



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2022 – 04:27 PM EDT

PDB ID : 7TIE
Title : Structure of oxidized bovine cytochrome c oxidase at 1.90 Angstrom resolution
obtained by synchrotron X-rays
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.
Deposited on : 2022-01-13
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

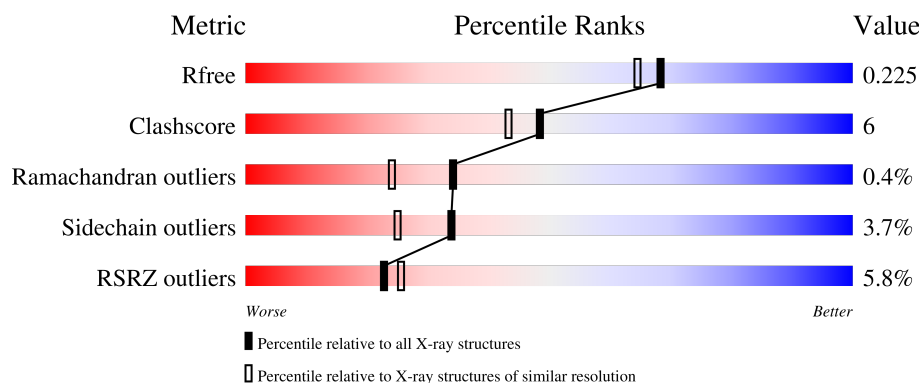
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.













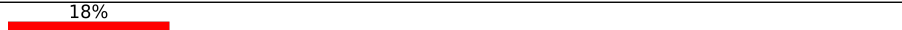

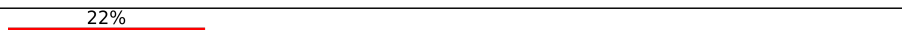
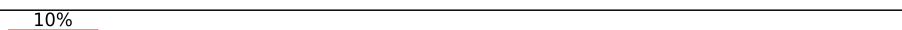
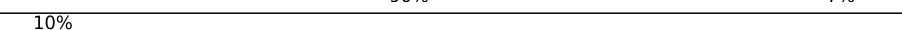






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	514	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> <div>.</div> </div>
1	N	514	<div> <div>2%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>.</div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> <div>.</div> </div>
2	O	227	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>11%</div> </div> <div>.</div> </div>
3	C	261	<div> <div></div> <div> <div></div> <div>92%</div> <div>7%</div> </div> <div>.</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	605	X	-	-	-
18	HEA	A	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	607	X	-	-	-
18	HEA	N	608	X	-	-	-
19	EDO	A	618	-	-	-	X
19	EDO	W	303	-	-	-	X
27	DMU	G	101	-	-	-	X
29	SAC	V	101	-	-	-	X

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32913 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	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	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	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	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	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	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 (three-letter code: 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		

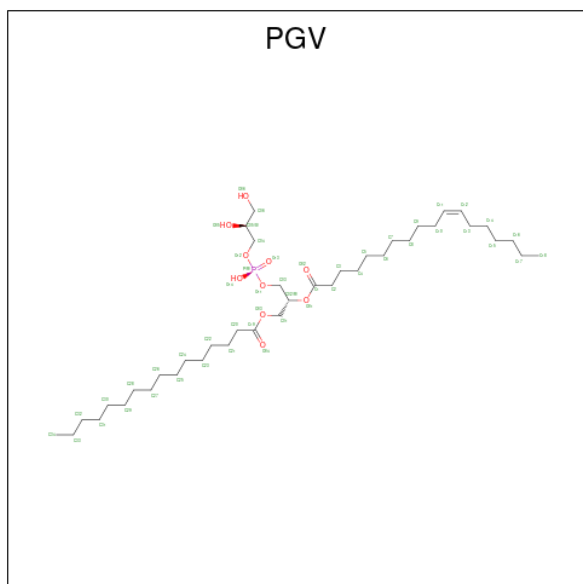
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: NA) (formula: Na).

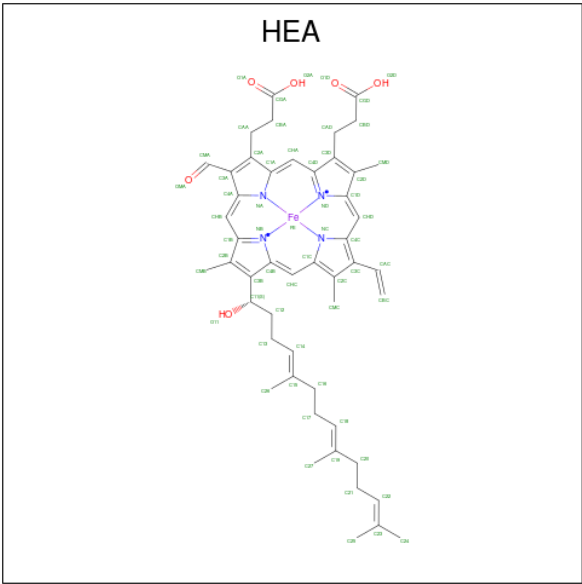
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	M	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	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆) (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 (three-letter code: EDO) (formula: C₂H₆O₂).



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		
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	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
19	E	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

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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	H	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	K	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	L	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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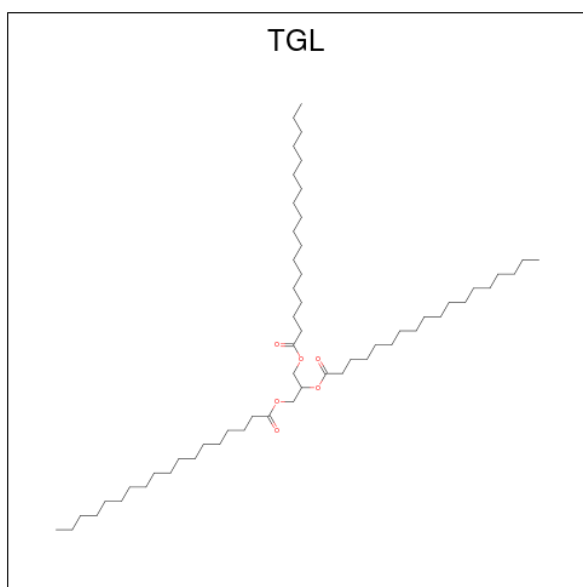
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	O	1	Total 4	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	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	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

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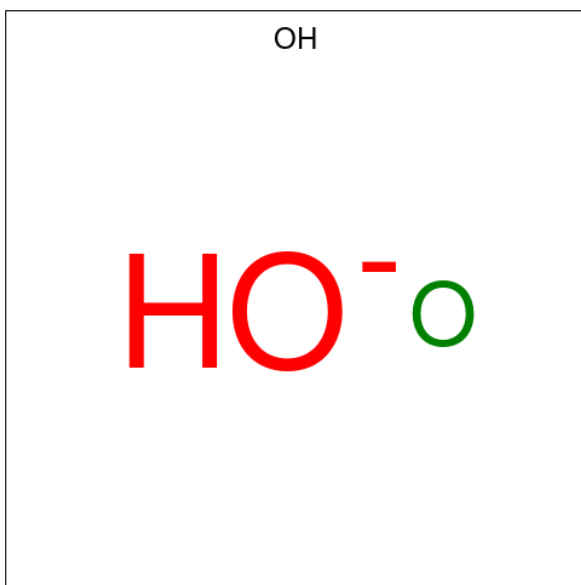
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	U	1	Total	C	O	0	0
			4	2	2		
19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

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



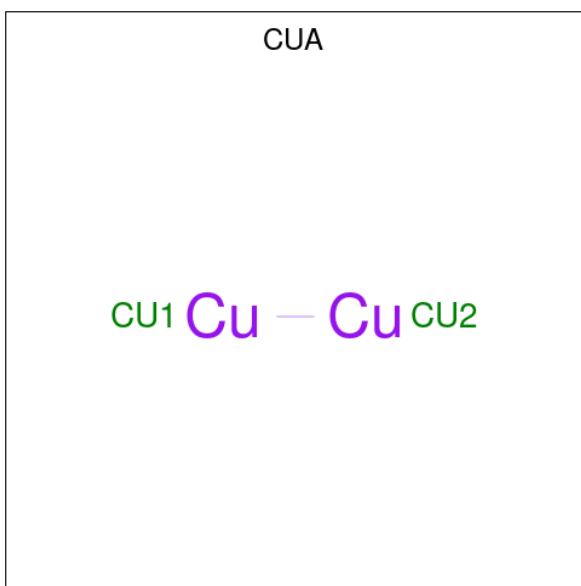
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



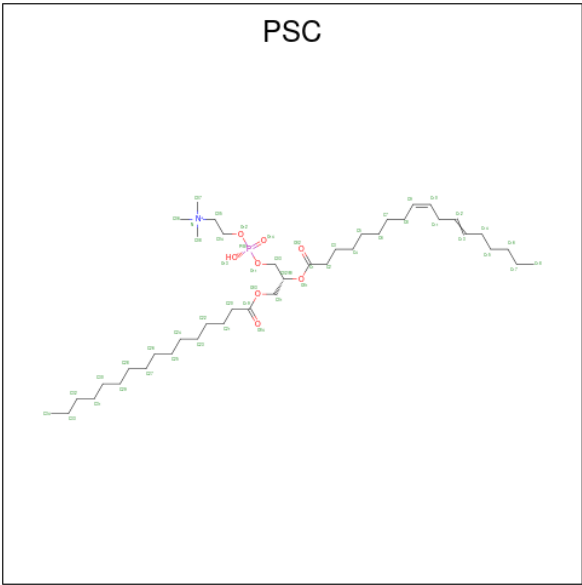
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

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



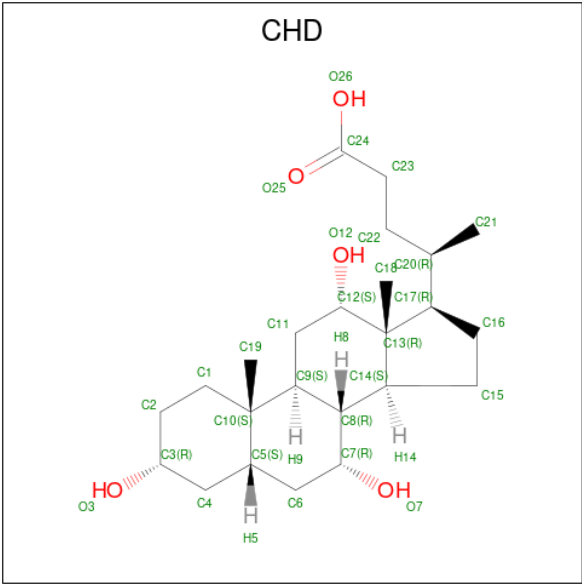
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

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



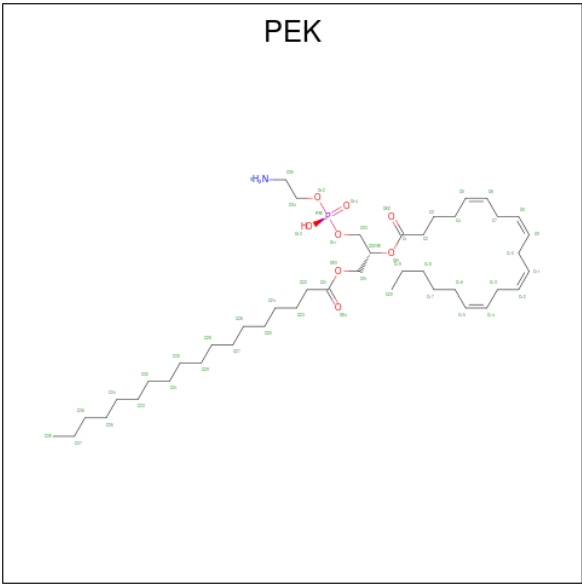
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C₂₄H₄₀O₅).



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

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



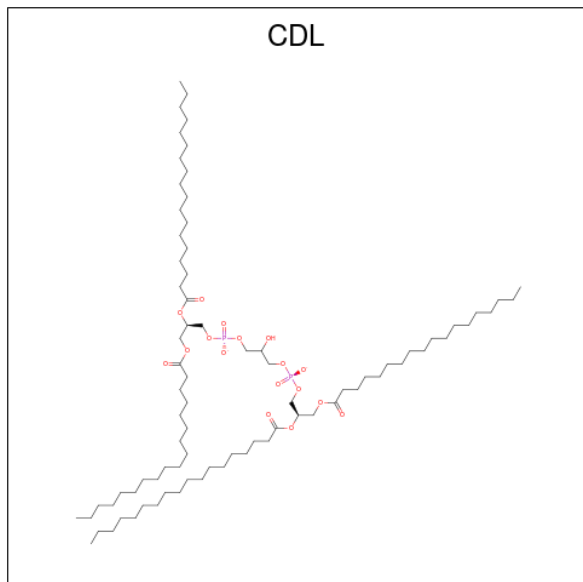
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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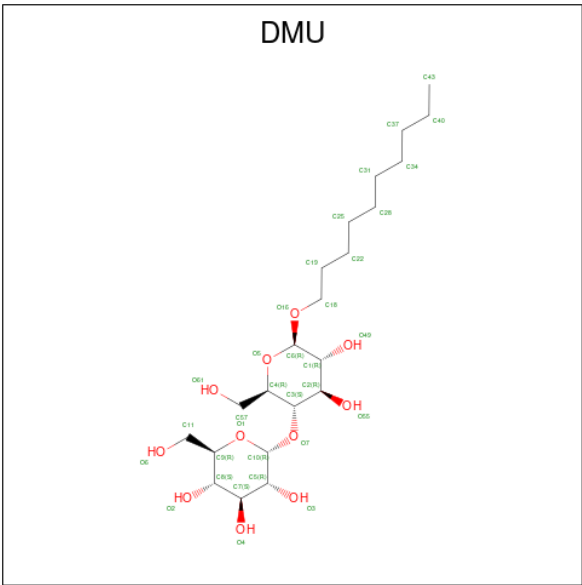
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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

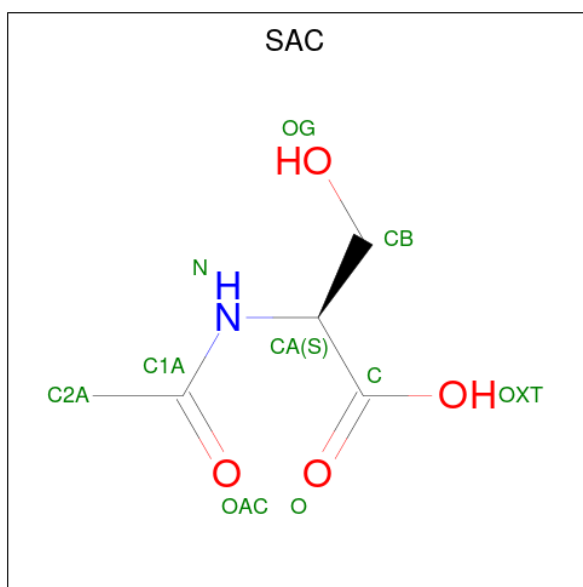


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	Z	1	Total	C	O	0	0
			33	22	11		

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

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

- Molecule 29 is N-ACETYL-SERINE (three-letter code: SAC) (formula: C₅H₉NO₄).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	215	Total	O	0	0
			215	215		
30	B	149	Total	O	0	0
			149	149		
30	C	111	Total	O	0	0
			111	111		
30	D	98	Total	O	0	0
			98	98		
30	E	81	Total	O	0	0
			81	81		
30	F	85	Total	O	0	0
			85	85		
30	G	45	Total	O	0	0
			45	45		
30	H	50	Total	O	0	0
			50	50		
30	I	31	Total	O	0	0
			31	31		
30	J	32	Total	O	0	0
			32	32		

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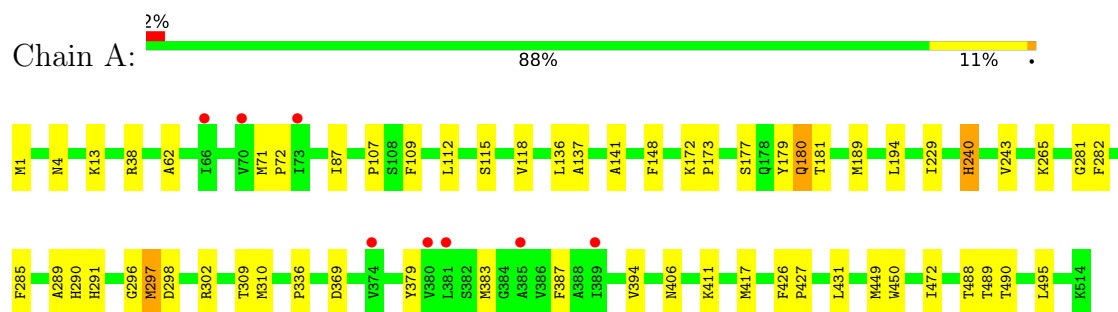
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	24	Total 24	O 24	0	0
30	L	24	Total 24	O 24	0	0
30	M	23	Total 23	O 23	0	0
30	N	184	Total 184	O 184	0	0
30	O	111	Total 111	O 111	0	0
30	P	96	Total 96	O 96	0	0
30	Q	59	Total 59	O 59	0	0
30	R	58	Total 58	O 58	0	0
30	S	73	Total 73	O 73	0	0
30	T	35	Total 35	O 35	0	0
30	U	47	Total 47	O 47	0	0
30	V	18	Total 18	O 18	0	0
30	W	18	Total 18	O 18	0	0
30	X	14	Total 14	O 14	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	6	Total 6	O 6	0	0

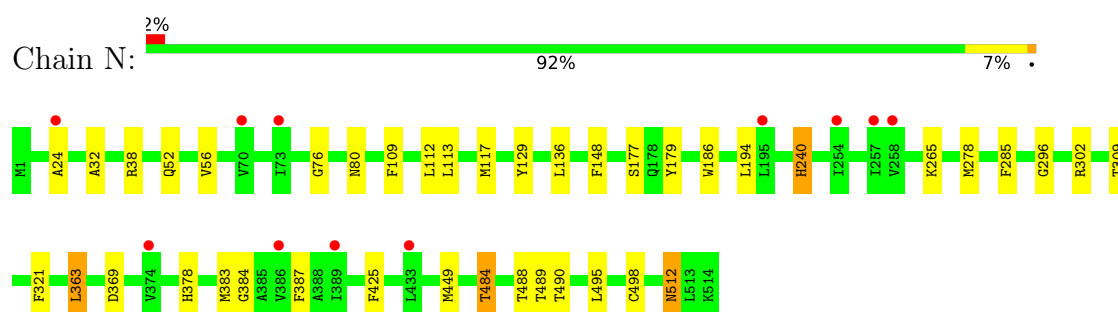
3 Residue-property plots

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

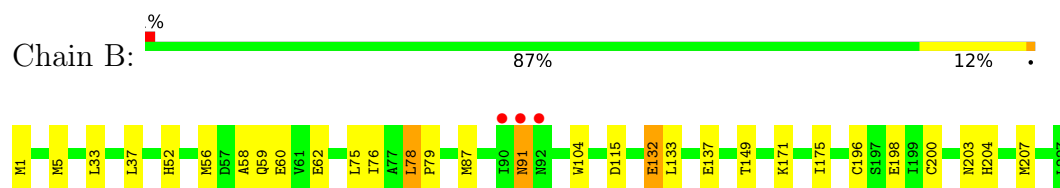
• Molecule 1: Cytochrome c oxidase subunit 1



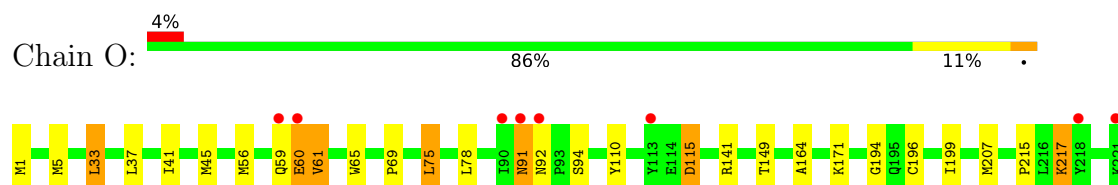
• Molecule 1: Cytochrome c oxidase subunit 1

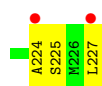


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 92% 7%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 89% 10%



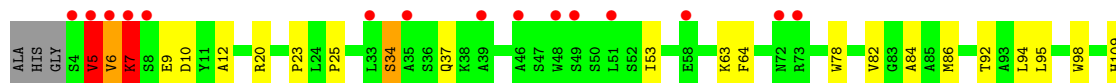
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 89% 7%



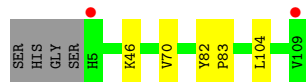
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain Q: 11% 82% 13%



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

Chain E: 2% 92% 5%

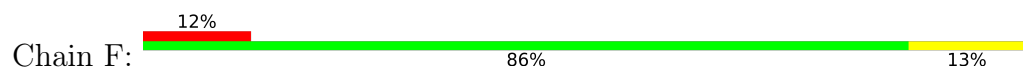


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

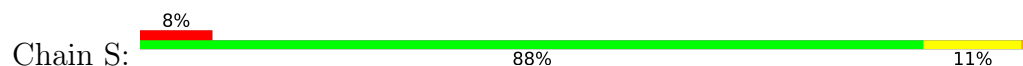
Chain R: 4% 90% 6%



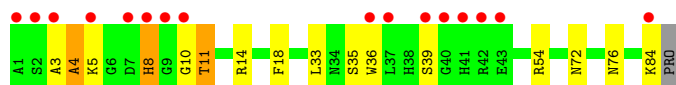
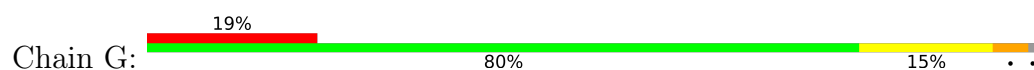
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



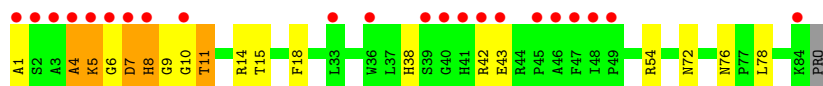
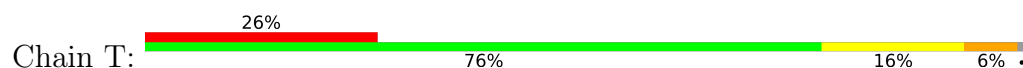
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



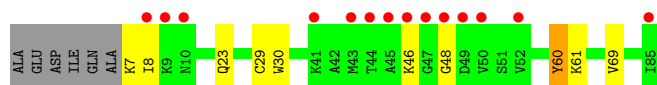
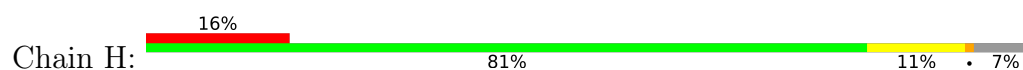
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



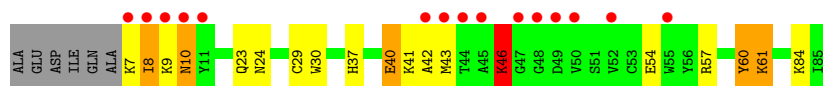
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



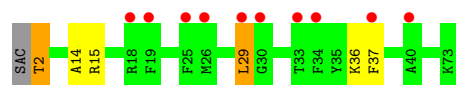
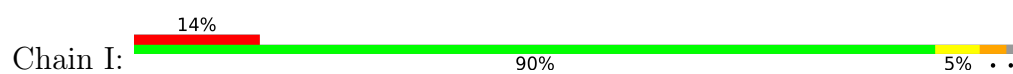
- Molecule 8: Cytochrome c oxidase subunit 6B1



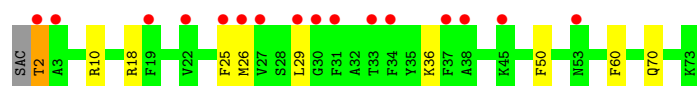
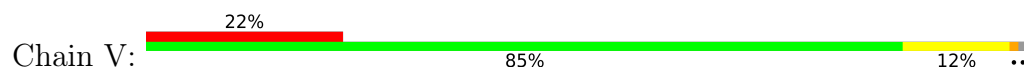
- Molecule 8: Cytochrome c oxidase subunit 6B1



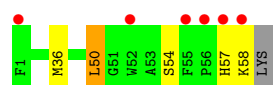
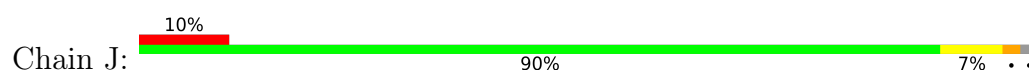
- Molecule 9: Cytochrome c oxidase subunit 6C



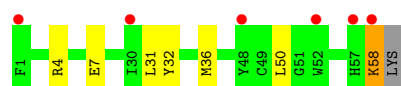
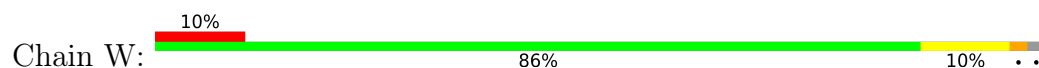
- Molecule 9: Cytochrome c oxidase subunit 6C



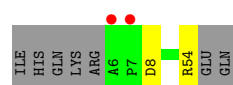
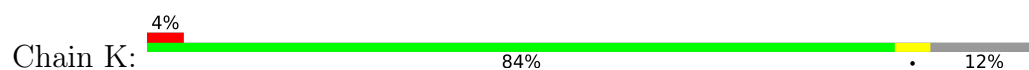
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



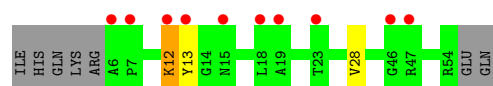
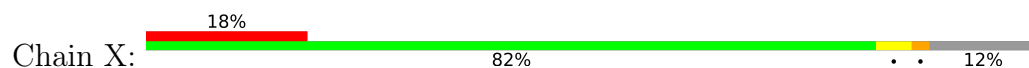
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



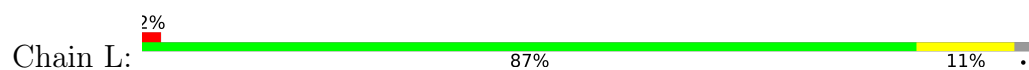
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



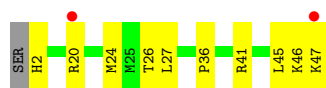
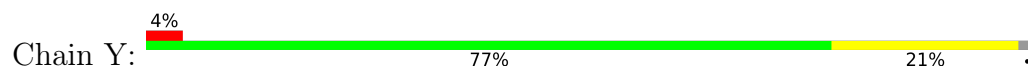
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



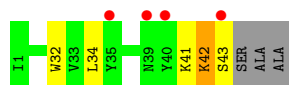
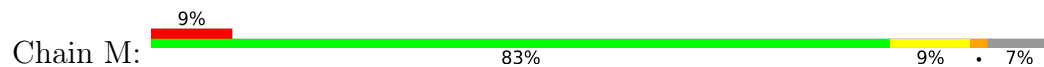
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



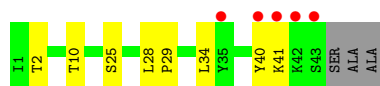
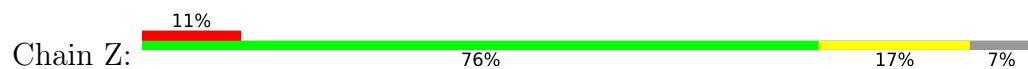
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	178.12Å 182.41Å 208.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 1.90 39.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.99-1.90) 99.8 (39.96-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.215 0.196 , 0.225	Depositor DCC
R_{free} test set	26755 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32913	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: ZN, PEK, TPO, TGL, PGV, CU, DMU, PSC, CDL, NA, FME, HEA, SAC, EDO, CUA, MG, OH, CHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/4156	0.84	1/5678 (0.0%)
1	N	0.77	0/4156	0.81	2/5678 (0.0%)
2	B	0.82	2/1860 (0.1%)	0.93	0/2534
2	O	0.74	0/1860	0.88	1/2534 (0.0%)
3	C	0.74	0/2197	0.79	2/3005 (0.1%)
3	P	0.79	0/2197	0.78	0/3005
4	D	0.76	0/1229	0.85	3/1658 (0.2%)
4	Q	0.73	0/1229	0.78	1/1658 (0.1%)
5	E	0.74	0/871	0.81	0/1182
5	R	0.70	0/871	0.80	0/1182
6	F	0.78	0/765	0.92	0/1038
6	S	0.76	0/765	0.85	0/1038
7	G	0.71	0/690	0.89	0/937
7	T	0.71	0/690	0.85	1/937 (0.1%)
8	H	0.74	0/682	0.85	0/921
8	U	0.68	0/682	0.86	0/921
9	I	0.74	0/605	0.87	0/802
9	V	0.69	0/605	0.86	0/802
10	J	0.66	0/471	0.81	1/636 (0.2%)
10	W	0.78	0/471	0.77	0/636
11	K	0.73	0/398	0.84	0/546
11	X	0.69	0/398	0.71	0/546
12	L	0.68	0/393	0.83	0/526
12	Y	0.73	0/393	0.80	0/526
13	M	0.76	0/345	0.85	0/470
13	Z	0.67	0/345	0.79	0/470
All	All	0.75	2/29324 (0.0%)	0.83	12/39866 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	132	GLU	CD-OE2	5.34	1.31	1.25
2	B	198	GLU	CD-OE2	-5.27	1.19	1.25

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH1	-7.77	116.41	120.30
4	Q	20	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	N	240	HIS	CA-CB-CG	-6.09	103.24	113.60
10	J	36	MET	CG-SD-CE	-6.04	90.53	100.20
2	O	92	ASN	CB-CA-C	5.45	121.31	110.40
1	A	240	HIS	CA-CB-CG	-5.44	104.35	113.60
4	D	20	ARG	CG-CD-NE	-5.44	100.38	111.80
4	D	20	ARG	NE-CZ-NH2	5.28	122.94	120.30
3	C	80	ARG	CG-CD-NE	-5.15	100.98	111.80
7	T	5	LYS	CB-CA-C	5.13	120.66	110.40
1	N	129	TYR	CB-CG-CD1	5.11	124.06	121.00
3	C	80	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	49	0
1	N	4027	0	4001	39	0
2	B	1824	0	1833	22	0
2	O	1824	0	1833	22	0
3	C	2110	0	2027	16	0
3	P	2110	0	2027	16	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	16	0
5	E	852	0	845	3	0
5	R	852	0	845	5	0
6	F	748	0	728	7	0
6	S	748	0	728	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	675	0	644	20	0
7	T	675	0	643	21	0
8	H	662	0	623	8	0
8	U	662	0	623	17	0
9	I	592	0	604	8	0
9	V	592	0	604	10	0
10	J	460	0	459	3	0
10	W	460	0	459	5	0
11	K	384	0	366	4	0
11	X	384	0	366	3	0
12	L	380	0	380	4	0
12	Y	380	0	380	13	0
13	M	335	0	352	5	0
13	Z	335	0	352	10	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	51	0	76	4	0
17	C	102	0	152	7	0
17	M	51	0	76	6	0
17	N	102	0	152	16	0
17	P	102	0	152	1	0
18	A	120	0	108	7	0
18	N	120	0	108	8	0
19	A	44	0	66	6	0
19	B	32	0	48	2	0
19	C	20	0	30	1	0
19	D	16	0	24	0	0
19	E	20	0	30	0	0
19	F	24	0	36	0	0
19	G	16	0	24	0	0
19	H	4	0	6	1	0
19	I	8	0	12	0	0
19	J	8	0	12	0	0
19	K	4	0	6	0	0
19	L	12	0	18	0	0
19	M	4	0	6	0	0
19	N	48	0	72	4	0
19	O	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	P	16	0	24	0	0
19	Q	16	0	24	0	0
19	R	8	0	12	1	0
19	S	24	0	36	1	0
19	T	8	0	12	0	0
19	U	4	0	6	3	0
19	V	12	0	18	1	0
19	W	8	0	12	0	0
20	A	63	0	110	0	0
20	D	63	0	110	10	0
20	L	63	0	110	3	0
20	N	189	0	330	11	0
21	A	1	0	0	1	0
21	N	1	0	0	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	8	0
23	R	52	0	80	6	0
24	B	29	0	39	1	0
24	C	58	0	78	1	0
24	G	29	0	39	0	0
24	J	29	0	39	2	0
24	P	58	0	78	1	0
24	T	29	0	39	4	0
24	W	29	0	39	1	0
24	Y	29	0	39	4	0
25	C	106	0	154	4	0
25	G	53	0	77	7	0
25	P	159	0	231	10	0
26	C	200	0	312	4	0
26	P	200	0	312	13	0
27	C	33	0	42	0	0
27	G	66	0	84	0	0
27	M	33	0	42	0	0
27	P	33	0	42	0	0
27	Z	33	0	42	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	2	0
29	V	9	0	8	3	0
30	A	215	0	0	7	0
30	B	149	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	C	111	0	0	1	0
30	D	98	0	0	2	0
30	E	81	0	0	0	0
30	F	85	0	0	0	0
30	G	45	0	0	0	0
30	H	50	0	0	2	0
30	I	31	0	0	1	0
30	J	32	0	0	1	0
30	K	24	0	0	2	0
30	L	24	0	0	3	0
30	M	23	0	0	3	0
30	N	184	0	0	7	0
30	O	111	0	0	1	0
30	P	96	0	0	2	0
30	Q	59	0	0	3	0
30	R	58	0	0	4	0
30	S	73	0	0	1	0
30	T	35	0	0	1	0
30	U	47	0	0	5	0
30	V	18	0	0	0	0
30	W	18	0	0	0	0
30	X	14	0	0	1	0
30	Y	6	0	0	1	0
30	Z	6	0	0	0	0
All	All	32913	0	32023	381	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (381) 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:P:44:MET:HG3	30:P:495:HOH:O	1.49	1.11
7:G:11:TPO:HA	7:G:11:TPO:O3P	1.51	1.05
1:N:484:THR:HG23	30:N:870:HOH:O	1.58	1.03
23:B:302:PSC:H42	9:I:14:ALA:HB2	1.35	1.01
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.46	0.97
25:P:304:PEK:H71	25:P:304:PEK:H32	1.48	0.95
7:G:72:ASN:H	7:G:76:ASN:HD22	1.14	0.93
26:C:305:CDL:OA5	26:C:305:CDL:H1	1.68	0.91
23:B:302:PSC:H61	23:B:302:PSC:H21	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:608:HEA:HMC1	18:N:608:HEA:HBC1	1.54	0.89
21:A:619:OH:O	30:A:701:HOH:O	1.90	0.88
2:B:56:MET:HA	23:B:302:PSC:H221	1.57	0.87
2:B:52:HIS:ND1	23:B:302:PSC:H31	1.90	0.86
30:B:527:HOH:O	17:C:304:PGV:H041	1.79	0.82
21:N:623:OH:O	30:N:701:HOH:O	1.98	0.81
26:C:310:CDL:H382	30:O:496:HOH:O	1.79	0.81
17:N:622:PGV:H241	17:N:622:PGV:H011	1.63	0.81
23:B:302:PSC:H42	9:I:14:ALA:CB	2.12	0.80
17:N:622:PGV:O02	17:N:622:PGV:H52	1.81	0.79
7:T:1:ALA:O	30:T:1401:HOH:O	2.01	0.77
8:U:10:ASN:HA	30:U:1643:HOH:O	1.84	0.75
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.32	0.75
11:K:54:ARG:NH2	30:K:301:HOH:O	2.20	0.74
7:T:72:ASN:H	7:T:76:ASN:HD22	1.36	0.73
5:R:90:ARG:HD3	30:R:338:HOH:O	1.88	0.72
7:G:11:TPO:HG23	7:G:14:ARG:H	1.53	0.72
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.69	0.72
18:N:607:HEA:HMC1	18:N:607:HEA:HBC1	1.71	0.72
25:P:304:PEK:HN2	7:T:76:ASN:HD21	1.38	0.72
6:S:75:HIS:H	6:S:80:GLN:HE22	1.34	0.71
9:V:2:THR:N	29:V:101:SAC:HG	1.88	0.71
4:D:78:TRP:N	20:D:201:TGL:HB32	2.05	0.71
2:O:217:LYS:H	2:O:217:LYS:CE	2.03	0.70
17:N:622:PGV:C1	17:N:622:PGV:C5	2.70	0.70
7:G:5:LYS:CD	1:N:278:MET:HB3	2.21	0.69
19:B:311:EDO:O1	30:B:401:HOH:O	2.09	0.69
7:G:72:ASN:H	7:G:76:ASN:ND2	1.89	0.69
20:N:618:TGL:HG2	20:N:618:TGL:HC22	1.74	0.68
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.23	0.68
25:P:305:PEK:H382	26:P:312:CDL:C25	2.24	0.67
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.93	0.67
19:N:615:EDO:H11	30:N:776:HOH:O	1.96	0.66
7:T:11:TPO:HG23	7:T:14:ARG:H	1.59	0.66
18:A:605:HEA:HBC1	18:A:605:HEA:HMC1	1.78	0.66
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.78	0.65
25:P:305:PEK:C38	26:P:312:CDL:H271	2.26	0.65
1:A:298:ASP:HB3	30:A:830:HOH:O	1.97	0.65
18:A:606:HEA:HBC1	18:A:606:HEA:HMC1	1.79	0.64
1:N:488:THR:HB	1:N:495:LEU:HD13	1.78	0.64
5:R:90:ARG:CD	30:R:338:HOH:O	2.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:201:PSC:H32	30:R:353:HOH:O	1.97	0.64
30:A:702:HOH:O	20:D:201:TGL:HG11	1.97	0.63
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.63
3:C:161:GLN:HE22	25:C:302:PEK:H031	1.63	0.63
2:B:1:FME:HE3	2:B:133:LEU:HD11	1.79	0.63
1:N:113:LEU:HB2	20:N:605:TGL:H323	1.81	0.63
17:A:604:PGV:H343	25:G:102:PEK:H371	1.81	0.62
2:O:56:MET:HA	23:R:201:PSC:H221	1.79	0.62
30:B:522:HOH:O	8:H:61:LYS:HE3	1.98	0.62
30:L:622:HOH:O	13:M:32:TRP:HH2	1.80	0.62
2:O:217:LYS:H	2:O:217:LYS:HE2	1.63	0.62
12:L:46:LYS:O	12:L:47:LYS:HD2	2.00	0.61
9:V:25:PHE:HD2	9:V:26:MET:HE2	1.64	0.61
17:N:622:PGV:H241	17:N:622:PGV:C01	2.29	0.61
7:G:10:GLY:HA2	1:N:177:SER:HB2	1.82	0.61
17:N:622:PGV:O02	17:N:622:PGV:C5	2.49	0.61
4:D:78:TRP:HA	20:D:201:TGL:HB52	1.82	0.61
25:P:305:PEK:H382	26:P:312:CDL:H251	1.84	0.60
19:B:305:EDO:O2	30:B:402:HOH:O	2.15	0.60
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.02	0.60
11:K:54:ARG:HG3	11:K:54:ARG:NH1	2.17	0.60
4:D:77:GLU:HB3	20:D:201:TGL:HB31	1.84	0.59
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.01	0.59
6:S:85:CYS:SG	6:S:87:THR:HG23	2.43	0.58
7:G:3:ALA:O	7:G:4:ALA:HB2	2.04	0.58
1:A:194:LEU:CD2	7:T:4:ALA:HB1	2.33	0.58
4:D:78:TRP:H	20:D:201:TGL:HB32	1.67	0.58
20:L:502:TGL:HC82	20:L:502:TGL:H363	1.85	0.58
7:G:8:HIS:HB2	1:N:179:TYR:OH	2.04	0.58
8:H:46:LYS:NZ	30:H:201:HOH:O	2.36	0.58
17:N:622:PGV:C1	17:N:622:PGV:C6	2.81	0.58
30:A:735:HOH:O	3:C:77:LYS:HE3	2.03	0.57
17:N:622:PGV:O12	17:N:622:PGV:H02	2.04	0.57
8:U:54:GLU:OE2	8:U:57:ARG:NH2	2.33	0.57
19:N:612:EDO:H12	30:N:743:HOH:O	2.04	0.57
2:B:1:FME:HE1	2:B:133:LEU:HD13	1.85	0.57
17:N:622:PGV:H52	17:N:622:PGV:C1	2.34	0.57
1:A:297:MET:CG	1:A:302:ARG:HG3	2.34	0.57
2:B:52:HIS:ND1	23:B:302:PSC:C3	2.66	0.57
4:Q:6:VAL:HG12	4:Q:6:VAL:O	2.05	0.57
8:U:24:ASN:HD21	19:U:1501:EDO:C1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:309:THR:HG22	18:N:607:HEA:HMB2	1.88	0.56
25:P:304:PEK:H71	25:P:304:PEK:C3	2.30	0.56
20:N:618:TGL:HB42	4:Q:78:TRP:HA	1.88	0.56
30:A:891:HOH:O	20:D:201:TGL:HC82	2.05	0.56
12:L:28:PHE:CD1	20:L:502:TGL:HA32	2.39	0.56
1:A:87:ILE:O	1:A:173:PRO:HD3	2.06	0.56
2:B:87:MET:HE2	30:B:404:HOH:O	2.06	0.56
1:A:336:PRO:HB2	1:A:394:VAL:HG11	1.86	0.56
20:N:618:TGL:HB22	30:Q:1742:HOH:O	2.06	0.55
20:N:605:TGL:HC42	12:Y:20:ARG:HH12	1.72	0.55
2:O:217:LYS:H	2:O:217:LYS:HE3	1.71	0.55
23:R:201:PSC:C1	23:R:201:PSC:H232	2.36	0.55
17:N:622:PGV:H011	17:N:622:PGV:C24	2.35	0.55
4:Q:5:VAL:O	4:Q:7:LYS:N	2.40	0.55
18:N:608:HEA:HHC	18:N:608:HEA:H122	1.88	0.55
9:V:25:PHE:HD2	9:V:26:MET:CE	2.19	0.55
7:G:35:SER:O	7:G:39:SER:HB3	2.06	0.54
9:V:25:PHE:CD2	9:V:26:MET:CE	2.90	0.54
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.37	0.54
19:A:614:EDO:H21	2:B:58:ALA:HB3	1.87	0.54
7:G:8:HIS:ND1	7:G:8:HIS:N	2.55	0.54
10:J:57:HIS:HA	30:J:228:HOH:O	2.06	0.54
17:C:304:PGV:H72	17:C:304:PGV:H22	1.89	0.54
23:R:201:PSC:C08	9:V:10:ARG:HH21	2.21	0.54
8:U:54:GLU:HA	8:U:54:GLU:OE1	2.07	0.54
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.54
1:A:309:THR:HG22	18:A:605:HEA:HMB2	1.89	0.54
1:N:449:MET:SD	2:O:5:MET:HG2	2.48	0.54
7:G:4:ALA:CB	1:N:285:PHE:CE2	2.91	0.54
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.90	0.54
19:C:312:EDO:H22	10:J:50:LEU:HB2	1.90	0.53
2:B:1:FME:CE	2:B:133:LEU:CD1	2.86	0.53
7:T:11:TPO:O1P	7:T:11:TPO:HA	2.07	0.53
1:N:512:ASN:C	1:N:512:ASN:HD22	2.10	0.53
30:A:735:HOH:O	3:C:77:LYS:CE	2.54	0.53
8:U:24:ASN:HD21	19:U:1501:EDO:H11	1.74	0.53
2:O:141:ARG:H	9:V:70:GLN:NE2	2.06	0.53
24:C:301:CHD:H212	24:C:301:CHD:H183	1.90	0.53
6:F:64:GLU:O	6:F:65:ASP:HB2	2.09	0.53
1:N:136:LEU:HD12	30:N:852:HOH:O	2.09	0.52
25:P:305:PEK:H383	26:P:312:CDL:H271	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.90	0.52
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.44	0.52
17:N:622:PGV:H151	4:Q:84:ALA:HB2	1.90	0.52
6:F:95:GLN:N	6:F:95:GLN:HE21	2.07	0.52
12:Y:41:ARG:HH12	24:Y:101:CHD:C18	2.22	0.52
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.91	0.52
1:N:113:LEU:HD13	20:N:605:TGL:H311	1.92	0.52
7:G:11:TPO:O3P	7:G:11:TPO:CA	2.43	0.52
1:N:24:ALA:HB2	18:N:608:HEA:H253	1.90	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.51
17:C:304:PGV:C18	7:T:1:ALA:HB2	2.41	0.51
17:C:304:PGV:H262	7:T:1:ALA:N	2.25	0.51
17:A:604:PGV:H343	25:G:102:PEK:C37	2.39	0.51
9:I:2:THR:OG1	29:I:101:SAC:H2A1	2.10	0.51
8:H:7:LYS:O	8:H:7:LYS:HD3	2.11	0.51
2:B:1:FME:HE1	2:B:133:LEU:CD1	2.41	0.51
1:N:302:ARG:NH1	30:N:706:HOH:O	2.44	0.51
17:N:622:PGV:C01	17:N:622:PGV:C24	2.88	0.51
8:U:10:ASN:CA	30:U:1643:HOH:O	2.52	0.51
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.91	0.51
23:B:302:PSC:H42	9:I:14:ALA:CA	2.41	0.51
25:P:304:PEK:H101	25:P:304:PEK:H31	1.93	0.51
4:D:19:ARG:HD3	4:D:21:ASP:OD1	2.10	0.50
1:N:383:MET:O	1:N:387:PHE:HB2	2.12	0.50
4:D:23:PRO:HB3	5:E:70:VAL:CG2	2.42	0.50
19:N:612:EDO:C1	30:N:743:HOH:O	2.58	0.50
6:S:92:VAL:O	6:S:92:VAL:HG23	2.11	0.50
3:P:246:ASP:HB2	30:P:484:HOH:O	2.11	0.50
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.75	0.50
9:I:36:LYS:NZ	30:I:203:HOH:O	2.45	0.50
18:N:607:HEA:HMC1	18:N:607:HEA:CBC	2.41	0.50
1:A:472:ILE:HG21	20:L:502:TGL:H202	1.92	0.50
1:A:406:ASN:HD21	17:M:101:PGV:H71	1.76	0.50
2:O:227:LEU:C	2:O:227:LEU:HD12	2.32	0.50
4:D:4:SER:HA	30:D:363:HOH:O	2.12	0.50
23:R:201:PSC:H011	23:R:201:PSC:H211	1.94	0.49
2:B:1:FME:CE	2:B:133:LEU:HD11	2.42	0.49
1:N:76:GLY:O	1:N:80:ASN:HB2	2.12	0.49
13:M:42:LYS:O	13:M:43:SER:HB2	2.12	0.49
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.95	0.49
1:A:417:MET:CE	18:A:606:HEA:H263	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:54:ARG:HG3	11:K:54:ARG:HH11	1.77	0.49
1:A:281:GLY:C	7:T:4:ALA:HB3	2.33	0.49
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.46	0.49
4:D:77:GLU:HB3	20:D:201:TGL:CB3	2.43	0.49
25:G:102:PEK:C12	25:G:102:PEK:H162	2.43	0.49
4:Q:5:VAL:HG13	4:Q:10:ASP:OD1	2.13	0.49
8:U:42:ALA:O	8:U:46:LYS:HB2	2.12	0.49
11:X:12:LYS:HB3	11:X:13:TYR:CD2	2.47	0.49
2:O:33:LEU:O	2:O:37:LEU:HD23	2.12	0.49
1:A:297:MET:SD	1:A:302:ARG:HG2	2.53	0.48
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.11	0.48
2:O:41:ILE:O	2:O:45:MET:HG2	2.13	0.48
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.96	0.48
1:N:309:THR:CG2	18:N:607:HEA:HMB2	2.44	0.48
1:A:177:SER:H	1:A:180:GLN:HE21	1.62	0.48
7:G:5:LYS:HG2	1:N:278:MET:O	2.13	0.48
9:I:2:THR:N	29:I:101:SAC:H	2.11	0.48
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
11:K:8:ASP:HB2	30:K:309:HOH:O	2.14	0.48
10:W:32:TYR:CZ	10:W:36:MET:HG3	2.48	0.48
3:C:161:GLN:NE2	25:C:302:PEK:H031	2.29	0.48
17:M:101:PGV:H062	30:M:219:HOH:O	2.13	0.48
1:A:179:TYR:OH	7:T:8:HIS:HB3	2.14	0.48
3:P:258:TRP:CD1	26:P:312:CDL:H781	2.49	0.48
7:G:4:ALA:CB	1:N:285:PHE:CD2	2.96	0.47
2:O:141:ARG:H	9:V:70:GLN:HE22	1.60	0.47
4:Q:92:THR:O	4:Q:95:LEU:HB2	2.13	0.47
12:Y:41:ARG:NH1	30:Y:201:HOH:O	2.41	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.15	0.47
4:D:78:TRP:CA	20:D:201:TGL:HB52	2.45	0.47
3:P:95:THR:HG21	17:P:307:PGV:H302	1.97	0.47
26:P:308:CDL:OA5	26:P:308:CDL:H1	2.14	0.47
7:T:15:THR:HG21	24:T:1302:CHD:H213	1.95	0.47
8:U:40:GLU:OE2	30:U:1601:HOH:O	2.20	0.47
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.96	0.47
3:P:40:MET:O	3:P:44:MET:HG2	2.14	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE2	2.50	0.46
8:U:8:ILE:O	8:U:8:ILE:CG2	2.62	0.46
17:M:101:PGV:H042	30:M:219:HOH:O	2.16	0.46
26:P:312:CDL:H872	26:P:312:CDL:H811	1.97	0.46
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:THR:HG22	25:C:302:PEK:H132	1.98	0.46
13:Z:28:LEU:HD23	27:Z:101:DMU:C18	2.45	0.46
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.79	0.46
26:P:312:CDL:OB7	26:P:312:CDL:CB6	2.62	0.46
9:V:50:PHE:O	19:V:103:EDO:H21	2.16	0.46
1:A:118:VAL:HG11	1:A:141:ALA:HB3	1.97	0.46
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.99	0.46
4:Q:98:TRP:CE2	27:Z:101:DMU:H11	2.51	0.46
4:D:29:HIS:HD2	4:D:61:ARG:O	1.99	0.46
7:G:4:ALA:HB1	1:N:194:LEU:CD2	2.45	0.45
9:V:2:THR:N	29:V:101:SAC:OG	2.48	0.45
13:Z:28:LEU:HD23	27:Z:101:DMU:H7	1.99	0.45
1:A:379:TYR:O	1:A:383:MET:HB2	2.17	0.45
20:D:201:TGL:HG11	20:D:201:TGL:HB42	1.98	0.45
2:O:60:GLU:HG2	2:O:61:VAL:N	2.30	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.45
24:W:302:CHD:H17	24:W:302:CHD:H232	1.81	0.45
4:D:23:PRO:CB	5:E:70:VAL:HG21	2.47	0.45
1:N:321:PHE:HB3	2:O:65:TRP:CE2	2.51	0.45
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.15	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
3:P:67:PHE:CE2	26:P:308:CDL:HB22	2.51	0.45
1:A:112:LEU:O	1:A:115:SER:HB3	2.16	0.45
19:S:106:EDO:H22	30:S:264:HOH:O	2.16	0.45
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.99	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.45
10:J:54:SER:O	12:L:46:LYS:HE2	2.16	0.45
4:D:147:LYS:CE	4:D:147:LYS:HA	2.47	0.45
30:L:622:HOH:O	13:M:32:TRP:CH2	2.56	0.45
17:N:622:PGV:O02	17:N:622:PGV:H61	2.16	0.45
1:A:411:LYS:NZ	30:A:702:HOH:O	2.48	0.45
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.99	0.44
3:C:210:ILE:HG21	17:C:303:PGV:H282	1.98	0.44
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.44
2:O:199:ILE:HG23	2:O:199:ILE:O	2.18	0.44
1:A:297:MET:HG3	1:A:302:ARG:HG3	1.98	0.44
24:J:101:CHD:H12	24:J:101:CHD:H212	1.98	0.44
19:A:615:EDO:H21	6:F:70:ILE:HD12	1.99	0.44
1:A:289:ALA:HB1	1:A:297:MET:HE1	2.00	0.44
20:N:618:TGL:HG31	20:N:618:TGL:CC3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:200:CYS:SG	2:B:204:HIS:HA	2.58	0.44
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.44
7:T:9:GLY:HA2	24:T:1302:CHD:C11	2.48	0.44
1:A:489:THR:HA	6:F:71:TRP:O	2.18	0.44
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.52	0.44
12:Y:41:ARG:HH12	24:Y:101:CHD:H182	1.81	0.44
1:A:194:LEU:HD21	7:T:4:ALA:HB1	2.00	0.44
8:U:41:LYS:O	8:U:42:ALA:C	2.56	0.44
8:H:69:VAL:HG11	19:H:101:EDO:C1	2.48	0.44
3:P:59:ARG:HA	26:P:308:CDL:H512	1.98	0.44
4:Q:109:HIS:HD2	30:Q:1737:HOH:O	2.00	0.44
8:U:24:ASN:HD21	19:U:1501:EDO:H12	1.82	0.44
20:D:201:TGL:HG32	20:D:201:TGL:HC52	1.99	0.43
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.91	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.53	0.43
17:N:622:PGV:H212	13:Z:10:THR:H	1.83	0.43
8:U:10:ASN:CB	30:U:1643:HOH:O	2.65	0.43
19:A:618:EDO:H12	13:M:41:LYS:HG3	2.00	0.43
2:B:115:ASP:HB2	30:H:223:HOH:O	2.18	0.43
1:N:52:GLN:O	1:N:56:VAL:HG23	2.18	0.43
1:N:498:CYS:H	4:Q:7:LYS:HE2	1.82	0.43
19:A:618:EDO:C1	13:M:41:LYS:HG3	2.48	0.43
3:C:76:GLN:O	3:C:80:ARG:HG3	2.17	0.43
3:C:246:ASP:HB2	30:C:483:HOH:O	2.18	0.43
20:N:605:TGL:HC42	12:Y:24:MET:SD	2.57	0.43
26:P:312:CDL:HB32	26:P:312:CDL:H151	1.99	0.43
11:X:12:LYS:NZ	30:X:101:HOH:O	2.50	0.43
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.07	0.43
2:O:115:ASP:OD1	8:U:61:LYS:HE3	2.19	0.43
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.43
3:P:54:MET:HB3	3:P:58:TRP:CZ3	2.54	0.43
17:M:101:PGV:C04	30:M:219:HOH:O	2.67	0.43
19:N:611:EDO:O2	4:Q:7:LYS:NZ	2.50	0.43
12:Y:45:LEU:HD13	24:Y:101:CHD:H5	2.00	0.43
12:L:24:MET:HG3	30:L:619:HOH:O	2.19	0.43
1:A:62:ALA:HB2	18:A:606:HEA:HBD1	2.01	0.43
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.43
1:N:112:LEU:HD23	1:N:112:LEU:C	2.39	0.43
7:T:9:GLY:HA2	24:T:1302:CHD:H112	2.00	0.43
8:U:37:HIS:HE1	30:U:1608:HOH:O	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:HIS:CD2	1:A:240:HIS:C	2.93	0.43
24:B:303:CHD:H12	24:B:303:CHD:H212	2.01	0.43
25:P:305:PEK:H02	25:P:305:PEK:H6	2.01	0.43
25:G:102:PEK:C12	25:G:102:PEK:C16	2.97	0.42
26:P:312:CDL:O1	26:P:312:CDL:H873	2.18	0.42
1:N:240:HIS:CD2	1:N:240:HIS:C	2.91	0.42
30:B:522:HOH:O	8:H:61:LYS:CE	2.62	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.93	0.42
10:W:32:TYR:CE1	10:W:36:MET:HG3	2.54	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.55	0.42
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.19	0.42
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.01	0.42
17:N:622:PGV:C1	17:N:622:PGV:H61	2.50	0.42
4:Q:12:ALA:O	6:S:75:HIS:NE2	2.51	0.42
1:A:488:THR:HB	1:A:495:LEU:HD13	2.02	0.42
17:N:622:PGV:O02	17:N:622:PGV:C6	2.68	0.42
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.20	0.42
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.00	0.42
1:A:309:THR:CG2	18:A:605:HEA:HMB2	2.50	0.42
1:A:449:MET:SD	2:B:5:MET:HG2	2.60	0.42
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.55	0.42
26:P:312:CDL:OB7	26:P:312:CDL:HB62	2.20	0.42
7:T:8:HIS:O	24:T:1302:CHD:H212	2.20	0.41
17:C:304:PGV:H72	17:C:304:PGV:C2	2.48	0.41
20:N:618:TGL:HB31	30:Q:1742:HOH:O	2.19	0.41
17:A:604:PGV:H183	25:G:102:PEK:H341	2.01	0.41
3:C:59:ARG:HA	26:C:305:CDL:H512	2.02	0.41
4:D:48:TRP:O	4:D:51:LEU:HB2	2.20	0.41
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.90	0.41
26:C:310:CDL:H671	26:C:310:CDL:HA31	2.01	0.41
9:I:36:LYS:HD3	9:I:36:LYS:HA	1.90	0.41
2:O:61:VAL:HG23	23:R:201:PSC:C8	2.51	0.41
25:P:301:PEK:H5	25:P:301:PEK:H241	2.03	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
2:B:91:ASN:HB2	2:B:149:THR:HG21	2.03	0.41
24:J:101:CHD:H213	24:J:101:CHD:H232	1.98	0.41
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.20	0.41
1:A:148:PHE:HB3	3:C:28:THR:HB	2.02	0.41
1:A:243:VAL:HB	18:A:605:HEA:C3C	2.50	0.41
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.95	0.41
3:C:248:VAL:HG22	25:C:314:PEK:H8	2.02	0.41
1:A:13:LYS:HD3	19:A:612:EDO:H22	2.01	0.41
17:C:304:PGV:H172	7:T:1:ALA:HB2	2.03	0.41
7:G:8:HIS:HB3	1:N:186:TRP:HH2	1.86	0.41
17:M:101:PGV:C4	17:M:101:PGV:H02	2.51	0.41
17:N:622:PGV:C18	17:N:622:PGV:H343	2.49	0.41
1:A:1:FME:HE3	1:A:4:ASN:HD22	1.85	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
24:P:303:CHD:H212	24:P:303:CHD:H12	2.01	0.41
10:W:58:LYS:HE3	10:W:58:LYS:N	2.36	0.41
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.55	0.41
17:A:604:PGV:C34	25:G:102:PEK:C37	2.99	0.41
18:N:608:HEA:H211	18:N:608:HEA:H271	1.88	0.41
2:O:65:TRP:O	2:O:69:PRO:HG2	2.21	0.41
2:O:75:LEU:HD12	2:O:75:LEU:HA	1.94	0.41
5:R:90:ARG:HD2	30:R:338:HOH:O	2.16	0.41
8:U:60:TYR:CD1	8:U:60:TYR:C	2.94	0.41
1:A:137:ALA:O	19:A:611:EDO:H21	2.21	0.41
20:N:605:TGL:CC4	12:Y:24:MET:SD	3.09	0.41
5:R:20:ASN:HD21	19:R:203:EDO:H12	1.86	0.41
3:P:186:PHE:HA	3:P:190:ASP:OD2	2.21	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.04	0.40
1:A:426:PHE:N	1:A:427:PRO:CD	2.84	0.40
23:B:302:PSC:H222	23:B:302:PSC:H012	2.03	0.40
17:M:101:PGV:O11	17:M:101:PGV:H31	2.21	0.40
1:N:113:LEU:HB2	20:N:605:TGL:C32	2.50	0.40
7:T:6:GLY:O	7:T:8:HIS:N	2.55	0.40
29:V:101:SAC:HA	29:V:101:SAC:H2A1	1.75	0.40
12:Y:45:LEU:CD1	24:Y:101:CHD:H7	2.51	0.40
13:Z:28:LEU:HA	27:Z:101:DMU:H7	2.03	0.40
4:D:109:HIS:HD2	30:D:340:HOH:O	2.03	0.40
1:N:148:PHE:HB3	3:P:28:THR:HB	2.02	0.40
1:N:378:HIS:CG	1:N:425:PHE:CE1	3.10	0.40
6:S:51:SER:O	6:S:93:PRO:HA	2.22	0.40
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.04	0.40
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.40
9:I:29:LEU:HD12	9:I:29:LEU:HA	1.85	0.40
3:P:16:TRP:N	3:P:17:PRO:CD	2.85	0.40
3:P:223:LEU:HD23	3:P:223:LEU:HA	1.89	0.40
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:6:GLY:O	7:T:7:ASP:C	2.60	0.40
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.56	0.40
2:O:224:ALA:O	2:O:227:LEU:HG	2.22	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%)	499 (98%)	12 (2%)	1 (0%)	47	38
2	B	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
2	O	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	4 (3%)	4 (3%)	5	1
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
7	G	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	13	4
7	T	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	3	0
8	H	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	12	4
8	U	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	3	0
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	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	3502/3614 (97%)	3393 (97%)	96 (3%)	13 (0%)	34	24

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
4	Q	6	VAL
4	Q	7	LYS
7	T	7	ASP
8	U	8	ILE
8	U	46	LYS
7	T	4	ALA
4	Q	34	SER
8	H	48	GLY
7	T	5	LYS
8	U	43	MET
1	N	384	GLY
4	Q	5	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	419 (98%)	7 (2%)	62	60
1	N	426/426 (100%)	419 (98%)	7 (2%)	62	60
2	B	210/210 (100%)	202 (96%)	8 (4%)	33	24
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	9
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	55
3	P	224/226 (99%)	220 (98%)	4 (2%)	59	55
4	D	128/129 (99%)	125 (98%)	3 (2%)	50	45
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	32
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	47
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	19
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	15
6	S	81/81 (100%)	77 (95%)	4 (5%)	25	15
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	3
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2
8	H	71/75 (95%)	68 (96%)	3 (4%)	30	20
8	U	71/75 (95%)	62 (87%)	9 (13%)	4	1
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	7
9	V	57/57 (100%)	53 (93%)	4 (7%)	15	7
10	J	49/50 (98%)	47 (96%)	2 (4%)	30	21
10	W	49/50 (98%)	47 (96%)	2 (4%)	30	21
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	39
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	35 (90%)	4 (10%)	7	2
13	M	37/38 (97%)	35 (95%)	2 (5%)	22	13
13	Z	37/38 (97%)	35 (95%)	2 (5%)	22	13
All	All	3040/3082 (99%)	2929 (96%)	111 (4%)	34	25

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	136	LEU
1	A	180	GLN
1	A	189	MET
1	A	297	MET
1	A	369	ASP
2	B	33	LEU
2	B	37	LEU
2	B	59	GLN
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
4	D	147	LYS
5	E	46	LYS
5	E	104	LEU
6	F	48	LEU
6	F	83	PRO
6	F	95	GLN
6	F	96	LEU
7	G	8	HIS
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
9	I	2	THR
9	I	15	ARG
9	I	29	LEU
9	I	37	PHE
10	J	50	LEU
10	J	58	LYS

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Mol	Chain	Res	Type
12	L	20	ARG
13	M	34	LEU
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	117	MET
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	512	ASN
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	61	VAL
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	171	LYS
2	O	217	LYS
2	O	225	SER
3	P	3	HIS
3	P	127	LEU
3	P	159	MET
3	P	230	ASN
4	Q	5	VAL
4	Q	7	LYS
4	Q	9	GLU
4	Q	53	ILE
5	R	14	ARG
5	R	80	GLU
5	R	108	LYS
5	R	109	VAL
6	S	43	LYS
6	S	48	LEU
6	S	54	ASN
6	S	80	GLN
7	T	8	HIS
7	T	18	PHE
7	T	38	HIS

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Mol	Chain	Res	Type
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
7	T	78	LEU
8	U	7	LYS
8	U	9	LYS
8	U	10	ASN
8	U	29	CYS
8	U	40	GLU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	2	THR
9	V	18	ARG
9	V	29	LEU
9	V	36	LYS
10	W	50	LEU
10	W	58	LYS
11	X	12	LYS
12	Y	2	HIS
12	Y	27	LEU
12	Y	46	LYS
12	Y	47	LYS
13	Z	34	LEU
13	Z	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
2	B	10	GLN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	101	HIS

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Mol	Chain	Res	Type
4	D	109	HIS
5	E	94	ASN
6	F	95	GLN
7	G	76	ASN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	232	GLN
1	N	512	ASN
2	O	10	GLN
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
4	Q	37	GLN
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
8	U	10	ASN
9	V	70	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	O	1	2	8,9,10	0.82	1 (12%)	7,9,11	1.25	1 (14%)
7	TPO	G	11	7	8,10,11	1.50	1 (12%)	10,14,16	1.03	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	0.41	0	7,9,11	0.97	0
2	FME	B	1	2	8,9,10	0.67	0	7,9,11	1.16	0
1	FME	A	1	1	8,9,10	0.52	0	7,9,11	0.94	0
7	TPO	T	11	7	8,10,11	1.52	1 (12%)	10,14,16	1.19	1 (10%)

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	O	1	2	-	0/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	4/7/9/11	-
1	FME	A	1	1	-	0/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	3.81	1.66	1.59
7	G	11	TPO	P-OG1	3.62	1.66	1.59
2	O	1	FME	CG-SD	-2.11	1.70	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	P-OG1-CB	2.83	131.76	123.21
2	O	1	FME	CG-CB-CA	-2.44	106.18	112.95
7	G	11	TPO	O-C-CA	-2.26	118.87	124.78

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FME	C-CA-CB-CG
2	B	1	FME	CA-CB-CG-SD
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1

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Mol	Chain	Res	Type	Atoms
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	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
2	B	1	FME	CB-CG-SD-CE
1	N	1	FME	CB-CG-SD-CE
2	B	1	FME	N-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	3	0
2	B	1	FME	5	0
1	A	1	FME	1	0
7	T	11	TPO	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - 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	A	612	-	3,3,3	0.28	0	2,2,2	0.21	0
19	EDO	V	104	-	3,3,3	0.57	0	2,2,2	0.83	0
19	EDO	B	308	-	3,3,3	0.29	0	2,2,2	0.20	0
17	PGV	N	606	-	50,50,50	0.50	0	53,56,56	0.68	1 (1%)
26	CDL	C	310	-	99,99,99	0.38	0	105,111,111	0.43	0
26	CDL	P	312	-	99,99,99	0.35	0	105,111,111	0.41	0
19	EDO	S	106	-	3,3,3	0.20	0	2,2,2	0.31	0
19	EDO	A	615	-	3,3,3	0.10	0	2,2,2	0.21	0
19	EDO	D	203	-	3,3,3	0.12	0	2,2,2	0.05	0
19	EDO	P	311	-	3,3,3	0.09	0	2,2,2	0.24	0
19	EDO	R	202	-	3,3,3	0.16	0	2,2,2	0.14	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.37	0
24	CHD	C	306	-	32,32,32	0.60	0	51,51,51	0.75	1 (1%)
29	SAC	V	101	-	7,8,9	0.53	0	8,9,11	1.38	1 (12%)
27	DMU	G	104	-	34,34,34	1.70	7 (20%)	45,45,45	1.77	15 (33%)
19	EDO	S	105	-	3,3,3	0.16	0	2,2,2	0.20	0
19	EDO	S	103	-	3,3,3	0.39	0	2,2,2	0.37	0
18	HEA	N	608	1	57,67,67	2.10	15 (26%)	61,103,103	2.48	25 (40%)
24	CHD	B	303	-	32,32,32	0.56	0	51,51,51	0.90	2 (3%)
19	EDO	W	303	-	3,3,3	0.10	0	2,2,2	0.17	0
19	EDO	R	203	-	3,3,3	0.01	0	2,2,2	0.10	0
18	HEA	N	607	1	57,67,67	1.85	15 (26%)	61,103,103	2.35	20 (32%)
24	CHD	Y	101	-	32,32,32	0.69	0	51,51,51	1.22	6 (11%)
19	EDO	N	617	-	3,3,3	0.23	0	2,2,2	0.34	0
19	EDO	C	309	-	3,3,3	0.12	0	2,2,2	0.28	0
19	EDO	N	613	-	3,3,3	0.21	0	2,2,2	0.09	0
19	EDO	B	306	-	3,3,3	0.35	0	2,2,2	0.28	0
29	SAC	I	101	-	7,8,9	0.62	0	8,9,11	0.89	0
19	EDO	G	103	-	3,3,3	0.39	0	2,2,2	0.57	0
19	EDO	M	103	-	3,3,3	0.11	0	2,2,2	0.33	0
19	EDO	S	104	-	3,3,3	0.22	0	2,2,2	0.15	0
20	TGL	N	618	-	62,62,62	0.31	0	65,65,65	0.39	0
19	EDO	A	616	-	3,3,3	0.12	0	2,2,2	0.47	0
19	EDO	I	102	-	3,3,3	0.07	0	2,2,2	0.11	0
20	TGL	N	605	-	62,62,62	0.37	0	65,65,65	0.49	1 (1%)
20	TGL	L	502	-	62,62,62	0.40	0	65,65,65	0.38	0
19	EDO	N	612	-	3,3,3	0.38	0	2,2,2	0.70	0
19	EDO	V	103	-	3,3,3	0.10	0	2,2,2	0.18	0
19	EDO	E	205	-	3,3,3	0.04	0	2,2,2	0.42	0
25	PEK	P	304	-	52,52,52	0.41	0	55,57,57	0.91	5 (9%)
19	EDO	A	607	-	3,3,3	0.40	0	2,2,2	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PGV	P	306	-	50,50,50	0.49	0	53,56,56	0.55	1 (1%)
19	EDO	P	314	-	3,3,3	0.05	0	2,2,2	0.25	0
19	EDO	Q	1604	-	3,3,3	0.30	0	2,2,2	0.43	0
17	PGV	N	622	-	50,50,50	0.44	0	53,56,56	0.53	0
19	EDO	N	614	-	3,3,3	0.13	0	2,2,2	0.47	0
19	EDO	D	202	-	3,3,3	0.17	0	2,2,2	0.21	0
24	CHD	C	301	-	32,32,32	0.68	0	51,51,51	0.82	1 (1%)
19	EDO	H	101	-	3,3,3	0.39	0	2,2,2	0.16	0
19	EDO	N	620	-	3,3,3	0.27	0	2,2,2	0.29	0
24	CHD	P	303	-	32,32,32	0.65	1 (3%)	51,51,51	0.70	0
19	EDO	A	610	-	3,3,3	0.11	0	2,2,2	0.08	0
19	EDO	B	310	-	3,3,3	0.08	0	2,2,2	0.18	0
19	EDO	A	611	-	3,3,3	0.35	0	2,2,2	0.31	0
23	PSC	R	201	-	51,51,51	0.39	0	57,59,59	0.50	0
19	EDO	L	501	-	3,3,3	0.16	0	2,2,2	0.15	0
17	PGV	A	604	-	50,50,50	0.57	0	53,56,56	0.70	1 (1%)
19	EDO	A	618	-	3,3,3	0.28	0	2,2,2	0.52	0
25	PEK	P	305	-	52,52,52	0.41	0	55,57,57	0.48	0
19	EDO	B	311	-	3,3,3	0.08	0	2,2,2	0.20	0
19	EDO	A	609	-	3,3,3	0.36	0	2,2,2	0.20	0
19	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.10	0
19	EDO	J	102	-	3,3,3	0.15	0	2,2,2	0.20	0
19	EDO	B	309	-	3,3,3	0.15	0	2,2,2	0.34	0
19	EDO	G	105	-	3,3,3	0.09	0	2,2,2	0.24	0
19	EDO	A	614	-	3,3,3	0.04	0	2,2,2	0.18	0
19	EDO	S	102	-	3,3,3	0.48	0	2,2,2	0.35	0
19	EDO	J	103	-	3,3,3	0.42	0	2,2,2	0.20	0
27	DMU	C	311	-	34,34,34	1.89	8 (23%)	45,45,45	2.16	12 (26%)
27	DMU	G	101	-	34,34,34	2.13	7 (20%)	45,45,45	2.00	11 (24%)
17	PGV	P	307	-	50,50,50	0.34	0	53,56,56	0.43	0
27	DMU	M	102	-	34,34,34	1.62	5 (14%)	45,45,45	1.69	9 (20%)
19	EDO	O	302	-	3,3,3	0.03	0	2,2,2	0.23	0
19	EDO	D	204	-	3,3,3	0.21	0	2,2,2	0.17	0
19	EDO	I	103	-	3,3,3	0.46	0	2,2,2	0.28	0
19	EDO	V	102	-	3,3,3	0.12	0	2,2,2	0.38	0
19	EDO	S	107	-	3,3,3	0.09	0	2,2,2	0.72	0
24	CHD	W	302	-	32,32,32	0.58	0	51,51,51	0.70	1 (1%)
19	EDO	G	108	-	3,3,3	0.07	0	2,2,2	0.23	0
23	PSC	B	302	-	51,51,51	0.50	0	57,59,59	0.58	0
19	EDO	F	702	-	3,3,3	0.27	0	2,2,2	0.10	0
19	EDO	D	205	-	3,3,3	0.10	0	2,2,2	0.31	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	0.31	0	2,2,2	0.40	0
19	EDO	B	307	-	3,3,3	0.27	0	2,2,2	0.29	0
25	PEK	C	302	-	52,52,52	0.43	0	55,57,57	0.55	1 (1%)
19	EDO	C	312	-	3,3,3	0.67	0	2,2,2	0.92	0
19	EDO	P	313	-	3,3,3	0.57	0	2,2,2	0.50	0
27	DMU	P	302	-	34,34,34	0.91	3 (8%)	45,45,45	1.65	8 (17%)
22	CUA	O	301	2	0,1,1	-	-	-	-	-
17	PGV	C	303	-	50,50,50	0.42	0	53,56,56	0.54	0
20	TGL	A	613	-	62,62,62	0.43	0	65,65,65	0.79	1 (1%)
19	EDO	E	203	-	3,3,3	0.15	0	2,2,2	0.08	0
19	EDO	W	301	-	3,3,3	0.09	0	2,2,2	0.04	0
26	CDL	C	305	-	99,99,99	0.38	0	105,111,111	0.69	4 (3%)
19	EDO	F	706	-	3,3,3	0.32	0	2,2,2	0.19	0
19	EDO	T	1301	-	3,3,3	0.36	0	2,2,2	0.18	0
19	EDO	F	707	-	3,3,3	0.13	0	2,2,2	0.13	0
19	EDO	L	504	-	3,3,3	0.12	0	2,2,2	0.23	0
24	CHD	P	309	-	32,32,32	0.65	0	51,51,51	1.09	3 (5%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
19	EDO	C	313	-	3,3,3	0.35	0	2,2,2	0.09	0
19	EDO	T	1303	-	3,3,3	0.31	0	2,2,2	0.15	0
19	EDO	N	611	-	3,3,3	0.23	0	2,2,2	0.31	0
19	EDO	Q	1603	-	3,3,3	0.15	0	2,2,2	0.23	0
19	EDO	F	704	-	3,3,3	0.10	0	2,2,2	0.27	0
19	EDO	B	304	-	3,3,3	0.27	0	2,2,2	0.32	0
19	EDO	F	701	-	3,3,3	0.23	0	2,2,2	0.52	0
19	EDO	P	310	-	3,3,3	0.07	0	2,2,2	0.19	0
27	DMU	Z	101	-	34,34,34	0.99	2 (5%)	45,45,45	1.46	9 (20%)
17	PGV	M	101	-	50,50,50	0.48	0	53,56,56	0.79	2 (3%)
19	EDO	C	307	-	3,3,3	0.46	0	2,2,2	0.39	0
19	EDO	E	204	-	3,3,3	0.10	0	2,2,2	0.07	0
26	CDL	P	308	-	99,99,99	0.37	0	105,111,111	0.49	1 (0%)
19	EDO	A	608	-	3,3,3	0.34	0	2,2,2	0.07	0
18	HEA	A	606	1	57,67,67	1.74	10 (17%)	61,103,103	2.68	27 (44%)
25	PEK	P	301	-	52,52,52	0.36	0	55,57,57	0.60	1 (1%)
19	EDO	N	609	-	3,3,3	0.15	0	2,2,2	0.51	0
19	EDO	Q	1601	-	3,3,3	0.11	0	2,2,2	0.07	0
24	CHD	G	107	-	32,32,32	0.64	0	51,51,51	0.75	0
19	EDO	E	202	-	3,3,3	0.18	0	2,2,2	0.35	0
17	PGV	C	304	-	50,50,50	0.50	0	53,56,56	0.65	0
19	EDO	N	619	-	3,3,3	0.12	0	2,2,2	0.12	0
19	EDO	C	308	-	3,3,3	0.13	0	2,2,2	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	O	303	-	3,3,3	0.39	0	2,2,2	0.05	0
19	EDO	N	616	-	3,3,3	0.16	0	2,2,2	0.31	0
25	PEK	C	314	-	52,52,52	0.41	0	55,57,57	0.59	0
19	EDO	A	617	-	3,3,3	0.30	0	2,2,2	0.58	0
19	EDO	E	201	-	3,3,3	0.08	0	2,2,2	0.11	0
19	EDO	N	621	-	3,3,3	0.31	0	2,2,2	0.52	0
24	CHD	J	101	-	32,32,32	0.62	1 (3%)	51,51,51	0.96	2 (3%)
25	PEK	G	102	-	52,52,52	0.47	0	55,57,57	0.66	0
19	EDO	K	201	-	3,3,3	0.10	0	2,2,2	0.15	0
18	HEA	A	605	1	57,67,67	1.64	10 (17%)	61,103,103	2.38	25 (40%)
19	EDO	F	705	-	3,3,3	0.35	0	2,2,2	0.36	0
19	EDO	N	615	-	3,3,3	0.63	0	2,2,2	0.66	0
19	EDO	N	610	-	3,3,3	0.43	0	2,2,2	0.09	0
19	EDO	Q	1602	-	3,3,3	0.17	0	2,2,2	0.21	0
19	EDO	L	503	-	3,3,3	0.09	0	2,2,2	0.10	0
20	TGL	N	604	-	62,62,62	0.34	0	65,65,65	0.59	1 (1%)
24	CHD	T	1302	-	32,32,32	0.63	0	51,51,51	0.99	1 (1%)
19	EDO	G	106	-	3,3,3	0.23	0	2,2,2	0.29	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	A	612	-	-	0/1/1/1	-
19	EDO	V	104	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
17	PGV	N	606	-	-	9/55/55/55	-
26	CDL	C	310	-	-	53/110/110/110	-
26	CDL	P	312	-	-	53/110/110/110	-
19	EDO	S	106	-	-	1/1/1/1	-
19	EDO	A	615	-	-	0/1/1/1	-
19	EDO	D	203	-	-	0/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
19	EDO	R	202	-	-	0/1/1/1	-
20	TGL	D	201	-	-	30/65/65/65	-
24	CHD	C	306	-	-	2/9/74/74	0/4/4/4
29	SAC	V	101	-	-	2/7/8/10	-
27	DMU	G	104	-	-	11/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	S	105	-	-	1/1/1/1	-
19	EDO	S	103	-	-	1/1/1/1	-
18	HEA	N	608	1	3/3/7/16	4/32/76/76	-
24	CHD	B	303	-	-	2/9/74/74	0/4/4/4
19	EDO	W	303	-	-	1/1/1/1	-
19	EDO	R	203	-	-	1/1/1/1	-
18	HEA	N	607	1	3/3/7/16	4/32/76/76	-
24	CHD	Y	101	-	-	9/9/74/74	1/4/4/4
19	EDO	N	617	-	-	1/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
19	EDO	N	613	-	-	0/1/1/1	-
19	EDO	B	306	-	-	0/1/1/1	-
29	SAC	I	101	-	-	5/7/8/10	-
19	EDO	G	103	-	-	0/1/1/1	-
19	EDO	M	103	-	-	1/1/1/1	-
19	EDO	S	104	-	-	0/1/1/1	-
20	TGL	N	618	-	-	38/65/65/65	-
19	EDO	A	616	-	-	1/1/1/1	-
19	EDO	I	102	-	-	1/1/1/1	-
20	TGL	N	605	-	-	34/65/65/65	-
20	TGL	L	502	-	-	39/65/65/65	-
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	V	103	-	-	1/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
25	PEK	P	304	-	-	19/56/56/56	-
19	EDO	A	607	-	-	0/1/1/1	-
17	PGV	P	306	-	-	15/55/55/55	-
19	EDO	P	314	-	-	0/1/1/1	-
19	EDO	Q	1604	-	-	1/1/1/1	-
17	PGV	N	622	-	-	25/55/55/55	-
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	D	202	-	-	1/1/1/1	-
24	CHD	C	301	-	-	1/9/74/74	0/4/4/4
19	EDO	H	101	-	-	1/1/1/1	-
19	EDO	N	620	-	-	1/1/1/1	-
24	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	A	610	-	-	1/1/1/1	-
19	EDO	B	310	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSC	R	201	-	-	35/55/55/55	-
19	EDO	L	501	-	-	1/1/1/1	-
17	PGV	A	604	-	-	14/55/55/55	-
19	EDO	A	618	-	-	0/1/1/1	-
25	PEK	P	305	-	-	30/56/56/56	-
19	EDO	B	311	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	J	102	-	-	0/1/1/1	-
19	EDO	B	309	-	-	1/1/1/1	-
19	EDO	G	105	-	-	1/1/1/1	-
19	EDO	A	614	-	-	0/1/1/1	-
19	EDO	S	102	-	-	1/1/1/1	-
19	EDO	J	103	-	-	0/1/1/1	-
27	DMU	C	311	-	-	7/19/59/59	0/2/2/2
27	DMU	G	101	-	-	14/19/59/59	0/2/2/2
17	PGV	P	307	-	-	30/55/55/55	-
27	DMU	M	102	-	-	7/19/59/59	0/2/2/2
19	EDO	O	302	-	-	1/1/1/1	-
19	EDO	D	204	-	-	0/1/1/1	-
19	EDO	I	103	-	-	0/1/1/1	-
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	S	107	-	-	0/1/1/1	-
24	CHD	W	302	-	-	1/9/74/74	0/4/4/4
19	EDO	G	108	-	-	1/1/1/1	-
23	PSC	B	302	-	-	28/55/55/55	-
19	EDO	F	702	-	-	1/1/1/1	-
19	EDO	D	205	-	-	0/1/1/1	-
19	EDO	U	1501	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
25	PEK	C	302	-	-	28/56/56/56	-
19	EDO	C	312	-	-	0/1/1/1	-
19	EDO	P	313	-	-	0/1/1/1	-
27	DMU	P	302	-	-	9/19/59/59	0/2/2/2
17	PGV	C	303	-	-	15/55/55/55	-
20	TGL	A	613	-	-	37/65/65/65	-
19	EDO	E	203	-	-	1/1/1/1	-
19	EDO	W	301	-	-	0/1/1/1	-
26	CDL	C	305	-	-	66/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	F	706	-	-	0/1/1/1	-
19	EDO	T	1301	-	-	1/1/1/1	-
19	EDO	F	707	-	-	0/1/1/1	-
19	EDO	L	504	-	-	0/1/1/1	-
24	CHD	P	309	-	-	2/9/74/74	0/4/4/4
19	EDO	C	313	-	-	1/1/1/1	-
19	EDO	T	1303	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	Q	1603	-	-	1/1/1/1	-
19	EDO	F	704	-	-	0/1/1/1	-
19	EDO	B	304	-	-	0/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-
19	EDO	P	310	-	-	1/1/1/1	-
27	DMU	Z	101	-	-	8/19/59/59	0/2/2/2
17	PGV	M	101	-	-	40/55/55/55	-
19	EDO	C	307	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
26	CDL	P	308	-	-	58/110/110/110	-
19	EDO	A	608	-	-	0/1/1/1	-
18	HEA	A	606	1	2/2/7/16	1/32/76/76	-
25	PEK	P	301	-	-	34/56/56/56	-
19	EDO	N	609	-	-	1/1/1/1	-
19	EDO	Q	1601	-	-	1/1/1/1	-
24	CHD	G	107	-	-	3/9/74/74	0/4/4/4
19	EDO	E	202	-	-	1/1/1/1	-
17	PGV	C	304	-	-	29/55/55/55	-
19	EDO	N	619	-	-	1/1/1/1	-
19	EDO	C	308	-	-	0/1/1/1	-
19	EDO	O	303	-	-	0/1/1/1	-
19	EDO	N	616	-	-	1/1/1/1	-
25	PEK	C	314	-	-	30/56/56/56	-
19	EDO	A	617	-	-	0/1/1/1	-
19	EDO	E	201	-	-	1/1/1/1	-
19	EDO	N	621	-	-	1/1/1/1	-
24	CHD	J	101	-	-	3/9/74/74	0/4/4/4
25	PEK	G	102	-	-	21/56/56/56	-
19	EDO	K	201	-	-	1/1/1/1	-
18	HEA	A	605	1	3/3/7/16	4/32/76/76	-
19	EDO	F	705	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	N	615	-	-	0/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	Q	1602	-	-	0/1/1/1	-
19	EDO	L	503	-	-	1/1/1/1	-
20	TGL	N	604	-	-	29/65/65/65	-
24	CHD	T	1302	-	-	6/9/74/74	1/4/4/4
19	EDO	G	106	-	-	1/1/1/1	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	101	DMU	O16-C6	8.88	1.55	1.40
27	C	311	DMU	O16-C6	6.77	1.51	1.40
27	M	102	DMU	O16-C6	6.43	1.51	1.40
18	N	608	HEA	C1D-ND	-5.43	1.31	1.40
18	N	608	HEA	C3C-C2C	4.90	1.47	1.40
18	N	608	HEA	C3A-C2A	4.90	1.47	1.40
27	G	104	DMU	O16-C6	4.83	1.48	1.40
18	N	608	HEA	C4B-NB	-4.81	1.32	1.40
18	A	605	HEA	C3B-C2B	4.51	1.44	1.34
18	A	606	HEA	C3D-C2D	4.46	1.46	1.36
18	N	608	HEA	C3B-C2B	4.45	1.44	1.34
18	N	607	HEA	CHD-C1D	4.37	1.46	1.35
18	A	605	HEA	C3D-C2D	4.36	1.46	1.36
18	A	606	HEA	C1D-ND	-4.31	1.32	1.40
18	N	607	HEA	C3B-C2B	4.25	1.44	1.34
18	N	607	HEA	C1D-ND	-4.22	1.33	1.40
18	A	606	HEA	C3C-C2C	4.18	1.46	1.40
18	N	607	HEA	C3A-C2A	4.15	1.46	1.40
27	C	311	DMU	O7-C10	4.07	1.53	1.41
18	N	607	HEA	C4B-NB	-4.02	1.33	1.40
18	N	608	HEA	C3D-C2D	3.89	1.45	1.36
18	A	605	HEA	CHD-C1D	3.83	1.44	1.35
18	N	608	HEA	C4B-C3B	3.74	1.50	1.44
27	G	104	DMU	O1-C10	3.60	1.51	1.41
18	A	606	HEA	CHD-C1D	3.59	1.44	1.35
18	A	606	HEA	C3B-C2B	3.57	1.42	1.34
18	N	608	HEA	CHD-C1D	3.53	1.44	1.35
18	N	608	HEA	C1B-NB	-3.51	1.31	1.38
27	C	311	DMU	C3-C4	3.45	1.62	1.52
18	N	607	HEA	CHC-C4B	3.42	1.43	1.35
18	A	605	HEA	C1D-ND	-3.42	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	606	HEA	C3A-C2A	3.40	1.45	1.40
18	A	605	HEA	CHC-C4B	3.33	1.43	1.35
18	A	605	HEA	C3C-C2C	3.29	1.44	1.40
18	A	606	HEA	CHC-C4B	3.24	1.43	1.35
18	N	608	HEA	FE-ND	3.19	2.12	1.96
18	N	608	HEA	C4D-ND	-3.17	1.32	1.38
27	G	104	DMU	C2-C1	3.16	1.60	1.52
18	A	606	HEA	C4B-NB	-3.08	1.35	1.40
27	C	311	DMU	O1-C10	3.00	1.49	1.41
18	A	605	HEA	C3A-C2A	3.00	1.44	1.40
18	A	606	HEA	C1B-NB	-2.98	1.32	1.38
27	G	104	DMU	C2-C3	2.98	1.60	1.52
18	N	607	HEA	C1B-NB	-2.97	1.32	1.38
27	M	102	DMU	C6-C1	-2.97	1.43	1.52
18	N	607	HEA	C1D-C2D	2.95	1.50	1.44
18	N	608	HEA	CHC-C4B	2.94	1.42	1.35
27	M	102	DMU	O1-C9	2.91	1.51	1.44
27	G	104	DMU	O1-C9	2.90	1.51	1.44
27	G	104	DMU	O5-C6	2.88	1.49	1.41
18	N	607	HEA	C4D-C3D	2.83	1.49	1.45
27	Z	101	DMU	O1-C10	2.82	1.49	1.41
18	A	605	HEA	C1B-NB	-2.81	1.33	1.38
27	G	101	DMU	C2-C1	2.79	1.59	1.52
18	A	606	HEA	C4C-NC	-2.66	1.30	1.36
27	C	311	DMU	O5-C4	2.66	1.50	1.44
18	A	605	HEA	C4B-C3B	2.63	1.49	1.44
27	C	311	DMU	O1-C9	2.62	1.50	1.44
27	Z	101	DMU	O1-C9	2.62	1.50	1.44
27	G	101	DMU	O7-C10	2.58	1.49	1.41
27	G	101	DMU	C7-C5	2.56	1.58	1.52
27	P	302	DMU	O55-C2	2.50	1.48	1.43
18	N	607	HEA	FE-ND	2.44	2.08	1.96
27	P	302	DMU	O1-C10	2.42	1.48	1.41
18	N	607	HEA	FE-NB	2.42	2.08	1.96
27	C	311	DMU	O5-C6	2.40	1.47	1.41
27	M	102	DMU	O5-C6	2.39	1.47	1.41
27	G	101	DMU	O5-C6	2.37	1.47	1.41
18	N	608	HEA	FE-NB	2.37	2.08	1.96
24	J	101	CHD	O26-C24	-2.35	1.22	1.30
27	G	101	DMU	C8-C7	2.34	1.58	1.52
18	N	607	HEA	C4B-C3B	2.34	1.48	1.44
27	G	104	DMU	O7-C10	2.26	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	P	302	DMU	O16-C6	2.21	1.44	1.40
18	N	608	HEA	C1B-C2B	2.20	1.48	1.44
18	N	607	HEA	C4D-ND	-2.19	1.34	1.38
24	P	303	CHD	O26-C24	-2.18	1.23	1.30
18	N	608	HEA	C4C-CHD	2.15	1.47	1.41
18	N	607	HEA	C3D-C2D	2.14	1.41	1.36
27	M	102	DMU	O7-C10	2.08	1.47	1.41
18	A	605	HEA	CHB-C1B	2.07	1.47	1.41
18	N	607	HEA	C18-C19	2.05	1.37	1.33
27	C	311	DMU	O7-C3	2.04	1.49	1.43
27	G	101	DMU	O3-C5	2.04	1.47	1.43

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	311	DMU	C18-O16-C6	8.17	127.38	113.84
27	G	101	DMU	C18-O16-C6	7.56	126.37	113.84
18	A	606	HEA	C3D-C4D-ND	7.45	117.58	110.36
18	N	607	HEA	CAD-CBD-CGD	-6.92	98.70	113.60
27	P	302	DMU	C6-O5-C4	6.21	125.87	113.69
18	N	608	HEA	C3D-C4D-ND	6.16	116.33	110.36
27	M	102	DMU	C18-O16-C6	-6.11	103.71	113.84
18	A	605	HEA	C2D-C1D-ND	5.94	116.88	109.84
18	N	607	HEA	C2D-C1D-ND	5.90	116.83	109.84
18	N	608	HEA	C3B-C4B-NB	5.75	116.65	109.84
18	N	608	HEA	C2B-C1B-NB	5.51	116.48	109.88
18	N	608	HEA	C13-C12-C11	-5.48	106.11	114.35
27	C	311	DMU	O1-C9-C11	5.40	119.86	106.44
18	A	605	HEA	C2B-C1B-NB	5.39	116.34	109.88
18	A	606	HEA	C2D-C1D-ND	5.36	116.20	109.84
18	A	605	HEA	C3D-C4D-ND	5.30	115.49	110.36
18	N	607	HEA	C2B-C1B-NB	5.23	116.14	109.88
20	A	613	TGL	OG2-CB1-CB2	5.11	122.51	111.50
18	A	606	HEA	C2B-C1B-NB	5.08	115.97	109.88
18	A	606	HEA	C3B-C4B-NB	5.03	115.80	109.84
18	A	605	HEA	C1D-C2D-C3D	-5.03	101.67	106.96
18	N	607	HEA	C1D-C2D-C3D	-5.00	101.70	106.96
18	A	606	HEA	CHA-C4D-C3D	-4.85	117.71	124.84
18	A	606	HEA	C13-C12-C11	-4.84	107.07	114.35
18	N	607	HEA	C3D-C4D-ND	4.80	115.01	110.36
18	N	608	HEA	C4A-CHB-C1B	4.77	128.85	122.56
18	A	605	HEA	C3B-C4B-NB	4.75	115.47	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	606	HEA	C4A-CHB-C1B	4.66	128.71	122.56
27	C	311	DMU	O5-C6-O16	4.63	120.93	109.97
27	M	102	DMU	O16-C6-C1	4.54	115.39	108.30
18	N	607	HEA	C3B-C4B-NB	4.40	115.05	109.84
18	A	606	HEA	C1D-C2D-C3D	-4.35	102.38	106.96
18	N	608	HEA	C2D-C1D-ND	4.22	114.84	109.84
18	A	605	HEA	CMB-C2B-C1B	4.07	131.23	125.04
18	N	608	HEA	C3C-C4C-NC	4.01	114.40	109.21
18	A	605	HEA	CMD-C2D-C1D	4.00	131.13	125.04
27	G	101	DMU	C8-C7-C5	3.99	117.79	110.82
18	N	608	HEA	C4D-C3D-C2D	-3.99	101.08	106.90
18	N	608	HEA	CAA-CBA-CGA	-3.96	102.66	113.76
18	N	608	HEA	CHB-C1B-C2B	-3.92	118.86	124.98
18	N	607	HEA	C1B-C2B-C3B	-3.90	102.14	106.80
27	G	104	DMU	C1-C2-C3	3.90	118.58	109.68
17	M	101	PGV	O01-C1-C2	3.89	119.89	111.50
18	N	607	HEA	C3C-C4C-NC	3.88	114.22	109.21
20	N	604	TGL	OG2-CB1-CB2	3.87	119.84	111.50
18	N	608	HEA	C4B-C3B-C2B	-3.85	100.83	107.41
18	A	606	HEA	C3C-C4C-NC	3.75	114.06	109.21
18	A	606	HEA	CMC-C2C-C3C	3.69	131.58	124.68
18	A	605	HEA	C3C-C4C-NC	3.68	113.96	109.21
27	G	101	DMU	O16-C6-C1	3.64	113.98	108.30
24	P	309	CHD	C1-C2-C3	3.60	115.09	110.47
27	Z	101	DMU	C18-O16-C6	3.60	119.80	113.84
27	G	104	DMU	O5-C6-O16	3.59	118.48	109.97
27	G	101	DMU	C1-C2-C3	3.56	117.81	109.68
27	G	101	DMU	C6-C1-C2	3.55	117.39	110.00
18	A	605	HEA	CAD-CBD-CGD	-3.54	105.98	113.60
27	G	104	DMU	O1-C9-C11	3.49	115.12	106.44
27	M	102	DMU	C28-C25-C22	-3.49	96.70	114.42
18	A	606	HEA	C1D-ND-C4D	-3.46	101.50	105.07
18	A	605	HEA	CHA-C4D-C3D	-3.45	119.76	124.84
27	G	104	DMU	C10-O1-C9	3.42	120.41	113.69
18	A	605	HEA	C4B-C3B-C2B	-3.38	101.63	107.41
18	A	606	HEA	CHC-C4B-NB	-3.37	120.22	124.38
18	A	606	HEA	C4D-C3D-C2D	-3.34	102.03	106.90
29	V	101	SAC	O-C-CA	-3.31	116.10	124.78
18	N	607	HEA	CHB-C1B-C2B	-3.26	119.89	124.98
18	N	608	HEA	C1B-C2B-C3B	-3.25	102.91	106.80
27	G	101	DMU	O5-C6-O16	3.25	117.67	109.97
18	N	608	HEA	C1D-C2D-C3D	-3.20	103.60	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	606	HEA	CAA-CBA-CGA	-3.19	104.81	113.76
18	A	606	HEA	C4B-C3B-C2B	-3.19	101.96	107.41
27	G	101	DMU	C7-C8-C9	3.17	115.90	110.24
18	N	607	HEA	CHA-C4D-C3D	-3.11	120.26	124.84
18	A	606	HEA	C27-C19-C20	3.08	120.45	115.27
27	Z	101	DMU	C10-O1-C9	3.08	119.72	113.69
18	A	605	HEA	CMB-C2B-C3B	-3.06	124.50	130.34
18	A	606	HEA	C21-C20-C19	2.99	122.80	112.98
24	Y	101	CHD	C13-C14-C8	2.96	118.52	114.74
27	C	311	DMU	O5-C4-C3	2.94	115.94	109.75
18	N	607	HEA	C4D-CHA-C1A	2.93	126.43	122.56
26	C	305	CDL	OA6-CA5-C11	2.93	117.81	111.50
18	A	605	HEA	CMC-C2C-C3C	2.92	130.15	124.68
18	A	605	HEA	CAD-C3D-C4D	2.92	129.75	124.66
18	N	607	HEA	C4A-CHB-C1B	2.91	126.39	122.56
20	N	605	TGL	OG2-CB1-CB2	2.88	117.70	111.50
24	C	301	CHD	C6-C7-C8	2.87	114.55	111.48
26	C	305	CDL	OB2-PB2-OB3	2.87	120.29	109.07
25	P	304	PEK	O11-P-O14	-2.83	98.00	109.07
18	A	605	HEA	CHD-C1D-C2D	-2.79	119.01	126.72
18	A	605	HEA	C1D-ND-C4D	-2.78	102.20	105.07
18	A	606	HEA	CMD-C2D-C1D	2.77	129.26	125.04
18	A	606	HEA	C25-C23-C22	-2.76	114.67	122.65
18	A	606	HEA	CAD-C3D-C4D	2.74	129.45	124.66
27	C	311	DMU	C11-C9-C8	-2.73	106.60	113.00
25	P	304	PEK	O01-C1-C2	-2.71	105.67	111.50
27	Z	101	DMU	O1-C9-C11	2.70	113.14	106.44
18	A	606	HEA	CMB-C2B-C1B	2.69	129.13	125.04
18	N	608	HEA	O2D-CGD-O1D	-2.68	116.63	123.30
17	N	606	PGV	O12-P-O13	2.67	119.49	109.07
18	N	607	HEA	C1D-ND-C4D	-2.66	102.32	105.07
18	A	605	HEA	CHB-C1B-C2B	-2.64	120.85	124.98
18	A	606	HEA	C4B-NB-C1B	-2.64	102.35	105.07
18	N	608	HEA	CAD-CBD-CGD	-2.64	107.93	113.60
27	G	104	DMU	O7-C10-O1	2.63	118.03	110.67
18	N	607	HEA	CMD-C2D-C1D	2.62	129.02	125.04
27	P	302	DMU	C7-C8-C9	-2.60	105.60	110.24
27	C	311	DMU	O7-C10-O1	2.60	117.93	110.67
24	Y	101	CHD	C18-C13-C14	2.59	115.27	111.21
24	B	303	CHD	C17-C13-C14	2.57	102.69	100.09
18	A	605	HEA	C4D-CHA-C1A	2.56	125.94	122.56
24	Y	101	CHD	C17-C13-C14	-2.56	97.51	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	607	HEA	C4B-C3B-C2B	-2.56	103.03	107.41
18	A	606	HEA	CHD-C1D-C2D	-2.56	119.64	126.72
27	P	302	DMU	C37-C34-C31	-2.56	101.44	114.42
18	N	608	HEA	C27-C19-C20	2.55	119.56	115.27
24	Y	101	CHD	C17-C13-C12	2.53	119.97	117.67
18	N	607	HEA	CMB-C2B-C1B	2.52	128.88	125.04
24	J	101	CHD	C5-C4-C3	2.51	116.45	112.76
27	G	104	DMU	O49-C1-C6	-2.51	103.95	110.05
18	A	605	HEA	C4B-NB-C1B	-2.51	102.48	105.07
27	G	104	DMU	C31-C28-C25	-2.51	101.70	114.42
27	Z	101	DMU	C6-O5-C4	-2.49	108.80	113.69
25	P	304	PEK	O02-C1-C2	2.46	133.34	123.73
18	N	608	HEA	CHC-C4B-NB	-2.45	121.36	124.38
27	G	101	DMU	O5-C4-C57	2.45	112.52	106.44
27	C	311	DMU	C6-O5-C4	2.44	118.48	113.69
18	A	606	HEA	C1B-C2B-C3B	-2.44	103.88	106.80
27	M	102	DMU	C10-O1-C9	2.44	118.48	113.69
27	C	311	DMU	C25-C22-C19	-2.44	102.04	114.42
18	N	608	HEA	CHA-C4D-C3D	-2.42	121.28	124.84
24	T	1302	CHD	C17-C13-C14	2.41	102.52	100.09
24	P	309	CHD	C2-C1-C10	2.38	116.87	112.78
27	P	302	DMU	O1-C9-C11	2.37	112.34	106.44
27	Z	101	DMU	C11-C9-C8	-2.36	107.47	113.00
24	Y	101	CHD	C18-C13-C12	-2.35	106.67	109.07
18	N	607	HEA	C13-C12-C11	-2.34	110.84	114.35
18	A	605	HEA	C4D-C3D-C2D	-2.34	103.49	106.90
27	Z	101	DMU	O5-C6-O16	-2.32	104.47	109.97
18	A	605	HEA	C1B-C2B-C3B	-2.32	104.03	106.80
18	N	607	HEA	C20-C19-C18	-2.32	116.42	121.12
27	M	102	DMU	O49-C1-C6	-2.32	104.41	110.05
25	P	301	PEK	O01-C1-C2	2.32	116.49	111.50
27	Z	101	DMU	C34-C31-C28	-2.31	102.70	114.42
24	B	303	CHD	C16-C17-C13	-2.29	101.31	103.55
18	A	605	HEA	CBA-CAA-C2A	-2.29	108.75	112.60
27	C	311	DMU	C31-C28-C25	-2.28	102.84	114.42
18	N	607	HEA	OMA-CMA-C3A	-2.27	119.97	124.91
17	P	306	PGV	O14-P-O13	2.26	123.42	112.24
27	M	102	DMU	O5-C4-C3	-2.26	104.99	109.75
25	P	304	PEK	O13-P-O14	2.26	123.40	112.24
18	A	606	HEA	CHB-C1B-C2B	-2.23	121.49	124.98
17	M	101	PGV	O01-C1-O02	-2.23	118.32	123.70
27	G	104	DMU	C6-O5-C4	-2.22	109.32	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	G	104	DMU	C25-C22-C19	-2.20	103.27	114.42
27	C	311	DMU	C8-C7-C5	-2.19	107.00	110.82
27	G	104	DMU	O16-C18-C19	-2.17	101.97	109.56
27	G	104	DMU	C10-C5-C7	2.16	114.50	110.00
18	N	608	HEA	CAD-C3D-C4D	2.16	128.43	124.66
27	P	302	DMU	C8-C7-C5	-2.16	107.05	110.82
27	C	311	DMU	C6-C1-C2	-2.15	105.52	110.00
27	P	302	DMU	O55-C2-C3	2.15	115.64	109.94
27	P	302	DMU	O4-C7-C8	2.14	115.31	110.35
18	A	605	HEA	CAA-CBA-CGA	-2.14	107.75	113.76
27	M	102	DMU	C34-C31-C28	-2.14	103.57	114.42
18	A	605	HEA	C13-C12-C11	-2.13	111.14	114.35
27	C	311	DMU	O5-C6-C1	-2.13	105.84	110.35
26	C	305	CDL	OB6-CB5-C51	2.13	116.09	111.50
24	C	306	CHD	C18-C13-C14	2.13	114.54	111.21
25	C	302	PEK	O01-C1-C2	2.12	116.08	111.50
18	N	607	HEA	CHD-C1D-C2D	-2.12	120.87	126.72
18	A	606	HEA	O2D-CGD-CBD	2.11	120.81	114.03
26	C	305	CDL	OB4-PB2-OB2	-2.11	97.95	107.75
18	N	608	HEA	O2A-CGA-O1A	-2.11	118.04	123.30
24	Y	101	CHD	C10-C9-C8	2.10	114.08	111.82
18	A	606	HEA	O2D-CGD-O1D	-2.10	118.06	123.30
18	N	608	HEA	CHA-C4D-ND	-2.10	122.15	124.43
27	P	302	DMU	C31-C28-C25	-2.10	103.78	114.42
24	W	302	CHD	C9-C8-C7	2.09	114.38	111.88
27	G	104	DMU	C6-C1-C2	2.09	114.34	110.00
27	Z	101	DMU	C8-C7-C5	-2.08	107.20	110.82
24	P	309	CHD	C18-C13-C12	-2.07	106.96	109.07
25	P	304	PEK	C2-C3-C4	2.07	116.92	113.23
27	G	104	DMU	C37-C34-C31	-2.06	103.97	114.42
27	Z	101	DMU	O16-C6-C1	2.05	111.51	108.30
27	G	101	DMU	C10-C5-C7	2.05	114.27	110.00
27	G	101	DMU	C28-C25-C22	-2.05	104.01	114.42
27	G	104	DMU	O5-C4-C57	2.05	111.53	106.44
27	M	102	DMU	O49-C1-C2	-2.05	105.61	110.35
24	J	101	CHD	C13-C17-C20	-2.05	117.05	119.50
27	G	101	DMU	C31-C28-C25	-2.04	104.06	114.42
27	G	104	DMU	C28-C25-C22	-2.04	104.06	114.42
18	N	608	HEA	C20-C19-C18	-2.04	117.00	121.12
18	N	608	HEA	C13-C14-C15	-2.03	122.77	127.66
27	M	102	DMU	O1-C9-C11	2.03	111.48	106.44
17	A	604	PGV	O03-C19-C20	2.02	118.25	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	308	CDL	OB6-CB5-OB7	-2.02	118.82	123.70
18	N	608	HEA	C21-C22-C23	-2.02	120.85	127.75
18	A	605	HEA	O2A-CGA-CBA	2.02	120.51	114.03
18	N	608	HEA	C4D-CHA-C1A	2.01	125.21	122.56

All (11) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	605	HEA	NA
18	A	605	HEA	NB
18	A	605	HEA	ND
18	A	606	HEA	NB
18	A	606	HEA	ND
18	N	607	HEA	NA
18	N	607	HEA	NB
18	N	607	HEA	ND
18	N	608	HEA	NA
18	N	608	HEA	NB
18	N	608	HEA	ND

All (999) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	304	PGV	C03-O11-P-O12
17	C	304	PGV	C03-O11-P-O14
17	C	304	PGV	C04-O12-P-O13
17	C	304	PGV	C04-O12-P-O14
17	M	101	PGV	O03-C01-C02-O01
17	M	101	PGV	C02-C03-O11-P
17	M	101	PGV	O02-C1-O01-C02
17	M	101	PGV	C2-C1-O01-C02
17	N	622	PGV	C04-O12-P-O13
17	N	622	PGV	C02-C03-O11-P
17	N	622	PGV	O02-C1-O01-C02
17	N	622	PGV	C2-C1-O01-C02
17	P	307	PGV	C03-O11-P-O13
17	P	307	PGV	C04-O12-P-O13
17	P	307	PGV	C04-C05-C06-O06
18	A	606	HEA	C19-C20-C21-C22
18	N	608	HEA	C12-C11-C3B-C2B
20	D	201	TGL	CB2-CB1-OG2-CG2
20	D	201	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
20	L	502	TGL	CB2-CB1-OG2-CG2
20	N	605	TGL	OB1-CB1-OG2-CG2
20	N	618	TGL	CC2-CC1-OG3-CG3
20	N	618	TGL	OC1-CC1-OG3-CG3
23	B	302	PSC	C03-O11-P-O13
23	B	302	PSC	C04-O12-P-O11
23	B	302	PSC	C04-O12-P-O13
23	B	302	PSC	C04-O12-P-O14
23	R	201	PSC	C03-O11-P-O14
23	R	201	PSC	O12-C04-C05-N
25	C	302	PEK	C03-O11-P-O13
25	C	302	PEK	O12-C04-C05-N
25	C	314	PEK	C03-O11-P-O12
25	C	314	PEK	C03-O11-P-O13
25	C	314	PEK	C03-O11-P-O14
25	C	314	PEK	O12-C04-C05-N
25	C	314	PEK	C9-C10-C11-C12
25	G	102	PEK	C6-C7-C8-C9
25	G	102	PEK	C12-C13-C14-C15
25	P	301	PEK	C03-O11-P-O14
25	P	301	PEK	C04-O12-P-O14
25	P	301	PEK	O02-C1-O01-C02
25	P	305	PEK	C03-O11-P-O14
25	P	305	PEK	O02-C1-O01-C02
25	P	305	PEK	C11-C12-C13-C14
26	C	305	CDL	C1-CA2-OA2-PA1
26	C	305	CDL	OA7-CA5-OA6-CA4
26	C	305	CDL	C11-CA5-OA6-CA4
26	C	310	CDL	CA2-OA2-PA1-OA4
26	C	310	CDL	CA3-OA5-PA1-OA3
26	C	310	CDL	C11-CA5-OA6-CA4
26	C	310	CDL	CB2-OB2-PB2-OB5
26	C	310	CDL	CB3-OB5-PB2-OB4
26	P	308	CDL	CB2-C1-CA2-OA2
26	P	308	CDL	C1-CA2-OA2-PA1
26	P	308	CDL	CA3-OA5-PA1-OA4
26	P	312	CDL	CB2-OB2-PB2-OB4
26	P	312	CDL	CB3-OB5-PB2-OB4
26	P	312	CDL	CB6-CB4-OB6-CB5
27	G	101	DMU	C1-C6-O16-C18
27	G	104	DMU	O5-C6-O16-C18
27	M	102	DMU	O5-C6-O16-C18

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Mol	Chain	Res	Type	Atoms
27	Z	101	DMU	C1-C6-O16-C18
27	Z	101	DMU	O5-C6-O16-C18
27	Z	101	DMU	C19-C18-O16-C6
29	I	101	SAC	C2A-C1A-N-CA
29	I	101	SAC	OAC-C1A-N-CA
29	I	101	SAC	O-C-CA-CB
29	I	101	SAC	N-CA-CB-OG
29	I	101	SAC	C-CA-CB-OG
29	V	101	SAC	C2A-C1A-N-CA
29	V	101	SAC	OAC-C1A-N-CA
23	R	201	PSC	O04-C19-O03-C01
23	R	201	PSC	C20-C19-O03-C01
17	N	622	PGV	O04-C19-O03-C01
26	P	308	CDL	OA9-CA7-OA8-CA6
27	G	104	DMU	O1-C10-O7-C3
20	L	502	TGL	OB1-CB1-OG2-CG2
23	B	302	PSC	O02-C1-O01-C02
26	C	310	CDL	OA7-CA5-OA6-CA4
17	N	622	PGV	C20-C19-O03-C01
27	G	104	DMU	O6-C11-C9-O1
20	N	605	TGL	CB2-CB1-OG2-CG2
23	B	302	PSC	C2-C1-O01-C02
25	P	301	PEK	C2-C1-O01-C02
25	P	305	PEK	C2-C1-O01-C02
27	C	311	DMU	C5-C10-O7-C3
24	T	1302	CHD	C21-C20-C22-C23
20	D	201	TGL	OC1-CC1-OG3-CG3
18	N	608	HEA	C27-C19-C20-C21
18	N	608	HEA	C18-C19-C20-C21
20	A	613	TGL	CC2-CC1-OG3-CG3
20	D	201	TGL	CC2-CC1-OG3-CG3
20	N	604	TGL	CC2-CC1-OG3-CG3
23	B	302	PSC	C20-C19-O03-C01
26	P	308	CDL	C31-CA7-OA8-CA6
20	N	604	TGL	OC1-CC1-OG3-CG3
27	C	311	DMU	O1-C10-O7-C3
17	C	304	PGV	O12-C04-C05-O05
26	C	310	CDL	O1-C1-CB2-OB2
26	P	308	CDL	O1-C1-CA2-OA2
26	P	312	CDL	C71-CB7-OB8-CB6
26	P	312	CDL	OB9-CB7-OB8-CB6
26	C	305	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
17	M	101	PGV	C1-C2-C3-C4
27	G	104	DMU	O6-C11-C9-C8
20	D	201	TGL	C14-C29-C30-C31
25	C	302	PEK	C23-C24-C25-C26
26	C	305	CDL	C82-C83-C84-C85
23	B	302	PSC	O04-C19-O03-C01
27	G	104	DMU	O5-C4-C57-O61
27	G	101	DMU	O5-C4-C57-O61
17	M	101	PGV	C05-C04-O12-P
27	G	101	DMU	O6-C11-C9-O1
20	A	613	TGL	OC1-CC1-OG3-CG3
24	T	1302	CHD	C17-C20-C22-C23
24	Y	101	CHD	C17-C20-C22-C23
17	C	304	PGV	O12-C04-C05-C06
17	M	101	PGV	O12-C04-C05-C06
26	C	310	CDL	CA2-C1-CB2-OB2
26	P	312	CDL	OA9-CA7-OA8-CA6
20	A	613	TGL	CA2-CA1-OG1-CG1
20	L	502	TGL	CC2-CC1-OG3-CG3
20	N	605	TGL	CA2-CA1-OG1-CG1
25	P	305	PEK	C22-C21-O03-C01
26	C	310	CDL	C71-CB7-OB8-CB6
26	P	312	CDL	C31-CA7-OA8-CA6
20	A	613	TGL	CA1-CA2-CA3-CA4
27	G	101	DMU	C3-C4-C57-O61
27	G	104	DMU	C3-C4-C57-O61
26	P	312	CDL	O1-C1-CA2-OA2
24	Y	101	CHD	C21-C20-C22-C23
25	C	302	PEK	C1-C2-C3-C4
20	L	502	TGL	C16-C15-CC9-CC8
23	B	302	PSC	C23-C24-C25-C26
27	P	302	DMU	C3-C4-C57-O61
17	N	622	PGV	C1-C2-C3-C4
26	P	312	CDL	CA5-C11-C12-C13
20	N	605	TGL	OA1-CA1-OG1-CG1
20	L	502	TGL	CC2-CC3-CC4-CC5
17	M	101	PGV	C20-C19-O03-C01
17	P	307	PGV	C1-C2-C3-C4
20	N	605	TGL	CA1-CA2-CA3-CA4
20	N	618	TGL	CC1-CC2-CC3-CC4
25	P	301	PEK	C1-C2-C3-C4
26	C	305	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
26	C	310	CDL	CA5-C11-C12-C13
20	D	201	TGL	C16-C17-C18-C19
17	P	307	PGV	O05-C05-C06-O06
17	N	622	PGV	C19-C20-C21-C22
20	N	605	TGL	CC1-CC2-CC3-CC4
26	C	310	CDL	CA7-C31-C32-C33
20	A	613	TGL	CA5-CA6-CA7-CA8
20	N	605	TGL	C20-C21-C22-C23
27	G	101	DMU	O6-C11-C9-C8
23	R	201	PSC	C04-C05-N-C07
20	D	201	TGL	CC1-CC2-CC3-CC4
20	N	618	TGL	CB1-CB2-CB3-CB4
25	G	102	PEK	C1-C2-C3-C4
19	T	1301	EDO	O1-C1-C2-O2
20	L	502	TGL	OC1-CC1-OG3-CG3
25	P	305	PEK	O04-C21-O03-C01
20	N	604	TGL	CB1-CB2-CB3-CB4
20	A	613	TGL	OA1-CA1-OG1-CG1
27	M	102	DMU	O6-C11-C9-O1
17	M	101	PGV	O12-C04-C05-O05
26	C	305	CDL	O1-C1-CA2-OA2
25	C	302	PEK	C22-C21-O03-C01
27	Z	101	DMU	O16-C18-C19-C22
26	C	310	CDL	OB9-CB7-OB8-CB6
27	M	102	DMU	O6-C11-C9-C8
27	P	302	DMU	O16-C18-C19-C22
25	P	301	PEK	C13-C14-C15-C16
27	Z	101	DMU	O6-C11-C9-O1
20	L	502	TGL	C17-C18-C19-C33
17	C	304	PGV	C04-O12-P-O11
17	P	307	PGV	C03-O11-P-O12
23	B	302	PSC	C03-O11-P-O12
23	R	201	PSC	C04-O12-P-O11
25	C	302	PEK	C03-O11-P-O12
25	C	314	PEK	C04-O12-P-O11
25	P	305	PEK	C03-O11-P-O12
26	C	305	CDL	CA3-OA5-PA1-OA2
26	C	310	CDL	CA2-OA2-PA1-OA5
26	C	310	CDL	CB3-OB5-PB2-OB2
26	P	308	CDL	CA3-OA5-PA1-OA2
26	P	308	CDL	CB2-OB2-PB2-OB5
26	P	312	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
26	P	312	CDL	CB3-OB5-PB2-OB2
26	C	305	CDL	CB2-C1-CA2-OA2
26	P	308	CDL	CA2-C1-CB2-OB2
26	C	305	CDL	OB7-CB5-OB6-CB4
24	J	101	CHD	C20-C22-C23-C24
17	C	303	PGV	C12-C13-C14-C15
23	B	302	PSC	C1-C2-C3-C4
17	M	101	PGV	C5-C6-C7-C8
17	N	622	PGV	C14-C15-C16-C17
20	D	201	TGL	C18-C19-C33-C34
20	D	201	TGL	C19-C33-C34-C35
26	C	310	CDL	C38-C39-C40-C41
20	A	613	TGL	CB2-CB1-OG2-CG2
17	M	101	PGV	C2-C3-C4-C5
20	A	613	TGL	C21-C22-C23-C24
20	D	201	TGL	CC4-CC5-CC6-CC7
20	L	502	TGL	CB6-CB7-CB8-CB9
20	L	502	TGL	CC9-C15-C16-C17
20	N	605	TGL	C13-C14-C29-C30
20	N	605	TGL	C24-C25-C26-C27
25	C	302	PEK	C28-C29-C30-C31
25	C	314	PEK	C29-C30-C31-C32
25	G	102	PEK	C24-C25-C26-C27
25	P	301	PEK	C23-C24-C25-C26
26	C	310	CDL	C12-C13-C14-C15
26	C	310	CDL	C73-C74-C75-C76
26	P	308	CDL	C36-C37-C38-C39
26	P	308	CDL	C55-C56-C57-C58
26	P	312	CDL	C33-C34-C35-C36
26	C	305	CDL	C31-CA7-OA8-CA6
17	M	101	PGV	C20-C21-C22-C23
17	N	622	PGV	C3-C4-C5-C6
20	N	605	TGL	C10-C11-C12-C13
20	N	618	TGL	C11-C12-C13-C14
23	R	201	PSC	C3-C4-C5-C6
26	C	305	CDL	C52-C53-C54-C55
26	C	310	CDL	C55-C56-C57-C58
26	P	312	CDL	C80-C81-C82-C83
23	R	201	PSC	C19-C20-C21-C22
20	A	613	TGL	C24-C25-C26-C27
23	B	302	PSC	C20-C21-C22-C23
26	P	312	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
25	C	314	PEK	C7-C8-C9-C10
25	P	304	PEK	C7-C8-C9-C10
25	P	305	PEK	C7-C8-C9-C10
17	A	604	PGV	C5-C6-C7-C8
17	C	303	PGV	C28-C29-C30-C31
17	P	307	PGV	C25-C26-C27-C28
20	A	613	TGL	CA3-CA4-CA5-CA6
20	D	201	TGL	CB4-CB5-CB6-CB7
20	N	605	TGL	CA9-C20-C21-C22
20	N	618	TGL	CB2-CB3-CB4-CB5
25	G	102	PEK	C22-C23-C24-C25
26	C	305	CDL	C37-C38-C39-C40
26	C	305	CDL	C59-C60-C61-C62
26	C	310	CDL	C13-C14-C15-C16
26	P	308	CDL	C56-C57-C58-C59
20	D	201	TGL	CA3-CA4-CA5-CA6
20	N	605	TGL	CC2-CC3-CC4-CC5
20	N	618	TGL	CC9-C15-C16-C17
26	C	310	CDL	C57-C58-C59-C60
17	M	101	PGV	C22-C23-C24-C25
17	M	101	PGV	C25-C26-C27-C28
17	N	606	PGV	C6-C7-C8-C9
17	N	622	PGV	C4-C5-C6-C7
20	D	201	TGL	CA6-CA7-CA8-CA9
20	N	605	TGL	C11-C12-C13-C14
20	N	618	TGL	CA4-CA5-CA6-CA7
25	P	305	PEK	C23-C24-C25-C26
26	C	305	CDL	C23-C24-C25-C26
26	C	305	CDL	C36-C37-C38-C39
27	M	102	DMU	C31-C34-C37-C40
25	C	302	PEK	O04-C21-O03-C01
17	C	304	PGV	C6-C7-C8-C9
20	D	201	TGL	CA9-C20-C21-C22
25	P	301	PEK	C33-C34-C35-C36
26	C	305	CDL	C21-C22-C23-C24
26	P	308	CDL	C61-C62-C63-C64
26	P	312	CDL	C74-C75-C76-C77
27	G	101	DMU	O16-C18-C19-C22
17	A	604	PGV	C6-C7-C8-C9
17	N	606	PGV	C7-C8-C9-C10
17	P	306	PGV	C6-C7-C8-C9
20	D	201	TGL	CC7-CC8-CC9-C15

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Mol	Chain	Res	Type	Atoms
20	L	502	TGL	CA9-C20-C21-C22
20	N	605	TGL	CB7-CB8-CB9-C10
20	N	618	TGL	C24-C25-C26-C27
23	B	302	PSC	C22-C23-C24-C25
26	C	310	CDL	C75-C76-C77-C78
26	P	308	CDL	C43-C44-C45-C46
26	P	308	CDL	C83-C84-C85-C86
24	W	302	CHD	C20-C22-C23-C24
17	M	101	PGV	O04-C19-O03-C01
17	P	306	PGV	C25-C26-C27-C28
20	A	613	TGL	CA4-CA5-CA6-CA7
20	A	613	TGL	C16-C15-CC9-CC8
20	L	502	TGL	C16-C17-C18-C19
26	C	305	CDL	C16-C17-C18-C19
26	P	308	CDL	C39-C40-C41-C42
26	P	308	CDL	C52-C53-C54-C55
26	P	312	CDL	C11-C12-C13-C14
26	P	312	CDL	C43-C44-C45-C46
20	A	613	TGL	OB1-CB1-OG2-CG2
17	P	306	PGV	C7-C8-C9-C10
17	P	307	PGV	C24-C25-C26-C27
20	A	613	TGL	C12-C13-C14-C29
20	A	613	TGL	C18-C19-C33-C34
20	L	502	TGL	CB7-CB8-CB9-C10
20	L	502	TGL	C14-C29-C30-C31
20	N	618	TGL	C16-C17-C18-C19
20	N	618	TGL	C23-C24-C25-C26
26	P	312	CDL	C12-C13-C14-C15
23	R	201	PSC	C1-C2-C3-C4
25	P	305	PEK	C21-C22-C23-C24
17	C	304	PGV	C24-C25-C26-C27
17	M	101	PGV	C27-C28-C29-C30
17	N	606	PGV	C5-C6-C7-C8
20	N	605	TGL	C18-C19-C33-C34
20	N	618	TGL	CB4-CB5-CB6-CB7
20	N	618	TGL	C13-C14-C29-C30
25	P	304	PEK	C24-C25-C26-C27
25	P	305	PEK	C16-C17-C18-C19
26	C	305	CDL	C76-C77-C78-C79
26	C	310	CDL	C78-C79-C80-C81
17	C	304	PGV	C22-C23-C24-C25
17	P	306	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
17	P	307	PGV	C22-C23-C24-C25
20	N	604	TGL	C10-C11-C12-C13
20	N	604	TGL	C22-C23-C24-C25
23	R	201	PSC	C25-C26-C27-C28
26	P	308	CDL	C22-C23-C24-C25
25	G	102	PEK	O12-C04-C05-N
17	C	303	PGV	C27-C28-C29-C30
17	M	101	PGV	C3-C4-C5-C6
17	M	101	PGV	C14-C15-C16-C17
26	P	312	CDL	C22-C23-C24-C25
20	N	604	TGL	C20-C21-C22-C23
20	N	605	TGL	CA3-CA4-CA5-CA6
20	N	605	TGL	CB2-CB3-CB4-CB5
20	N	618	TGL	C20-C21-C22-C23
26	P	312	CDL	C18-C19-C20-C21
26	P	312	CDL	C40-C41-C42-C43
27	G	104	DMU	O16-C18-C19-C22
20	A	613	TGL	C11-C12-C13-C14
27	G	101	DMU	C18-C19-C22-C25
27	M	102	DMU	C18-C19-C22-C25
27	C	311	DMU	C19-C18-O16-C6
17	C	304	PGV	C30-C31-C32-C33
17	M	101	PGV	C6-C7-C8-C9
20	L	502	TGL	CB2-CB3-CB4-CB5
20	N	604	TGL	CA9-C20-C21-C22
20	N	605	TGL	CB9-C10-C11-C12
20	N	618	TGL	CC5-CC6-CC7-CC8
25	P	305	PEK	C30-C31-C32-C33
26	C	305	CDL	C43-C44-C45-C46
26	P	308	CDL	C77-C78-C79-C80
20	A	613	TGL	CC4-CC5-CC6-CC7
20	L	502	TGL	C24-C25-C26-C27
23	B	302	PSC	C4-C5-C6-C7
25	P	305	PEK	C28-C29-C30-C31
27	G	104	DMU	C18-C19-C22-C25
25	C	302	PEK	C13-C14-C15-C16
25	C	314	PEK	C13-C14-C15-C16
25	P	301	PEK	C7-C8-C9-C10
20	N	604	TGL	CA5-CA6-CA7-CA8
25	G	102	PEK	C23-C24-C25-C26
26	C	305	CDL	C22-C23-C24-C25
26	C	305	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
26	P	308	CDL	C78-C79-C80-C81
26	P	308	CDL	CA7-C31-C32-C33
26	P	312	CDL	CA7-C31-C32-C33
23	R	201	PSC	C27-C28-C29-C30
26	C	305	CDL	C41-C42-C43-C44
26	P	312	CDL	C35-C36-C37-C38
25	C	314	PEK	C22-C21-O03-C01
25	P	301	PEK	C22-C21-O03-C01
25	C	314	PEK	C2-C1-O01-C02
20	A	613	TGL	CC7-CC8-CC9-C15
17	C	303	PGV	C24-C25-C26-C27
17	M	101	PGV	C24-C25-C26-C27
17	N	622	PGV	C26-C27-C28-C29
20	N	605	TGL	CB5-CB6-CB7-CB8
26	C	310	CDL	C77-C78-C79-C80
26	P	312	CDL	C60-C61-C62-C63
24	Y	101	CHD	C13-C17-C20-C22
26	C	305	CDL	OA9-CA7-OA8-CA6
17	C	304	PGV	C20-C21-C22-C23
17	M	101	PGV	C23-C24-C25-C26
26	P	308	CDL	C12-C13-C14-C15
26	P	308	CDL	C19-C20-C21-C22
17	A	604	PGV	C30-C31-C32-C33
25	C	302	PEK	C31-C32-C33-C34
20	N	618	TGL	C16-C15-CC9-CC8
20	A	613	TGL	CA9-C20-C21-C22
26	P	312	CDL	C78-C79-C80-C81
20	N	618	TGL	OB1-CB1-OG2-CG2
25	C	314	PEK	O02-C1-O01-C02
20	L	502	TGL	CC6-CC7-CC8-CC9
23	R	201	PSC	C22-C23-C24-C25
25	P	304	PEK	C25-C26-C27-C28
26	C	305	CDL	C61-C62-C63-C64
17	A	604	PGV	C4-C5-C6-C7
20	N	605	TGL	C17-C18-C19-C33
25	G	102	PEK	C31-C32-C33-C34
25	P	301	PEK	C28-C29-C30-C31
26	C	305	CDL	C56-C57-C58-C59
17	A	604	PGV	C19-C20-C21-C22
19	A	610	EDO	O1-C1-C2-O2
19	B	308	EDO	O1-C1-C2-O2
19	B	310	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	B	311	EDO	O1-C1-C2-O2
19	C	313	EDO	O1-C1-C2-O2
19	F	702	EDO	O1-C1-C2-O2
19	G	106	EDO	O1-C1-C2-O2
19	G	108	EDO	O1-C1-C2-O2
19	N	617	EDO	O1-C1-C2-O2
19	N	620	EDO	O1-C1-C2-O2
19	P	310	EDO	O1-C1-C2-O2
19	Q	1604	EDO	O1-C1-C2-O2
19	V	103	EDO	O1-C1-C2-O2
19	W	303	EDO	O1-C1-C2-O2
27	C	311	DMU	O5-C4-C57-O61
17	M	101	PGV	C26-C27-C28-C29
20	L	502	TGL	C18-C19-C33-C34
26	C	310	CDL	C34-C35-C36-C37
20	N	604	TGL	CB3-CB4-CB5-CB6
20	N	604	TGL	C11-C12-C13-C14
20	N	604	TGL	CC7-CC8-CC9-C15
25	C	314	PEK	C27-C28-C29-C30
25	P	305	PEK	C27-C28-C29-C30
26	C	305	CDL	C63-C64-C65-C66
20	A	613	TGL	CB4-CB5-CB6-CB7
26	P	312	CDL	C34-C35-C36-C37
17	P	307	PGV	C4-C5-C6-C7
20	D	201	TGL	C23-C24-C25-C26
20	L	502	TGL	C12-C13-C14-C29
20	N	618	TGL	C17-C18-C19-C33
20	A	613	TGL	C33-C34-C35-C36
17	N	606	PGV	C12-C13-C14-C15
25	C	302	PEK	C2-C3-C4-C5
25	P	301	PEK	C2-C3-C4-C5
17	C	304	PGV	O02-C1-O01-C02
27	G	101	DMU	C31-C34-C37-C40
23	R	201	PSC	C2-C3-C4-C5
26	C	305	CDL	C11-C12-C13-C14
26	C	310	CDL	C52-C53-C54-C55
26	C	305	CDL	CB5-C51-C52-C53
17	N	622	PGV	C21-C22-C23-C24
25	C	302	PEK	C25-C26-C27-C28
25	P	301	PEK	C34-C35-C36-C37
26	C	305	CDL	C81-C82-C83-C84
20	N	618	TGL	CC3-CC4-CC5-CC6

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Mol	Chain	Res	Type	Atoms
27	G	101	DMU	O5-C6-O16-C18
25	P	301	PEK	C25-C26-C27-C28
27	G	101	DMU	C28-C31-C34-C37
20	N	604	TGL	CA1-CA2-CA3-CA4
17	C	304	PGV	C2-C1-O01-C02
20	N	618	TGL	CB2-CB1-OG2-CG2
26	P	308	CDL	C51-CB5-OB6-CB4
27	G	104	DMU	C1-C6-O16-C18
20	N	604	TGL	CB4-CB5-CB6-CB7
25	P	305	PEK	C24-C25-C26-C27
26	C	305	CDL	C83-C84-C85-C86
26	P	308	CDL	C59-C60-C61-C62
23	R	201	PSC	C04-C05-N-C06
23	R	201	PSC	C04-C05-N-C08
17	A	604	PGV	C7-C8-C9-C10
20	A	613	TGL	CB5-CB6-CB7-CB8
23	R	201	PSC	C13-C14-C15-C16
20	A	613	TGL	CC9-C15-C16-C17
20	N	605	TGL	C14-C29-C30-C31
25	G	102	PEK	C25-C26-C27-C28
26	P	312	CDL	C31-C32-C33-C34
24	J	101	CHD	C17-C20-C22-C23
25	P	301	PEK	C4-C5-C6-C7
25	P	304	PEK	C34-C35-C36-C37
26	C	305	CDL	C14-C15-C16-C17
26	C	305	CDL	C60-C61-C62-C63
26	P	308	CDL	OB7-CB5-OB6-CB4
17	C	304	PGV	C23-C24-C25-C26
17	P	306	PGV	C11-C12-C13-C14
17	N	622	PGV	C04-O12-P-O11
17	P	307	PGV	C04-O12-P-O11
20	D	201	TGL	OA1-CA1-OG1-CG1
17	M	101	PGV	C01-C02-C03-O11
17	P	307	PGV	C01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-CA6
24	Y	101	CHD	C13-C17-C20-C21
20	N	618	TGL	CB7-CB8-CB9-C10
17	P	307	PGV	C3-C4-C5-C6
25	P	304	PEK	C15-C16-C17-C18
26	C	305	CDL	C80-C81-C82-C83
20	D	201	TGL	CA2-CA1-OG1-CG1
26	C	305	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
17	N	622	PGV	C6-C7-C8-C9
20	D	201	TGL	C12-C13-C14-C29
25	P	301	PEK	O04-C21-O03-C01
24	Y	101	CHD	C16-C17-C20-C21
26	P	308	CDL	C72-C73-C74-C75
24	Y	101	CHD	C20-C22-C23-C24
17	M	101	PGV	O03-C01-C02-C03
20	L	502	TGL	CB9-C10-C11-C12
20	N	605	TGL	C22-C23-C24-C25
26	C	305	CDL	CA3-CA4-CA6-OA8
26	C	305	CDL	CB3-CB4-CB6-OB8
25	C	302	PEK	C24-C25-C26-C27
25	G	102	PEK	C35-C36-C37-C38
17	N	606	PGV	C19-C20-C21-C22
25	C	314	PEK	O04-C21-O03-C01
20	D	201	TGL	C15-C16-C17-C18
25	P	301	PEK	C29-C30-C31-C32
17	C	304	PGV	C31-C32-C33-C34
20	N	604	TGL	C29-C30-C31-C32
25	P	305	PEK	C35-C36-C37-C38
24	Y	101	CHD	C16-C17-C20-C22
20	N	605	TGL	C33-C34-C35-C36
26	P	312	CDL	C20-C21-C22-C23
27	Z	101	DMU	C19-C22-C25-C28
17	A	604	PGV	C12-C13-C14-C15
23	B	302	PSC	C6-C7-C8-C9
25	P	305	PEK	C2-C3-C4-C5
20	L	502	TGL	C11-C12-C13-C14
25	C	314	PEK	C24-C25-C26-C27
25	C	302	PEK	C35-C36-C37-C38
25	P	301	PEK	C22-C23-C24-C25
26	C	310	CDL	C44-C45-C46-C47
20	L	502	TGL	C21-C22-C23-C24
20	N	605	TGL	C21-C22-C23-C24
25	G	102	PEK	C28-C29-C30-C31
17	P	306	PGV	C27-C28-C29-C30
20	N	604	TGL	C12-C13-C14-C29
20	N	604	TGL	C21-C22-C23-C24
20	N	618	TGL	C29-C30-C31-C32
17	P	306	PGV	C19-C20-C21-C22
20	N	604	TGL	CB5-CB6-CB7-CB8
27	M	102	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
25	C	302	PEK	C14-C15-C16-C17
25	P	301	PEK	C14-C15-C16-C17
17	P	307	PGV	C27-C28-C29-C30
25	P	305	PEK	C17-C18-C19-C20
26	C	305	CDL	C18-C19-C20-C21
26	C	305	CDL	C44-C45-C46-C47
26	P	308	CDL	C57-C58-C59-C60
17	N	622	PGV	O01-C02-C03-O11
26	P	312	CDL	OB5-CB3-CB4-OB6
17	C	304	PGV	C5-C6-C7-C8
26	P	312	CDL	C24-C25-C26-C27
27	P	302	DMU	O5-C4-C57-O61
20	N	605	TGL	C29-C30-C31-C32
17	A	604	PGV	C29-C30-C31-C32
27	C	311	DMU	C1-C6-O16-C18
17	C	304	PGV	O03-C01-C02-O01
26	P	308	CDL	OB6-CB4-CB6-OB8
20	N	604	TGL	C15-C16-C17-C18
26	P	308	CDL	C42-C43-C44-C45
17	M	101	PGV	C4-C5-C6-C7
26	C	310	CDL	C22-C23-C24-C25
27	G	101	DMU	C34-C37-C40-C43
20	L	502	TGL	C22-C23-C24-C25
26	P	308	CDL	C37-C38-C39-C40
26	P	312	CDL	C23-C24-C25-C26
26	P	312	CDL	CB2-C1-CA2-OA2
20	N	604	TGL	CB2-CB1-OG2-CG2
17	C	303	PGV	C22-C23-C24-C25
25	P	304	PEK	C4-C5-C6-C7
25	C	314	PEK	C17-C18-C19-C20
25	P	301	PEK	C16-C17-C18-C19
25	P	305	PEK	C3-C4-C5-C6
17	C	304	PGV	C7-C8-C9-C10
26	P	312	CDL	C56-C57-C58-C59
25	P	301	PEK	C35-C36-C37-C38
25	C	314	PEK	C35-C36-C37-C38
26	P	308	CDL	C64-C65-C66-C67
25	C	314	PEK	C1-C2-C3-C4
25	C	314	PEK	C16-C17-C18-C19
26	C	310	CDL	C31-C32-C33-C34
27	Z	101	DMU	C18-C19-C22-C25
17	N	606	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	P	302	DMU	C19-C18-O16-C6
17	N	622	PGV	C27-C28-C29-C30
17	P	307	PGV	C28-C29-C30-C31
25	P	301	PEK	C17-C18-C19-C20
25	C	314	PEK	C30-C31-C32-C33
20	N	604	TGL	CA2-CA1-OG1-CG1
20	L	502	TGL	CG1-CG2-CG3-OG3
20	N	618	TGL	OG1-CG1-CG2-CG3
23	B	302	PSC	O03-C01-C02-C03
25	C	302	PEK	O03-C01-C02-C03
26	C	310	CDL	CB3-CB4-CB6-OB8
26	P	308	CDL	CB3-CB4-CB6-OB8
25	C	302	PEK	C10-C11-C12-C13
25	G	102	PEK	C4-C5-C6-C7
26	P	312	CDL	C83-C84-C85-C86
23	B	302	PSC	C9-C10-C11-C12
23	B	302	PSC	C10-C11-C12-C13
23	R	201	PSC	C9-C10-C11-C12
23	R	201	PSC	C10-C11-C12-C13
25	C	302	PEK	C6-C7-C8-C9
25	C	302	PEK	C11-C10-C9-C8
25	C	302	PEK	C11-C12-C13-C14
25	C	314	PEK	C5-C6-C7-C8
25	C	314	PEK	C6-C7-C8-C9
25	C	314	PEK	C12-C13-C14-C15
25	P	301	PEK	C5-C6-C7-C8
25	P	301	PEK	C9-C10-C11-C12
25	P	301	PEK	C11-C12-C13-C14
25	P	304	PEK	C9-C10-C11-C12
25	P	305	PEK	C5-C6-C7-C8
25	P	305	PEK	C12-C13-C14-C15
20	N	604	TGL	CC6-CC7-CC8-CC9
17	C	303	PGV	C7-C8-C9-C10
17	C	304	PGV	C2-C3-C4-C5
25	C	314	PEK	C28-C29-C30-C31
26	C	305	CDL	C77-C78-C79-C80
26	C	310	CDL	C71-C72-C73-C74
17	M	101	PGV	O01-C02-C03-O11
26	C	310	CDL	OB5-CB3-CB4-OB6
26	P	308	CDL	OB5-CB3-CB4-OB6
25	P	305	PEK	C15-C16-C17-C18
27	P	302	DMU	O6-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
26	C	310	CDL	O1-C1-CA2-OA2
17	M	101	PGV	C21-C22-C23-C24
25	C	302	PEK	O03-C01-C02-O01
26	C	305	CDL	OA6-CA4-CA6-OA8
26	C	310	CDL	OB6-CB4-CB6-OB8
20	L	502	TGL	CC7-CC8-CC9-C15
20	N	618	TGL	CA3-CA4-CA5-CA6
25	P	305	PEK	C33-C34-C35-C36
26	P	308	CDL	C11-C12-C13-C14
26	C	310	CDL	C60-C61-C62-C63
26	C	310	CDL	C61-C62-C63-C64
20	D	201	TGL	CB2-CB3-CB4-CB5
26	C	305	CDL	C15-C16-C17-C18
20	N	605	TGL	CA6-CA7-CA8-CA9
26	P	308	CDL	C1-CB2-OB2-PB2
17	C	304	PGV	C11-C10-C9-C8
17	A	604	PGV	C13-C14-C15-C16
26	C	305	CDL	C40-C41-C42-C43
20	N	604	TGL	C19-C33-C34-C35
25	P	304	PEK	C3-C4-C5-C6
19	B	309	EDO	O1-C1-C2-O2
19	G	105	EDO	O1-C1-C2-O2
19	L	503	EDO	O1-C1-C2-O2
19	N	621	EDO	O1-C1-C2-O2
19	Q	1603	EDO	O1-C1-C2-O2
19	R	203	EDO	O1-C1-C2-O2
17	P	307	PGV	C13-C14-C15-C16
20	N	605	TGL	CC4-CC5-CC6-CC7
17	C	304	PGV	C4-C5-C6-C7
20	L	502	TGL	CB1-CB2-CB3-CB4
27	G	101	DMU	C19-C22-C25-C28
23	R	201	PSC	C24-C25-C26-C27
26	P	308	CDL	OB5-CB3-CB4-CB6
25	P	305	PEK	C31-C32-C33-C34
25	G	102	PEK	C3-C4-C5-C6
27	G	104	DMU	C31-C34-C37-C40
20	N	618	TGL	CB6-CB7-CB8-CB9
17	M	101	PGV	C19-C20-C21-C22
26	C	310	CDL	C72-C73-C74-C75
27	C	311	DMU	C34-C37-C40-C43
25	P	305	PEK	C25-C26-C27-C28
23	R	201	PSC	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
26	P	308	CDL	C80-C81-C82-C83
24	G	107	CHD	C17-C20-C22-C23
23	B	302	PSC	C31-C32-C33-C34
20	A	613	TGL	C25-C26-C27-C28
17	C	304	PGV	C02-C03-O11-P
20	D	201	TGL	OG1-CG1-CG2-CG3
20	D	201	TGL	CG1-CG2-CG3-OG3
25	P	301	PEK	C02-C03-O11-P
26	P	312	CDL	C1-CA2-OA2-PA1
26	P	312	CDL	CA3-CA4-CA6-OA8
26	P	308	CDL	C74-C75-C76-C77
25	C	314	PEK	O01-C02-C03-O11
26	C	305	CDL	OB5-CB3-CB4-OB6
17	C	304	PGV	C29-C30-C31-C32
20	L	502	TGL	C11-C10-CB9-CB8
26	C	305	CDL	C51-C52-C53-C54
26	C	310	CDL	C21-C22-C23-C24
17	P	306	PGV	C23-C24-C25-C26
20	D	201	TGL	C21-C20-CA9-CA8
26	C	305	CDL	C24-C25-C26-C27
26	P	308	CDL	C16-C17-C18-C19
26	C	305	CDL	C62-C63-C64-C65
20	N	604	TGL	OB1-CB1-OG2-CG2
26	P	312	CDL	C62-C63-C64-C65
26	C	310	CDL	C11-C12-C13-C14
20	N	604	TGL	C13-C14-C29-C30
26	P	308	CDL	C17-C18-C19-C20
20	L	502	TGL	OG2-CG2-CG3-OG3
23	B	302	PSC	C24-C25-C26-C27
20	N	604	TGL	OA1-CA1-OG1-CG1
25	P	304	PEK	C30-C31-C32-C33
17	M	101	PGV	C12-C13-C14-C15
20	N	618	TGL	C11-C10-CB9-CB8
26	P	312	CDL	C84-C85-C86-C87
26	P	308	CDL	C21-C22-C23-C24
20	N	618	TGL	C21-C20-CA9-CA8
25	G	102	PEK	C7-C8-C9-C10
25	P	301	PEK	O01-C1-C2-C3
20	N	618	TGL	CA6-CA7-CA8-CA9
26	C	310	CDL	C56-C57-C58-C59
26	P	312	CDL	C81-C82-C83-C84
17	C	304	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
20	N	605	TGL	C25-C26-C27-C28
17	N	606	PGV	C23-C24-C25-C26
23	R	201	PSC	C03-O11-P-O12
25	P	301	PEK	C03-O11-P-O12
25	P	301	PEK	C04-O12-P-O11
26	C	310	CDL	CA3-OA5-PA1-OA2
26	P	308	CDL	C20-C21-C22-C23
26	P	312	CDL	C57-C58-C59-C60
26	P	308	CDL	O1-C1-CB2-OB2
25	P	305	PEK	C1-C2-C3-C4
20	D	201	TGL	C22-C23-C24-C25
17	C	303	PGV	C02-C03-O11-P
17	P	306	PGV	C02-C03-O11-P
17	P	307	PGV	C05-C04-O12-P
26	C	305	CDL	CA4-CA3-OA5-PA1
26	P	312	CDL	CA4-CA3-OA5-PA1
17	N	622	PGV	C04-O12-P-O14
17	P	307	PGV	C03-O11-P-O14
17	P	307	PGV	C04-O12-P-O14
23	R	201	PSC	C04-O12-P-O14
25	C	314	PEK	C04-O12-P-O14
25	P	301	PEK	C03-O11-P-O13
26	C	305	CDL	CA3-OA5-PA1-OA3
26	C	310	CDL	CB2-OB2-PB2-OB4
26	C	310	CDL	CB3-OB5-PB2-OB3
26	P	308	CDL	CB2-OB2-PB2-OB3
26	P	308	CDL	CB2-OB2-PB2-OB4
26	P	312	CDL	CB2-OB2-PB2-OB3
26	C	305	CDL	C74-C75-C76-C77
27	P	302	DMU	C2-C3-O7-C10
17	N	622	PGV	C01-C02-C03-O11
25	C	314	PEK	C01-C02-C03-O11
26	P	312	CDL	OB5-CB3-CB4-CB6
26	P	312	CDL	C73-C74-C75-C76
19	M	103	EDO	O1-C1-C2-O2
27	M	102	DMU	C34-C37-C40-C43
23	B	302	PSC	C5-C6-C7-C8
26	P	308	CDL	C81-C82-C83-C84
25	C	302	PEK	C05-C04-O12-P
17	P	306	PGV	C1-C2-C3-C4
27	Z	101	DMU	C22-C25-C28-C31
17	C	304	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	P	312	CDL	C42-C43-C44-C45
17	M	101	PGV	C11-C10-C9-C8
17	C	303	PGV	C13-C14-C15-C16
26	C	310	CDL	C63-C64-C65-C66
17	M	101	PGV	C30-C31-C32-C33
20	L	502	TGL	CA2-CA3-CA4-CA5
17	P	307	PGV	O01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-OA6
20	D	201	TGL	CC9-C15-C16-C17
25	G	102	PEK	C2-C1-O01-C02
17	M	101	PGV	C7-C8-C9-C10
17	C	304	PGV	O03-C01-C02-C03
23	B	302	PSC	O12-C04-C05-N
23	R	201	PSC	O03-C01-C02-O01
26	C	305	CDL	OB6-CB4-CB6-OB8
20	L	502	TGL	C19-C33-C34-C35
26	P	308	CDL	C62-C63-C64-C65
20	A	613	TGL	CA6-CA7-CA8-CA9
27	P	302	DMU	C34-C37-C40-C43
17	P	306	PGV	C21-C22-C23-C24
17	N	606	PGV	O03-C19-C20-C21
25	P	304	PEK	C23-C24-C25-C26
26	P	312	CDL	C63-C64-C65-C66
20	N	605	TGL	C16-C17-C18-C19
17	C	304	PGV	C1-C2-C3-C4
26	C	305	CDL	C17-C18-C19-C20
26	P	312	CDL	C71-C72-C73-C74
17	P	306	PGV	C10-C11-C12-C13
27	G	101	DMU	C25-C28-C31-C34
23	R	201	PSC	C26-C27-C28-C29
20	N	604	TGL	CC5-CC6-CC7-CC8
26	P	308	CDL	C44-C45-C46-C47
26	P	308	CDL	C63-C64-C65-C66
17	P	307	PGV	C15-C16-C17-C18
20	D	201	TGL	C13-C14-C29-C30
26	C	305	CDL	C42-C43-C44-C45
26	C	310	CDL	C83-C84-C85-C86
20	A	613	TGL	CC2-CC3-CC4-CC5
20	A	613	TGL	C16-C17-C18-C19
17	N	622	PGV	C03-C02-O01-C1
25	C	302	PEK	C03-C02-O01-C1
25	P	305	PEK	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
23	R	201	PSC	C4-C5-C6-C7
26	C	305	CDL	C57-C58-C59-C60
17	A	604	PGV	O03-C19-C20-C21
25	G	102	PEK	C17-C18-C19-C20
25	P	301	PEK	O03-C21-C22-C23
20	N	605	TGL	CC7-CC8-CC9-C15
19	B	307	EDO	O1-C1-C2-O2
19	C	307	EDO	O1-C1-C2-O2
19	E	201	EDO	O1-C1-C2-O2
19	K	201	EDO	O1-C1-C2-O2
19	P	311	EDO	O1-C1-C2-O2
19	V	102	EDO	O1-C1-C2-O2
27	P	302	DMU	C4-C3-O7-C10
20	A	613	TGL	C11-C10-CB9-CB8
17	C	303	PGV	C11-C12-C13-C14
17	P	306	PGV	C9-C10-C11-C12
23	R	201	PSC	C7-C8-C9-C10
25	P	304	PEK	O03-C21-C22-C23
20	D	201	TGL	OG1-CG1-CG2-OG2
23	B	302	PSC	O03-C01-C02-O01
26	C	305	CDL	C31-C32-C33-C34
17	M	101	PGV	C03-O11-P-O12
25	C	302	PEK	C04-O12-P-O11
17	A	604	PGV	C26-C27-C28-C29
26	C	310	CDL	CB5-C51-C52-C53
20	A	613	TGL	CC3-CC4-CC5-CC6
20	A	613	TGL	C21-C20-CA9-CA8
27	C	311	DMU	C31-C34-C37-C40
17	N	622	PGV	C7-C8-C9-C10
26	C	310	CDL	C19-C20-C21-C22
26	P	308	CDL	CA4-CA3-OA5-PA1
17	C	304	PGV	C9-C10-C11-C12
17	C	303	PGV	C29-C30-C31-C32
20	L	502	TGL	CA4-CA5-CA6-CA7
25	P	304	PEK	C2-C3-C4-C5
17	M	101	PGV	C10-C11-C12-C13
25	C	314	PEK	C10-C11-C12-C13
20	L	502	TGL	CC3-CC4-CC5-CC6
17	N	622	PGV	C13-C14-C15-C16
26	P	312	CDL	C16-C17-C18-C19
20	A	613	TGL	C29-C30-C31-C32
23	B	302	PSC	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C35-C36-C37-C38
25	P	304	PEK	C14-C15-C16-C17
20	A	613	TGL	CC6-CC7-CC8-CC9
26	C	310	CDL	C84-C85-C86-C87
17	P	306	PGV	C15-C16-C17-C18
20	N	605	TGL	C16-C15-CC9-CC8
23	R	201	PSC	C15-C16-C17-C18
26	C	305	CDL	C20-C21-C22-C23
19	A	611	EDO	O1-C1-C2-O2
19	A	616	EDO	O1-C1-C2-O2
19	C	309	EDO	O1-C1-C2-O2
19	E	202	EDO	O1-C1-C2-O2
19	E	205	EDO	O1-C1-C2-O2
19	N	609	EDO	O1-C1-C2-O2
26	P	312	CDL	C59-C60-C61-C62
20	N	618	TGL	CC7-CC8-CC9-C15
26	C	305	CDL	C34-C35-C36-C37
18	A	605	HEA	CAA-CBA-CGA-O1A
23	B	302	PSC	C21-C22-C23-C24
25	P	305	PEK	C32-C33-C34-C35
26	P	312	CDL	C61-C62-C63-C64
24	B	303	CHD	C22-C23-C24-O25
24	G	107	CHD	C22-C23-C24-O26
24	P	309	CHD	C22-C23-C24-O25
27	G	104	DMU	C5-C10-O7-C3
17	P	307	PGV	C21-C22-C23-C24
25	C	302	PEK	C30-C31-C32-C33
26	C	305	CDL	C79-C80-C81-C82
26	C	310	CDL	C74-C75-C76-C77
24	P	309	CHD	C22-C23-C24-O26
20	N	618	TGL	CG1-CG2-OG2-CB1
20	N	604	TGL	C11-C10-CB9-CB8
24	B	303	CHD	C22-C23-C24-O26
24	C	306	CHD	C22-C23-C24-O25
25	P	301	PEK	C6-C7-C8-C9
25	P	305	PEK	C9-C10-C11-C12
17	C	303	PGV	C31-C32-C33-C34
20	D	201	TGL	C24-C25-C26-C27
25	P	301	PEK	C30-C31-C32-C33
23	R	201	PSC	C28-C29-C30-C31
20	A	613	TGL	CB9-C10-C11-C12
25	C	314	PEK	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
26	C	305	CDL	C64-C65-C66-C67
26	C	305	CDL	OB5-CB3-CB4-CB6
26	C	310	CDL	OB5-CB3-CB4-CB6
26	C	310	CDL	C51-C52-C53-C54
26	P	308	CDL	C58-C59-C60-C61
18	A	605	HEA	CAA-CBA-CGA-O2A
18	A	605	HEA	CAD-CBD-CGD-O1D
20	L	502	TGL	OG1-CG1-CG2-OG2
25	P	304	PEK	C28-C29-C30-C31
17	C	303	PGV	C20-C21-C22-C23
18	A	605	HEA	CAD-CBD-CGD-O2D
24	T	1302	CHD	C22-C23-C24-O26
20	L	502	TGL	CC4-CC5-CC6-CC7
20	N	618	TGL	CB5-CB6-CB7-CB8
24	G	107	CHD	C22-C23-C24-O25
26	P	312	CDL	C32-C31-CA7-OA8
23	R	201	PSC	C30-C31-C32-C33
17	P	306	PGV	C26-C27-C28-C29
26	C	305	CDL	O1-C1-CB2-OB2
17	A	604	PGV	C31-C32-C33-C34
17	N	606	PGV	C9-C10-C11-C12
17	M	101	PGV	C29-C30-C31-C32
20	A	613	TGL	CB2-CB3-CB4-CB5
25	P	304	PEK	C22-C23-C24-C25
19	E	204	EDO	O1-C1-C2-O2
19	N	612	EDO	O1-C1-C2-O2
19	N	616	EDO	O1-C1-C2-O2
19	S	105	EDO	O1-C1-C2-O2
20	N	604	TGL	C24-C25-C26-C27
24	T	1302	CHD	C22-C23-C24-O25
24	Y	101	CHD	C22-C23-C24-O25
26	C	305	CDL	C58-C59-C60-C61
27	P	302	DMU	O6-C11-C9-O1
17	N	622	PGV	C25-C26-C27-C28
17	P	307	PGV	C26-C27-C28-C29
20	L	502	TGL	C13-C14-C29-C30
25	C	302	PEK	O03-C21-C22-C23
20	A	613	TGL	CB3-CB4-CB5-CB6
17	P	307	PGV	O03-C01-C02-O01
20	N	618	TGL	OG1-CG1-CG2-OG2
26	C	310	CDL	OA6-CA4-CA6-OA8
25	G	102	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	P	312	CDL	C13-C14-C15-C16
26	P	308	CDL	C24-C25-C26-C27
18	N	607	HEA	CAD-CBD-CGD-O2D
26	P	308	CDL	C75-C76-C77-C78
17	P	307	PGV	C20-C21-C22-C23
17	P	307	PGV	O04-C19-O03-C01
20	N	618	TGL	OG3-CC1-CC2-CC3
17	N	622	PGV	C11-C12-C13-C14
23	B	302	PSC	C27-C28-C29-C30
20	N	618	TGL	CG3-CG2-OG2-CB1
25	C	302	PEK	C01-C02-O01-C1
25	P	305	PEK	C01-C02-O01-C1
26	C	310	CDL	CA3-CA4-OA6-CA5
20	N	605	TGL	C23-C24-C25-C26
20	L	502	TGL	C23-C24-C25-C26
20	D	201	TGL	OG2-CB1-CB2-CB3
17	M	101	PGV	O03-C19-C20-C21
25	G	102	PEK	O01-C1-C2-C3
25	C	302	PEK	C3-C4-C5-C6
23	B	302	PSC	C25-C26-C27-C28
23	R	201	PSC	O03-C01-C02-C03
18	N	607	HEA	CAD-CBD-CGD-O1D
24	Y	101	CHD	C22-C23-C24-O26
20	N	618	TGL	CA1-CA2-CA3-CA4
19	I	102	EDO	O1-C1-C2-O2
19	L	501	EDO	O1-C1-C2-O2
19	N	614	EDO	O1-C1-C2-O2
19	N	619	EDO	O1-C1-C2-O2
19	O	302	EDO	O1-C1-C2-O2
19	Q	1601	EDO	O1-C1-C2-O2
19	S	106	EDO	O1-C1-C2-O2
19	T	1303	EDO	O1-C1-C2-O2
19	U	1501	EDO	O1-C1-C2-O2
20	A	613	TGL	C13-C14-C29-C30
17	A	604	PGV	C9-C10-C11-C12
25	C	314	PEK	C14-C15-C16-C17
17	N	622	PGV	O12-C04-C05-C06
24	C	301	CHD	C22-C23-C24-O25
17	A	604	PGV	C27-C28-C29-C30
25	P	304	PEK	C17-C18-C19-C20
25	P	304	PEK	C35-C36-C37-C38
20	N	605	TGL	CA7-CA8-CA9-C20

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Mol	Chain	Res	Type	Atoms
26	P	308	CDL	OA6-CA4-CA6-OA8
18	N	607	HEA	CAA-CBA-CGA-O2A
17	P	307	PGV	O01-C1-C2-C3
24	P	303	CHD	C22-C23-C24-O25
20	N	604	TGL	CC1-CC2-CC3-CC4
20	L	502	TGL	CA3-CA4-CA5-CA6
24	T	1302	CHD	C16-C17-C20-C22
23	R	201	PSC	O03-C19-C20-C21
24	P	303	CHD	C22-C23-C24-O26
23	B	302	PSC	C26-C27-C28-C29
17	M	101	PGV	C15-C16-C17-C18
24	C	306	CHD	C22-C23-C24-O26
24	T	1302	CHD	C20-C22-C23-C24
25	G	102	PEK	C26-C27-C28-C29
24	J	101	CHD	C22-C23-C24-O25
20	N	605	TGL	CB3-CB4-CB5-CB6
26	P	308	CDL	C71-CB7-OB8-CB6
20	L	502	TGL	OG1-CG1-CG2-CG3
23	R	201	PSC	O02-C1-O01-C02
17	C	303	PGV	C05-C04-O12-P
17	P	307	PGV	C02-C03-O11-P
17	P	307	PGV	O02-C1-C2-C3
17	M	101	PGV	C03-O11-P-O13
26	C	305	CDL	CB2-OB2-PB2-OB3
20	A	613	TGL	OG1-CA1-CA2-CA3
25	P	301	PEK	O12-C04-C05-N
19	D	202	EDO	O1-C1-C2-O2
19	E	203	EDO	O1-C1-C2-O2
19	F	701	EDO	O1-C1-C2-O2
19	H	101	EDO	O1-C1-C2-O2
19	S	102	EDO	O1-C1-C2-O2
19	S	103	EDO	O1-C1-C2-O2
25	G	102	PEK	O03-C21-C22-C23
18	N	607	HEA	CAA-CBA-CGA-O1A
17	M	101	PGV	O04-C19-C20-C21
17	M	101	PGV	C9-C10-C11-C12
17	C	303	PGV	C23-C24-C25-C26
20	N	618	TGL	OC1-CC1-CC2-CC3
23	R	201	PSC	C05-C04-O12-P
17	C	303	PGV	C1-C2-C3-C4
26	P	308	CDL	OB9-CB7-OB8-CB6
20	L	502	TGL	OG3-CC1-CC2-CC3

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Mol	Chain	Res	Type	Atoms
20	N	618	TGL	OG2-CB1-CB2-CB3
25	P	304	PEK	O01-C1-C2-C3
26	C	310	CDL	C81-C82-C83-C84
25	G	102	PEK	O02-C1-C2-C3
26	P	308	CDL	C53-C54-C55-C56
23	R	201	PSC	O01-C1-C2-C3
18	N	608	HEA	O11-C11-C3B-C2B
20	L	502	TGL	OC1-CC1-CC2-CC3
23	R	201	PSC	O04-C19-C20-C21
25	P	304	PEK	O02-C1-C2-C3
17	P	307	PGV	C23-C24-C25-C26
27	G	101	DMU	C19-C18-O16-C6
26	P	312	CDL	C72-C71-CB7-OB8
20	N	618	TGL	OB1-CB1-CB2-CB3

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	Y	101	CHD	C1-C10-C2-C3-C4-C5
24	T	1302	CHD	C1-C10-C2-C3-C4-C5

52 monomers are involved in 160 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	612	EDO	1	0
26	C	310	CDL	2	0
26	P	312	CDL	10	0
19	S	106	EDO	1	0
19	A	615	EDO	1	0
20	D	201	TGL	10	0
29	V	101	SAC	3	0
18	N	608	HEA	4	0
24	B	303	CHD	1	0
19	R	203	EDO	1	0
18	N	607	HEA	4	0
24	Y	101	CHD	4	0
29	I	101	SAC	2	0
20	N	618	TGL	5	0
20	N	605	TGL	6	0
20	L	502	TGL	3	0
19	N	612	EDO	2	0
19	V	103	EDO	1	0

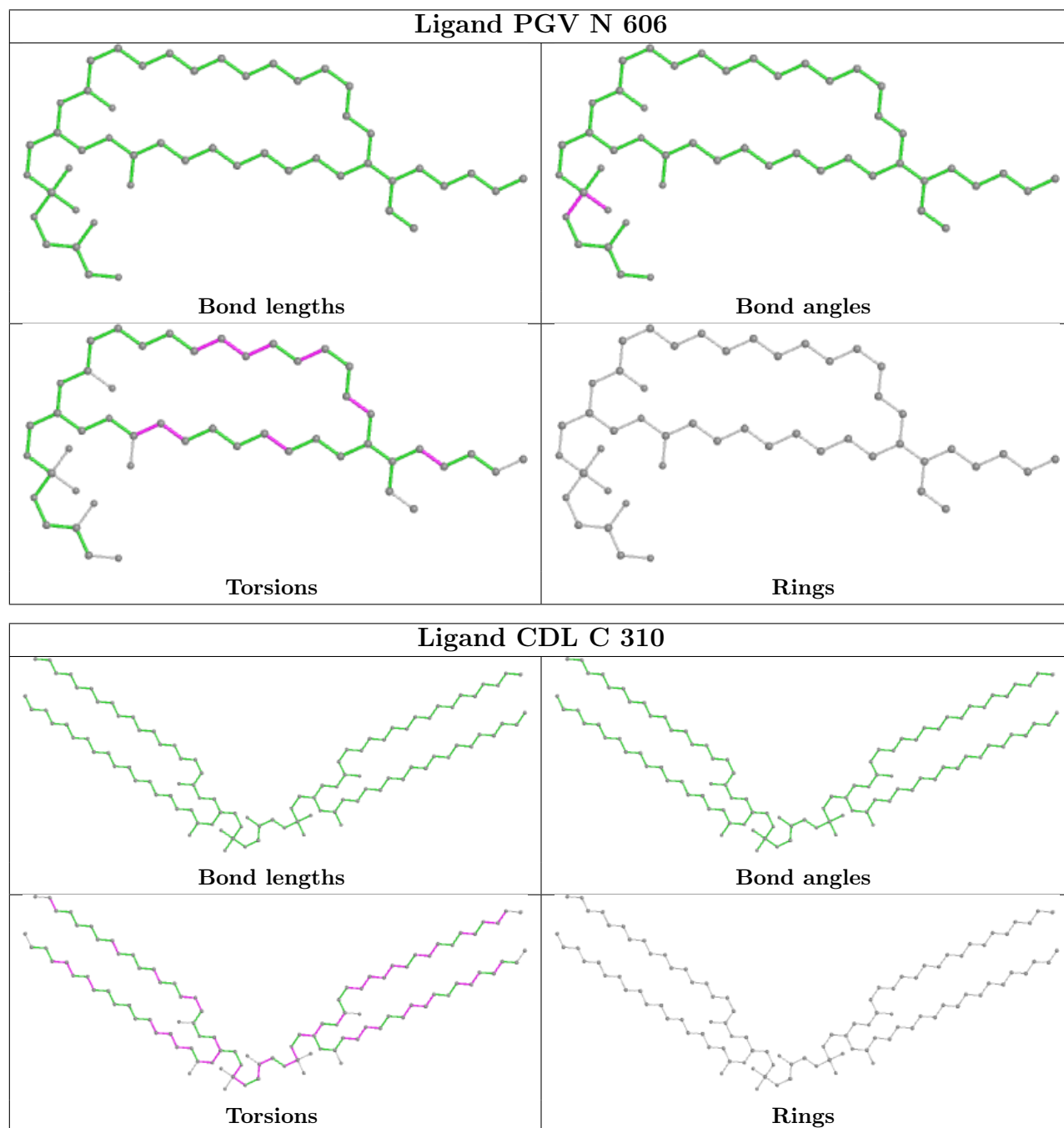
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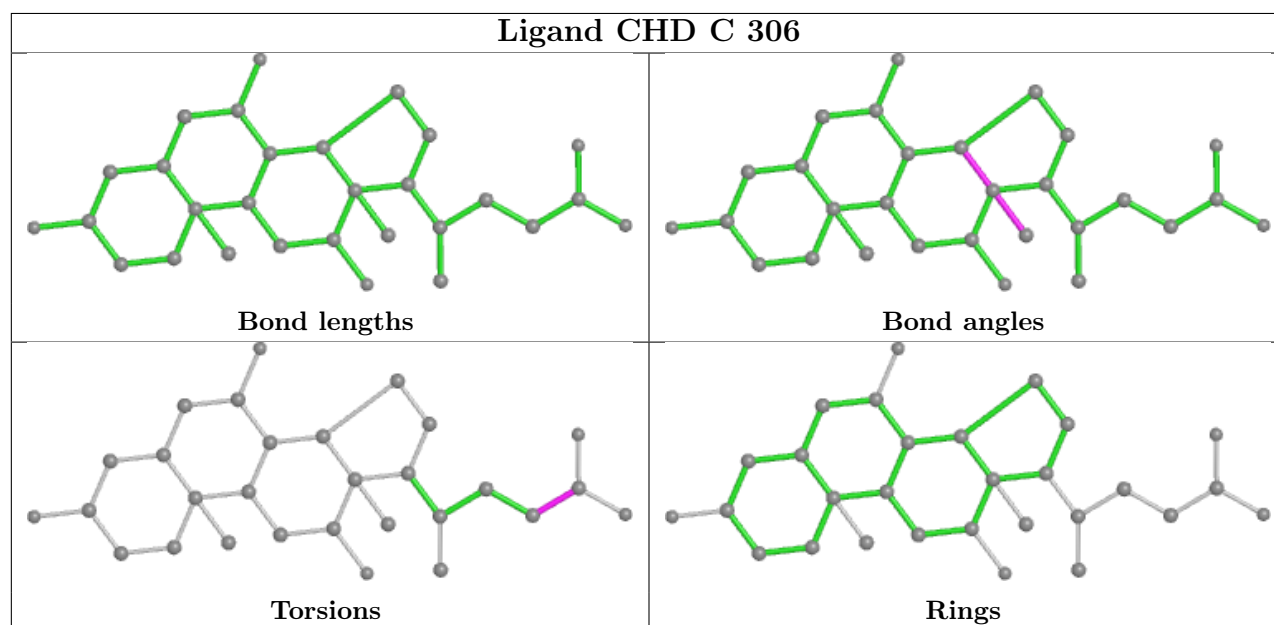
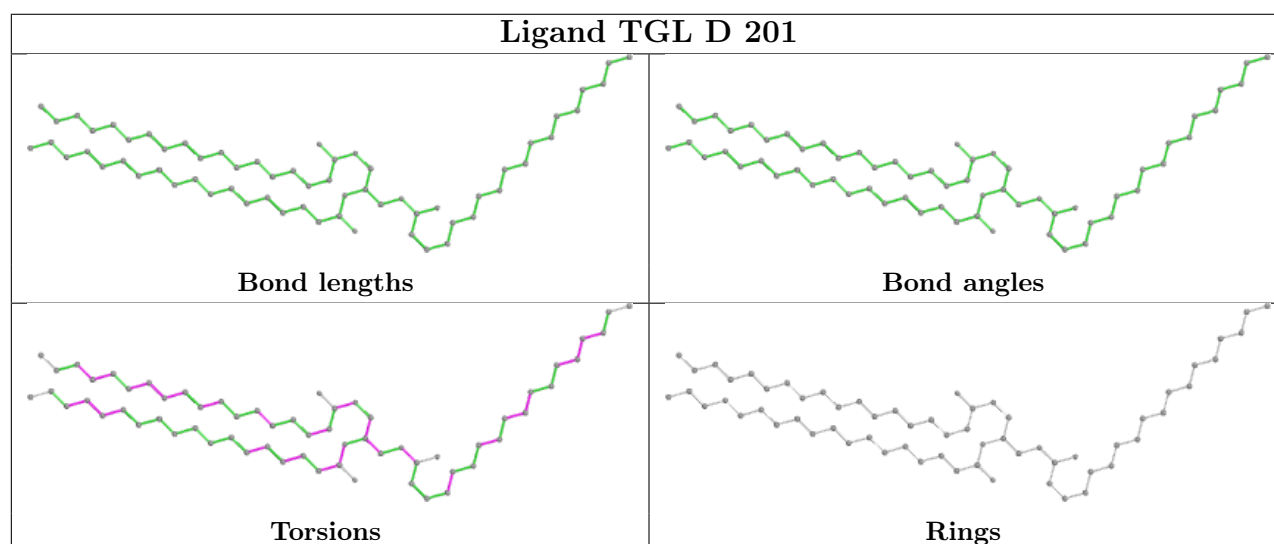
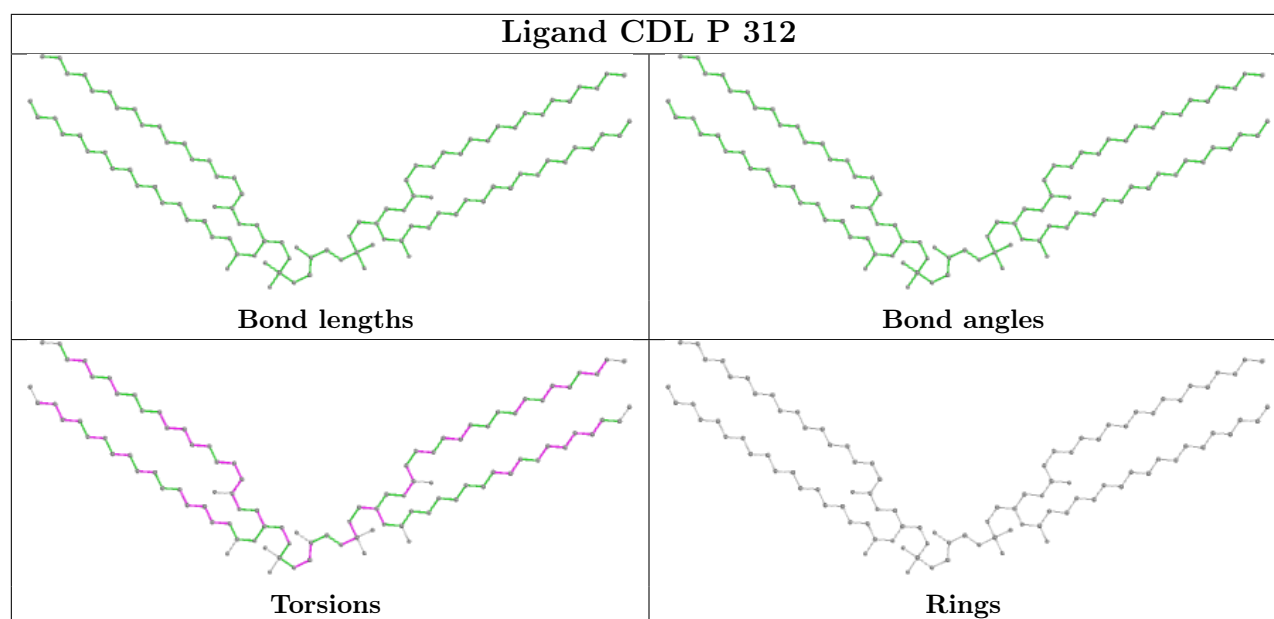
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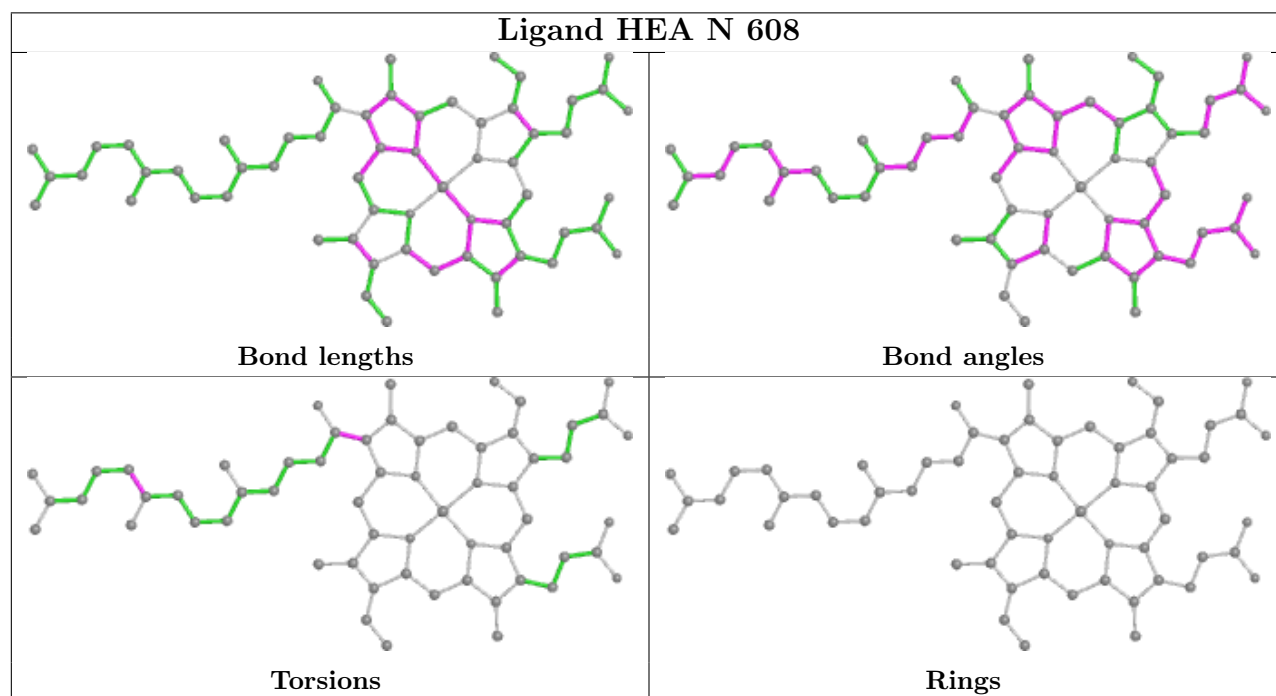
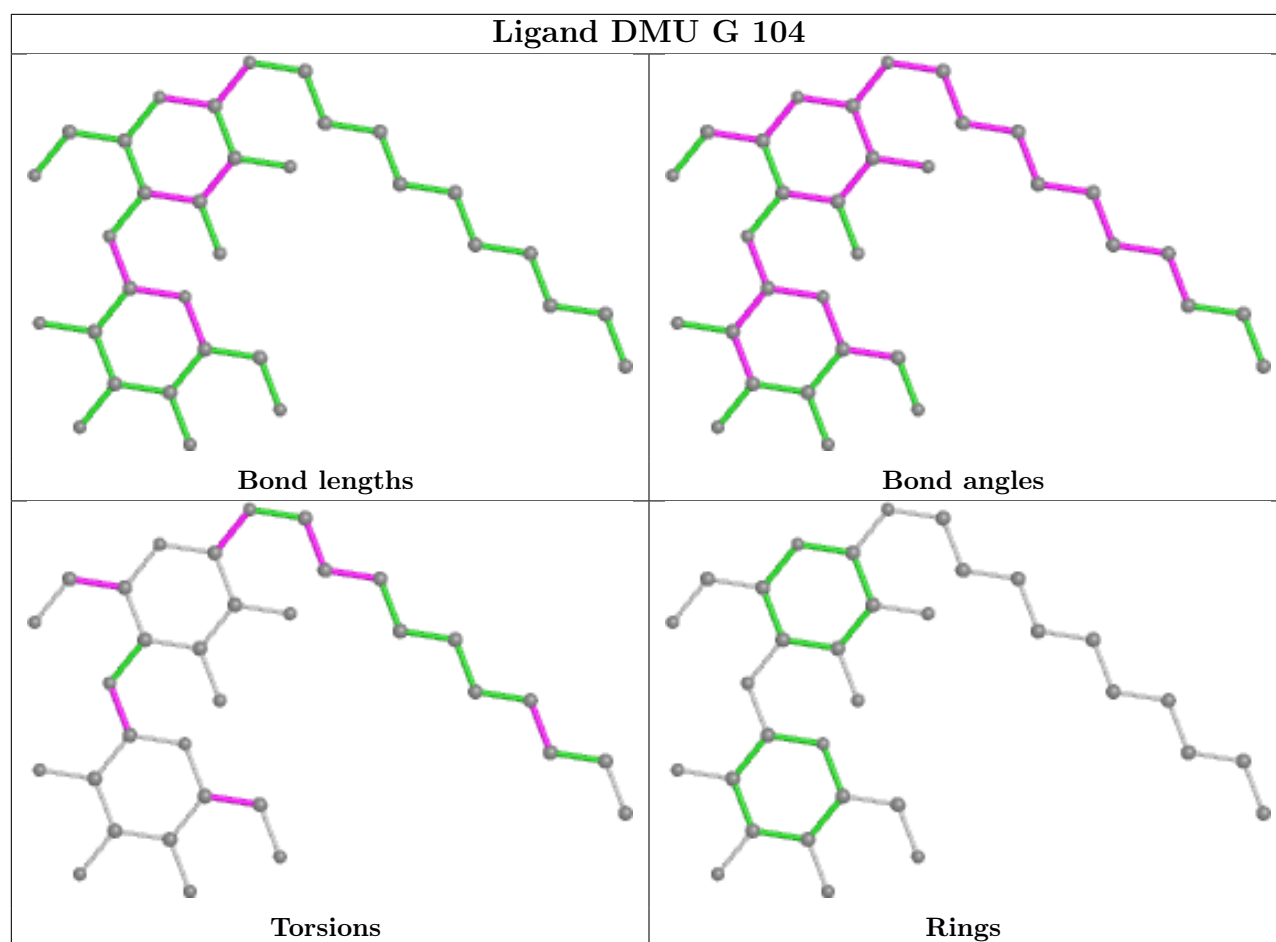
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	P	304	PEK	4	0
17	N	622	PGV	16	0
24	C	301	CHD	1	0
19	H	101	EDO	1	0
24	P	303	CHD	1	0
19	A	611	EDO	1	0
23	R	201	PSC	6	0
17	A	604	PGV	4	0
19	A	618	EDO	2	0
25	P	305	PEK	5	0
19	B	311	EDO	1	0
19	B	305	EDO	1	0
19	A	614	EDO	1	0
17	P	307	PGV	1	0
24	W	302	CHD	1	0
23	B	302	PSC	8	0
19	U	1501	EDO	3	0
25	C	302	PEK	3	0
19	C	312	EDO	1	0
17	C	303	PGV	1	0
26	C	305	CDL	2	0
19	N	611	EDO	1	0
27	Z	101	DMU	4	0
17	M	101	PGV	6	0
26	P	308	CDL	3	0
18	A	606	HEA	3	0
25	P	301	PEK	1	0
17	C	304	PGV	6	0
25	C	314	PEK	1	0
24	J	101	CHD	2	0
25	G	102	PEK	7	0
18	A	605	HEA	4	0
19	N	615	EDO	1	0
24	T	1302	CHD	4	0

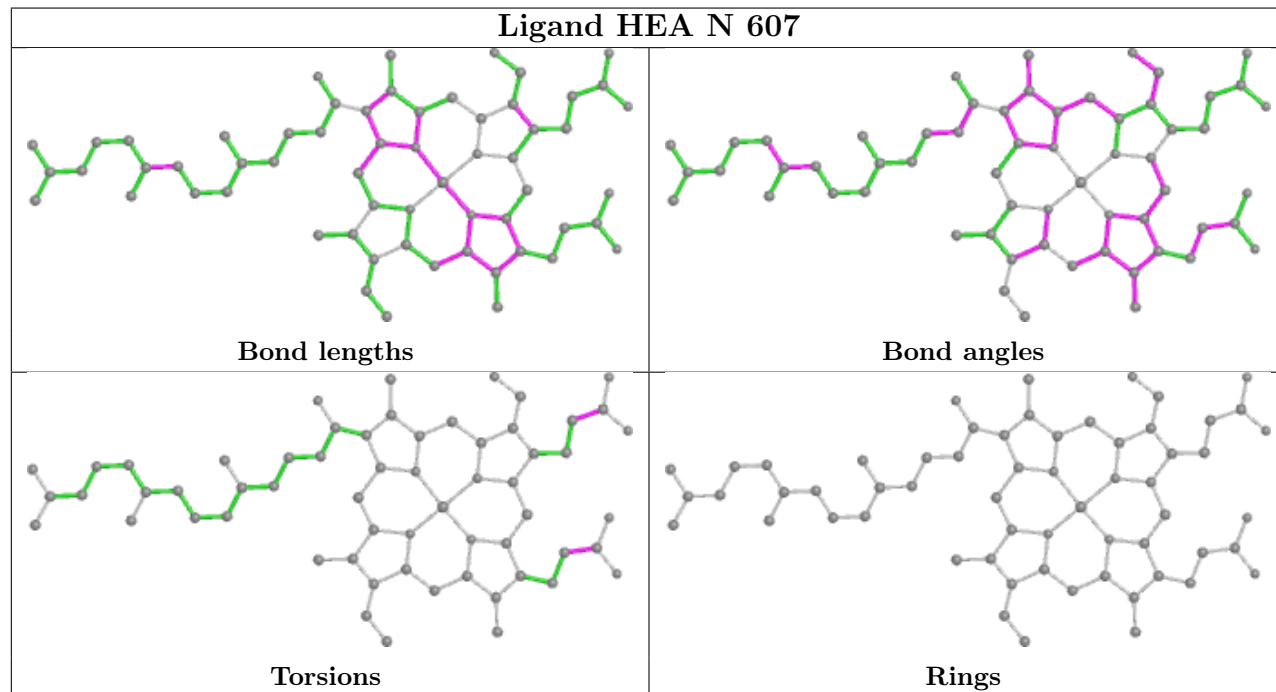
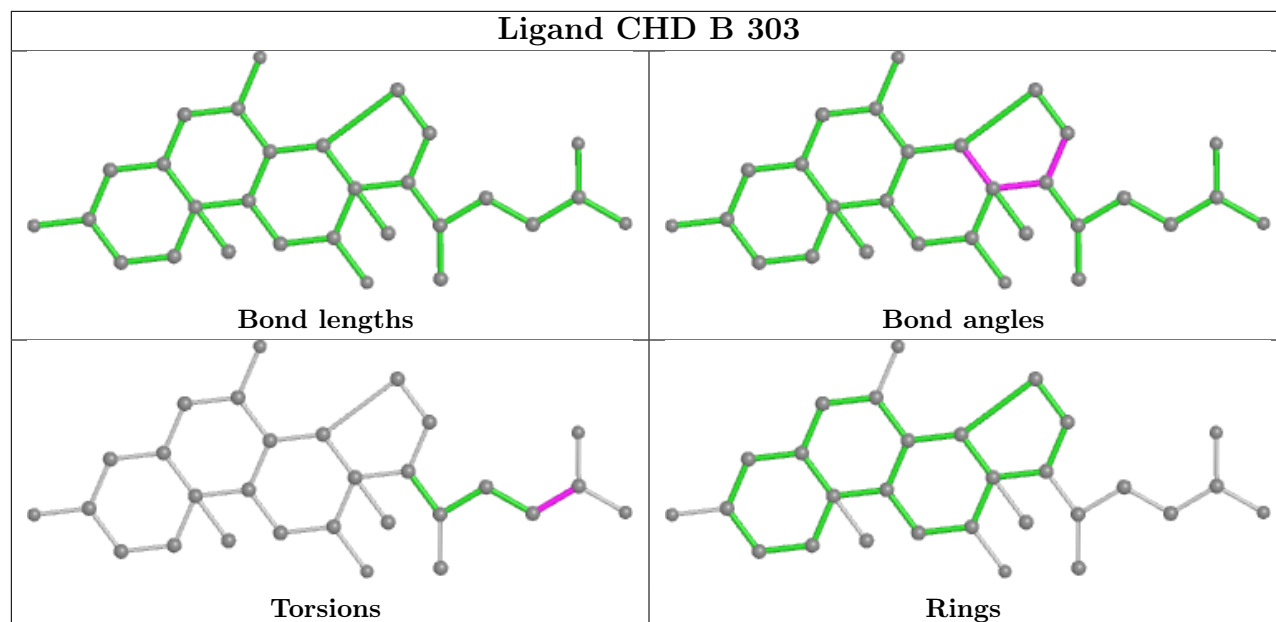
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

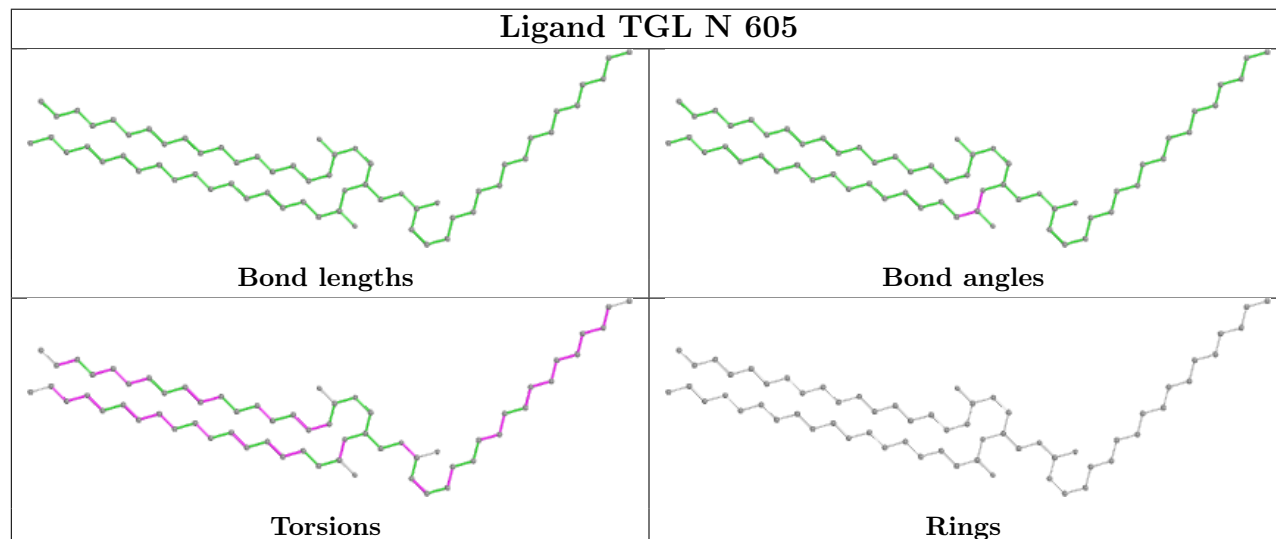
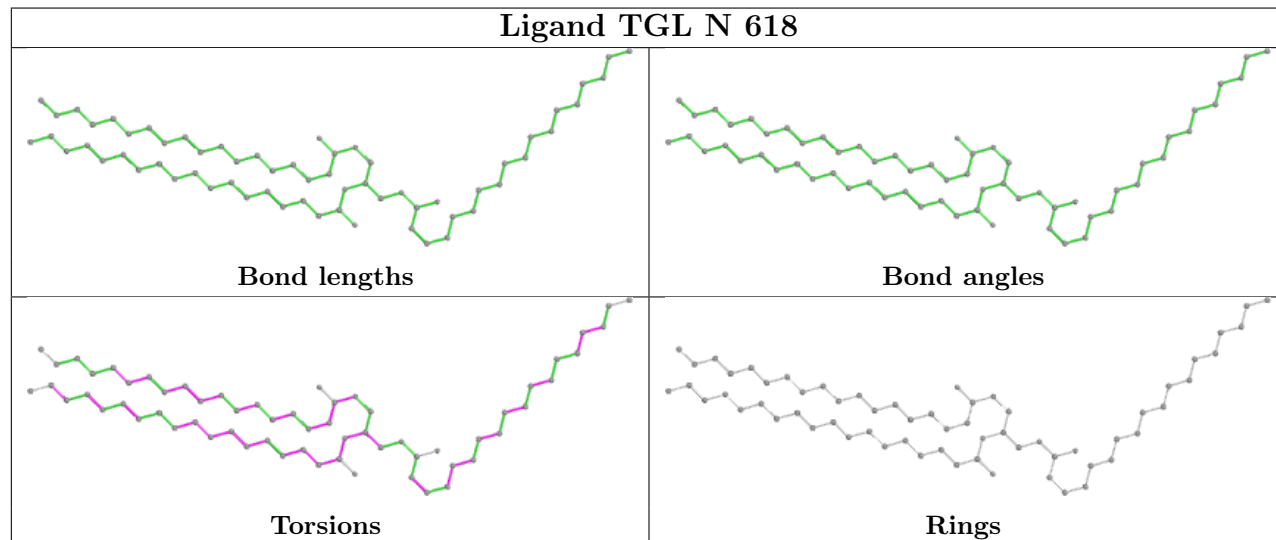
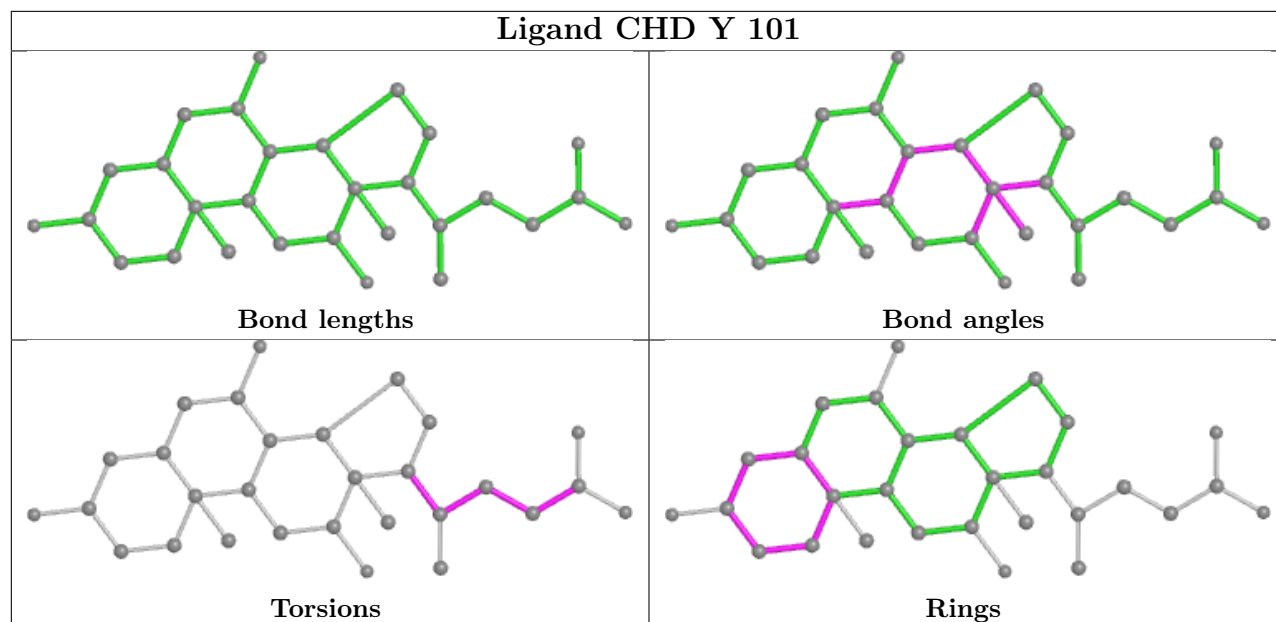
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

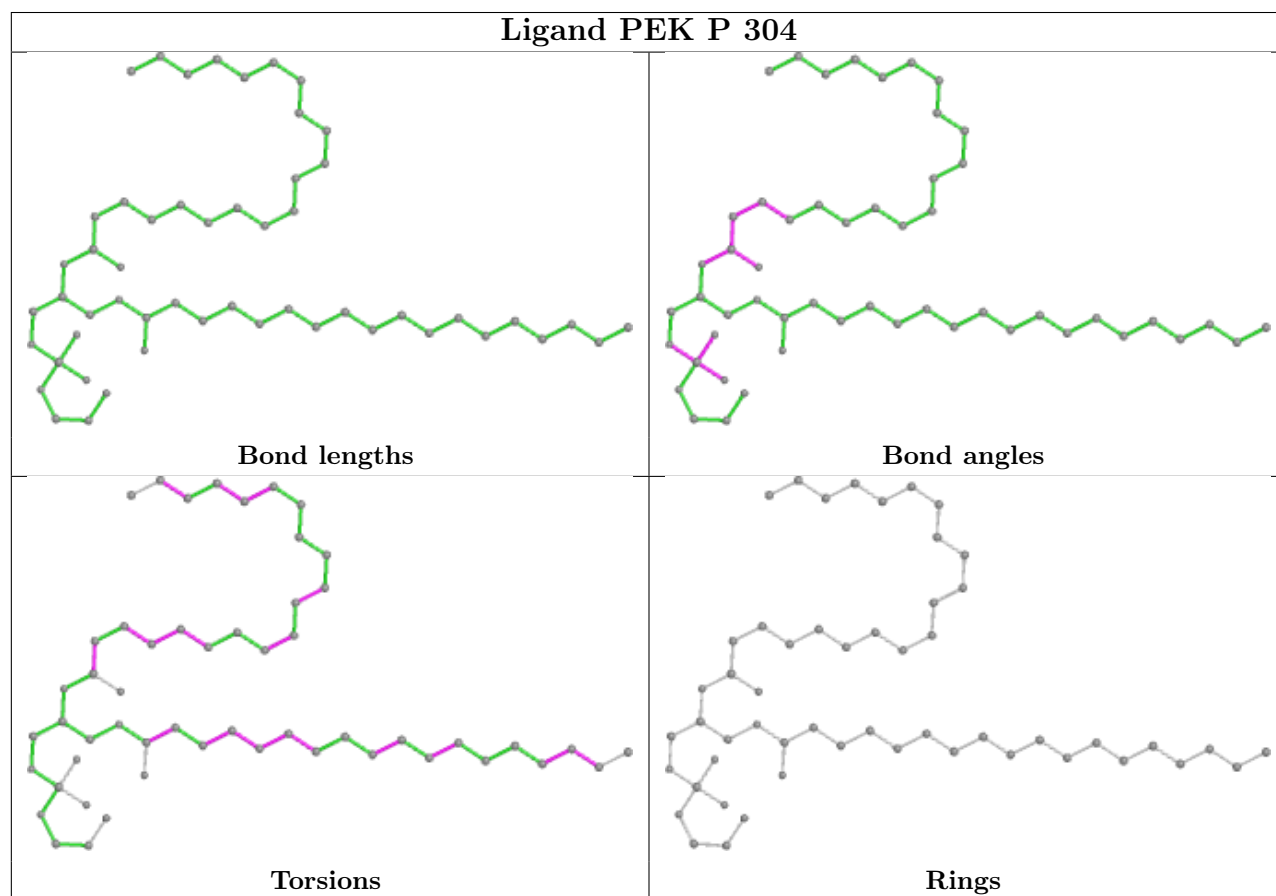
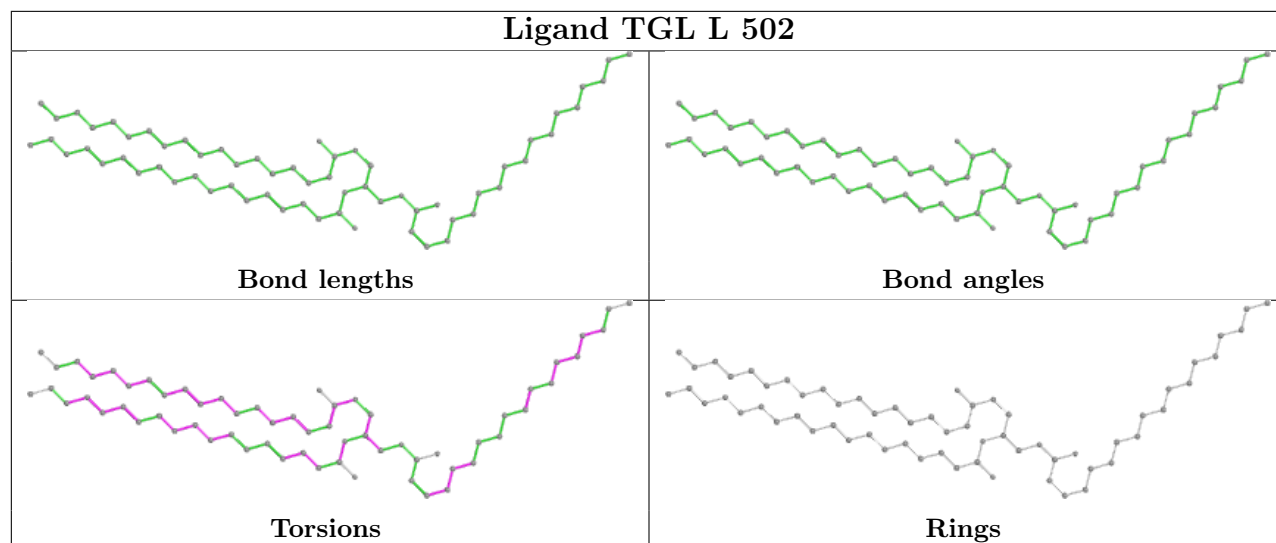




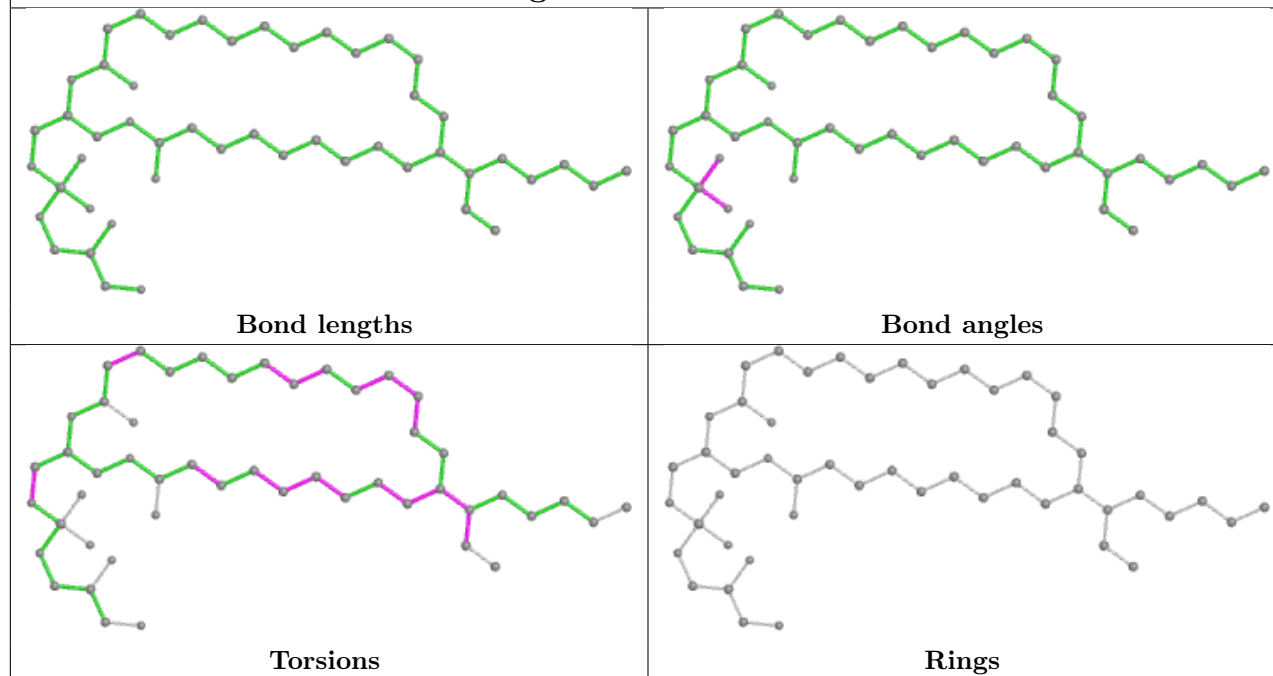




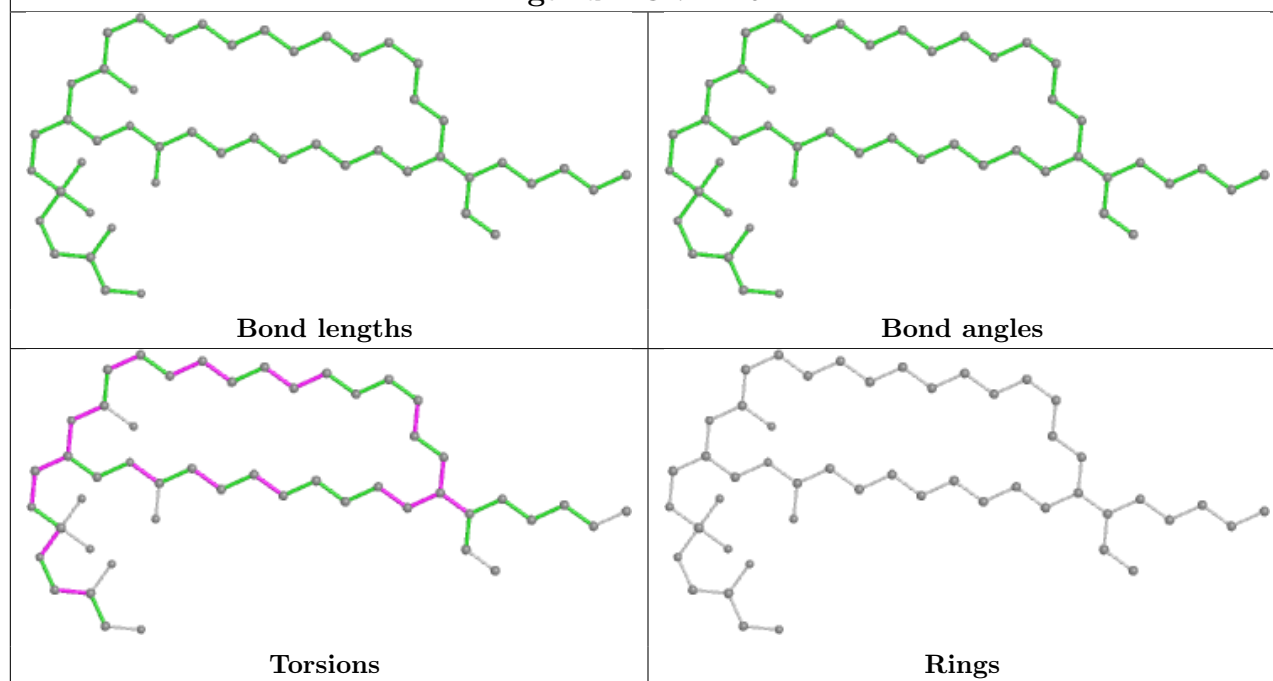


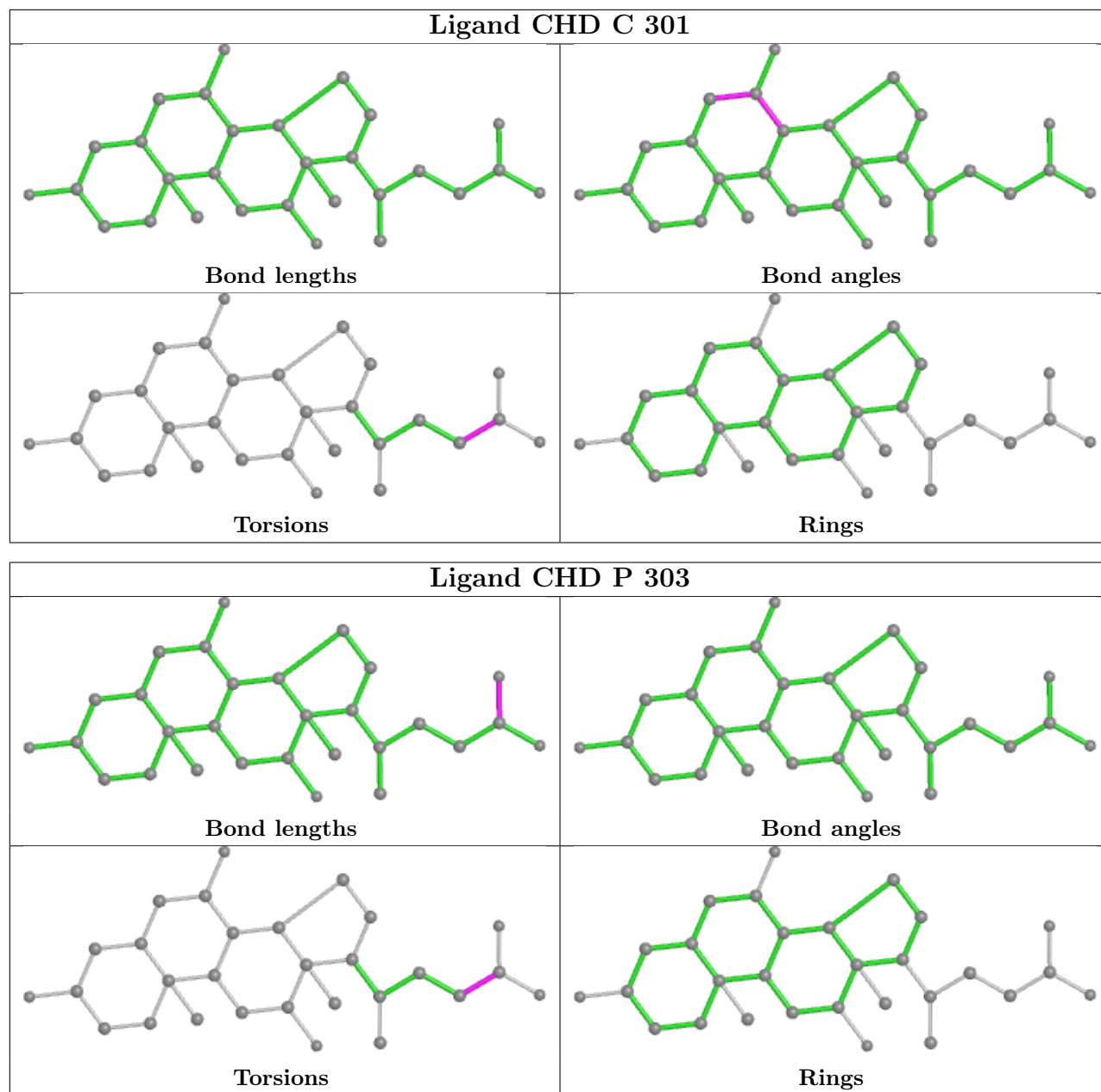


Ligand PGV P 306

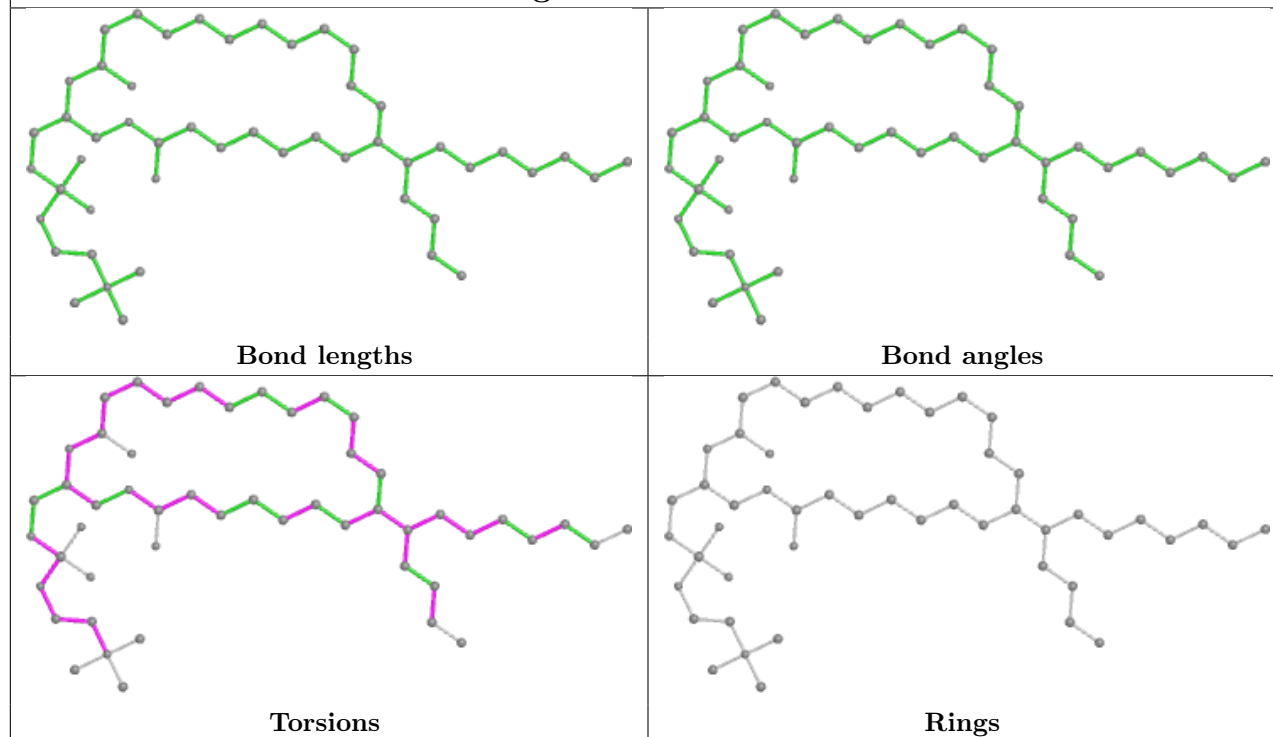


Ligand PGV N 622

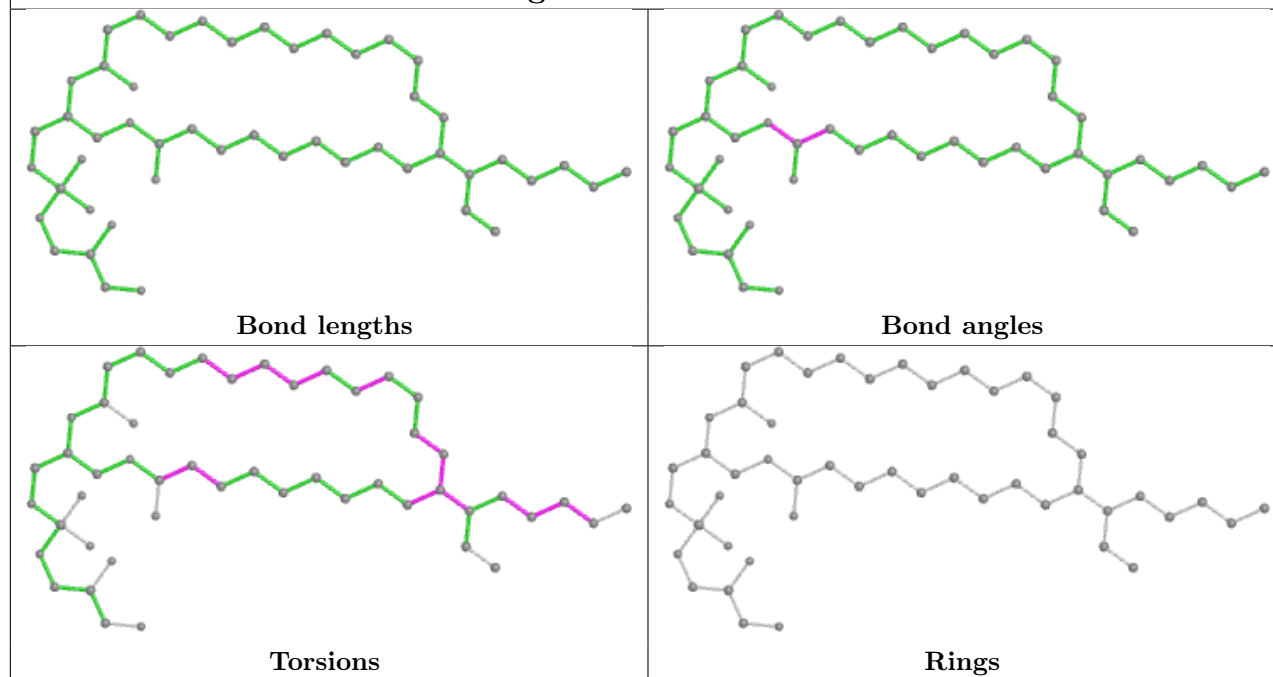


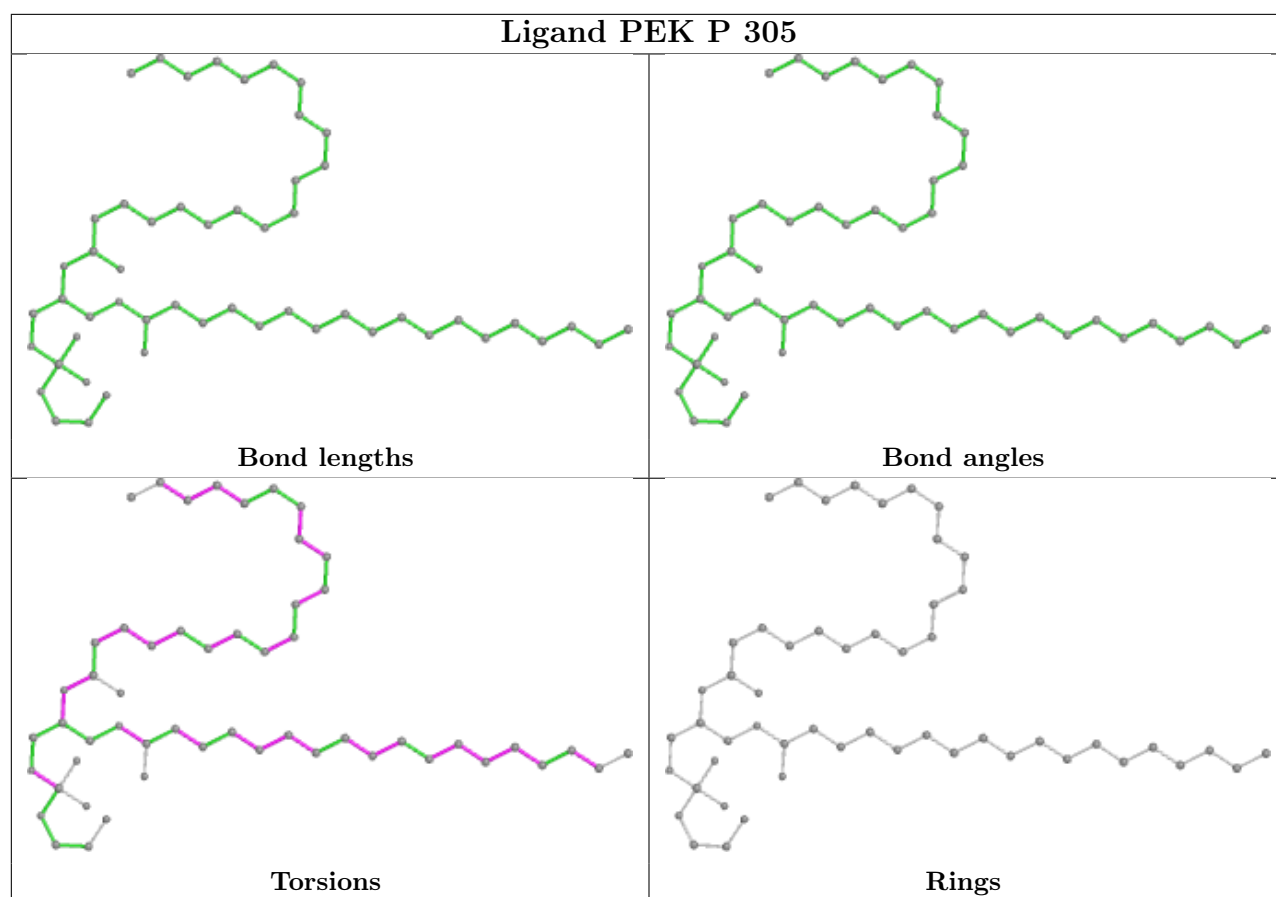


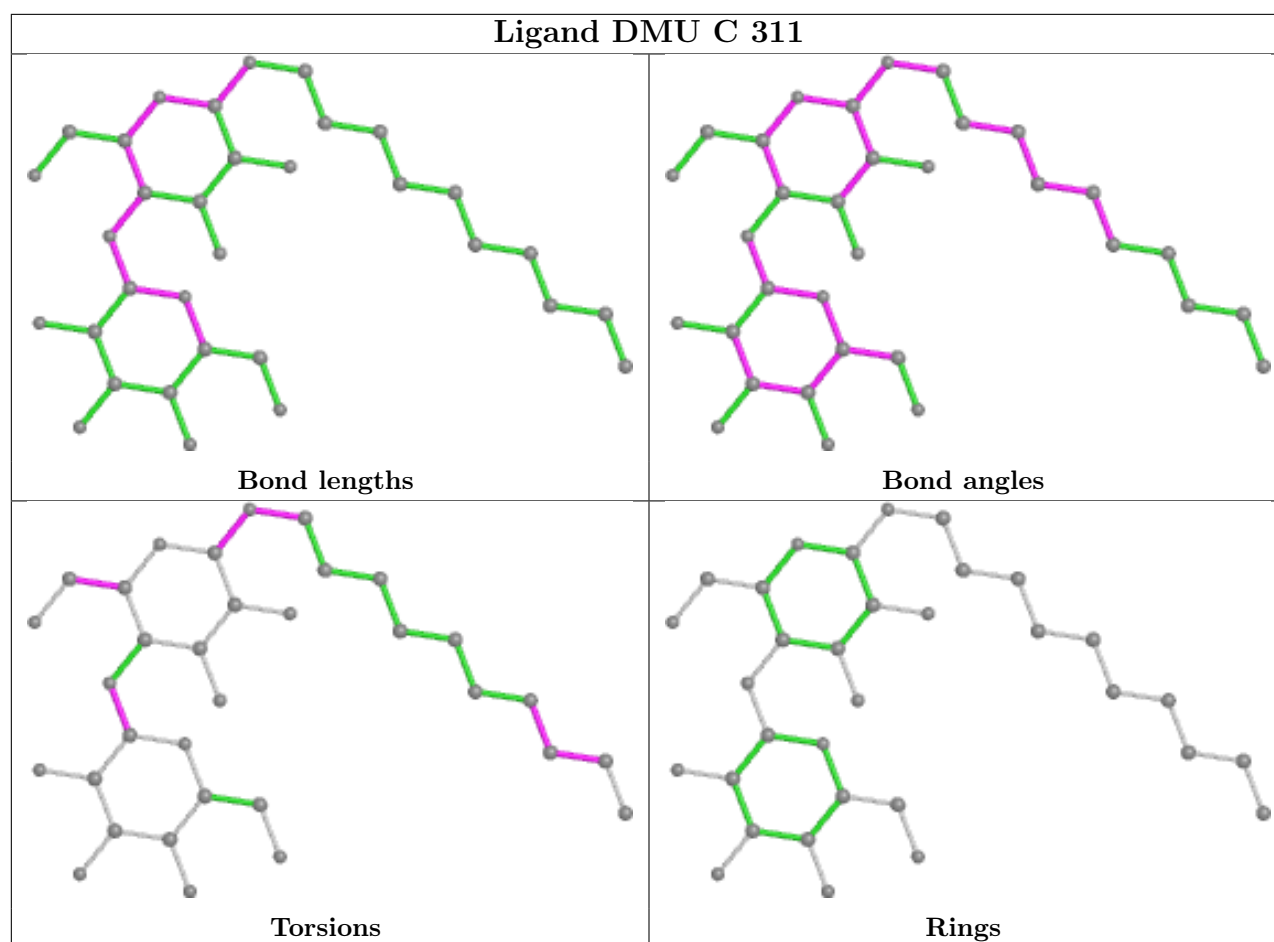
Ligand PSC R 201



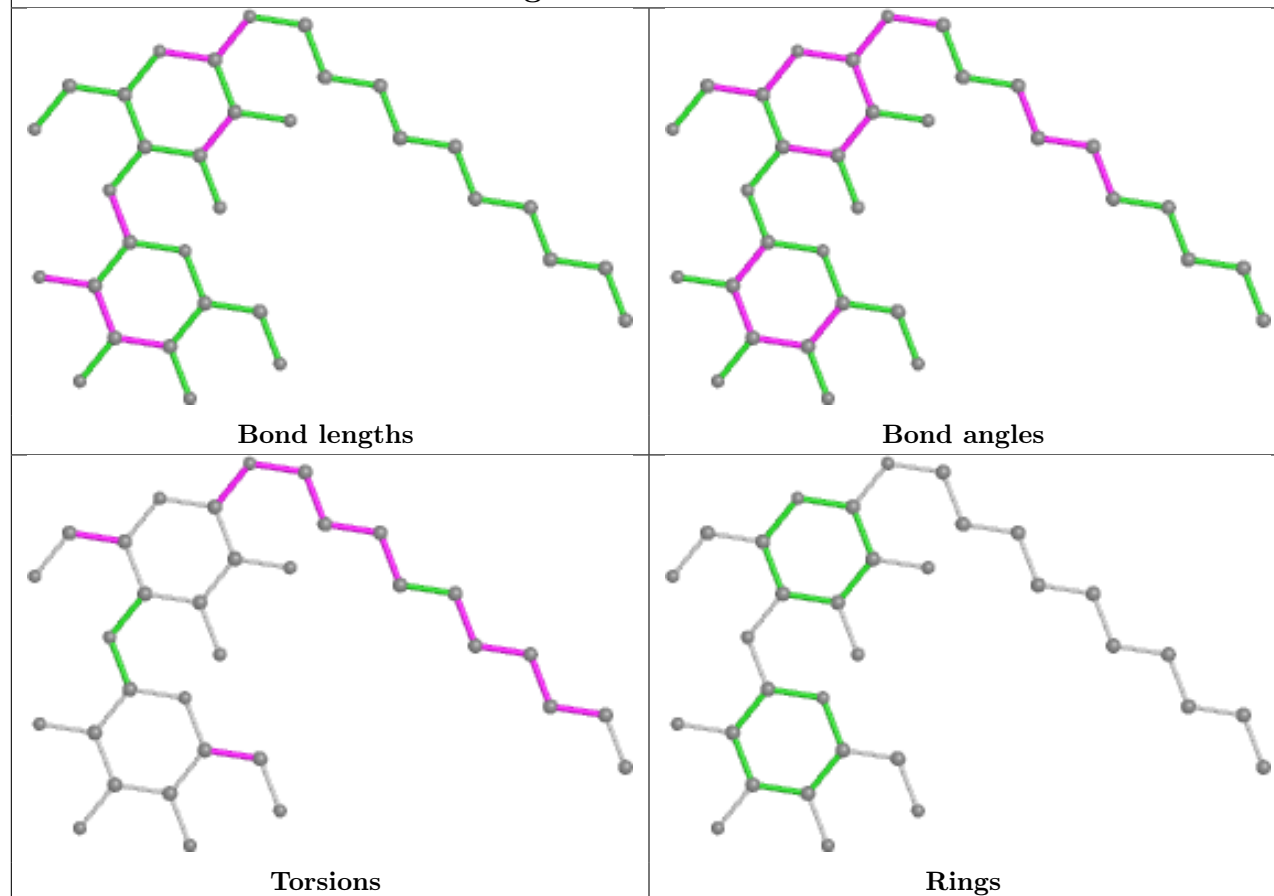
Ligand PGV A 604



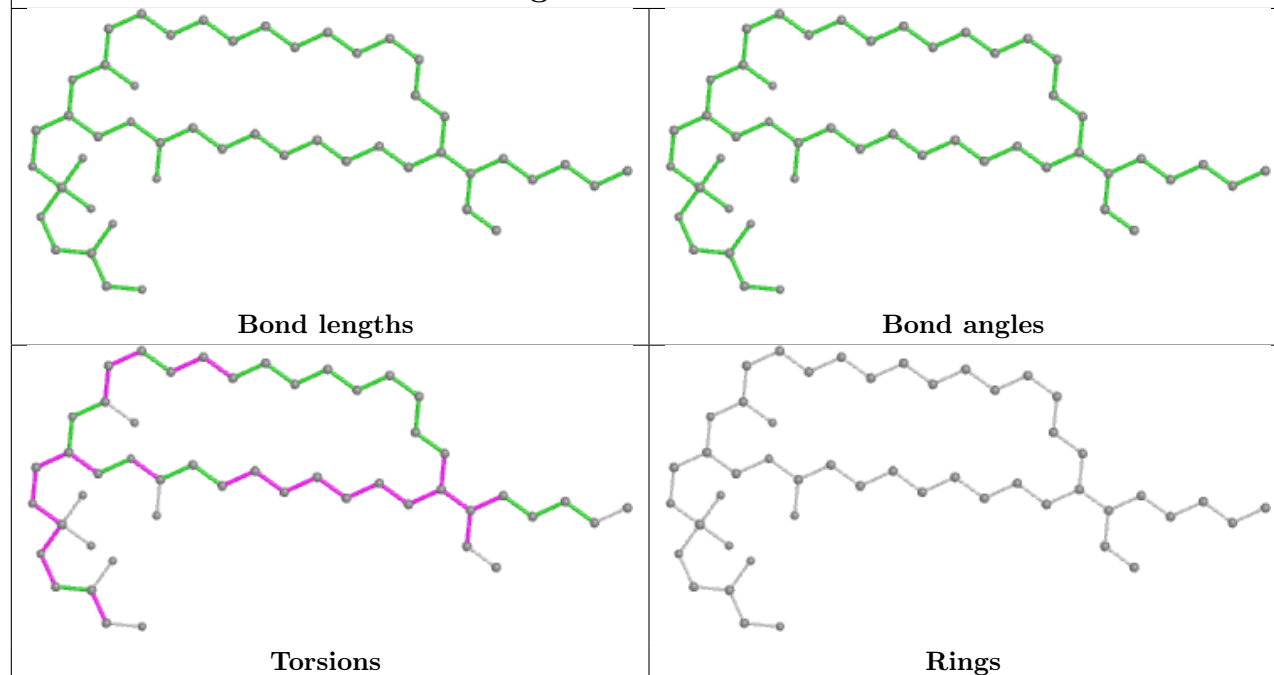




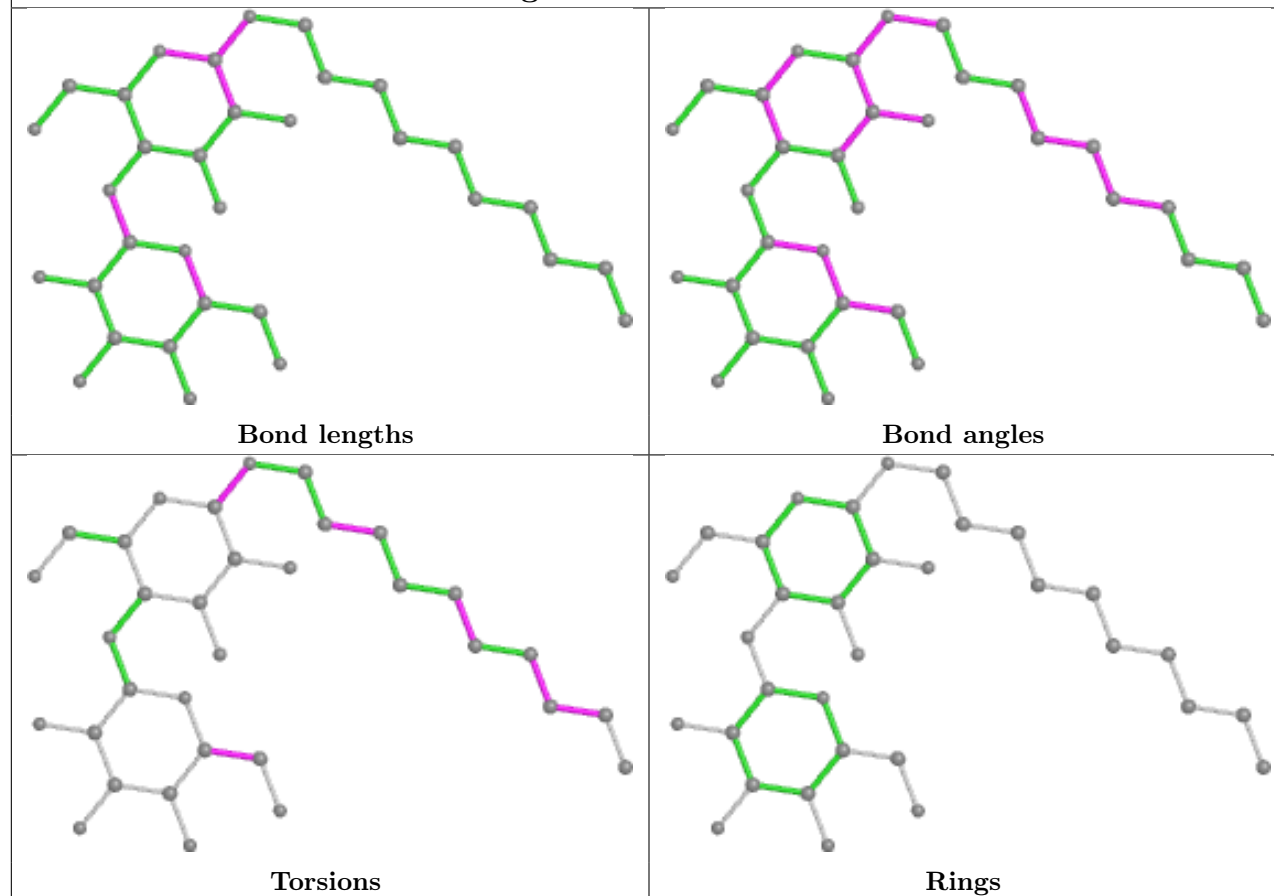
Ligand DMU G 101



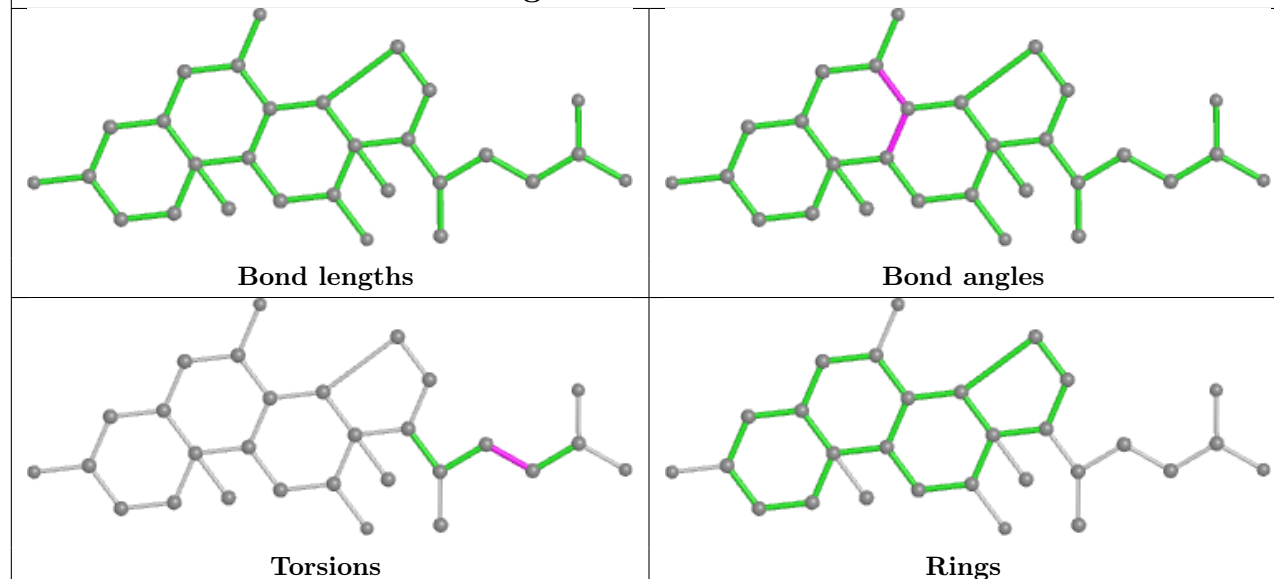
Ligand PGV P 307

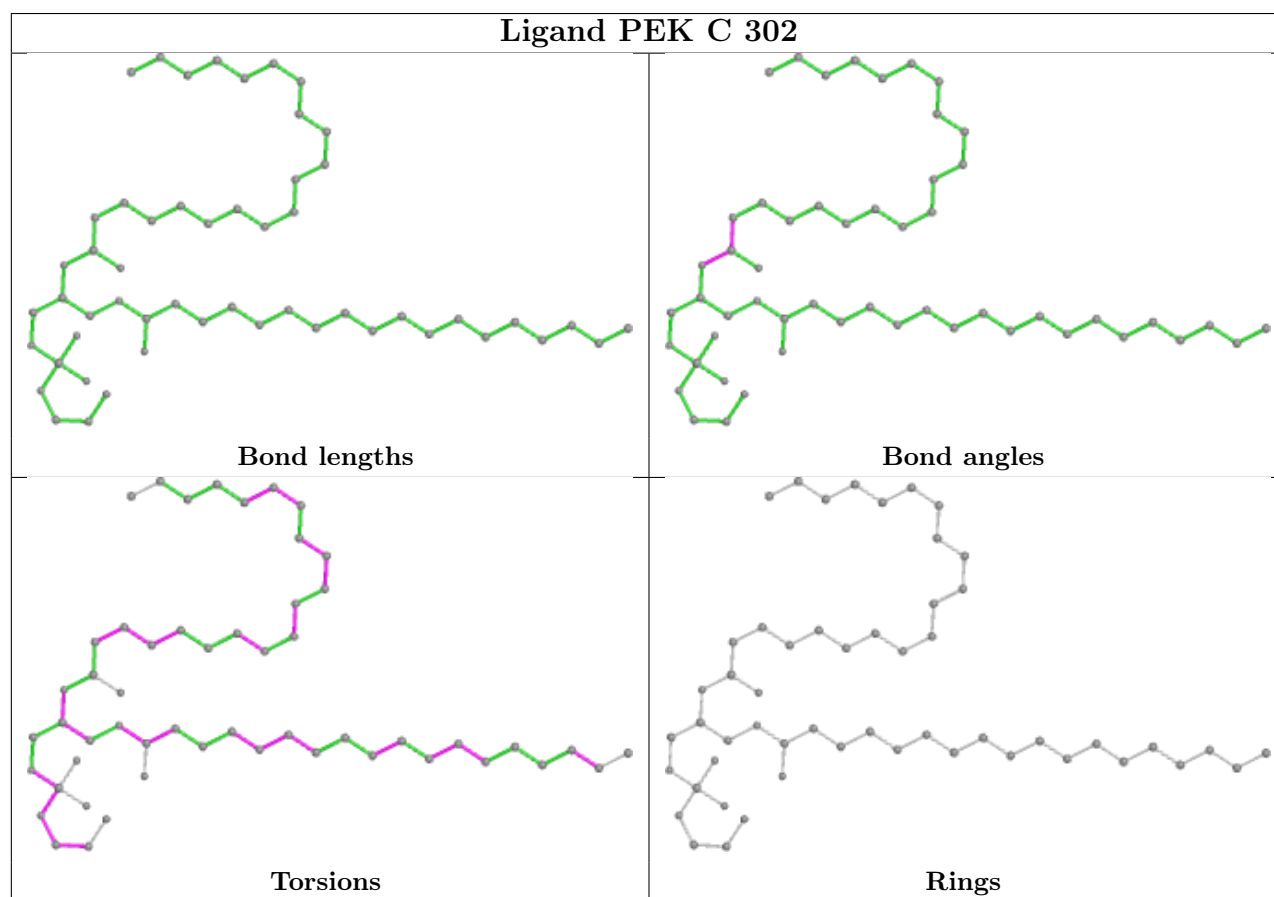
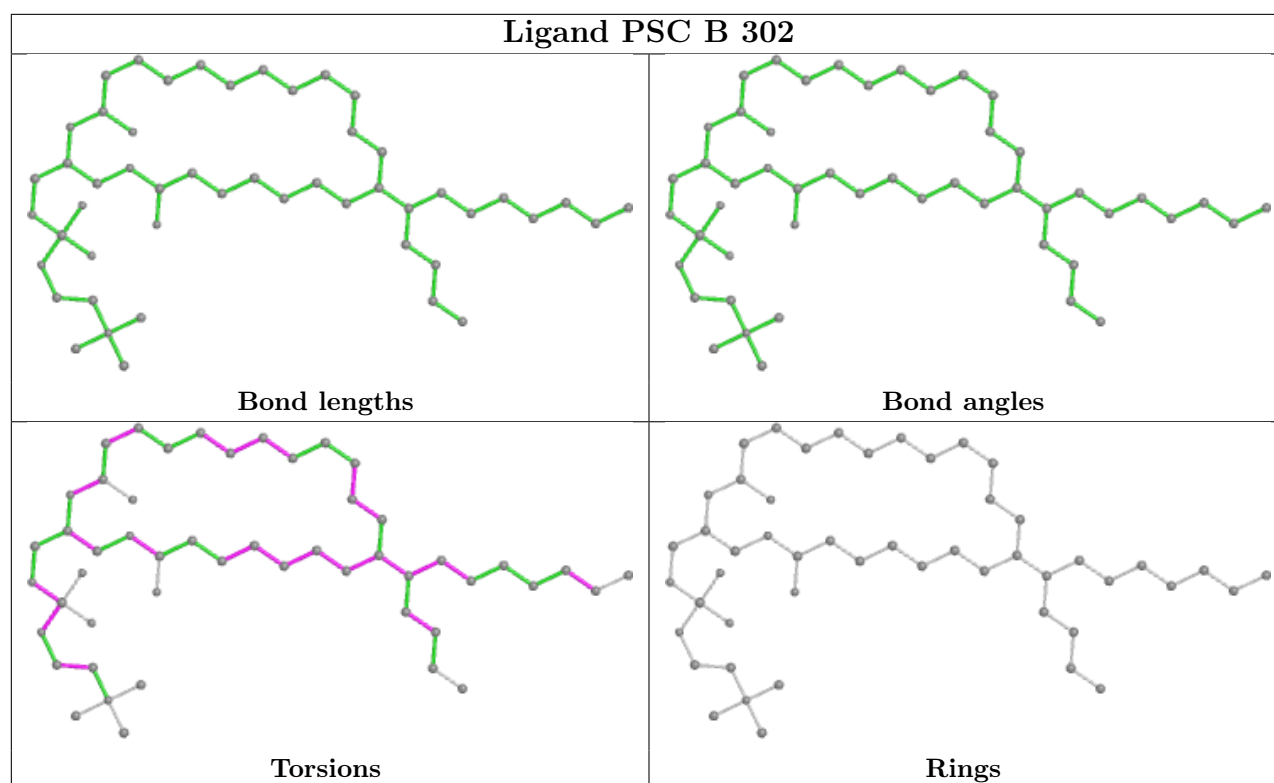


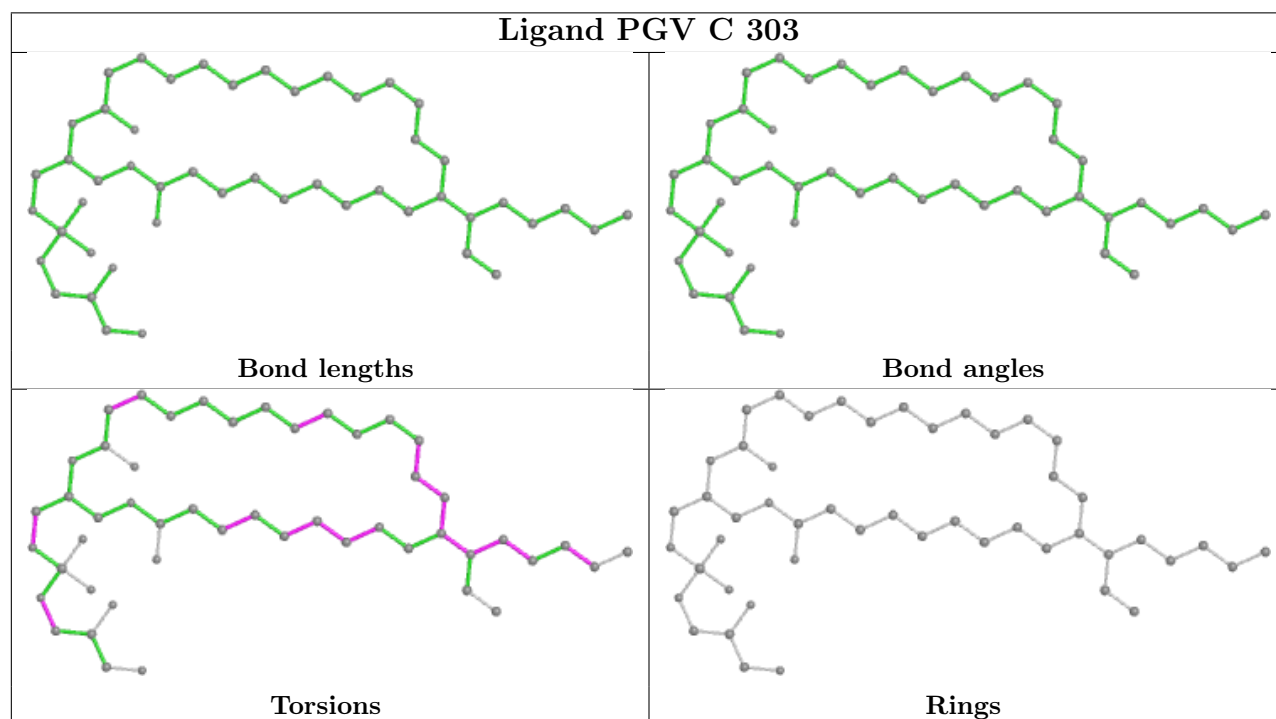
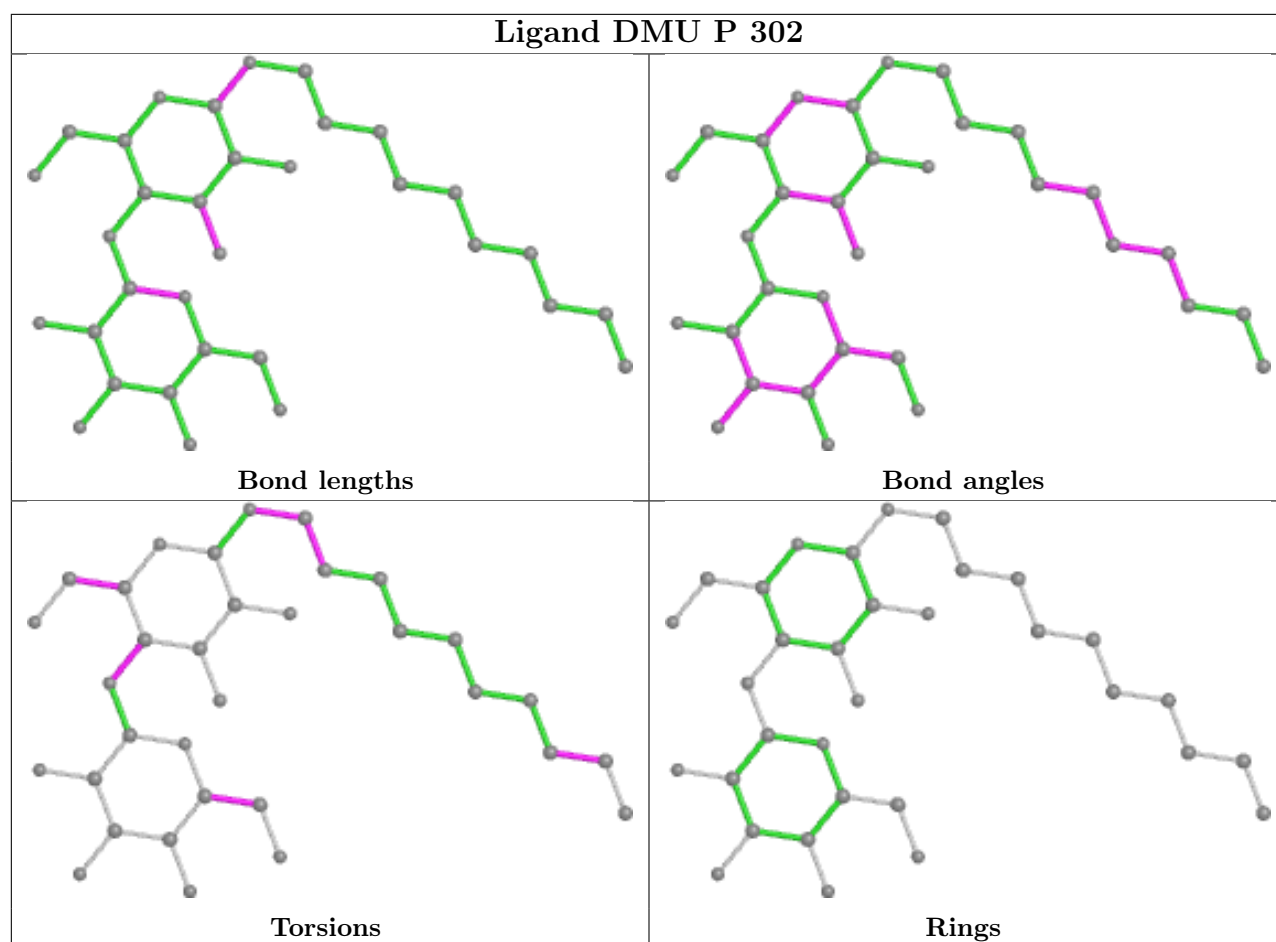
Ligand DMU M 102

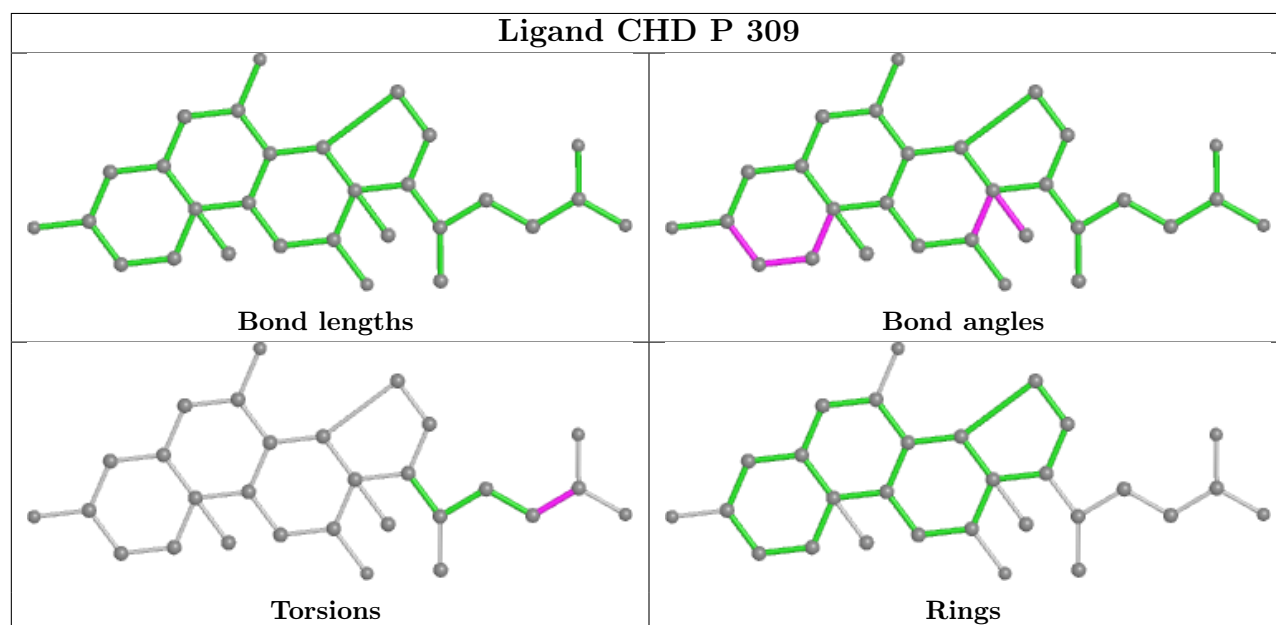
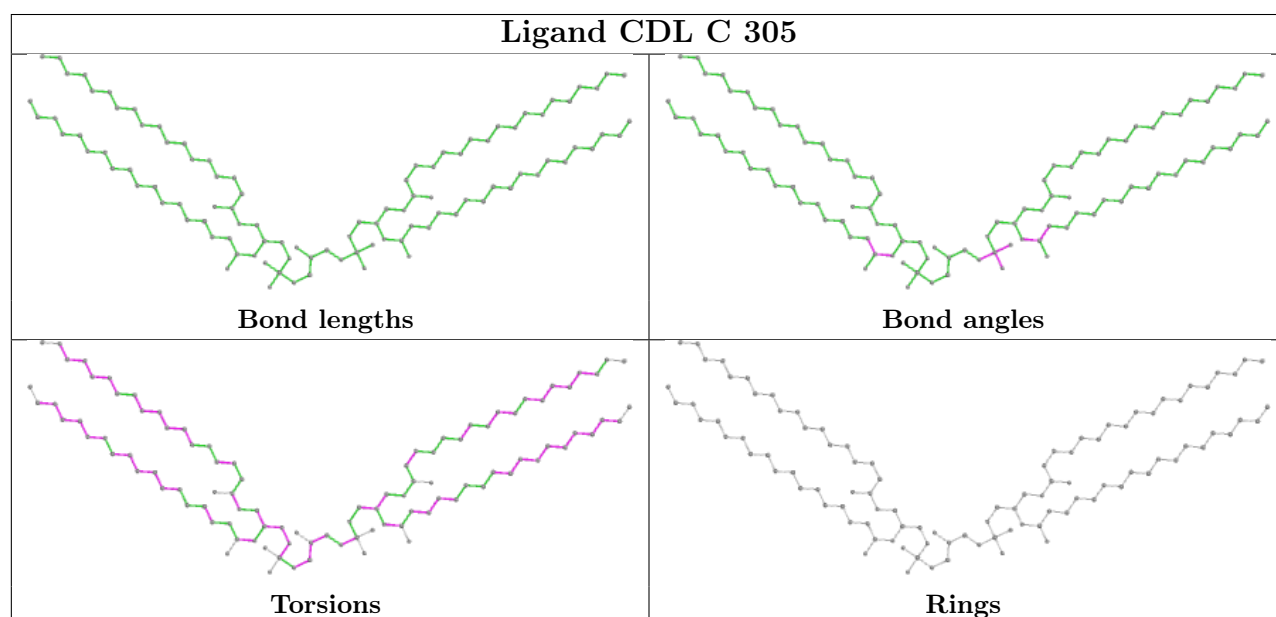
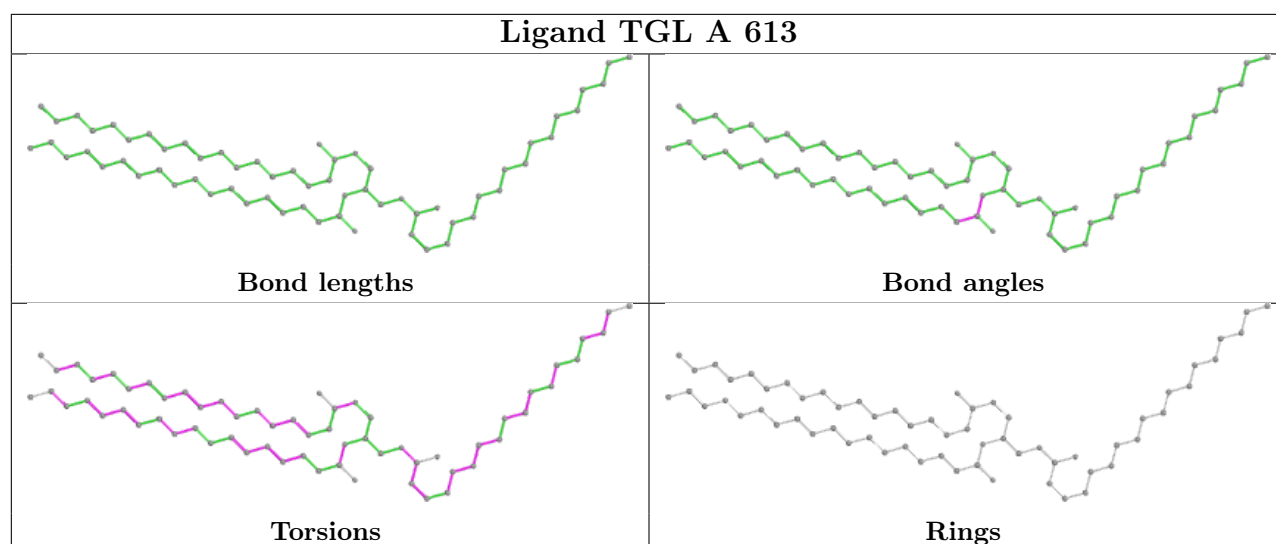


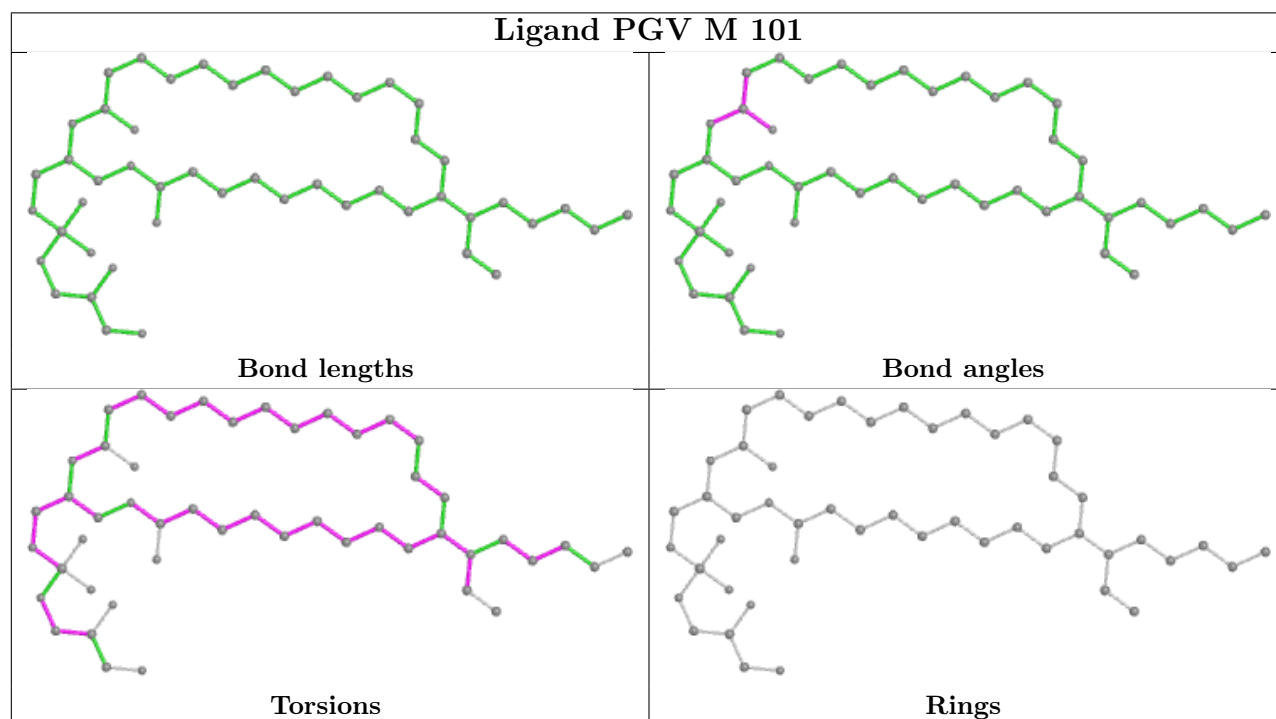
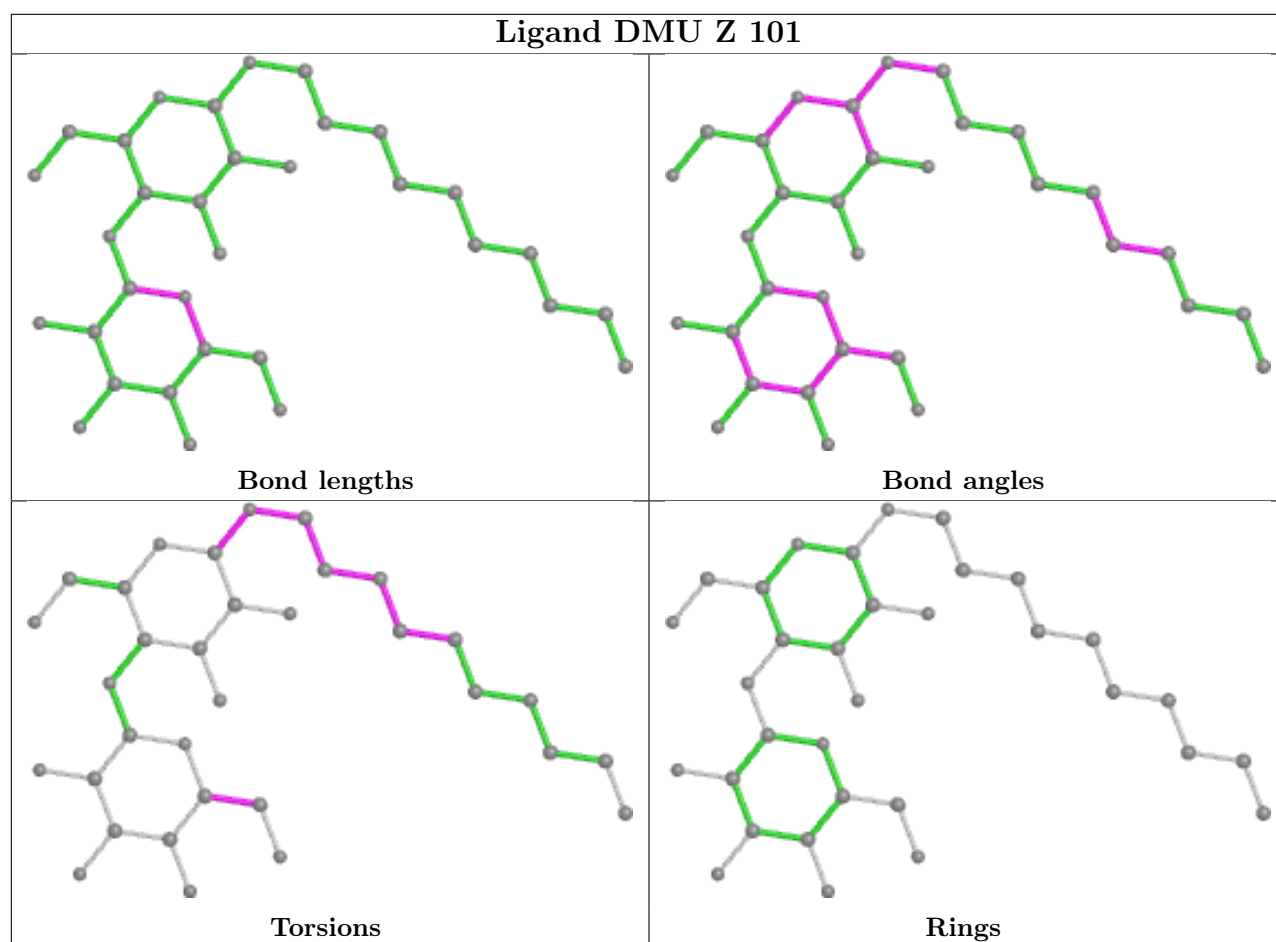
Ligand CHD W 302

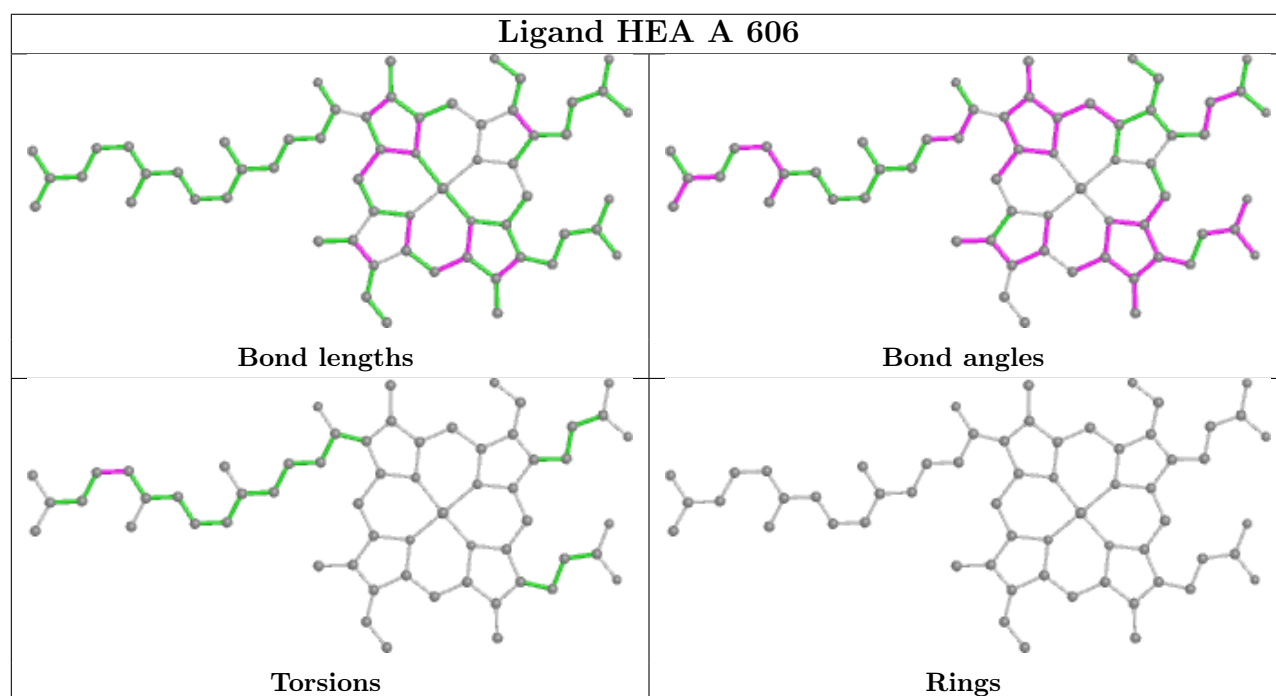
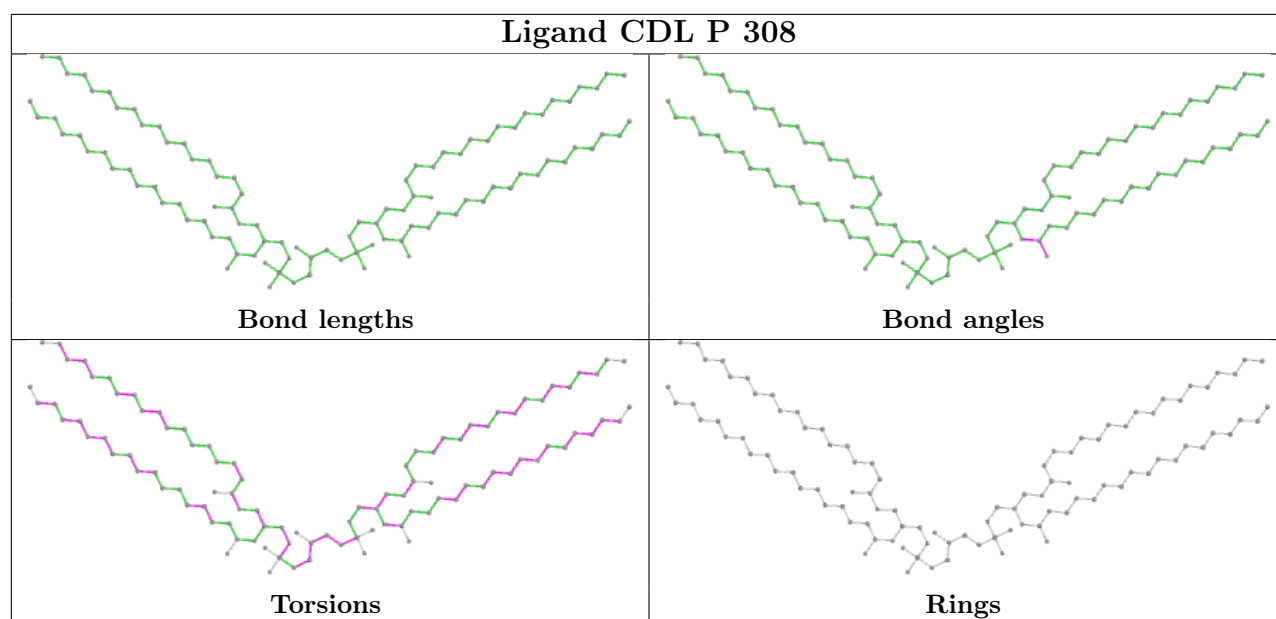




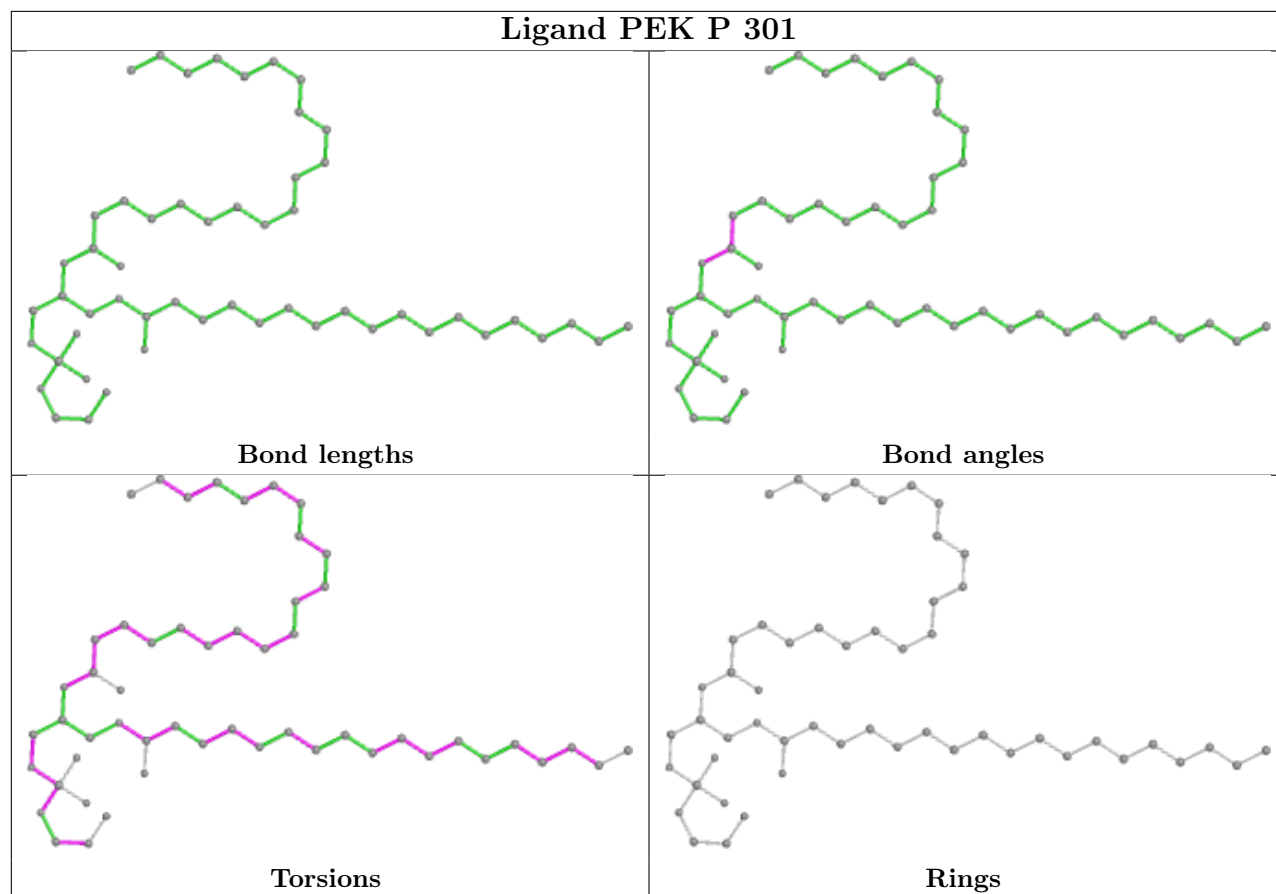




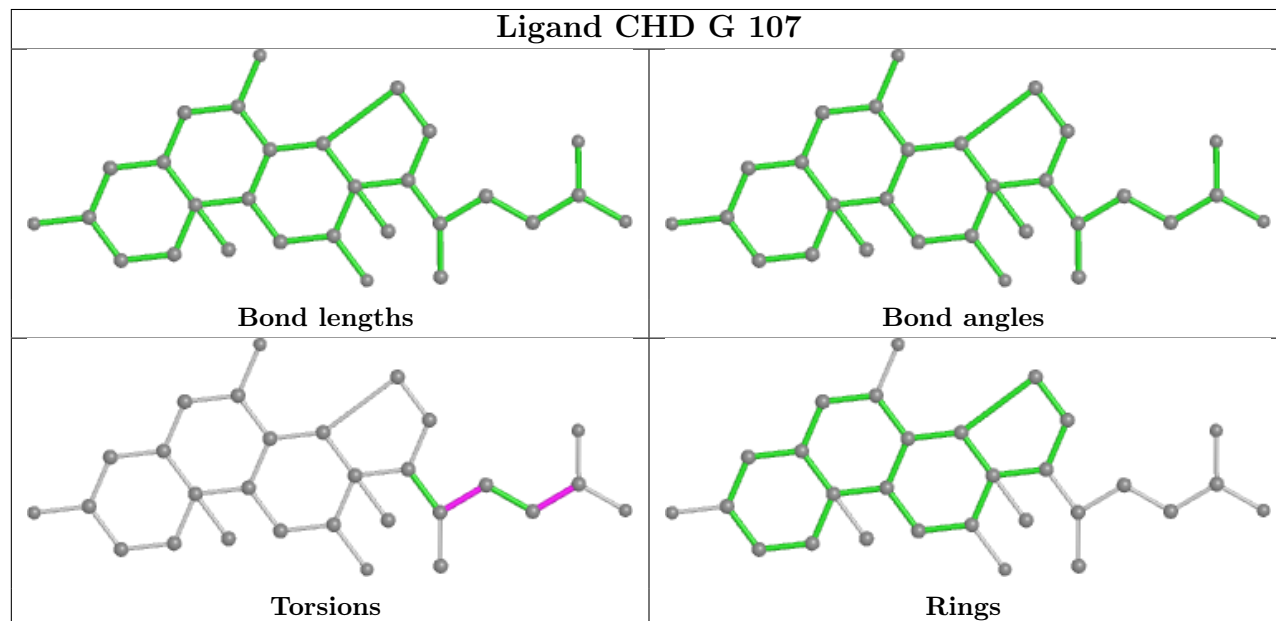


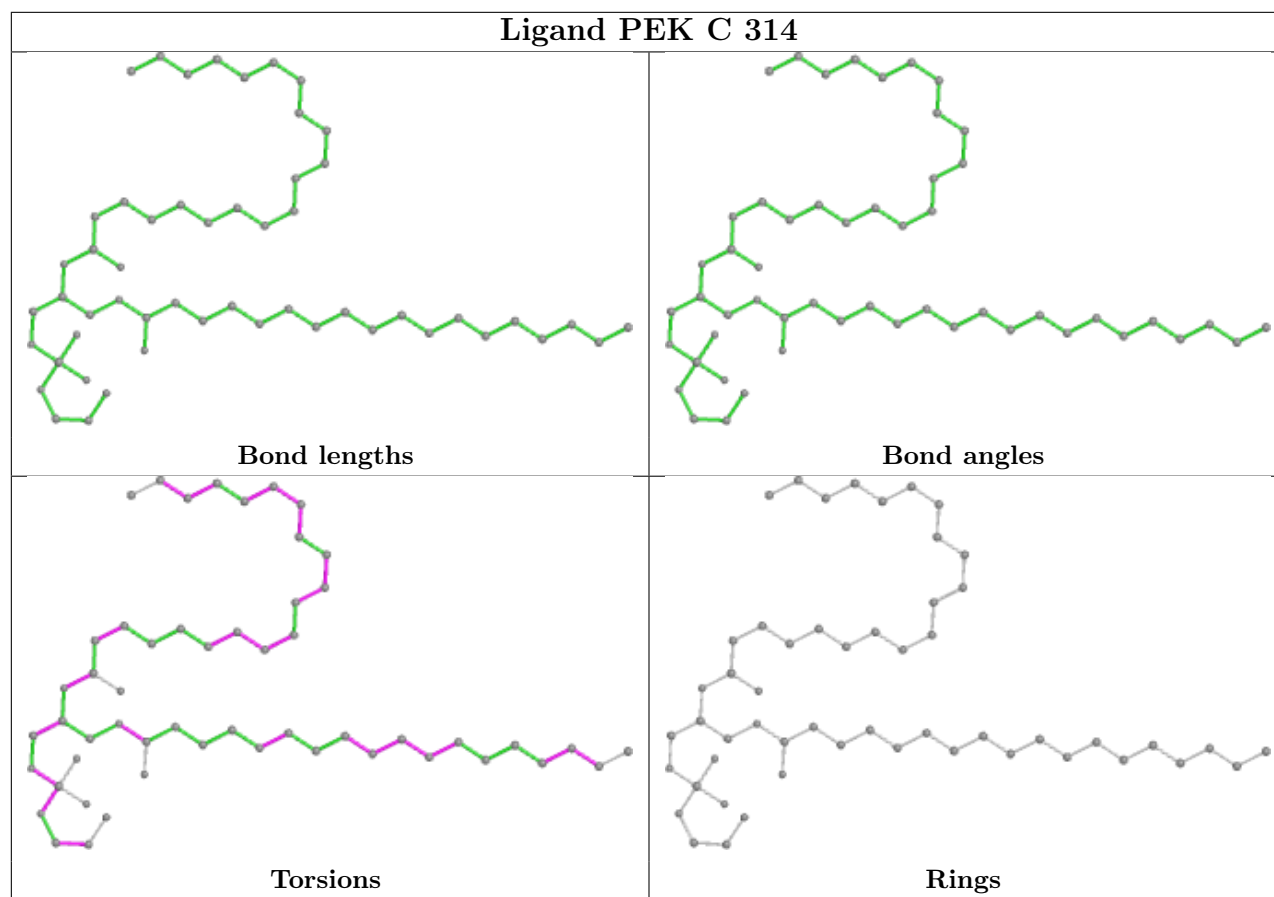
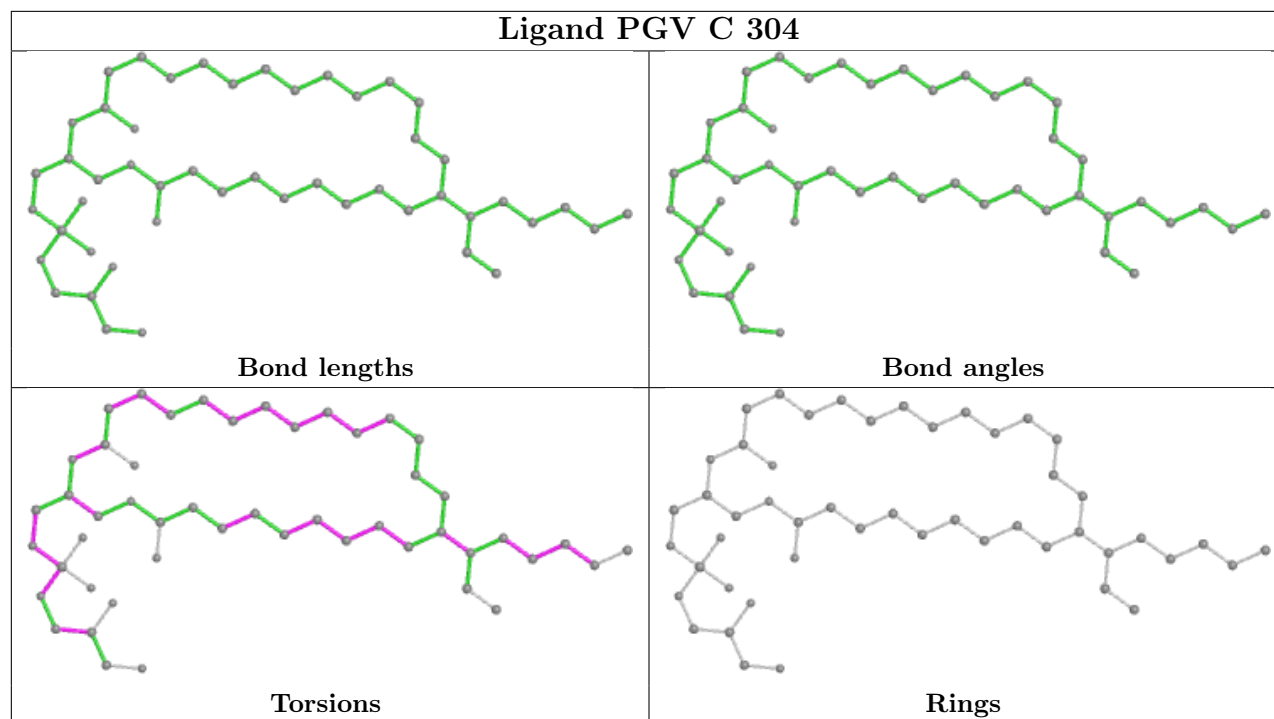


Ligand PEK P 301

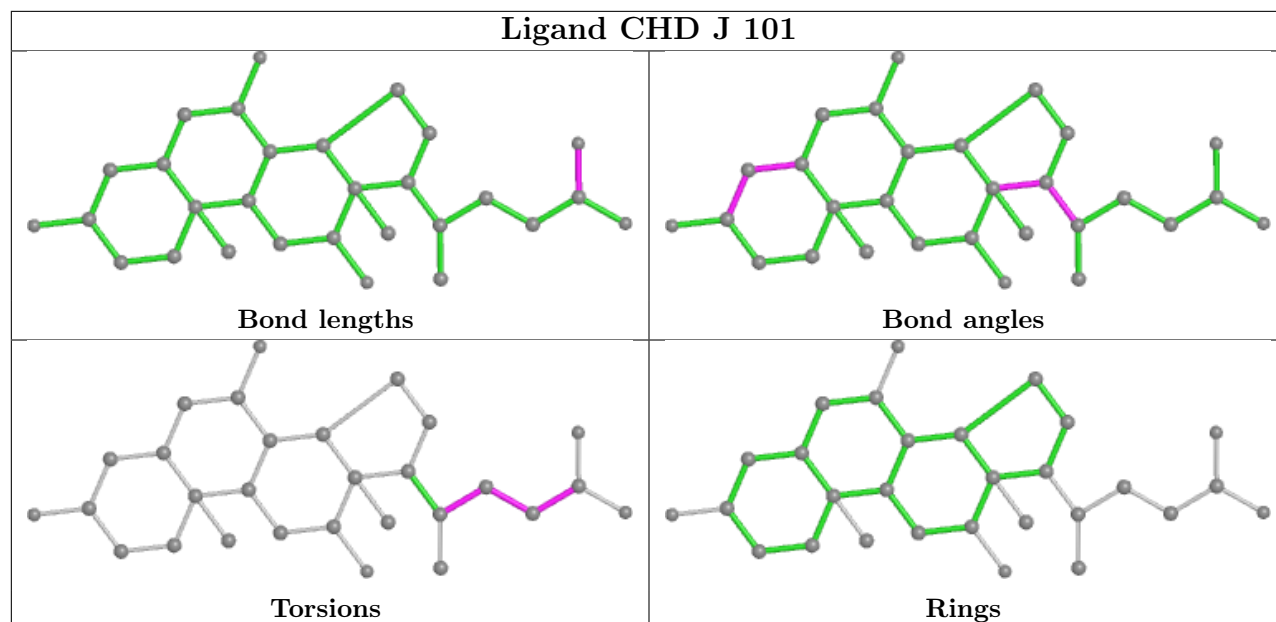


Ligand CHD G 107

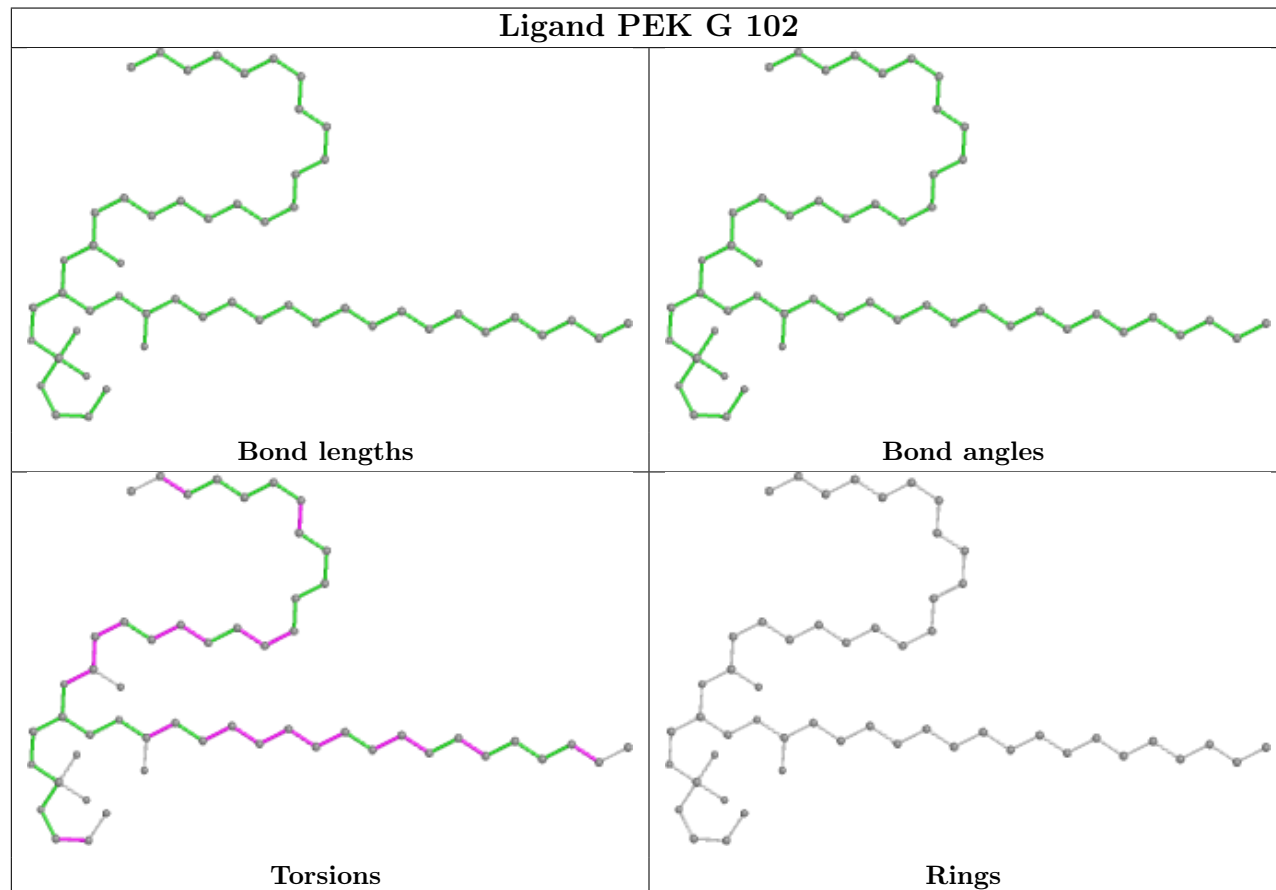


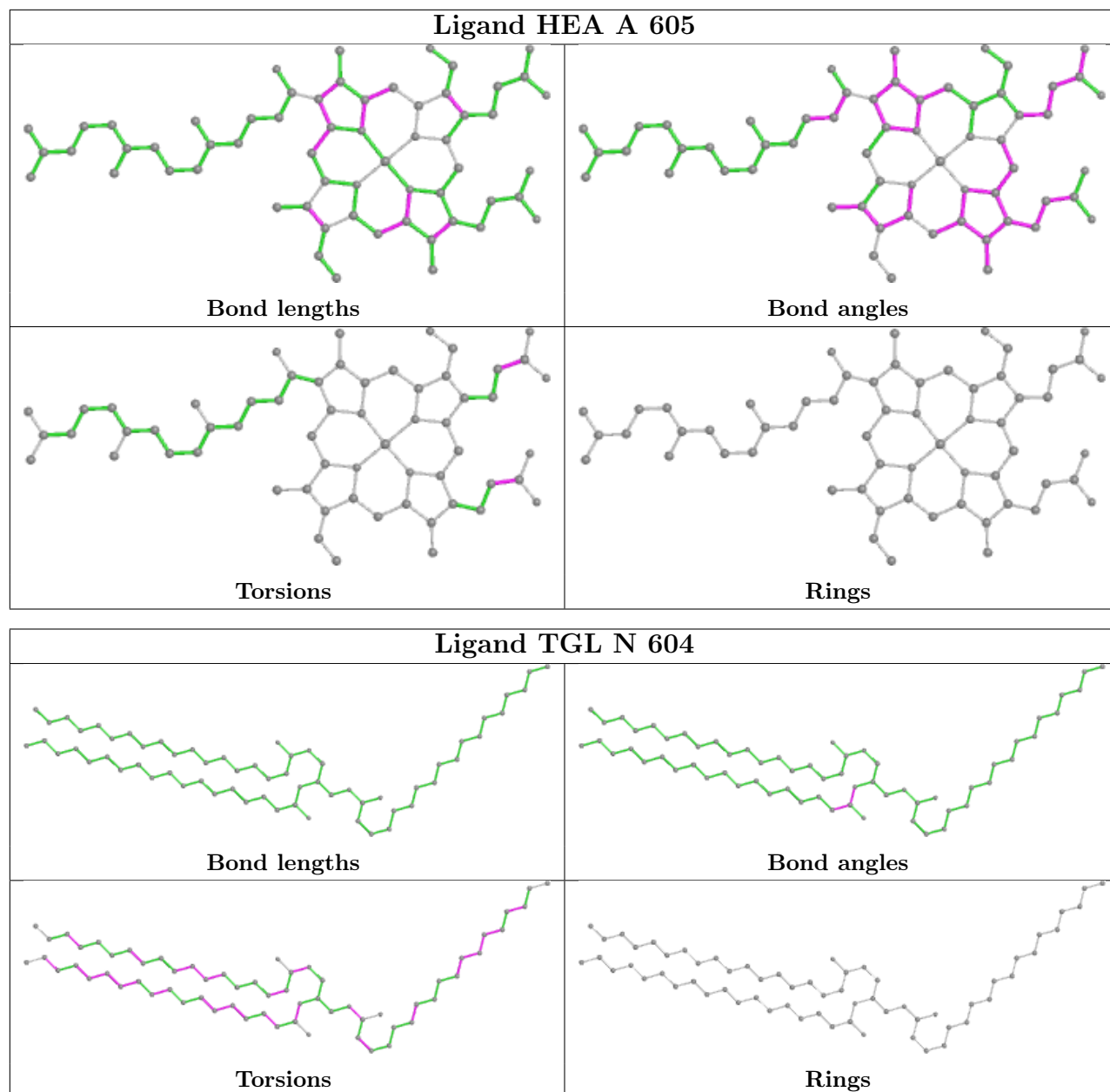


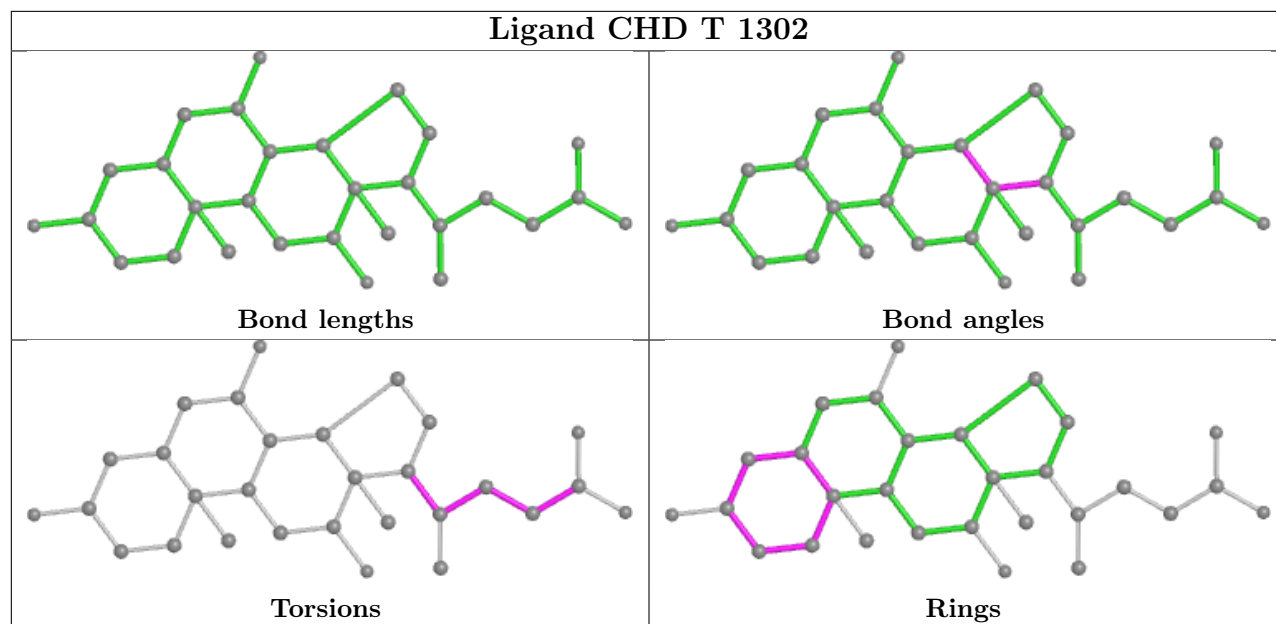
Ligand CHD J 101



Ligand PEK G 102







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%)	0.09	8 (1%) 72 74	23, 29, 37, 72	0
1	N	513/514 (99%)	0.10	11 (2%) 63 66	28, 35, 46, 77	0
2	B	226/227 (99%)	-0.24	3 (1%) 77 79	25, 35, 57, 78	0
2	O	226/227 (99%)	-0.06	10 (4%) 34 37	33, 43, 70, 90	0
3	C	259/261 (99%)	-0.41	1 (0%) 92 93	27, 33, 45, 81	0
3	P	259/261 (99%)	-0.46	1 (0%) 92 93	29, 37, 51, 84	0
4	D	144/147 (97%)	-0.35	2 (1%) 75 77	32, 39, 54, 80	0
4	Q	144/147 (97%)	0.73	16 (11%) 5 6	41, 55, 81, 164	0
5	E	105/109 (96%)	-0.18	2 (1%) 66 69	34, 42, 67, 120	0
5	R	105/109 (96%)	0.23	4 (3%) 40 43	39, 51, 69, 119	0
6	F	98/98 (100%)	0.58	12 (12%) 4 4	30, 40, 82, 140	0
6	S	98/98 (100%)	0.26	8 (8%) 11 13	32, 44, 81, 118	0
7	G	83/85 (97%)	0.75	16 (19%) 1 1	31, 40, 110, 119	0
7	T	83/85 (97%)	1.02	22 (26%) 0 0	32, 46, 108, 117	0
8	H	79/85 (92%)	0.51	14 (17%) 1 1	31, 43, 92, 105	0
8	U	79/85 (92%)	0.84	15 (18%) 1 1	40, 49, 104, 130	0
9	I	72/73 (98%)	0.61	10 (13%) 2 3	32, 48, 69, 83	0
9	V	72/73 (98%)	0.82	16 (22%) 0 0	38, 54, 77, 100	0
10	J	58/59 (98%)	0.21	6 (10%) 6 7	33, 44, 71, 119	0
10	W	58/59 (98%)	0.39	6 (10%) 6 7	39, 50, 77, 122	0
11	K	49/56 (87%)	0.29	2 (4%) 37 40	32, 42, 59, 81	0
11	X	49/56 (87%)	1.06	10 (20%) 1 1	47, 54, 74, 111	0
12	L	46/47 (97%)	-0.37	1 (2%) 62 64	30, 36, 57, 99	0
12	Y	46/47 (97%)	-0.08	2 (4%) 35 38	39, 47, 75, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.05	4 (9%) 8 10	33, 36, 64, 99	0
13	Z	43/46 (93%)	0.55	5 (11%) 4 5	43, 50, 76, 112	0
All	All	3550/3614 (98%)	0.11	207 (5%) 23 25	23, 39, 71, 164	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	18.1
4	Q	6	VAL	15.4
6	F	97	ALA	14.0
6	F	98	HIS	12.2
4	Q	4	SER	10.9
8	U	8	ILE	10.8
6	S	96	LEU	9.9
6	F	96	LEU	9.6
8	H	45	ALA	9.3
7	T	36	TRP	9.3
5	R	109	VAL	9.2
7	G	3	ALA	9.1
7	T	10	GLY	9.0
11	X	6	ALA	8.8
9	I	37	PHE	7.8
8	U	7	LYS	7.8
7	T	3	ALA	7.2
13	Z	43	SER	7.2
8	U	45	ALA	7.1
5	E	5	HIS	7.0
5	R	5	HIS	7.0
7	G	2	SER	6.9
6	F	1	ALA	6.8
7	G	7	ASP	6.7
9	V	37	PHE	6.7
2	O	90	ILE	6.6
10	J	1	PHE	6.3
6	S	98	HIS	6.2
8	U	10	ASN	6.1
11	K	7	PRO	6.1
10	W	58	LYS	6.1
11	X	7	PRO	6.0
7	G	10	GLY	6.0
8	U	44	THR	6.0

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Mol	Chain	Res	Type	RSRZ
7	G	40	GLY	5.8
10	J	58	LYS	5.8
7	T	40	GLY	5.7
9	I	25	PHE	5.5
5	E	109	VAL	5.4
4	Q	33	LEU	5.3
4	Q	7	LYS	5.2
7	G	9	GLY	5.2
13	Z	42	LYS	5.2
7	G	36	TRP	5.2
10	W	57	HIS	5.2
7	T	7	ASP	5.1
8	U	9	LYS	5.1
7	G	42	ARG	5.0
2	O	113	TYR	5.0
6	S	95	GLN	4.9
11	X	13	TYR	4.9
13	M	43	SER	4.8
10	J	57	HIS	4.8
8	H	9	LYS	4.8
8	H	48	GLY	4.7
7	T	42	ARG	4.7
6	F	95	GLN	4.7
9	V	2	THR	4.6
10	W	52	TRP	4.6
9	I	33	THR	4.5
8	H	47	GLY	4.5
7	G	5	LYS	4.4
7	T	41	HIS	4.3
9	I	34	PHE	4.3
4	Q	147	LYS	4.3
5	R	108	LYS	4.2
8	U	48	GLY	4.2
4	Q	46	ALA	4.2
6	S	97	ALA	4.1
4	D	147	LYS	4.1
2	O	227	LEU	4.0
6	S	94	HIS	4.0
9	V	34	PHE	4.0
7	T	84	LYS	4.0
7	G	43	GLU	4.0
4	Q	51	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	4.0
2	O	224	ALA	4.0
8	H	44	THR	3.9
8	H	8	ILE	3.9
8	H	46	LYS	3.8
10	W	48	TYR	3.7
4	Q	48	TRP	3.7
13	Z	40	TYR	3.7
11	K	6	ALA	3.7
9	I	29	LEU	3.6
2	B	90	ILE	3.6
10	W	1	PHE	3.6
6	F	2	SER	3.6
12	Y	47	LYS	3.6
7	G	84	LYS	3.6
9	V	25	PHE	3.5
7	T	1	ALA	3.5
8	U	47	GLY	3.5
7	T	47	PHE	3.5
7	T	5	LYS	3.4
11	X	12	LYS	3.4
4	Q	39	ALA	3.4
7	T	45	PRO	3.3
10	J	55	PHE	3.3
7	T	8	HIS	3.3
2	O	59	GLN	3.2
7	T	43	GLU	3.2
7	G	8	HIS	3.2
7	T	46	ALA	3.2
6	F	94	HIS	3.2
7	G	37	LEU	3.2
13	M	39	ASN	3.1
4	Q	8	SER	3.1
8	U	49	ASP	3.1
7	T	2	SER	3.1
13	Z	35	TYR	3.1
11	X	19	ALA	3.0
9	V	31	PHE	3.0
7	G	39	SER	3.0
8	U	42	ALA	3.0
11	X	47	ARG	3.0
7	G	41	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
8	U	52	VAL	2.9
10	J	56	PRO	2.9
9	V	45	LYS	2.9
2	O	218	TYR	2.9
9	V	33	THR	2.9
3	P	3	HIS	2.9
12	L	2	HIS	2.9
1	A	70	VAL	2.9
9	I	30	GLY	2.9
1	A	66	ILE	2.8
4	Q	35	ALA	2.8
6	S	22	LEU	2.8
2	O	91	ASN	2.8
8	U	50	VAL	2.8
4	Q	73	ARG	2.8
9	V	26	MET	2.8
1	A	381	LEU	2.7
13	Z	41	LYS	2.7
12	Y	20	ARG	2.7
6	F	28	GLN	2.7
2	B	91	ASN	2.7
2	O	60	GLU	2.7
7	T	6	GLY	2.6
4	D	78	TRP	2.6
8	H	50	VAL	2.6
9	V	22	VAL	2.6
8	H	10	ASN	2.6
4	Q	49	SER	2.6
6	F	27	GLY	2.6
1	N	195	LEU	2.6
7	T	33	LEU	2.6
6	S	93	PRO	2.6
1	N	254	ILE	2.5
11	X	18	LEU	2.5
1	N	73	ILE	2.5
9	V	27	VAL	2.5
3	C	3	HIS	2.5
1	N	24	ALA	2.5
6	F	22	LEU	2.5
6	F	3	GLY	2.4
7	T	48	ILE	2.4
2	B	92	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
4	Q	58	GLU	2.4
7	T	39	SER	2.4
8	U	43	MET	2.4
9	I	26	MET	2.4
8	U	11	TYR	2.4
5	R	106	LEU	2.4
1	A	389	ILE	2.4
1	A	73	ILE	2.3
13	M	40	TYR	2.3
8	H	43	MET	2.3
9	V	3	ALA	2.3
1	A	380	VAL	2.3
4	Q	72	ASN	2.3
1	A	374	VAL	2.3
2	O	221	LYS	2.2
9	I	19	PHE	2.2
2	O	92	ASN	2.2
8	H	52	VAL	2.2
6	F	26	LYS	2.2
7	T	49	PRO	2.2
1	N	433	LEU	2.2
13	M	35	TYR	2.2
1	N	70	VAL	2.2
1	N	374	VAL	2.2
10	J	52	TRP	2.2
9	V	30	GLY	2.1
8	H	41	LYS	2.1
9	I	40	ALA	2.1
9	V	19	PHE	2.1
9	V	53	ASN	2.1
1	A	385	ALA	2.1
7	T	4	ALA	2.1
9	I	18	ARG	2.1
1	N	389	ILE	2.1
10	W	30	ILE	2.1
1	N	386	VAL	2.1
9	V	38	ALA	2.1
11	X	46	GLY	2.1
11	X	23	THR	2.0
6	S	1	ALA	2.0
8	U	55	TRP	2.0
8	H	49	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	N	258	VAL	2.0
1	N	257	ILE	2.0
8	H	85	ILE	2.0
9	V	29	LEU	2.0
11	X	15	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	T	11	11/12	0.63	0.33	42,81,138,146	0
7	TPO	G	11	11/12	0.77	0.24	45,80,126,126	0
1	FME	A	1	10/11	0.95	0.15	43,47,72,89	0
2	FME	O	1	10/11	0.97	0.13	37,42,53,65	0
1	FME	N	1	10/11	0.97	0.20	51,56,89,89	0
2	FME	B	1	10/11	0.98	0.11	31,34,50,51	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
27	DMU	G	101	33/33	0.21	0.50	79,121,140,147	0
29	SAC	V	101	9/10	0.26	0.55	95,103,113,114	0
29	SAC	I	101	9/10	0.32	0.37	81,96,103,109	0
19	EDO	W	303	4/4	0.45	0.50	90,96,96,99	0
19	EDO	G	108	4/4	0.56	0.20	90,90,94,98	0
19	EDO	J	102	4/4	0.62	0.14	73,74,74,78	0
25	PEK	C	302	53/53	0.63	0.24	65,84,142,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
25	PEK	P	301	53/53	0.65	0.24	55,83,136,152	0
23	PSC	B	302	52/52	0.65	0.33	47,82,154,167	0
26	CDL	C	310	100/100	0.66	0.30	65,91,146,163	0
24	CHD	Y	101	29/29	0.66	0.33	91,127,145,177	0
19	EDO	P	310	4/4	0.67	0.29	73,73,73,75	0
20	TGL	N	605	63/63	0.67	0.24	52,72,118,136	0
17	PGV	C	304	51/51	0.68	0.26	43,82,124,144	0
25	PEK	P	305	53/53	0.68	0.25	52,87,152,165	0
26	CDL	P	312	100/100	0.69	0.24	68,96,141,163	0
25	PEK	C	314	53/53	0.70	0.27	59,83,139,159	0
26	CDL	P	308	100/100	0.70	0.23	48,88,121,129	0
20	TGL	N	618	63/63	0.71	0.21	64,82,103,110	0
23	PSC	R	201	52/52	0.72	0.32	44,100,157,168	0
20	TGL	A	613	63/63	0.72	0.26	51,74,117,120	0
17	PGV	N	622	51/51	0.73	0.33	54,89,159,169	0
17	PGV	P	307	51/51	0.73	0.27	64,96,123,143	0
20	TGL	N	604	63/63	0.75	0.27	58,83,114,119	0
27	DMU	G	104	33/33	0.75	0.23	64,106,127,137	0
27	DMU	Z	101	33/33	0.76	0.28	58,69,87,94	0
19	EDO	A	618	4/4	0.76	0.46	58,69,77,79	0
24	CHD	T	1302	29/29	0.76	0.36	97,136,151,152	0
19	EDO	V	103	4/4	0.77	0.23	75,79,82,83	0
20	TGL	D	201	63/63	0.77	0.20	49,79,97,114	0
19	EDO	P	311	4/4	0.77	0.27	55,68,74,84	0
19	EDO	N	621	4/4	0.78	0.21	57,60,61,70	0
26	CDL	C	305	100/100	0.78	0.25	45,82,118,125	0
20	TGL	L	502	63/63	0.79	0.19	45,65,91,99	0
27	DMU	P	302	33/33	0.80	0.33	59,101,117,119	0
17	PGV	M	101	51/51	0.80	0.25	48,92,149,181	0
19	EDO	B	307	4/4	0.81	0.19	58,67,71,76	0
19	EDO	P	314	4/4	0.81	0.23	70,71,74,81	0
19	EDO	A	610	4/4	0.83	0.18	56,65,66,69	0
19	EDO	N	615	4/4	0.83	0.15	55,59,61,74	0
19	EDO	B	308	4/4	0.84	0.25	50,57,66,69	0
27	DMU	C	311	33/33	0.84	0.24	60,85,105,107	0
19	EDO	D	202	4/4	0.84	0.14	60,61,70,75	0
19	EDO	K	201	4/4	0.84	0.16	61,64,65,71	0
19	EDO	L	503	4/4	0.84	0.21	58,63,64,71	0
19	EDO	M	103	4/4	0.84	0.19	65,68,69,69	0
24	CHD	W	302	29/29	0.84	0.30	61,76,89,94	0
19	EDO	V	102	4/4	0.84	0.13	69,70,71,77	0
19	EDO	H	101	4/4	0.85	0.35	66,68,68,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	O	302	4/4	0.85	0.22	62,71,72,86	0
19	EDO	Q	1603	4/4	0.85	0.23	72,72,77,81	0
19	EDO	A	611	4/4	0.85	0.17	49,55,61,69	0
19	EDO	N	614	4/4	0.87	0.21	55,67,68,76	0
27	DMU	M	102	33/33	0.87	0.22	43,52,65,81	0
19	EDO	C	308	4/4	0.87	0.10	71,72,73,76	0
19	EDO	G	105	4/4	0.88	0.18	75,75,80,101	0
19	EDO	I	102	4/4	0.88	0.10	74,76,76,80	0
19	EDO	B	311	4/4	0.88	0.27	65,71,77,89	0
19	EDO	N	612	4/4	0.88	0.24	59,63,65,74	0
19	EDO	S	103	4/4	0.88	0.13	53,66,68,69	0
19	EDO	U	1501	4/4	0.88	0.25	57,60,62,68	0
19	EDO	T	1301	4/4	0.89	0.23	56,59,64,66	0
19	EDO	R	203	4/4	0.89	0.32	64,68,71,77	0
19	EDO	B	309	4/4	0.89	0.11	62,68,69,74	0
19	EDO	S	104	4/4	0.89	0.13	52,55,59,61	0
24	CHD	J	101	29/29	0.89	0.28	56,70,84,95	0
19	EDO	V	104	4/4	0.89	0.15	51,65,68,72	0
19	EDO	C	313	4/4	0.90	0.22	58,60,62,71	0
19	EDO	S	105	4/4	0.90	0.21	44,58,64,69	0
19	EDO	G	106	4/4	0.90	0.10	65,65,65,69	0
19	EDO	Q	1604	4/4	0.90	0.15	59,70,72,89	0
19	EDO	B	305	4/4	0.90	0.15	50,57,64,68	0
19	EDO	F	702	4/4	0.90	0.22	57,69,73,86	0
19	EDO	I	103	4/4	0.91	0.12	58,60,62,67	0
19	EDO	Q	1602	4/4	0.91	0.18	70,73,76,83	0
19	EDO	N	613	4/4	0.91	0.18	65,67,75,77	0
19	EDO	A	617	4/4	0.92	0.17	56,59,61,63	0
19	EDO	S	106	4/4	0.92	0.14	65,68,69,75	0
19	EDO	E	203	4/4	0.92	0.25	63,70,73,77	0
19	EDO	E	204	4/4	0.92	0.18	72,74,78,81	0
19	EDO	A	612	4/4	0.92	0.20	55,56,59,61	0
19	EDO	N	616	4/4	0.92	0.11	47,55,60,62	0
19	EDO	C	309	4/4	0.92	0.12	73,74,77,78	0
19	EDO	C	312	4/4	0.92	0.15	52,55,57,62	0
19	EDO	B	310	4/4	0.92	0.17	55,64,65,74	0
24	CHD	P	309	29/29	0.93	0.18	51,60,67,72	0
19	EDO	S	107	4/4	0.93	0.11	49,54,60,61	0
19	EDO	D	205	4/4	0.93	0.33	60,70,70,78	0
19	EDO	N	620	4/4	0.93	0.14	45,56,59,69	0
19	EDO	A	609	4/4	0.93	0.22	34,36,42,43	0
19	EDO	N	617	4/4	0.94	0.15	44,61,71,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
19	EDO	N	619	4/4	0.94	0.18	48,52,56,61	0
19	EDO	A	607	4/4	0.94	0.14	42,48,54,55	0
19	EDO	J	103	4/4	0.94	0.25	57,60,62,63	0
19	EDO	R	202	4/4	0.94	0.14	49,50,51,51	0
19	EDO	A	614	4/4	0.94	0.12	42,59,61,65	0
19	EDO	E	201	4/4	0.94	0.11	47,48,49,50	0
19	EDO	A	615	4/4	0.94	0.26	50,56,58,64	0
25	PEK	P	304	53/53	0.94	0.18	36,57,87,100	0
19	EDO	W	301	4/4	0.94	0.30	55,71,76,82	0
24	CHD	C	306	29/29	0.94	0.20	46,55,60,61	0
19	EDO	L	504	4/4	0.95	0.11	55,63,64,66	0
19	EDO	E	205	4/4	0.95	0.12	56,62,65,65	0
19	EDO	N	611	4/4	0.95	0.11	51,52,53,54	0
15	MG	N	602	1/1	0.95	0.12	35,35,35,35	0
25	PEK	G	102	53/53	0.95	0.20	31,53,79,97	0
19	EDO	B	306	4/4	0.95	0.09	37,42,49,51	0
19	EDO	E	202	4/4	0.95	0.16	43,47,52,53	0
19	EDO	A	616	4/4	0.95	0.14	53,61,63,72	0
19	EDO	L	501	4/4	0.95	0.26	49,62,63,65	0
19	EDO	D	203	4/4	0.95	0.29	53,62,67,70	0
19	EDO	C	307	4/4	0.96	0.07	39,42,46,47	0
17	PGV	P	306	51/51	0.96	0.15	29,45,86,96	0
19	EDO	Q	1601	4/4	0.96	0.12	44,57,57,59	0
17	PGV	N	606	51/51	0.96	0.19	31,50,77,82	0
17	PGV	A	604	51/51	0.96	0.18	26,42,71,76	0
19	EDO	F	704	4/4	0.96	0.12	56,56,59,63	0
19	EDO	F	706	4/4	0.96	0.12	39,43,48,49	0
19	EDO	F	707	4/4	0.96	0.15	49,61,64,65	0
24	CHD	C	301	29/29	0.96	0.07	29,33,39,42	0
19	EDO	O	303	4/4	0.96	0.10	39,40,42,43	0
19	EDO	A	608	4/4	0.96	0.16	28,28,28,29	0
24	CHD	B	303	29/29	0.97	0.07	30,34,41,46	0
19	EDO	D	204	4/4	0.97	0.20	63,65,71,78	0
18	HEA	N	608	60/60	0.97	0.16	27,33,49,63	0
19	EDO	P	313	4/4	0.97	0.09	37,46,48,53	0
24	CHD	P	303	29/29	0.97	0.07	33,36,42,43	0
19	EDO	G	103	4/4	0.97	0.10	33,34,41,43	0
17	PGV	C	303	51/51	0.97	0.20	26,39,103,112	0
19	EDO	S	102	4/4	0.97	0.11	31,32,33,36	0
19	EDO	T	1303	4/4	0.97	0.19	36,40,43,44	0
18	HEA	A	606	60/60	0.98	0.14	20,26,54,64	0
19	EDO	N	609	4/4	0.98	0.11	36,37,38,41	0

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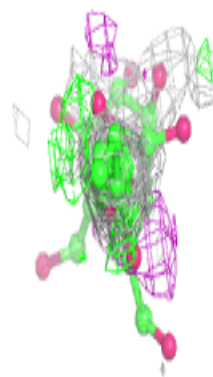
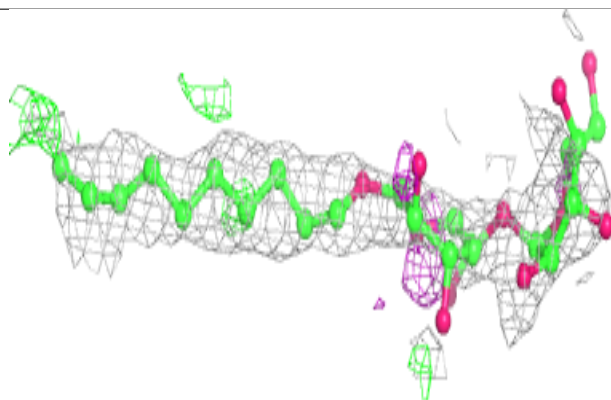
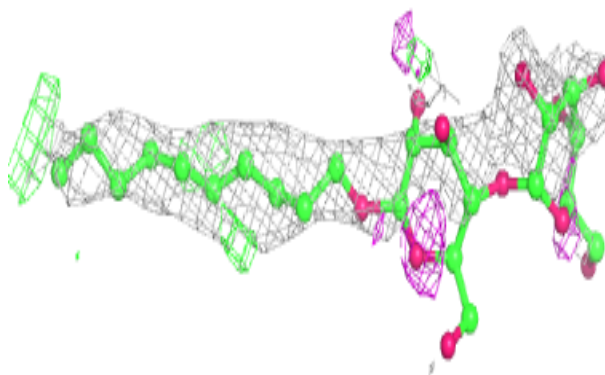
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CHD	G	107	29/29	0.98	0.05	31,35,39,42	0
19	EDO	N	610	4/4	0.98	0.23	36,40,43,43	0
18	HEA	N	607	60/60	0.98	0.13	25,29,36,43	0
19	EDO	F	705	4/4	0.98	0.20	28,30,30,31	0
19	EDO	B	304	4/4	0.98	0.13	27,29,30,34	0
16	NA	N	603	1/1	0.98	0.05	40,40,40,40	0
19	EDO	F	701	4/4	0.98	0.14	38,39,41,42	0
15	MG	A	602	1/1	0.99	0.10	28,28,28,28	0
18	HEA	A	605	60/60	0.99	0.13	21,26,32,37	0
16	NA	A	603	1/1	0.99	0.04	25,25,25,25	0
21	OH	A	619	1/1	0.99	0.20	24,24,24,24	0
28	ZN	F	703	1/1	0.99	0.05	34,34,34,34	0
28	ZN	S	101	1/1	0.99	0.06	38,38,38,38	0
21	OH	N	623	1/1	0.99	0.18	31,31,31,31	0
22	CUA	O	301	2/2	0.99	0.06	34,34,34,35	0
14	CU	N	601	1/1	1.00	0.11	34,34,34,34	0
14	CU	A	601	1/1	1.00	0.10	28,28,28,28	0
22	CUA	B	301	2/2	1.00	0.07	26,26,26,26	0

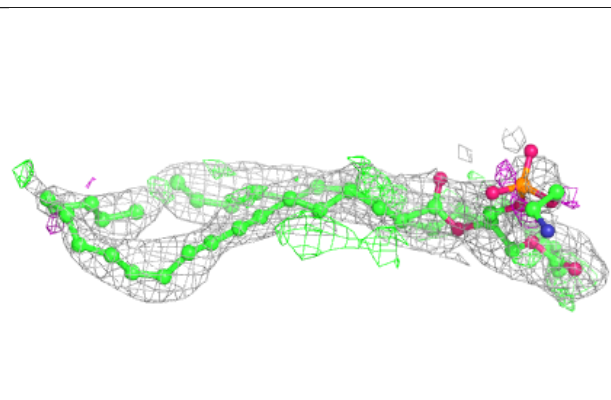
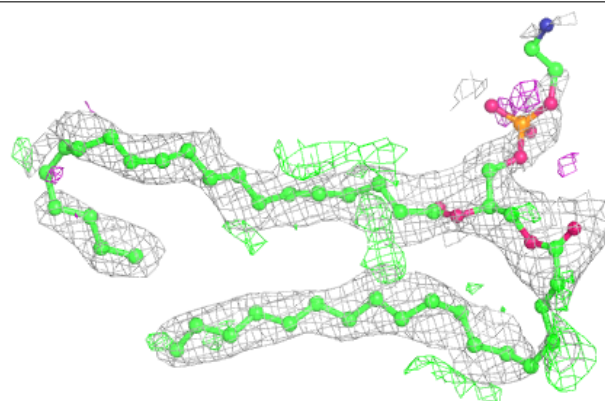
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU G 101:

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

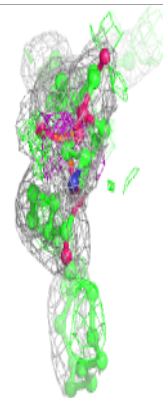
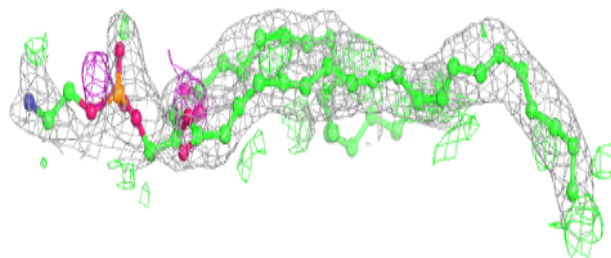
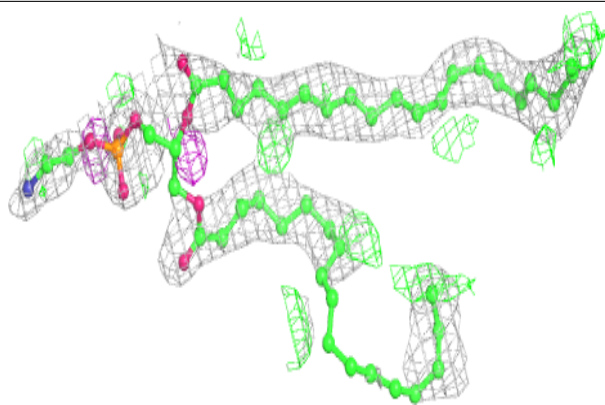
**Electron density around PEK C 302:**

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

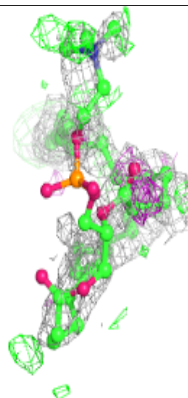
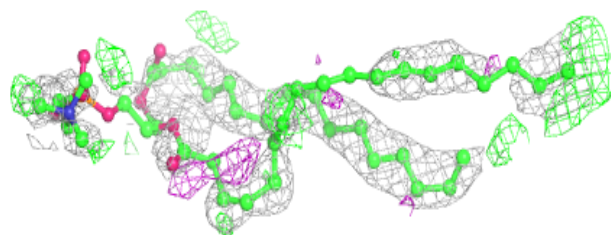
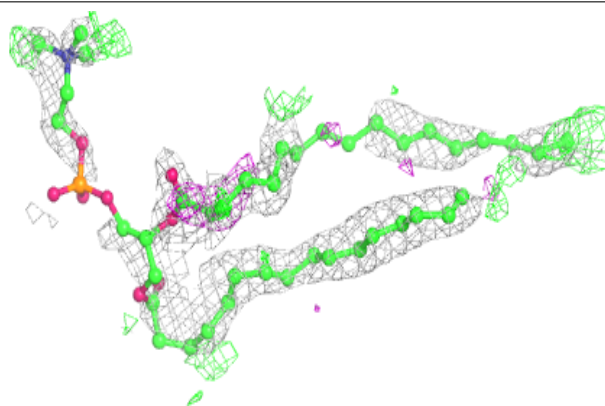


Electron density around PEK P 301:

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

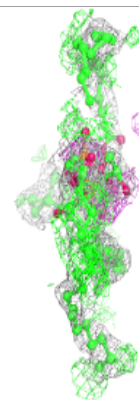
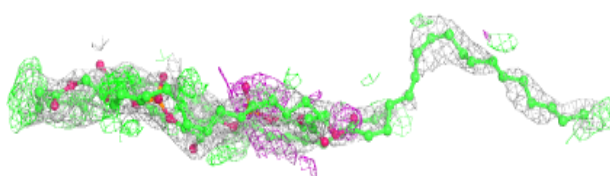
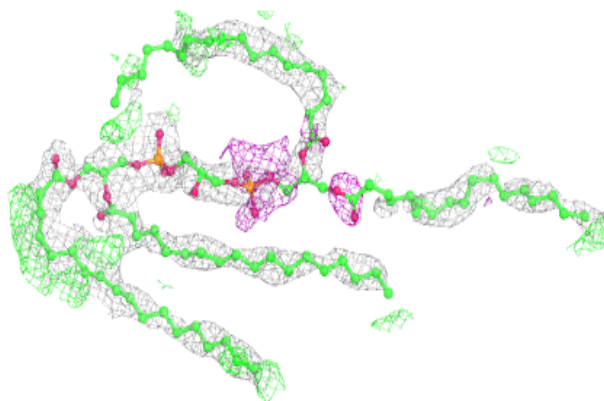
**Electron density around PSC B 302:**

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

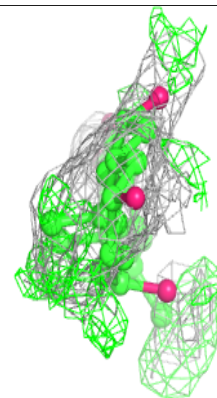
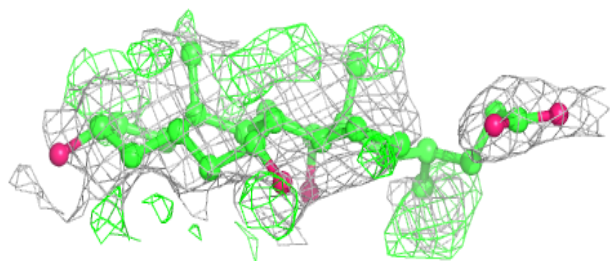
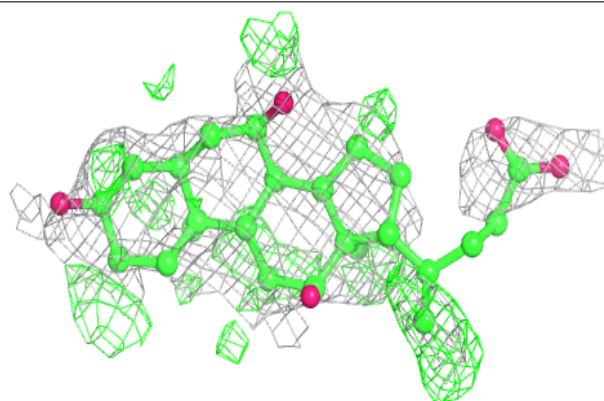


Electron density around CDL C 310:

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

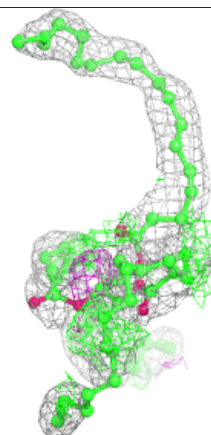
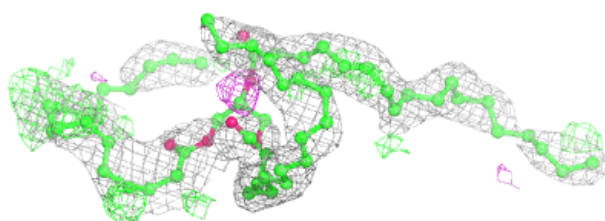
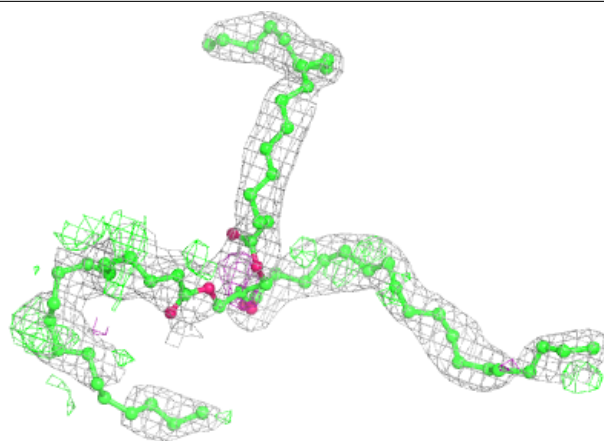
**Electron density around CHD Y 101:**

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

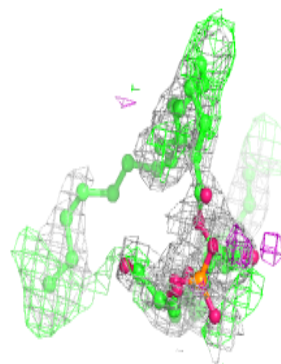
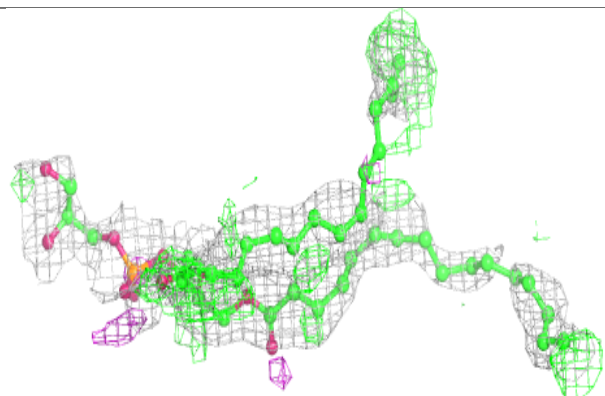
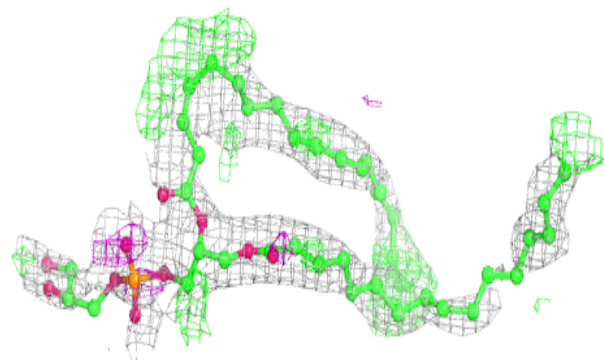


Electron density around TGL N 605:

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

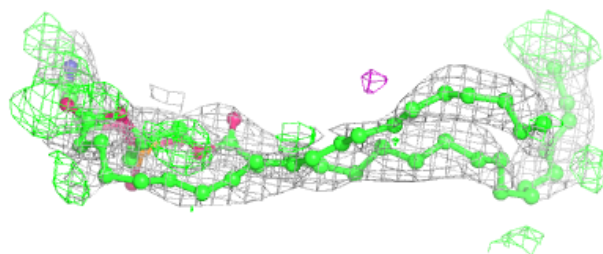
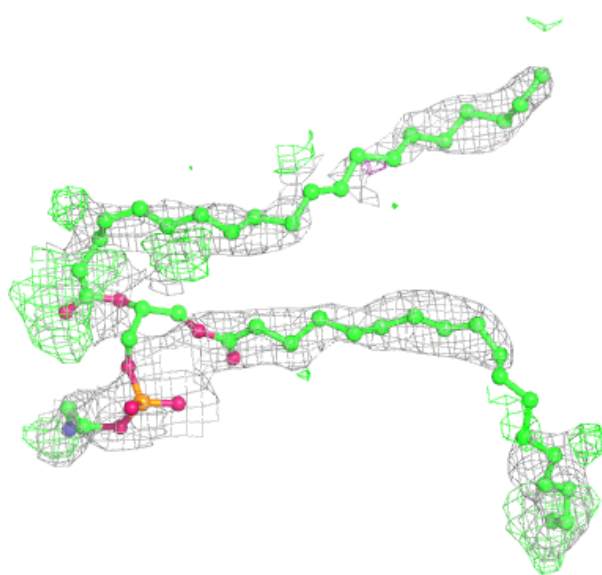
**Electron density around PGV C 304:**

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



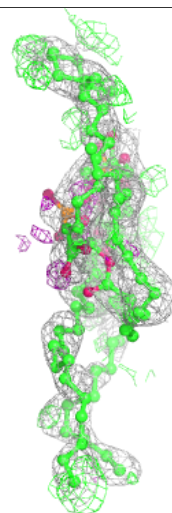
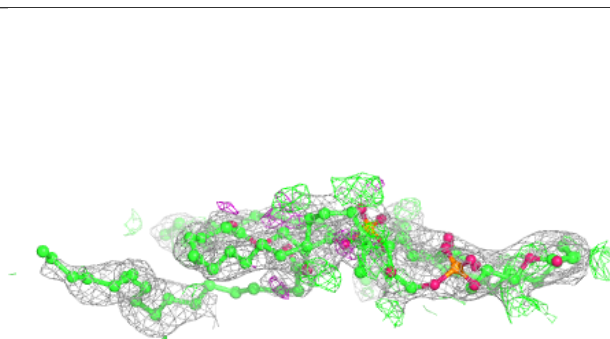
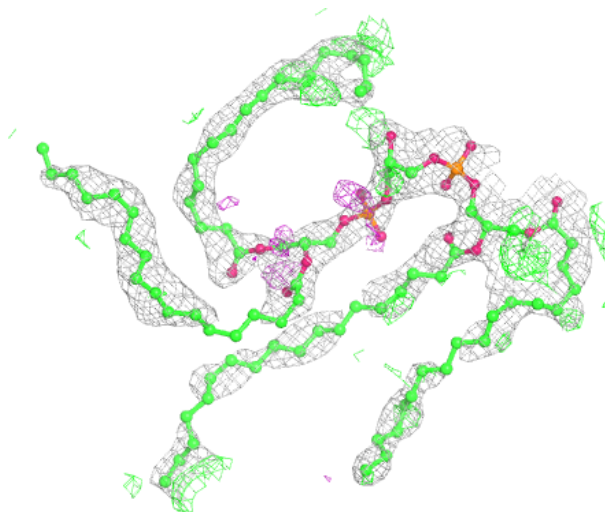
Electron density around PEK P 305:

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



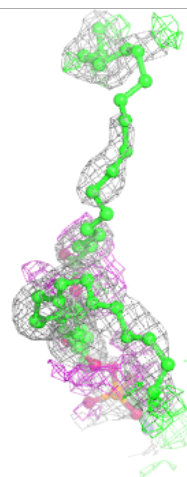
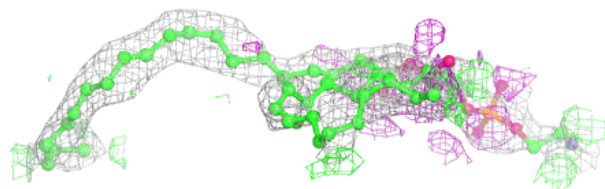
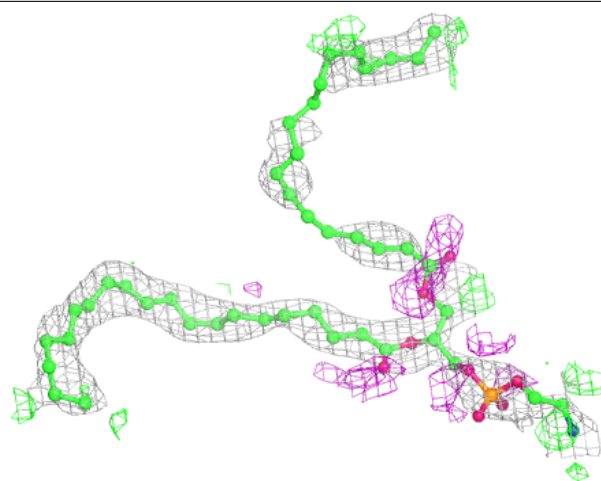
Electron density around CDL P 312:

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



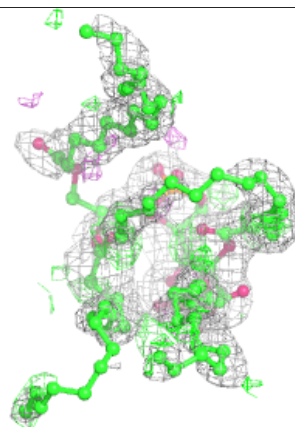
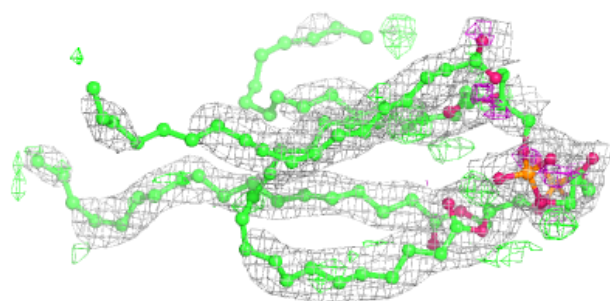
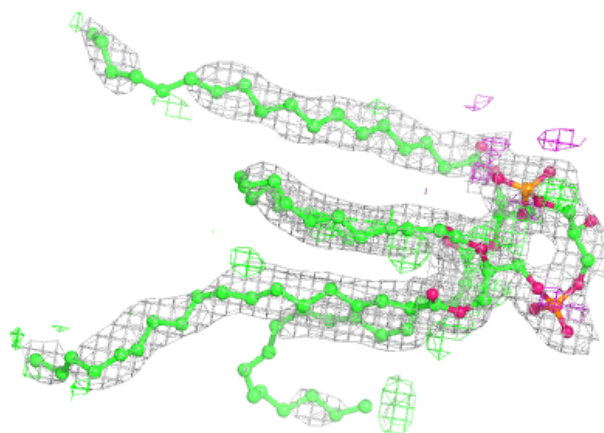
Electron density around PEK C 314:

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

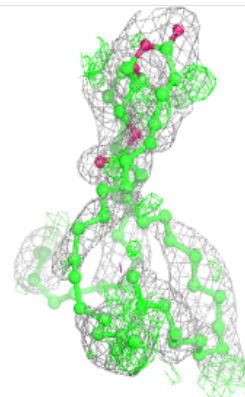
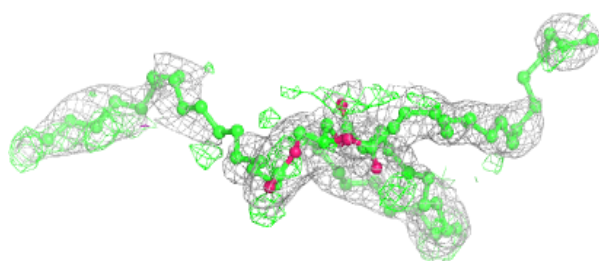
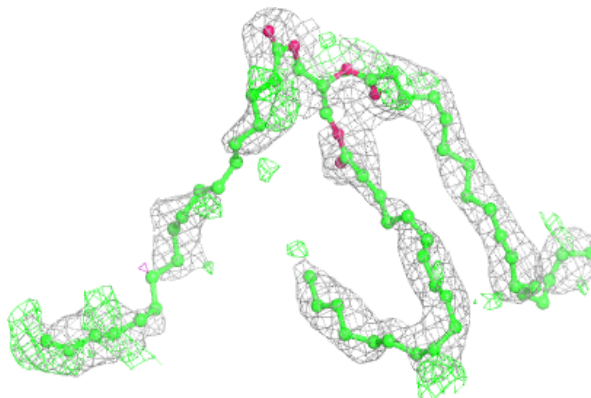


Electron density around CDL P 308:

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

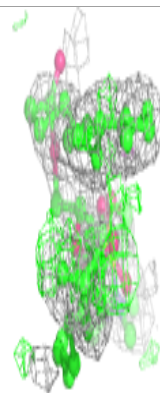
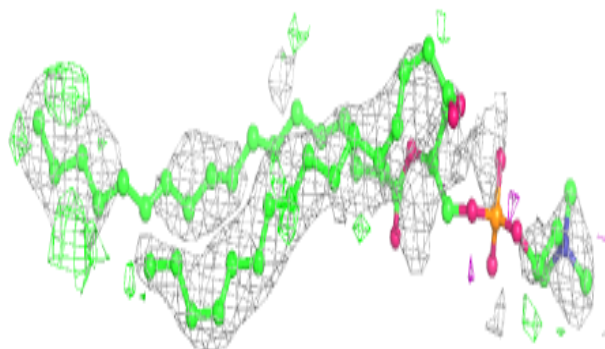
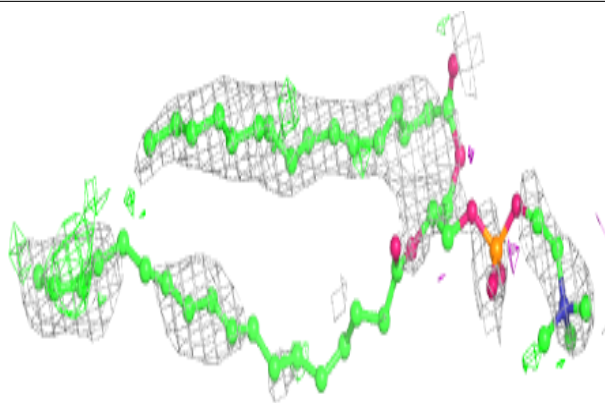
**Electron density around TGL N 618:**

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

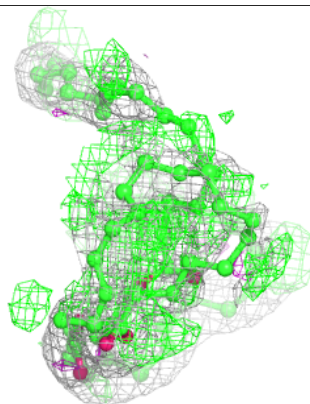
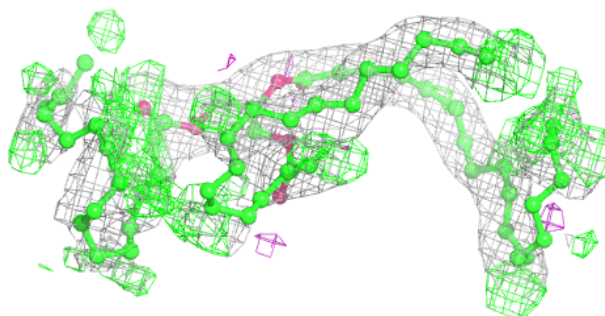
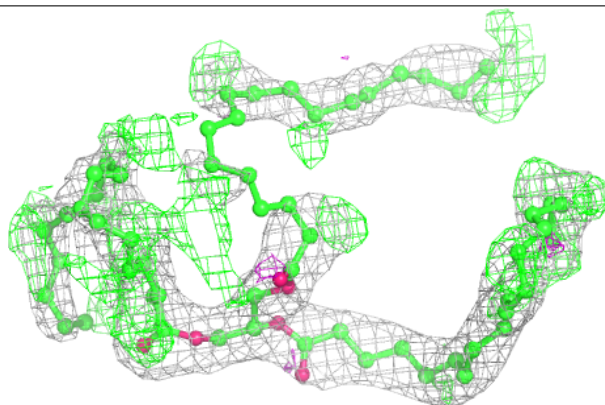


Electron density around PSC R 201:

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

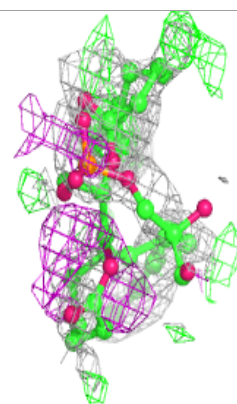
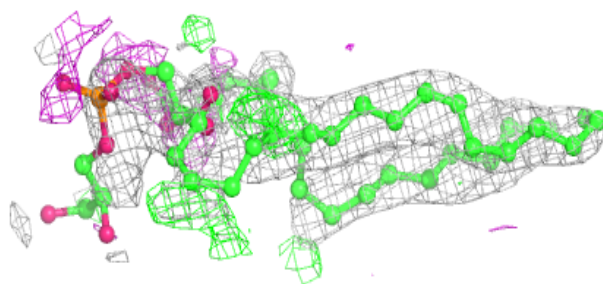
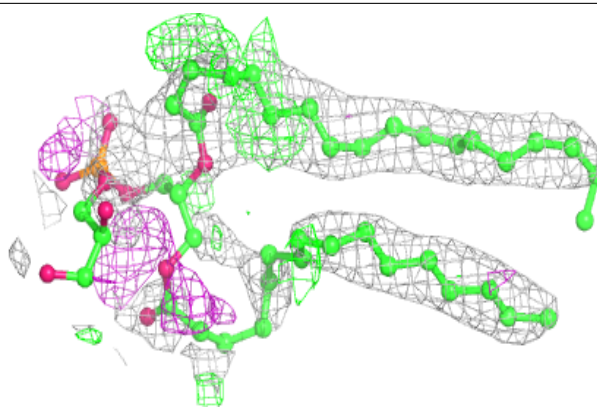
**Electron density around TGL A 613:**

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

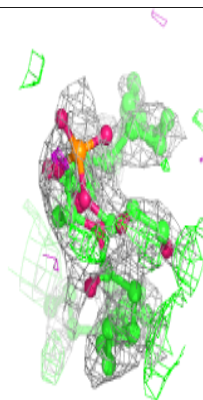
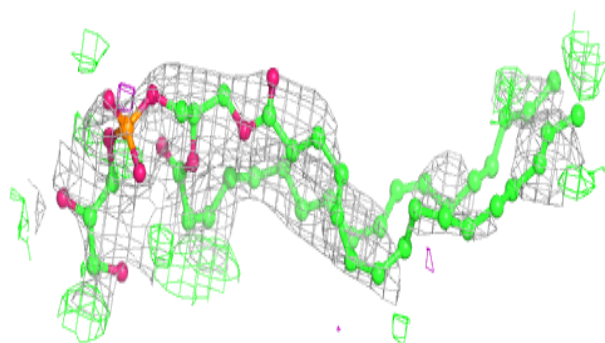
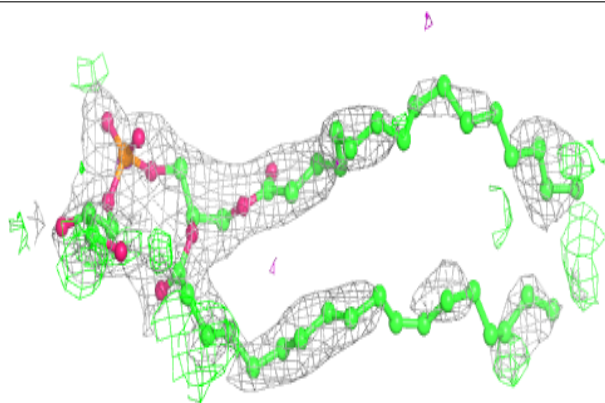


Electron density around PGV N 622:

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

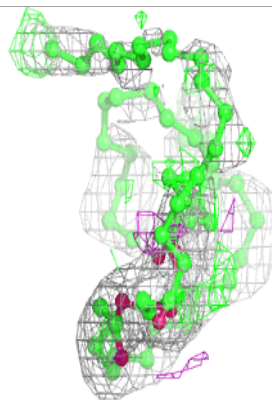
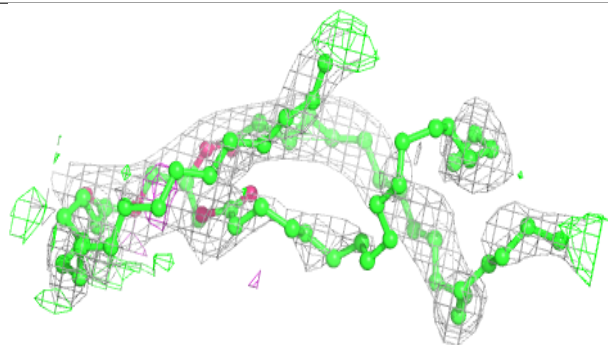
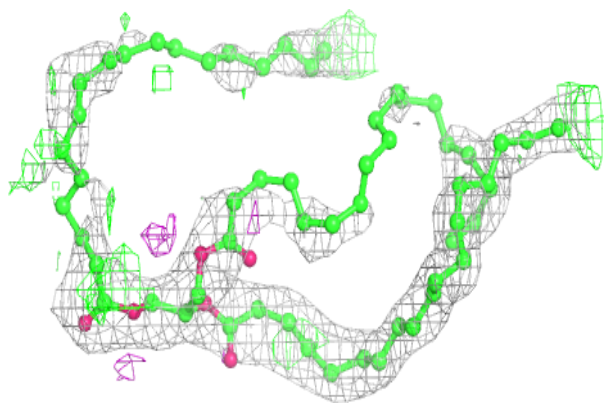
**Electron density around PGV P 307:**

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

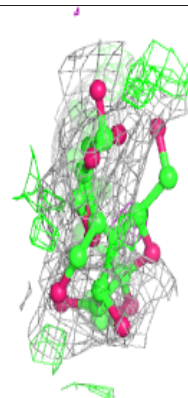
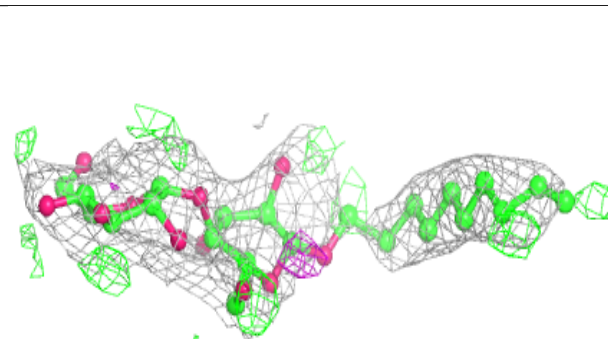
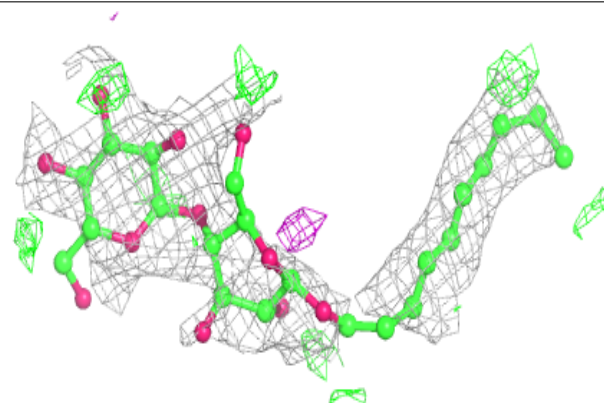


Electron density around TGL N 604:

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

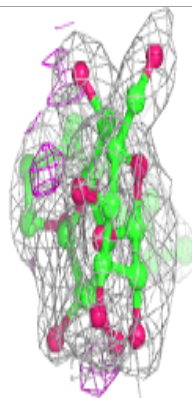
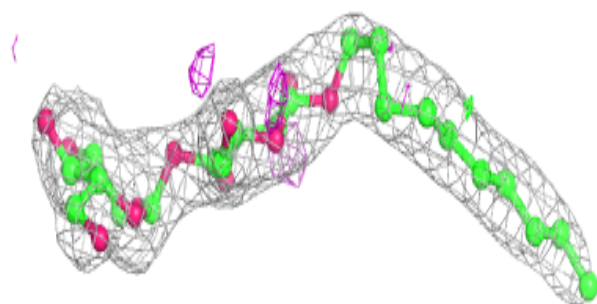
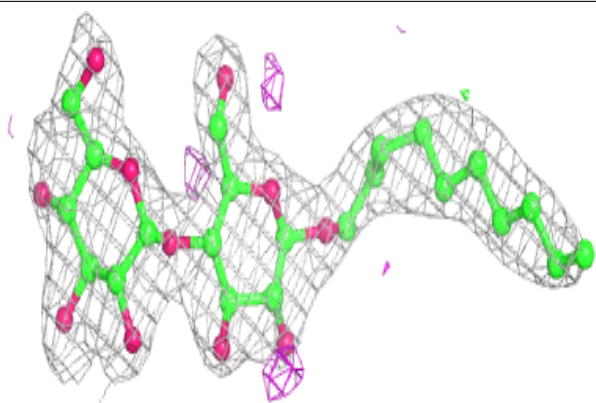
**Electron density around DMU G 104:**

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

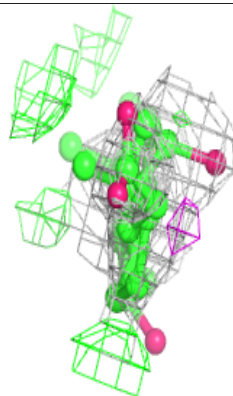
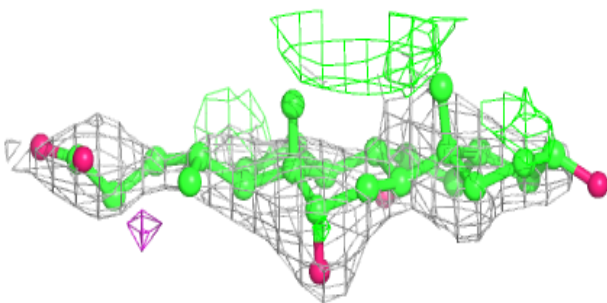
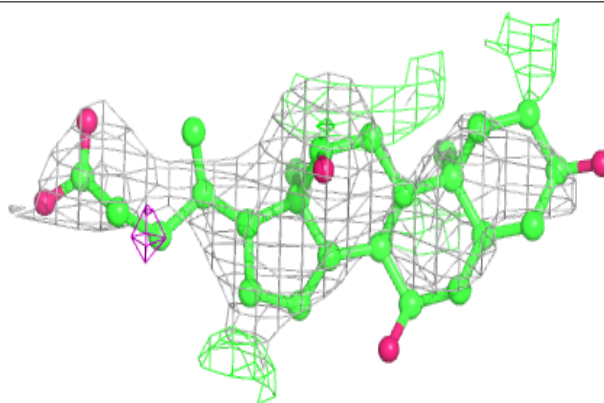


Electron density around DMU Z 101:

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

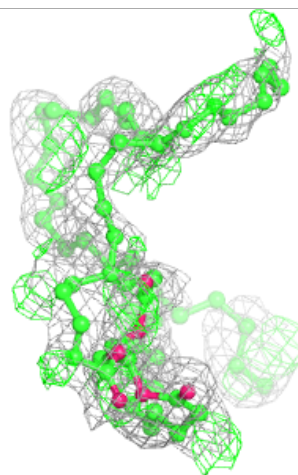
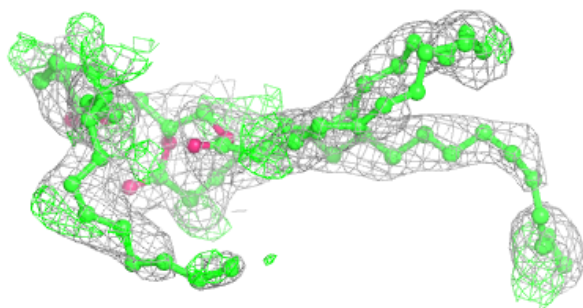
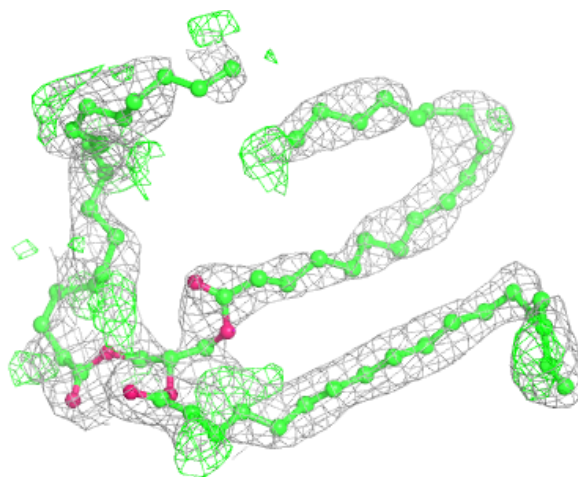
**Electron density around CHD T 1302:**

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



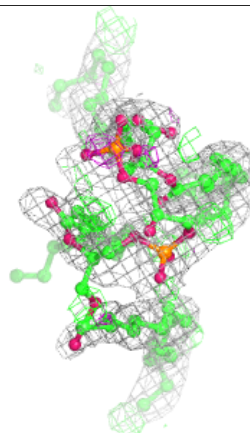
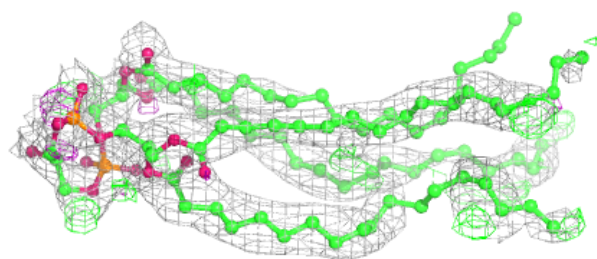
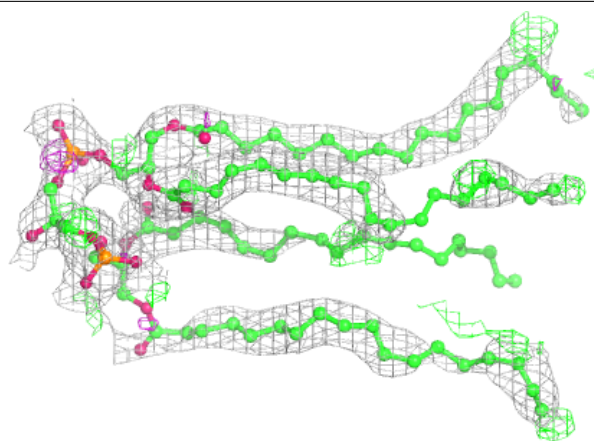
Electron density around TGL D 201:

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



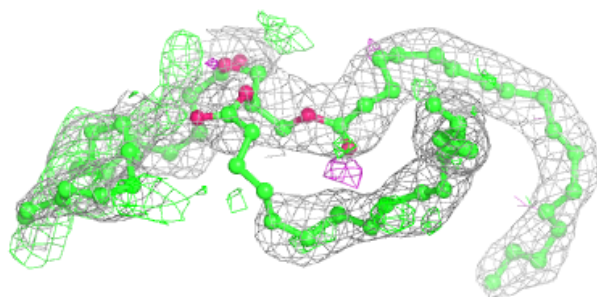
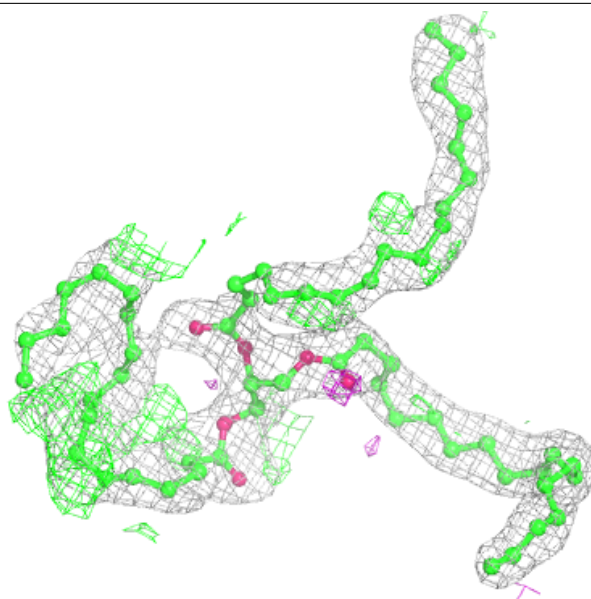
Electron density around CDL C 305:

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



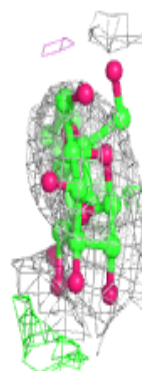
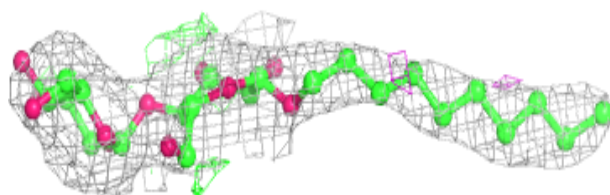
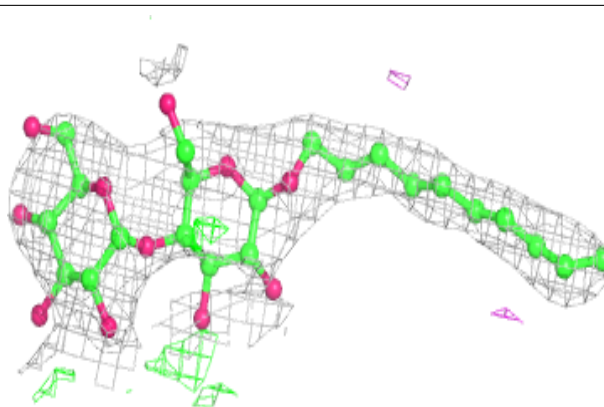
Electron density around TGL L 502:

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

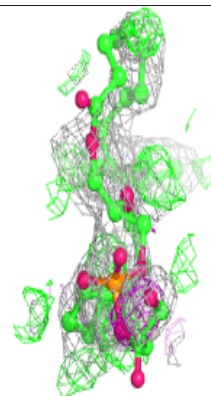
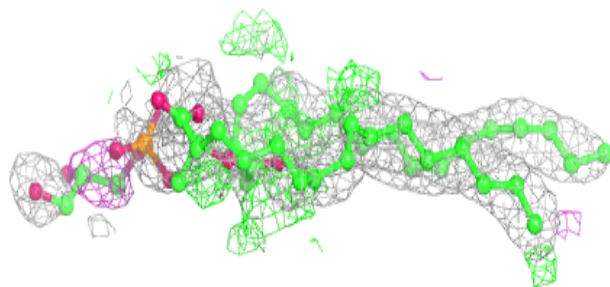
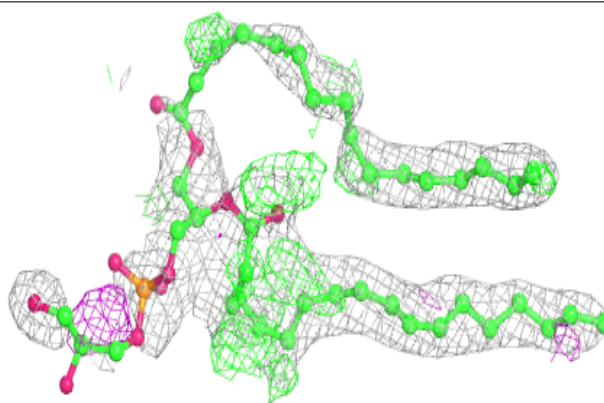


Electron density around DMU P 302:

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

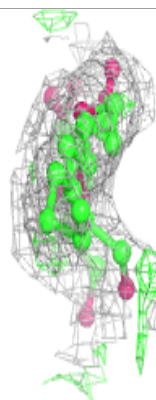
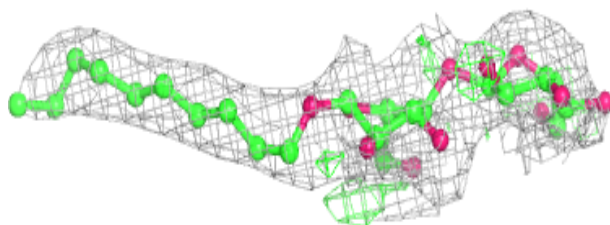
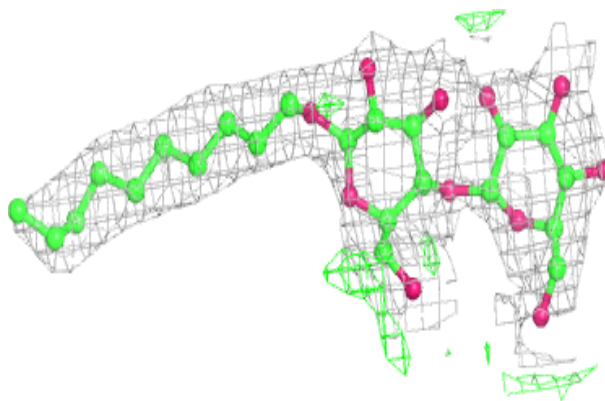
**Electron density around PGV M 101:**

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

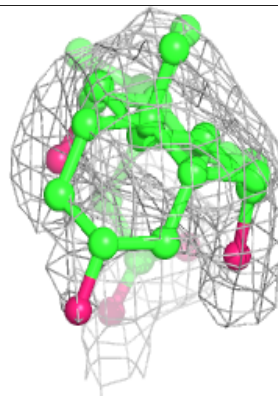
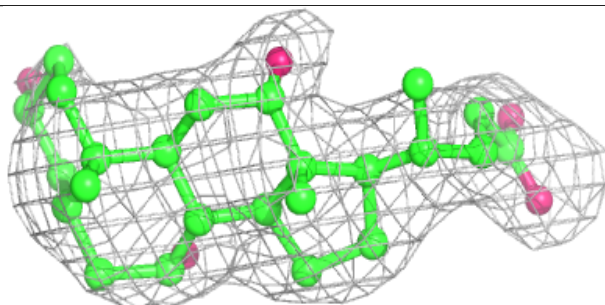
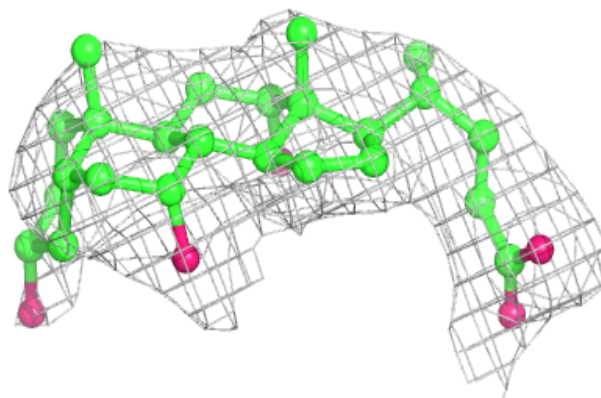


Electron density around DMU C 311:

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

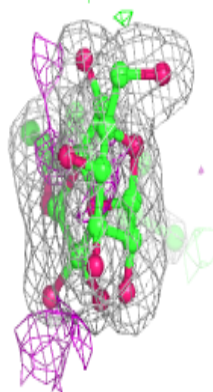
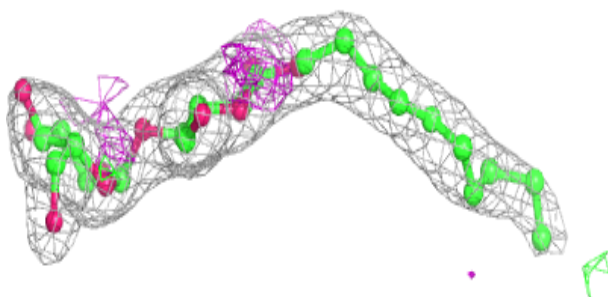
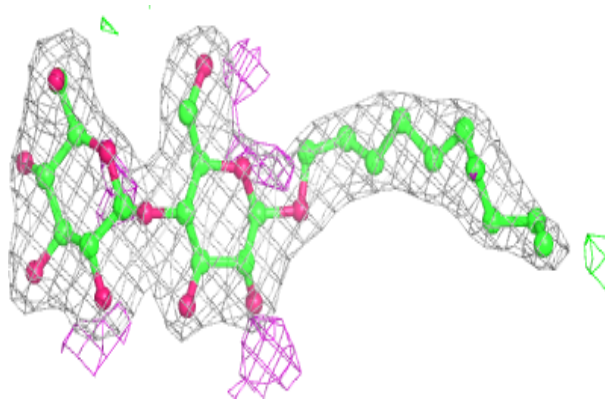
**Electron density around CHD W 302:**

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

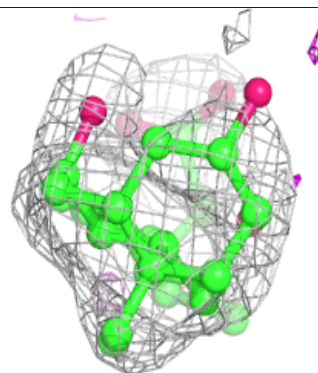
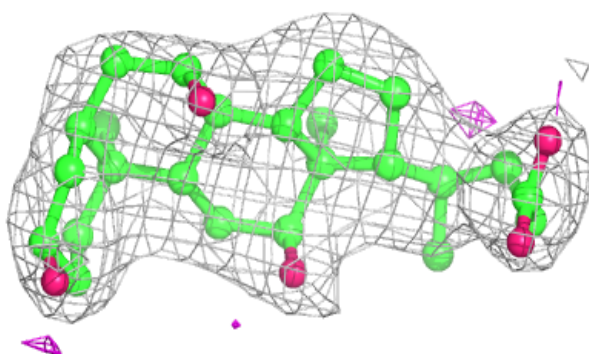
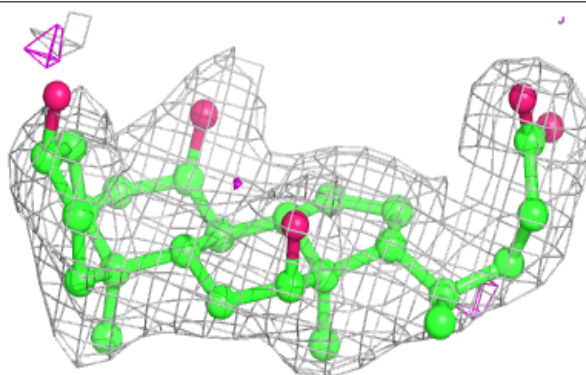


Electron density around DMU M 102:

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

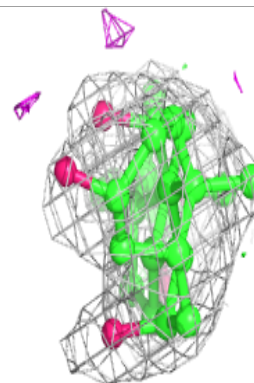
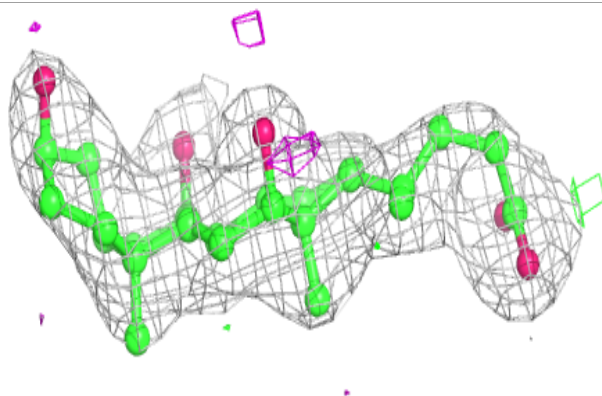
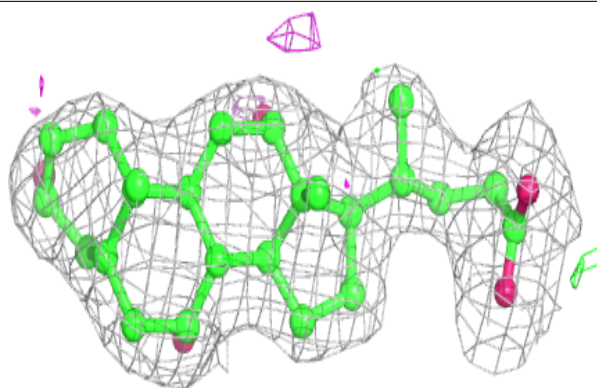
**Electron density around CHD J 101:**

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

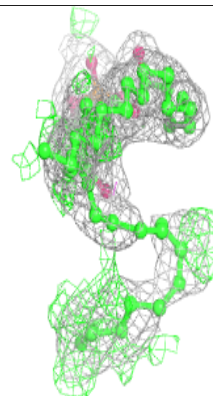
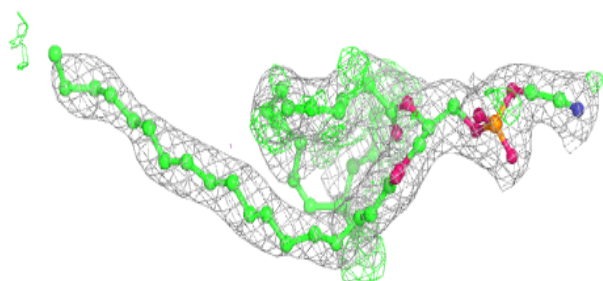
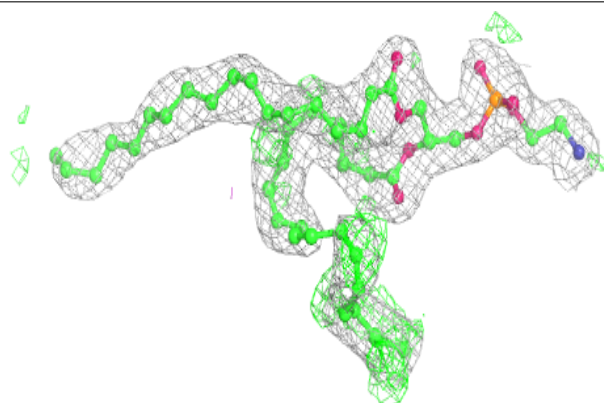


Electron density around CHD P 309:

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

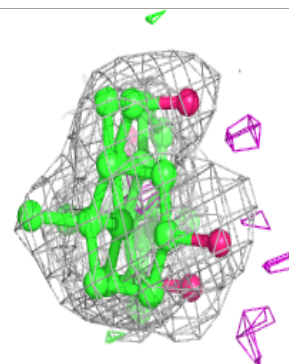
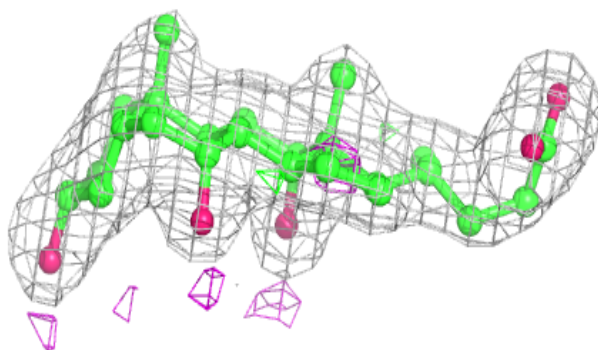
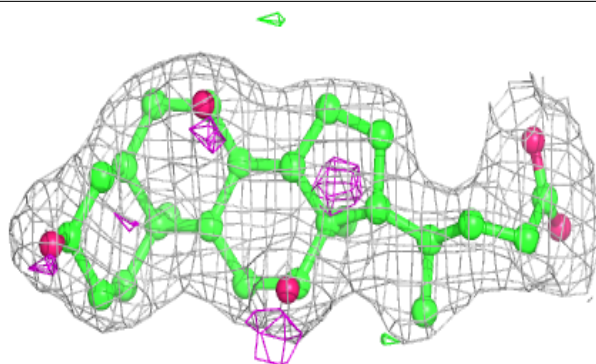
**Electron density around PEK P 304:**

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

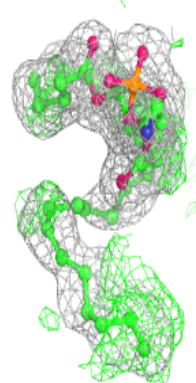
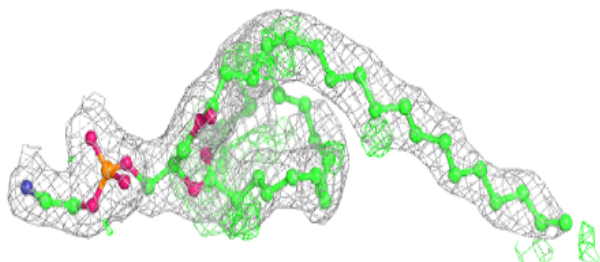
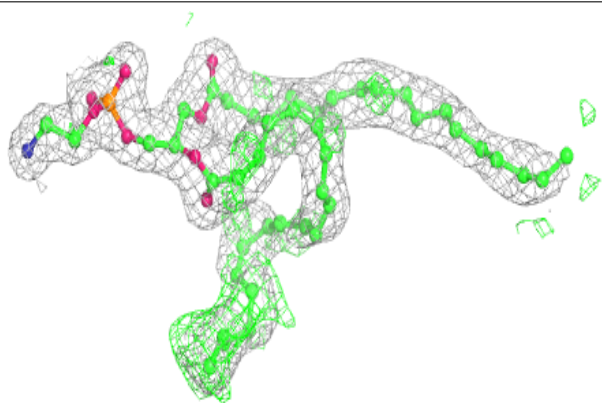


Electron density around CHD C 306:

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

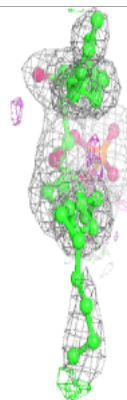
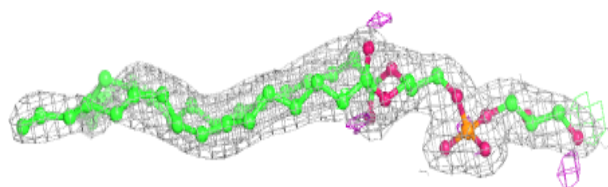
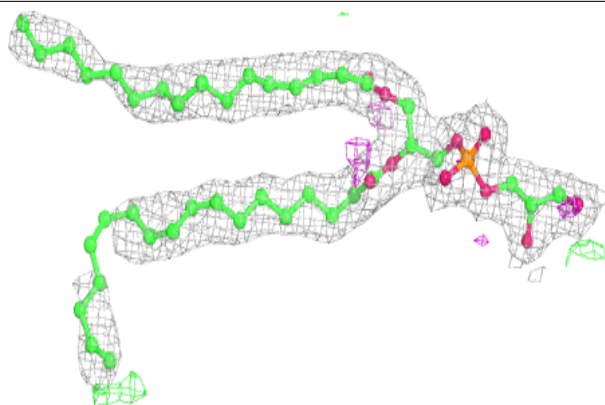
**Electron density around PEK G 102:**

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

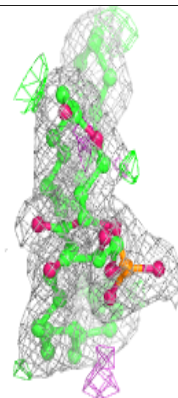
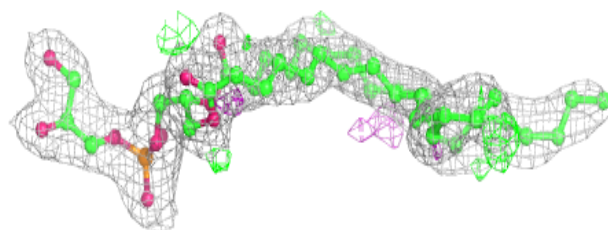
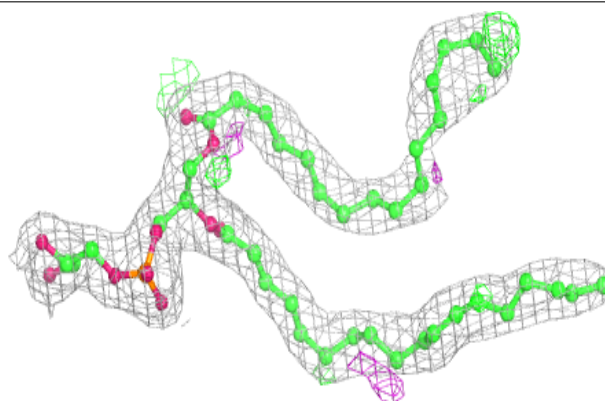


Electron density around PGV P 306:

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

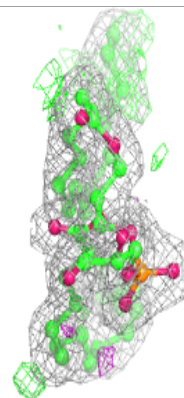
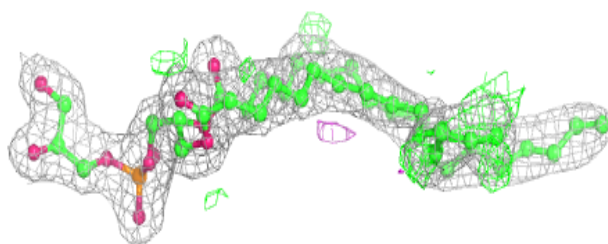
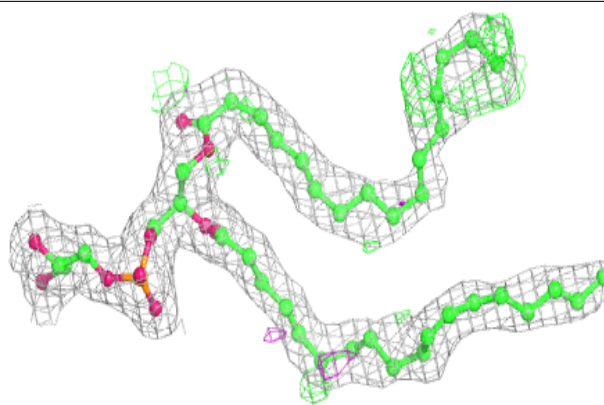
**Electron density around PGV N 606:**

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

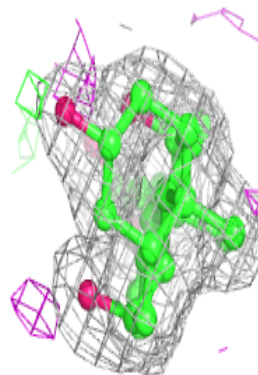
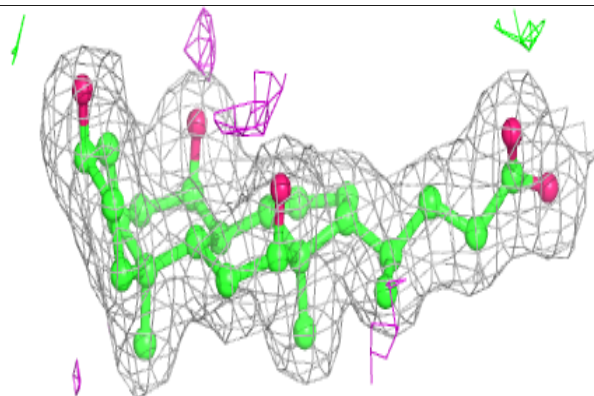
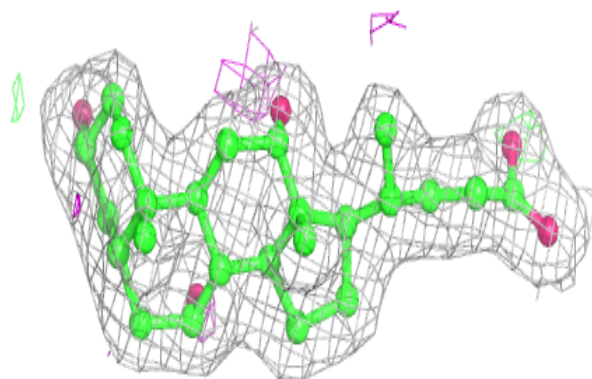


Electron density around PGV A 604:

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

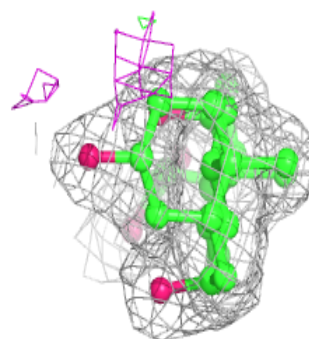
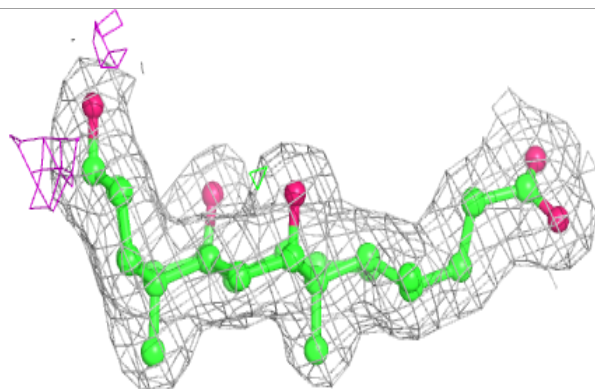
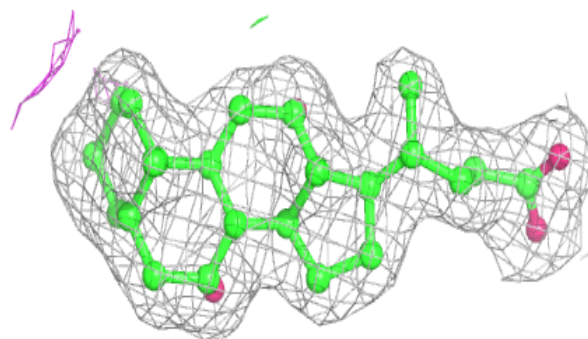
**Electron density around CHD C 301:**

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

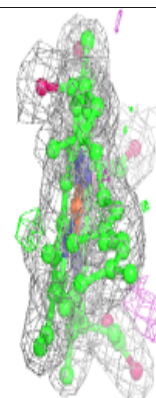
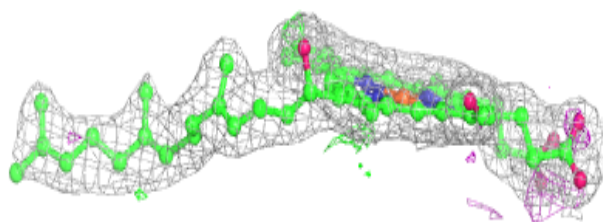
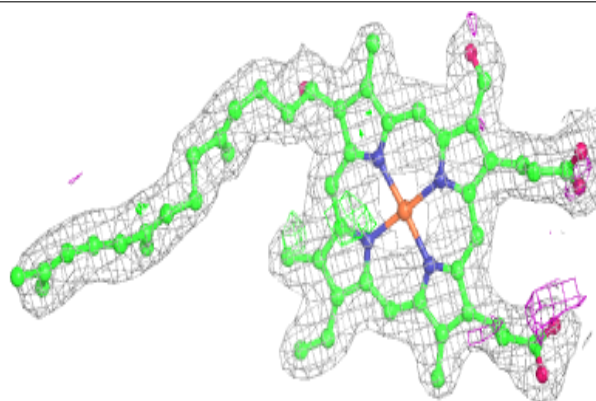


Electron density around CHD B 303:

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

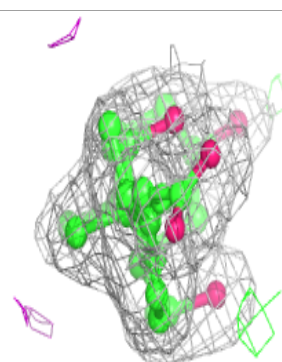
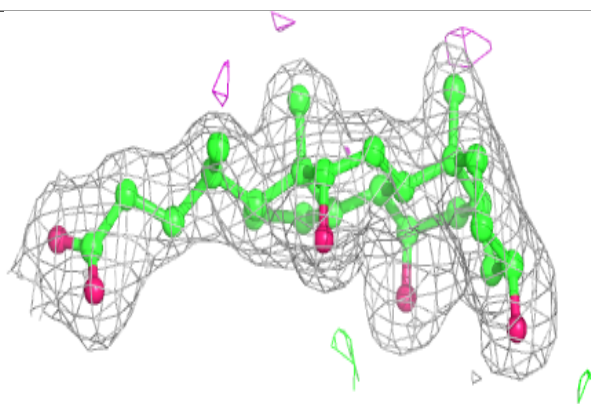
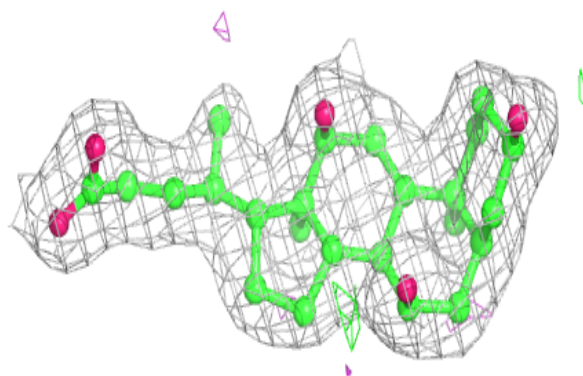
**Electron density around HEA N 608:**

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

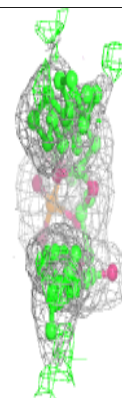
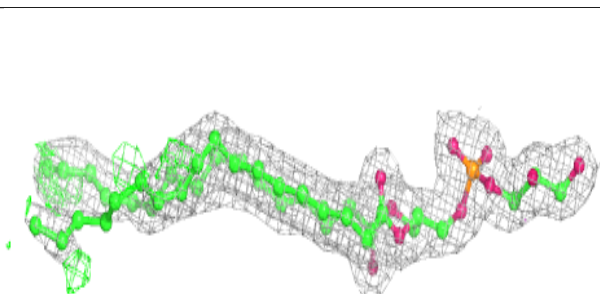
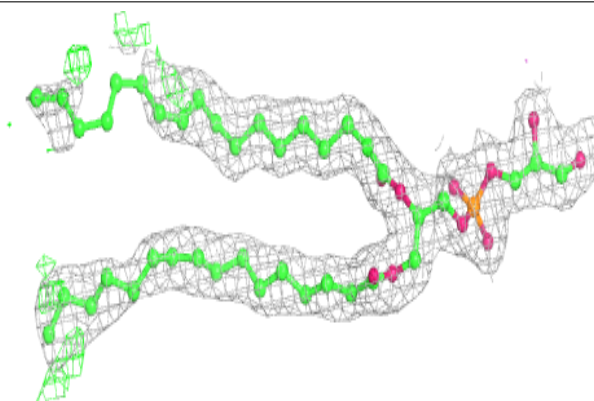


Electron density around CHD P 303:

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

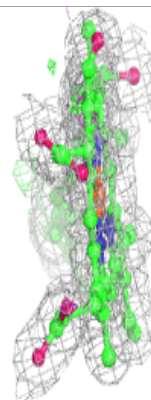
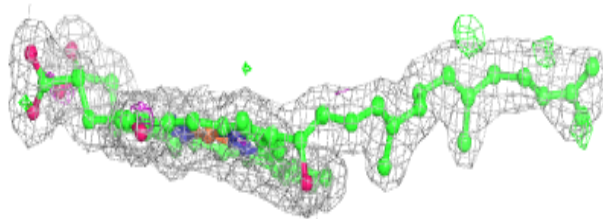
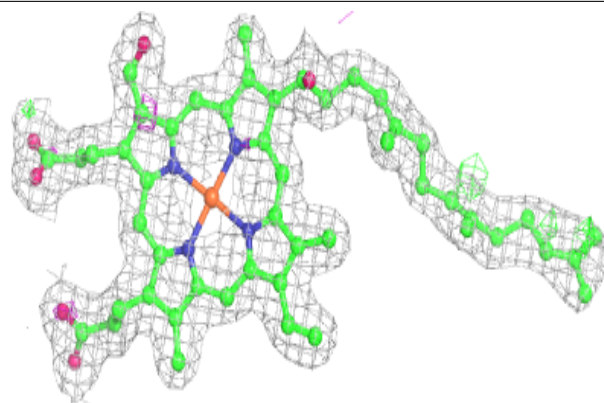
**Electron density around PGV C 303:**

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

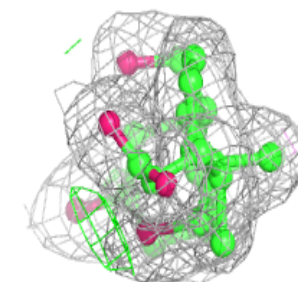
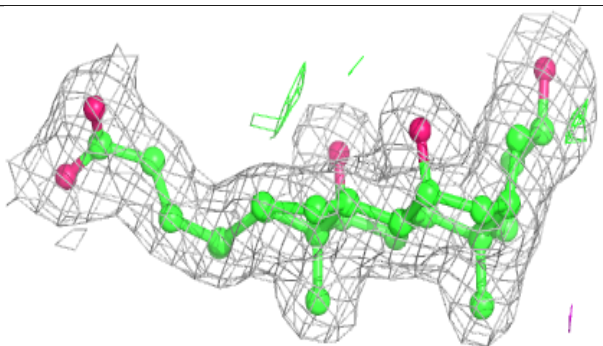
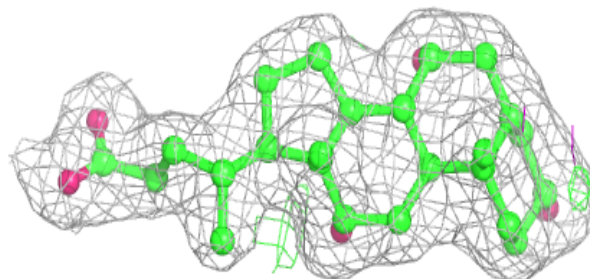


Electron density around HEA A 606:

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

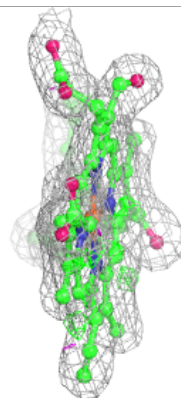
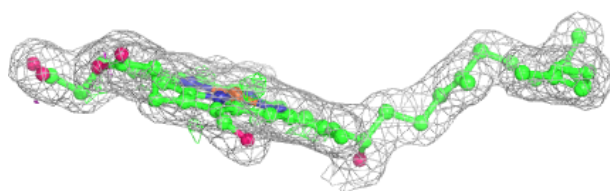
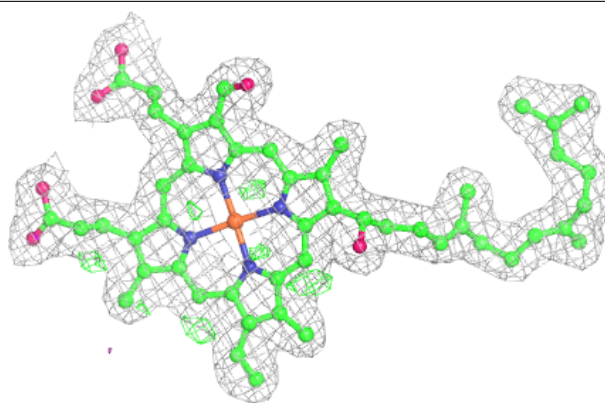
**Electron density around CHD G 107:**

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

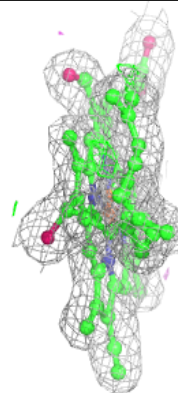
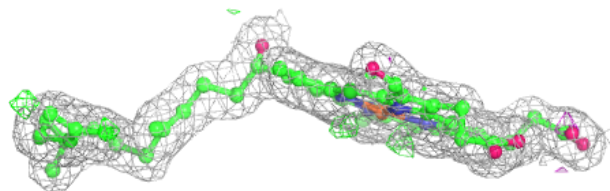
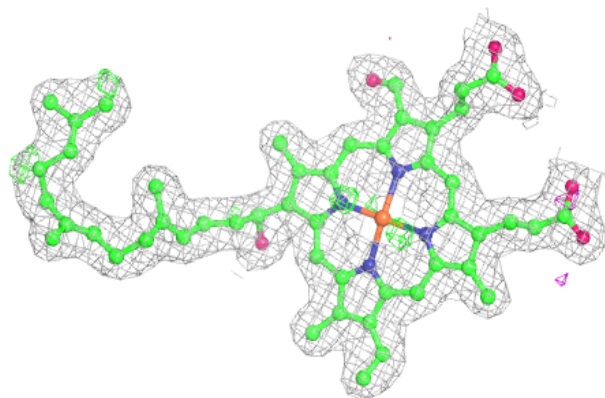


Electron density around HEA N 607:

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

**Electron density around HEA A 605:**

$2mF_o-DF_c$ (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.