	53/53	0.78	0.28	64,89,138,146	0
19	EDO	N	613	4/4	0.78	0.29	61,65,69,80	0
19	EDO	W	304	4/4	0.79	0.23	88,88,91,100	0
23	DMU	G	1302	33/33	0.79	0.19	62,110,125,125	0
17	PGV	T	101	51/51	0.79	0.26	56,90,115,134	0
19	EDO	D	204	4/4	0.79	0.18	60,76,76,78	0
19	EDO	F	702	4/4	0.79	0.20	70,84,89,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	J	1103	4/4	0.80	0.20	77,77,78,85	0
20	TGL	N	604	63/63	0.80	0.28	65,97,118,130	0
19	EDO	A	611	4/4	0.80	0.24	63,81,82,84	0
19	EDO	A	614	4/4	0.81	0.24	41,44,46,52	0
23	DMU	P	302	33/33	0.81	0.16	73,106,128,133	0
19	EDO	C	311	4/4	0.81	0.23	83,85,90,99	0
20	TGL	A	615	63/63	0.81	0.28	59,87,139,151	0
19	EDO	G	1306	4/4	0.81	0.20	90,90,93,95	0
17	PGV	N	616	51/51	0.82	0.23	66,87,140,156	0
25	CDL	T	102	100/100	0.82	0.28	67,112,154,170	0
19	EDO	V	103	4/4	0.82	0.20	81,81,90,95	0
20	TGL	D	201	63/63	0.83	0.25	55,86,101,108	0
19	EDO	N	617	4/4	0.83	0.20	87,88,92,93	0
19	EDO	S	2201	4/4	0.83	0.22	58,63,63,78	0
24	PEK	P	305	53/53	0.83	0.25	59,92,159,171	0
19	EDO	T	103	4/4	0.83	0.21	57,66,69,71	0
19	EDO	S	2206	4/4	0.84	0.17	55,60,63,70	0
19	EDO	S	2207	4/4	0.84	0.22	75,81,84,85	0
20	TGL	Q	201	63/63	0.84	0.25	67,91,111,119	0
20	TGL	Y	101	63/63	0.84	0.26	55,79,120,132	0
19	EDO	B	309	4/4	0.84	0.23	75,91,97,105	0
25	CDL	P	307	100/100	0.85	0.23	52,96,128,136	0
19	EDO	V	104	4/4	0.85	0.20	50,74,76,77	0
19	EDO	I	102	4/4	0.85	0.19	88,88,94,94	0
19	EDO	S	2204	4/4	0.86	0.18	50,66,66,68	0
19	EDO	Z	103	4/4	0.86	0.16	86,94,94,96	0
19	EDO	P	309	4/4	0.86	0.15	81,82,85,87	0
20	TGL	L	101	63/63	0.87	0.22	47,77,104,109	0
19	EDO	B	308	4/4	0.87	0.18	59,62,69,85	0
25	CDL	C	306	100/100	0.87	0.21	48,89,122,127	0
19	EDO	W	303	4/4	0.87	0.19	60,74,75,76	0
19	EDO	G	1303	4/4	0.87	0.17	71,83,83,89	0
19	EDO	D	205	4/4	0.88	0.16	64,77,78,81	0
19	EDO	D	206	4/4	0.88	0.17	74,79,83,88	0
19	EDO	J	1105	4/4	0.88	0.14	56,73,74,88	0
19	EDO	N	611	4/4	0.88	0.17	67,71,73,81	0
19	EDO	N	612	4/4	0.88	0.18	67,73,74,82	0
19	EDO	E	204	4/4	0.88	0.17	73,75,75,78	0
19	EDO	U	1501	4/4	0.88	0.20	55,66,68,72	0
19	EDO	A	610	4/4	0.88	0.16	38,43,46,50	0
19	EDO	O	303	4/4	0.88	0.16	53,74,76,77	0
19	EDO	D	202	4/4	0.88	0.15	62,72,77,81	0

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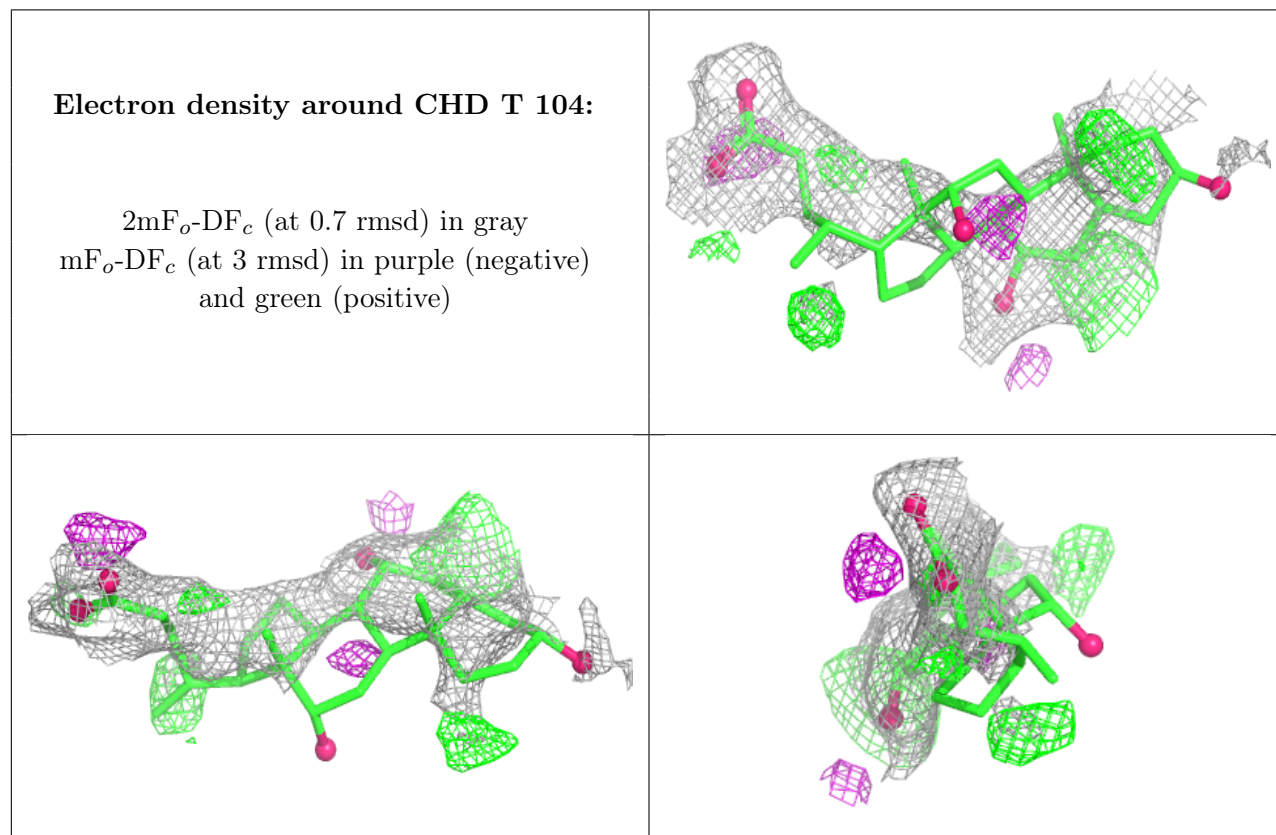
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	EDO	A	612	4/4	0.88	0.18	55,56,56,62	0
19	EDO	Q	204	4/4	0.88	0.17	73,73,75,75	0
19	EDO	B	306	4/4	0.89	0.22	70,76,78,81	0
19	EDO	F	704	4/4	0.89	0.19	61,61,69,71	0
19	EDO	N	614	4/4	0.89	0.26	41,45,46,47	0
23	DMU	Z	101	33/33	0.89	0.14	54,72,82,84	0
22	CHD	J	1102	29/29	0.89	0.13	59,74,86,97	0
19	EDO	C	309	4/4	0.89	0.17	75,80,83,84	0
19	EDO	N	620	4/4	0.89	0.19	65,66,69,79	0
19	EDO	B	304	4/4	0.89	0.15	51,59,64,72	0
19	EDO	L	102	4/4	0.90	0.17	68,69,72,75	0
19	EDO	B	307	4/4	0.90	0.19	65,67,68,84	0
19	EDO	S	2205	4/4	0.90	0.14	56,59,69,70	0
19	EDO	E	205	4/4	0.90	0.20	81,82,82,86	0
22	CHD	P	308	29/29	0.90	0.12	57,64,73,78	0
19	EDO	A	616	4/4	0.90	0.15	54,66,68,68	0
19	EDO	E	203	4/4	0.91	0.11	51,52,57,59	0
22	CHD	W	302	29/29	0.91	0.12	78,88,98,106	0
22	CHD	C	307	29/29	0.91	0.11	53,60,67,73	0
19	EDO	A	618	4/4	0.91	0.14	56,62,64,73	0
19	EDO	G	1304	4/4	0.91	0.18	75,79,80,80	0
19	EDO	V	102	4/4	0.92	0.18	78,79,80,83	0
19	EDO	C	314	4/4	0.92	0.14	62,70,71,79	0
19	EDO	P	311	4/4	0.92	0.14	42,51,51,60	0
19	EDO	Q	202	4/4	0.92	0.14	44,56,58,60	0
19	EDO	M	102	4/4	0.92	0.13	72,75,80,83	0
19	EDO	D	208	4/4	0.93	0.16	62,64,70,74	0
19	EDO	Q	203	4/4	0.93	0.15	73,77,82,86	0
19	EDO	A	620	4/4	0.93	0.11	45,47,52,52	0
19	EDO	N	618	4/4	0.93	0.13	54,56,62,64	0
24	PEK	P	304	53/53	0.93	0.18	41,64,101,108	0
19	EDO	W	301	4/4	0.93	0.16	62,74,75,76	0
19	EDO	N	610	4/4	0.93	0.14	52,55,58,59	0
19	EDO	I	103	4/4	0.94	0.11	58,63,64,67	0
19	EDO	A	613	4/4	0.94	0.14	45,52,57,59	0
19	EDO	A	608	4/4	0.94	0.14	50,56,63,68	0
19	EDO	K	101	4/4	0.94	0.13	74,75,76,77	0
19	EDO	D	203	4/4	0.94	0.15	61,66,75,83	0
19	EDO	A	619	4/4	0.94	0.16	66,67,70,78	0
19	EDO	N	609	4/4	0.94	0.13	50,53,54,55	0
19	EDO	N	619	4/4	0.94	0.12	51,60,68,77	0
19	EDO	R	201	4/4	0.94	0.10	54,54,55,56	0

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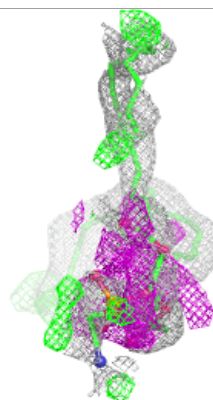
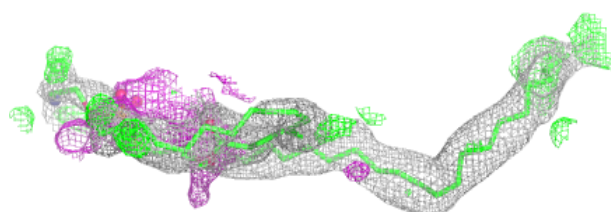
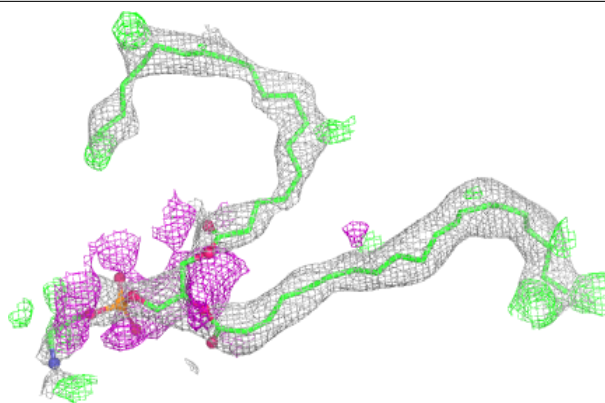
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	PEK	C	303	53/53	0.95	0.15	37,62,93,113	0
22	CHD	C	302	29/29	0.95	0.08	35,38,41,42	0
19	EDO	A	617	4/4	0.95	0.14	56,61,62,69	0
19	EDO	S	2203	4/4	0.95	0.12	35,36,37,40	0
19	EDO	J	1104	4/4	0.95	0.13	55,55,58,62	0
19	EDO	E	202	4/4	0.95	0.09	51,52,52,54	0
17	PGV	A	605	51/51	0.95	0.13	28,48,85,90	0
19	EDO	N	615	4/4	0.95	0.15	55,68,73,83	0
19	EDO	B	305	4/4	0.95	0.10	44,54,60,62	0
19	EDO	T	105	4/4	0.95	0.13	44,46,47,49	0
17	PGV	N	605	51/51	0.95	0.14	34,49,85,93	0
23	DMU	M	101	33/33	0.95	0.09	46,54,68,74	0
19	EDO	D	207	4/4	0.95	0.12	60,63,63,70	0
19	EDO	J	1101	4/4	0.95	0.10	52,61,64,68	0
17	PGV	P	306	51/51	0.96	0.12	35,49,96,106	0
16	NA	A	603	1/1	0.96	0.12	35,35,35,35	0
19	EDO	N	608	4/4	0.96	0.08	42,42,45,50	0
22	CHD	P	303	29/29	0.96	0.07	35,40,44,46	0
19	EDO	C	308	4/4	0.96	0.11	43,49,53,61	0
19	EDO	K	102	4/4	0.96	0.10	66,68,74,75	0
19	EDO	O	304	4/4	0.96	0.19	44,45,48,50	0
17	PGV	C	305	51/51	0.97	0.12	32,43,94,101	0
19	EDO	A	609	4/4	0.97	0.07	33,34,35,36	0
22	CHD	B	302	29/29	0.97	0.07	33,37,43,46	0
19	EDO	F	701	4/4	0.97	0.09	46,48,50,55	0
15	MG	A	602	1/1	0.97	0.04	32,32,32,32	0
22	CHD	G	1305	29/29	0.97	0.07	35,39,43,46	0
16	NA	N	603	1/1	0.97	0.11	49,49,49,49	0
19	EDO	B	303	4/4	0.97	0.14	32,33,34,37	0
18	HEA	N	606	60/60	0.98	0.06	27,34,43,49	0
19	EDO	F	705	4/4	0.98	0.09	34,36,37,37	0
19	EDO	G	1301	4/4	0.98	0.07	39,40,49,51	0
18	HEA	N	607	60/60	0.98	0.07	31,36,53,61	0
15	MG	N	602	1/1	0.98	0.05	39,39,39,39	0
18	HEA	A	607	60/60	0.99	0.06	24,29,48,55	0
27	ZN	F	703	1/1	0.99	0.03	38,38,38,38	0
18	HEA	A	606	60/60	0.99	0.05	24,29,37,43	0
21	CUA	O	301	2/2	0.99	0.02	37,37,37,38	0
21	CUA	B	301	2/2	1.00	0.02	30,30,30,30	0
27	ZN	S	2202	1/1	1.00	0.03	42,42,42,42	0
14	CU	N	601	1/1	1.00	0.02	35,35,35,35	0
14	CU	A	601	1/1	1.00	0.01	29,29,29,29	0

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

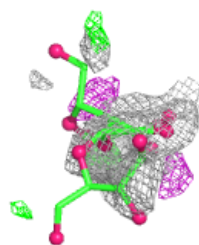
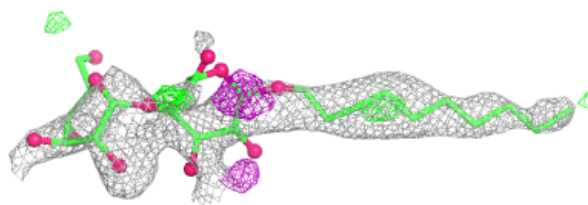
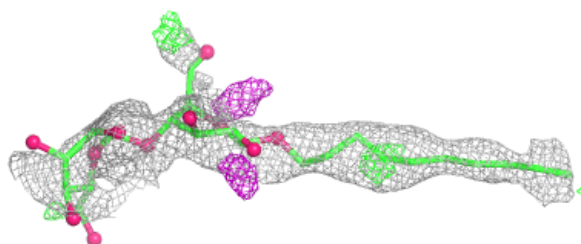


Electron density around PEK C 315:

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

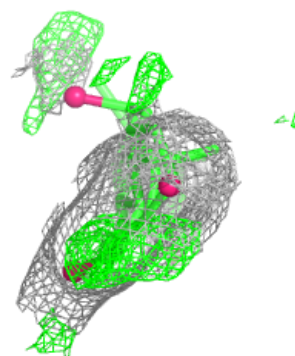
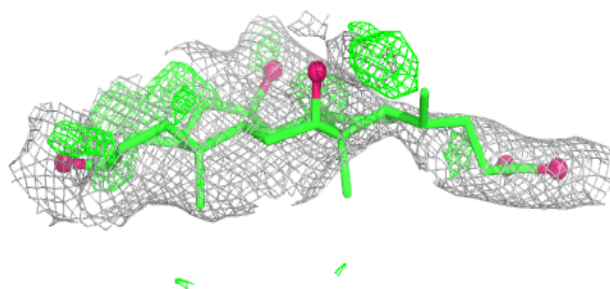
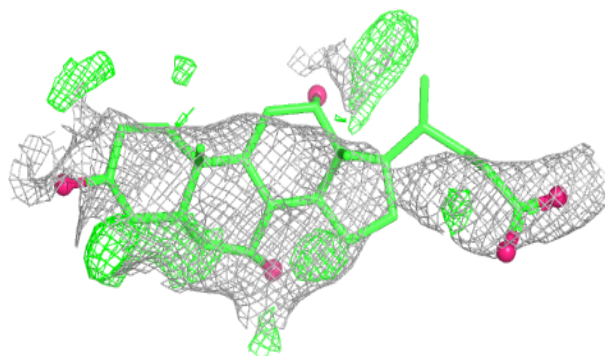
**Electron density around DMU C 301:**

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

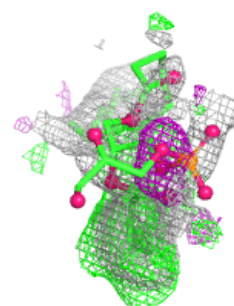
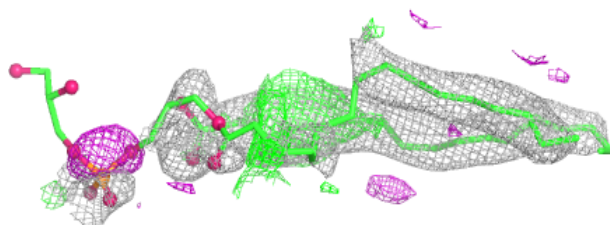
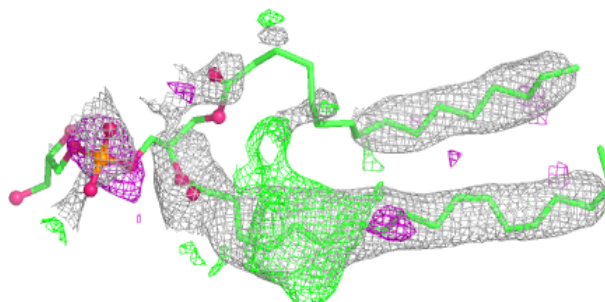


Electron density around CHD Y 102:

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

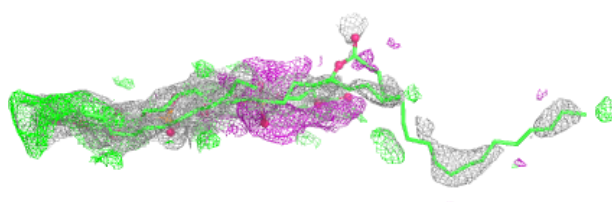
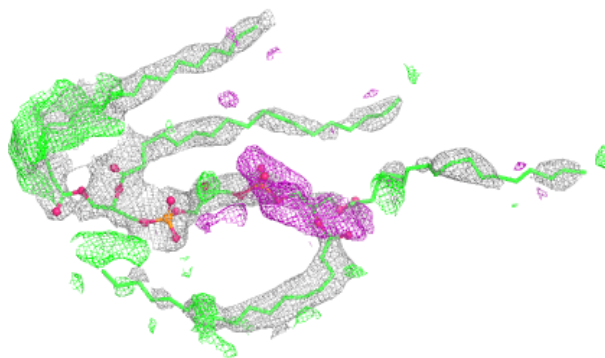
**Electron density around PGV Z 102:**

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

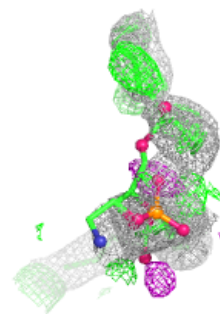
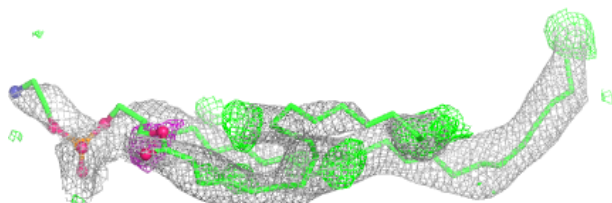
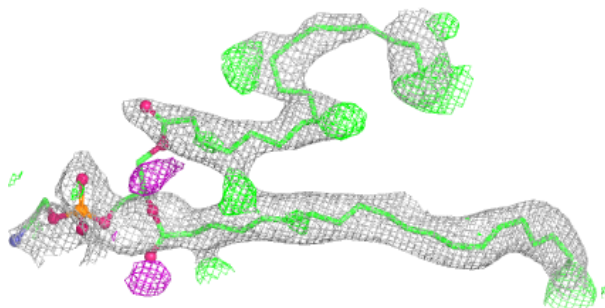


Electron density around CDL C 312:

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

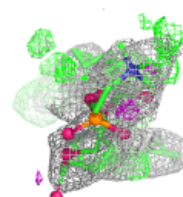
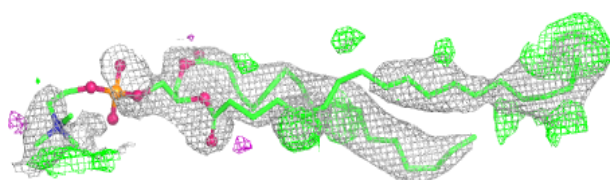
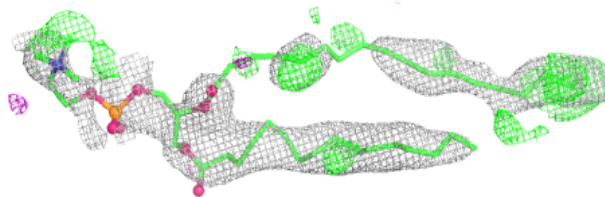
**Electron density around PEK P 301:**

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

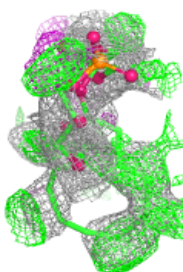
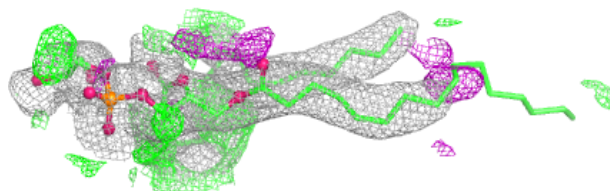
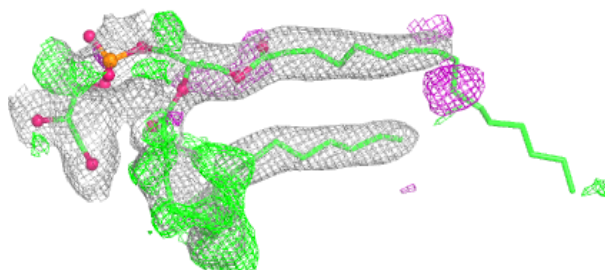


Electron density around PSC O 302:

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

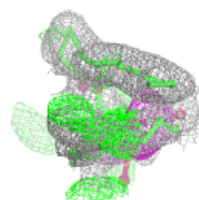
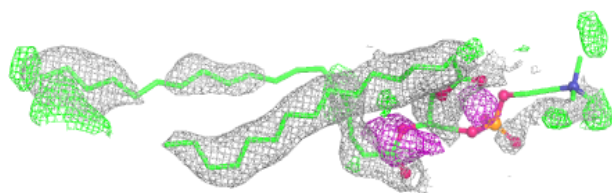
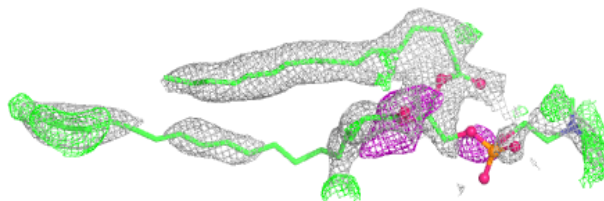
**Electron density around PGV A 604:**

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

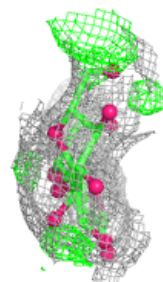
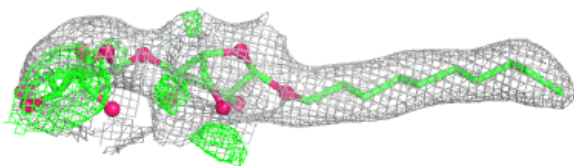
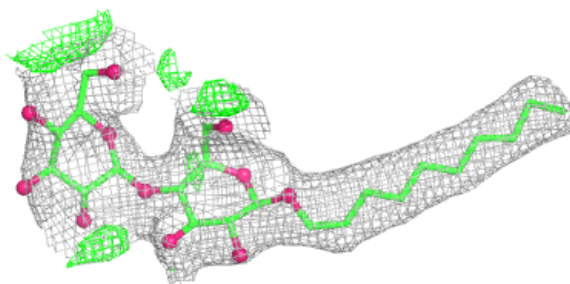


Electron density around PSC E 201:

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

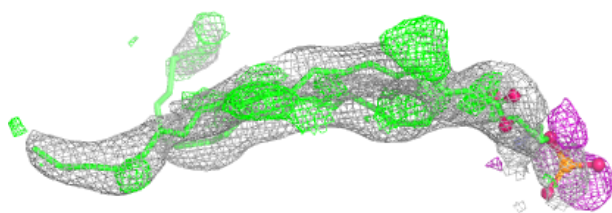
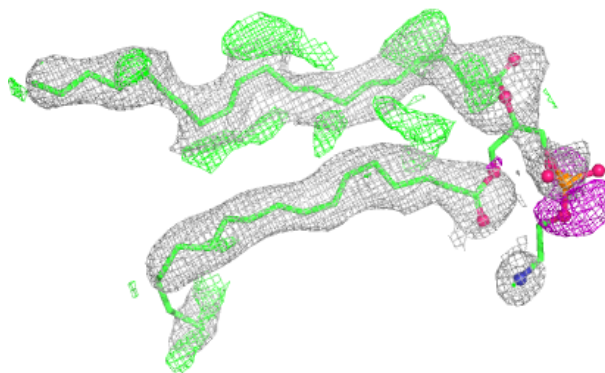
**Electron density around DMU C 313:**

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

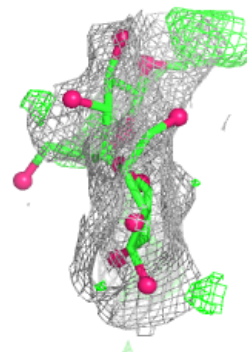
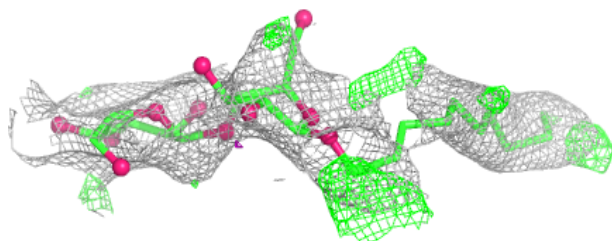
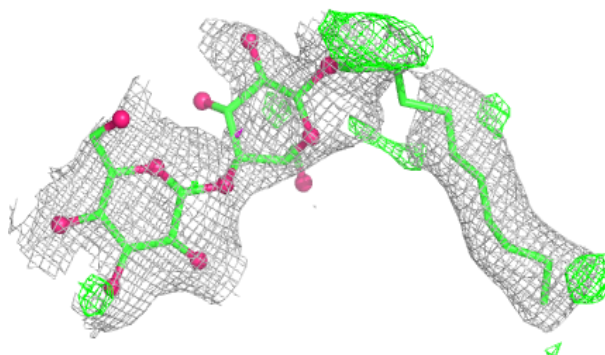


Electron density around PEK C 304:

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

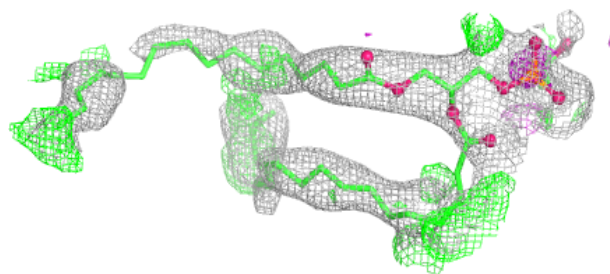
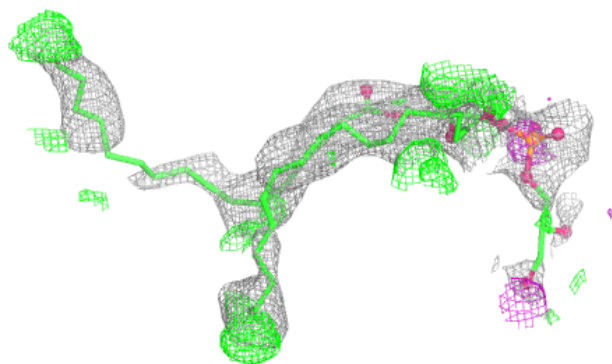
**Electron density around DMU G 1302:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

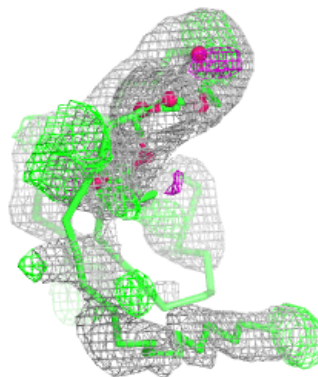
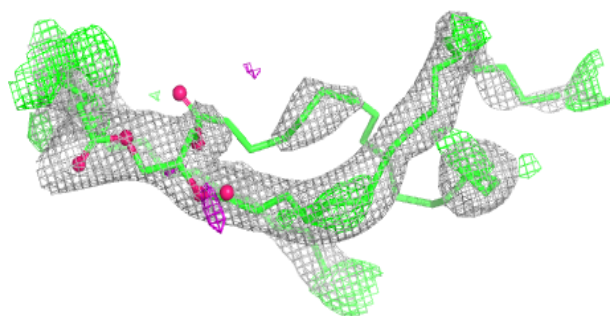
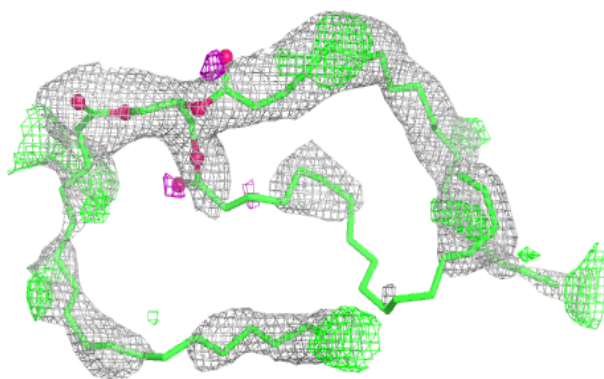


Electron density around PGV T 101:

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

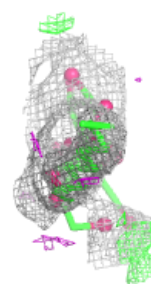
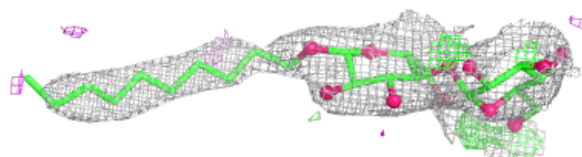
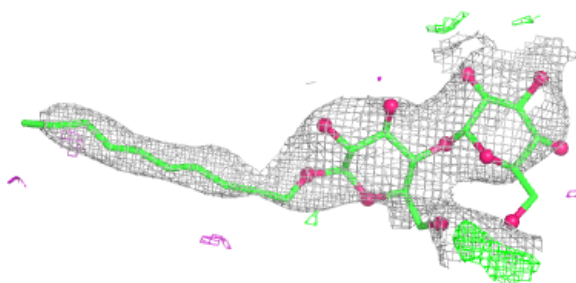
**Electron density around TGL N 604:**

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

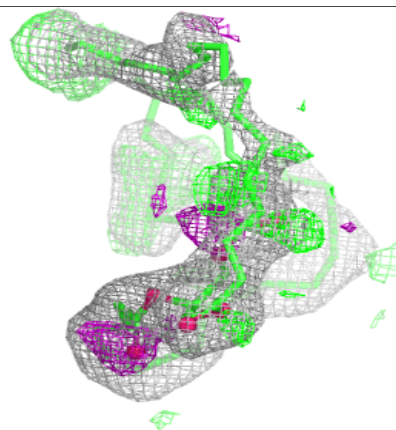
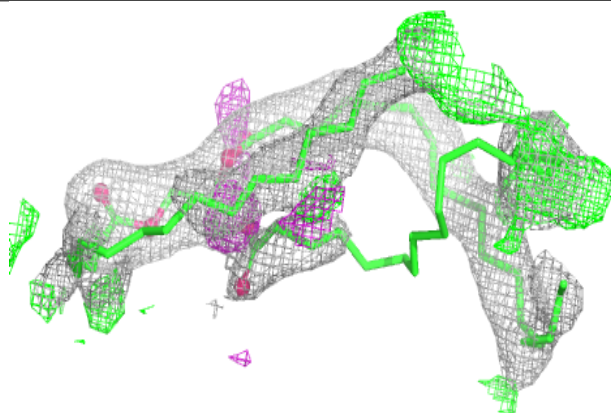
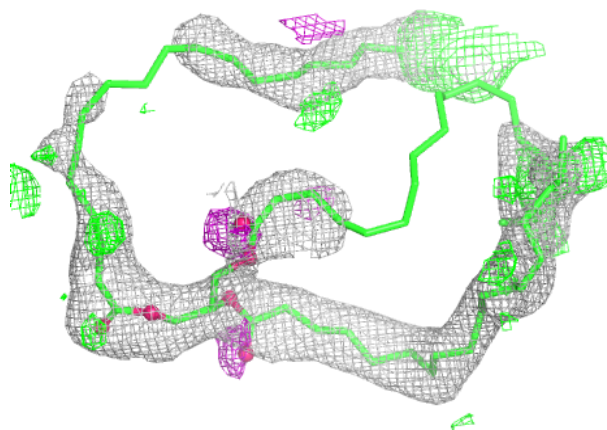


Electron density around DMU P 302:

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

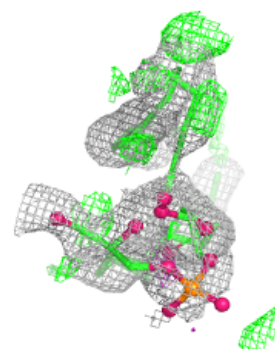
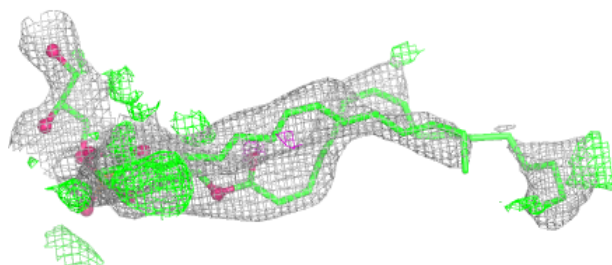
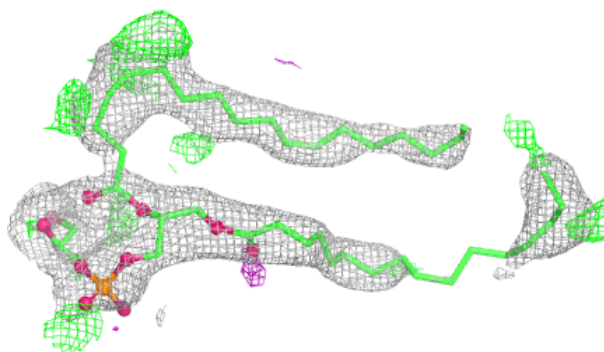
**Electron density around TGL A 615:**

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and green (positive)

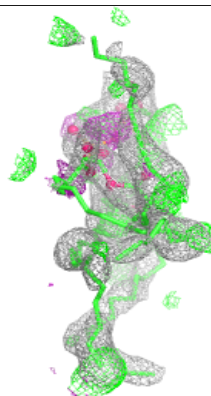
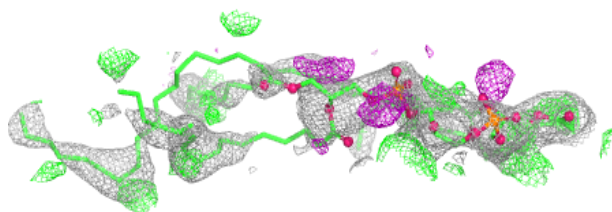
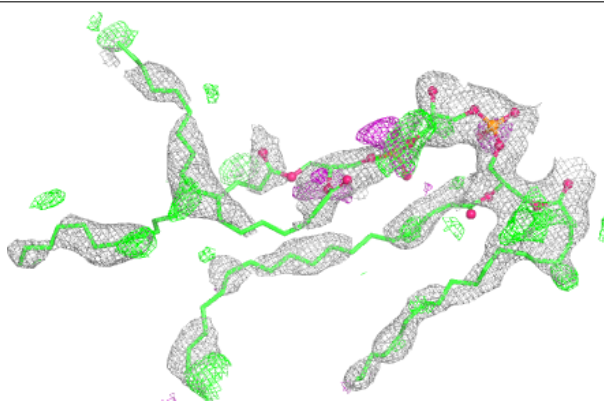


Electron density around PGV N 616:

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

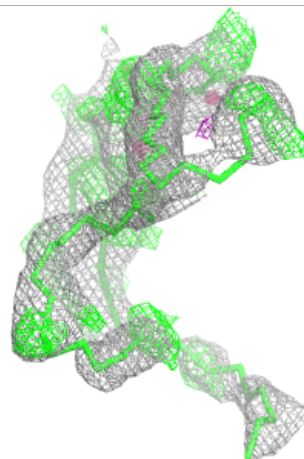
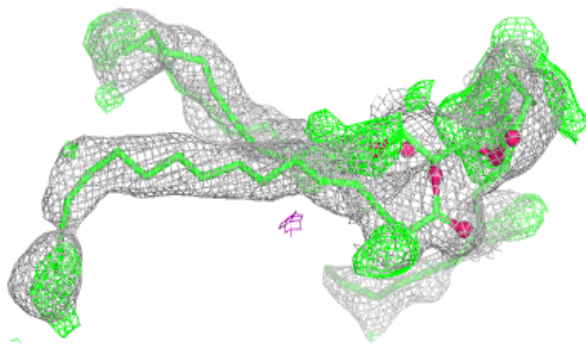
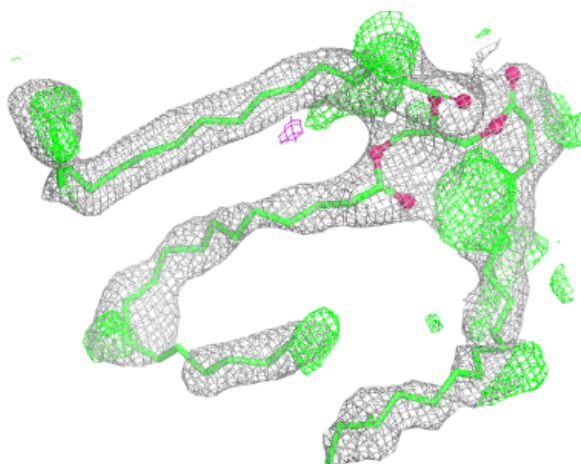
**Electron density around CDL T 102:**

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



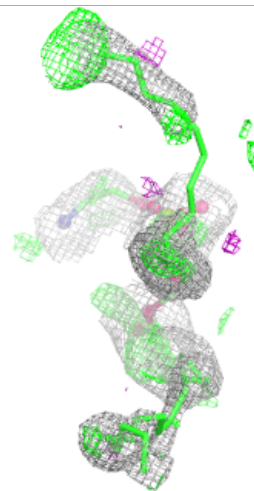
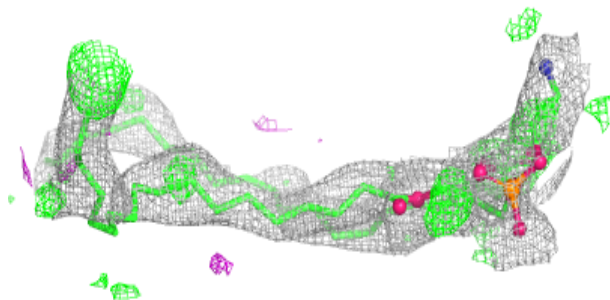
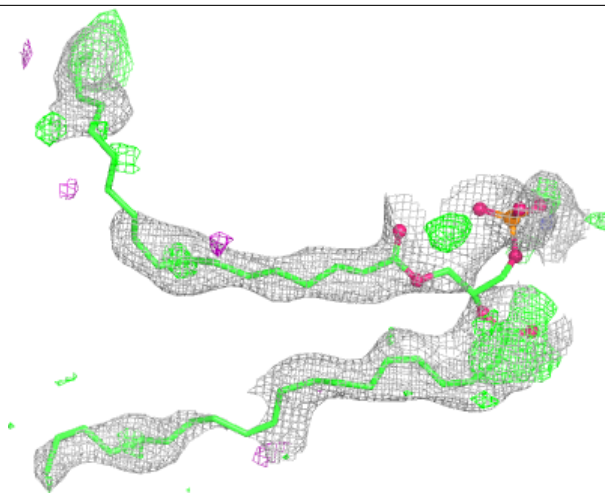
Electron density around TGL D 201:

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



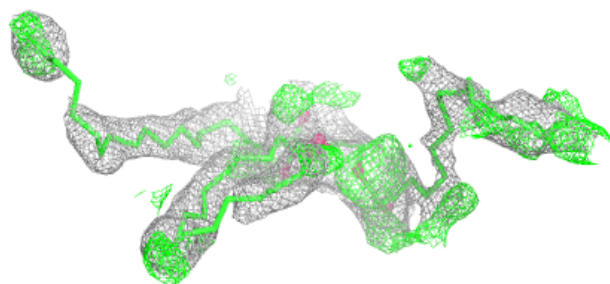
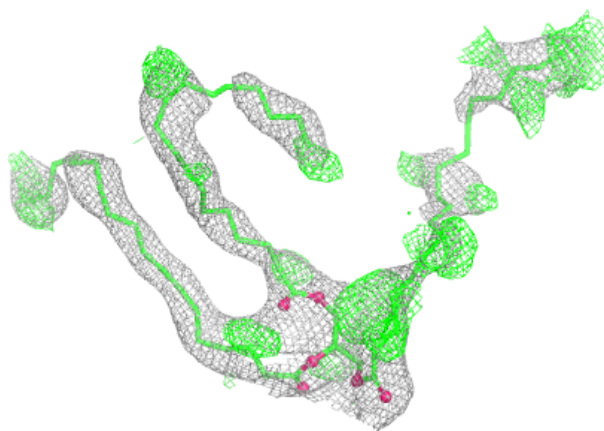
Electron density around PEK P 305:

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

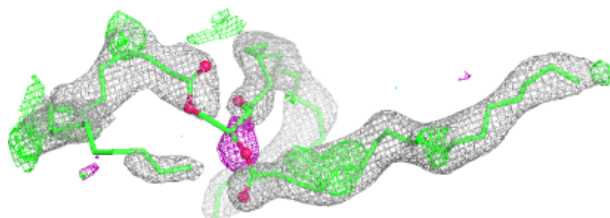
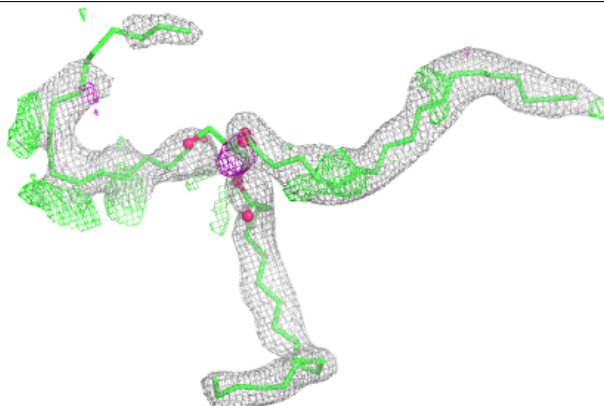


Electron density around TGL Q 201:

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and green (positive)

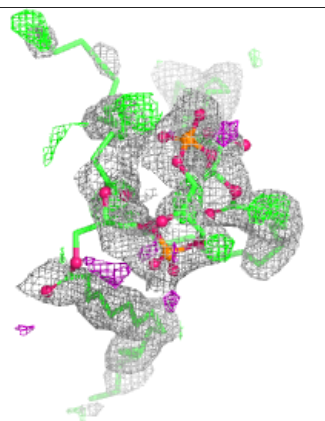
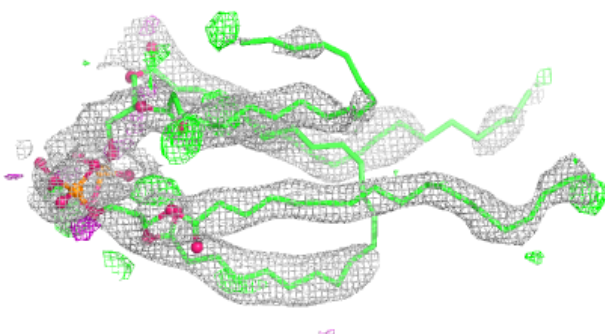
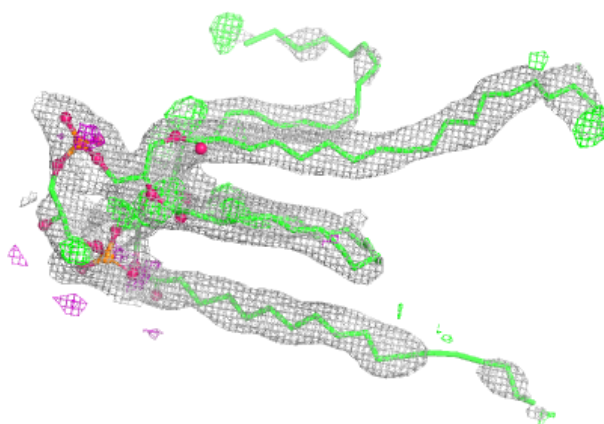
**Electron density around TGL Y 101:**

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



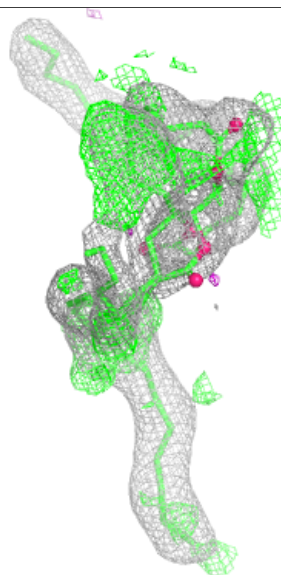
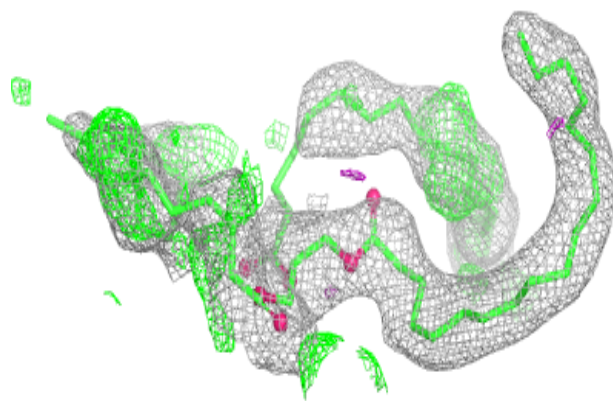
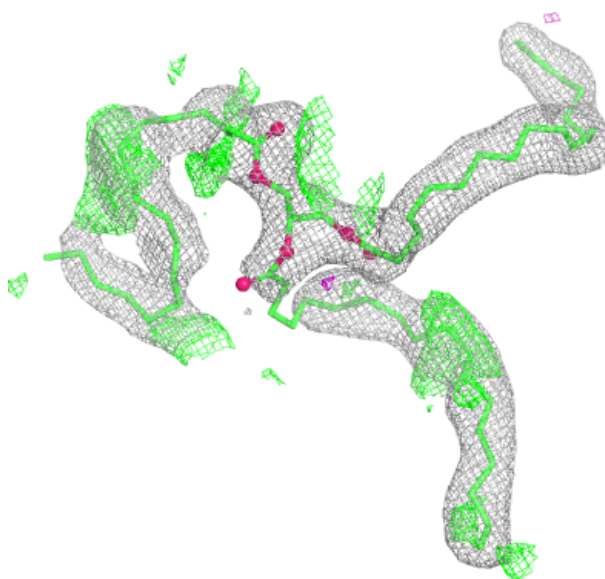
Electron density around CDL P 307:

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



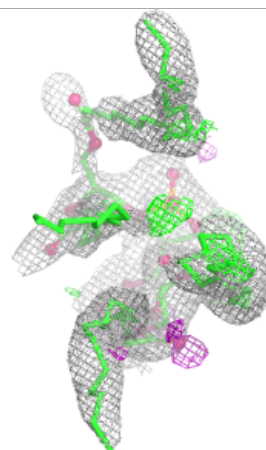
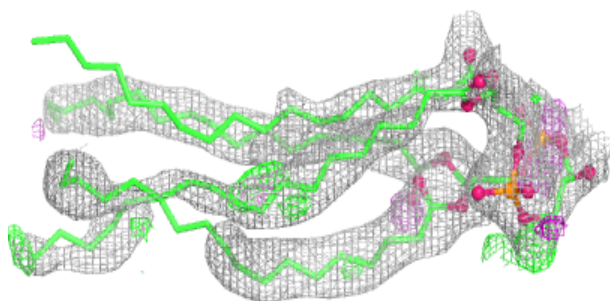
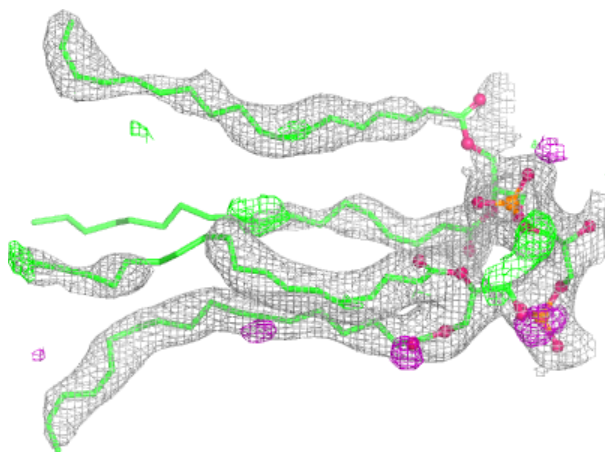
Electron density around TGL L 101:

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



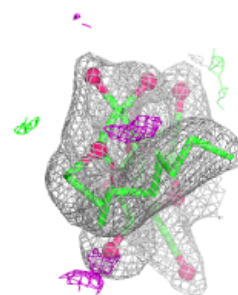
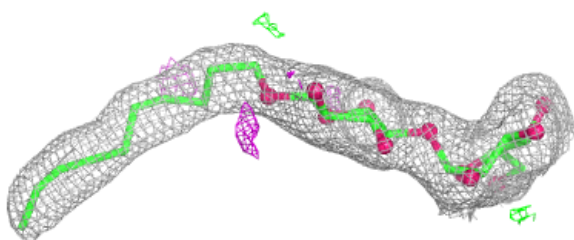
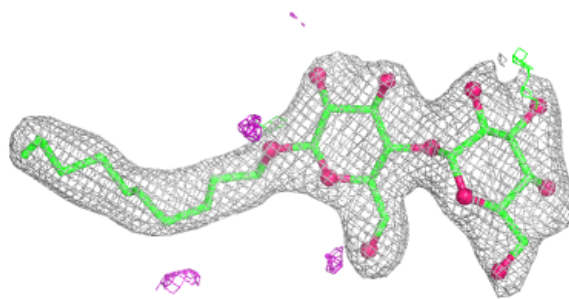
Electron density around CDL C 306:

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

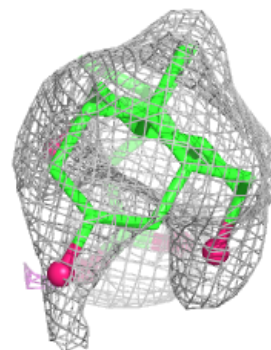
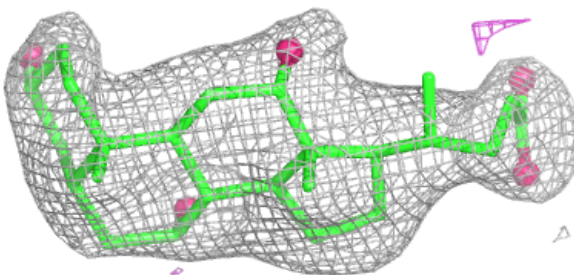
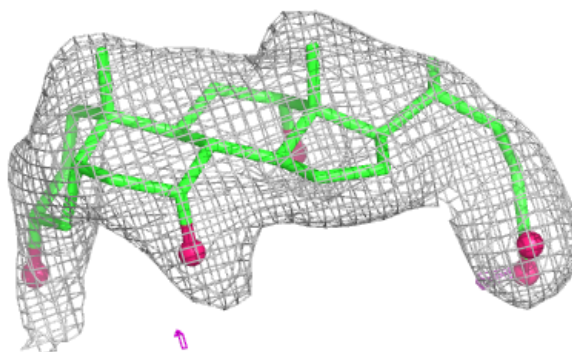


Electron density around DMU Z 101:

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

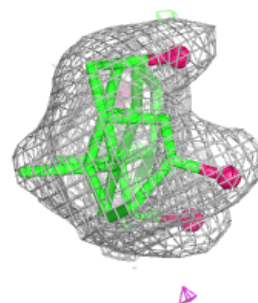
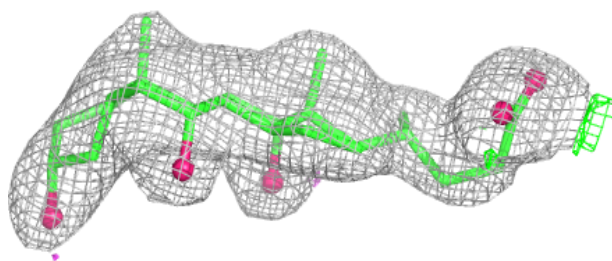
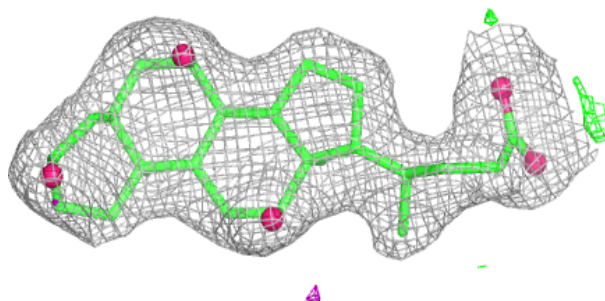
**Electron density around CHD J 1102:**

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

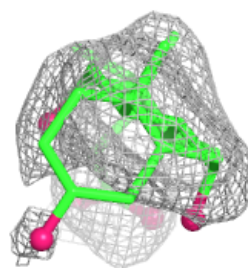
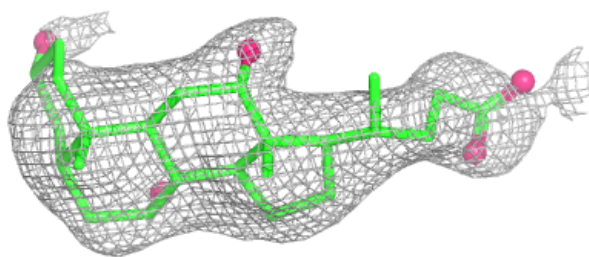
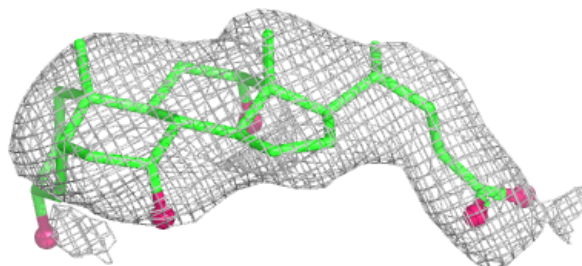


Electron density around CHD P 308:

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

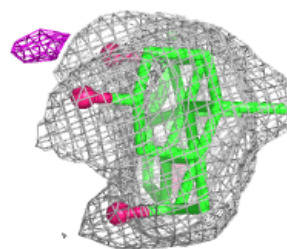
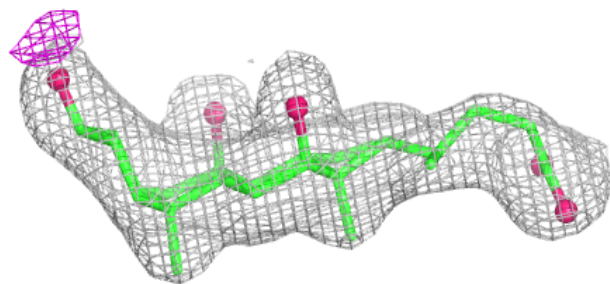
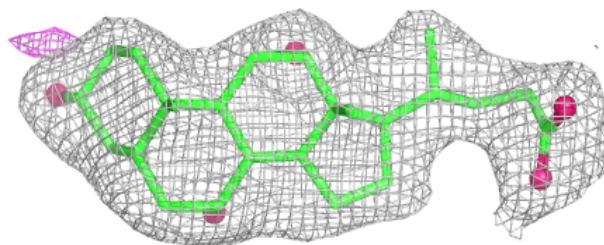
**Electron density around CHD W 302:**

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

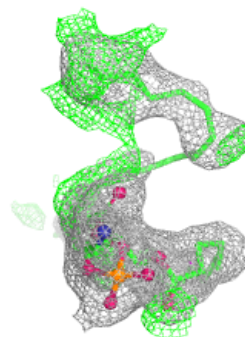
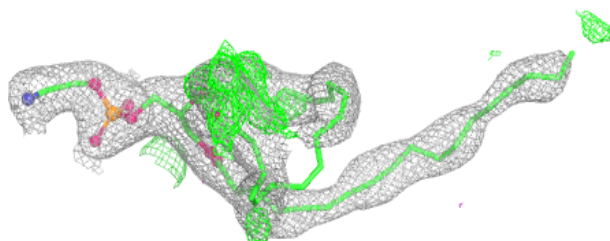
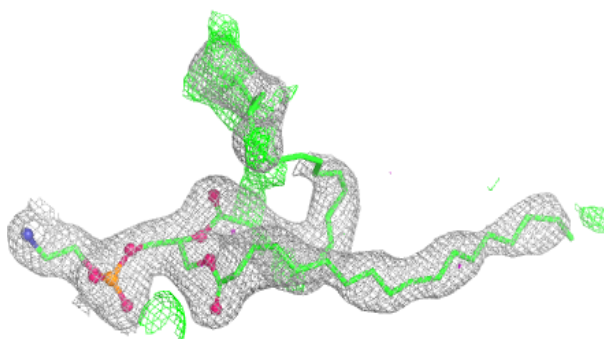


Electron density around CHD C 307:

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

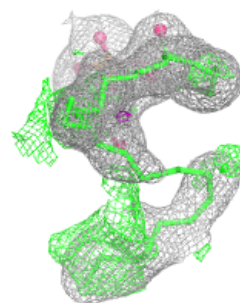
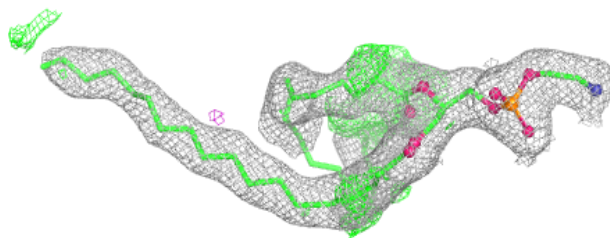
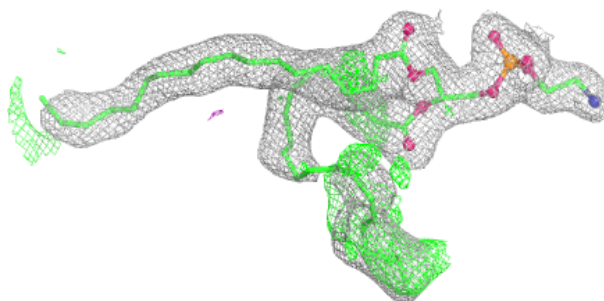
**Electron density around PEK P 304:**

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

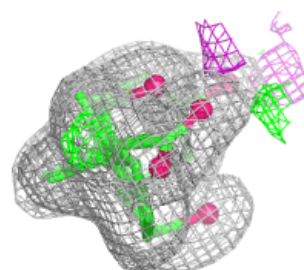
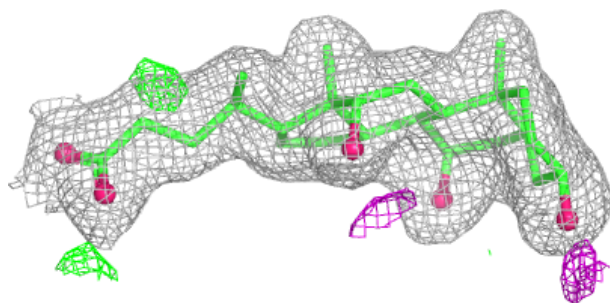
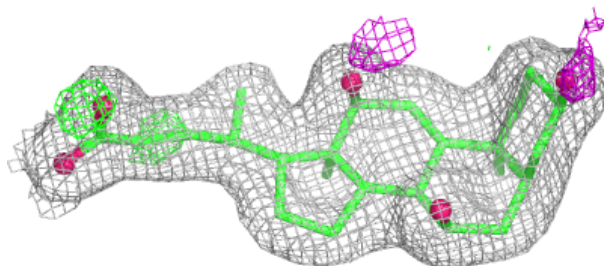


Electron density around PEK C 303:

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

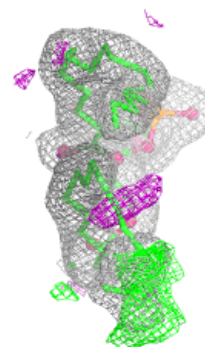
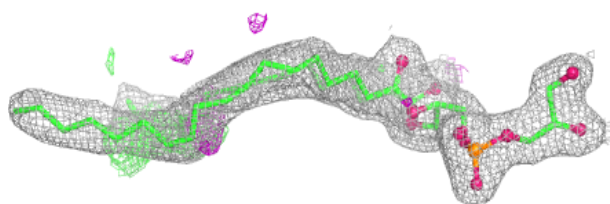
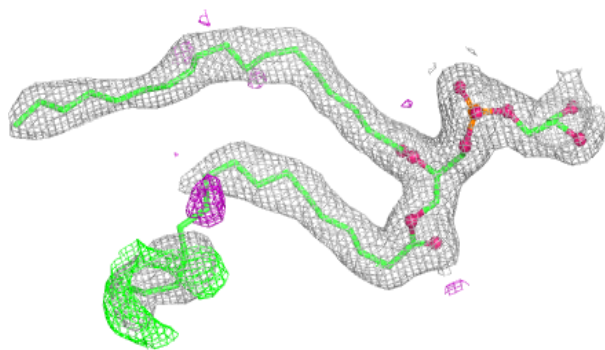
**Electron density around CHD C 302:**

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

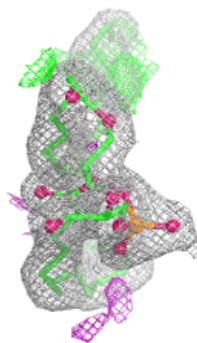
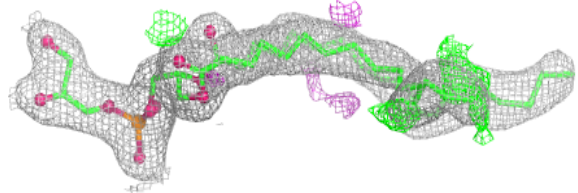
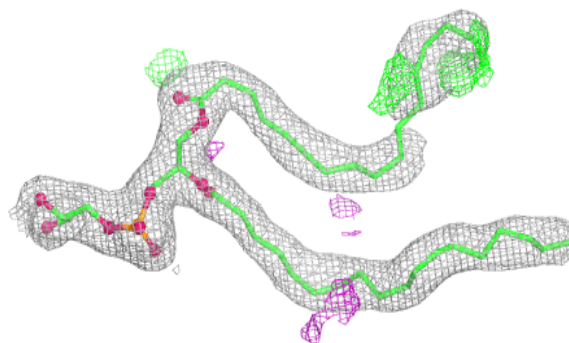


Electron density around PGV A 605:

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

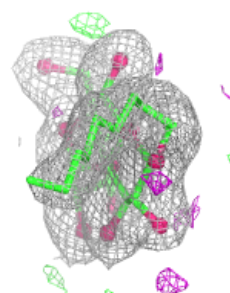
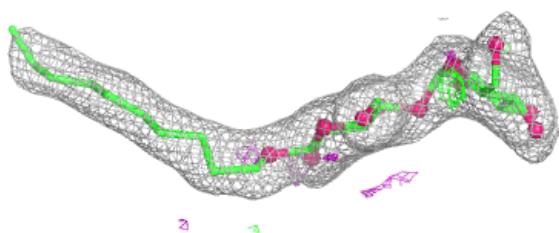
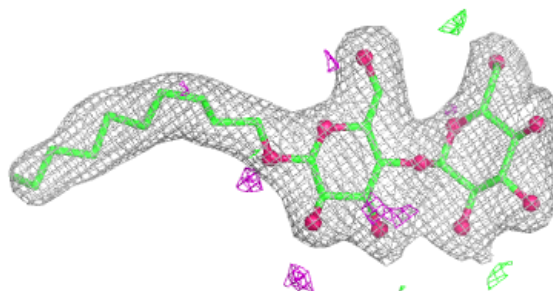
**Electron density around PGV N 605:**

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

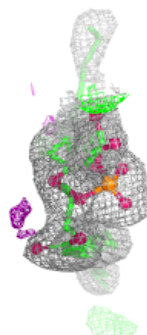
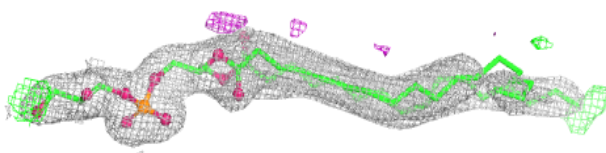
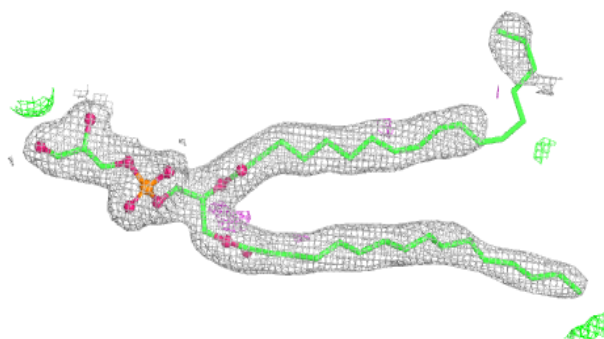


Electron density around DMU M 101:

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

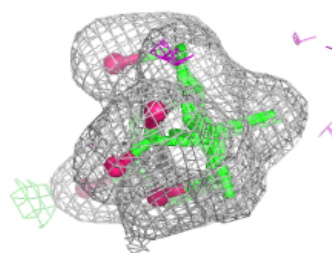
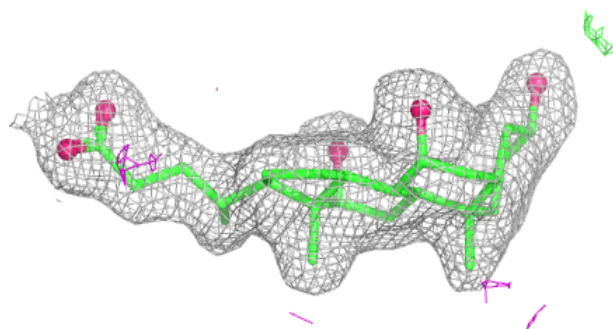
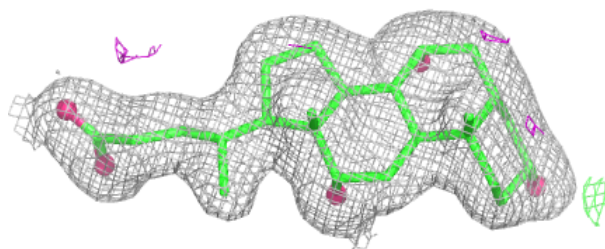
**Electron density around PGV P 306:**

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

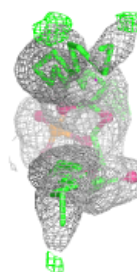
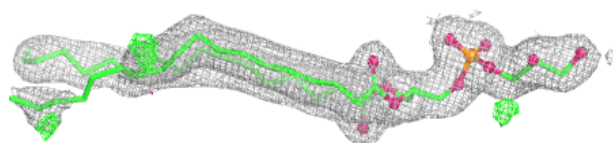
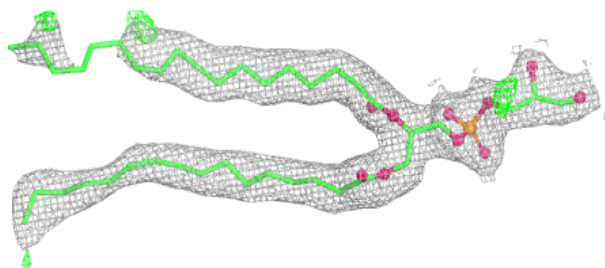


Electron density around CHD P 303:

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

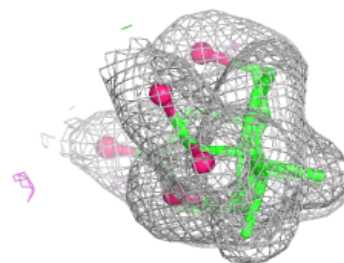
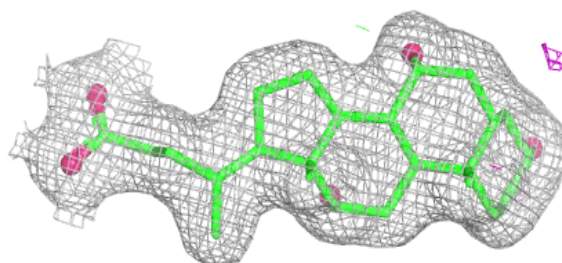
**Electron density around PGV C 305:**

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

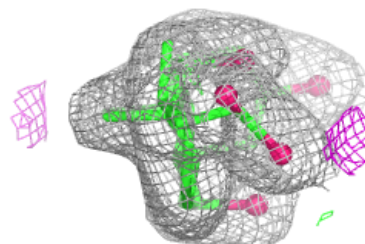
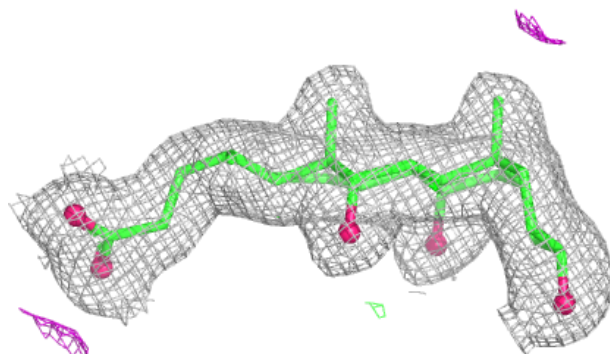
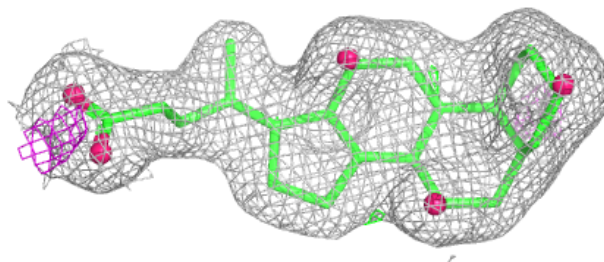


Electron density around CHD B 302:

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

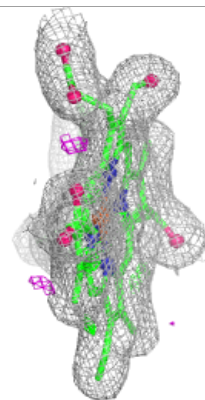
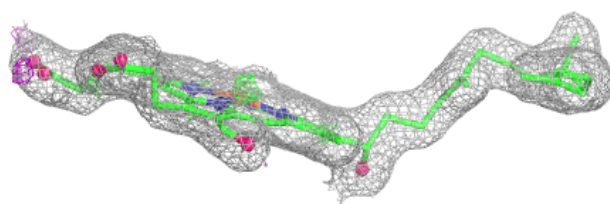
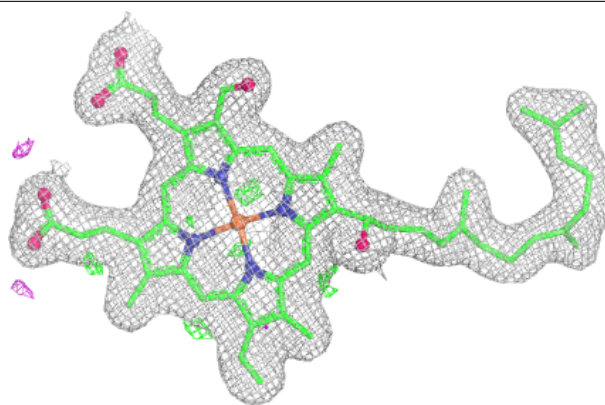
**Electron density around CHD G 1305:**

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

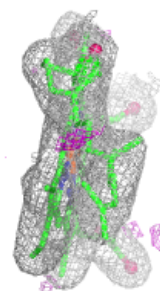
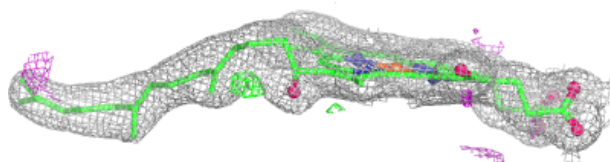
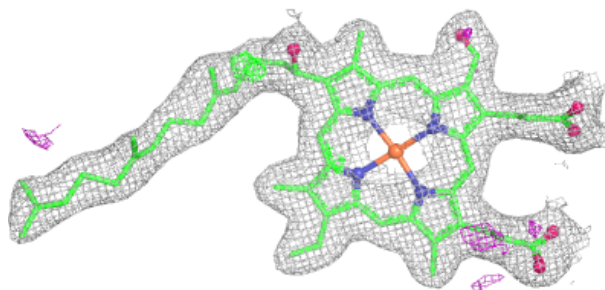


Electron density around HEA N 606:

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

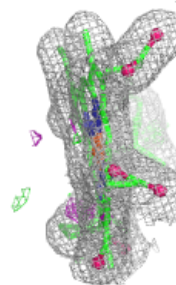
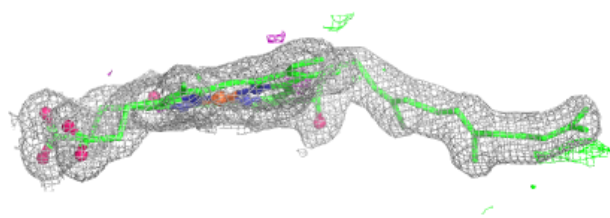
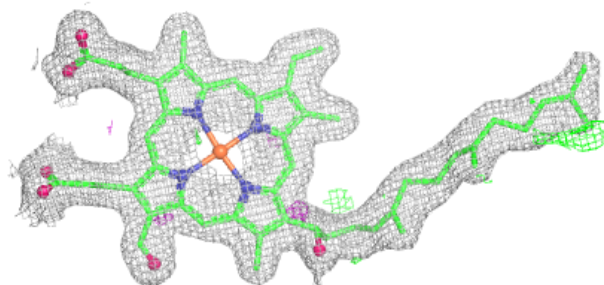
**Electron density around HEA N 607:**

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

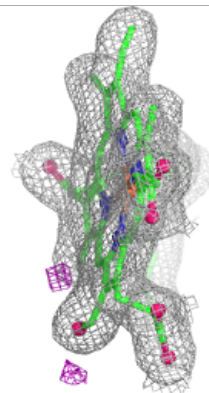
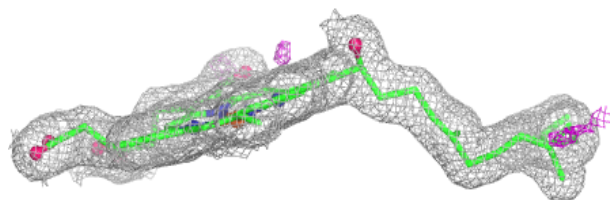
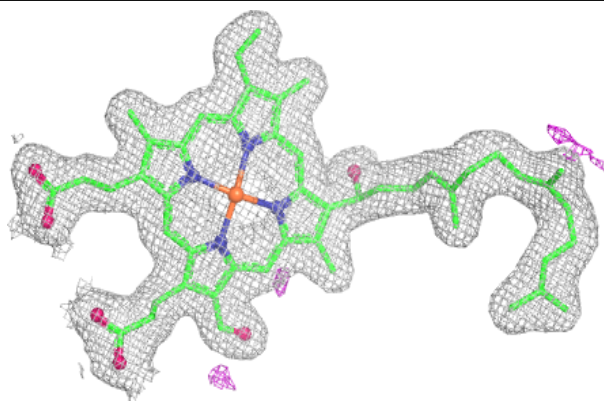


Electron density around HEA A 607:

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

**Electron density around HEA A 606:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.