



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:37 PM UTC

PDB ID : 7EV7 / pdb_00007ev7
Title : Bovine heart cytochrome c oxidase in the carbon monoxide-bound fully reduced state at a 50 K
Authors : Shimada, A.; Yoshikawa, S.; Tsukihara, T.
Deposited on : 2021-05-20
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

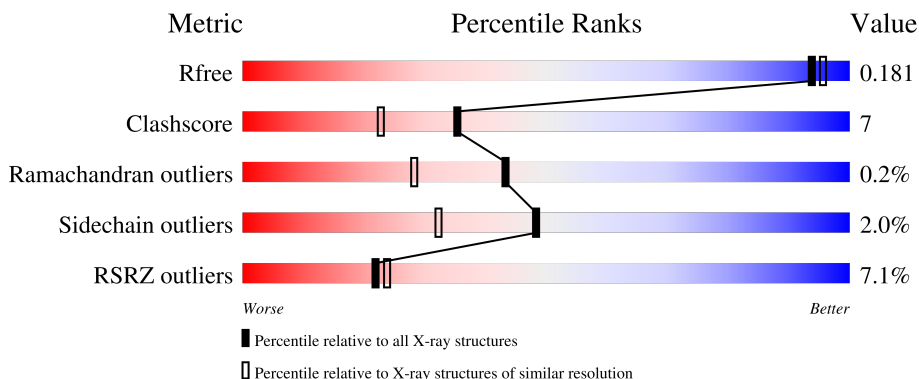
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



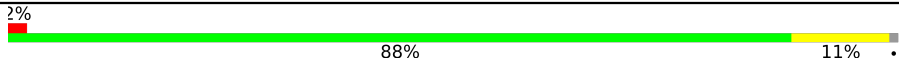
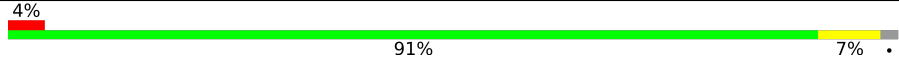
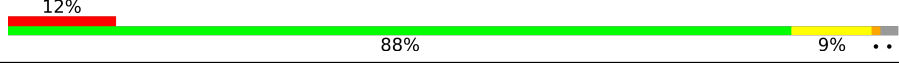
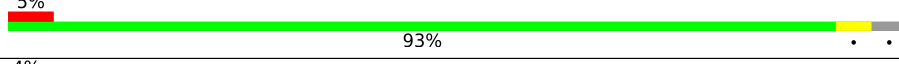
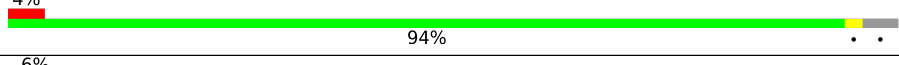
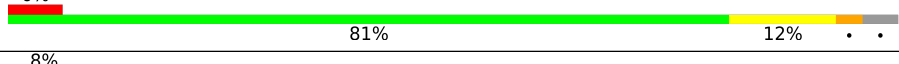


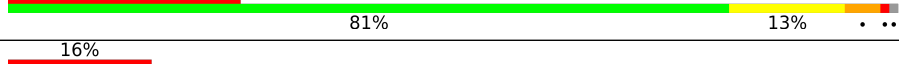


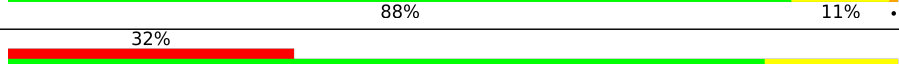

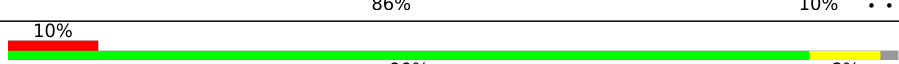
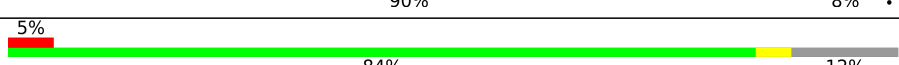
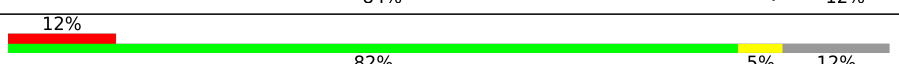
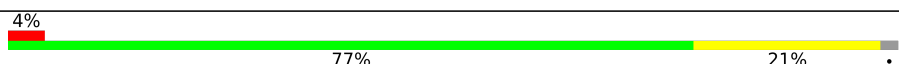
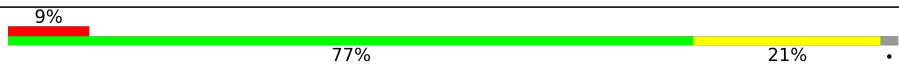
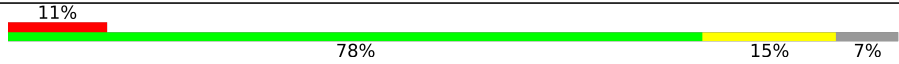


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	514	 88% 11%
1	N	514	 87% 13%
2	B	227	 82% 17%
2	O	227	 81% 19%
3	C	261	 92% 8%

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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
20	EDO	B	309	-	-	-	X
20	EDO	B	314	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	D	206	-	-	-	X
20	EDO	H	103	-	-	X	-
20	EDO	N	612	-	-	X	-
20	EDO	N	630	-	-	-	X
20	EDO	O	305	-	-	-	X
20	EDO	W	104	-	-	-	X

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 34489 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
			Total	C	N	O	S			
1	A	514	Total	C	N	O	S	0	30	0
			4124	2750	635	698	41			
1	N	514	Total	C	N	O	S	0	28	0
			4116	2741	635	699	41			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	Total	C	N	O	S	0	11	0
			1869	1218	284	348	19			
2	O	227	Total	C	N	O	S	0	10	0
			1865	1216	284	346	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	Total	C	N	O	S	0	9	0
			2131	1422	337	357	15			
3	P	259	Total	C	N	O	S	0	11	0
			2141	1428	341	357	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	Total	C	N	O	S	0	5	0
			1214	787	202	221	4			
4	Q	144	Total	C	N	O	S	0	3	0
			1206	785	199	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	3	0
			723	447	129	142	5			
6	S	94	Total	C	N	O	S	0	3	0
			723	448	128	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	1	0
			678	432	129	115	1	1			

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

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

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

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

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

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

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

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

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			

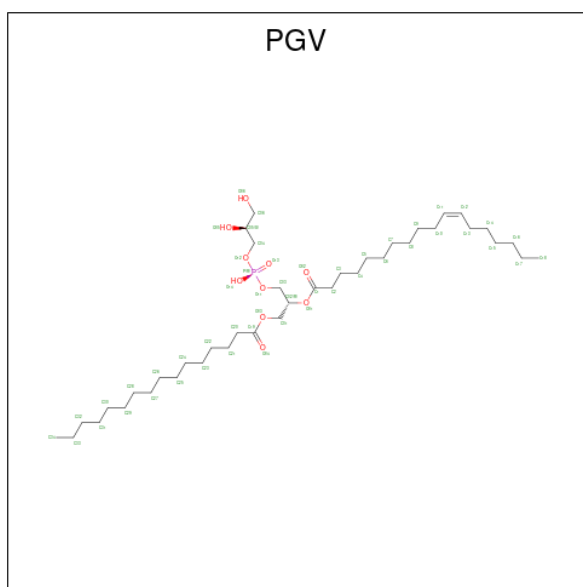
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			388	259	66	60	3			
12	Y	46	Total	C	N	O	S	0	4	0
			394	261	66	64	3			

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

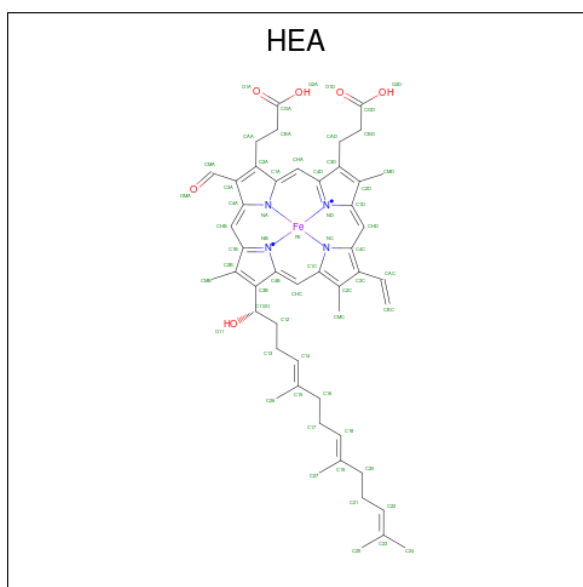
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



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

- Molecule 15 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

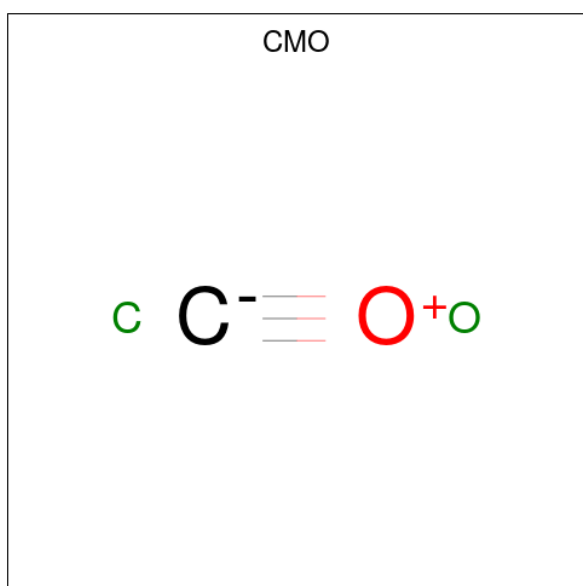
- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is SODIUM ION (CCD ID: NA) (formula: Na).

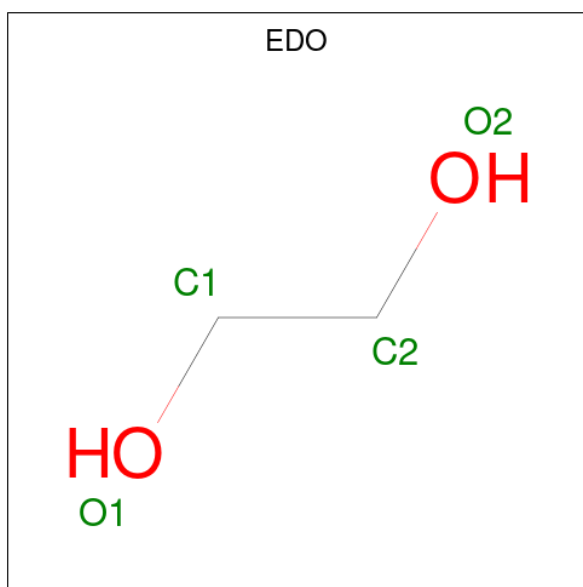
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Na	0	0
			1	1		
18	C	1	Total	Na	0	0
			1	1		
18	N	1	Total	Na	0	0
			1	1		
18	P	1	Total	Na	0	0
			1	1		

- Molecule 19 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



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

- Molecule 20 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

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

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

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

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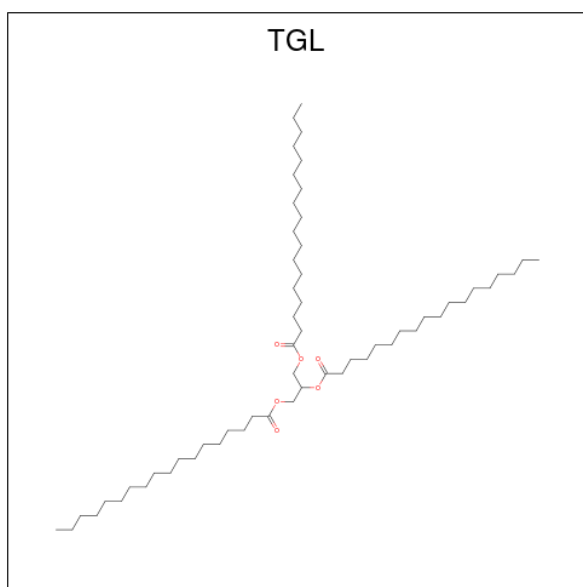
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20	P	1	Total	C	O	0	0
			4	2	2		
20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

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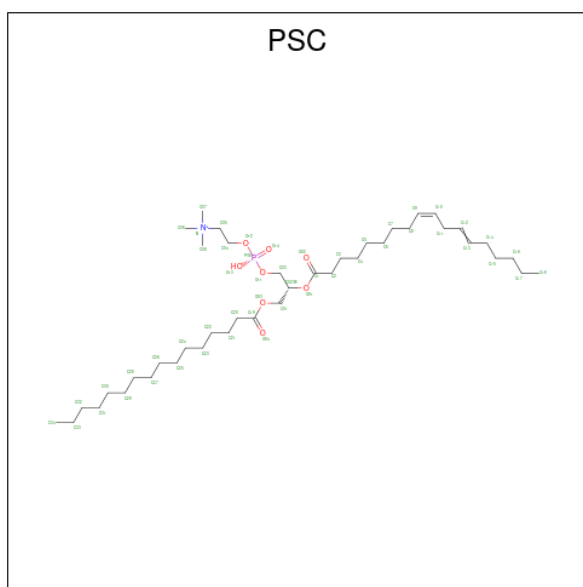
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	S	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20	T	1	Total	C	O	0	0
			4	2	2		
20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

- Molecule 21 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



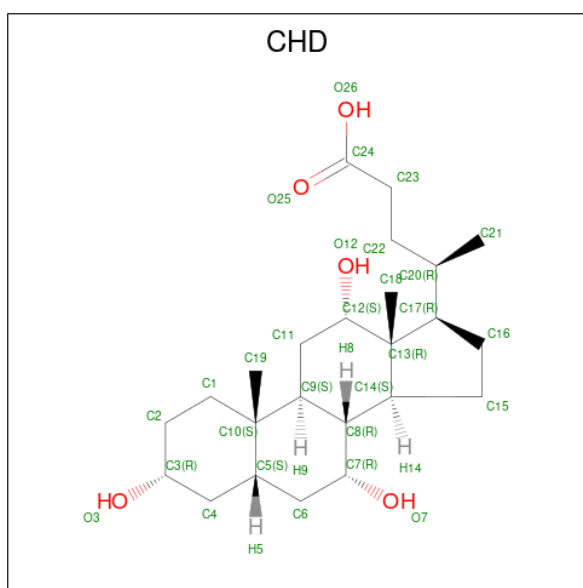
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		
21	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



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

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



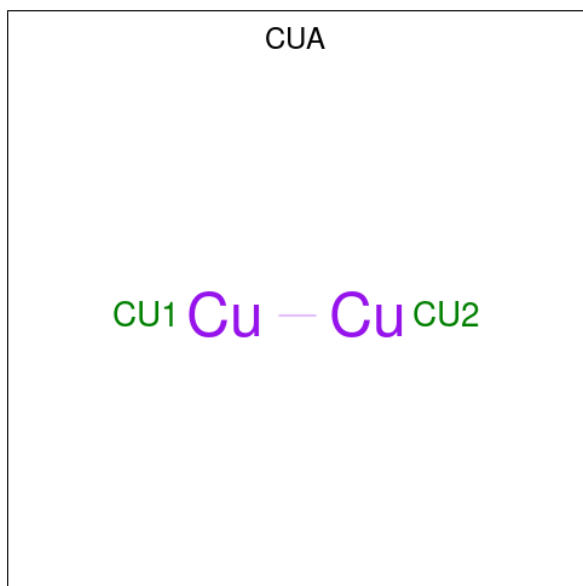
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		

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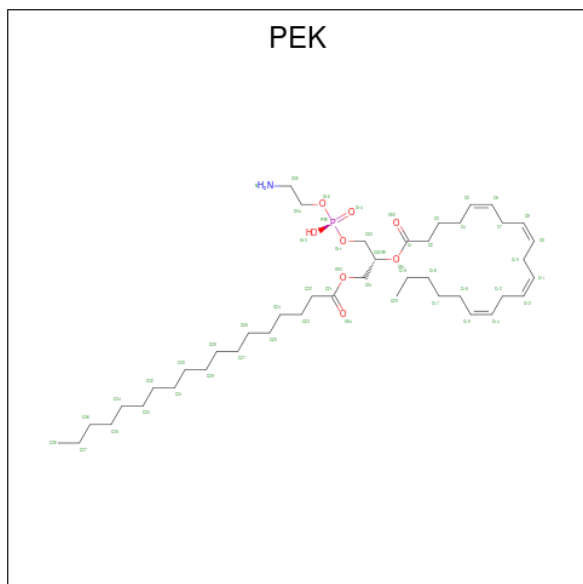
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	C	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0
23	G	1	Total C O 29 24 5	0	0
23	J	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	P	1	Total C O 29 24 5	0	0
23	W	1	Total C O 29 24 5	0	0
23	Y	1	Total C O 29 24 5	0	0

- Molecule 24 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



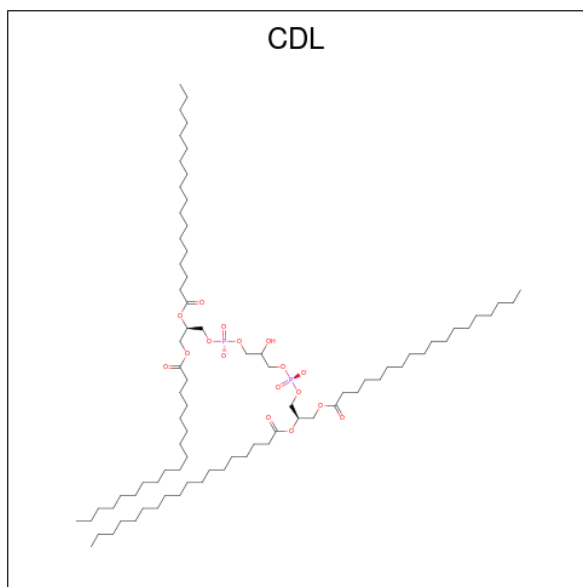
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Cu 2 2	0	0
24	O	1	Total Cu 2 2	0	0

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



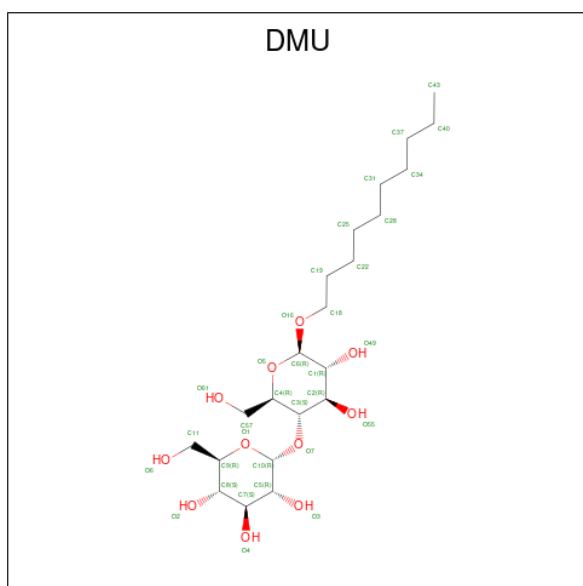
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
25	C	1	Total 53	43	1	8	1	0	0
25	C	1	Total 53	43	1	8	1	0	0
25	C	1	Total 53	43	1	8	1	0	0
25	P	1	Total 53	43	1	8	1	0	0
25	P	1	Total 53	43	1	8	1	0	0
25	P	1	Total 53	43	1	8	1	0	0

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



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

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

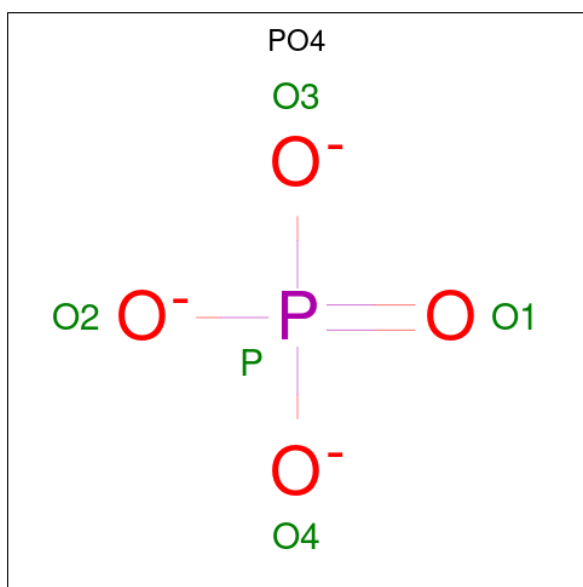


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			33	22	11		
27	C	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	V	1	Total	C	O	0	0
			33	22	11		
27	Z	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 (CCD ID: 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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	255	Total	O	0	0
			255	255		
30	B	194	Total	O	0	2
			195	195		
30	C	142	Total	O	0	0
			142	142		
30	D	167	Total	O	0	0
			167	167		
30	E	120	Total	O	0	0
			120	120		
30	F	130	Total	O	0	0
			130	130		
30	G	67	Total	O	0	0
			67	67		
30	H	78	Total	O	0	0
			78	78		
30	I	53	Total	O	0	0
			53	53		
30	J	39	Total	O	0	0
			39	39		

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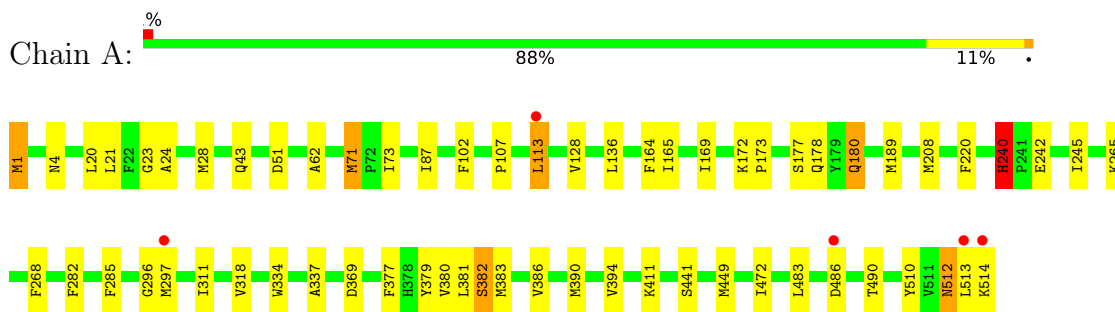
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	43	Total 43	O 43	0	0
30	L	38	Total 38	O 38	0	0
30	M	32	Total 32	O 32	0	0
30	N	240	Total 240	O 240	0	0
30	O	163	Total 164	O 164	0	1
30	P	138	Total 138	O 138	0	0
30	Q	85	Total 85	O 85	0	0
30	R	96	Total 96	O 96	0	0
30	S	129	Total 129	O 129	0	0
30	T	65	Total 65	O 65	0	0
30	U	72	Total 72	O 72	0	0
30	V	40	Total 40	O 40	0	0
30	W	45	Total 45	O 45	0	0
30	X	33	Total 33	O 33	0	0
30	Y	27	Total 27	O 27	0	0
30	Z	21	Total 21	O 21	0	0

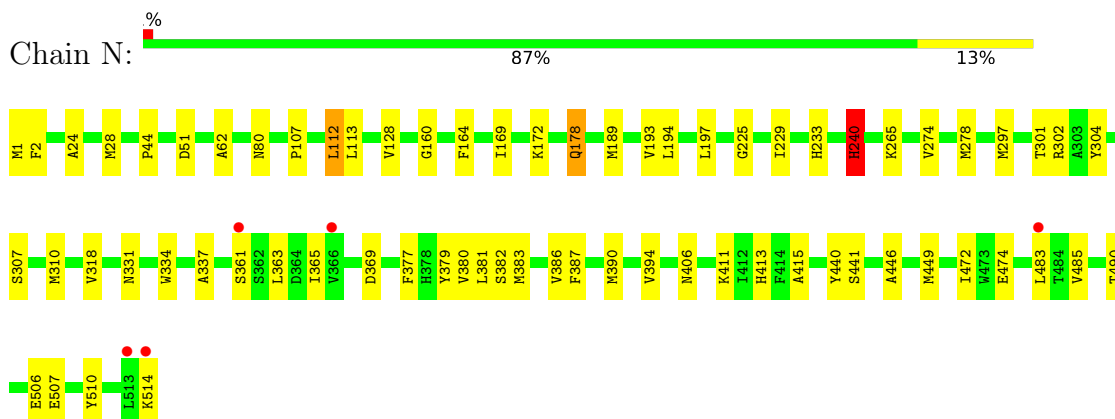
3 Residue-property plots [i](#)

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

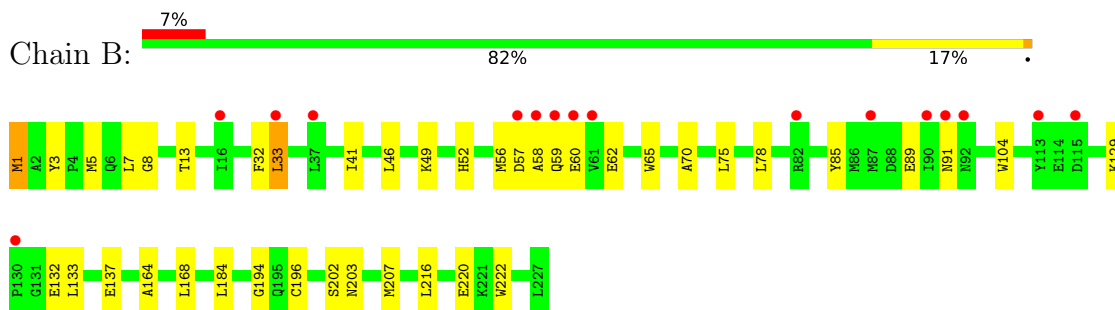
- Molecule 1: Cytochrome c oxidase subunit 1



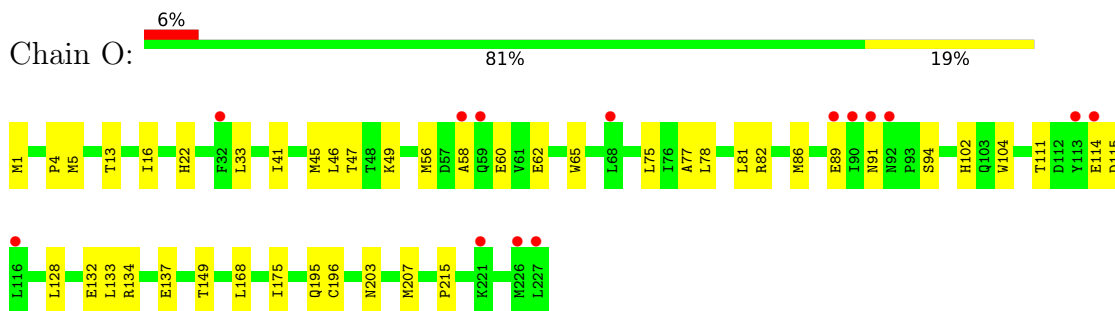
- Molecule 1: Cytochrome c oxidase subunit 1



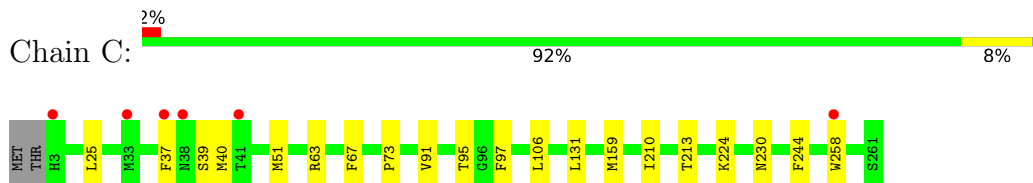
- Molecule 2: Cytochrome c oxidase subunit 2



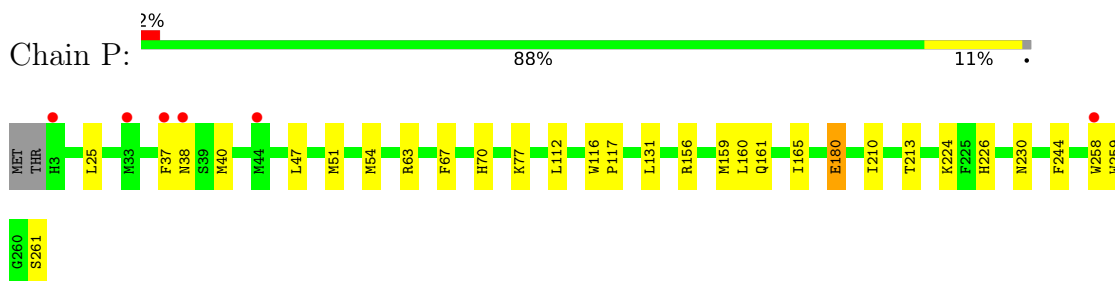
- Molecule 2: Cytochrome c oxidase subunit 2



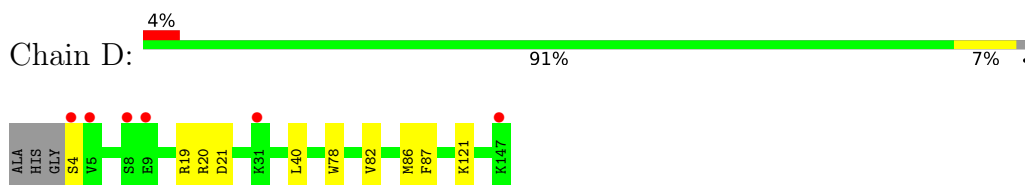
- Molecule 3: Cytochrome c oxidase subunit 3



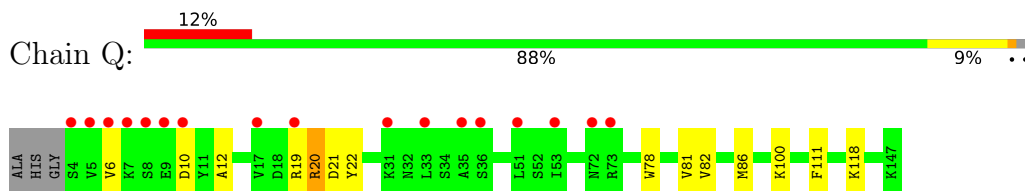
- Molecule 3: Cytochrome c oxidase subunit 3



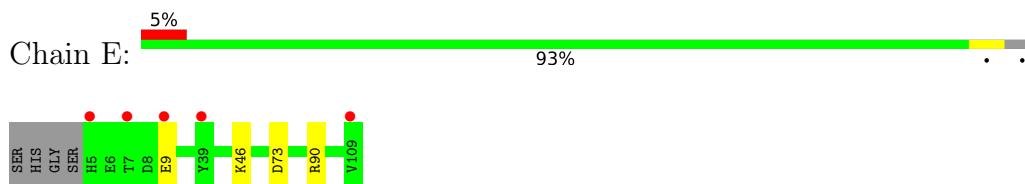
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



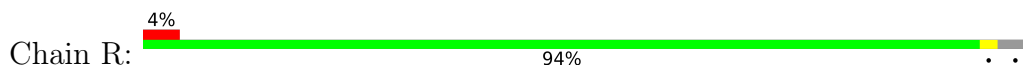
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



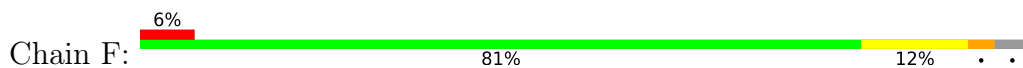
- Molecule 5: Cytochrome c oxidase subunit 5A



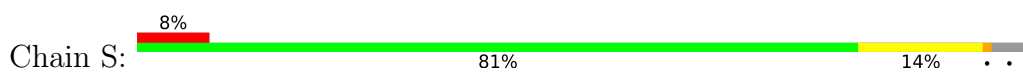
- Molecule 5: Cytochrome c oxidase subunit 5A



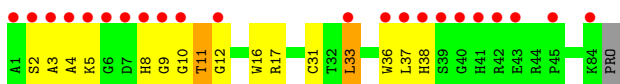
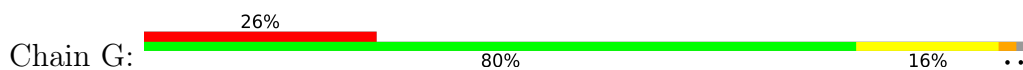
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



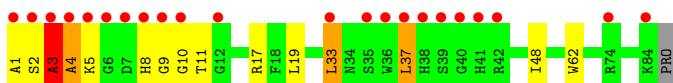
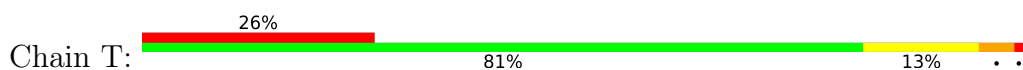
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



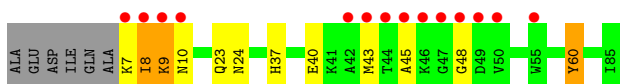
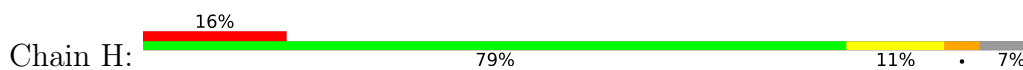
- Molecule 7: Cytochrome c oxidase subunit 6A2



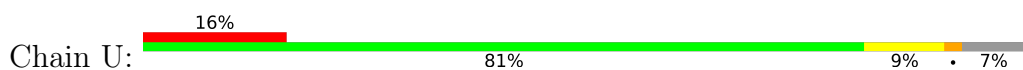
- Molecule 7: Cytochrome c oxidase subunit 6A2



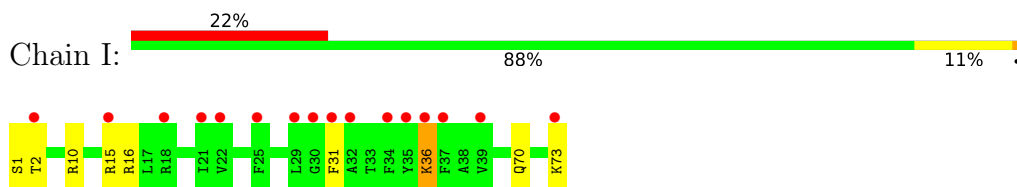
- Molecule 8: Cytochrome c oxidase subunit 6B1



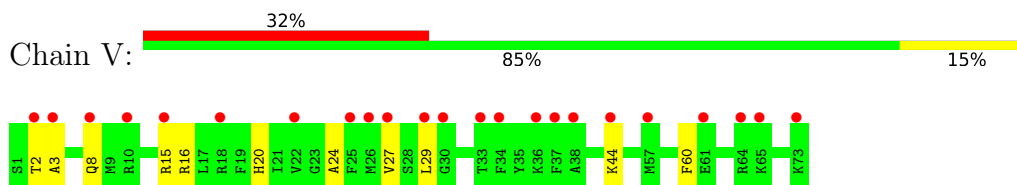
- Molecule 8: Cytochrome c oxidase subunit 6B1



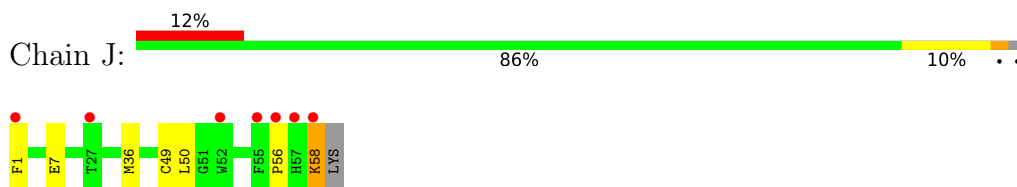
- Molecule 9: Cytochrome c oxidase subunit 6C



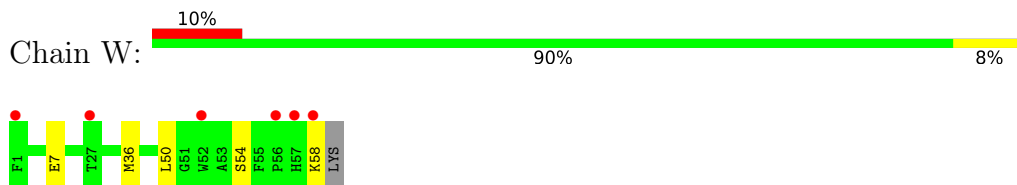
- Molecule 9: Cytochrome c oxidase subunit 6C



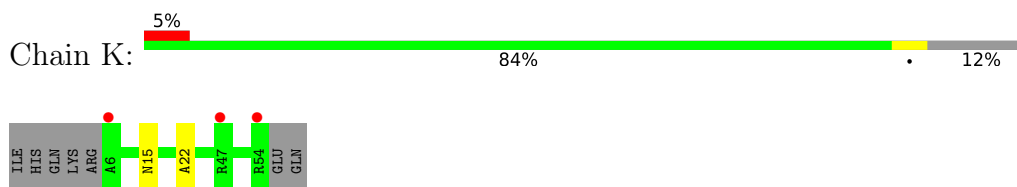
- Molecule 10: Cytochrome c oxidase subunit 7A1



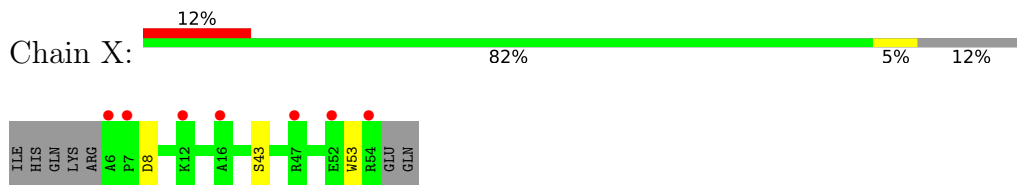
- Molecule 10: Cytochrome c oxidase subunit 7A1



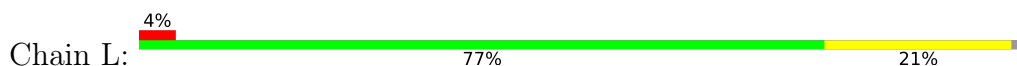
- Molecule 11: Cytochrome c oxidase subunit 7B



- Molecule 11: Cytochrome c oxidase subunit 7B

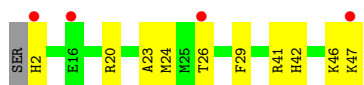
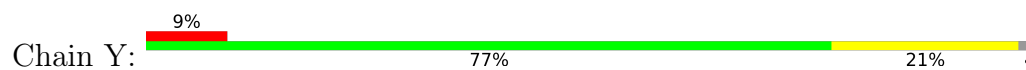


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

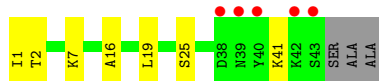
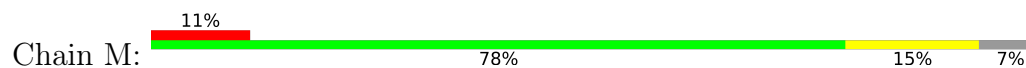




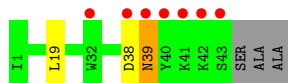
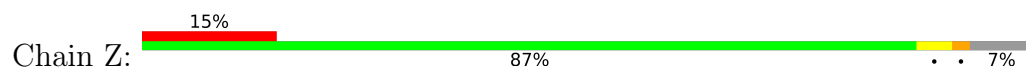
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 13: Cytochrome c oxidase subunit 8B



- Molecule 13: Cytochrome c oxidase subunit 8B



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.54Å 203.66Å 177.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 1.70 39.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.74-1.70) 99.6 (39.74-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 1.70Å)	Xtrriage
Refinement program	PHENIX (1.13-2998-000)	Depositor
R, R_{free}	0.159 , 0.178 0.163 , 0.181	Depositor DCC
R_{free} test set	35759 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.782	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34489	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: NA, DMU, FME, TPO, ZN, SAC, CDL, CMO, TGL, HEA, CUA, EDO, CU, MG, PGV, CHD, PO4, PSC, PEK

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	0.99	0/4390	0.97	5/5989 (0.1%)
1	N	0.91	0/4371	0.90	1/5964 (0.0%)
2	B	0.85	0/1961	0.94	0/2672
2	O	0.76	0/1952	0.85	0/2660
3	C	0.88	0/2268	0.84	0/3099
3	P	0.92	0/2289	0.84	0/3126
4	D	0.76	0/1273	0.78	0/1716
4	Q	0.55	0/1258	0.64	0/1696
5	E	0.72	0/871	0.71	0/1182
5	R	0.58	0/871	0.63	0/1182
6	F	0.81	0/755	0.89	0/1026
6	S	0.76	0/755	0.81	0/1025
7	G	0.75	0/690	0.70	0/937
7	T	0.67	0/698	0.75	2/948 (0.2%)
8	H	0.79	0/682	0.81	0/921
8	U	0.66	0/682	0.73	0/921
9	I	0.63	0/605	0.71	0/802
9	V	0.51	0/605	0.62	0/802
10	J	0.63	0/471	0.66	0/636
10	W	0.54	0/471	0.63	0/636
11	K	0.70	0/398	0.71	0/546
11	X	0.52	0/398	0.55	0/546
12	L	0.82	0/412	0.77	0/551
12	Y	0.68	0/430	0.67	0/575
13	M	0.76	0/345	0.74	0/470
13	Z	0.61	0/345	0.62	0/470
All	All	0.82	0/30246	0.83	8/41098 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
All	All	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-13.06	72.16	100.90
1	N	240	HIS	CA-CB-CG	-7.80	106.00	113.80
1	A	240	HIS	CA-CB-CG	-7.22	106.58	113.80
1	A	102	PHE	CA-CB-CG	-5.97	107.83	113.80
7	T	3	ALA	CA-C-N	5.60	131.78	121.70
7	T	3	ALA	C-N-CA	5.60	131.78	121.70
1	A	512[A]	ASN	N-CA-CB	5.29	118.46	110.42
1	A	512[B]	ASN	N-CA-CB	5.29	118.46	110.42

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain

5.2 Too-close contacts [i](#)

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	4124	0	4092	62	0
1	N	4116	0	4070	67	0
2	B	1869	0	1872	37	0
2	O	1865	0	1874	39	0
3	C	2131	0	2039	23	0
3	P	2141	0	2056	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1214	0	1205	17	0
4	Q	1206	0	1196	16	0
5	E	852	0	845	3	0
5	R	852	0	845	1	0
6	F	723	0	702	9	0
6	S	723	0	705	14	0
7	G	675	0	644	20	0
7	T	678	0	644	14	0
8	H	662	0	623	8	0
8	U	662	0	623	8	0
9	I	601	0	613	7	0
9	V	601	0	613	9	0
10	J	460	0	459	6	0
10	W	460	0	459	3	0
11	K	384	0	366	4	0
11	X	384	0	366	3	0
12	L	388	0	389	14	0
12	Y	394	0	385	9	0
13	M	335	0	352	9	0
13	Z	335	0	352	2	0
14	A	102	0	152	3	0
14	C	102	0	152	4	0
14	N	102	0	152	4	0
14	P	102	0	152	8	0
15	A	139	0	112	5	0
15	N	139	0	112	3	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	N	1	0	0	0	0
18	A	1	0	0	0	0
18	C	1	0	0	0	0
18	N	1	0	0	0	0
18	P	1	0	0	1	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	76	0	114	9	0
20	B	40	0	60	10	2
20	C	28	0	42	3	0
20	D	24	0	33	3	2
20	E	12	0	18	0	0
20	F	24	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	G	20	0	30	4	0
20	H	12	0	18	5	0
20	J	8	0	12	2	0
20	K	8	0	12	2	0
20	L	16	0	24	0	0
20	M	16	0	24	3	0
20	N	84	0	126	13	0
20	O	20	0	30	2	0
20	P	44	0	66	5	0
20	Q	8	0	12	0	0
20	R	20	0	30	1	0
20	S	44	0	66	3	0
20	T	8	0	12	0	0
20	U	4	0	6	1	0
20	V	4	0	6	0	0
20	W	12	0	18	2	0
20	Y	8	0	12	0	0
21	B	63	0	110	4	0
21	D	63	0	110	9	0
21	L	63	0	110	11	0
21	N	63	0	110	2	0
21	Q	63	0	110	7	0
21	Y	63	0	110	11	0
22	B	52	0	80	10	0
22	O	52	0	80	5	0
23	B	29	0	39	0	0
23	C	87	0	117	3	0
23	G	29	0	39	1	0
23	J	29	0	39	3	0
23	P	87	0	117	9	0
23	W	29	0	39	3	0
23	Y	29	0	39	4	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	C	159	0	231	8	0
25	P	159	0	231	15	0
26	C	100	0	156	13	0
26	G	100	0	156	18	0
26	P	100	0	156	20	0
26	T	100	0	156	11	0
27	C	66	0	84	3	0
27	G	33	0	42	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	M	66	0	84	0	0
27	P	99	0	124	8	0
27	V	33	0	42	4	0
27	Z	66	0	84	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	255	0	0	7	0
30	B	195	0	0	3	2
30	C	142	0	0	1	0
30	D	167	0	0	1	2
30	E	120	0	0	1	0
30	F	130	0	0	2	0
30	G	67	0	0	1	0
30	H	78	0	0	1	0
30	I	53	0	0	1	0
30	J	39	0	0	1	0
30	K	43	0	0	0	0
30	L	38	0	0	1	0
30	M	32	0	0	0	0
30	N	240	0	0	5	0
30	O	164	0	0	3	0
30	P	138	0	0	4	0
30	Q	85	0	0	5	0
30	R	96	0	0	1	0
30	S	129	0	0	6	0
30	T	65	0	0	0	0
30	U	72	0	0	2	0
30	V	40	0	0	1	0
30	W	45	0	0	3	0
30	X	33	0	0	1	0
30	Y	27	0	0	1	0
30	Z	21	0	0	0	0
All	All	34489	0	32823	482	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (482) 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)
8:H:24:ASN:HD21	20:H:103:EDO:H21	1.24	0.98
6:F:75:HIS:H	6:F:80[A]:GLN:HE22	1.12	0.97
1:N:178[B]:GLN:NE2	30:N:701:HOH:O	1.99	0.95
6:S:75:HIS:H	6:S:80[A]:GLN:HE22	1.14	0.93
25:P:305:PEK:H041	7:T:17:ARG:HH22	1.32	0.93
11:K:15:ASN:H	20:K:102:EDO:H12	1.34	0.91
7:T:3:ALA:HA	7:T:4:ALA:HB2	1.55	0.89
22:B:302:PSC:H071	9:I:10:ARG:HH21	1.39	0.87
12:L:24[B]:MET:SD	30:L:223:HOH:O	2.33	0.86
21:D:201:TGL:H342	9:I:16:ARG:HE	1.42	0.85
20:A:609:EDO:H22	30:A:790:HOH:O	1.77	0.84
12:Y:42:HIS:HB2	23:Y:104:CHD:H12	1.59	0.83
12:L:13:PHE:HA	21:L:101:TGL:HC21	1.61	0.83
12:L:20:ARG:HH22	21:L:101:TGL:HC61	1.42	0.81
20:A:627:EDO:H12	30:A:756:HOH:O	1.81	0.80
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.63	0.80
2:B:8:GLY:H	20:B:310:EDO:H21	1.46	0.78
4:Q:100:LYS:NZ	30:Q:301:HOH:O	2.16	0.78
26:P:308:CDL:H862	26:P:308:CDL:H822	1.65	0.77
20:A:619:EDO:H12	20:F:103:EDO:H11	1.67	0.76
3:P:161[A]:GLN:HE22	25:P:305:PEK:H22	1.52	0.75
3:P:63:ARG:HE	26:P:308:CDL:HA21	1.52	0.75
3:P:67:PHE:HE2	26:P:308:CDL:H1	1.52	0.74
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.28	0.74
25:C:305:PEK:H042	7:G:17:ARG:HH12	1.53	0.73
1:N:390:MET:O	1:N:394[B]:VAL:HG12	1.89	0.72
1:A:318:VAL:HG22	2:B:65[A]:TRP:CD1	2.25	0.72
4:D:19[B]:ARG:NH1	30:D:301:HOH:O	2.22	0.71
2:B:7:LEU:HD11	21:B:301:TGL:H152	1.72	0.71
7:G:5:LYS:NZ	20:G:103:EDO:O2	2.21	0.71
1:N:164:PHE:CE2	20:N:612:EDO:H22	2.26	0.70
3:C:213:THR:HG23	26:C:308:CDL:H771	1.72	0.70
1:A:411:LYS:NZ	30:A:701:HOH:O	2.26	0.69
6:F:3:GLY:O	30:F:201:HOH:O	2.09	0.69
12:L:20:ARG:NH2	21:L:101:TGL:HC61	2.08	0.68
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.34	0.68
2:O:89:GLU:O	2:O:91:ASN:ND2	2.26	0.68
9:V:8:GLN:NE2	30:V:202:HOH:O	2.26	0.68
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.76	0.68
21:N:608:TGL:HA81	21:N:608:TGL:H141	1.75	0.68
3:P:70:HIS:HE1	20:P:319:EDO:H11	1.59	0.68
1:N:318:VAL:HG22	2:O:65[A]:TRP:CD1	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TYR:OH	1:A:512[B]:ASN:OD1	2.03	0.67
13:M:1:ILE:HG23	20:M:103:EDO:H22	1.77	0.66
1:N:233:HIS:HE2	20:N:623:EDO:H22	1.61	0.65
7:G:8:HIS:CD2	7:G:9:GLY:H	2.14	0.65
14:P:306:PGV:H161	26:P:308:CDL:H651	1.78	0.65
3:C:67:PHE:HE2	26:C:308:CDL:H1	1.60	0.65
5:R:90:ARG:NH2	30:R:302:HOH:O	2.29	0.65
4:D:40:LEU:HB2	20:D:205:EDO:H21	1.79	0.65
3:P:180[B]:GLU:OE2	30:P:401:HOH:O	2.15	0.65
1:A:381[B]:LEU:HB2	15:A:603:HEA:CAC	2.27	0.64
18:P:302:NA:NA	30:P:505:HOH:O	1.70	0.64
1:N:80:ASN:HD21	20:N:612:EDO:H12	1.62	0.64
20:P:314:EDO:O2	30:P:402:HOH:O	2.15	0.64
13:M:7:LYS:NZ	20:M:104:EDO:H11	2.12	0.64
3:P:165:ILE:HG12	25:P:305:PEK:H9	1.77	0.64
6:S:80[B]:GLN:NE2	30:S:204:HOH:O	2.32	0.63
1:A:285:PHE:HB2	7:T:3:ALA:HB2	1.79	0.63
26:G:101:CDL:H322	26:G:101:CDL:HA62	1.80	0.63
10:J:36:MET:HG2	23:J:101:CHD:H222	1.79	0.62
14:P:306:PGV:H131	26:P:308:CDL:H591	1.81	0.62
7:T:8:HIS:CD2	7:T:9:GLY:H	2.17	0.62
2:B:85:TYR:CE2	26:T:101:CDL:H111	2.34	0.62
25:C:305:PEK:H042	7:G:17:ARG:NH1	2.15	0.62
1:N:415:ALA:HB1	21:Q:201:TGL:H121	1.80	0.62
2:O:13:THR:HB	2:O:168:LEU:HD23	1.81	0.62
26:G:101:CDL:H561	26:G:101:CDL:H771	1.82	0.62
3:P:51[B]:MET:SD	26:P:308:CDL:H621	2.40	0.61
1:A:113[B]:LEU:HD12	21:L:101:TGL:H131	1.81	0.61
27:C:310:DMU:H11	10:J:49:CYS:HB3	1.80	0.61
2:O:91:ASN:HB3	2:O:149:THR:HG21	1.82	0.61
3:C:39:SER:OG	27:C:319:DMU:H30	2.00	0.61
3:P:213:THR:HG23	26:P:308:CDL:H761	1.82	0.61
12:Y:42:HIS:HB2	23:Y:104:CHD:H212	1.82	0.61
7:T:48:ILE:HG12	20:U:101:EDO:H12	1.81	0.61
26:C:308:CDL:H192	26:C:308:CDL:H622	1.83	0.61
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.82	0.60
1:N:474:GLU:OE2	20:N:619:EDO:H22	2.00	0.60
4:Q:20[A]:ARG:HG2	30:Q:362:HOH:O	2.01	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.46	0.60
1:N:507:GLU:H	20:N:618:EDO:H12	1.66	0.60
20:A:624:EDO:H22	21:L:101:TGL:HC51	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:VAL:O	3:C:95[B]:THR:HG23	2.01	0.60
9:V:27:VAL:HG21	27:V:102:DMU:H7	1.83	0.60
6:S:94:HIS:O	30:S:201:HOH:O	2.16	0.60
4:D:78:TRP:CA	21:D:201:TGL:HB22	2.31	0.59
1:N:51[C]:ASP:OD2	1:N:441:SER:OG	2.19	0.59
1:N:446:ALA:H	20:N:630:EDO:H21	1.67	0.59
2:O:56:MET:HB3	22:O:301:PSC:H231	1.85	0.59
23:J:101:CHD:H221	20:J:102:EDO:H22	1.84	0.59
2:B:222:TRP:HE1	20:B:312:EDO:C2	2.16	0.58
1:A:311[A]:ILE:HD13	26:T:101:CDL:H441	1.85	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.84	0.58
30:Q:312:HOH:O	20:R:203:EDO:H21	2.04	0.58
26:G:101:CDL:H141	26:G:101:CDL:H381	1.86	0.58
14:P:307:PGV:H032	30:P:499:HOH:O	2.03	0.58
7:G:12:GLY:HA3	20:G:107:EDO:H11	1.86	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.85	0.57
3:P:37:PHE:CE2	27:P:309:DMU:H12	2.38	0.57
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.86	0.57
3:C:210:ILE:HD13	14:C:306:PGV:H302	1.85	0.57
8:H:8:ILE:HG22	8:H:9:LYS:HD2	1.86	0.57
10:J:58:LYS:H	10:J:58:LYS:HD2	1.70	0.57
25:C:305:PEK:N	30:C:402:HOH:O	2.15	0.57
1:N:472:ILE:HG21	21:Y:101:TGL:H201	1.87	0.57
20:N:612:EDO:H11	30:N:922:HOH:O	2.05	0.57
1:A:28[A]:MET:HE3	12:L:29:PHE:CD1	2.40	0.56
11:K:15:ASN:N	20:K:102:EDO:H12	2.13	0.56
1:A:169:ILE:HD12	7:T:8:HIS:HB3	1.86	0.56
20:N:630:EDO:H11	2:O:133:LEU:HD22	1.87	0.56
3:P:210:ILE:HD13	14:P:306:PGV:H302	1.88	0.56
8:U:43:MET:HE3	8:U:48:GLY:HA3	1.86	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.56
3:P:161[A]:GLN:NE2	25:P:305:PEK:H5	2.20	0.56
1:N:381[B]:LEU:HB2	15:N:603:HEA:CAC	2.36	0.56
2:B:203:ASN:ND2	30:B:405[A]:HOH:O	2.37	0.56
1:N:169:ILE:HG12	1:N:189[A]:MET:HE1	1.87	0.56
14:N:601:PGV:H301	13:Z:19:LEU:HD23	1.88	0.56
20:O:306:EDO:H21	8:U:24:ASN:HD21	1.70	0.56
12:Y:23:ALA:HB2	27:Z:102:DMU:H15	1.88	0.56
2:B:13:THR:HB	2:B:168:LEU:HD23	1.88	0.56
1:N:318:VAL:HG22	2:O:65[A]:TRP:HD1	1.68	0.56
3:C:224:LYS:CD	26:C:308:CDL:HB31	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:TRP:CD1	23:C:311:CHD:H161	2.41	0.55
20:A:614:EDO:H22	13:M:2:THR:HG23	1.89	0.55
12:Y:20:ARG:HH22	21:Y:101:TGL:HC62	1.72	0.55
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.88	0.55
12:L:24[B]:MET:HG2	21:L:101:TGL:HA22	1.89	0.55
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.87	0.55
1:A:510:TYR:HE1	1:A:512[B]:ASN:ND2	2.06	0.54
7:G:5:LYS:HB3	1:N:278[B]:MET:HE1	1.89	0.54
25:C:303:PEK:H381	7:T:19:LEU:HD21	1.88	0.54
1:N:382[B]:SER:O	1:N:386:VAL:HB	2.08	0.54
26:T:101:CDL:H531	26:T:101:CDL:H262	1.89	0.54
1:A:24:ALA:HB2	15:A:602[A]:HEA:H253	1.89	0.54
1:N:112:LEU:HD23	1:N:112:LEU:C	2.33	0.54
4:Q:19[B]:ARG:HD3	4:Q:21:ASP:OD1	2.07	0.54
3:P:67:PHE:CE2	26:P:308:CDL:H1	2.39	0.54
25:P:305:PEK:H041	7:T:17:ARG:NH2	2.13	0.54
3:C:40[A]:MET:SD	27:G:108:DMU:O49	2.66	0.53
13:M:7:LYS:HZ1	20:M:104:EDO:H11	1.72	0.53
12:Y:24[A]:MET:SD	21:Y:101:TGL:H172	2.47	0.53
1:N:112:LEU:HG	30:N:916:HOH:O	2.06	0.53
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.07	0.53
1:A:165:ILE:HG23	1:A:189[B]:MET:HE1	1.89	0.53
1:A:486[A]:ASP:OD1	4:D:19[A]:ARG:HD2	2.09	0.53
30:F:214:HOH:O	20:J:103:EDO:H11	2.08	0.53
3:P:261:SER:OXT	23:P:310:CHD:H21	2.08	0.53
20:P:315:EDO:H11	20:W:104:EDO:H22	1.90	0.53
7:T:33:LEU:HD13	7:T:37:LEU:HD22	1.91	0.53
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.91	0.53
7:G:33:LEU:HB3	20:G:104:EDO:H22	1.91	0.53
4:D:19[B]:ARG:HH21	4:D:21:ASP:CG	2.17	0.53
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.91	0.53
2:O:62:GLU:HG2	2:O:65[A]:TRP:CE2	2.43	0.53
3:P:156:ARG:HE	23:P:311:CHD:C24	2.21	0.53
27:P:324:DMU:H1	7:T:62:TRP:HB2	1.91	0.53
1:N:411:LYS:NZ	30:N:704:HOH:O	2.42	0.53
3:P:259:TRP:O	23:P:310:CHD:O12	2.27	0.53
1:A:379:TYR:O	1:A:383[B]:MET:HB2	2.09	0.52
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.91	0.52
1:A:318:VAL:HG22	2:B:65[A]:TRP:HD1	1.71	0.52
4:D:78:TRP:CB	21:D:201:TGL:HB22	2.40	0.52
12:L:2[A]:HIS:CG	12:L:3:TYR:H	2.28	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	1.92	0.52
20:P:320:EDO:H12	6:S:52:ILE:HD11	1.92	0.51
30:A:763:HOH:O	20:H:103:EDO:H11	2.09	0.51
26:G:101:CDL:HB32	1:N:304:TYR:HD1	1.75	0.51
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.08	0.51
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.46	0.51
8:H:24:ASN:ND2	20:H:103:EDO:H21	2.09	0.51
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.75	0.51
12:Y:20:ARG:HH12	21:Y:101:TGL:HC42	1.76	0.51
20:C:316:EDO:O2	20:H:102:EDO:H22	2.10	0.51
26:G:101:CDL:H381	2:O:81:LEU:HD12	1.93	0.51
4:Q:81:VAL:HG11	21:Q:201:TGL:HB62	1.91	0.51
3:P:258:TRP:CD1	23:P:310:CHD:H161	2.45	0.51
1:N:406:ASN:HD21	14:N:601:PGV:H22	1.76	0.51
14:N:609:PGV:H343	25:P:304:PEK:H381	1.93	0.51
3:P:51[A]:MET:SD	26:P:308:CDL:H612	2.50	0.51
8:U:8:ILE:HG22	8:U:9:LYS:HD2	1.93	0.51
25:C:305:PEK:H383	26:G:101:CDL:C27	2.42	0.51
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.92	0.50
3:C:51[A]:MET:SD	26:C:308:CDL:H611	2.51	0.50
10:W:36:MET:HG2	23:W:101:CHD:H222	1.93	0.50
1:N:113:LEU:HB2	21:Y:101:TGL:H301	1.92	0.50
1:N:297[B]:MET:HE3	1:N:301:THR:HG21	1.93	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.93	0.50
4:Q:10:ASP:HB2	30:Q:302:HOH:O	2.10	0.50
10:W:54:SER:O	12:Y:46:LYS:HD3	2.10	0.50
1:A:382[B]:SER:O	1:A:386:VAL:HB	2.11	0.50
30:A:734:HOH:O	12:L:7:PRO:HG3	2.11	0.50
3:C:73:PRO:O	20:C:317:EDO:H12	2.12	0.50
1:N:28[A]:MET:HE3	12:Y:29:PHE:CD1	2.46	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.93	0.50
25:C:303:PEK:H282	25:C:303:PEK:H322	1.93	0.50
2:O:82:ARG:NH2	30:O:404:HOH:O	2.44	0.50
3:C:106:LEU:HD13	14:C:307:PGV:H21	1.94	0.50
5:E:46:LYS:NZ	30:E:303:HOH:O	2.44	0.50
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.93	0.50
7:G:31:CYS:SG	26:G:101:CDL:H532	2.52	0.49
6:S:19:GLU:HG2	30:S:297:HOH:O	2.12	0.49
21:L:101:TGL:H231	21:L:101:TGL:HA92	1.94	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.49
2:B:49:LYS:HD2	4:D:20[B]:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:507:GLU:H	20:N:618:EDO:C1	2.24	0.49
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.94	0.49
7:G:4:ALA:HB1	1:N:194:LEU:HD12	1.95	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.49
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.47	0.49
3:P:54:MET:HE1	14:P:306:PGV:H132	1.94	0.49
8:U:37:HIS:HD2	30:U:201:HOH:O	1.96	0.49
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.94	0.49
12:L:26:THR:HG23	13:M:25:SER:CB	2.43	0.49
2:B:58:ALA:H	20:B:311:EDO:H21	1.78	0.49
20:B:309:EDO:H12	30:B:566:HOH:O	2.11	0.49
7:G:4:ALA:CB	1:N:194:LEU:HD12	2.43	0.49
1:A:1:FME:HE2	1:A:4:ASN:HD22	1.78	0.48
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.11	0.48
3:P:224:LYS:HE3	26:P:308:CDL:H131	1.95	0.48
3:P:224:LYS:CD	26:P:308:CDL:HB31	2.42	0.48
25:P:304:PEK:H101	25:P:304:PEK:H42	1.95	0.48
2:O:82:ARG:HD2	30:O:401:HOH:O	2.13	0.48
3:P:40[A]:MET:HE2	27:P:324:DMU:H32	1.95	0.48
4:D:20[B]:ARG:NE	5:E:73:ASP:OD2	2.42	0.48
26:G:101:CDL:H172	1:N:307:SER:CB	2.44	0.48
1:N:514:LYS:NZ	30:N:705:HOH:O	2.47	0.48
6:S:10:GLU:OE1	6:S:25:ARG:NH2	2.43	0.48
21:B:301:TGL:HC31	20:B:310:EDO:H12	1.96	0.48
3:C:131:LEU:HD21	26:G:101:CDL:HB61	1.96	0.48
7:G:4:ALA:HB2	1:N:197:LEU:HD12	1.96	0.48
3:C:224:LYS:HD3	26:C:308:CDL:HB31	1.94	0.48
7:G:38:HIS:CE1	26:G:101:CDL:H122	2.49	0.48
7:G:11:TPO:O2P	7:G:16:TRP:NE1	2.34	0.47
20:S:107:EDO:H11	30:S:278:HOH:O	2.14	0.47
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.95	0.47
2:B:52:HIS:HE1	22:B:302:PSC:H012	1.79	0.47
26:G:101:CDL:H181	20:G:104:EDO:O1	2.13	0.47
3:P:40[A]:MET:HE2	27:P:324:DMU:H3	1.83	0.47
7:G:8:HIS:HD2	7:G:9:GLY:H	1.58	0.47
23:J:101:CHD:H193	23:J:101:CHD:H111	1.58	0.47
2:B:3:TYR:OH	20:B:310:EDO:H22	2.13	0.47
2:O:41:ILE:HD13	22:O:301:PSC:C34	2.44	0.47
2:O:22[A]:HIS:CE1	9:V:44:LYS:HG3	2.49	0.47
25:P:305:PEK:H203	25:P:305:PEK:H162	1.96	0.47
1:A:208[B]:MET:HE3	1:A:220:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:601:PGV:H311	13:M:19:LEU:HD23	1.97	0.47
1:A:43:GLN:HG3	20:A:623:EDO:H11	1.96	0.47
1:A:472:ILE:HG21	21:L:101:TGL:HA91	1.96	0.47
2:B:33[A]:LEU:HD13	9:I:31:PHE:CD2	2.50	0.47
3:C:37:PHE:CD2	27:C:310:DMU:H13	2.50	0.47
2:O:49:LYS:HD3	21:Q:201:TGL:HC71	1.96	0.47
2:O:82:ARG:NH1	30:O:401:HOH:O	2.25	0.47
3:P:161[A]:GLN:HE21	25:P:305:PEK:H5	1.77	0.47
1:A:449[A]:MET:SD	2:B:5:MET:HG2	2.55	0.47
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.95	0.47
1:A:51[C]:ASP:HB2	2:B:202:SER:O	2.15	0.47
1:A:71:MET:HB3	1:A:71:MET:HE2	1.82	0.47
30:B:552:HOH:O	21:D:201:TGL:HC61	2.15	0.47
3:P:259:TRP:HD1	23:P:310:CHD:H213	1.80	0.47
4:Q:78:TRP:N	21:Q:201:TGL:HB22	2.30	0.47
21:Y:101:TGL:HC71	21:Y:101:TGL:HC22	1.97	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
2:B:129:LYS:HG3	20:B:309:EDO:H21	1.97	0.46
9:V:2:THR:OG1	9:V:3:ALA:N	2.46	0.46
9:V:24:ALA:HA	27:V:102:DMU:H8	1.97	0.46
27:P:324:DMU:H32	27:P:324:DMU:H3	1.67	0.46
6:S:94:HIS:HD2	30:S:314:HOH:O	1.99	0.46
1:A:240:HIS:C	1:A:240:HIS:CD2	2.93	0.46
8:H:37:HIS:HD2	8:H:40:GLU:OE2	1.99	0.46
23:P:310:CHD:H182	23:P:310:CHD:H8	1.60	0.46
1:A:510:TYR:CE1	1:A:512[B]:ASN:ND2	2.83	0.46
12:L:24[B]:MET:HE3	12:L:24[B]:MET:HB2	1.82	0.46
1:N:24:ALA:HB2	15:N:602[A]:HEA:H253	1.96	0.46
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.97	0.46
8:U:60:TYR:CD1	8:U:60:TYR:C	2.93	0.46
1:A:390:MET:O	1:A:394[A]:VAL:HG22	2.15	0.46
4:D:121:LYS:NZ	20:D:207:EDO:O2	2.49	0.46
4:Q:82:VAL:HG12	4:Q:86:MET:HE2	1.97	0.46
2:O:58:ALA:O	2:O:62:GLU:HG3	2.16	0.46
10:J:56:PRO:HD3	12:L:46:LYS:HD2	1.97	0.46
1:N:510:TYR:HD2	20:S:107:EDO:H21	1.80	0.46
2:O:16:ILE:HD11	2:O:86:MET:HG2	1.97	0.46
3:P:67:PHE:HE2	26:P:308:CDL:C1	2.23	0.46
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.16	0.46
20:A:620:EDO:H11	12:L:10:ASN:HD22	1.80	0.46
8:H:43:MET:HE3	8:H:48:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:101:CDL:H511	26:T:101:CDL:H231	1.98	0.46
2:B:56:MET:HA	22:B:302:PSC:H212	1.97	0.46
7:G:38:HIS:NE2	26:G:101:CDL:O1	2.35	0.46
3:P:160:LEU:HD13	23:P:311:CHD:H181	1.98	0.46
1:A:510:TYR:CZ	1:A:512[B]:ASN:OD1	2.69	0.46
14:A:601:PGV:H312	13:M:16:ALA:HA	1.97	0.46
1:A:164:PHE:CE2	20:A:609:EDO:H21	2.51	0.45
20:W:104:EDO:H21	30:W:216:HOH:O	2.16	0.45
22:O:301:PSC:H21	22:O:301:PSC:H02	1.86	0.45
4:Q:19[B]:ARG:HG2	4:Q:22:TYR:HB3	1.98	0.45
1:A:20:LEU:HB3	21:L:101:TGL:H221	1.98	0.45
6:S:48:LEU:H	20:S:103:EDO:HO2	1.63	0.45
21:B:301:TGL:H242	21:B:301:TGL:HA91	1.98	0.45
23:C:311:CHD:H111	23:C:311:CHD:H193	1.79	0.45
12:L:26:THR:HG23	13:M:25:SER:HB3	1.99	0.45
26:G:101:CDL:H651	26:G:101:CDL:H622	1.77	0.45
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.17	0.45
10:W:7:GLU:HG3	30:W:231:HOH:O	2.16	0.45
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.69	0.45
2:B:52:HIS:CE1	22:B:302:PSC:H012	2.51	0.45
1:A:381[B]:LEU:HB2	15:A:603:HEA:HAC	1.98	0.45
23:C:309:CHD:O25	10:J:1:PHE:N	2.43	0.45
1:N:160:GLY:CA	20:N:612:EDO:H21	2.47	0.45
6:F:51:SER:O	6:F:94:HIS:N	2.48	0.45
26:G:101:CDL:H422	26:G:101:CDL:H451	1.55	0.45
1:N:80:ASN:ND2	20:N:612:EDO:H12	2.30	0.45
20:N:630:EDO:H11	2:O:133:LEU:CD2	2.47	0.45
3:P:226:HIS:CE1	26:P:308:CDL:HB32	2.52	0.45
1:A:311[A]:ILE:CD1	26:T:101:CDL:H441	2.47	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.98	0.45
8:H:60:TYR:CD1	8:H:60:TYR:C	2.95	0.45
25:P:304:PEK:H42	25:P:304:PEK:H72	1.58	0.45
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.44
21:D:201:TGL:H241	21:D:201:TGL:HA92	2.00	0.44
7:G:4:ALA:HB1	1:N:193:VAL:HG12	2.00	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.44
1:A:51[A]:ASP:OD2	1:A:441:SER:OG	2.27	0.44
2:B:89:GLU:O	2:B:91:ASN:ND2	2.50	0.44
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.48	0.44
3:P:131:LEU:HD21	26:T:101:CDL:HB61	1.99	0.44
1:A:136[B]:LEU:HD11	30:A:945:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:1:ALA:HA	7:T:2:SER:HA	1.75	0.44
26:T:101:CDL:H771	26:T:101:CDL:H561	2.00	0.44
1:A:164:PHE:HE2	20:A:609:EDO:H21	1.82	0.44
4:D:78:TRP:HA	21:D:201:TGL:HB22	1.98	0.44
8:U:9:LYS:HB3	8:U:10:ASN:H	1.62	0.44
14:C:307:PGV:H272	14:C:307:PGV:H241	1.71	0.44
3:P:37:PHE:CD2	27:P:309:DMU:H12	2.53	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.52	0.44
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	1.99	0.44
3:C:244:PHE:HA	25:C:303:PEK:H101	1.98	0.44
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.99	0.44
1:A:334:TRP:CZ3	21:D:201:TGL:HA62	2.52	0.44
2:B:56:MET:HB3	22:B:302:PSC:H252	1.99	0.44
26:G:101:CDL:HB32	1:N:304:TYR:CD1	2.52	0.44
1:N:2:PHE:HZ	21:Y:101:TGL:HG32	1.82	0.44
6:F:53:THR:HG23	6:F:55:LYS:H	1.83	0.44
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.17	0.44
8:U:40:GLU:OE2	30:U:201:HOH:O	2.21	0.44
3:C:63:ARG:HH21	26:C:308:CDL:HA21	1.82	0.44
14:C:306:PGV:H172	26:C:308:CDL:H652	2.00	0.44
14:N:601:PGV:H042	14:N:601:PGV:H031	2.00	0.44
2:O:65[B]:TRP:HE1	22:O:301:PSC:H12	1.83	0.44
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.53	0.43
7:G:36:TRP:NE1	30:G:203:HOH:O	2.51	0.43
12:L:24[A]:MET:SD	21:L:101:TGL:H162	2.57	0.43
1:N:310:MET:HE1	2:O:77:ALA:HB2	2.00	0.43
3:P:70:HIS:CE1	20:P:319:EDO:H11	2.46	0.43
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.00	0.43
25:P:305:PEK:H042	6:S:1:ALA:HA	2.00	0.43
26:T:101:CDL:H651	26:T:101:CDL:H622	1.77	0.43
1:A:297[B]:MET:HE3	1:A:297[B]:MET:HB2	1.85	0.43
26:G:101:CDL:H511	26:G:101:CDL:H202	2.00	0.43
9:I:36:LYS:NZ	9:I:36:LYS:HB3	2.33	0.43
1:N:240:HIS:C	1:N:240:HIS:CD2	2.96	0.43
2:O:62:GLU:HG2	2:O:65[A]:TRP:CZ2	2.54	0.43
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.53	0.43
3:C:73:PRO:HB3	20:C:317:EDO:H11	1.98	0.43
26:G:101:CDL:H522	26:G:101:CDL:H231	2.00	0.43
14:P:307:PGV:H242	14:P:307:PGV:H101	2.00	0.43
26:P:308:CDL:H711	26:P:308:CDL:H172	1.99	0.43
23:P:310:CHD:H232	23:P:310:CHD:H211	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:ASN:OD1	20:B:308:EDO:H21	2.18	0.43
8:H:9:LYS:HB3	8:H:10:ASN:H	1.53	0.43
3:P:244:PHE:HA	25:P:303:PEK:H101	2.01	0.43
3:C:40[B]:MET:HE2	3:C:40[B]:MET:HB2	1.57	0.43
3:P:40[B]:MET:HE3	3:P:40[B]:MET:HB3	1.95	0.43
21:Y:101:TGL:H182	21:Y:101:TGL:H342	1.89	0.43
23:Y:104:CHD:H193	23:Y:104:CHD:H111	1.86	0.43
2:O:4:PRO:HB2	11:X:43:SER:HA	2.01	0.43
9:V:20:HIS:HD2	27:V:102:DMU:H1	1.83	0.43
25:C:304:PEK:H71	25:C:304:PEK:H42	1.69	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.53	0.43
23:W:101:CHD:H221	30:W:218:HOH:O	2.19	0.43
1:A:334:TRP:HZ3	21:D:201:TGL:HA62	1.84	0.43
26:C:308:CDL:H822	26:C:308:CDL:H851	1.62	0.43
7:G:2:SER:HB3	25:P:303:PEK:H331	2.01	0.43
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.99	0.42
2:B:49:LYS:O	4:D:20[B]:ARG:NH2	2.50	0.42
3:P:37:PHE:CD2	27:P:309:DMU:H9	2.53	0.42
2:B:62:GLU:HA	2:B:65[A]:TRP:CD1	2.54	0.42
3:C:67:PHE:HE2	26:C:308:CDL:C1	2.31	0.42
3:C:67:PHE:CE2	26:C:308:CDL:H1	2.48	0.42
26:C:308:CDL:H451	26:C:308:CDL:H421	1.73	0.42
10:J:7:GLU:HG3	30:J:227:HOH:O	2.18	0.42
20:O:306:EDO:C2	8:U:24:ASN:HD21	2.31	0.42
6:S:94:HIS:NE2	30:S:205:HOH:O	2.36	0.42
23:W:101:CHD:H211	23:W:101:CHD:H231	1.69	0.42
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.54	0.42
9:I:15:ARG:HG3	30:I:128:HOH:O	2.20	0.42
14:P:306:PGV:H172	26:P:308:CDL:H632	2.02	0.42
20:H:103:EDO:H22	30:H:248:HOH:O	2.18	0.42
23:P:310:CHD:H193	23:P:310:CHD:H111	1.79	0.42
1:A:21:LEU:HD23	21:L:101:TGL:H211	2.02	0.42
23:G:102:CHD:H12	23:G:102:CHD:H212	2.01	0.42
1:N:506:GLU:N	20:N:618:EDO:H11	2.35	0.42
25:P:305:PEK:C04	7:T:17:ARG:HH22	2.17	0.42
6:S:21[B]:MET:HE2	6:S:21[B]:MET:HB3	1.79	0.42
1:A:208[A]:MET:HE2	3:C:97:PHE:CD1	2.55	0.42
2:B:216:LEU:O	2:B:220:GLU:HG3	2.20	0.42
2:B:222:TRP:HE1	20:B:312:EDO:H22	1.84	0.42
20:B:312:EDO:H11	9:I:70:GLN:OE1	2.20	0.42
2:O:5:MET:HE2	2:O:5:MET:HB3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:101:CDL:H312	26:T:101:CDL:HA62	1.67	0.42
2:B:41:ILE:HG21	22:B:302:PSC:H332	2.02	0.42
1:N:449:MET:SD	2:O:5:MET:HG2	2.60	0.42
3:C:51[B]:MET:SD	26:C:308:CDL:H232	2.60	0.41
6:F:64:GLU:O	6:F:65:ASP:HB2	2.20	0.41
1:N:331[B]:ASN:HD21	4:Q:21:ASP:HB3	1.84	0.41
2:O:111:THR:HA	2:O:114:GLU:O	2.19	0.41
4:Q:20[B]:ARG:HG3	30:Q:362:HOH:O	2.19	0.41
1:A:87:ILE:O	1:A:173:PRO:HD3	2.19	0.41
21:B:301:TGL:H241	21:B:301:TGL:H272	1.80	0.41
5:E:9:GLU:H	5:E:9:GLU:CD	2.28	0.41
7:G:8:HIS:HA	7:G:11:TPO:HG23	2.02	0.41
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.81	0.41
2:O:102:HIS:O	2:O:104:TRP:HA	2.20	0.41
21:Y:101:TGL:H232	21:Y:101:TGL:H202	1.57	0.41
1:A:379:TYR:CZ	1:A:383[A]:MET:HE1	2.54	0.41
1:A:242:GLU:HA	1:A:245:ILE:HD12	2.02	0.41
2:B:70:ALA:HB1	26:T:101:CDL:H471	2.03	0.41
2:O:47:THR:HA	21:Q:201:TGL:HC81	2.01	0.41
6:S:64:GLU:O	6:S:65:ASP:HB2	2.19	0.41
1:A:268:PHE:HE2	22:B:302:PSC:H251	1.85	0.41
3:P:38:ASN:O	27:P:323:DMU:O3	2.36	0.41
9:V:27:VAL:HG11	27:V:102:DMU:H11	2.01	0.41
13:Z:39:ASN:OD1	13:Z:39:ASN:N	2.52	0.41
1:N:302[A]:ARG:NH2	1:N:365:ILE:HD11	2.35	0.41
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.35	0.41
1:A:483:LEU:HD23	1:A:483:LEU:HA	1.95	0.41
2:B:32[B]:PHE:CD2	9:I:31:PHE:CZ	3.09	0.41
22:B:302:PSC:H042	22:B:302:PSC:H063	1.77	0.41
4:D:86:MET:CE	11:K:22:ALA:HB2	2.51	0.41
1:N:2:PHE:CZ	21:Y:101:TGL:HG32	2.56	0.41
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.56	0.41
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	2.02	0.41
1:N:334:TRP:CE3	21:Q:201:TGL:HA31	2.55	0.41
1:N:383[A]:MET:HA	1:N:387:PHE:CD1	2.56	0.41
3:P:224:LYS:HD2	26:P:308:CDL:HB31	2.02	0.41
3:P:224:LYS:CE	26:P:308:CDL:H131	2.51	0.41
26:P:308:CDL:H161	26:P:308:CDL:H132	1.86	0.41
4:Q:19[A]:ARG:HG2	4:Q:21:ASP:OD1	2.21	0.41
26:T:101:CDL:H832	26:T:101:CDL:H801	1.83	0.41
11:X:8:ASP:HB2	30:X:116:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ASP:H	22:B:302:PSC:C21	2.34	0.41
3:P:116:TRP:HA	3:P:117:PRO:C	2.46	0.41
21:Q:201:TGL:H363	9:V:16:ARG:HH21	1.86	0.41
12:Y:41:ARG:HH12	23:Y:104:CHD:H9	1.85	0.41
26:P:308:CDL:H452	26:P:308:CDL:H421	1.84	0.40
15:A:602[A]:HEA:H211	15:A:602[A]:HEA:H271	1.96	0.40
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.03	0.40
7:G:2:SER:OG	7:G:3:ALA:O	2.32	0.40
1:N:440:TYR:OH	2:O:195:GLN:HB3	2.21	0.40
22:O:301:PSC:H261	22:O:301:PSC:H232	1.49	0.40
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.02	0.40
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.21	0.40
1:A:510:TYR:HE1	1:A:512[B]:ASN:HD21	1.70	0.40
30:A:899:HOH:O	13:M:41:LYS:HG2	2.21	0.40
22:B:302:PSC:H252	22:B:302:PSC:H221	1.74	0.40
14:P:307:PGV:H62	14:P:307:PGV:H31	1.85	0.40
4:Q:10:ASP:C	4:Q:12:ALA:N	2.79	0.40
14:A:601:PGV:H131	4:D:87:PHE:CD2	2.56	0.40
26:G:101:CDL:H381	2:O:81:LEU:CD1	2.50	0.40
21:N:608:TGL:HA91	21:N:608:TGL:H252	2.02	0.40
3:P:77:LYS:NZ	25:P:303:PEK:HN1	2.20	0.40
1:N:472:ILE:HD13	21:Y:101:TGL:H201	2.03	0.40
3:P:226:HIS:HE1	26:P:308:CDL:HB32	1.86	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:314:EDO:C2	20:D:206:EDO:C1[2_584]	1.49	0.71
30:B:479:HOH:O	30:D:306:HOH:O[2_584]	1.96	0.24
20:B:314:EDO:O2	20:D:206:EDO:C1[2_584]	1.97	0.23
30:B:551:HOH:O	30:D:426:HOH:O[2_584]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	543/514 (106%)	532 (98%)	11 (2%)	0	100	100
1	N	541/514 (105%)	532 (98%)	9 (2%)	0	100	100
2	B	236/227 (104%)	231 (98%)	5 (2%)	0	100	100
2	O	235/227 (104%)	228 (97%)	7 (3%)	0	100	100
3	C	266/261 (102%)	260 (98%)	6 (2%)	0	100	100
3	P	268/261 (103%)	263 (98%)	5 (2%)	0	100	100
4	D	147/147 (100%)	144 (98%)	3 (2%)	0	100	100
4	Q	145/147 (99%)	140 (97%)	5 (3%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
6	S	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	73 (90%)	7 (9%)	1 (1%)	10	2
7	T	82/85 (96%)	73 (89%)	6 (7%)	3 (4%)	2	0
8	H	77/85 (91%)	71 (92%)	3 (4%)	3 (4%)	2	0
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	9	2
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
12	Y	47/47 (100%)	46 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3616/3614 (100%)	3521 (97%)	87 (2%)	8 (0%)	43	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	T	4	ALA
7	G	10	GLY
8	H	8	ILE
8	H	9	LYS
7	T	3	ALA
8	H	45	ALA
7	T	10	GLY
8	U	8	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/426 (107%)	447 (98%)	8 (2%)	51	36
1	N	453/426 (106%)	445 (98%)	8 (2%)	51	36
2	B	221/210 (105%)	214 (97%)	7 (3%)	34	17
2	O	220/210 (105%)	212 (96%)	8 (4%)	31	14
3	C	233/226 (103%)	231 (99%)	2 (1%)	70	62
3	P	235/226 (104%)	231 (98%)	4 (2%)	53	38
4	D	133/129 (103%)	132 (99%)	1 (1%)	73	65
4	Q	131/129 (102%)	129 (98%)	2 (2%)	57	43
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	54
5	R	92/95 (97%)	91 (99%)	1 (1%)	65	54
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	3
6	S	81/81 (100%)	79 (98%)	2 (2%)	42	24
7	G	67/68 (98%)	65 (97%)	2 (3%)	36	19
7	T	68/68 (100%)	65 (96%)	3 (4%)	25	10
8	H	71/75 (95%)	69 (97%)	2 (3%)	38	21
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	21
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	7
9	V	57/57 (100%)	55 (96%)	2 (4%)	32	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	11
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	11
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	41/40 (102%)	41 (100%)	0	100	100
12	Y	43/40 (108%)	39 (91%)	4 (9%)	8	2
13	M	37/38 (97%)	37 (100%)	0	100	100
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	6
All	All	3152/3082 (102%)	3078 (98%)	74 (2%)	48	27

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113[A]	LEU
1	A	113[B]	LEU
1	A	128	VAL
1	A	180	GLN
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER
1	A	382[C]	SER
2	B	33[A]	LEU
2	B	33[B]	LEU
2	B	59	GLN
2	B	60[A]	GLU
2	B	60[B]	GLU
2	B	75	LEU
2	B	78	LEU
3	C	159	MET
3	C	230	ASN
4	D	4	SER
5	E	90	ARG
6	F	2	SER
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80[A]	GLN
6	F	80[B]	GLN
6	F	94	HIS
7	G	33	LEU

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Mol	Chain	Res	Type
7	G	37	LEU
8	H	7	LYS
8	H	60	TYR
9	I	2	THR
9	I	36	LYS
9	I	73	LYS
10	J	50	LEU
10	J	58	LYS
1	N	112	LEU
1	N	128	VAL
1	N	178[A]	GLN
1	N	178[B]	GLN
1	N	361	SER
1	N	363	LEU
1	N	369	ASP
1	N	485	VAL
2	O	33[A]	LEU
2	O	33[B]	LEU
2	O	60	GLU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	115[A]	ASP
2	O	115[B]	ASP
3	P	159	MET
3	P	180[A]	GLU
3	P	180[B]	GLU
3	P	230	ASN
4	Q	20[A]	ARG
4	Q	20[B]	ARG
5	R	80	GLU
6	S	80[A]	GLN
6	S	80[B]	GLN
7	T	5	LYS
7	T	33	LEU
7	T	37	LEU
8	U	7	LYS
8	U	60	TYR
9	V	15	ARG
9	V	29	LEU
10	W	50	LEU
10	W	58	LYS

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Mol	Chain	Res	Type
12	Y	2[A]	HIS
12	Y	2[B]	HIS
12	Y	26	THR
12	Y	47	LYS
13	Z	38	ASP
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	170	ASN
1	A	180	GLN
1	A	422	ASN
2	B	10	GLN
2	B	59	GLN
3	C	68	GLN
3	C	76	GLN
4	D	29	HIS
4	D	109	HIS
4	D	119	GLN
7	G	8	HIS
8	H	25	GLN
8	H	28	ASN
8	H	31	GLN
8	H	32	ASN
8	H	37	HIS
10	J	57	HIS
13	M	39	ASN
1	N	170	ASN
1	N	422	ASN
2	O	10	GLN
2	O	91	ASN
2	O	140	ASN
4	Q	32	ASN
4	Q	101	HIS
4	Q	109	HIS
6	S	94	HIS
7	T	8	HIS
8	U	10	ASN
8	U	25	GLN
8	U	28	ASN

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Mol	Chain	Res	Type
8	U	31	GLN
8	U	32	ASN
8	U	37	HIS
9	V	8	GLN
9	V	20	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	V	1	9	7,8,9	0.65	0	7,9,11	0.86	0
7	TPO	T	11	7	8,10,11	1.36	1 (12%)	10,14,16	0.85	0
1	FME	N	1	1	8,9,10	0.44	0	8,9,11	1.16	1 (12%)
2	FME	B	1	2	8,9,10	0.94	0	8,9,11	1.33	1 (12%)
1	FME	A	1	1	8,9,10	0.48	0	8,9,11	1.60	1 (12%)
9	SAC	I	1	9	7,8,9	0.68	0	7,9,11	1.03	1 (14%)
2	FME	O	1	2	8,9,10	0.88	0	8,9,11	0.95	0
7	TPO	G	11	7	8,10,11	1.37	1 (12%)	10,14,16	0.91	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
9	SAC	V	1	9	-	4/7/8/10	-

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.94	1.59	1.50
7	G	11	TPO	P-O1P	2.93	1.59	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	C-CA-N	3.32	115.91	109.50
2	B	1	FME	O-C-CA	-2.23	119.03	124.77
1	N	1	FME	O-C-CA	-2.05	119.50	124.77
9	I	1	SAC	O-C-CA	-2.02	119.57	124.77

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 209 ligands modelled in this entry, 10 are monoatomic - leaving 199 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	$\# Z > 2$
20	EDO	S	108	-	3,3,3	0.70	0	2,2,2	0.39	0
20	EDO	M	104	-	3,3,3	0.61	0	2,2,2	0.51	0
23	CHD	G	102	-	32,32,32	0.97	0	51,51,51	1.38	7 (13%)
20	EDO	S	112	-	3,3,3	0.47	0	2,2,2	1.61	1 (50%)
20	EDO	B	306	-	3,3,3	0.77	0	2,2,2	0.38	0
20	EDO	B	313	-	3,3,3	0.53	0	2,2,2	0.40	0
26	CDL	G	101	-	99,99,99	1.41	12 (12%)	105,111,111	1.47	12 (11%)
20	EDO	B	309	-	3,3,3	0.39	0	2,2,2	0.15	0
20	EDO	R	204	-	3,3,3	0.48	0	2,2,2	0.30	0
27	DMU	V	102	-	34,34,34	0.55	1 (2%)	45,45,45	1.05	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	P	308	-	99,99,99	1.43	12 (12%)	105,111,111	1.34	9 (8%)
20	EDO	K	101	-	3,3,3	0.66	0	2,2,2	0.17	0
20	EDO	F	107	-	3,3,3	0.34	0	2,2,2	0.60	0
20	EDO	A	615	-	3,3,3	0.61	0	2,2,2	0.11	0
20	EDO	O	305	-	3,3,3	0.44	0	2,2,2	0.17	0
20	EDO	P	322	-	3,3,3	0.50	0	2,2,2	0.28	0
23	CHD	C	301	-	32,32,32	1.13	4 (12%)	51,51,51	1.54	8 (15%)
20	EDO	P	321	-	3,3,3	0.56	0	2,2,2	0.53	0
20	EDO	A	623	-	3,3,3	0.57	0	2,2,2	0.33	0
20	EDO	D	202	-	3,3,3	0.57	0	2,2,2	0.18	0
20	EDO	A	624	-	3,3,3	0.37	0	2,2,2	0.66	0
20	EDO	L	103	-	3,3,3	0.55	0	2,2,2	0.16	0
20	EDO	S	111	-	3,3,3	0.74	0	2,2,2	0.22	0
21	TGL	B	301	-	62,62,62	1.13	3 (4%)	65,65,65	1.30	6 (9%)
20	EDO	N	613	-	3,3,3	0.41	0	2,2,2	0.50	0
20	EDO	S	110	-	3,3,3	0.60	0	2,2,2	0.69	0
20	EDO	F	106	-	3,3,3	0.86	0	2,2,2	0.46	0
20	EDO	H	102	-	3,3,3	0.50	0	2,2,2	0.21	0
20	EDO	A	617	-	3,3,3	0.65	0	2,2,2	0.12	0
20	EDO	N	623	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	N	629	-	3,3,3	0.38	0	2,2,2	0.39	0
14	PGV	N	609	-	50,50,50	1.03	5 (10%)	53,56,56	1.14	3 (5%)
27	DMU	Z	102	-	34,34,34	0.48	0	45,45,45	1.15	3 (6%)
20	EDO	C	317	-	3,3,3	0.37	0	2,2,2	0.05	0
20	EDO	M	105	-	3,3,3	1.15	0	2,2,2	0.62	0
20	EDO	P	317	-	3,3,3	0.64	0	2,2,2	0.19	0
20	EDO	C	316	-	3,3,3	0.87	0	2,2,2	0.57	0
20	EDO	P	320	-	3,3,3	0.44	0	2,2,2	0.34	0
20	EDO	H	101	-	3,3,3	0.40	0	2,2,2	0.56	0
20	EDO	N	617	-	3,3,3	0.30	0	2,2,2	0.82	0
21	TGL	Y	101	-	62,62,62	1.03	3 (4%)	65,65,65	1.16	4 (6%)
20	EDO	P	316	-	3,3,3	0.63	0	2,2,2	0.35	0
20	EDO	P	318	-	3,3,3	0.70	0	2,2,2	0.15	0
20	EDO	C	314	-	3,3,3	0.51	0	2,2,2	0.42	0
20	EDO	A	621	-	3,3,3	0.58	0	2,2,2	0.42	0
20	EDO	J	103	-	3,3,3	0.37	0	2,2,2	0.52	0
20	EDO	P	313	-	3,3,3	0.41	0	2,2,2	0.34	0
23	CHD	Y	104	-	32,32,32	0.86	1 (3%)	51,51,51	1.78	13 (25%)
20	EDO	D	206	20	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	Y	103	-	3,3,3	0.40	0	2,2,2	0.29	0
15	HEA	A	602[B]	-	67,67,67	1.80	18 (26%)	81,103,103	1.83	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	P	312	-	3,3,3	0.43	0	2,2,2	1.02	0
20	EDO	N	612	-	3,3,3	0.51	0	2,2,2	0.65	0
20	EDO	D	205	-	3,3,3	0.65	0	2,2,2	0.35	0
20	EDO	S	105	-	3,3,3	0.50	0	2,2,2	0.18	0
20	EDO	F	105	-	3,3,3	0.50	0	2,2,2	0.17	0
24	CUA	O	302	2	0,1,1	-	-	-	-	-
19	CMO	N	607[A]	-	0,1,1	-	-	-	-	-
20	EDO	A	625	-	3,3,3	0.51	0	2,2,2	0.84	0
20	EDO	L	102	-	3,3,3	0.51	0	2,2,2	0.14	0
20	EDO	B	311	-	3,3,3	0.51	0	2,2,2	0.16	0
27	DMU	Z	101	-	34,34,34	0.38	0	45,45,45	0.87	2 (4%)
20	EDO	G	106	-	3,3,3	0.59	0	2,2,2	0.71	0
20	EDO	W	103	-	3,3,3	0.82	0	2,2,2	0.38	0
20	EDO	A	620	-	3,3,3	0.61	0	2,2,2	1.04	0
20	EDO	F	104	-	3,3,3	0.86	0	2,2,2	0.11	0
20	EDO	H	103	-	3,3,3	0.48	0	2,2,2	0.17	0
20	EDO	A	616	-	3,3,3	0.39	0	2,2,2	0.67	0
15	HEA	N	602[B]	-	67,67,67	1.76	21 (31%)	81,103,103	2.08	24 (29%)
20	EDO	F	103	-	3,3,3	0.41	0	2,2,2	0.21	0
20	EDO	F	102	-	3,3,3	0.94	0	2,2,2	0.59	0
29	PO4	H	104	-	4,4,4	0.97	0	6,6,6	0.39	0
20	EDO	B	314	20	3,3,3	0.44	0	2,2,2	0.43	0
20	EDO	D	207	-	3,3,3	0.46	0	2,2,2	0.79	0
21	TGL	L	101	-	62,62,62	1.06	3 (4%)	65,65,65	1.21	8 (12%)
23	CHD	C	309	-	32,32,32	0.73	0	51,51,51	1.11	4 (7%)
20	EDO	G	105	-	3,3,3	0.51	0	2,2,2	0.08	0
25	PEK	C	303	-	52,52,52	0.93	2 (3%)	55,57,57	1.32	5 (9%)
21	TGL	Q	201	-	62,62,62	1.04	3 (4%)	65,65,65	1.02	6 (9%)
20	EDO	N	622	-	3,3,3	0.52	0	2,2,2	0.55	0
20	EDO	B	310	-	3,3,3	0.42	0	2,2,2	0.29	0
20	EDO	N	619	-	3,3,3	0.52	0	2,2,2	0.20	0
20	EDO	N	624	-	3,3,3	0.59	0	2,2,2	0.32	0
14	PGV	N	601	-	50,50,50	0.93	2 (4%)	53,56,56	1.21	5 (9%)
20	EDO	V	101	-	3,3,3	0.45	0	2,2,2	0.45	0
14	PGV	P	306	-	50,50,50	0.78	1 (2%)	53,56,56	1.25	4 (7%)
20	EDO	A	619	-	3,3,3	0.36	0	2,2,2	0.86	0
14	PGV	C	307	-	50,50,50	0.96	2 (4%)	53,56,56	1.60	8 (15%)
27	DMU	P	323	-	34,34,34	0.45	0	45,45,45	0.90	3 (6%)
23	CHD	P	310	-	32,32,32	0.82	1 (3%)	51,51,51	1.87	11 (21%)
20	EDO	O	306	-	3,3,3	0.49	0	2,2,2	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PGV	A	601	-	50,50,50	0.96	2 (4%)	53,56,56	1.09	4 (7%)
20	EDO	N	630	-	3,3,3	0.36	0	2,2,2	0.14	0
20	EDO	A	618	-	3,3,3	0.41	0	2,2,2	0.52	0
20	EDO	N	614	-	3,3,3	0.78	0	2,2,2	0.35	0
20	EDO	R	201	-	3,3,3	0.57	0	2,2,2	0.52	0
20	EDO	K	102	-	3,3,3	0.46	0	2,2,2	0.26	0
15	HEA	A	603	1	67,67,67	1.82	16 (23%)	81,103,103	1.92	21 (25%)
22	PSC	B	302	-	51,51,51	1.10	3 (5%)	57,59,59	1.35	7 (12%)
20	EDO	A	610	-	3,3,3	0.90	0	2,2,2	1.04	0
25	PEK	P	303	-	52,52,52	0.94	2 (3%)	55,57,57	1.16	5 (9%)
23	CHD	P	301	-	32,32,32	0.96	2 (6%)	51,51,51	1.42	10 (19%)
27	DMU	C	319	-	34,34,34	0.47	0	45,45,45	1.06	6 (13%)
20	EDO	S	102	-	3,3,3	0.90	0	2,2,2	0.79	0
20	EDO	O	307	-	3,3,3	0.45	0	2,2,2	0.31	0
23	CHD	B	303	-	32,32,32	1.20	2 (6%)	51,51,51	1.75	11 (21%)
24	CUA	B	304	2	0,1,1	-	-	-	-	-
20	EDO	C	313	-	3,3,3	0.74	0	2,2,2	0.23	0
20	EDO	M	103	-	3,3,3	0.42	0	2,2,2	0.19	0
20	EDO	S	103	-	3,3,3	0.78	0	2,2,2	0.09	0
20	EDO	B	307	-	3,3,3	0.57	0	2,2,2	0.27	0
20	EDO	M	102	-	3,3,3	0.43	0	2,2,2	0.38	0
26	CDL	T	101	-	99,99,99	1.40	12 (12%)	105,111,111	1.12	6 (5%)
14	PGV	C	306	-	50,50,50	0.81	2 (4%)	53,56,56	0.95	3 (5%)
20	EDO	E	202	-	3,3,3	0.62	0	2,2,2	0.12	0
20	EDO	A	622	-	3,3,3	0.30	0	2,2,2	0.60	0
20	EDO	O	303	-	3,3,3	0.83	0	2,2,2	0.50	0
27	DMU	G	108	-	34,34,34	0.49	0	45,45,45	1.17	3 (6%)
20	EDO	E	203	-	3,3,3	0.52	0	2,2,2	0.54	0
14	PGV	A	608	-	50,50,50	0.89	2 (4%)	53,56,56	0.89	1 (1%)
20	EDO	S	106	-	3,3,3	0.42	0	2,2,2	0.59	0
20	EDO	Y	102	-	3,3,3	0.50	0	2,2,2	0.42	0
20	EDO	N	620	-	3,3,3	0.56	0	2,2,2	0.46	0
20	EDO	P	314	-	3,3,3	0.38	0	2,2,2	0.80	0
20	EDO	B	308	-	3,3,3	0.56	0	2,2,2	0.40	0
21	TGL	D	201	-	62,62,62	1.21	4 (6%)	65,65,65	0.95	5 (7%)
20	EDO	E	201	-	3,3,3	0.38	0	2,2,2	0.50	0
20	EDO	J	102	-	3,3,3	0.37	0	2,2,2	0.39	0
19	CMO	A	607[B]	16	0,1,1	-	-	-	-	-
29	PO4	U	102	-	4,4,4	1.02	0	6,6,6	0.43	0
15	HEA	N	602[A]	-	67,67,67	1.73	20 (29%)	81,103,103	2.22	26 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DMU	P	309	-	34,34,34	0.47	0	45,45,45	0.71	0
20	EDO	D	203	-	3,3,3	0.47	0	2,2,2	0.19	0
23	CHD	J	101	-	32,32,32	0.77	1 (3%)	51,51,51	1.72	13 (25%)
20	EDO	Q	202	-	3,3,3	0.39	0	2,2,2	0.38	0
20	EDO	S	107	-	3,3,3	0.46	0	2,2,2	0.39	0
26	CDL	C	308	-	99,99,99	1.41	12 (12%)	105,111,111	1.24	9 (8%)
27	DMU	C	310	-	34,34,34	0.43	0	45,45,45	0.89	1 (2%)
20	EDO	N	628	-	3,3,3	0.42	0	2,2,2	1.08	0
25	PEK	C	304	-	52,52,52	0.86	2 (3%)	55,57,57	1.07	4 (7%)
20	EDO	N	610	-	3,3,3	1.10	0	2,2,2	0.55	0
20	EDO	S	109	-	3,3,3	0.43	0	2,2,2	0.47	0
27	DMU	P	324	-	34,34,34	0.55	0	45,45,45	0.75	1 (2%)
23	CHD	P	311	-	32,32,32	0.79	0	51,51,51	1.16	5 (9%)
20	EDO	N	616	-	3,3,3	0.50	0	2,2,2	0.43	0
23	CHD	C	311	-	32,32,32	0.85	1 (3%)	51,51,51	1.77	10 (19%)
20	EDO	G	104	-	3,3,3	0.41	0	2,2,2	0.55	0
25	PEK	P	305	-	52,52,52	0.96	2 (3%)	55,57,57	1.24	5 (9%)
20	EDO	N	611	-	3,3,3	0.64	0	2,2,2	0.58	0
20	EDO	G	107	-	3,3,3	0.70	0	2,2,2	0.18	0
20	EDO	N	615	-	3,3,3	0.49	0	2,2,2	0.41	0
20	EDO	N	627	-	3,3,3	0.41	0	2,2,2	0.52	0
20	EDO	A	627	-	3,3,3	0.82	0	2,2,2	0.49	0
20	EDO	G	103	-	3,3,3	0.52	0	2,2,2	0.26	0
20	EDO	N	621	-	3,3,3	0.56	0	2,2,2	0.28	0
20	EDO	A	613	-	3,3,3	0.69	0	2,2,2	0.40	0
20	EDO	Q	203	-	3,3,3	0.40	0	2,2,2	0.44	0
20	EDO	C	312	-	3,3,3	0.71	0	2,2,2	0.17	0
20	EDO	C	315	-	3,3,3	0.57	0	2,2,2	0.45	0
15	HEA	N	603	1	67,67,67	1.76	18 (26%)	81,103,103	1.77	23 (28%)
20	EDO	A	609	-	3,3,3	0.42	0	2,2,2	0.46	0
20	EDO	C	318	-	3,3,3	0.68	0	2,2,2	0.15	0
20	EDO	U	101	-	3,3,3	0.58	0	2,2,2	0.20	0
15	HEA	A	602[A]	-	67,67,67	1.75	18 (26%)	81,103,103	1.97	21 (25%)
20	EDO	L	105	-	3,3,3	0.54	0	2,2,2	0.33	0
22	PSC	O	301	-	51,51,51	1.11	3 (5%)	57,59,59	1.27	5 (8%)
20	EDO	A	611	-	3,3,3	0.65	0	2,2,2	0.62	0
27	DMU	M	101	-	34,34,34	0.51	0	45,45,45	1.10	4 (8%)
27	DMU	M	106	-	34,34,34	0.59	1 (2%)	45,45,45	1.21	5 (11%)
20	EDO	A	626	-	3,3,3	0.64	0	2,2,2	1.02	0
20	EDO	N	618	-	3,3,3	0.75	0	2,2,2	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	EDO	N	625	-	3,3,3	0.70	0	2,2,2	0.24	0
20	EDO	R	205	-	3,3,3	0.50	0	2,2,2	0.23	0
20	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.23	0
20	EDO	R	203	-	3,3,3	0.52	0	2,2,2	0.29	0
20	EDO	B	312	-	3,3,3	0.55	0	2,2,2	0.17	0
25	PEK	P	304	-	52,52,52	0.70	2 (3%)	55,57,57	1.13	5 (9%)
20	EDO	W	102	-	3,3,3	0.27	0	2,2,2	0.70	0
20	EDO	R	202	-	3,3,3	0.58	0	2,2,2	0.27	0
20	EDO	S	104	-	3,3,3	0.76	0	2,2,2	0.75	0
20	EDO	T	102	-	3,3,3	0.64	0	2,2,2	0.95	0
20	EDO	W	104	-	3,3,3	0.49	0	2,2,2	0.33	0
20	EDO	T	103	-	3,3,3	0.54	0	2,2,2	0.53	0
23	CHD	W	101	-	32,32,32	0.73	1 (3%)	51,51,51	1.59	7 (13%)
25	PEK	C	305	-	52,52,52	0.95	2 (3%)	55,57,57	1.20	5 (9%)
20	EDO	P	315	-	3,3,3	1.03	0	2,2,2	0.47	0
20	EDO	A	612	-	3,3,3	0.58	0	2,2,2	0.68	0
21	TGL	N	608	-	62,62,62	1.02	3 (4%)	65,65,65	1.21	4 (6%)
20	EDO	L	104	-	3,3,3	0.79	0	2,2,2	0.20	0
20	EDO	N	626	-	3,3,3	0.33	0	2,2,2	0.38	0
19	CMO	A	607[A]	-	0,1,1	-	-	-	-	-
19	CMO	N	607[B]	16	0,1,1	-	-	-	-	-
20	EDO	O	304	-	3,3,3	0.47	0	2,2,2	0.18	0
20	EDO	P	319	-	3,3,3	0.92	0	2,2,2	0.42	0
20	EDO	B	305	-	3,3,3	0.44	0	2,2,2	0.70	0
14	PGV	P	307	-	50,50,50	0.98	2 (4%)	53,56,56	1.38	8 (15%)

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
20	EDO	S	108	-	-	1/1/1/1	-
20	EDO	M	104	-	-	1/1/1/1	-
23	CHD	G	102	-	-	2/9/74/74	0/4/4/4
20	EDO	S	112	-	-	1/1/1/1	-
20	EDO	B	306	-	-	0/1/1/1	-
20	EDO	B	313	-	-	1/1/1/1	-
26	CDL	G	101	-	-	29/110/110/110	-
20	EDO	B	309	-	-	0/1/1/1	-
20	EDO	R	204	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	V	102	-	-	11/19/59/59	0/2/2/2
26	CDL	P	308	-	-	34/110/110/110	-
20	EDO	K	101	-	-	0/1/1/1	-
20	EDO	F	107	-	-	1/1/1/1	-
20	EDO	A	615	-	-	0/1/1/1	-
20	EDO	O	305	-	-	1/1/1/1	-
20	EDO	P	322	-	-	1/1/1/1	-
23	CHD	C	301	-	-	1/9/74/74	0/4/4/4
20	EDO	P	321	-	-	1/1/1/1	-
20	EDO	A	623	-	-	0/1/1/1	-
20	EDO	D	202	-	-	1/1/1/1	-
20	EDO	A	624	-	-	0/1/1/1	-
20	EDO	L	103	-	-	0/1/1/1	-
20	EDO	S	111	-	-	1/1/1/1	-
21	TGL	B	301	-	-	20/65/65/65	-
20	EDO	N	613	-	-	0/1/1/1	-
20	EDO	S	110	-	-	0/1/1/1	-
20	EDO	F	106	-	-	0/1/1/1	-
20	EDO	H	102	-	-	0/1/1/1	-
20	EDO	A	617	-	-	1/1/1/1	-
20	EDO	N	623	-	-	1/1/1/1	-
20	EDO	N	629	-	-	1/1/1/1	-
14	PGV	N	609	-	-	5/55/55/55	-
27	DMU	Z	102	-	-	9/19/59/59	0/2/2/2
20	EDO	C	317	-	-	0/1/1/1	-
20	EDO	M	105	-	-	1/1/1/1	-
20	EDO	P	317	-	-	0/1/1/1	-
20	EDO	C	316	-	-	0/1/1/1	-
20	EDO	P	320	-	-	0/1/1/1	-
20	EDO	H	101	-	-	0/1/1/1	-
20	EDO	N	617	-	-	0/1/1/1	-
21	TGL	Y	101	-	-	30/65/65/65	-
20	EDO	P	316	-	-	1/1/1/1	-
20	EDO	P	318	-	-	0/1/1/1	-
20	EDO	C	314	-	-	0/1/1/1	-
20	EDO	A	621	-	-	0/1/1/1	-
20	EDO	J	103	-	-	1/1/1/1	-
20	EDO	P	313	-	-	1/1/1/1	-
23	CHD	Y	104	-	-	7/9/74/74	0/4/4/4
20	EDO	D	206	20	-	0/1/1/1	-
20	EDO	Y	103	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEA	A	602[B]	-	-	5/36/76/76	-
20	EDO	P	312	-	-	0/1/1/1	-
20	EDO	N	612	-	-	1/1/1/1	-
20	EDO	D	205	-	-	1/1/1/1	-
20	EDO	S	105	-	-	0/1/1/1	-
20	EDO	F	105	-	-	0/1/1/1	-
20	EDO	A	625	-	-	0/1/1/1	-
20	EDO	L	102	-	-	1/1/1/1	-
20	EDO	B	311	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	2/19/59/59	0/2/2/2
20	EDO	G	106	-	-	0/1/1/1	-
20	EDO	W	103	-	-	1/1/1/1	-
20	EDO	A	620	-	-	1/1/1/1	-
20	EDO	F	104	-	-	0/1/1/1	-
20	EDO	H	103	-	-	0/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
15	HEA	N	602[B]	-	-	4/36/76/76	-
20	EDO	F	103	-	-	0/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	B	314	20	-	0/1/1/1	-
20	EDO	D	207	-	-	0/1/1/1	-
21	TGL	L	101	-	-	29/65/65/65	-
23	CHD	C	309	-	-	5/9/74/74	0/4/4/4
20	EDO	G	105	-	-	0/1/1/1	-
25	PEK	C	303	-	-	21/56/56/56	-
21	TGL	Q	201	-	-	21/65/65/65	-
20	EDO	N	622	-	-	1/1/1/1	-
20	EDO	B	310	-	-	0/1/1/1	-
20	EDO	N	619	-	-	0/1/1/1	-
20	EDO	N	624	-	-	1/1/1/1	-
14	PGV	N	601	-	-	20/55/55/55	-
20	EDO	V	101	-	-	0/1/1/1	-
14	PGV	P	306	-	-	8/55/55/55	-
20	EDO	A	619	-	-	0/1/1/1	-
14	PGV	C	307	-	-	12/55/55/55	-
27	DMU	P	323	-	-	3/19/59/59	0/2/2/2
23	CHD	P	310	-	-	1/9/74/74	0/4/4/4
20	EDO	O	306	-	-	1/1/1/1	-
14	PGV	A	601	-	-	11/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	N	630	-	-	0/1/1/1	-
20	EDO	A	618	-	-	0/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	R	201	-	-	0/1/1/1	-
20	EDO	K	102	-	-	0/1/1/1	-
15	HEA	A	603	1	-	4/36/76/76	-
22	PSC	B	302	-	-	20/55/55/55	-
20	EDO	A	610	-	-	0/1/1/1	-
25	PEK	P	303	-	-	18/56/56/56	-
23	CHD	P	301	-	-	2/9/74/74	0/4/4/4
27	DMU	C	319	-	-	9/19/59/59	0/2/2/2
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	O	307	-	-	0/1/1/1	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
20	EDO	C	313	-	-	0/1/1/1	-
20	EDO	M	103	-	-	0/1/1/1	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	B	307	-	-	1/1/1/1	-
20	EDO	M	102	-	-	0/1/1/1	-
26	CDL	T	101	-	-	34/110/110/110	-
14	PGV	C	306	-	-	10/55/55/55	-
20	EDO	E	202	-	-	0/1/1/1	-
20	EDO	A	622	-	-	0/1/1/1	-
20	EDO	O	303	-	-	0/1/1/1	-
27	DMU	G	108	-	-	6/19/59/59	0/2/2/2
20	EDO	E	203	-	-	0/1/1/1	-
14	PGV	A	608	-	-	8/55/55/55	-
20	EDO	S	106	-	-	0/1/1/1	-
20	EDO	Y	102	-	-	0/1/1/1	-
20	EDO	N	620	-	-	0/1/1/1	-
20	EDO	P	314	-	-	0/1/1/1	-
20	EDO	B	308	-	-	0/1/1/1	-
21	TGL	D	201	-	-	19/65/65/65	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
15	HEA	N	602[A]	-	-	3/36/76/76	-
27	DMU	P	309	-	-	5/19/59/59	0/2/2/2
20	EDO	D	203	-	-	0/1/1/1	-
23	CHD	J	101	-	-	9/9/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	Q	202	-	-	1/1/1/1	-
20	EDO	S	107	-	-	1/1/1/1	-
26	CDL	C	308	-	-	34/110/110/110	-
27	DMU	C	310	-	-	4/19/59/59	0/2/2/2
20	EDO	N	628	-	-	1/1/1/1	-
25	PEK	C	304	-	-	12/56/56/56	-
20	EDO	N	610	-	-	0/1/1/1	-
20	EDO	S	109	-	-	0/1/1/1	-
27	DMU	P	324	-	-	13/19/59/59	0/2/2/2
23	CHD	P	311	-	-	5/9/74/74	0/4/4/4
20	EDO	N	616	-	-	1/1/1/1	-
23	CHD	C	311	-	-	1/9/74/74	0/4/4/4
20	EDO	G	104	-	-	0/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
20	EDO	G	107	-	-	0/1/1/1	-
20	EDO	N	615	-	-	0/1/1/1	-
20	EDO	N	627	-	-	0/1/1/1	-
20	EDO	A	627	-	-	0/1/1/1	-
20	EDO	G	103	-	-	1/1/1/1	-
20	EDO	N	621	-	-	0/1/1/1	-
20	EDO	A	613	-	-	0/1/1/1	-
20	EDO	Q	203	-	-	1/1/1/1	-
20	EDO	C	312	-	-	0/1/1/1	-
20	EDO	C	315	-	-	0/1/1/1	-
15	HEA	N	603	1	-	5/36/76/76	-
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	C	318	-	-	0/1/1/1	-
20	EDO	U	101	-	-	0/1/1/1	-
15	HEA	A	602[A]	-	-	7/36/76/76	-
20	EDO	L	105	-	-	0/1/1/1	-
22	PSC	O	301	-	-	19/55/55/55	-
20	EDO	A	611	-	-	0/1/1/1	-
27	DMU	M	101	-	-	7/19/59/59	0/2/2/2
27	DMU	M	106	-	-	7/19/59/59	0/2/2/2
20	EDO	A	626	-	-	1/1/1/1	-
20	EDO	N	618	-	-	1/1/1/1	-
20	EDO	N	625	-	-	1/1/1/1	-
20	EDO	R	205	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	R	203	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	B	312	-	-	0/1/1/1	-
25	PEK	P	304	-	-	9/56/56/56	-
20	EDO	W	102	-	-	1/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
20	EDO	S	104	-	-	0/1/1/1	-
20	EDO	T	102	-	-	0/1/1/1	-
20	EDO	W	104	-	-	1/1/1/1	-
20	EDO	T	103	-	-	1/1/1/1	-
23	CHD	W	101	-	-	8/9/74/74	0/4/4/4
25	PEK	C	305	-	-	19/56/56/56	-
20	EDO	P	315	-	-	0/1/1/1	-
20	EDO	A	612	-	-	0/1/1/1	-
21	TGL	N	608	-	-	19/65/65/65	-
20	EDO	L	104	-	-	1/1/1/1	-
20	EDO	N	626	-	-	0/1/1/1	-
20	EDO	P	319	-	-	0/1/1/1	-
25	PEK	P	305	-	-	21/56/56/56	-
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
14	PGV	P	307	-	-	9/55/55/55	-

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OG2-CB1	5.05	1.48	1.34
21	B	301	TGL	OG3-CC1	4.92	1.47	1.33
21	B	301	TGL	OG1-CA1	4.84	1.47	1.33
26	G	101	CDL	OA8-CA7	4.63	1.46	1.33
14	A	601	PGV	O03-C19	4.61	1.46	1.33
26	P	308	CDL	OA8-CA7	4.59	1.46	1.33
25	P	303	PEK	O03-C21	4.56	1.46	1.33
21	Q	201	TGL	OG1-CA1	4.54	1.46	1.33
14	N	601	PGV	O03-C19	4.53	1.46	1.33
25	C	303	PEK	O03-C21	4.52	1.46	1.33
14	P	307	PGV	O03-C19	4.52	1.46	1.33
21	L	101	TGL	OG2-CB1	4.50	1.47	1.34
26	P	308	CDL	OB6-CB5	4.49	1.47	1.34
21	Y	101	TGL	OG1-CA1	4.49	1.46	1.33
26	P	308	CDL	OA6-CA5	4.48	1.46	1.34
21	N	608	TGL	OG2-CB1	4.47	1.46	1.34
21	B	301	TGL	OG2-CB1	4.46	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	201	TGL	OG1-CA1	4.45	1.46	1.33
21	Y	101	TGL	OG2-CB1	4.45	1.46	1.34
21	L	101	TGL	OG3-CC1	4.44	1.46	1.33
25	P	305	PEK	O03-C21	4.36	1.46	1.33
25	C	305	PEK	O03-C21	4.33	1.46	1.33
22	O	301	PSC	O01-C1	4.33	1.46	1.34
21	L	101	TGL	OG1-CA1	4.32	1.45	1.33
21	N	608	TGL	OG3-CC1	4.30	1.45	1.33
14	C	307	PGV	O01-C1	4.29	1.46	1.34
26	T	101	CDL	OB8-CB7	4.28	1.45	1.33
26	C	308	CDL	OB8-CB7	4.27	1.45	1.33
25	P	305	PEK	O01-C1	4.27	1.46	1.34
14	C	307	PGV	O03-C19	4.26	1.45	1.33
21	Q	201	TGL	OG2-CB1	4.25	1.46	1.34
21	N	608	TGL	OG1-CA1	4.25	1.45	1.33
26	T	101	CDL	OB6-CB5	4.25	1.46	1.34
26	G	101	CDL	OB8-CB7	4.24	1.45	1.33
26	T	101	CDL	OA8-CA7	4.23	1.45	1.33
26	G	101	CDL	OB6-CB5	4.23	1.46	1.34
26	C	308	CDL	OA8-CA7	4.20	1.45	1.33
26	P	308	CDL	OB8-CB7	4.20	1.45	1.33
25	C	305	PEK	O01-C1	4.20	1.46	1.34
22	B	302	PSC	O01-C1	4.19	1.46	1.34
26	C	308	CDL	OB6-CB5	4.19	1.46	1.34
14	P	307	PGV	O01-C1	4.18	1.46	1.34
21	Y	101	TGL	OG3-CC1	4.14	1.45	1.33
15	A	602[A]	HEA	CHA-C1A	4.11	1.46	1.38
15	A	602[B]	HEA	CHA-C1A	4.11	1.46	1.38
25	P	303	PEK	O01-C1	4.11	1.45	1.34
26	C	308	CDL	OA6-CA5	4.10	1.45	1.34
26	G	101	CDL	OA6-CA5	4.09	1.45	1.34
22	B	302	PSC	O03-C19	4.07	1.45	1.33
21	D	201	TGL	OG3-CC1	4.03	1.45	1.33
15	A	603	HEA	CHC-C4B	4.02	1.46	1.38
22	O	301	PSC	O03-C19	4.02	1.45	1.33
21	Q	201	TGL	OG3-CC1	4.01	1.45	1.33
26	G	101	CDL	C42-C41	-3.96	1.32	1.51
21	D	201	TGL	OB1-CB1	3.93	1.34	1.22
26	T	101	CDL	OA6-CA5	3.93	1.45	1.34
25	C	303	PEK	O01-C1	3.92	1.45	1.34
15	A	603	HEA	FE-NC	3.89	2.08	1.95
26	C	308	CDL	C59-C58	-3.89	1.32	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601	PGV	O01-C1	3.89	1.45	1.34
26	C	308	CDL	C82-C81	-3.88	1.32	1.51
26	P	308	CDL	C79-C78	-3.87	1.32	1.51
22	B	302	PSC	C13-C12	3.86	1.53	1.31
15	A	603	HEA	CHD-C1D	3.83	1.46	1.38
26	P	308	CDL	C82-C81	-3.82	1.32	1.51
22	O	301	PSC	C13-C12	3.81	1.53	1.31
26	G	101	CDL	C82-C81	-3.80	1.32	1.51
26	C	308	CDL	C62-C61	-3.80	1.32	1.51
26	T	101	CDL	C82-C81	-3.79	1.32	1.51
14	N	601	PGV	O01-C1	3.76	1.44	1.34
26	T	101	CDL	C62-C61	-3.76	1.33	1.51
26	T	101	CDL	C59-C58	-3.76	1.33	1.51
26	C	308	CDL	C79-C78	-3.75	1.33	1.51
26	P	308	CDL	C59-C58	-3.73	1.33	1.51
26	T	101	CDL	C22-C21	-3.72	1.33	1.51
26	C	308	CDL	C39-C38	-3.69	1.33	1.51
26	G	101	CDL	C62-C61	-3.68	1.33	1.51
26	G	101	CDL	C39-C38	-3.66	1.33	1.51
15	N	602[A]	HEA	CHA-C1A	3.66	1.45	1.38
15	N	602[B]	HEA	CHA-C1A	3.66	1.45	1.38
26	G	101	CDL	C79-C78	-3.66	1.33	1.51
15	N	603	HEA	CHC-C4B	3.65	1.45	1.38
26	G	101	CDL	C59-C58	-3.65	1.33	1.51
26	P	308	CDL	C19-C18	-3.64	1.33	1.51
26	T	101	CDL	C79-C78	-3.64	1.33	1.51
26	P	308	CDL	C39-C38	-3.64	1.33	1.51
26	C	308	CDL	C42-C41	-3.63	1.33	1.51
26	T	101	CDL	C19-C18	-3.62	1.33	1.51
26	C	308	CDL	C22-C21	-3.62	1.33	1.51
26	P	308	CDL	C62-C61	-3.60	1.33	1.51
26	C	308	CDL	C19-C18	-3.59	1.33	1.51
26	P	308	CDL	C22-C21	-3.58	1.34	1.51
26	P	308	CDL	C42-C41	-3.58	1.34	1.51
26	G	101	CDL	C22-C21	-3.57	1.34	1.51
15	N	603	HEA	CHB-C4A	3.53	1.45	1.38
26	G	101	CDL	C19-C18	-3.53	1.34	1.51
14	N	609	PGV	O01-C1	3.53	1.44	1.34
15	A	603	HEA	CHB-C4A	3.52	1.45	1.38
23	B	303	CHD	C11-C12	3.52	1.59	1.53
26	T	101	CDL	C42-C41	-3.50	1.34	1.51
26	T	101	CDL	C39-C38	-3.50	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	602[A]	HEA	C1A-C2A	-3.49	1.39	1.45
15	A	602[B]	HEA	C1A-C2A	-3.49	1.39	1.45
15	A	602[A]	HEA	C1D-ND	-3.48	1.34	1.40
15	A	602[B]	HEA	C1D-ND	-3.48	1.34	1.40
15	A	602[A]	HEA	CHD-C1D	3.38	1.45	1.38
15	A	602[B]	HEA	CHD-C1D	3.38	1.45	1.38
15	A	603	HEA	CMC-C2C	3.37	1.57	1.50
15	A	602[B]	HEA	O11-C11	3.27	1.50	1.42
15	N	602[A]	HEA	C4C-NC	-3.26	1.33	1.39
15	N	602[B]	HEA	C4C-NC	-3.26	1.33	1.39
15	N	603	HEA	CHA-C1A	3.24	1.44	1.38
15	A	602[A]	HEA	C1D-C2D	-3.23	1.38	1.44
15	A	602[B]	HEA	C1D-C2D	-3.23	1.38	1.44
25	C	304	PEK	O03-C21	3.22	1.42	1.33
25	C	304	PEK	O01-C1	3.22	1.43	1.34
15	N	602[A]	HEA	CHC-C4B	3.21	1.44	1.38
15	N	602[B]	HEA	CHC-C4B	3.21	1.44	1.38
15	A	603	HEA	FE-NA	3.18	2.05	1.95
15	N	603	HEA	FE-NA	3.17	2.05	1.95
15	N	603	HEA	FE-NC	3.10	2.05	1.95
15	A	602[A]	HEA	C4D-C3D	-3.09	1.39	1.45
15	A	602[B]	HEA	C4D-C3D	-3.09	1.39	1.45
15	N	603	HEA	C3A-C4A	-3.08	1.40	1.46
15	A	603	HEA	FE-NB	3.05	2.04	1.94
15	A	602[A]	HEA	C1B-NB	-3.04	1.32	1.38
15	A	602[B]	HEA	C1B-NB	-3.04	1.32	1.38
15	N	603	HEA	FE-NB	3.03	2.04	1.94
15	A	603	HEA	C4A-NA	-2.98	1.34	1.39
23	B	303	CHD	C11-C9	2.98	1.58	1.53
15	A	603	HEA	CHA-C1A	2.97	1.44	1.38
15	N	602[A]	HEA	FE-NA	2.94	2.04	1.95
15	N	602[B]	HEA	FE-NA	2.94	2.04	1.95
15	N	602[A]	HEA	CHA-C4D	2.93	1.45	1.39
15	N	602[B]	HEA	CHA-C4D	2.93	1.45	1.39
15	N	602[A]	HEA	C1A-C2A	-2.82	1.40	1.45
15	N	602[B]	HEA	C1A-C2A	-2.82	1.40	1.45
15	N	602[A]	HEA	C1A-NA	-2.82	1.34	1.39
15	N	602[B]	HEA	C1A-NA	-2.82	1.34	1.39
15	A	603	HEA	C11-C3B	2.79	1.54	1.51
14	A	608	PGV	O01-C1	2.78	1.42	1.34
15	N	603	HEA	C4D-C3D	-2.77	1.40	1.45
15	N	602[A]	HEA	CHB-C4A	2.76	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	602[B]	HEA	CHB-C4A	2.76	1.43	1.38
14	N	609	PGV	O03-C19	2.76	1.41	1.33
15	A	602[A]	HEA	CAA-C2A	2.75	1.58	1.51
15	A	602[B]	HEA	CAA-C2A	2.75	1.58	1.51
15	N	603	HEA	CHC-C1C	2.72	1.45	1.39
15	A	602[A]	HEA	C4A-NA	-2.72	1.34	1.39
15	A	602[B]	HEA	C4A-NA	-2.72	1.34	1.39
15	N	602[B]	HEA	O11-C11	2.72	1.48	1.42
15	N	603	HEA	O11-C11	2.70	1.48	1.42
15	N	602[A]	HEA	C3A-C4A	-2.65	1.41	1.46
15	N	602[B]	HEA	C3A-C4A	-2.65	1.41	1.46
25	P	304	PEK	O03-C21	2.64	1.41	1.33
15	A	602[A]	HEA	CHC-C4B	2.62	1.43	1.38
15	A	602[B]	HEA	CHC-C4B	2.62	1.43	1.38
15	A	603	HEA	CHC-C1C	2.61	1.45	1.39
15	N	603	HEA	CHD-C1D	2.60	1.43	1.38
14	A	608	PGV	O01-C02	-2.55	1.40	1.46
15	A	602[A]	HEA	FE-NC	2.51	2.03	1.95
15	A	602[B]	HEA	FE-NC	2.51	2.03	1.95
14	C	306	PGV	O01-C1	2.47	1.41	1.34
14	N	609	PGV	O01-C02	-2.45	1.40	1.46
15	N	602[A]	HEA	C1D-C2D	-2.45	1.39	1.44
15	N	602[B]	HEA	C1D-C2D	-2.45	1.39	1.44
15	N	603	HEA	CHA-C4D	2.44	1.44	1.39
15	N	602[A]	HEA	CHD-C1D	2.44	1.43	1.38
15	N	602[B]	HEA	CHD-C1D	2.44	1.43	1.38
15	A	603	HEA	FE-ND	2.43	2.02	1.94
15	A	602[A]	HEA	CHD-C4C	2.41	1.44	1.39
15	A	602[B]	HEA	CHD-C4C	2.41	1.44	1.39
27	M	106	DMU	O16-C6	2.40	1.44	1.40
15	A	602[A]	HEA	C12-C11	-2.39	1.49	1.53
15	N	602[A]	HEA	C4A-NA	-2.38	1.35	1.39
15	N	602[B]	HEA	C4A-NA	-2.38	1.35	1.39
15	N	603	HEA	C12-C11	2.36	1.57	1.53
23	C	311	CHD	C13-C14	-2.35	1.51	1.55
15	A	603	HEA	C4D-C3D	-2.33	1.41	1.45
15	A	602[A]	HEA	C3D-C2D	2.33	1.41	1.36
15	A	602[B]	HEA	C3D-C2D	2.33	1.41	1.36
23	C	301	CHD	C11-C9	2.31	1.57	1.53
14	P	306	PGV	P-O14	-2.30	1.44	1.55
15	N	603	HEA	C1A-NA	-2.29	1.35	1.39
23	J	101	CHD	C13-C14	-2.28	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	310	CHD	C13-C14	-2.28	1.51	1.55
25	P	304	PEK	C05-C04	2.27	1.59	1.49
14	C	306	PGV	O01-C02	-2.26	1.41	1.46
15	A	602[A]	HEA	CBD-CGD	2.25	1.55	1.50
15	A	602[B]	HEA	CBD-CGD	2.25	1.55	1.50
15	N	603	HEA	CMC-C2C	2.24	1.55	1.50
15	N	603	HEA	CAD-C3D	2.23	1.57	1.51
14	N	609	PGV	O03-C01	2.22	1.50	1.45
15	N	603	HEA	FE-ND	2.22	2.01	1.94
15	N	602[A]	HEA	C4B-NB	-2.21	1.36	1.40
15	N	602[B]	HEA	C4B-NB	-2.21	1.36	1.40
15	A	603	HEA	C1D-C2D	-2.19	1.40	1.44
15	N	602[A]	HEA	CBA-CGA	2.16	1.55	1.50
15	N	602[B]	HEA	CBA-CGA	2.16	1.55	1.50
15	N	602[A]	HEA	C1C-NC	-2.16	1.35	1.39
15	N	602[B]	HEA	C1C-NC	-2.16	1.35	1.39
23	Y	104	CHD	C13-C14	-2.16	1.51	1.55
15	N	602[A]	HEA	CMD-C2D	2.16	1.55	1.50
15	N	602[B]	HEA	CMD-C2D	2.16	1.55	1.50
15	N	602[A]	HEA	OMA-CMA	2.15	1.26	1.22
15	N	602[B]	HEA	OMA-CMA	2.15	1.26	1.22
23	C	301	CHD	O12-C12	2.14	1.47	1.43
15	A	602[A]	HEA	C4C-NC	-2.13	1.35	1.39
15	A	602[B]	HEA	C4C-NC	-2.13	1.35	1.39
23	P	301	CHD	C11-C9	2.13	1.57	1.53
15	N	603	HEA	C4B-C3B	-2.13	1.41	1.44
15	N	602[A]	HEA	C1B-C2B	-2.12	1.40	1.44
15	N	602[B]	HEA	C1B-C2B	-2.12	1.40	1.44
15	A	602[A]	HEA	CAD-C3D	2.12	1.56	1.51
15	A	602[B]	HEA	CAD-C3D	2.12	1.56	1.51
15	A	603	HEA	C1A-C2A	-2.11	1.41	1.45
15	N	602[A]	HEA	O2D-CGD	-2.11	1.23	1.30
15	N	602[B]	HEA	O2D-CGD	-2.11	1.23	1.30
23	W	101	CHD	C13-C14	-2.11	1.52	1.55
15	N	602[A]	HEA	CMC-C2C	2.09	1.55	1.50
15	N	602[B]	HEA	CMC-C2C	2.09	1.55	1.50
23	C	301	CHD	C13-C12	-2.08	1.51	1.54
27	V	102	DMU	O16-C6	2.08	1.43	1.40
15	A	603	HEA	O11-C11	2.06	1.47	1.42
23	P	301	CHD	C2-C3	2.05	1.56	1.51
15	A	602[A]	HEA	CMB-C2B	2.04	1.55	1.50
15	A	602[B]	HEA	CMB-C2B	2.04	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	609	PGV	C03-C02	2.03	1.57	1.50
23	C	301	CHD	O25-C24	2.00	1.28	1.22

All (413) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[A]	HEA	C13-C12-C11	-7.80	101.93	114.39
23	P	310	CHD	C13-C14-C8	-6.52	106.46	114.72
15	A	602[A]	HEA	C13-C12-C11	-6.15	104.56	114.39
15	N	602[A]	HEA	C2B-C1B-NB	6.12	116.97	109.90
15	N	602[B]	HEA	C2B-C1B-NB	6.12	116.97	109.90
26	G	101	CDL	OA6-CA5-C11	5.93	124.31	111.48
14	C	307	PGV	O01-C1-C2	5.90	124.25	111.48
15	A	603	HEA	CHB-C4A-NA	5.80	130.77	124.45
15	A	603	HEA	CHC-C4B-NB	5.67	131.38	124.37
15	N	602[A]	HEA	C2D-C1D-ND	5.53	116.20	109.84
15	N	602[B]	HEA	C2D-C1D-ND	5.53	116.20	109.84
21	B	301	TGL	OG2-CB1-CB2	5.49	123.36	111.48
14	P	307	PGV	O03-C19-C20	5.35	128.15	111.83
23	C	311	CHD	C13-C14-C8	-5.29	108.02	114.72
14	N	601	PGV	O01-C1-C2	5.16	122.64	111.48
23	B	303	CHD	C11-C9-C10	-5.15	108.47	113.70
14	C	307	PGV	O03-C19-C20	5.14	127.50	111.83
22	B	302	PSC	O01-C1-C2	5.13	122.58	111.48
23	W	101	CHD	C1-C10-C5	5.11	115.08	107.75
22	O	301	PSC	O01-C1-C2	5.07	122.45	111.48
25	C	305	PEK	O01-C1-C2	5.06	122.42	111.48
21	N	608	TGL	OG2-CB1-CB2	5.03	122.37	111.48
25	C	303	PEK	O01-C1-C2	4.85	121.97	111.48
26	G	101	CDL	OA8-CA7-C31	4.85	126.62	111.83
26	G	101	CDL	OB6-CB5-C51	4.76	121.77	111.48
26	C	308	CDL	OB6-CB5-C51	4.76	121.77	111.48
26	P	308	CDL	OB6-CB5-C51	4.73	121.72	111.48
15	A	602[A]	HEA	C2B-C1B-NB	4.70	115.34	109.90
15	A	602[B]	HEA	C2B-C1B-NB	4.70	115.34	109.90
23	P	310	CHD	C11-C12-C13	4.69	116.03	111.26
26	T	101	CDL	OB6-CB5-C51	4.64	121.53	111.48
23	C	311	CHD	C11-C12-C13	4.60	115.94	111.26
15	N	603	HEA	C3D-C4D-ND	4.59	114.79	110.35
15	N	602[A]	HEA	C3D-C4D-ND	4.57	114.77	110.35
15	N	602[B]	HEA	C3D-C4D-ND	4.57	114.77	110.35
25	C	303	PEK	C02-O01-C1	-4.56	106.88	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	101	CHD	C11-C9-C10	-4.45	109.19	113.70
26	P	308	CDL	OA6-CA5-C11	4.44	121.08	111.48
15	N	602[A]	HEA	C4B-NB-C1B	-4.41	99.99	105.21
15	N	602[B]	HEA	C4B-NB-C1B	-4.41	99.99	105.21
15	N	602[A]	HEA	C1D-ND-C4D	-4.40	100.00	105.21
15	N	602[B]	HEA	C1D-ND-C4D	-4.40	100.00	105.21
23	C	301	CHD	C18-C13-C12	4.39	113.45	109.06
15	A	602[A]	HEA	CHA-C4D-C3D	-4.39	118.37	124.77
15	A	602[B]	HEA	CHA-C4D-C3D	-4.39	118.37	124.77
26	P	308	CDL	OB8-CB7-C71	4.31	124.99	111.83
25	P	305	PEK	O01-C1-C2	4.26	120.70	111.48
14	P	307	PGV	O01-C1-C2	4.26	120.70	111.48
21	L	101	TGL	OG2-CB1-CB2	4.17	120.50	111.48
23	C	301	CHD	C22-C20-C17	-4.14	101.75	110.33
15	A	602[A]	HEA	CHA-C4D-ND	4.14	128.88	124.42
15	A	602[B]	HEA	CHA-C4D-ND	4.14	128.88	124.42
25	P	305	PEK	O03-C21-C22	4.08	124.28	111.83
21	Y	101	TGL	OG2-CB1-CB2	4.08	120.31	111.48
15	A	602[B]	HEA	C13-C12-C11	-4.05	107.93	114.39
14	P	306	PGV	O01-C1-O02	-4.04	114.26	123.70
27	V	102	DMU	O1-C10-C5	4.03	118.66	110.37
25	P	303	PEK	O01-C1-C2	4.03	120.20	111.48
15	N	603	HEA	CAD-C3D-C4D	3.98	131.63	124.70
23	Y	104	CHD	C13-C17-C20	-3.96	114.69	119.48
15	A	602[A]	HEA	C2D-C1D-ND	3.96	114.39	109.84
15	A	602[B]	HEA	C2D-C1D-ND	3.96	114.39	109.84
23	J	101	CHD	C6-C5-C4	-3.93	106.73	111.23
23	J	101	CHD	C19-C10-C9	-3.83	106.03	111.18
23	Y	104	CHD	C5-C4-C3	-3.79	106.98	112.71
23	P	310	CHD	C11-C9-C10	-3.79	109.86	113.70
23	J	101	CHD	C13-C17-C20	-3.77	114.92	119.48
23	W	101	CHD	C1-C10-C9	-3.76	105.50	111.34
21	B	301	TGL	OG3-CC1-CC2	3.76	123.29	111.83
22	O	301	PSC	C03-C02-C01	-3.75	103.03	111.78
23	W	101	CHD	C11-C9-C10	-3.70	109.94	113.70
15	N	602[A]	HEA	C1B-C2B-C3B	-3.67	102.54	106.80
15	N	602[B]	HEA	C1B-C2B-C3B	-3.67	102.54	106.80
26	P	308	CDL	OA8-CA7-C31	3.66	122.99	111.83
15	N	602[A]	HEA	CHA-C1A-NA	3.66	128.44	124.45
15	N	602[B]	HEA	CHA-C1A-NA	3.66	128.44	124.45
23	P	310	CHD	C9-C11-C12	3.65	119.08	114.29
26	C	308	CDL	OB8-CB7-C71	3.65	122.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[B]	HEA	C13-C12-C11	-3.65	108.56	114.39
14	N	609	PGV	O01-C1-O02	-3.65	115.18	123.70
26	G	101	CDL	CA6-OA8-CA7	3.64	130.42	117.12
23	C	311	CHD	C11-C9-C10	-3.63	110.02	113.70
21	Q	201	TGL	OG1-CA1-CA2	3.62	122.88	111.83
23	C	311	CHD	C9-C11-C12	3.61	119.02	114.29
15	N	602[A]	HEA	C3B-C4B-NB	3.60	113.98	109.84
15	N	602[B]	HEA	C3B-C4B-NB	3.60	113.98	109.84
23	C	301	CHD	C1-C2-C3	-3.59	105.73	110.48
23	J	101	CHD	C10-C9-C8	-3.59	107.84	111.84
15	N	602[B]	HEA	C12-C11-C3B	3.59	117.73	112.12
14	A	601	PGV	O01-C1-C2	3.58	119.22	111.48
27	Z	102	DMU	O1-C10-C5	3.55	117.67	110.37
15	A	602[A]	HEA	CAA-CBA-CGA	-3.54	104.28	113.67
15	A	602[B]	HEA	CAA-CBA-CGA	-3.54	104.28	113.67
25	P	303	PEK	O03-C21-C22	3.53	122.61	111.83
26	G	101	CDL	OA6-CA5-OA7	-3.53	115.46	123.70
23	Y	104	CHD	C17-C13-C14	3.52	103.65	100.11
15	A	602[A]	HEA	O11-C11-C3B	-3.48	104.88	111.26
27	Z	102	DMU	C10-C5-C7	3.48	117.32	110.01
26	P	308	CDL	CB4-OB6-CB5	-3.46	109.51	117.80
26	G	101	CDL	CA4-OA6-CA5	-3.45	109.54	117.80
22	B	302	PSC	O01-C02-C03	3.45	120.71	108.34
23	G	102	CHD	C11-C9-C10	-3.44	110.21	113.70
15	A	602[A]	HEA	C1A-CHA-C4D	-3.42	118.76	126.02
15	A	602[B]	HEA	C1A-CHA-C4D	-3.42	118.76	126.02
23	W	101	CHD	C6-C5-C4	-3.42	107.32	111.23
15	A	602[A]	HEA	C26-C15-C16	3.39	121.11	115.23
15	A	603	HEA	CAD-CBD-CGD	-3.37	104.73	113.67
14	N	601	PGV	O01-C1-O02	-3.36	115.85	123.70
15	A	603	HEA	C2B-C1B-NB	3.34	113.76	109.90
15	A	603	HEA	CMD-C2D-C1D	3.33	130.23	125.03
21	L	101	TGL	OG3-CC1-OC1	-3.31	115.36	123.63
23	B	303	CHD	C19-C10-C5	-3.30	104.91	110.44
14	P	306	PGV	C03-C02-C01	-3.30	104.08	111.78
23	Y	104	CHD	C1-C2-C3	3.30	114.86	110.48
21	B	301	TGL	OG1-CA1-CA2	3.30	121.88	111.83
25	C	303	PEK	O03-C21-C22	3.29	121.88	111.83
26	G	101	CDL	OA8-CA7-OA9	-3.28	115.41	123.63
15	N	603	HEA	C1D-ND-C4D	-3.28	101.32	105.21
27	M	106	DMU	C10-O7-C3	-3.28	110.21	117.98
15	N	602[A]	HEA	CHB-C4A-NA	3.27	128.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[B]	HEA	CHB-C4A-NA	3.27	128.02	124.45
15	N	603	HEA	C13-C12-C11	-3.27	109.17	114.39
23	B	303	CHD	C9-C11-C12	-3.26	110.03	114.29
14	C	306	PGV	C21-C20-C19	-3.25	101.79	113.69
23	Y	104	CHD	C9-C8-C7	-3.22	107.80	111.86
15	A	603	HEA	CHC-C4B-C3B	-3.22	117.69	125.80
14	C	307	PGV	C01-O03-C19	3.21	128.85	117.12
15	N	603	HEA	CHD-C4C-NC	3.20	129.66	123.86
25	C	304	PEK	O03-C21-C22	3.19	121.56	111.83
23	Y	104	CHD	C6-C5-C10	3.18	116.05	112.66
15	N	602[A]	HEA	C3C-C4C-NC	3.18	112.48	109.80
15	N	602[B]	HEA	C3C-C4C-NC	3.18	112.48	109.80
23	Y	104	CHD	C10-C9-C8	-3.15	108.33	111.84
14	C	307	PGV	C02-O01-C1	-3.15	110.27	117.80
26	C	308	CDL	CB4-OB6-CB5	-3.13	110.31	117.80
21	D	201	TGL	OG1-CA1-CA2	3.10	121.28	111.83
15	N	602[A]	HEA	C1A-CHA-C4D	-3.10	119.44	126.02
15	N	602[B]	HEA	C1A-CHA-C4D	-3.10	119.44	126.02
21	N	608	TGL	OG3-CC1-CC2	3.10	121.27	111.83
23	G	102	CHD	C13-C17-C20	-3.09	115.74	119.48
25	C	305	PEK	O03-C21-C22	3.08	121.21	111.83
22	O	301	PSC	C21-C20-C19	-3.06	102.48	113.69
23	B	303	CHD	C6-C5-C4	-3.05	107.74	111.23
15	A	603	HEA	C4C-CHD-C1D	-3.05	119.08	126.25
27	G	108	DMU	C7-C8-C9	3.05	115.76	110.23
25	C	305	PEK	C02-O01-C1	-3.05	110.50	117.80
23	Y	104	CHD	C13-C14-C8	-3.04	110.86	114.72
15	A	603	HEA	C1C-CHC-C4B	-3.04	119.11	126.25
25	C	303	PEK	O01-C1-O02	-3.03	116.62	123.70
26	T	101	CDL	OA6-CA5-C11	3.02	118.00	111.48
15	A	603	HEA	C27-C19-C20	3.01	120.44	115.23
15	A	603	HEA	CHB-C1B-NB	-2.98	121.22	124.42
27	V	102	DMU	C10-C5-C7	2.97	116.25	110.01
23	B	303	CHD	O12-C12-C13	-2.96	106.02	111.02
26	C	308	CDL	OA8-CA7-C31	2.96	120.85	111.83
15	N	602[A]	HEA	CHB-C1B-NB	-2.95	121.25	124.42
15	N	602[B]	HEA	CHB-C1B-NB	-2.95	121.25	124.42
15	A	602[A]	HEA	O2A-CGA-CBA	2.95	123.32	114.00
15	A	602[B]	HEA	O2A-CGA-CBA	2.95	123.32	114.00
23	J	101	CHD	C1-C2-C3	2.93	114.37	110.48
14	N	609	PGV	O03-C19-O04	-2.93	116.30	123.63
25	P	305	PEK	O03-C21-O04	-2.93	116.31	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	307	PGV	O03-C19-O04	-2.91	116.35	123.63
23	P	301	CHD	C21-C20-C22	-2.91	105.84	110.34
21	Q	201	TGL	OG2-CB1-CB2	2.91	117.77	111.48
15	N	603	HEA	C27-C19-C20	2.91	120.28	115.23
26	G	101	CDL	CB6-CB4-CB3	-2.90	105.01	111.78
25	P	304	PEK	O11-P-O14	-2.90	97.44	108.94
21	N	608	TGL	OG1-CA1-CA2	2.89	120.63	111.83
14	N	601	PGV	O03-C19-C20	2.88	120.63	111.83
23	C	311	CHD	C14-C13-C12	2.88	110.05	107.42
15	A	603	HEA	CHD-C4C-NC	2.88	129.08	123.86
15	N	603	HEA	CHA-C4D-C3D	-2.87	120.59	124.77
15	N	602[B]	HEA	C27-C19-C20	2.86	120.19	115.23
14	A	601	PGV	O03-C19-C20	2.85	120.51	111.83
15	N	603	HEA	CAD-CBD-CGD	-2.85	106.12	113.67
27	G	108	DMU	C10-O7-C3	-2.84	111.25	117.98
23	C	311	CHD	C14-C8-C9	-2.84	105.78	109.75
15	N	602[A]	HEA	CAD-C3D-C2D	2.83	133.17	127.87
15	N	602[B]	HEA	CAD-C3D-C2D	2.83	133.17	127.87
15	N	603	HEA	C4C-CHD-C1D	-2.82	119.61	126.25
15	A	602[A]	HEA	C25-C23-C24	2.82	121.08	114.59
23	B	303	CHD	O12-C12-C11	2.82	114.85	109.12
15	A	603	HEA	CHA-C4D-C3D	-2.82	120.67	124.77
14	C	307	PGV	O01-C1-O02	-2.80	117.16	123.70
25	P	304	PEK	O03-C21-C22	2.80	120.36	111.83
15	A	602[B]	HEA	C13-C14-C15	-2.80	121.22	127.62
26	P	308	CDL	OB8-CB7-OB9	-2.79	116.65	123.63
15	N	602[A]	HEA	O11-C11-C3B	-2.79	106.15	111.26
21	Y	101	TGL	OG3-CC1-CC2	2.78	120.31	111.83
23	W	101	CHD	C4-C5-C10	2.78	115.62	112.66
21	L	101	TGL	CC3-CC2-CC1	2.78	123.88	113.69
22	B	302	PSC	C04-C05-N	-2.78	106.91	115.82
27	G	108	DMU	C8-C7-C5	2.77	115.70	110.83
15	N	603	HEA	CMB-C2B-C1B	2.77	129.36	125.03
14	P	307	PGV	C21-C20-C19	-2.76	103.56	113.69
23	P	310	CHD	C14-C13-C12	2.75	109.93	107.42
21	Y	101	TGL	OG1-CA1-CA2	2.75	120.21	111.83
15	A	602[A]	HEA	O1A-CGA-CBA	-2.74	114.40	123.09
15	A	602[B]	HEA	O1A-CGA-CBA	-2.74	114.40	123.09
15	N	603	HEA	C3B-C4B-NB	2.73	112.98	109.84
23	G	102	CHD	C6-C5-C4	-2.72	108.11	111.23
23	W	101	CHD	C4-C3-C2	-2.72	107.30	110.62
15	N	603	HEA	C4B-NB-C1B	-2.72	101.99	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	602[A]	HEA	CHA-C4D-C3D	-2.72	120.81	124.77
15	N	602[B]	HEA	CHA-C4D-C3D	-2.72	120.81	124.77
15	N	603	HEA	C2D-C1D-ND	2.72	112.96	109.84
25	P	305	PEK	C02-O01-C1	-2.71	111.31	117.80
27	P	324	DMU	O7-C10-C5	2.71	114.75	108.09
23	B	303	CHD	C16-C17-C13	2.70	106.16	103.54
27	M	101	DMU	C18-O16-C6	-2.68	109.10	113.68
15	N	603	HEA	CMD-C2D-C1D	2.68	129.22	125.03
15	A	603	HEA	CHB-C4A-C3A	-2.66	120.72	125.21
15	A	603	HEA	C4A-CHB-C1B	-2.66	120.36	126.02
15	N	602[A]	HEA	C26-C15-C16	2.66	119.84	115.23
21	L	101	TGL	OG1-CA1-CA2	2.65	119.91	111.83
27	Z	102	DMU	C10-O7-C3	-2.63	111.75	117.98
21	L	101	TGL	OG3-CC1-CC2	2.62	119.82	111.83
27	C	319	DMU	C10-O1-C9	2.62	118.83	113.72
15	A	602[A]	HEA	C4C-CHD-C1D	-2.61	120.10	126.25
15	A	602[B]	HEA	C4C-CHD-C1D	-2.61	120.10	126.25
26	G	101	CDL	CB4-OB6-CB5	-2.60	111.56	117.80
26	T	101	CDL	OA8-CA7-C31	2.60	119.77	111.83
23	B	303	CHD	C1-C10-C5	2.59	111.47	107.75
15	A	603	HEA	CHA-C4D-ND	2.58	127.20	124.42
23	Y	104	CHD	C9-C10-C5	2.58	112.09	108.51
15	A	603	HEA	C1B-C2B-C3B	-2.57	103.82	106.80
23	P	301	CHD	C6-C7-C8	-2.57	108.70	111.50
23	C	309	CHD	C16-C17-C13	2.57	106.03	103.54
23	P	301	CHD	O12-C12-C11	2.56	114.34	109.12
21	N	608	TGL	CG3-CG2-CG1	-2.55	105.83	111.78
15	A	602[A]	HEA	CHD-C4C-NC	2.55	128.49	123.86
15	A	602[B]	HEA	CHD-C4C-NC	2.55	128.49	123.86
15	N	602[B]	HEA	C13-C14-C15	-2.55	121.80	127.62
25	C	304	PEK	O11-P-O14	-2.54	98.85	108.94
23	P	310	CHD	C17-C13-C14	2.53	102.65	100.11
26	P	308	CDL	OA8-CA7-OA9	-2.53	117.30	123.63
26	T	101	CDL	CB6-CB4-CB3	-2.53	105.89	111.78
21	Q	201	TGL	CG2-OG2-CB1	-2.53	111.75	117.80
15	A	603	HEA	C20-C19-C18	-2.52	115.50	121.17
15	A	602[A]	HEA	CHB-C1B-NB	-2.52	121.71	124.42
15	A	602[B]	HEA	CHB-C1B-NB	-2.52	121.71	124.42
15	N	603	HEA	C2B-C1B-NB	2.52	112.81	109.90
26	C	308	CDL	OA6-CA5-C11	2.51	116.92	111.48
14	P	307	PGV	O03-C19-O04	-2.51	117.35	123.63
21	Q	201	TGL	OG1-CA1-OA1	-2.51	117.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	D	201	TGL	OG1-CA1-OA1	-2.49	117.41	123.63
23	G	102	CHD	C19-C10-C1	-2.48	104.36	108.31
23	P	301	CHD	C6-C5-C4	-2.48	108.39	111.23
27	M	106	DMU	C10-C5-C7	2.48	115.22	110.01
15	A	602[A]	HEA	CHD-C1D-C2D	-2.48	119.91	126.95
15	A	602[B]	HEA	CHD-C1D-C2D	-2.48	119.91	126.95
22	O	301	PSC	C14-C13-C12	-2.47	106.33	124.83
25	C	305	PEK	O03-C21-O04	-2.47	117.45	123.63
15	A	602[A]	HEA	C4B-NB-C1B	-2.46	102.29	105.21
15	A	602[B]	HEA	C4B-NB-C1B	-2.46	102.29	105.21
14	A	601	PGV	C02-O01-C1	-2.46	111.91	117.80
22	O	301	PSC	O01-C1-O02	-2.46	117.96	123.70
23	P	301	CHD	C22-C20-C17	-2.46	105.24	110.33
26	T	101	CDL	CB4-OB6-CB5	-2.45	111.92	117.80
23	J	101	CHD	C4-C3-C2	-2.45	107.63	110.62
21	L	101	TGL	CG3-CG2-CG1	-2.45	106.08	111.78
15	A	602[A]	HEA	C3D-C4D-ND	2.44	112.71	110.35
15	A	602[B]	HEA	C3D-C4D-ND	2.44	112.71	110.35
15	N	602[A]	HEA	CAA-CBA-CGA	-2.44	107.19	113.67
15	N	602[B]	HEA	CAA-CBA-CGA	-2.44	107.19	113.67
25	C	304	PEK	O01-C1-C2	2.43	116.75	111.48
25	P	303	PEK	O03-C21-O04	-2.43	117.54	123.63
21	B	301	TGL	CG3-CG2-CG1	-2.43	106.11	111.78
22	B	302	PSC	C3-C2-C1	-2.43	104.79	113.69
21	Q	201	TGL	OG3-CC1-CC2	2.43	119.24	111.83
21	D	201	TGL	CB3-CB2-CB1	2.43	122.59	113.69
23	C	311	CHD	C16-C17-C20	-2.43	108.50	112.18
23	G	102	CHD	C11-C12-C13	2.43	113.73	111.26
14	P	306	PGV	O01-C1-C2	2.41	116.69	111.48
23	P	311	CHD	C13-C14-C8	-2.41	111.67	114.72
23	P	311	CHD	C15-C14-C13	2.40	105.86	103.54
23	P	311	CHD	C16-C17-C13	2.39	105.86	103.54
15	N	602[A]	HEA	C12-C11-C3B	2.39	115.86	112.12
15	N	602[A]	HEA	CHD-C1D-C2D	-2.39	120.17	126.95
15	N	602[B]	HEA	CHD-C1D-C2D	-2.39	120.17	126.95
15	A	602[A]	HEA	CAD-C3D-C4D	2.38	128.84	124.70
15	A	602[B]	HEA	CAD-C3D-C4D	2.38	128.84	124.70
14	P	307	PGV	O04-C19-C20	-2.38	114.48	123.78
26	T	101	CDL	OB6-CB5-OB7	-2.38	118.15	123.70
15	N	603	HEA	CAD-C3D-C2D	-2.37	123.42	127.87
22	B	302	PSC	O01-C1-O02	-2.37	118.16	123.70
21	D	201	TGL	CG3-OG3-CC1	2.36	125.74	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	304	PEK	C03-C02-C01	-2.36	106.29	111.78
23	B	303	CHD	C22-C23-C24	-2.36	106.21	112.49
23	J	101	CHD	C13-C14-C8	-2.35	111.74	114.72
15	A	602[B]	HEA	C21-C20-C19	-2.35	105.39	113.19
15	N	603	HEA	C21-C22-C23	-2.35	119.81	127.64
15	A	602[B]	HEA	O11-C11-C12	2.35	115.36	109.14
23	P	310	CHD	C14-C8-C9	-2.34	106.47	109.75
15	N	603	HEA	O2A-CGA-CBA	2.34	121.40	114.00
21	L	101	TGL	OG2-CB1-OB1	-2.34	118.23	123.70
26	C	308	CDL	OB6-CB5-OB7	-2.34	118.23	123.70
15	N	602[A]	HEA	C1D-C2D-C3D	-2.34	104.52	106.98
15	N	602[B]	HEA	C1D-C2D-C3D	-2.34	104.52	106.98
23	P	301	CHD	C22-C23-C24	-2.33	106.28	112.49
26	C	308	CDL	OB8-CB7-OB9	-2.33	117.80	123.63
23	J	101	CHD	C1-C10-C5	2.33	111.09	107.75
26	G	101	CDL	OB6-CB5-OB7	-2.33	118.27	123.70
25	C	305	PEK	O01-C1-O02	-2.32	118.27	123.70
21	Q	201	TGL	OG3-CC1-OC1	-2.32	117.82	123.63
15	N	603	HEA	CMB-C2B-C3B	-2.32	125.80	130.28
27	M	101	DMU	C31-C28-C25	-2.31	102.69	114.37
26	C	308	CDL	C80-C79-C78	2.31	126.03	114.37
14	P	307	PGV	C02-O01-C1	-2.30	112.28	117.80
15	A	602[A]	HEA	C1B-C2B-C3B	-2.30	104.13	106.80
15	A	602[B]	HEA	C1B-C2B-C3B	-2.30	104.13	106.80
23	C	311	CHD	C1-C10-C5	2.29	111.03	107.75
25	P	304	PEK	O13-P-O14	2.29	123.08	112.44
27	Z	101	DMU	C10-O7-C3	-2.29	112.56	117.98
14	P	306	PGV	C21-C20-C19	-2.28	105.33	113.69
23	W	101	CHD	C13-C17-C20	-2.28	116.72	119.48
14	P	307	PGV	C3-C2-C1	-2.28	105.34	113.69
23	Y	104	CHD	C19-C10-C9	-2.28	108.11	111.18
26	P	308	CDL	C72-C71-CB7	-2.28	105.34	113.69
20	S	112	EDO	O2-C2-C1	-2.27	95.08	112.39
23	B	303	CHD	C13-C17-C20	-2.27	116.73	119.48
23	J	101	CHD	C14-C8-C9	2.27	112.92	109.75
21	B	301	TGL	CB3-CB2-CB1	-2.27	105.38	113.69
23	P	310	CHD	C1-C10-C5	2.27	111.00	107.75
27	P	323	DMU	C10-O1-C9	2.26	118.13	113.72
23	C	309	CHD	C13-C14-C8	-2.26	111.86	114.72
15	A	603	HEA	C21-C20-C19	2.25	120.66	113.19
15	N	602[A]	HEA	CHA-C1A-C2A	-2.25	121.32	124.86
15	N	602[B]	HEA	CHA-C1A-C2A	-2.25	121.32	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	302	PSC	O03-C01-C02	-2.24	101.93	108.40
15	A	603	HEA	C2D-C1D-ND	2.24	112.41	109.84
23	P	310	CHD	C16-C17-C20	-2.24	108.79	112.18
14	C	307	PGV	C21-C20-C19	-2.24	105.50	113.69
15	N	603	HEA	C1C-CHC-C4B	-2.23	121.01	126.25
15	N	603	HEA	O1D-CGD-CBD	-2.22	116.04	123.09
27	V	102	DMU	C10-O1-C9	2.22	118.05	113.72
23	C	301	CHD	O3-C3-C2	-2.21	104.39	110.17
23	J	101	CHD	C9-C8-C7	-2.21	109.08	111.86
15	N	602[A]	HEA	C4C-C3C-C2C	-2.21	104.56	107.30
15	N	602[B]	HEA	C4C-C3C-C2C	-2.21	104.56	107.30
22	B	302	PSC	C01-O03-C19	2.21	125.18	117.12
14	C	306	PGV	O01-C02-C03	-2.20	100.45	108.34
23	P	311	CHD	C19-C10-C9	-2.20	108.23	111.18
23	C	311	CHD	C22-C20-C17	-2.19	105.79	110.33
23	B	303	CHD	C16-C17-C20	-2.19	108.86	112.18
25	P	304	PEK	O03-C21-O04	-2.19	118.15	123.63
23	P	301	CHD	C9-C11-C12	-2.19	111.43	114.29
14	N	609	PGV	O03-C19-C20	2.19	118.50	111.83
23	C	309	CHD	C15-C14-C13	2.18	105.66	103.54
23	P	310	CHD	O25-C24-C23	-2.18	116.19	123.09
15	N	603	HEA	C21-C20-C19	2.17	120.37	113.19
23	G	102	CHD	C13-C14-C8	-2.17	111.97	114.72
27	M	106	DMU	O7-C3-C4	2.16	115.15	109.48
25	C	303	PEK	O03-C21-O04	-2.16	118.22	123.63
27	M	101	DMU	C22-C19-C18	-2.16	104.08	113.47
15	A	602[A]	HEA	CHB-C4A-NA	2.16	126.80	124.45
15	A	602[B]	HEA	CHB-C4A-NA	2.16	126.80	124.45
14	A	601	PGV	C4-C3-C2	-2.16	105.20	113.13
27	P	323	DMU	O1-C9-C8	2.15	113.58	109.70
15	N	602[A]	HEA	C16-C15-C14	-2.15	116.33	121.17
27	M	106	DMU	C2-C3-C4	-2.15	106.16	110.93
15	A	603	HEA	C16-C15-C14	-2.15	116.34	121.17
23	C	301	CHD	C6-C7-C8	-2.15	109.15	111.50
21	L	101	TGL	C21-C20-CA9	-2.14	103.53	114.37
23	C	309	CHD	C14-C8-C9	-2.14	106.76	109.75
25	P	303	PEK	C03-C02-C01	-2.14	106.80	111.78
23	P	311	CHD	C11-C9-C10	-2.13	111.54	113.70
23	P	301	CHD	O12-C12-C13	-2.13	107.42	111.02
21	D	201	TGL	OG3-CG3-CG2	-2.13	102.25	108.40
23	Y	104	CHD	O12-C12-C11	2.13	113.45	109.12
14	N	601	PGV	C02-O01-C1	-2.12	112.72	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	319	DMU	O1-C9-C8	2.12	113.52	109.70
23	P	310	CHD	C9-C8-C7	2.12	114.52	111.86
14	A	608	PGV	O03-C19-C20	2.12	118.29	111.83
23	C	301	CHD	C19-C10-C1	-2.11	104.96	108.31
23	Y	104	CHD	C11-C9-C10	-2.10	111.57	113.70
23	P	301	CHD	C10-C9-C8	-2.10	109.49	111.84
23	P	301	CHD	C19-C10-C1	-2.09	104.97	108.31
23	J	101	CHD	C17-C13-C14	2.09	102.21	100.11
27	M	106	DMU	O7-C10-C5	2.09	113.23	108.09
14	P	307	PGV	C01-O03-C19	2.09	124.76	117.12
27	C	319	DMU	C6-C1-C2	2.09	114.41	110.01
14	C	306	PGV	O01-C1-C2	2.09	115.99	111.48
21	Y	101	TGL	OG3-CC1-OC1	-2.08	118.43	123.63
25	P	305	PEK	C01-O03-C21	2.08	124.71	117.12
23	C	301	CHD	O12-C12-C13	-2.08	107.51	111.02
26	C	308	CDL	OA6-CA4-CA3	2.07	115.79	108.34
14	C	307	PGV	O14-P-O13	2.07	122.09	112.44
27	C	319	DMU	O7-C10-C5	2.07	113.19	108.09
15	N	602[A]	HEA	C25-C23-C24	2.06	119.34	114.59
15	N	602[A]	HEA	CHB-C1B-C2B	-2.06	121.77	125.03
15	N	602[B]	HEA	CHB-C1B-C2B	-2.06	121.77	125.03
26	P	308	CDL	CA6-CA4-CA3	-2.06	106.99	111.78
27	M	101	DMU	C10-O7-C3	-2.06	113.10	117.98
15	A	603	HEA	C13-C12-C11	-2.05	111.11	114.39
27	Z	101	DMU	C34-C31-C28	-2.04	104.04	114.37
15	N	603	HEA	C4A-CHB-C1B	-2.04	121.68	126.02
27	C	319	DMU	C10-O7-C3	-2.04	113.14	117.98
14	N	601	PGV	O01-C02-C03	2.04	115.64	108.34
23	C	301	CHD	C19-C10-C9	2.03	113.91	111.18
25	P	303	PEK	C01-O03-C21	2.03	124.54	117.12
25	C	304	PEK	C02-O01-C1	-2.03	112.94	117.80
26	G	101	CDL	OA8-CA6-CA4	-2.02	102.56	108.40
23	J	101	CHD	C18-C13-C12	2.02	111.08	109.06
27	C	319	DMU	C57-C4-C3	-2.02	107.70	113.38
27	P	323	DMU	C10-O7-C3	-2.02	113.20	117.98
23	Y	104	CHD	C14-C13-C12	-2.01	105.57	107.42
26	G	101	CDL	C39-C38-C37	2.01	124.54	114.37
27	C	310	DMU	C10-O7-C3	-2.01	113.22	117.98
23	G	102	CHD	C17-C13-C12	2.01	119.47	117.67
21	B	301	TGL	CG3-OG3-CC1	2.00	124.45	117.12
23	C	311	CHD	O25-C24-C23	-2.00	116.74	123.09

There are no chirality outliers.

All (679) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601	PGV	O04-C19-O03-C01
14	A	601	PGV	C20-C19-O03-C01
14	C	307	PGV	C04-O12-P-O11
14	C	307	PGV	C04-O12-P-O13
14	C	307	PGV	O04-C19-O03-C01
14	C	307	PGV	C20-C19-O03-C01
14	N	601	PGV	C2-C1-O01-C02
14	N	601	PGV	O04-C19-O03-C01
14	N	601	PGV	C20-C19-O03-C01
14	P	307	PGV	O04-C19-O03-C01
14	P	307	PGV	C20-C19-O03-C01
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
21	Y	101	TGL	CB2-CB1-OG2-CG2
22	B	302	PSC	C04-O12-P-O11
22	B	302	PSC	C04-O12-P-O13
22	B	302	PSC	C04-O12-P-O14
22	B	302	PSC	C2-C1-O01-C02
22	O	301	PSC	C03-O11-P-O12
22	O	301	PSC	C03-O11-P-O13
22	O	301	PSC	C03-O11-P-O14
22	O	301	PSC	O02-C1-O01-C02
22	O	301	PSC	C2-C1-O01-C02
25	C	303	PEK	C03-O11-P-O12
25	C	303	PEK	C03-O11-P-O13
25	C	303	PEK	C03-O11-P-O14
25	C	303	PEK	O04-C21-O03-C01
25	C	303	PEK	C22-C21-O03-C01
25	C	305	PEK	O04-C21-O03-C01
25	C	305	PEK	C22-C21-O03-C01
25	C	305	PEK	C5-C6-C7-C8
25	P	303	PEK	O04-C21-O03-C01
25	P	303	PEK	C22-C21-O03-C01
25	P	305	PEK	O04-C21-O03-C01
25	P	305	PEK	C22-C21-O03-C01
26	C	308	CDL	CA2-OA2-PA1-OA3
26	C	308	CDL	C11-CA5-OA6-CA4
26	C	308	CDL	OA9-CA7-OA8-CA6
26	C	308	CDL	C31-CA7-OA8-CA6
26	C	308	CDL	CB3-OB5-PB2-OB2
26	C	308	CDL	CB3-OB5-PB2-OB4
26	G	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
26	G	101	CDL	CB3-OB5-PB2-OB4
26	P	308	CDL	CA2-OA2-PA1-OA3
26	P	308	CDL	CA3-OA5-PA1-OA3
26	P	308	CDL	OA9-CA7-OA8-CA6
26	P	308	CDL	C31-CA7-OA8-CA6
26	P	308	CDL	CB2-OB2-PB2-OB3
26	P	308	CDL	CB3-OB5-PB2-OB2
26	P	308	CDL	CB3-OB5-PB2-OB4
26	T	101	CDL	CA2-OA2-PA1-OA4
26	T	101	CDL	CA2-OA2-PA1-OA5
26	T	101	CDL	CA3-OA5-PA1-OA2
26	T	101	CDL	CA3-OA5-PA1-OA4
26	T	101	CDL	OA9-CA7-OA8-CA6
26	T	101	CDL	C31-CA7-OA8-CA6
27	P	324	DMU	O5-C6-O16-C18
27	P	324	DMU	C5-C10-O7-C3
27	Z	102	DMU	C1-C6-O16-C18
27	Z	102	DMU	O5-C6-O16-C18
27	Z	102	DMU	C19-C18-O16-C6
26	G	101	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	C31-CA7-OA8-CA6
23	J	101	CHD	C21-C20-C22-C23
27	P	324	DMU	O1-C10-O7-C3
27	V	102	DMU	C5-C10-O7-C3
14	A	601	PGV	O02-C1-O01-C02
14	N	601	PGV	O02-C1-O01-C02
21	Y	101	TGL	OB1-CB1-OG2-CG2
22	B	302	PSC	O02-C1-O01-C02
26	C	308	CDL	OA7-CA5-OA6-CA4
27	P	324	DMU	O6-C11-C9-O1
23	W	101	CHD	C21-C20-C22-C23
23	Y	104	CHD	C21-C20-C22-C23
27	V	102	DMU	O6-C11-C9-O1
14	N	601	PGV	C10-C11-C12-C13
14	P	306	PGV	C10-C11-C12-C13
25	C	305	PEK	C13-C14-C15-C16
25	P	303	PEK	C4-C5-C6-C7
23	C	309	CHD	C17-C20-C22-C23
27	P	324	DMU	O6-C11-C9-C8
27	G	108	DMU	O5-C4-C57-O61
14	A	601	PGV	C2-C1-O01-C02
27	V	102	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
23	P	311	CHD	C17-C20-C22-C23
27	M	106	DMU	O5-C4-C57-O61
27	P	324	DMU	C3-C4-C57-O61
27	V	102	DMU	O6-C11-C9-C8
27	V	102	DMU	O1-C10-O7-C3
23	C	309	CHD	C21-C20-C22-C23
23	P	311	CHD	C21-C20-C22-C23
25	C	303	PEK	C4-C5-C6-C7
25	C	305	PEK	C4-C5-C6-C7
27	M	106	DMU	C3-C4-C57-O61
21	Y	101	TGL	CA2-CA1-OG1-CG1
27	P	324	DMU	O5-C4-C57-O61
21	L	101	TGL	CC3-CC4-CC5-CC6
26	P	308	CDL	C80-C81-C82-C83
27	Z	102	DMU	O5-C4-C57-O61
26	C	308	CDL	C57-C58-C59-C60
27	V	102	DMU	C3-C4-C57-O61
21	Y	101	TGL	OA1-CA1-OG1-CG1
25	C	303	PEK	C7-C8-C9-C10
25	C	305	PEK	C10-C11-C12-C13
25	P	305	PEK	C13-C14-C15-C16
26	G	101	CDL	CA7-C31-C32-C33
23	Y	104	CHD	C17-C20-C22-C23
20	M	105	EDO	O1-C1-C2-O2
14	P	307	PGV	C1-C2-C3-C4
27	C	319	DMU	O6-C11-C9-C8
21	Y	101	TGL	CC1-CC2-CC3-CC4
27	G	108	DMU	C3-C4-C57-O61
14	C	307	PGV	O12-C04-C05-O05
27	M	106	DMU	O16-C18-C19-C22
27	C	310	DMU	O16-C18-C19-C22
27	P	309	DMU	O16-C18-C19-C22
27	Z	102	DMU	O16-C18-C19-C22
27	P	324	DMU	O16-C18-C19-C22
21	Q	201	TGL	CB2-CB1-OG2-CG2
21	Q	201	TGL	OB1-CB1-OG2-CG2
25	C	303	PEK	O02-C1-O01-C02
14	C	307	PGV	O12-C04-C05-C06
23	Y	104	CHD	C20-C22-C23-C24
21	L	101	TGL	CC6-CC7-CC8-CC9
21	Q	201	TGL	CA9-C20-C21-C22
22	O	301	PSC	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
27	C	319	DMU	O5-C4-C57-O61
21	L	101	TGL	CC2-CC1-OG3-CG3
27	C	319	DMU	O6-C11-C9-O1
26	C	308	CDL	C42-C43-C44-C45
25	C	303	PEK	C2-C1-O01-C02
22	B	302	PSC	C11-C10-C9-C8
25	P	304	PEK	C7-C8-C9-C10
21	L	101	TGL	CA2-CA1-OG1-CG1
26	G	101	CDL	C80-C81-C82-C83
27	P	309	DMU	C5-C10-O7-C3
27	C	319	DMU	C3-C4-C57-O61
21	N	608	TGL	OB1-CB1-OG2-CG2
27	V	102	DMU	O5-C6-O16-C18
21	N	608	TGL	CB2-CB1-OG2-CG2
26	P	308	CDL	C51-CB5-OB6-CB4
26	T	101	CDL	C51-CB5-OB6-CB4
27	Z	102	DMU	C28-C31-C34-C37
21	D	201	TGL	CA9-C20-C21-C22
21	Y	101	TGL	CC4-CC5-CC6-CC7
26	P	308	CDL	C57-C58-C59-C60
26	T	101	CDL	OB7-CB5-OB6-CB4
21	Y	101	TGL	CB2-CB3-CB4-CB5
21	Y	101	TGL	C12-C13-C14-C29
21	D	201	TGL	CB1-CB2-CB3-CB4
21	L	101	TGL	C11-C10-CB9-CB8
21	B	301	TGL	CB2-CB1-OG2-CG2
26	G	101	CDL	C51-CB5-OB6-CB4
21	L	101	TGL	CC2-CC3-CC4-CC5
21	L	101	TGL	CA9-C20-C21-C22
26	T	101	CDL	C77-C78-C79-C80
21	N	608	TGL	CB1-CB2-CB3-CB4
21	D	201	TGL	CA6-CA7-CA8-CA9
27	P	309	DMU	O1-C10-O7-C3
26	T	101	CDL	CA5-C11-C12-C13
21	Q	201	TGL	C20-C21-C22-C23
21	L	101	TGL	OA1-CA1-OG1-CG1
21	B	301	TGL	C11-C12-C13-C14
21	N	608	TGL	CB4-CB5-CB6-CB7
21	B	301	TGL	OB1-CB1-OG2-CG2
27	G	108	DMU	C28-C31-C34-C37
14	P	306	PGV	C24-C25-C26-C27
21	B	301	TGL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
21	L	101	TGL	CB3-CB4-CB5-CB6
21	L	101	TGL	CB7-CB8-CB9-C10
21	Q	201	TGL	CC5-CC6-CC7-CC8
21	Y	101	TGL	CB7-CB8-CB9-C10
26	C	308	CDL	C20-C21-C22-C23
20	A	620	EDO	O1-C1-C2-O2
20	N	618	EDO	O1-C1-C2-O2
20	N	629	EDO	O1-C1-C2-O2
20	O	305	EDO	O1-C1-C2-O2
20	P	313	EDO	O1-C1-C2-O2
20	W	102	EDO	O1-C1-C2-O2
23	P	310	CHD	C21-C20-C22-C23
21	L	101	TGL	CC9-C15-C16-C17
26	C	308	CDL	C17-C18-C19-C20
26	C	308	CDL	C40-C41-C42-C43
27	C	310	DMU	C31-C34-C37-C40
27	M	106	DMU	C28-C31-C34-C37
14	C	307	PGV	C2-C1-O01-C02
14	C	306	PGV	C7-C8-C9-C10
14	P	306	PGV	C7-C8-C9-C10
26	P	308	CDL	C77-C78-C79-C80
21	D	201	TGL	C11-C10-CB9-CB8
21	L	101	TGL	CB9-C10-C11-C12
23	W	101	CHD	C20-C22-C23-C24
14	N	601	PGV	C1-C2-C3-C4
21	Q	201	TGL	CC1-CC2-CC3-CC4
21	Y	101	TGL	CC3-CC4-CC5-CC6
21	L	101	TGL	OC1-CC1-OG3-CG3
21	D	201	TGL	CC7-CC8-CC9-C15
21	Y	101	TGL	CC5-CC6-CC7-CC8
26	C	308	CDL	OB7-CB5-OB6-CB4
26	G	101	CDL	OB7-CB5-OB6-CB4
26	P	308	CDL	OB7-CB5-OB6-CB4
14	N	601	PGV	C2-C3-C4-C5
21	N	608	TGL	CB3-CB4-CB5-CB6
25	P	304	PEK	C22-C23-C24-C25
26	G	101	CDL	C13-C14-C15-C16
27	V	102	DMU	C25-C28-C31-C34
21	B	301	TGL	CC2-CC1-OG3-CG3
26	G	101	CDL	C20-C21-C22-C23
21	N	608	TGL	C10-C11-C12-C13
27	M	106	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
27	C	319	DMU	C22-C25-C28-C31
21	D	201	TGL	CB2-CB1-OG2-CG2
25	C	305	PEK	C2-C1-O01-C02
26	C	308	CDL	C51-CB5-OB6-CB4
26	G	101	CDL	C11-CA5-OA6-CA4
21	B	301	TGL	CB1-CB2-CB3-CB4
25	C	304	PEK	C26-C27-C28-C29
21	D	201	TGL	OB1-CB1-OG2-CG2
26	G	101	CDL	OA7-CA5-OA6-CA4
21	B	301	TGL	CA5-CA6-CA7-CA8
21	Q	201	TGL	C18-C19-C33-C34
27	Z	102	DMU	C3-C4-C57-O61
14	C	306	PGV	C10-C11-C12-C13
21	B	301	TGL	C20-C21-C22-C23
21	Q	201	TGL	C21-C22-C23-C24
22	O	301	PSC	C30-C31-C32-C33
26	G	101	CDL	C37-C38-C39-C40
25	C	305	PEK	O02-C1-O01-C02
25	P	303	PEK	C2-C1-O01-C02
21	L	101	TGL	C12-C13-C14-C29
27	G	108	DMU	O6-C11-C9-O1
21	L	101	TGL	CA3-CA4-CA5-CA6
14	C	307	PGV	O02-C1-O01-C02
21	Y	101	TGL	C19-C33-C34-C35
21	D	201	TGL	CA3-CA4-CA5-CA6
26	T	101	CDL	C54-C55-C56-C57
21	Y	101	TGL	C21-C22-C23-C24
14	N	609	PGV	C10-C11-C12-C13
14	C	306	PGV	C20-C21-C22-C23
26	C	308	CDL	C77-C78-C79-C80
25	C	304	PEK	C16-C17-C18-C19
21	Y	101	TGL	C22-C23-C24-C25
21	D	201	TGL	C20-C21-C22-C23
27	C	319	DMU	C25-C28-C31-C34
26	G	101	CDL	C60-C61-C62-C63
23	P	311	CHD	C20-C22-C23-C24
26	T	101	CDL	C20-C21-C22-C23
22	O	301	PSC	C20-C19-O03-C01
25	P	304	PEK	C13-C14-C15-C16
26	G	101	CDL	C55-C56-C57-C58
14	N	601	PGV	O03-C01-C02-C03
25	P	305	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
26	C	308	CDL	CB3-CB4-CB6-OB8
26	T	101	CDL	C60-C61-C62-C63
26	P	308	CDL	CA5-C11-C12-C13
27	P	309	DMU	O6-C11-C9-O1
27	M	106	DMU	C31-C34-C37-C40
20	D	202	EDO	O1-C1-C2-O2
20	R	204	EDO	O1-C1-C2-O2
20	S	111	EDO	O1-C1-C2-O2
20	S	112	EDO	O1-C1-C2-O2
27	P	323	DMU	O6-C11-C9-C8
26	C	308	CDL	C36-C37-C38-C39
14	P	307	PGV	C2-C1-O01-C02
21	Q	201	TGL	C16-C17-C18-C19
27	C	319	DMU	C19-C22-C25-C28
21	L	101	TGL	C21-C22-C23-C24
23	Y	104	CHD	C13-C17-C20-C21
27	M	106	DMU	C25-C28-C31-C34
21	D	201	TGL	CC6-CC7-CC8-CC9
25	P	303	PEK	C30-C31-C32-C33
27	G	108	DMU	C31-C34-C37-C40
21	Y	101	TGL	C11-C12-C13-C14
15	A	602[A]	HEA	C2A-C3A-CMA-OMA
15	A	602[B]	HEA	C2A-C3A-CMA-OMA
14	A	608	PGV	C10-C11-C12-C13
25	C	304	PEK	C7-C8-C9-C10
21	Q	201	TGL	C11-C10-CB9-CB8
21	Y	101	TGL	CC6-CC7-CC8-CC9
21	Y	101	TGL	C24-C25-C26-C27
14	N	609	PGV	C27-C28-C29-C30
21	D	201	TGL	CC4-CC5-CC6-CC7
22	O	301	PSC	C22-C23-C24-C25
25	C	303	PEK	C29-C30-C31-C32
26	C	308	CDL	C41-C42-C43-C44
21	B	301	TGL	C12-C13-C14-C29
25	P	303	PEK	C33-C34-C35-C36
22	B	302	PSC	O03-C01-C02-O01
25	P	305	PEK	C34-C35-C36-C37
21	Y	101	TGL	CA3-CA4-CA5-CA6
27	C	319	DMU	C34-C37-C40-C43
27	P	323	DMU	C34-C37-C40-C43
21	L	101	TGL	C17-C18-C19-C33
23	Y	104	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
21	B	301	TGL	CA9-C20-C21-C22
26	T	101	CDL	CA7-C31-C32-C33
25	C	304	PEK	C4-C5-C6-C7
25	P	305	PEK	C10-C11-C12-C13
25	P	303	PEK	O02-C1-O01-C02
23	W	101	CHD	C17-C20-C22-C23
14	P	306	PGV	C02-C03-O11-P
14	A	601	PGV	C20-C21-C22-C23
14	A	601	PGV	C01-C02-C03-O11
25	P	305	PEK	C01-C02-C03-O11
26	P	308	CDL	OA5-CA3-CA4-CA6
21	B	301	TGL	C25-C26-C27-C28
21	B	301	TGL	CC4-CC5-CC6-CC7
21	B	301	TGL	OC1-CC1-OG3-CG3
26	G	101	CDL	C32-C31-CA7-OA8
21	N	608	TGL	C29-C30-C31-C32
22	O	301	PSC	O04-C19-O03-C01
25	C	304	PEK	C13-C14-C15-C16
27	Z	101	DMU	O16-C18-C19-C22
26	G	101	CDL	C57-C58-C59-C60
21	Q	201	TGL	CB2-CB3-CB4-CB5
21	Q	201	TGL	CG1-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-C03
26	T	101	CDL	CA3-CA4-CA6-OA8
21	N	608	TGL	C20-C21-C22-C23
21	Y	101	TGL	C23-C24-C25-C26
26	G	101	CDL	C61-C62-C63-C64
20	G	103	EDO	O1-C1-C2-O2
26	C	308	CDL	C60-C61-C62-C63
26	P	308	CDL	C41-C42-C43-C44
21	D	201	TGL	OG3-CC1-CC2-CC3
26	P	308	CDL	OA5-CA3-CA4-OA6
23	J	101	CHD	C13-C17-C20-C22
23	Y	104	CHD	C13-C17-C20-C22
26	T	101	CDL	C61-C62-C63-C64
25	C	303	PEK	C33-C34-C35-C36
14	N	601	PGV	O03-C01-C02-O01
21	Q	201	TGL	OG2-CG2-CG3-OG3
26	C	308	CDL	OB6-CB4-CB6-OB8
22	B	302	PSC	C9-C10-C11-C12
22	B	302	PSC	C10-C11-C12-C13
22	O	301	PSC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	O	301	PSC	C10-C11-C12-C13
25	C	303	PEK	C5-C6-C7-C8
25	C	303	PEK	C11-C10-C9-C8
25	C	303	PEK	C9-C10-C11-C12
25	C	303	PEK	C11-C12-C13-C14
25	C	303	PEK	C12-C13-C14-C15
25	C	304	PEK	C9-C10-C11-C12
25	C	304	PEK	C11-C12-C13-C14
25	C	304	PEK	C12-C13-C14-C15
25	C	305	PEK	C6-C7-C8-C9
25	C	305	PEK	C11-C10-C9-C8
25	C	305	PEK	C9-C10-C11-C12
25	C	305	PEK	C11-C12-C13-C14
25	C	305	PEK	C12-C13-C14-C15
25	P	303	PEK	C5-C6-C7-C8
25	P	303	PEK	C6-C7-C8-C9
25	P	303	PEK	C11-C10-C9-C8
25	P	303	PEK	C9-C10-C11-C12
25	P	303	PEK	C11-C12-C13-C14
25	P	303	PEK	C12-C13-C14-C15
25	P	304	PEK	C6-C7-C8-C9
25	P	304	PEK	C9-C10-C11-C12
25	P	304	PEK	C11-C12-C13-C14
25	P	304	PEK	C12-C13-C14-C15
25	P	305	PEK	C5-C6-C7-C8
25	P	305	PEK	C6-C7-C8-C9
25	P	305	PEK	C11-C10-C9-C8
25	P	305	PEK	C9-C10-C11-C12
25	P	305	PEK	C11-C12-C13-C14
25	P	305	PEK	C12-C13-C14-C15
26	P	308	CDL	C36-C37-C38-C39
26	P	308	CDL	C12-C13-C14-C15
14	A	601	PGV	C19-C20-C21-C22
26	G	101	CDL	CB5-C51-C52-C53
21	L	101	TGL	CA5-CA6-CA7-CA8
21	Q	201	TGL	CC3-CC4-CC5-CC6
26	C	308	CDL	CB7-C71-C72-C73
26	G	101	CDL	C42-C43-C44-C45
14	P	307	PGV	O02-C1-O01-C02
23	J	101	CHD	C13-C17-C20-C21
23	C	311	CHD	C21-C20-C22-C23
14	N	601	PGV	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
22	B	302	PSC	C03-C02-O01-C1
25	P	303	PEK	C32-C33-C34-C35
21	D	201	TGL	CC2-CC3-CC4-CC5
25	P	305	PEK	O02-C1-O01-C02
26	G	101	CDL	OB5-CB3-CB4-OB6
23	J	101	CHD	C16-C17-C20-C22
23	Y	104	CHD	C16-C17-C20-C22
21	L	101	TGL	OG1-CG1-CG2-CG3
22	B	302	PSC	C24-C25-C26-C27
26	P	308	CDL	C52-C53-C54-C55
27	P	323	DMU	O16-C18-C19-C22
22	O	301	PSC	C11-C10-C9-C8
21	L	101	TGL	OG1-CG1-CG2-OG2
21	L	101	TGL	OG2-CG2-CG3-OG3
21	Y	101	TGL	OG1-CG1-CG2-OG2
21	Y	101	TGL	OG2-CG2-CG3-OG3
25	P	305	PEK	O03-C01-C02-O01
26	P	308	CDL	OB6-CB4-CB6-OB8
26	T	101	CDL	OA6-CA4-CA6-OA8
27	M	101	DMU	O6-C11-C9-C8
27	Z	101	DMU	C22-C25-C28-C31
14	A	608	PGV	C29-C30-C31-C32
25	C	303	PEK	C34-C35-C36-C37
22	B	302	PSC	O12-C04-C05-N
25	C	305	PEK	C01-C02-C03-O11
21	N	608	TGL	CA5-CA6-CA7-CA8
27	C	310	DMU	C18-C19-C22-C25
21	Y	101	TGL	CA6-CA7-CA8-CA9
14	P	307	PGV	C3-C4-C5-C6
25	P	303	PEK	C7-C8-C9-C10
25	P	304	PEK	C4-C5-C6-C7
26	G	101	CDL	O1-C1-CB2-OB2
21	L	101	TGL	C15-C16-C17-C18
14	A	601	PGV	O01-C02-C03-O11
26	T	101	CDL	OB5-CB3-CB4-OB6
21	Q	201	TGL	C16-C15-CC9-CC8
23	C	309	CHD	C20-C22-C23-C24
21	Y	101	TGL	CB9-C10-C11-C12
21	Q	201	TGL	C33-C34-C35-C36
25	P	305	PEK	C33-C34-C35-C36
15	A	602[A]	HEA	C4A-C3A-CMA-OMA
15	A	602[B]	HEA	C4A-C3A-CMA-OMA

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Mol	Chain	Res	Type	Atoms
23	J	101	CHD	C16-C17-C20-C21
25	C	304	PEK	C10-C11-C12-C13
21	D	201	TGL	C18-C19-C33-C34
21	Y	101	TGL	CC7-CC8-CC9-C15
21	L	101	TGL	CG1-CG2-CG3-OG3
21	Y	101	TGL	CG1-CG2-CG3-OG3
26	P	308	CDL	CB3-CB4-CB6-OB8
27	P	324	DMU	C28-C31-C34-C37
27	P	309	DMU	C22-C25-C28-C31
20	M	104	EDO	O1-C1-C2-O2
20	N	623	EDO	O1-C1-C2-O2
20	Q	203	EDO	O1-C1-C2-O2
27	V	102	DMU	C2-C3-O7-C10
21	D	201	TGL	C16-C15-CC9-CC8
27	V	102	DMU	C4-C3-O7-C10
25	P	305	PEK	C17-C18-C19-C20
14	C	307	PGV	C03-O11-P-O12
14	C	307	PGV	C04-O12-P-O14
26	C	308	CDL	CA3-OA5-PA1-OA3
26	C	308	CDL	CB2-OB2-PB2-OB3
26	G	101	CDL	CA2-OA2-PA1-OA3
26	G	101	CDL	CB3-OB5-PB2-OB2
26	P	308	CDL	CB2-OB2-PB2-OB4
26	P	308	CDL	CB2-OB2-PB2-OB5
14	C	306	PGV	C02-C03-O11-P
27	P	324	DMU	C18-C19-C22-C25
27	P	324	DMU	C19-C22-C25-C28
27	M	101	DMU	C19-C22-C25-C28
21	N	608	TGL	CC7-CC8-CC9-C15
21	N	608	TGL	CA4-CA5-CA6-CA7
14	N	609	PGV	C11-C12-C13-C14
21	Y	101	TGL	C29-C30-C31-C32
14	N	601	PGV	C01-C02-C03-O11
26	C	308	CDL	OA5-CA3-CA4-CA6
27	M	101	DMU	C34-C37-C40-C43
22	B	302	PSC	C7-C8-C9-C10
22	O	301	PSC	C19-C20-C21-C22
25	P	305	PEK	O01-C02-C03-O11
21	N	608	TGL	C12-C13-C14-C29
23	J	101	CHD	C17-C20-C22-C23
14	C	306	PGV	C25-C26-C27-C28
26	T	101	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
26	T	101	CDL	C12-C11-CA5-OA6
26	P	308	CDL	C60-C61-C62-C63
27	C	319	DMU	C28-C31-C34-C37
25	P	305	PEK	C2-C1-O01-C02
22	O	301	PSC	O03-C01-C02-C03
22	O	301	PSC	O03-C19-C20-C21
20	F	107	EDO	O1-C1-C2-O2
20	N	624	EDO	O1-C1-C2-O2
21	B	301	TGL	C11-C10-CB9-CB8
14	N	601	PGV	C19-C20-C21-C22
26	T	101	CDL	C43-C44-C45-C46
15	N	602[B]	HEA	C26-C15-C16-C17
26	T	101	CDL	C37-C38-C39-C40
26	T	101	CDL	OA5-CA3-CA4-OA6
14	N	601	PGV	C11-C12-C13-C14
22	B	302	PSC	C12-C13-C14-C15
26	P	308	CDL	C31-C32-C33-C34
27	M	101	DMU	C25-C28-C31-C34
14	N	601	PGV	O12-C04-C05-O05
26	C	308	CDL	C76-C77-C78-C79
21	Y	101	TGL	C15-C16-C17-C18
14	C	306	PGV	C1-C2-C3-C4
22	O	301	PSC	O03-C01-C02-O01
26	T	101	CDL	C17-C18-C19-C20
14	A	601	PGV	C23-C24-C25-C26
26	T	101	CDL	C11-C12-C13-C14
14	N	609	PGV	C26-C27-C28-C29
21	N	608	TGL	CB9-C10-C11-C12
23	G	102	CHD	C22-C23-C24-O25
23	G	102	CHD	C22-C23-C24-O26
14	C	307	PGV	O03-C01-C02-C03
21	Y	101	TGL	C20-C21-C22-C23
26	C	308	CDL	C37-C38-C39-C40
21	B	301	TGL	C15-C16-C17-C18
22	B	302	PSC	C3-C4-C5-C6
26	P	308	CDL	C75-C76-C77-C78
23	W	101	CHD	C22-C23-C24-O26
21	L	101	TGL	CC4-CC5-CC6-CC7
23	W	101	CHD	C13-C17-C20-C21
23	J	101	CHD	C22-C23-C24-O25
25	C	305	PEK	C34-C35-C36-C37
20	A	617	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
20	L	102	EDO	O1-C1-C2-O2
20	N	612	EDO	O1-C1-C2-O2
20	O	306	EDO	O1-C1-C2-O2
20	P	316	EDO	O1-C1-C2-O2
20	P	321	EDO	O1-C1-C2-O2
23	B	303	CHD	C22-C23-C24-O26
23	C	309	CHD	C22-C23-C24-O26
27	P	324	DMU	C34-C37-C40-C43
26	P	308	CDL	C17-C18-C19-C20
14	C	306	PGV	C24-C25-C26-C27
15	A	602[A]	HEA	CAD-CBD-CGD-O1D
15	A	602[B]	HEA	CAD-CBD-CGD-O1D
23	W	101	CHD	C22-C23-C24-O25
21	B	301	TGL	CC2-CC3-CC4-CC5
21	N	608	TGL	CC5-CC6-CC7-CC8
23	J	101	CHD	C22-C23-C24-O26
26	G	101	CDL	OB5-CB3-CB4-CB6
26	T	101	CDL	OB5-CB3-CB4-CB6
23	C	301	CHD	C22-C23-C24-O25
21	L	101	TGL	C22-C23-C24-C25
21	B	301	TGL	OG1-CG1-CG2-OG2
25	P	303	PEK	O03-C01-C02-O01
26	G	101	CDL	OB6-CB4-CB6-OB8
22	B	302	PSC	C29-C30-C31-C32
26	T	101	CDL	C81-C82-C83-C84
25	C	303	PEK	C6-C7-C8-C9
25	C	304	PEK	C5-C6-C7-C8
15	A	603	HEA	CAD-CBD-CGD-O2D
26	P	308	CDL	C37-C38-C39-C40
23	C	309	CHD	C22-C23-C24-O25
14	N	601	PGV	C21-C22-C23-C24
22	B	302	PSC	C20-C21-C22-C23
14	P	306	PGV	C1-C2-C3-C4
14	A	608	PGV	C23-C24-C25-C26
23	B	303	CHD	C22-C23-C24-O25
15	A	602[A]	HEA	C27-C19-C20-C21
27	M	101	DMU	C22-C25-C28-C31
27	Z	102	DMU	O6-C11-C9-O1
21	L	101	TGL	CA1-CA2-CA3-CA4
21	D	201	TGL	CC3-CC4-CC5-CC6
26	T	101	CDL	C80-C81-C82-C83
15	N	603	HEA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	P	303	PEK	O03-C01-C02-C03
21	Q	201	TGL	CC9-C15-C16-C17
26	P	308	CDL	C83-C84-C85-C86
27	V	102	DMU	C22-C25-C28-C31
25	C	305	PEK	O01-C02-C03-O11
26	C	308	CDL	OA5-CA3-CA4-OA6
26	C	308	CDL	C82-C83-C84-C85
15	N	603	HEA	CAA-CBA-CGA-O1A
26	C	308	CDL	C39-C40-C41-C42
20	A	609	EDO	O1-C1-C2-O2
20	B	307	EDO	O1-C1-C2-O2
20	D	205	EDO	O1-C1-C2-O2
20	N	625	EDO	O1-C1-C2-O2
20	Q	202	EDO	O1-C1-C2-O2
20	S	107	EDO	O1-C1-C2-O2
20	S	108	EDO	O1-C1-C2-O2
20	W	103	EDO	O1-C1-C2-O2
23	P	311	CHD	C22-C23-C24-O25
26	G	101	CDL	C40-C41-C42-C43
14	P	306	PGV	C9-C10-C11-C12
25	C	304	PEK	C14-C15-C16-C17
21	D	201	TGL	OC1-CC1-CC2-CC3
21	B	301	TGL	CC9-C15-C16-C17
21	N	608	TGL	C16-C15-CC9-CC8
14	P	307	PGV	C9-C10-C11-C12
26	P	308	CDL	C58-C59-C60-C61
21	B	301	TGL	C24-C25-C26-C27
15	A	602[A]	HEA	CAD-CBD-CGD-O2D
15	A	602[B]	HEA	CAD-CBD-CGD-O2D
23	P	301	CHD	C22-C23-C24-O25
14	A	608	PGV	C25-C26-C27-C28
14	A	608	PGV	O03-C19-C20-C21
14	A	608	PGV	C31-C32-C33-C34
21	N	608	TGL	C13-C14-C29-C30
15	A	603	HEA	CAA-CBA-CGA-O2A
15	A	603	HEA	CAD-CBD-CGD-O1D
14	N	609	PGV	O03-C19-C20-C21
21	Q	201	TGL	C12-C13-C14-C29
23	P	311	CHD	C22-C23-C24-O26
14	A	608	PGV	C11-C12-C13-C14
25	P	305	PEK	C14-C15-C16-C17
26	T	101	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
23	W	101	CHD	C13-C17-C20-C22
22	B	302	PSC	C1-C2-C3-C4
21	N	608	TGL	C14-C29-C30-C31
14	N	601	PGV	C9-C10-C11-C12
25	C	305	PEK	C3-C4-C5-C6
21	L	101	TGL	C16-C15-CC9-CC8
26	G	101	CDL	C15-C16-C17-C18
27	M	101	DMU	C28-C31-C34-C37
25	P	303	PEK	C3-C4-C5-C6
15	N	602[A]	HEA	CAD-CBD-CGD-O1D
15	N	602[B]	HEA	CAD-CBD-CGD-O1D
15	N	603	HEA	CAD-CBD-CGD-O2D
21	Y	101	TGL	OG1-CG1-CG2-CG3
15	A	603	HEA	CAA-CBA-CGA-O1A
26	G	101	CDL	C52-C53-C54-C55
14	A	601	PGV	C15-C16-C17-C18
25	P	304	PEK	C14-C15-C16-C17
23	W	101	CHD	C16-C17-C20-C22
26	P	308	CDL	C13-C14-C15-C16
21	N	608	TGL	C21-C22-C23-C24
27	C	310	DMU	C22-C25-C28-C31
27	P	324	DMU	C31-C34-C37-C40
21	Y	101	TGL	C10-C11-C12-C13
20	B	313	EDO	O1-C1-C2-O2
20	N	616	EDO	O1-C1-C2-O2
20	T	103	EDO	O1-C1-C2-O2
20	W	104	EDO	O1-C1-C2-O2
21	N	608	TGL	OG2-CG2-CG3-OG3
14	C	306	PGV	C11-C12-C13-C14
22	O	301	PSC	C7-C8-C9-C10
25	P	305	PEK	C3-C4-C5-C6
21	Q	201	TGL	CB3-CB4-CB5-CB6
21	D	201	TGL	CB5-CB6-CB7-CB8
15	N	603	HEA	CAD-CBD-CGD-O1D
26	T	101	CDL	C57-C58-C59-C60
22	O	301	PSC	C12-C13-C14-C15
25	C	305	PEK	C14-C15-C16-C17
27	M	101	DMU	O16-C18-C19-C22
14	C	306	PGV	C9-C10-C11-C12
14	P	307	PGV	C11-C12-C13-C14
14	C	307	PGV	C1-C2-C3-C4
26	C	308	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
27	G	108	DMU	C4-C3-O7-C10
25	C	303	PEK	O03-C21-C22-C23
26	C	308	CDL	C35-C36-C37-C38
14	N	601	PGV	O03-C19-C20-C21
26	P	308	CDL	C52-C51-CB5-OB6
26	T	101	CDL	C32-C31-CA7-OA8
23	J	101	CHD	C20-C22-C23-C24
22	B	302	PSC	C22-C23-C24-C25
20	A	626	EDO	O1-C1-C2-O2
20	L	104	EDO	O1-C1-C2-O2
20	N	622	EDO	O1-C1-C2-O2
20	N	628	EDO	O1-C1-C2-O2
14	A	608	PGV	C26-C27-C28-C29
14	P	307	PGV	C28-C29-C30-C31
26	C	308	CDL	C52-C51-CB5-OB6
14	P	306	PGV	C27-C28-C29-C30
14	P	306	PGV	C05-C04-O12-P
15	N	602[A]	HEA	CAD-CBD-CGD-O2D
15	N	602[B]	HEA	CAD-CBD-CGD-O2D
25	C	305	PEK	C23-C24-C25-C26
15	A	602[A]	HEA	C18-C19-C20-C21
27	Z	102	DMU	C22-C25-C28-C31
26	C	308	CDL	C55-C56-C57-C58
26	P	308	CDL	C52-C51-CB5-OB7
15	A	602[A]	HEA	CAA-CBA-CGA-O2A
15	A	602[B]	HEA	CAA-CBA-CGA-O2A
25	C	304	PEK	C22-C23-C24-C25
21	D	201	TGL	OC1-CC1-OG3-CG3
26	P	308	CDL	C61-C62-C63-C64
14	A	601	PGV	O03-C19-C20-C21
21	Q	201	TGL	OG3-CC1-CC2-CC3
21	Q	201	TGL	CA4-CA5-CA6-CA7
15	N	603	HEA	C26-C15-C16-C17
14	C	306	PGV	C05-C04-O12-P
25	C	303	PEK	C02-C03-O11-P
26	T	101	CDL	C52-C51-CB5-OB6
26	T	101	CDL	C31-C32-C33-C34
23	P	301	CHD	C16-C17-C20-C22
26	T	101	CDL	C32-C31-CA7-OA9
14	N	601	PGV	C11-C10-C9-C8
25	C	303	PEK	O04-C21-C22-C23
26	C	308	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
20	J	103	EDO	O1-C1-C2-O2
20	P	322	EDO	O1-C1-C2-O2
21	B	301	TGL	C10-C11-C12-C13
14	N	601	PGV	O01-C1-C2-C3
15	N	602[A]	HEA	CAA-CBA-CGA-O1A
15	N	602[B]	HEA	CAA-CBA-CGA-O1A
14	N	601	PGV	O04-C19-C20-C21

There are no ring outliers.

90 monomers are involved in 269 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	M	104	EDO	2	0
23	G	102	CHD	1	0
26	G	101	CDL	18	0
20	B	309	EDO	2	0
27	V	102	DMU	4	0
26	P	308	CDL	20	0
20	A	623	EDO	1	0
20	D	202	EDO	1	0
20	A	624	EDO	1	0
21	B	301	TGL	4	0
20	H	102	EDO	1	0
20	N	623	EDO	1	0
14	N	609	PGV	1	0
27	Z	102	DMU	1	0
20	C	317	EDO	2	0
20	C	316	EDO	1	0
20	P	320	EDO	1	0
21	Y	101	TGL	11	0
20	J	103	EDO	1	0
23	Y	104	CHD	4	0
20	D	206	EDO	0	2
20	N	612	EDO	5	0
20	D	205	EDO	1	0
20	B	311	EDO	1	0
20	A	620	EDO	1	0
20	H	103	EDO	4	0
20	F	103	EDO	1	0
20	B	314	EDO	0	2
20	D	207	EDO	1	0
21	L	101	TGL	11	0

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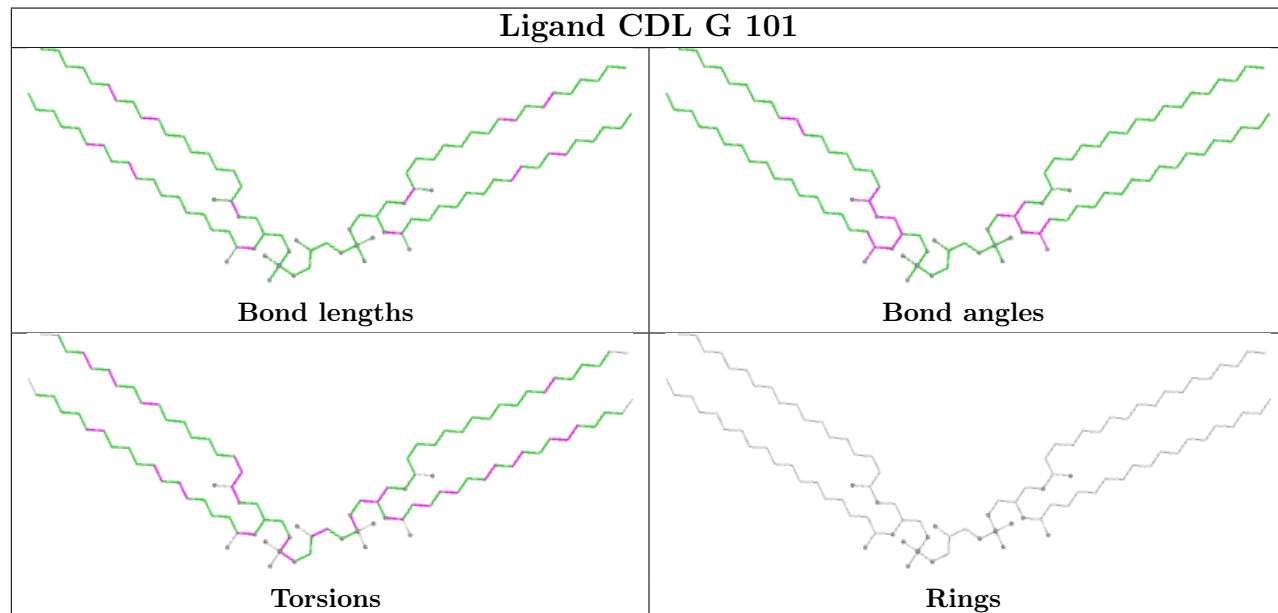
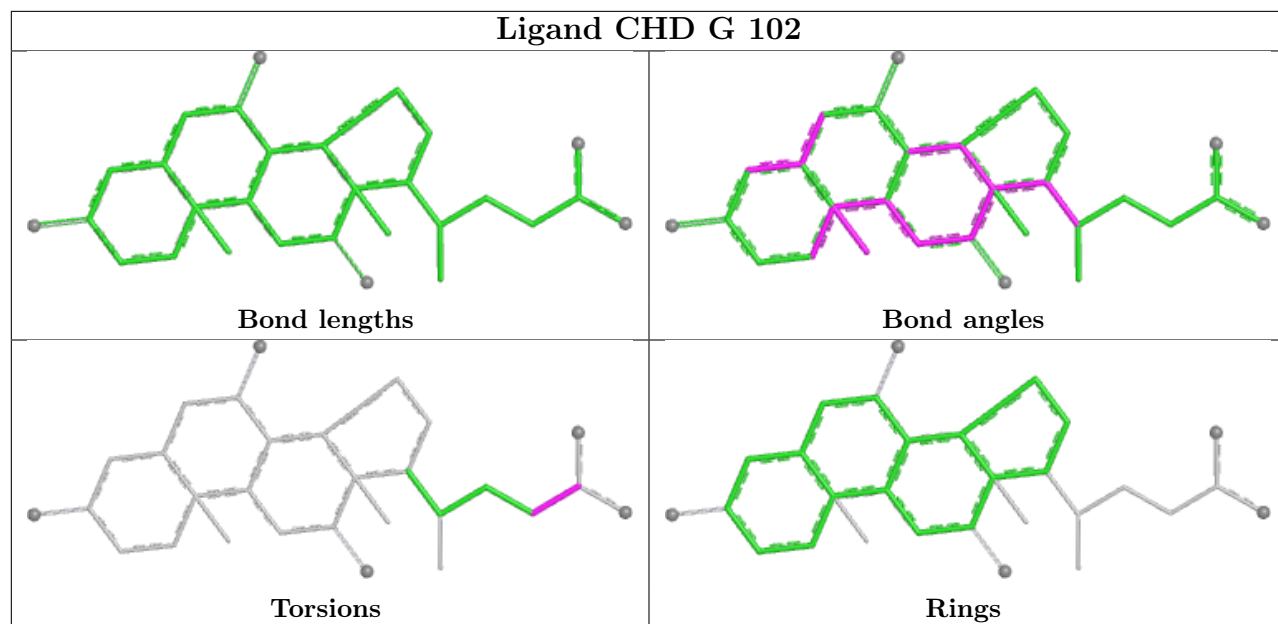
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	309	CHD	1	0
25	C	303	PEK	3	0
21	Q	201	TGL	7	0
20	B	310	EDO	3	0
20	N	619	EDO	1	0
14	N	601	PGV	3	0
14	P	306	PGV	5	0
20	A	619	EDO	1	0
14	C	307	PGV	2	0
27	P	323	DMU	1	0
23	P	310	CHD	7	0
20	O	306	EDO	2	0
14	A	601	PGV	3	0
20	N	630	EDO	3	0
20	K	102	EDO	2	0
15	A	603	HEA	2	0
22	B	302	PSC	10	0
25	P	303	PEK	3	0
27	C	319	DMU	1	0
20	M	103	EDO	1	0
20	S	103	EDO	1	0
26	T	101	CDL	11	0
14	C	306	PGV	2	0
27	G	108	DMU	1	0
20	P	314	EDO	1	0
20	B	308	EDO	1	0
21	D	201	TGL	9	0
20	J	102	EDO	1	0
15	N	602[A]	HEA	2	0
27	P	309	DMU	3	0
23	J	101	CHD	3	0
20	S	107	EDO	2	0
26	C	308	CDL	13	0
27	C	310	DMU	2	0
25	C	304	PEK	1	0
27	P	324	DMU	4	0
23	P	311	CHD	2	0
23	C	311	CHD	2	0
20	G	104	EDO	2	0
25	P	305	PEK	9	0
20	G	107	EDO	1	0
20	A	627	EDO	1	0

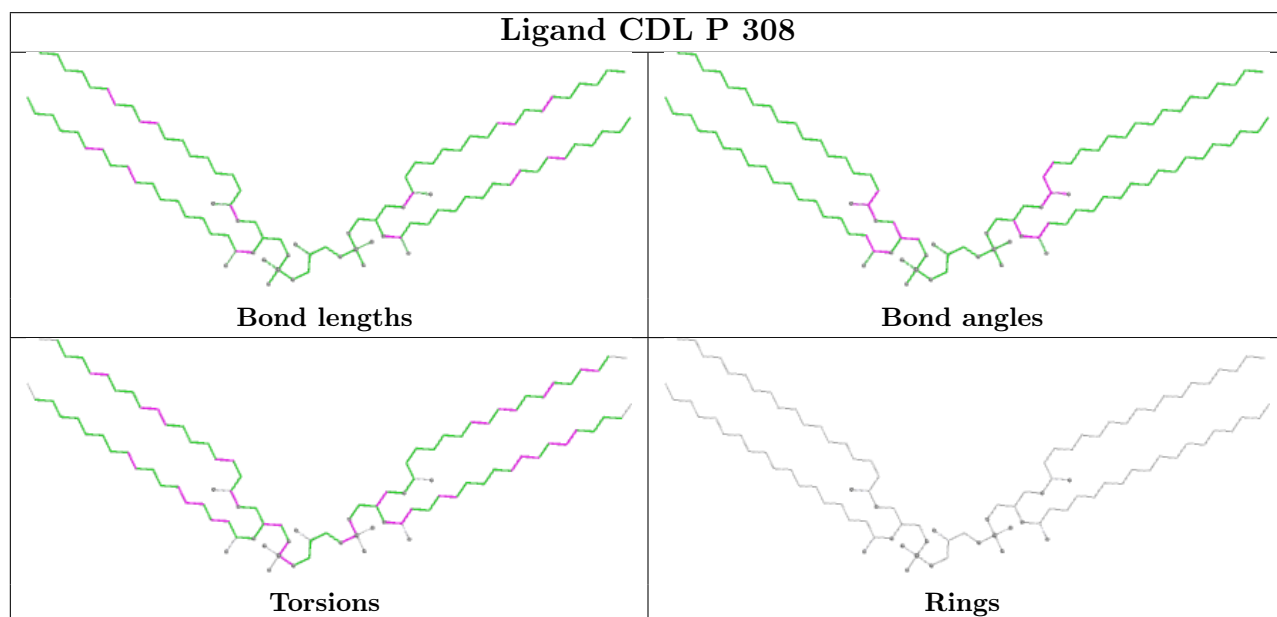
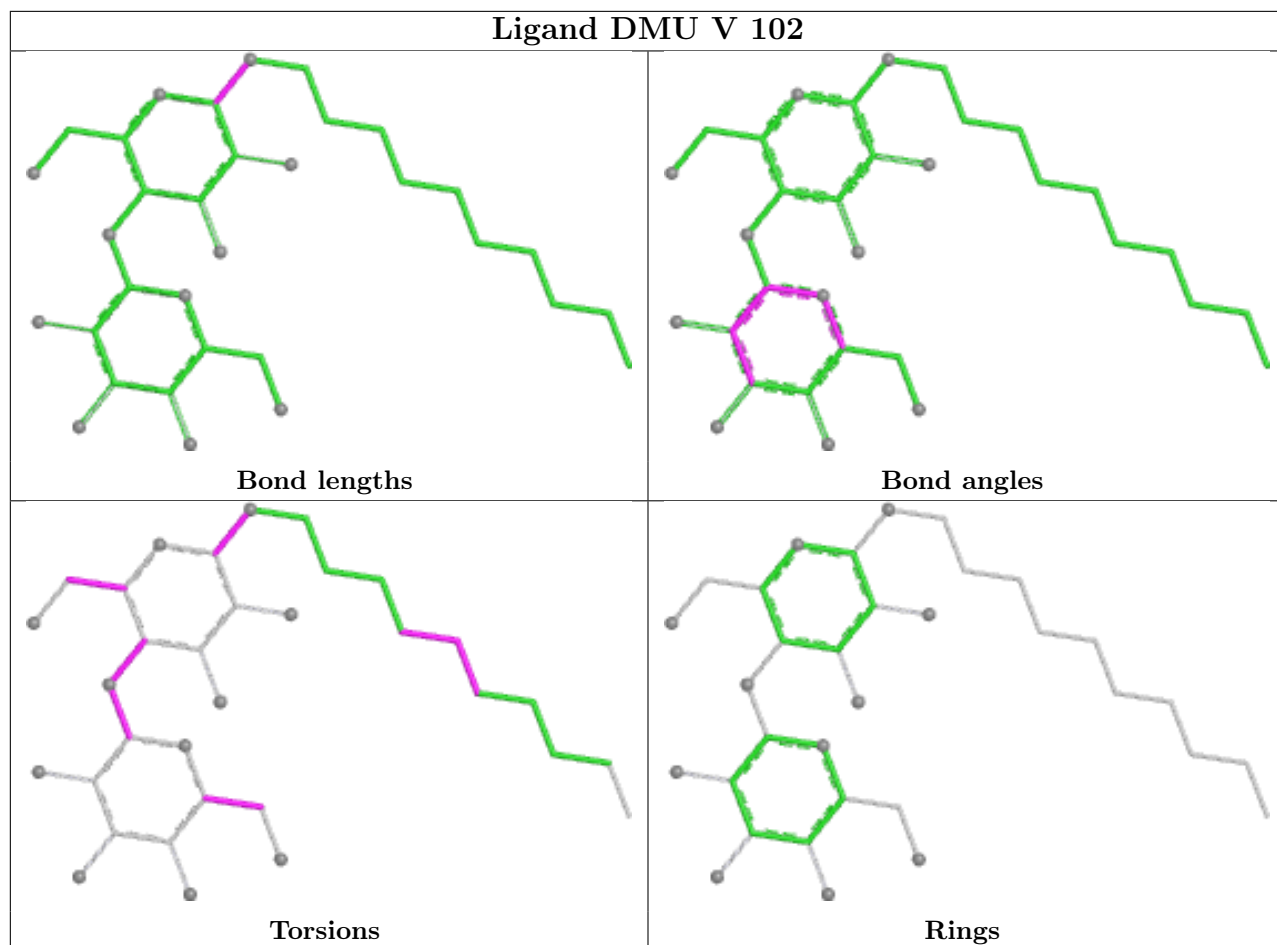
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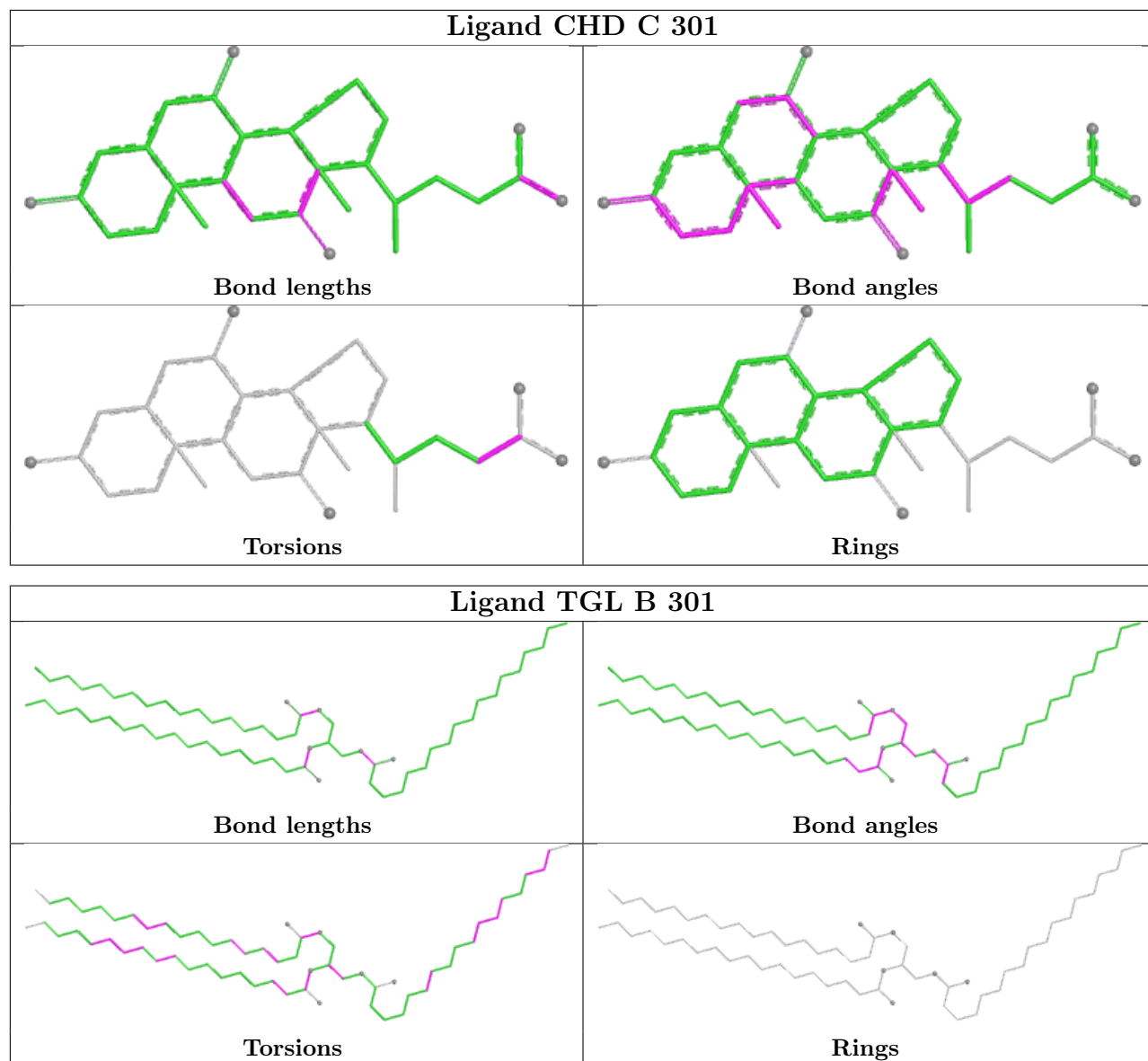
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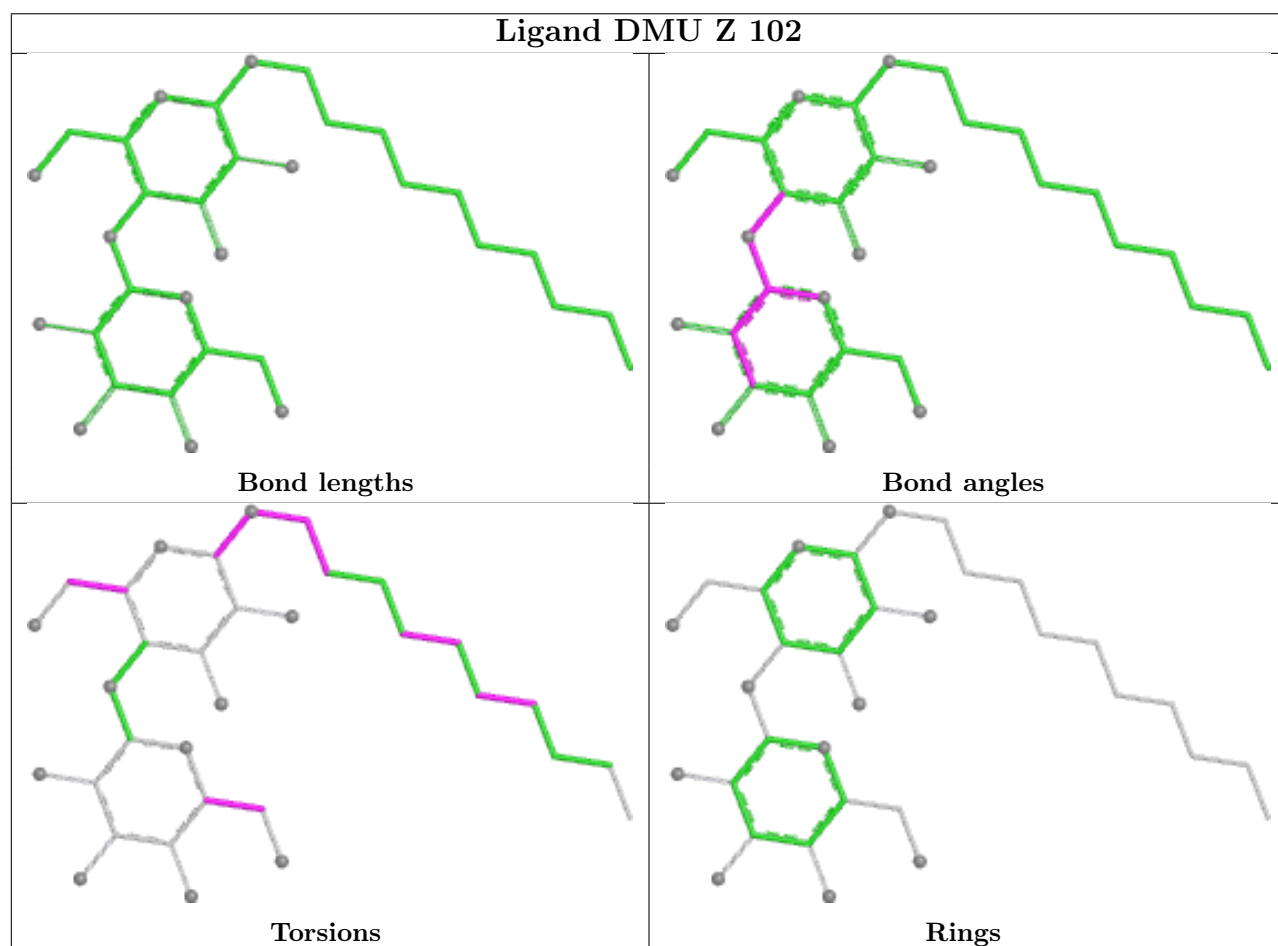
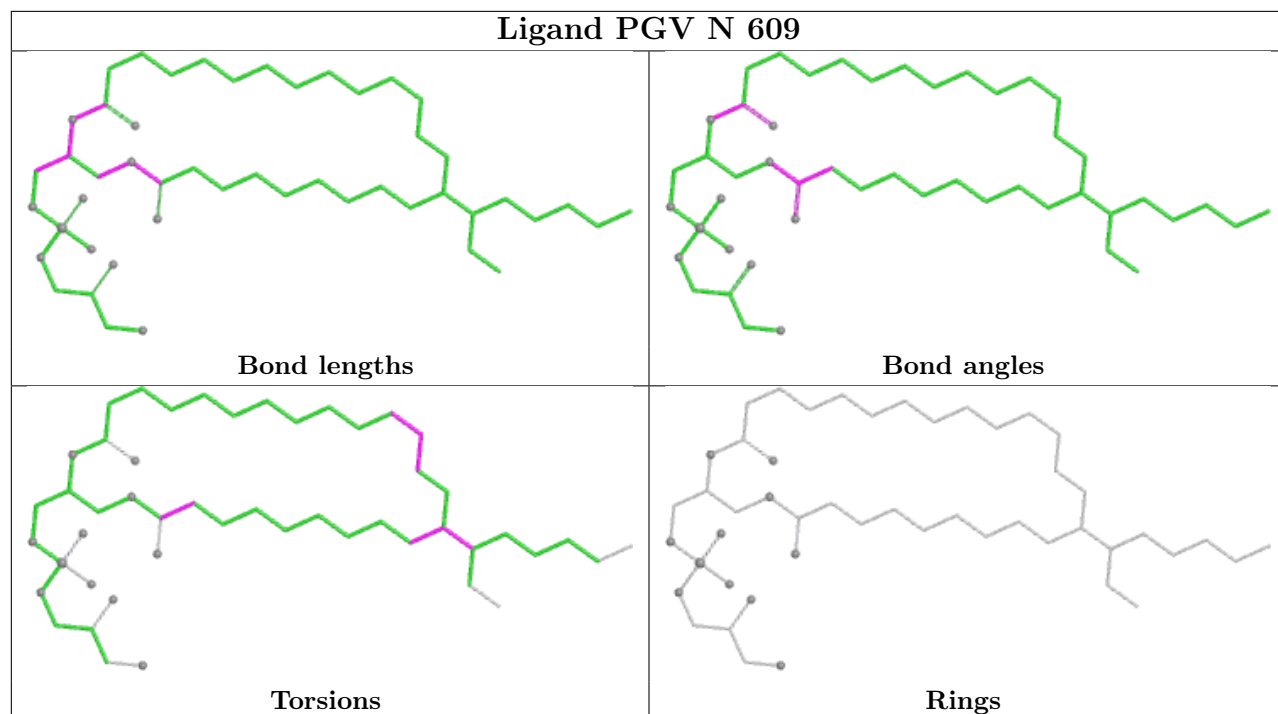
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	G	103	EDO	1	0
15	N	603	HEA	1	0
20	A	609	EDO	3	0
20	U	101	EDO	1	0
15	A	602[A]	HEA	3	0
22	O	301	PSC	5	0
20	N	618	EDO	3	0
20	A	614	EDO	1	0
20	R	203	EDO	1	0
20	B	312	EDO	3	0
25	P	304	PEK	3	0
20	W	104	EDO	2	0
23	W	101	CHD	3	0
25	C	305	PEK	4	0
20	P	315	EDO	1	0
21	N	608	TGL	2	0
20	P	319	EDO	2	0
14	P	307	PGV	3	0

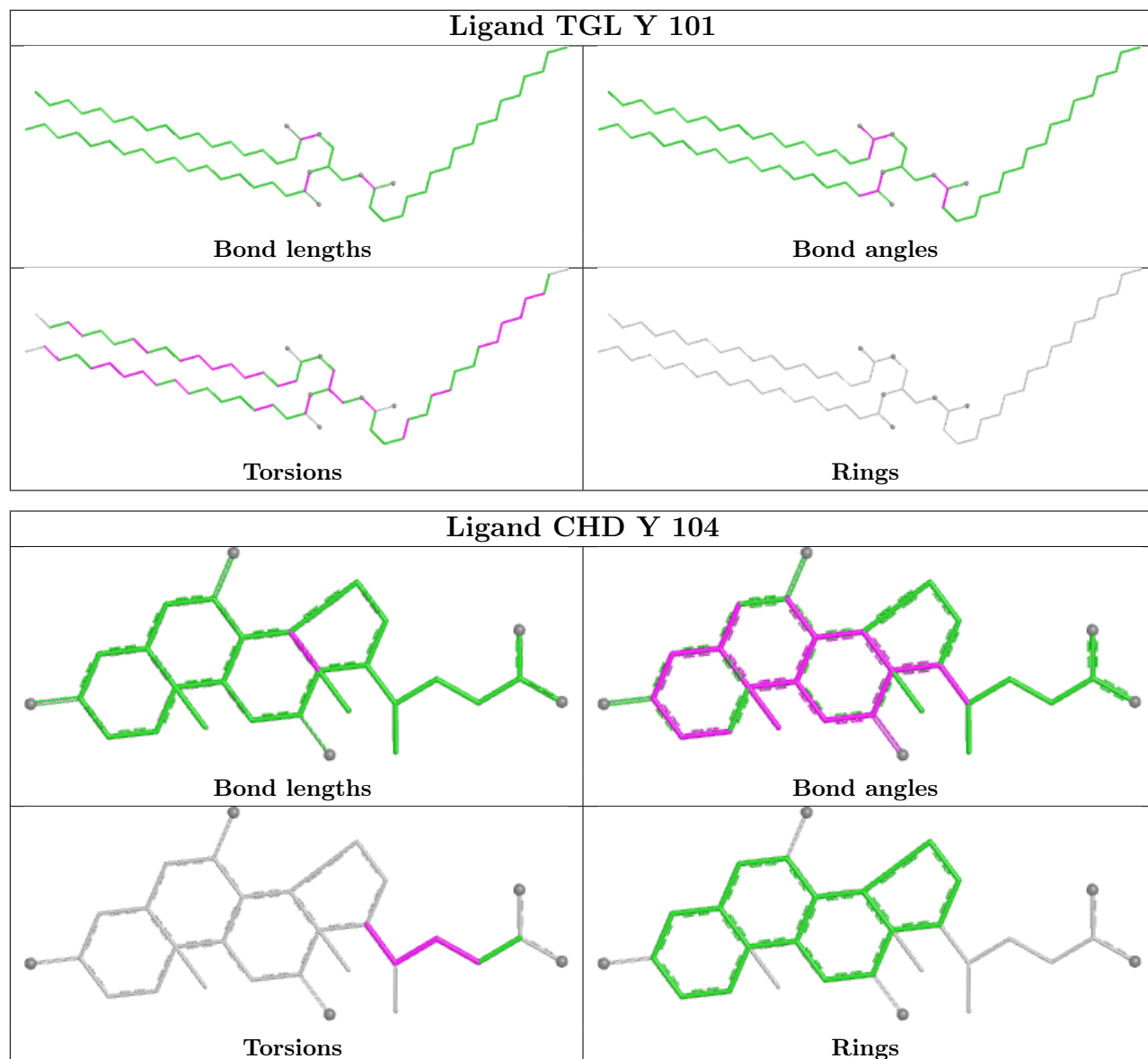
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

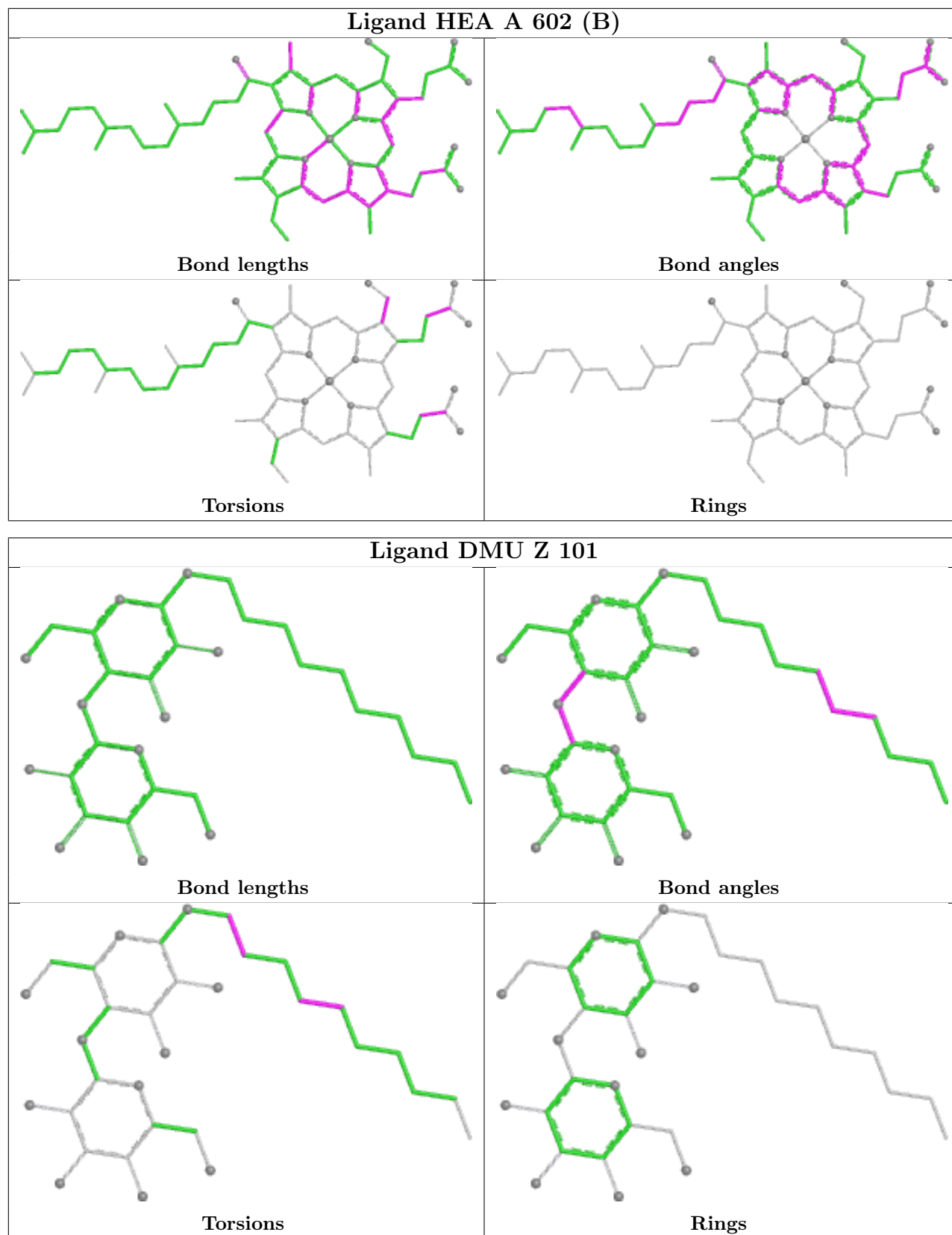


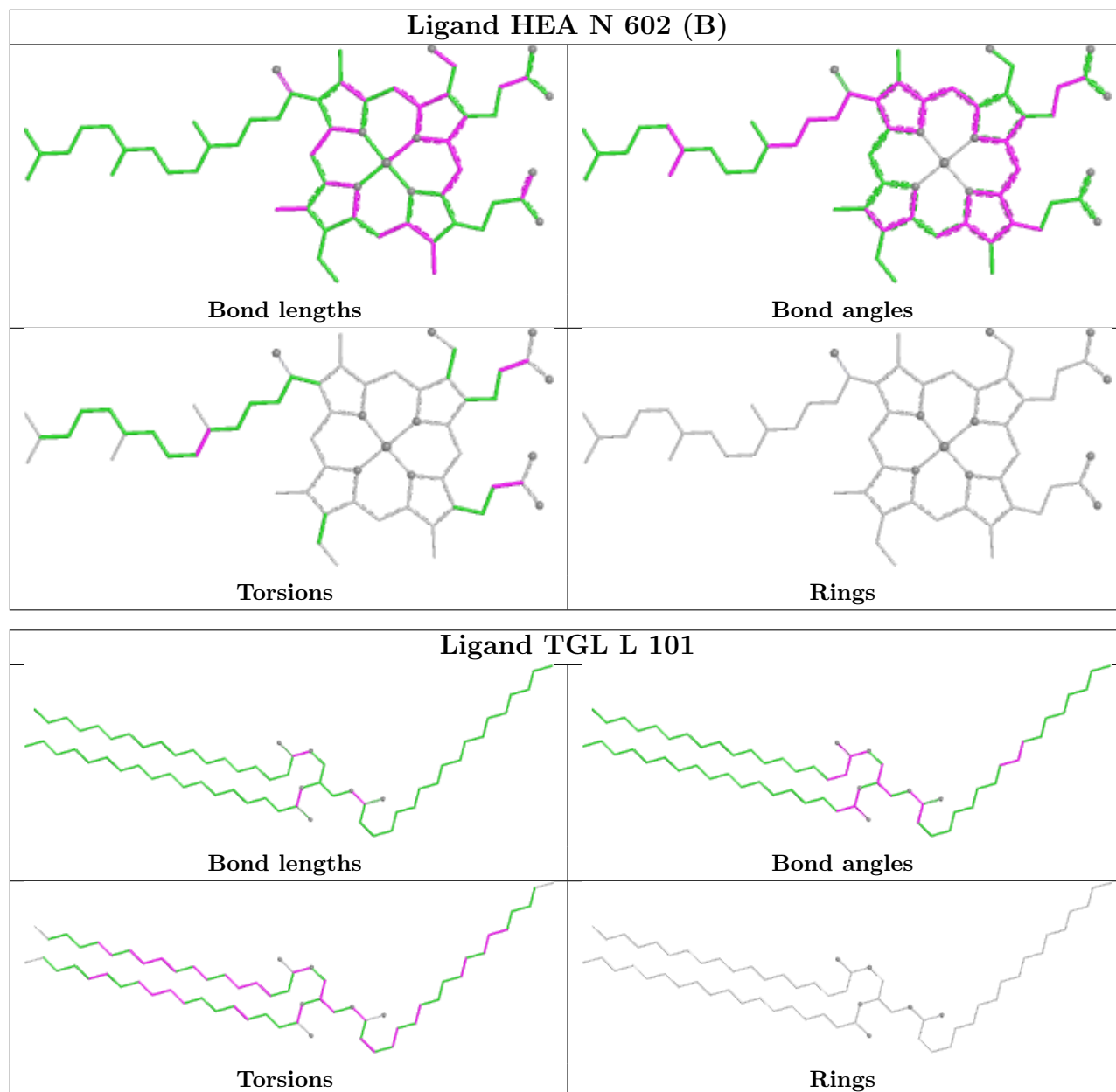


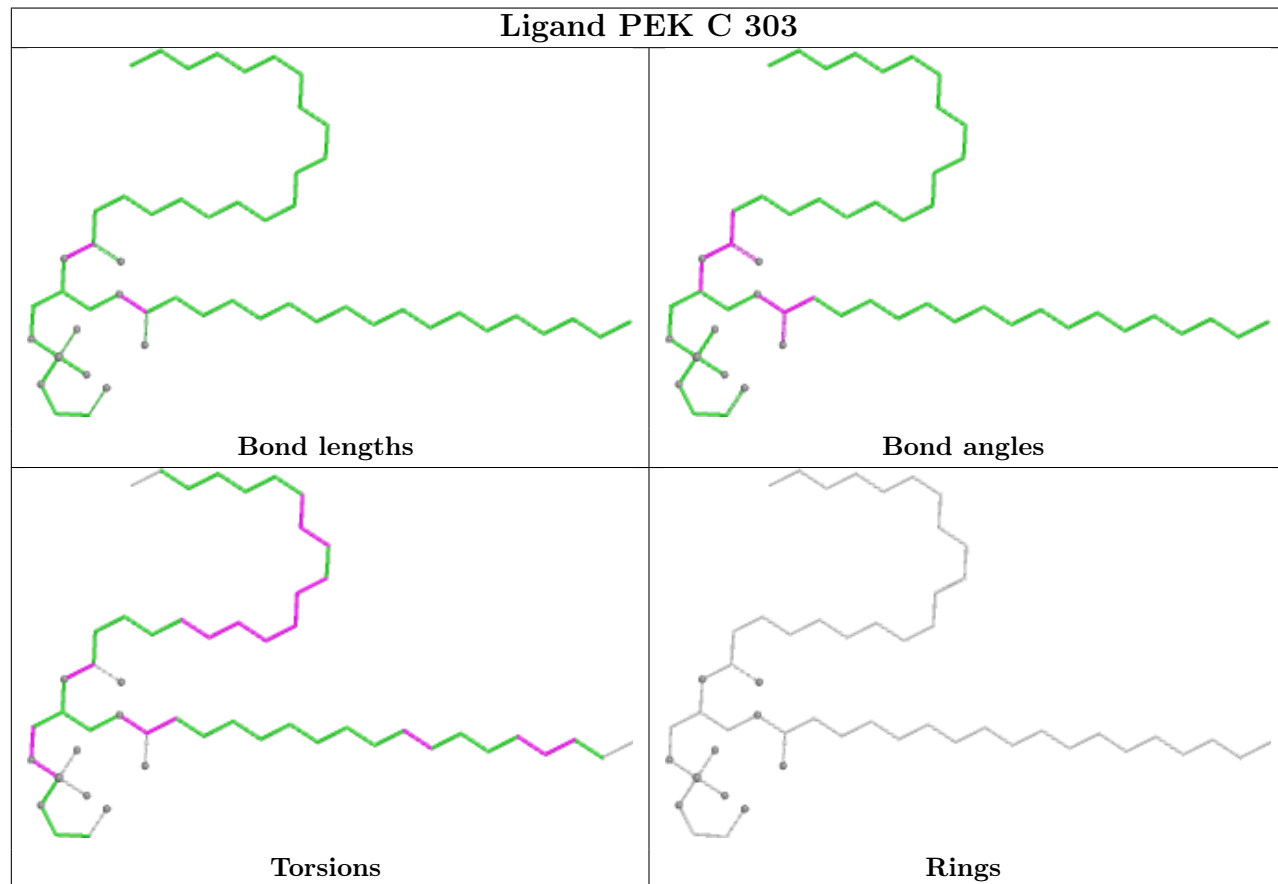
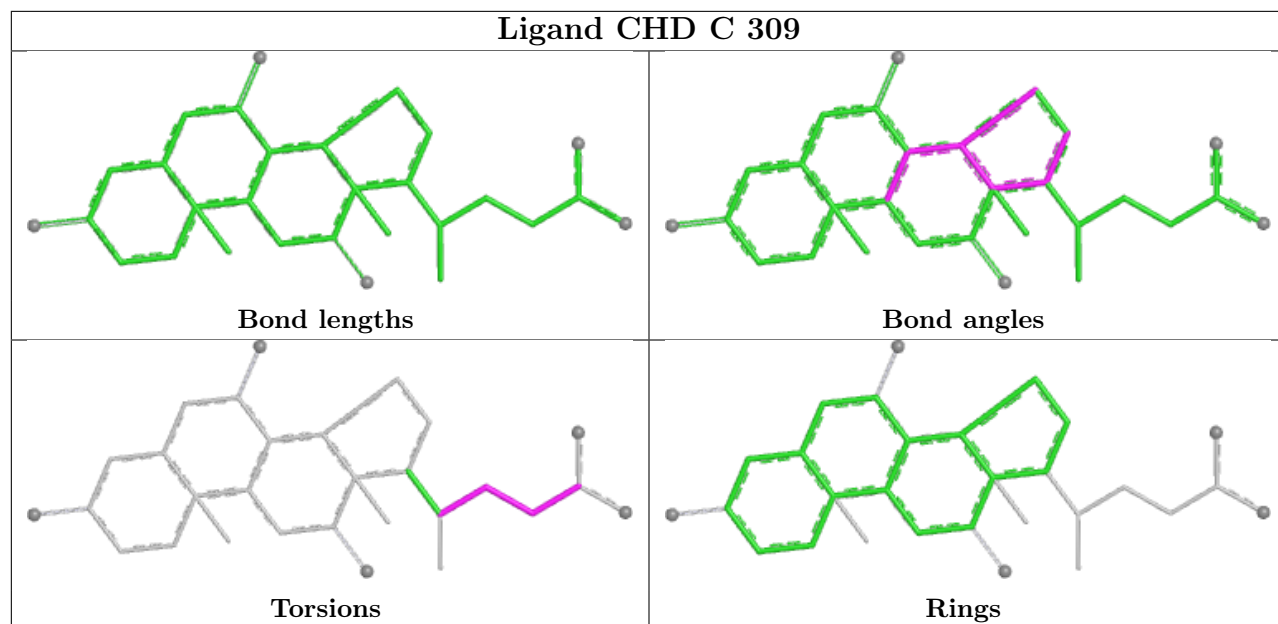


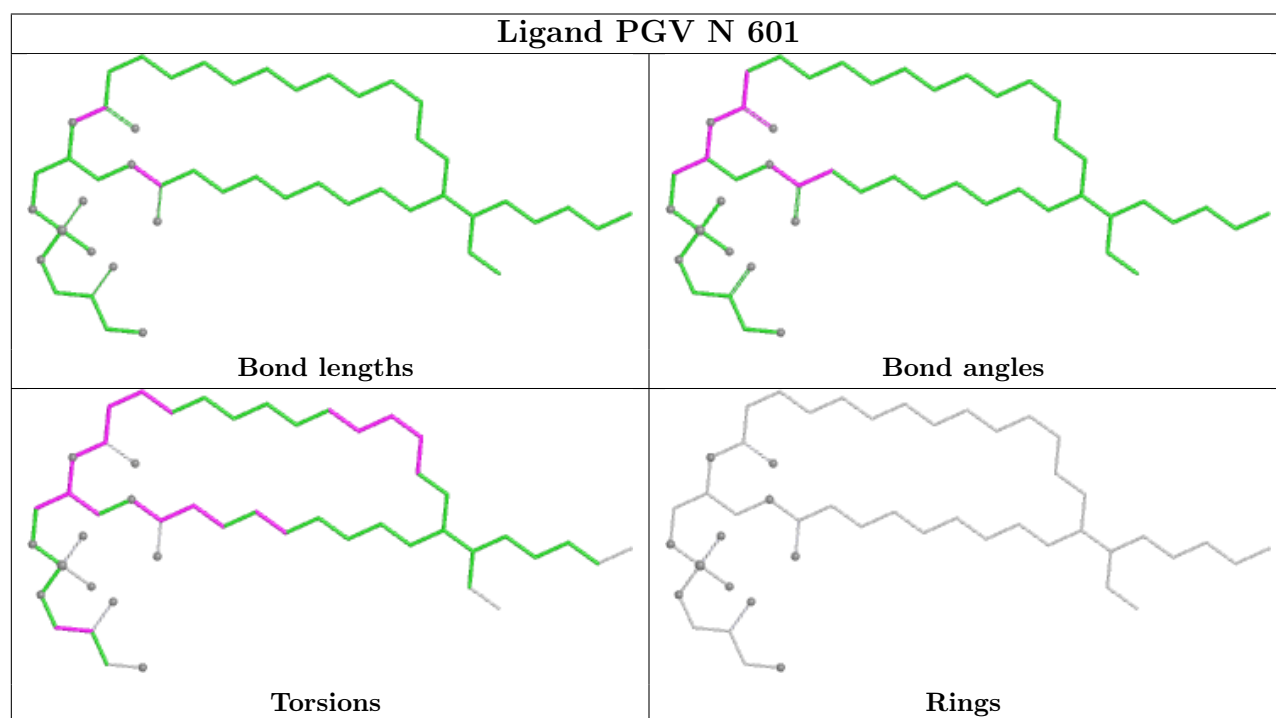
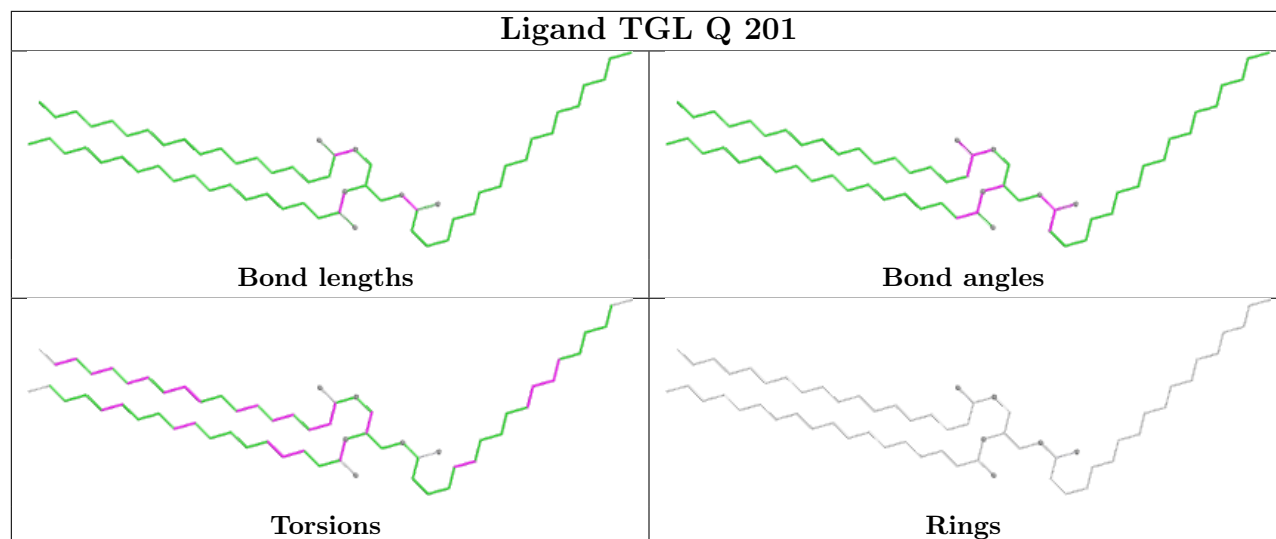


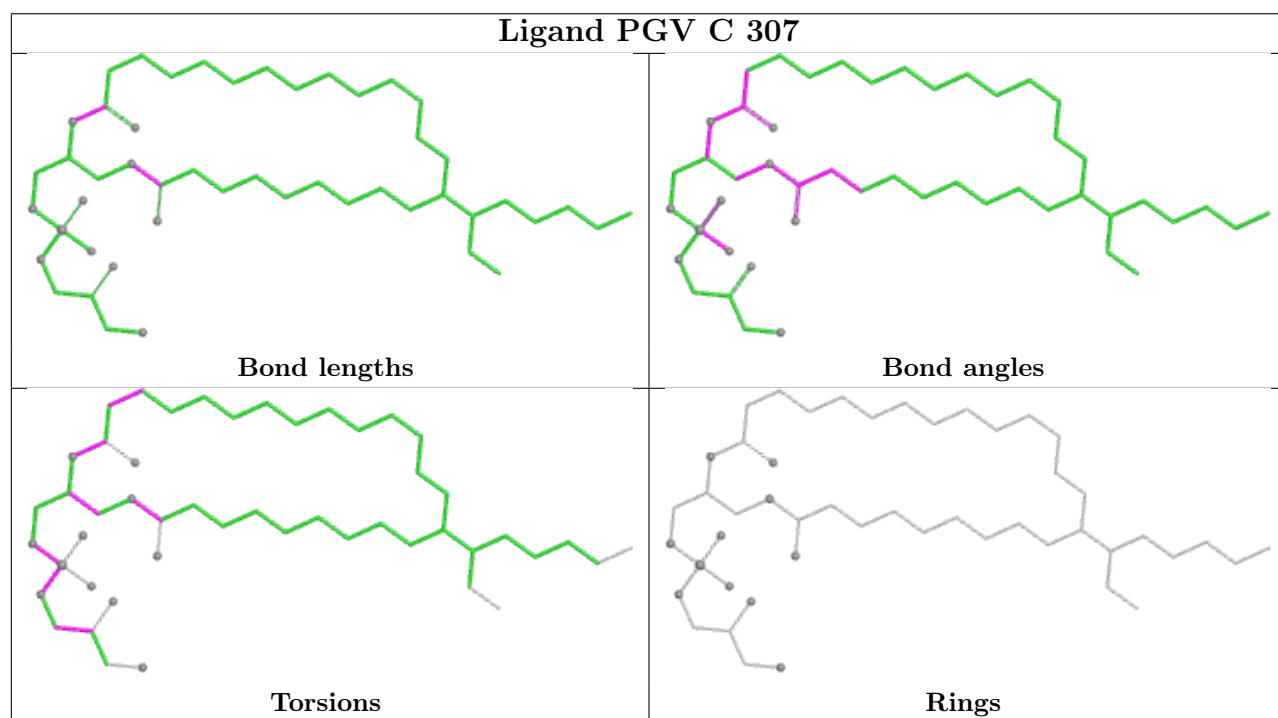
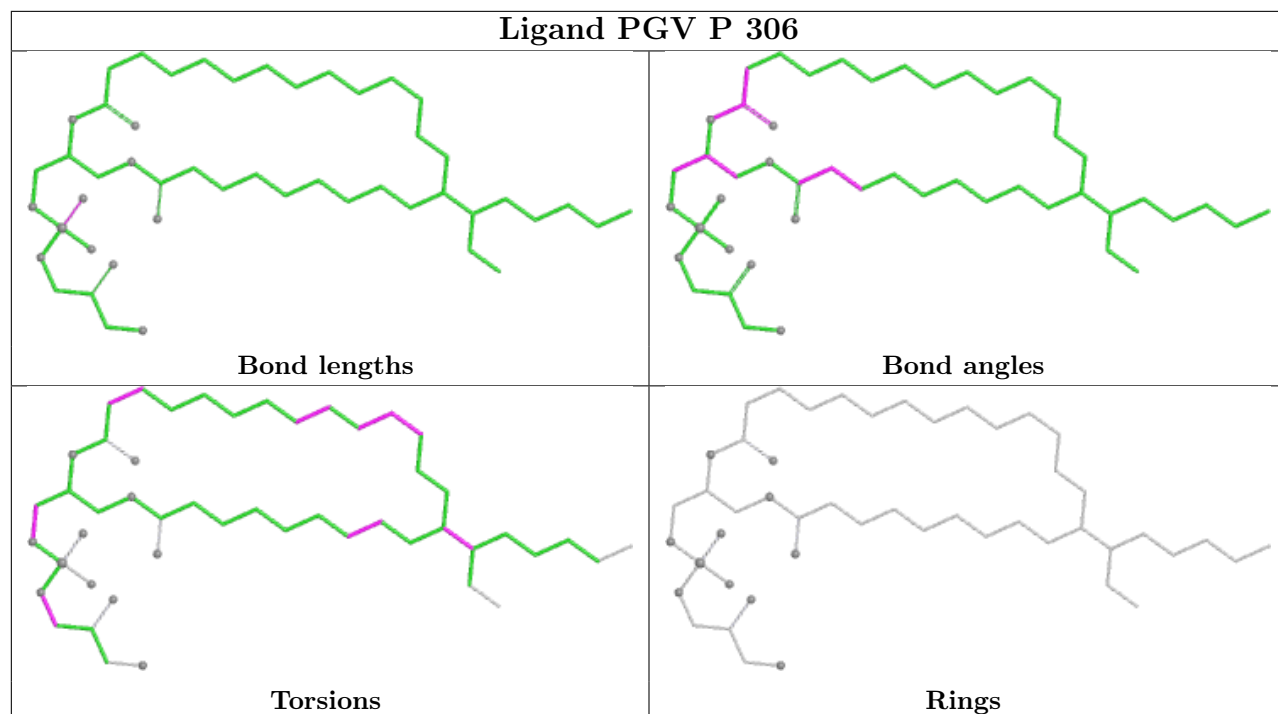


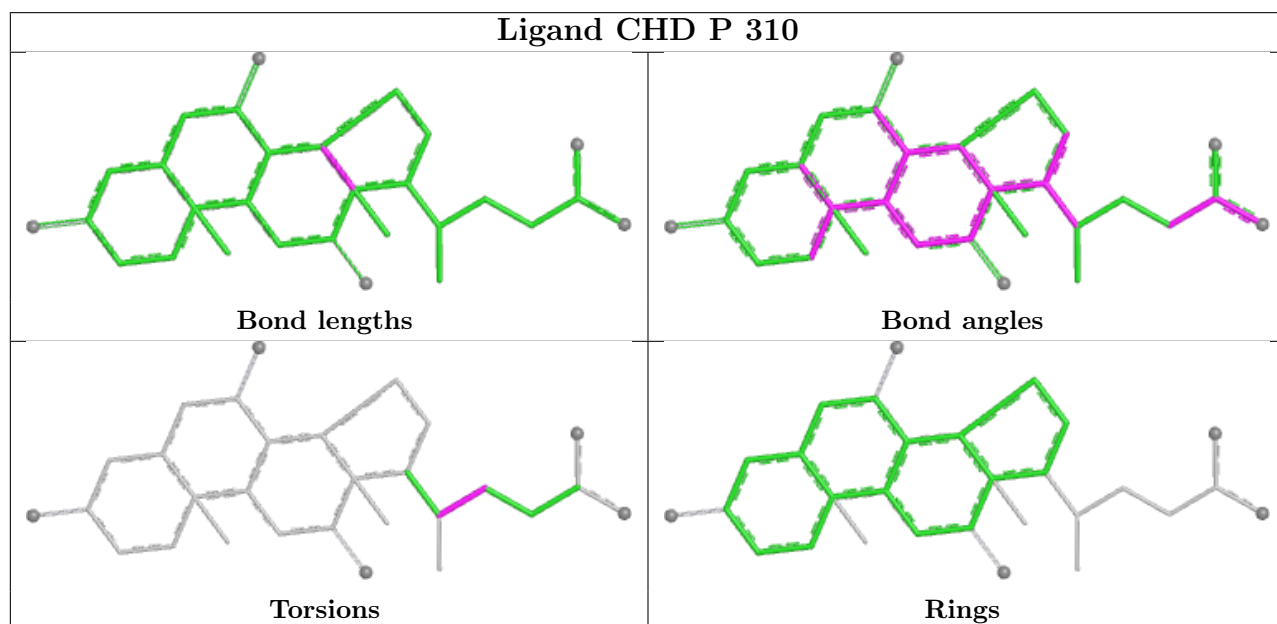
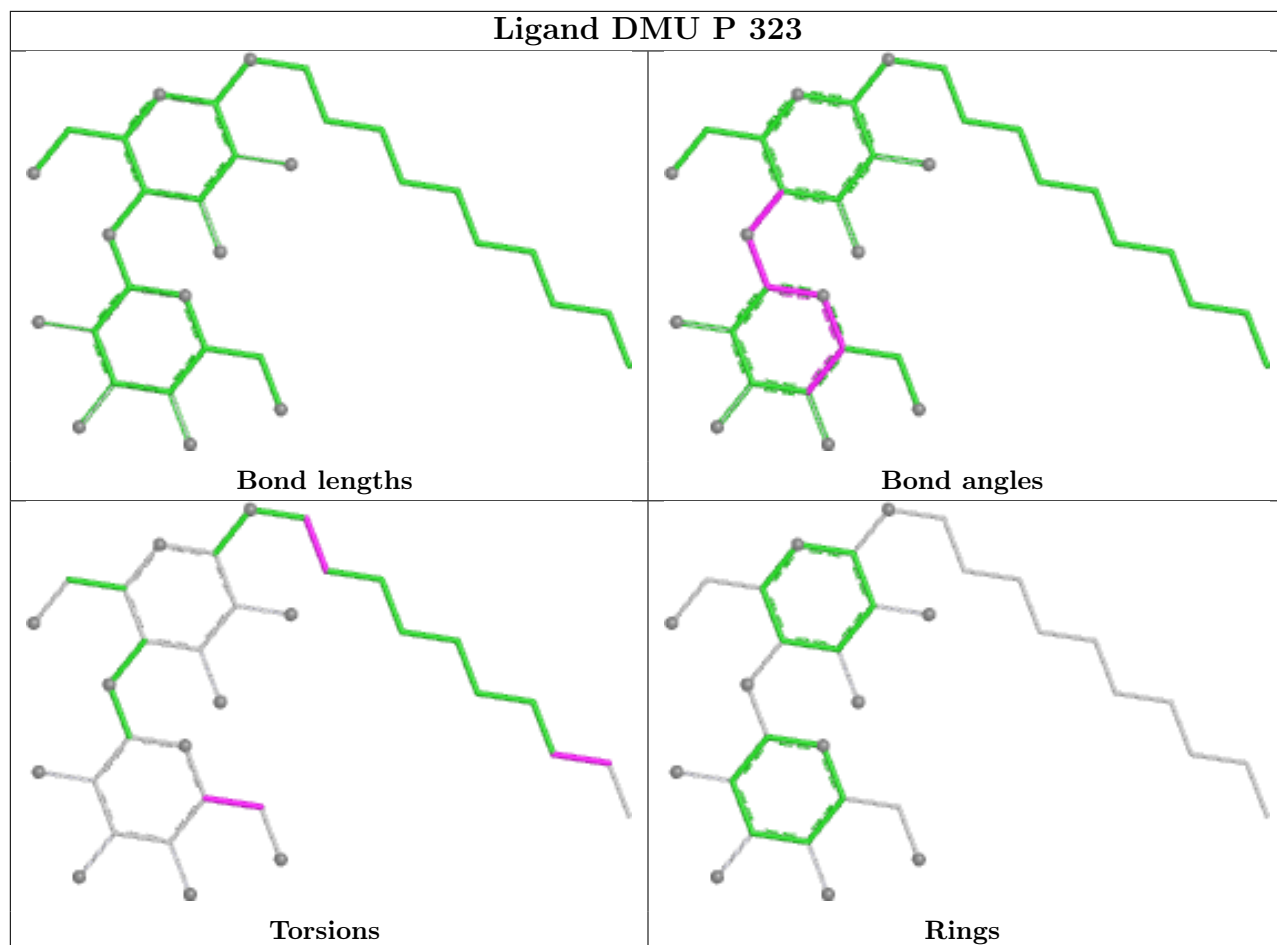


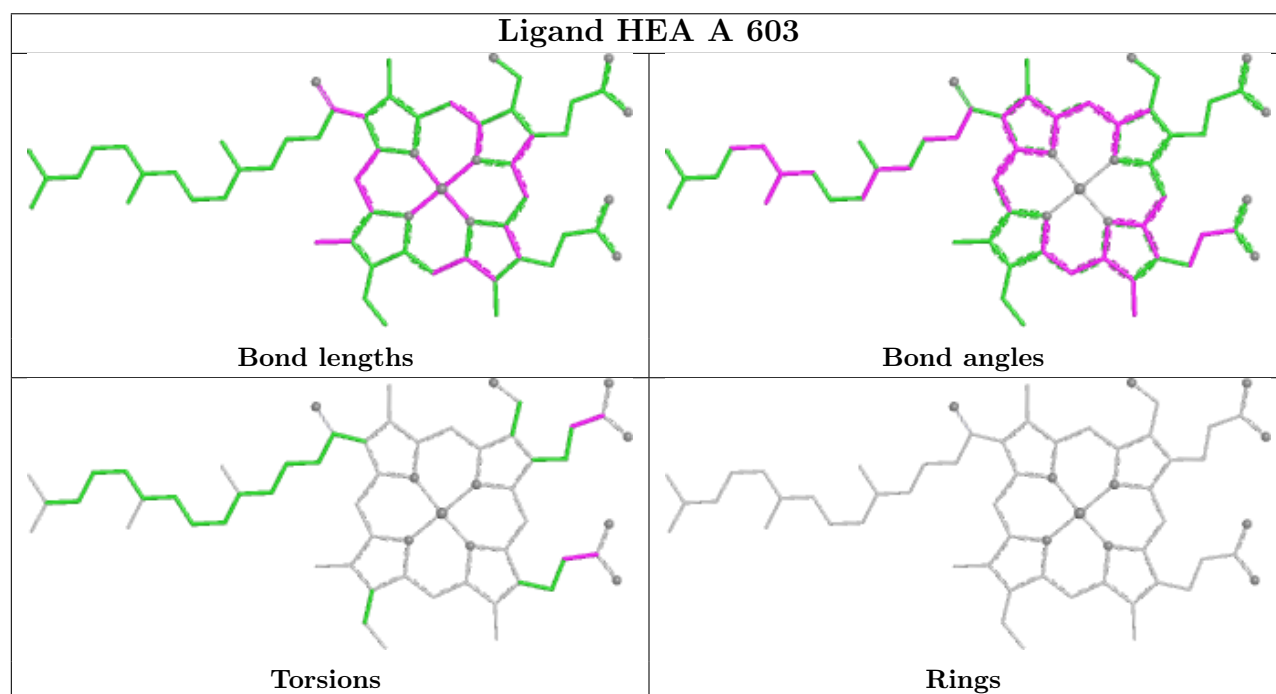
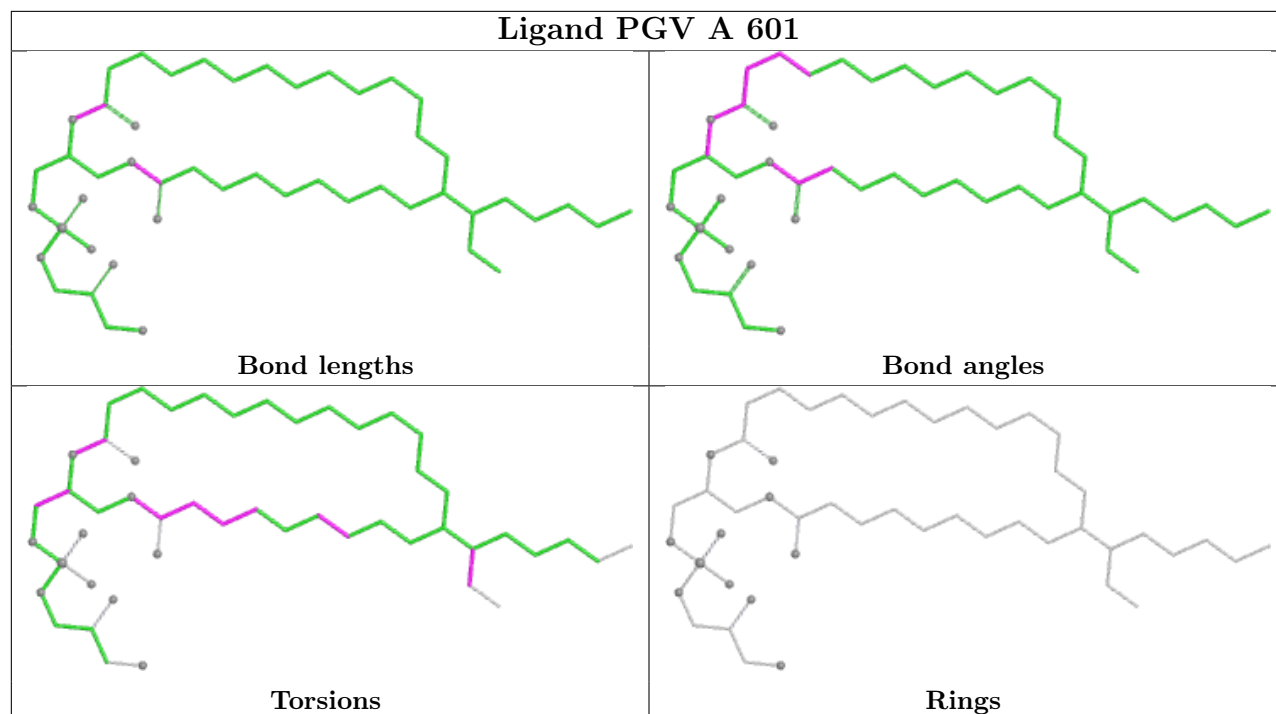


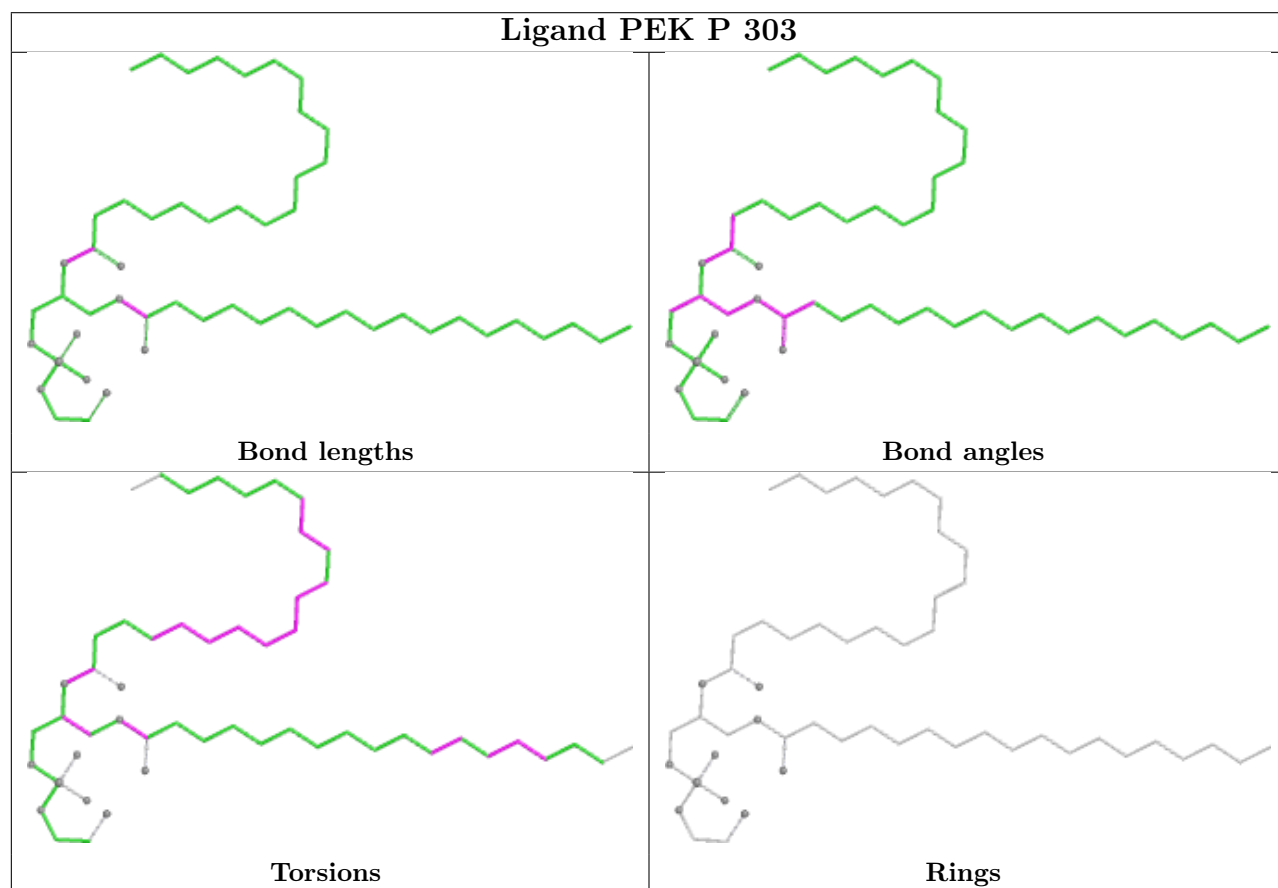
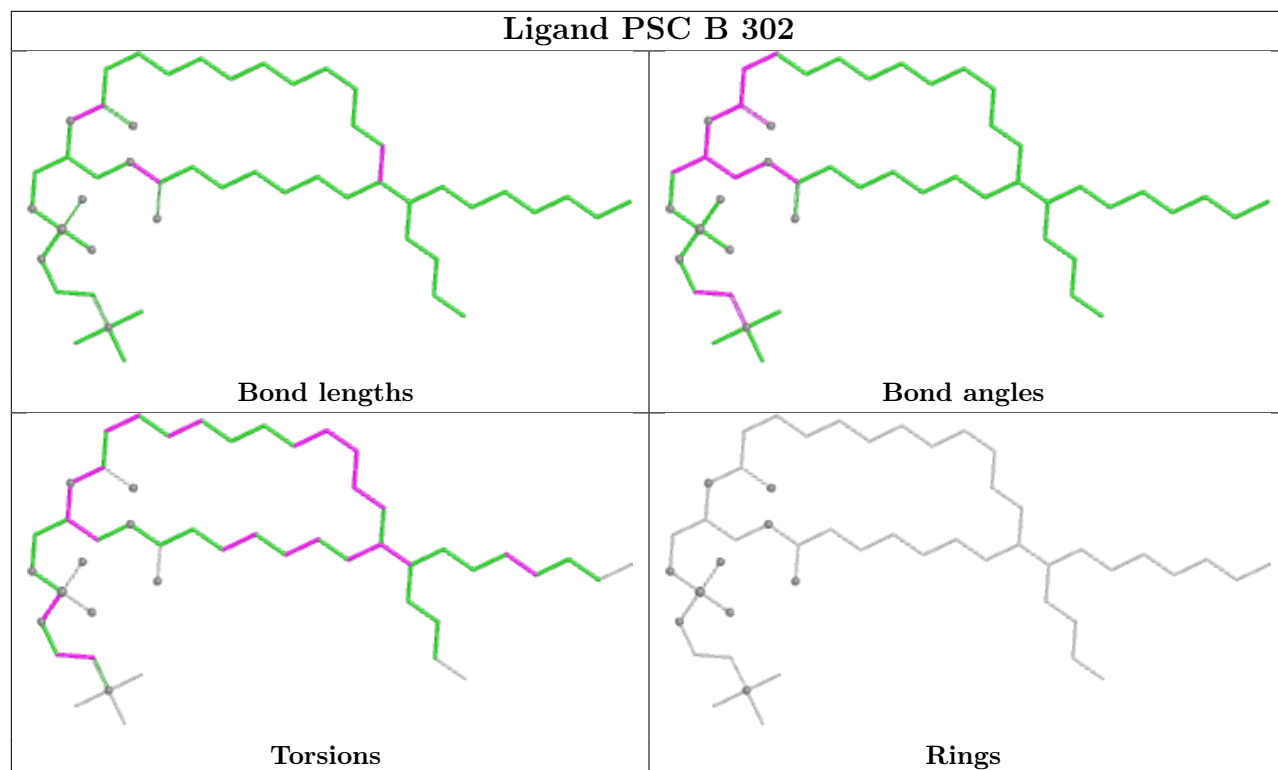


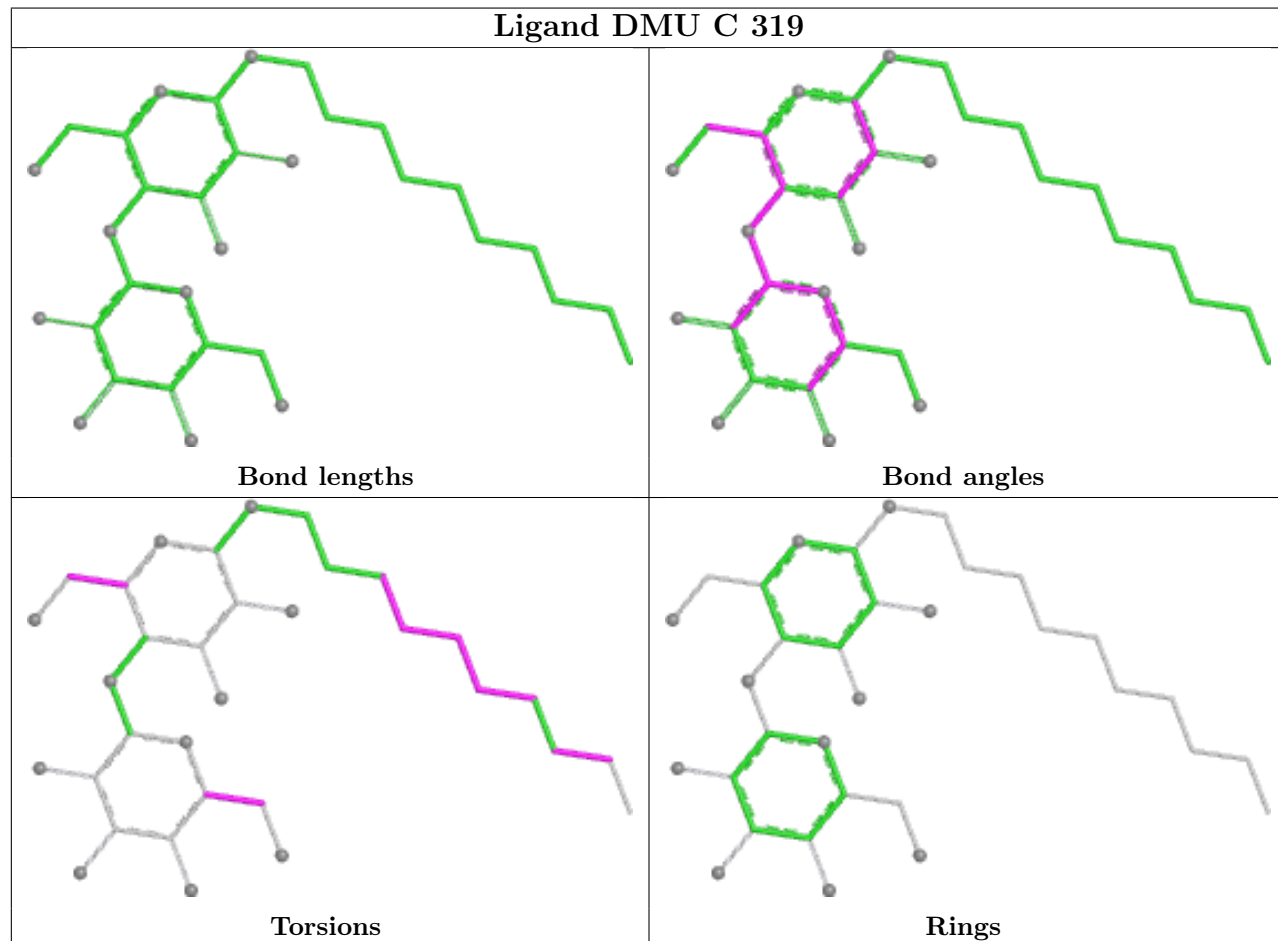
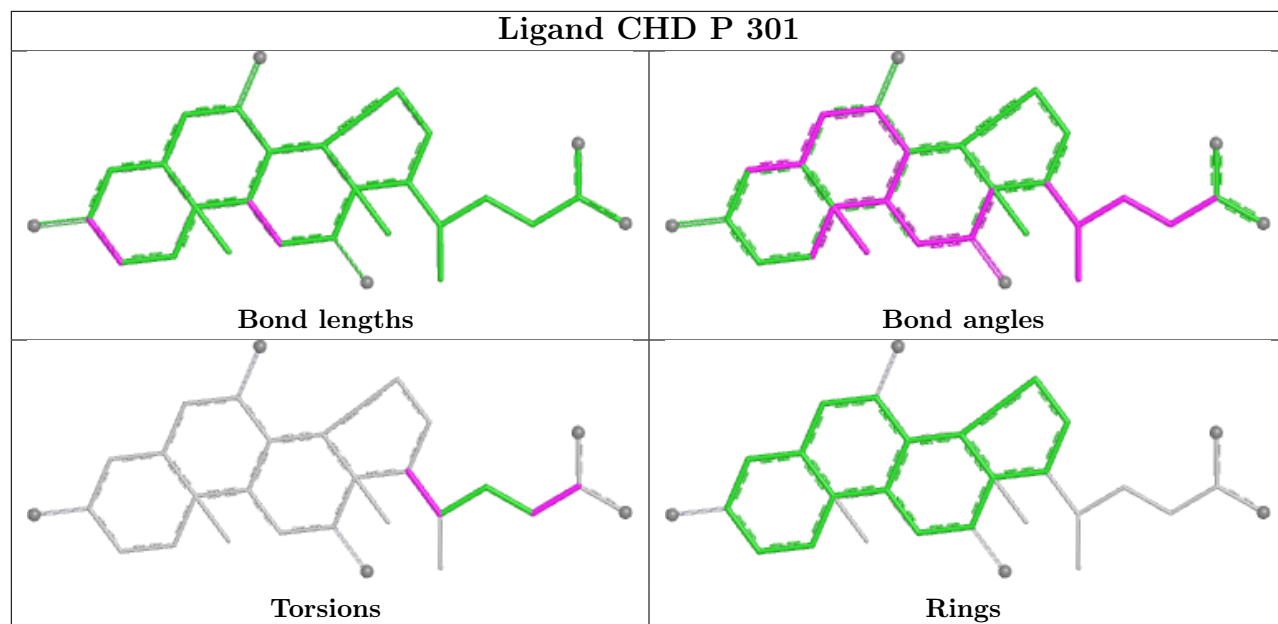


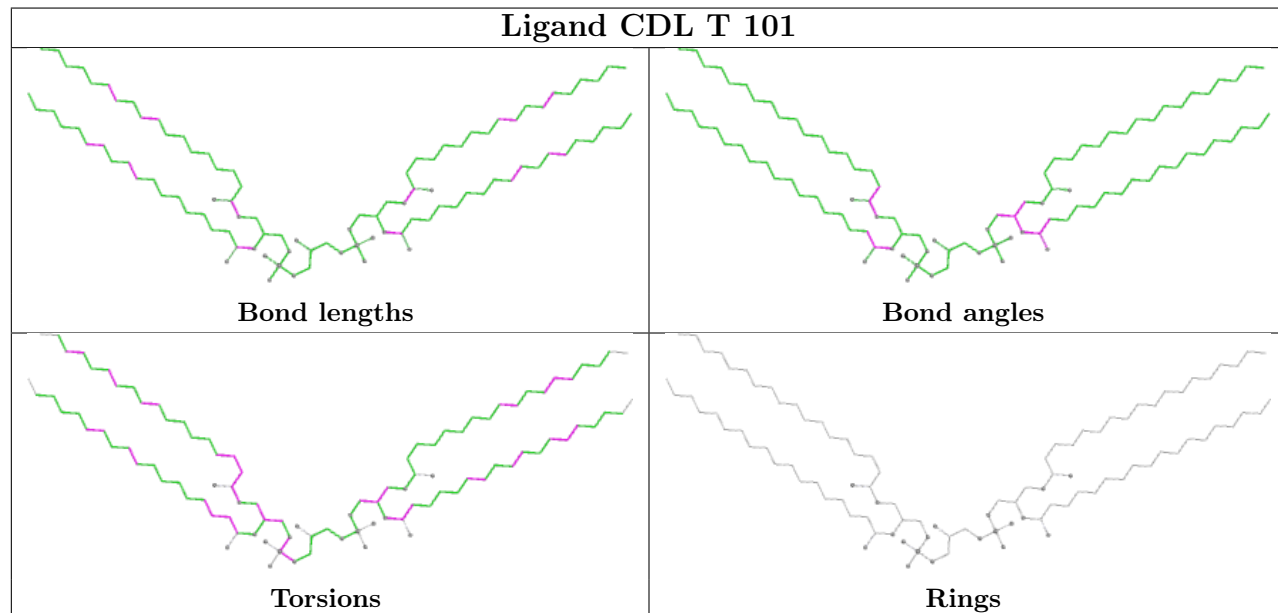
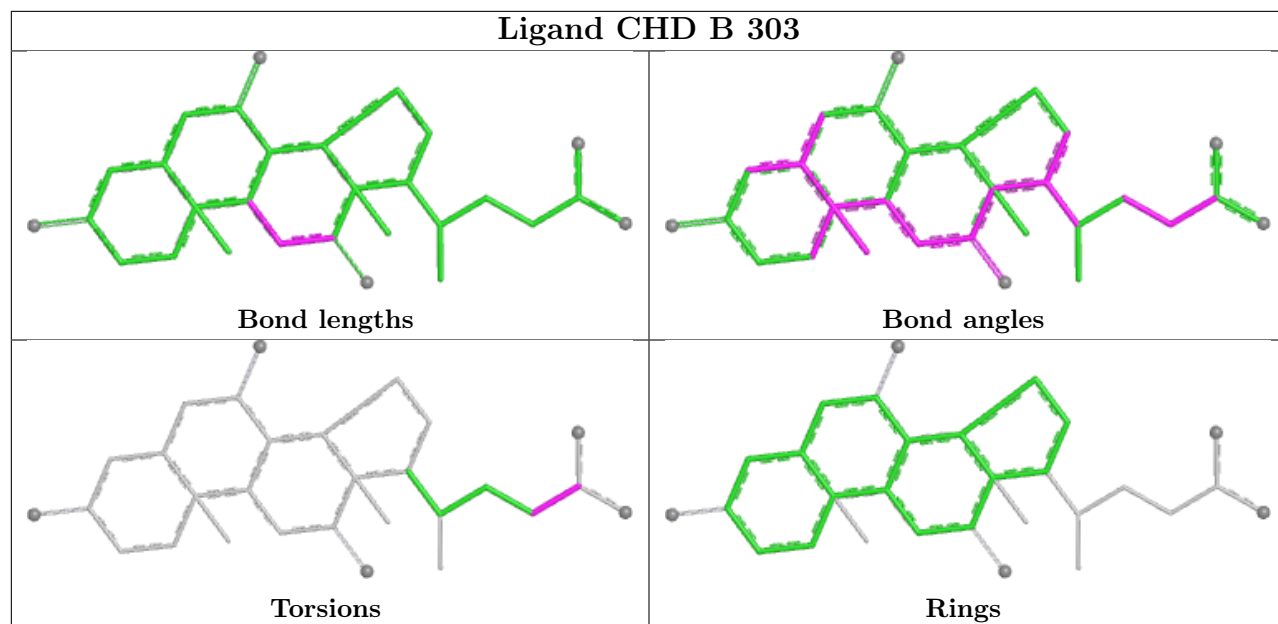


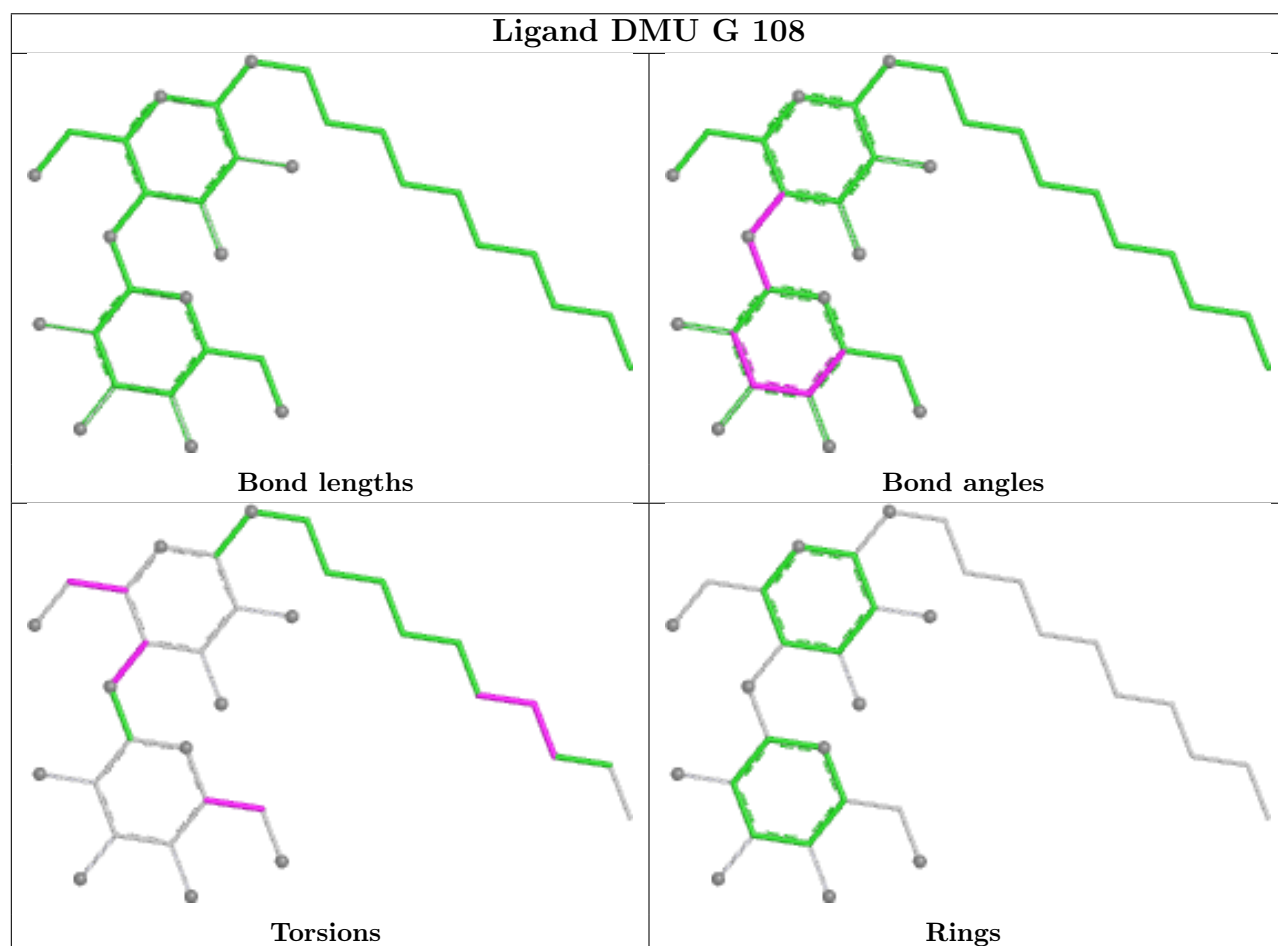
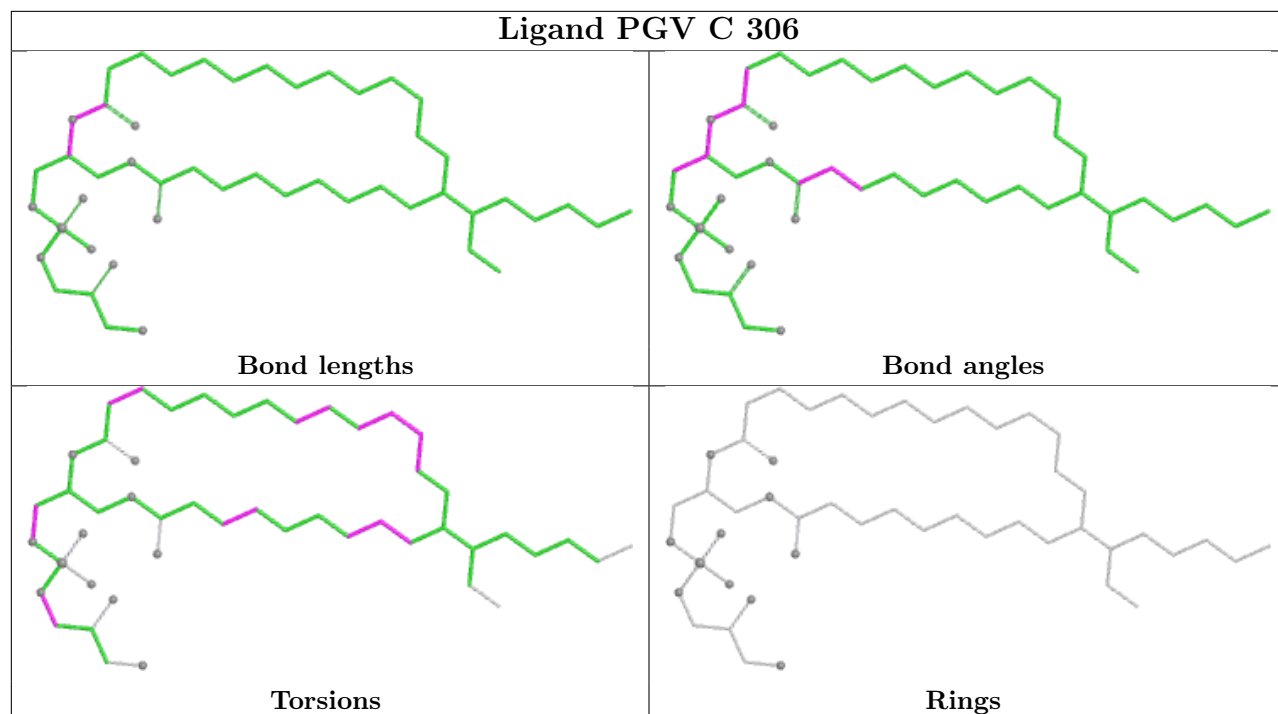


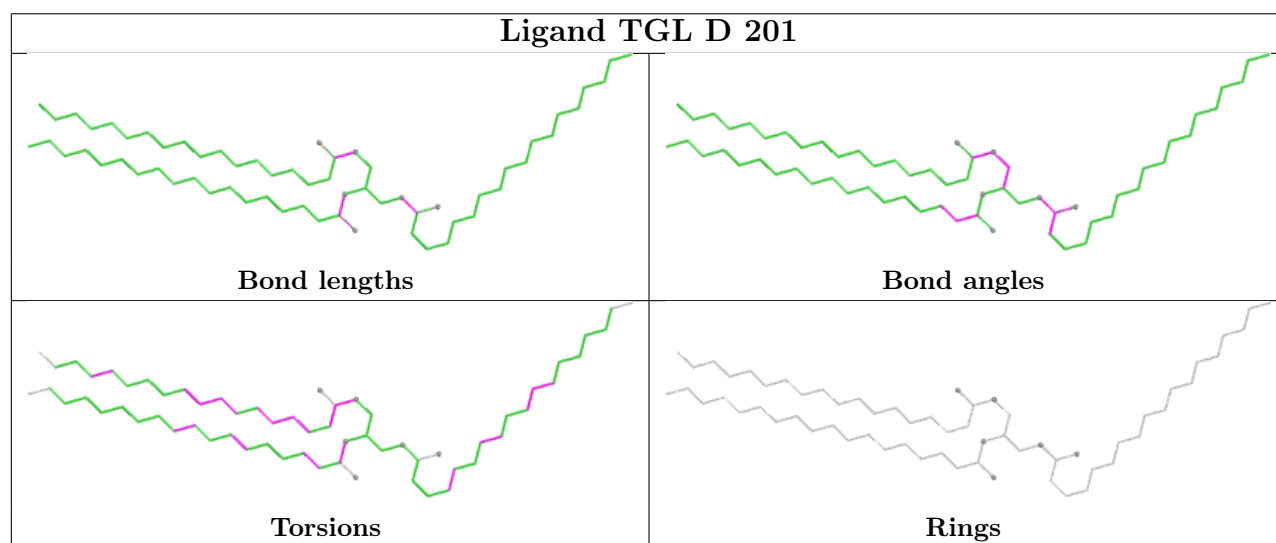
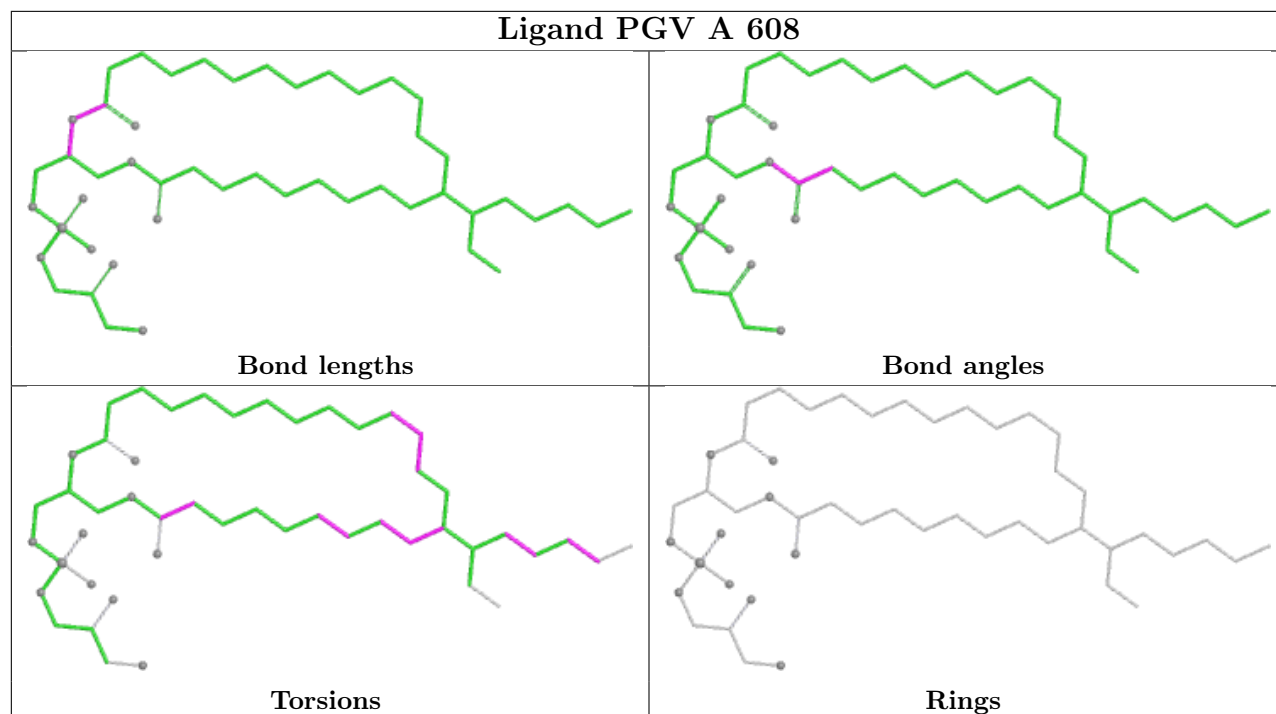


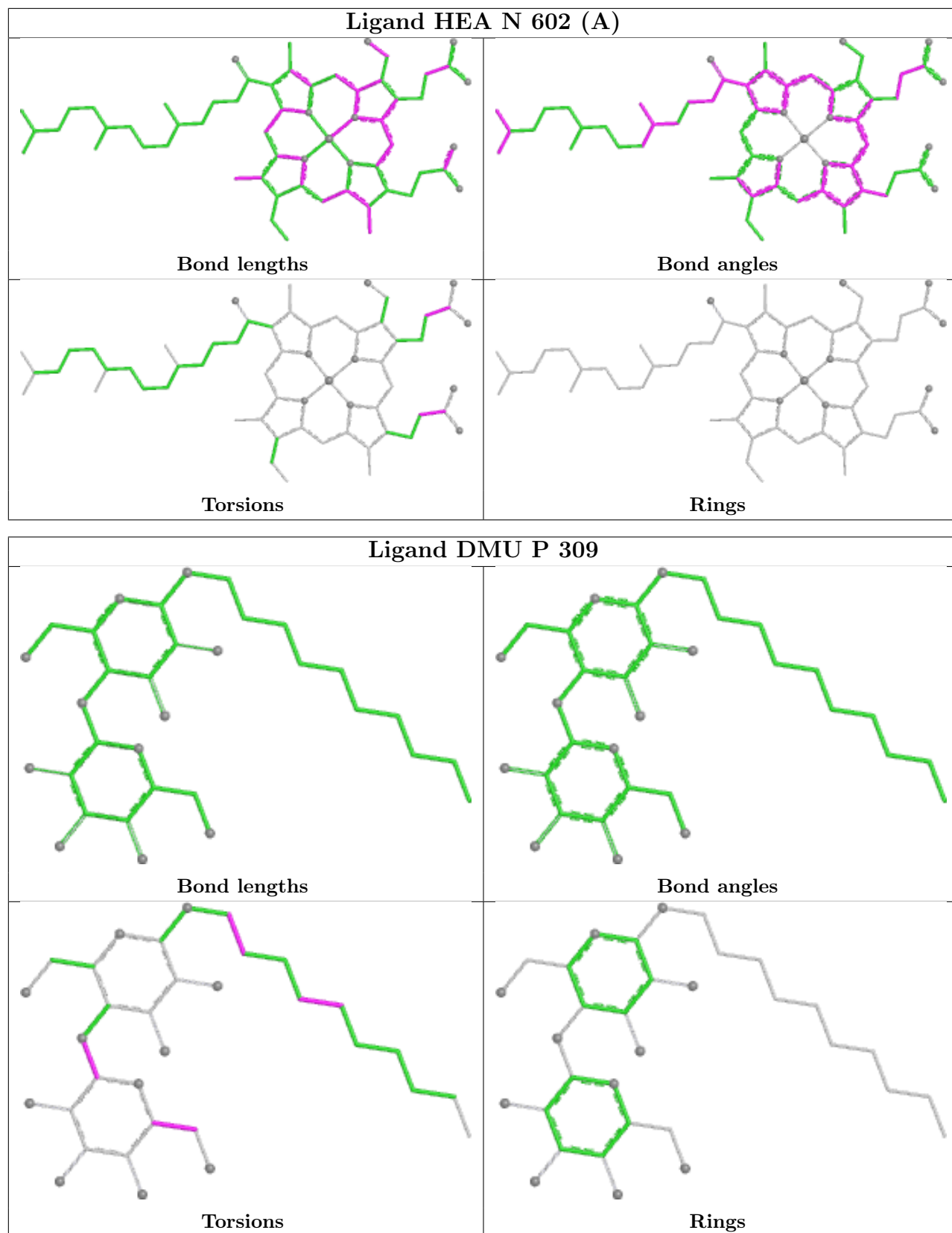


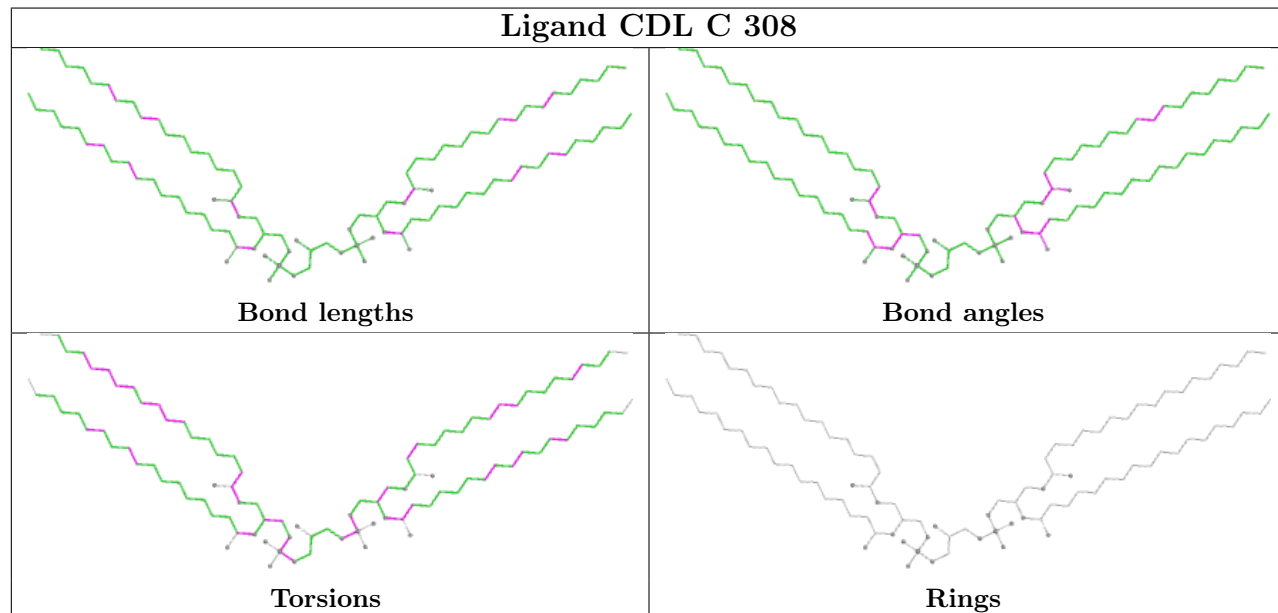
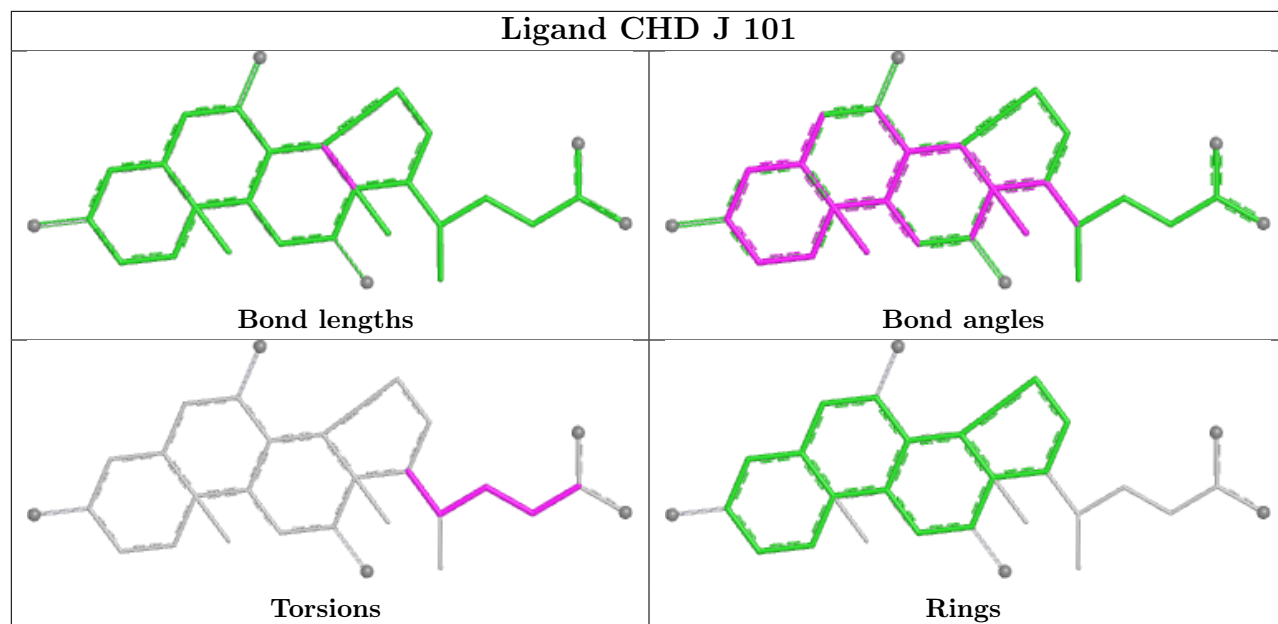


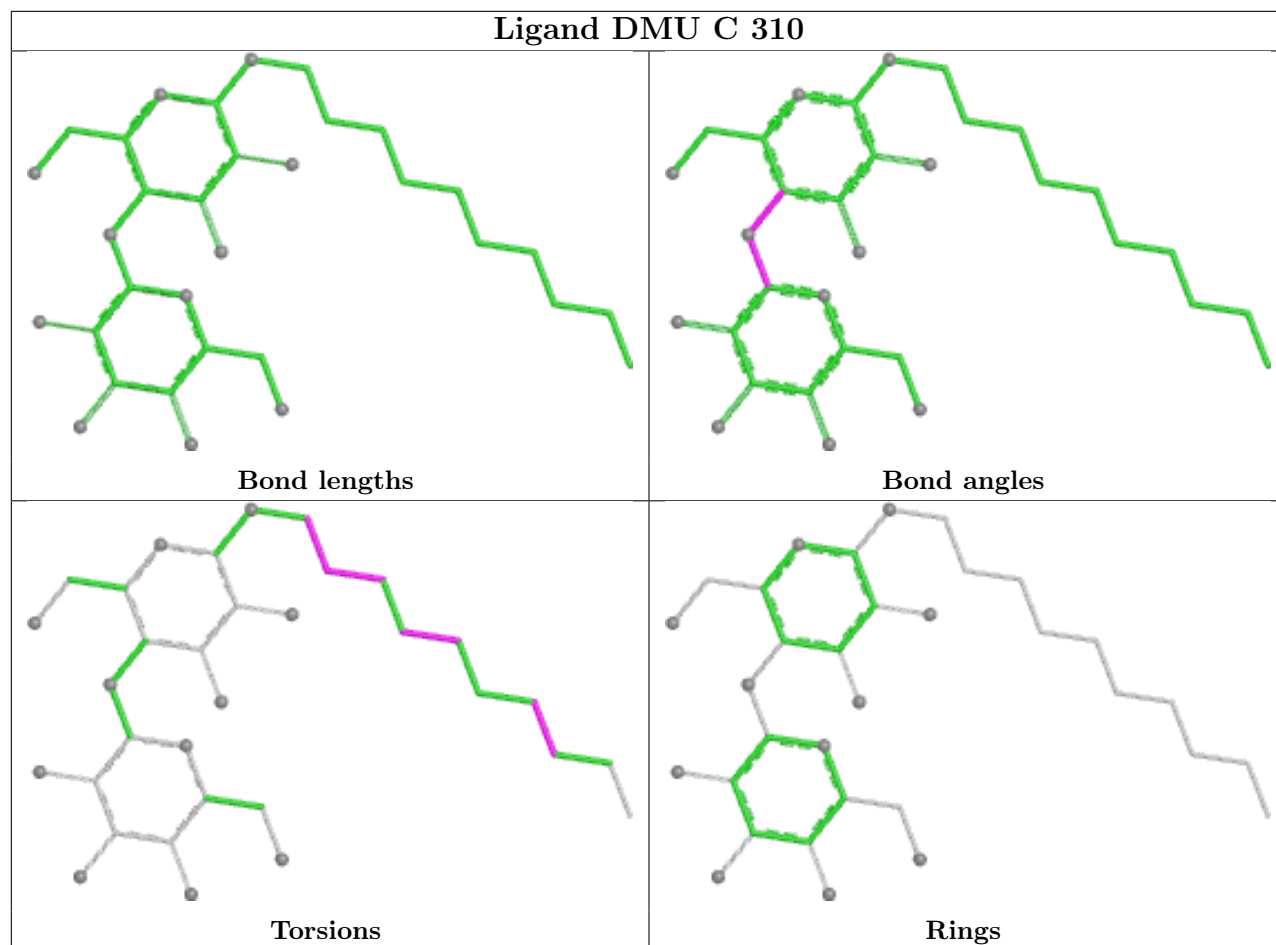


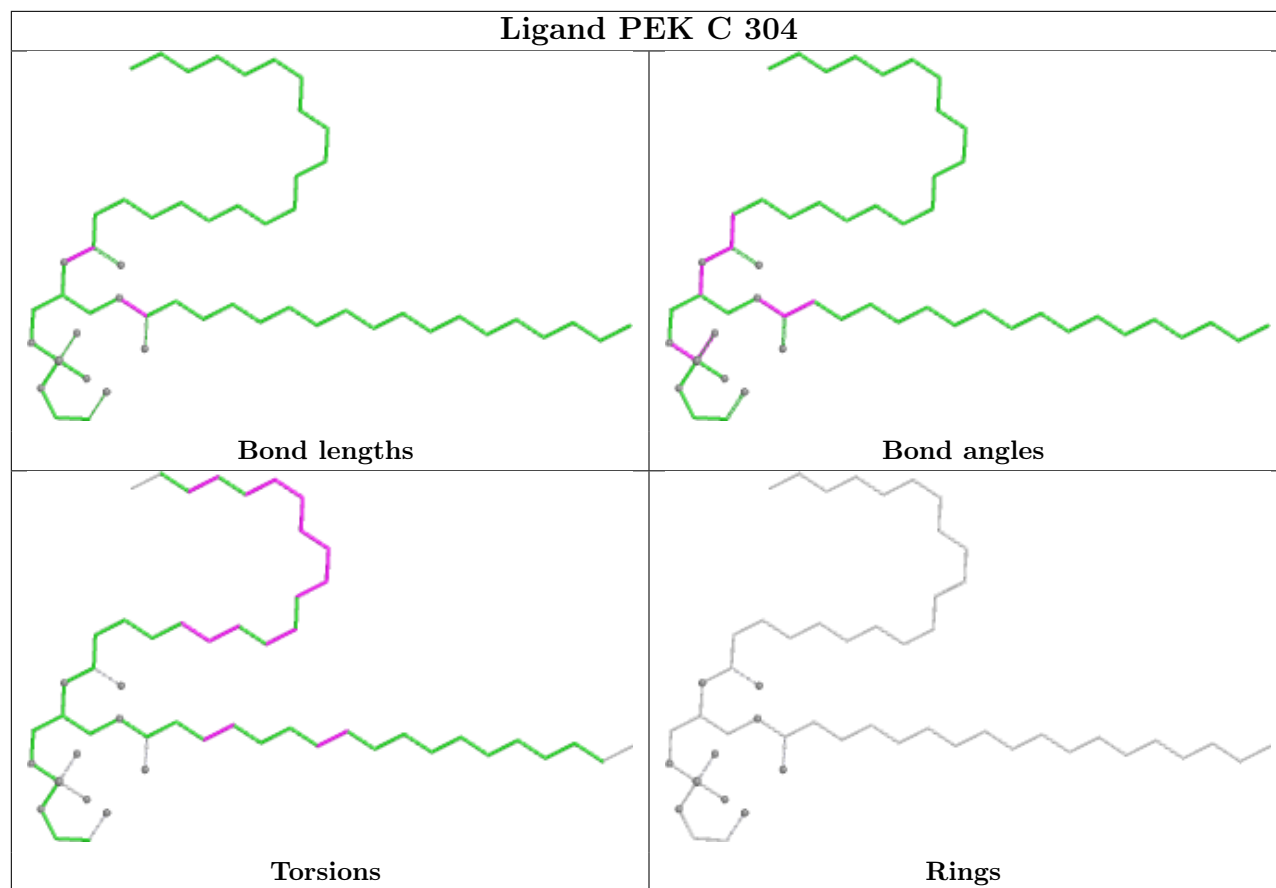


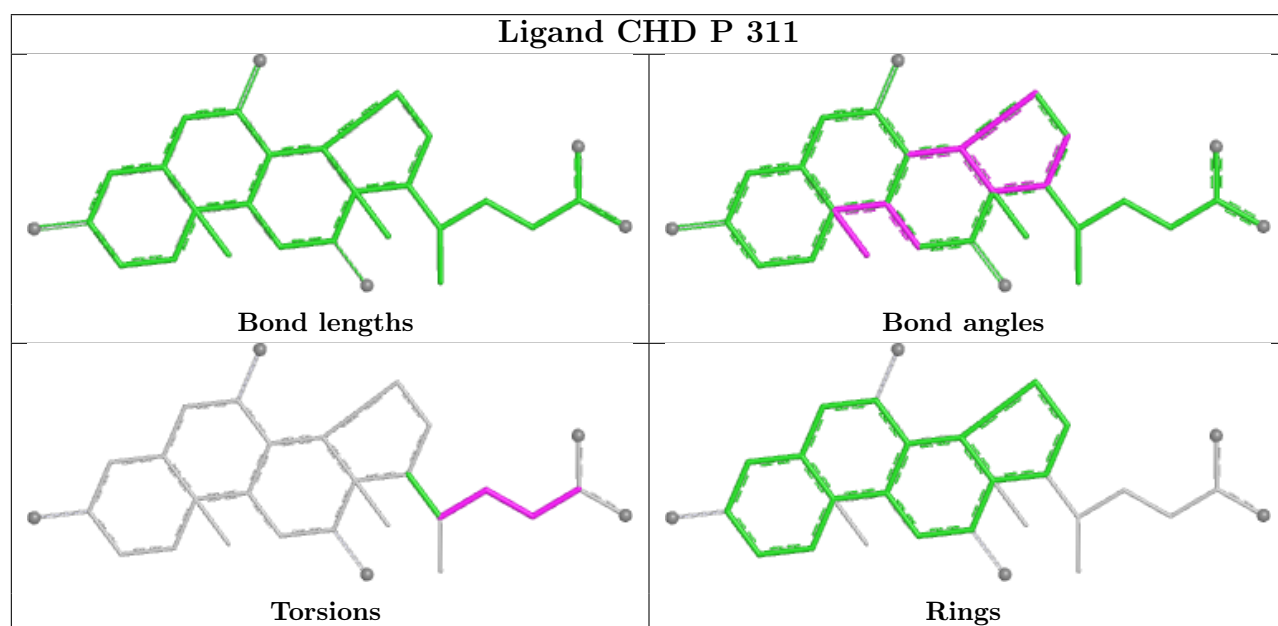
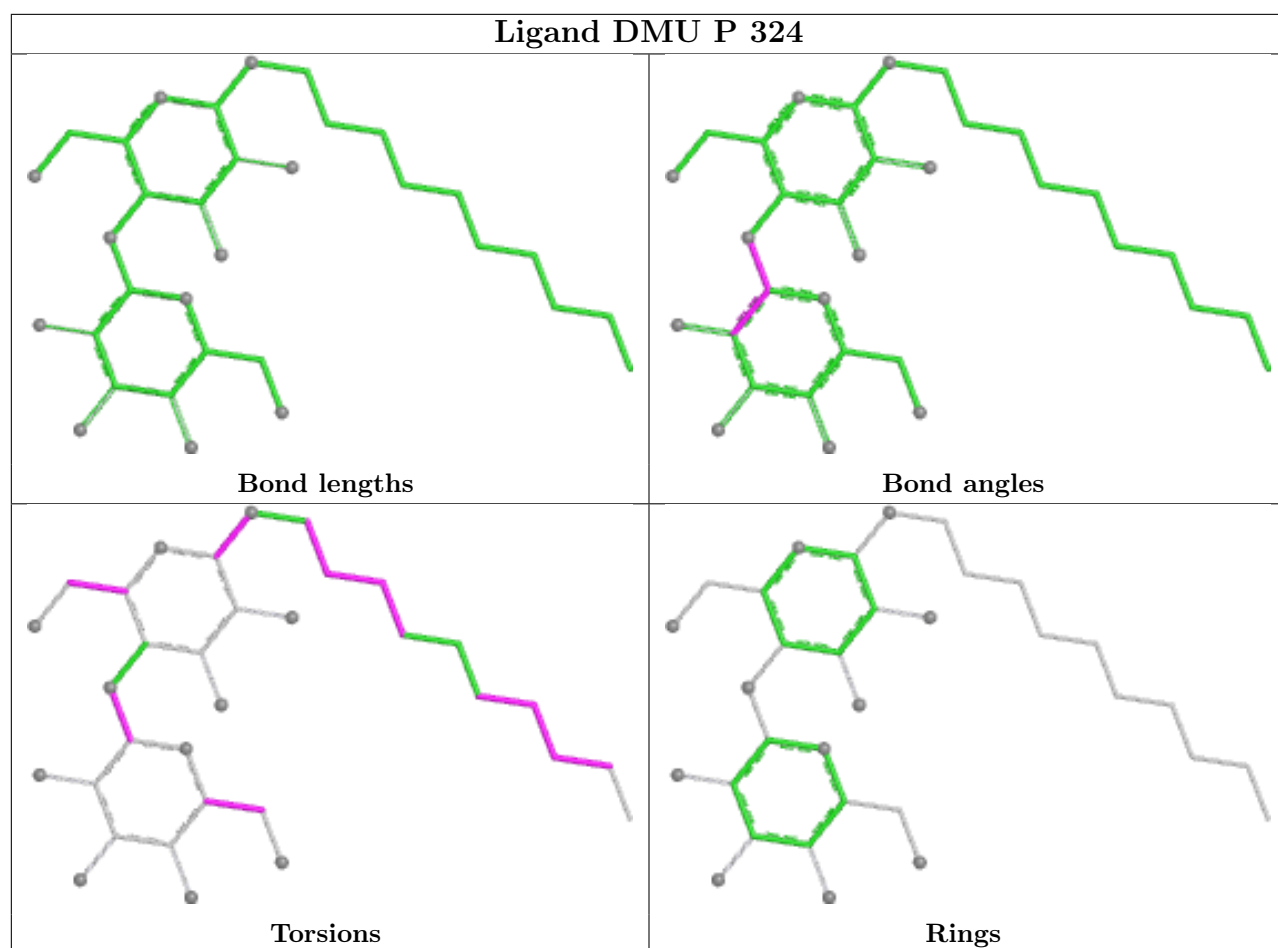


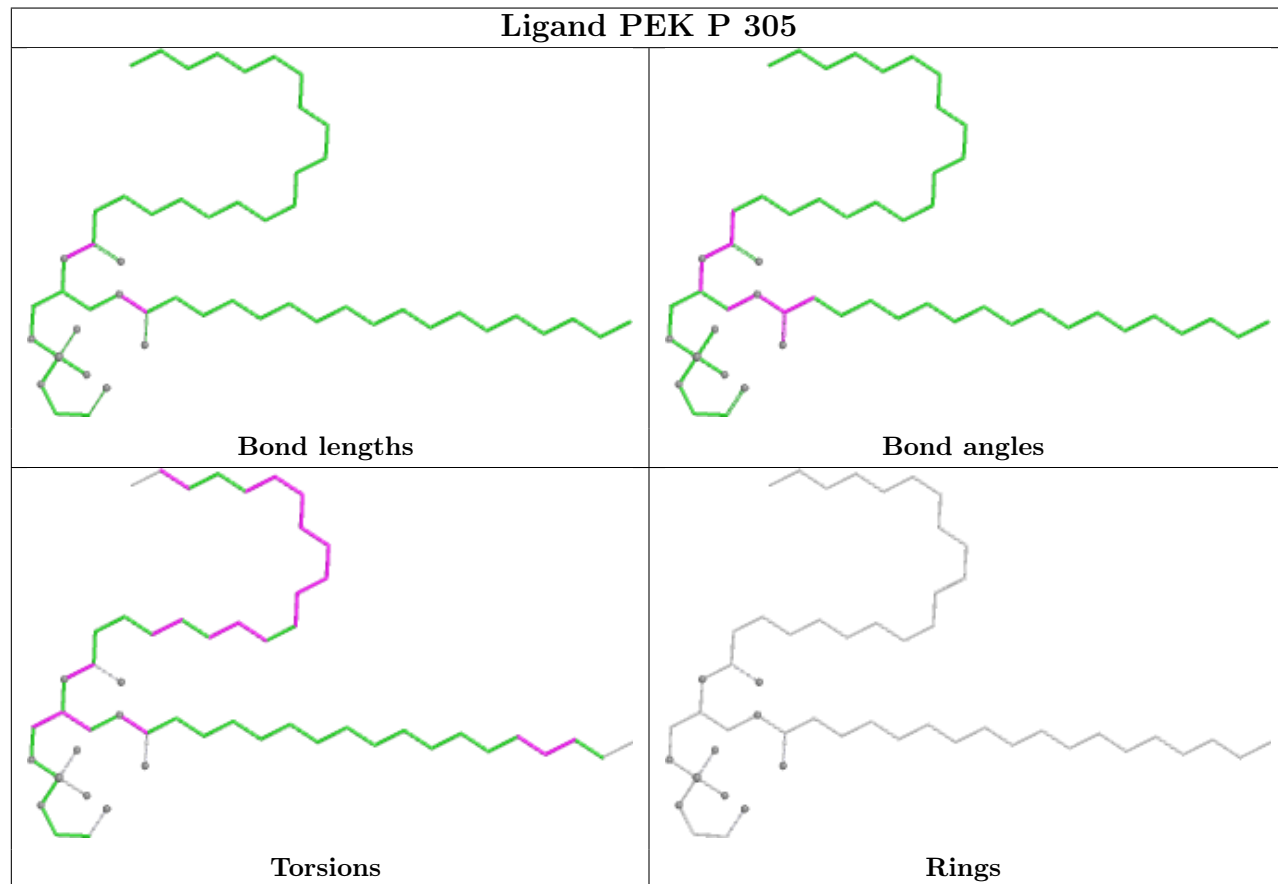
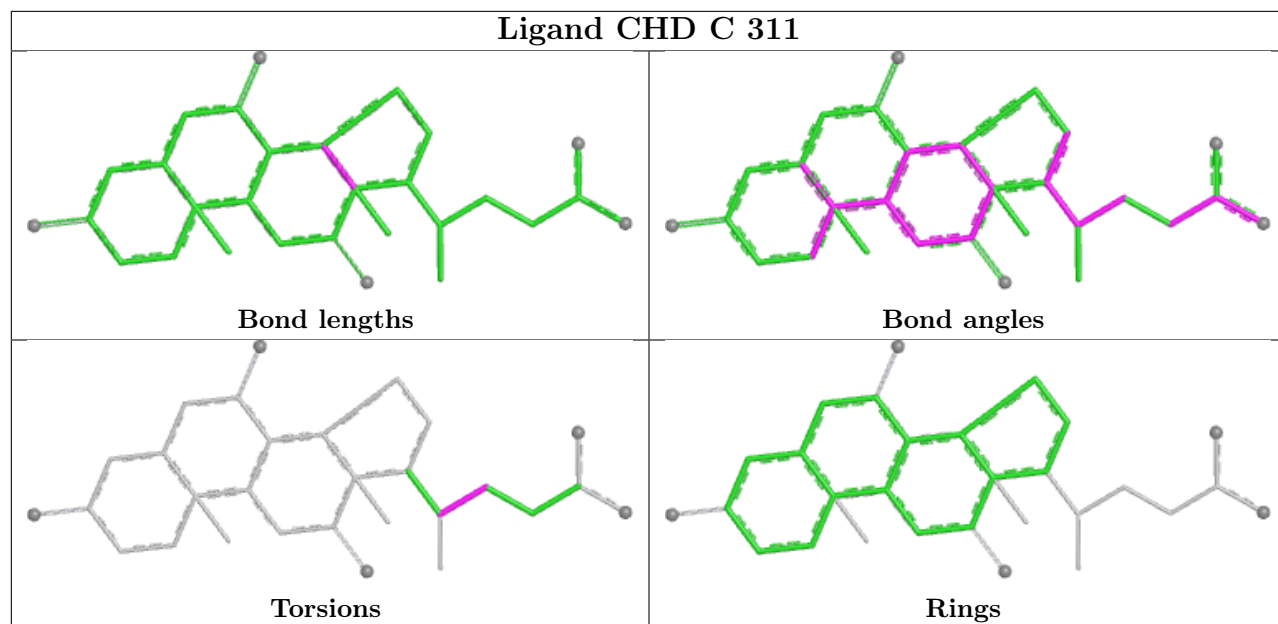


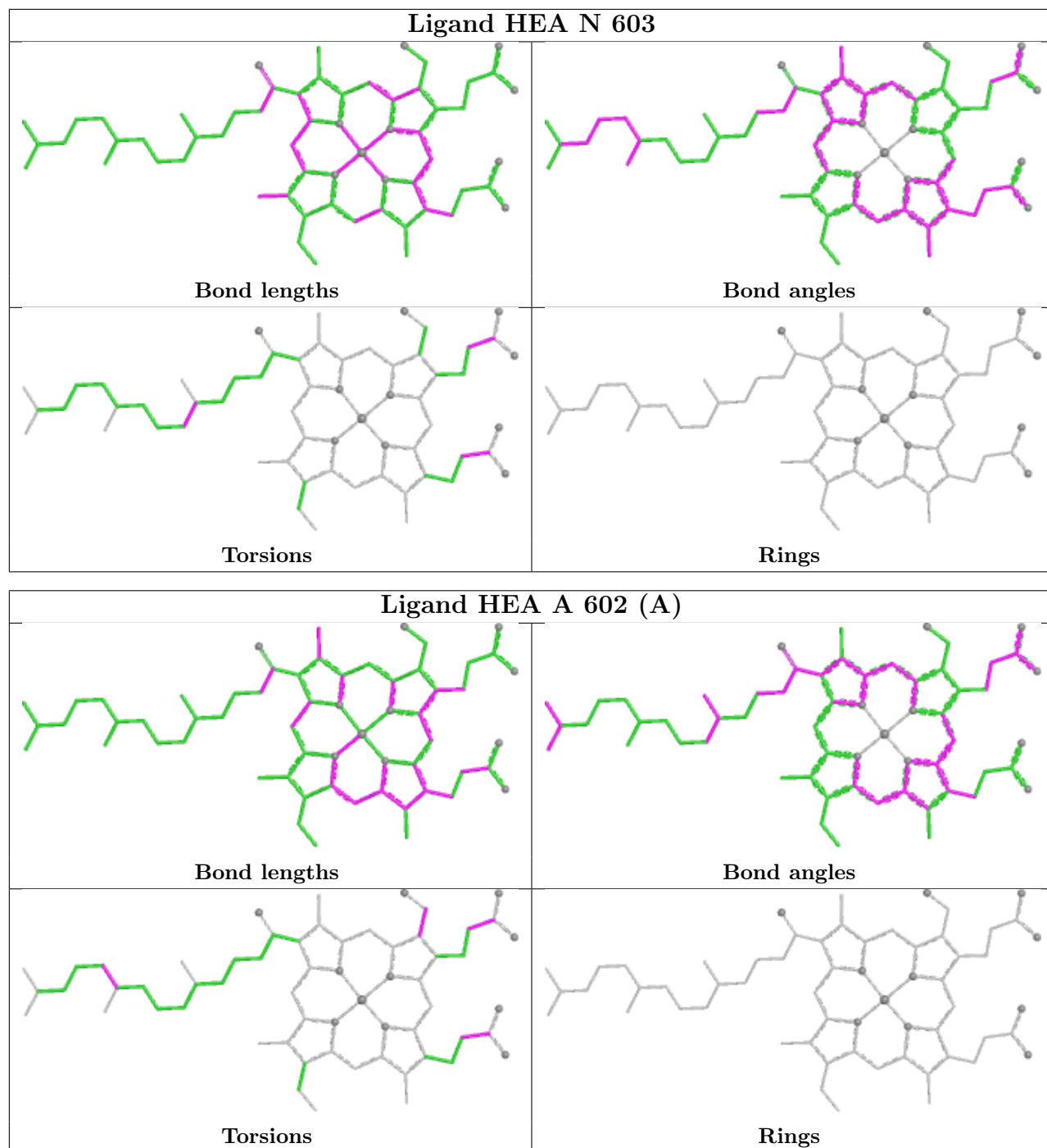


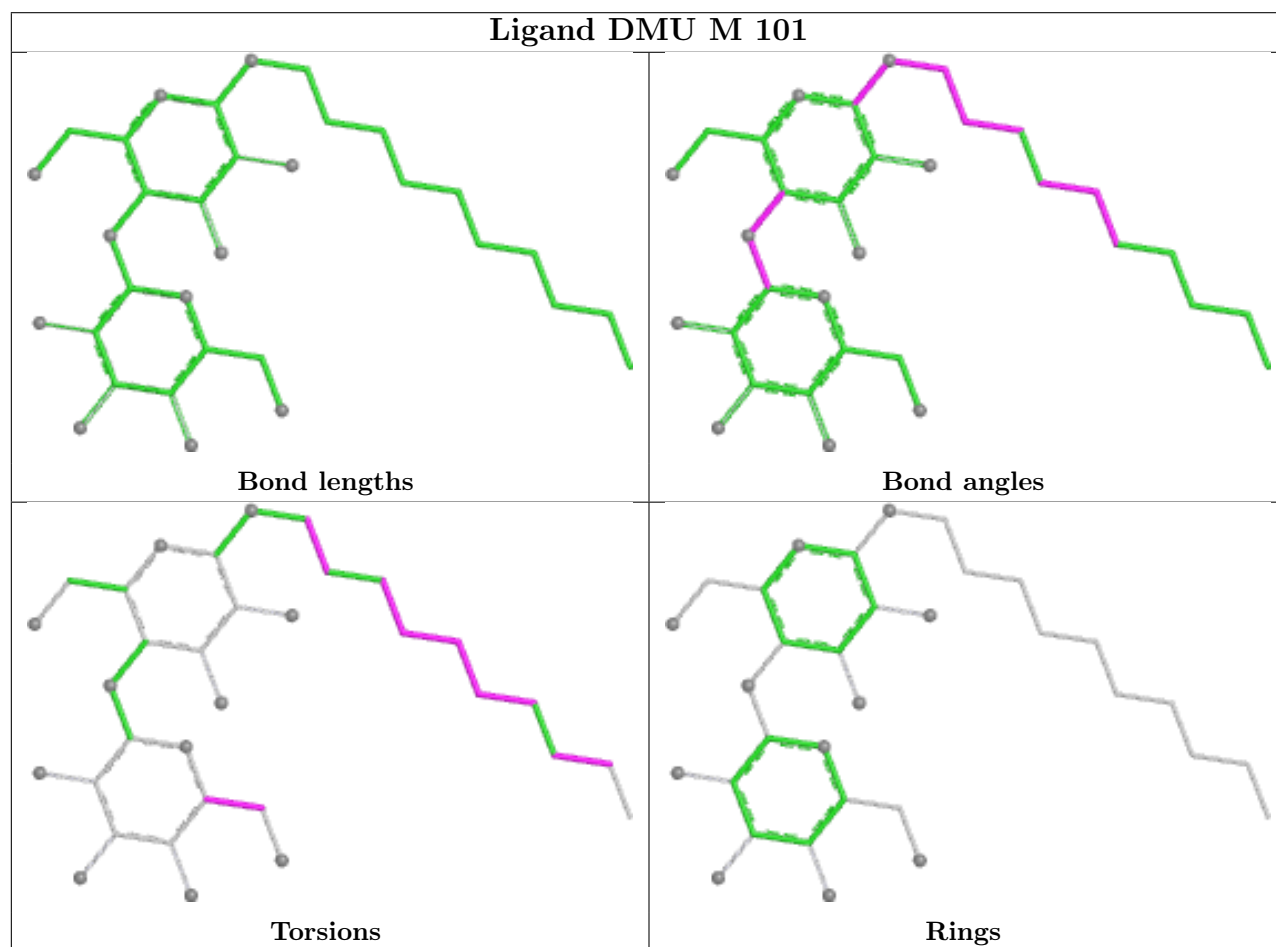
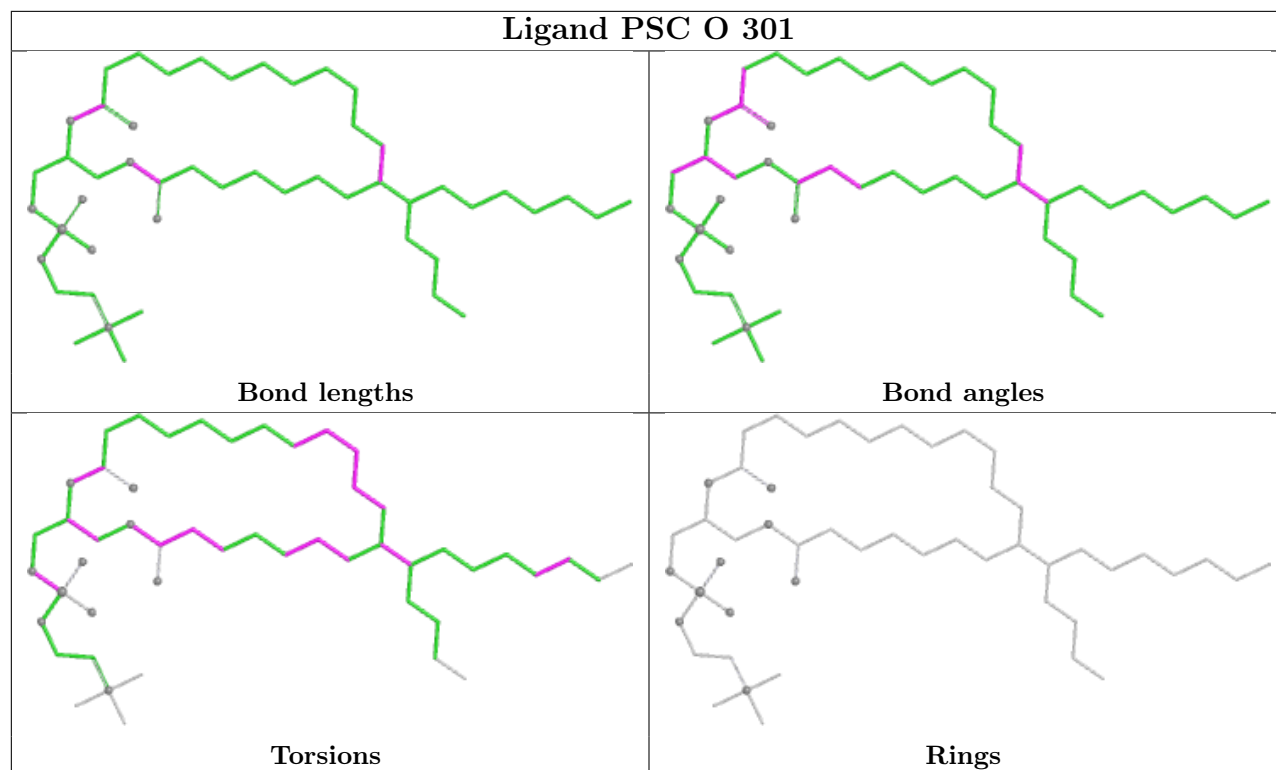


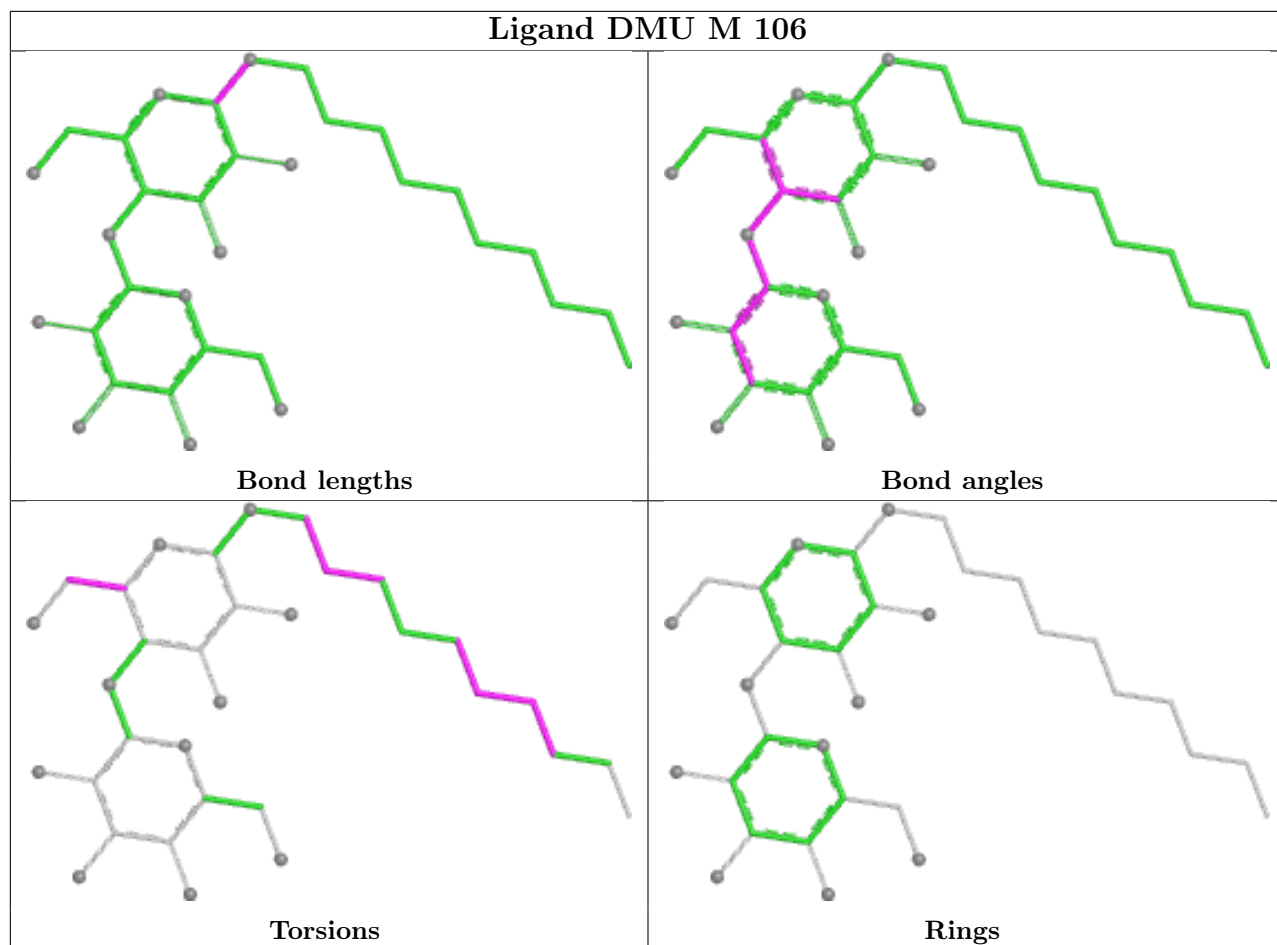


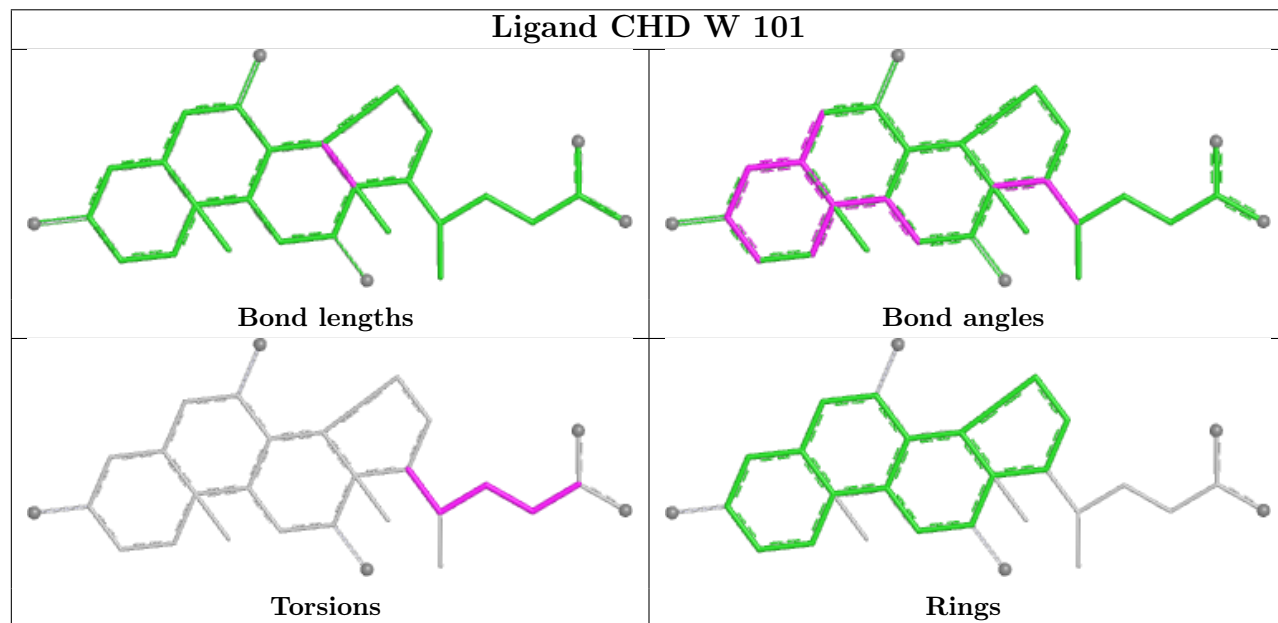
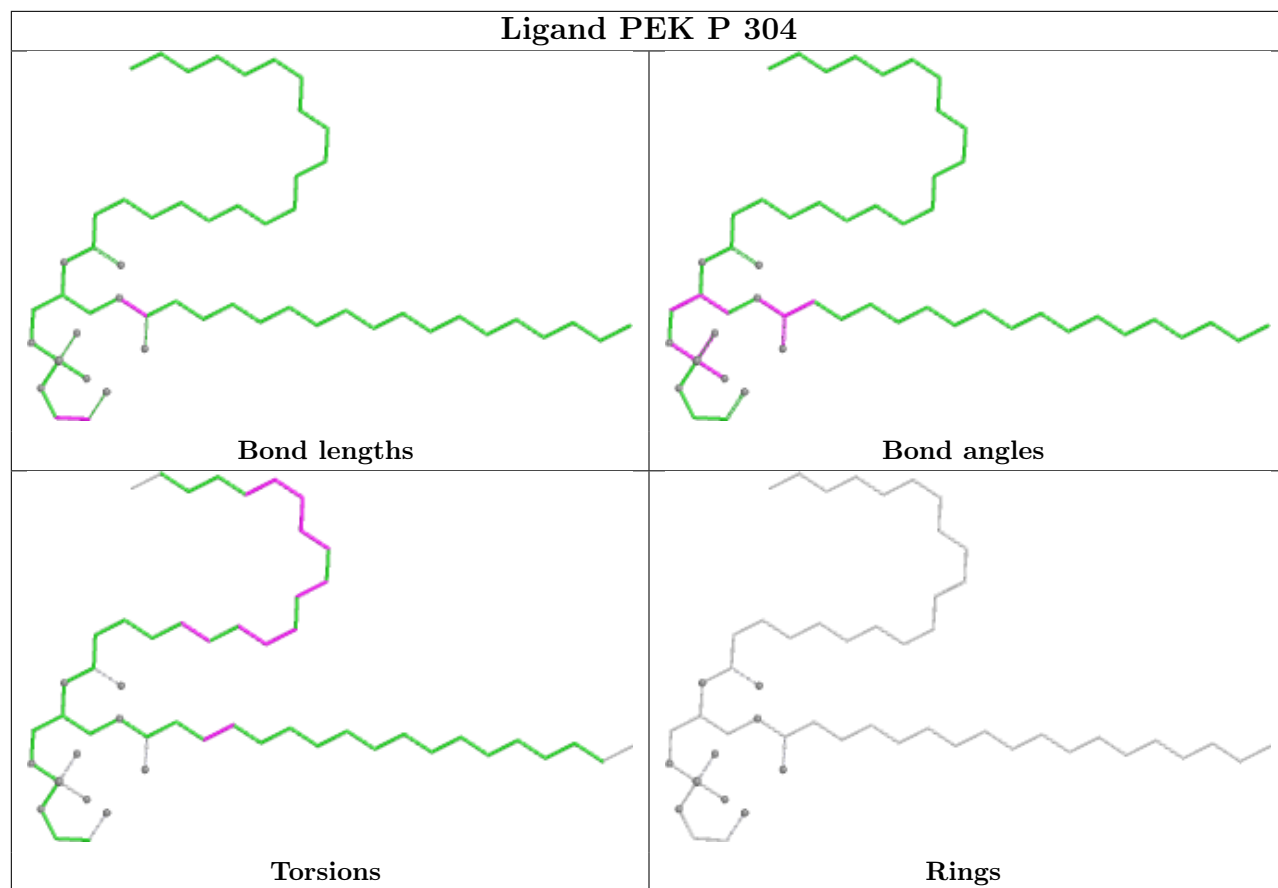


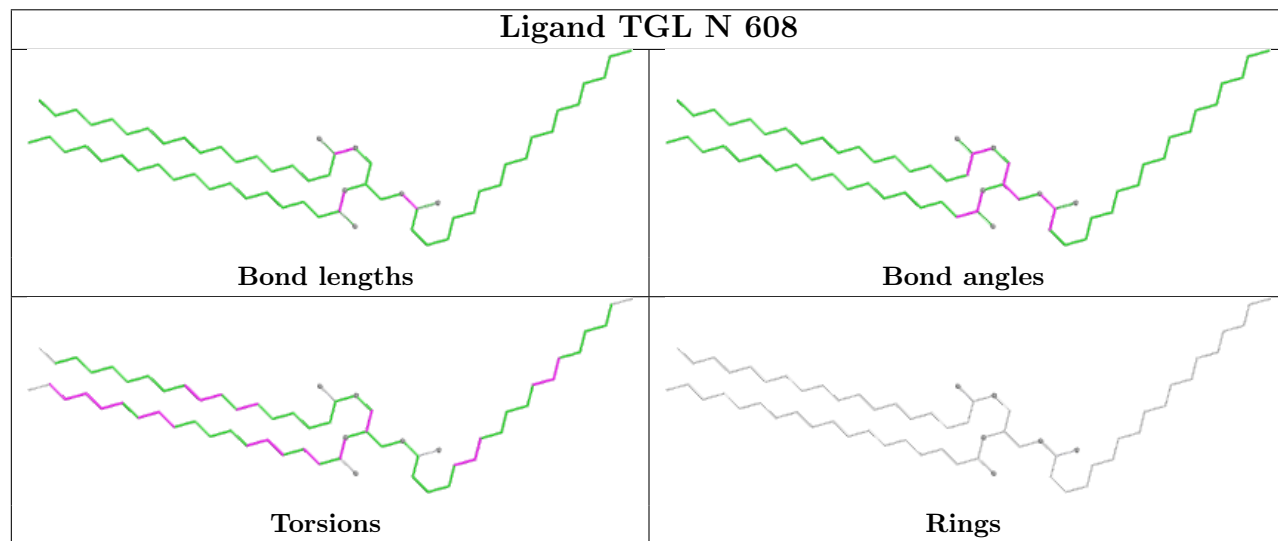
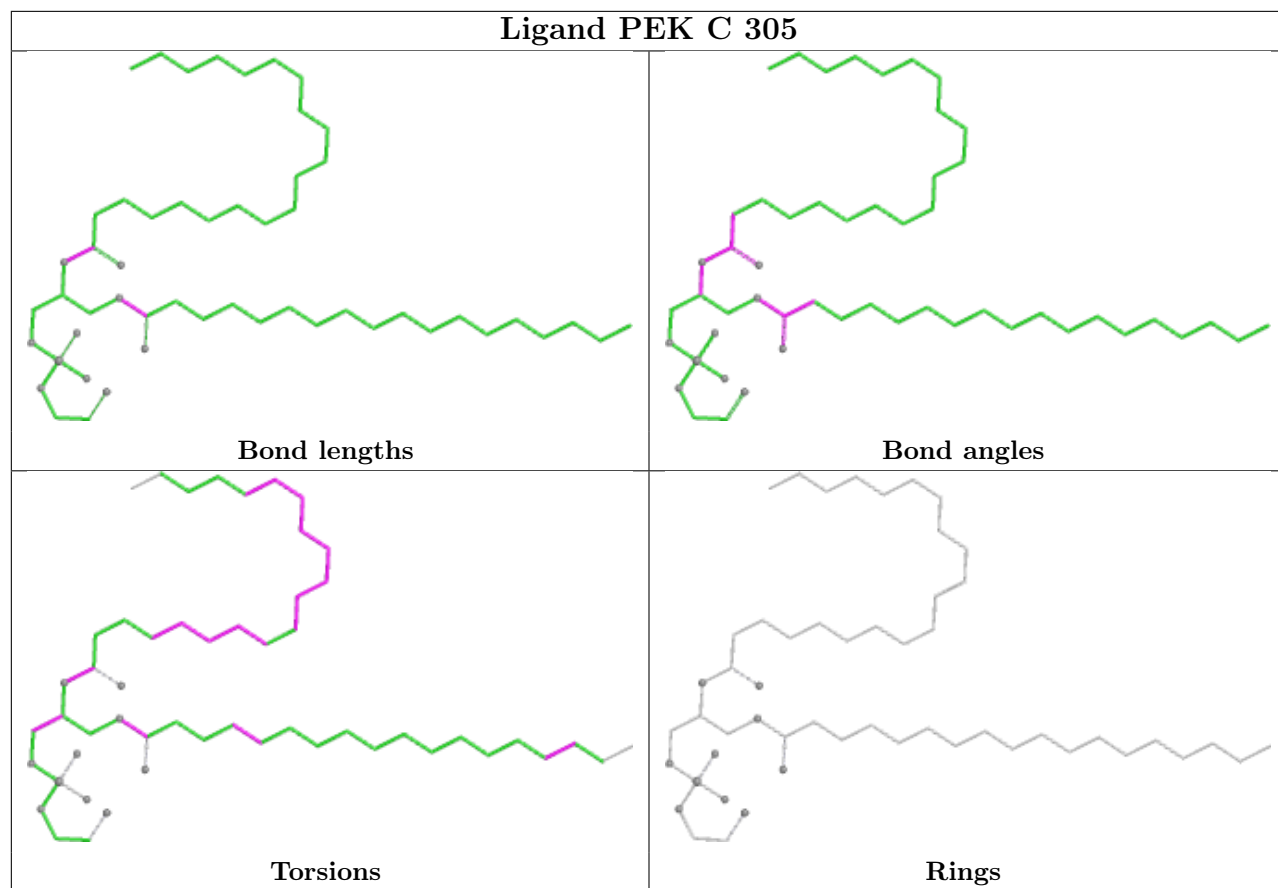


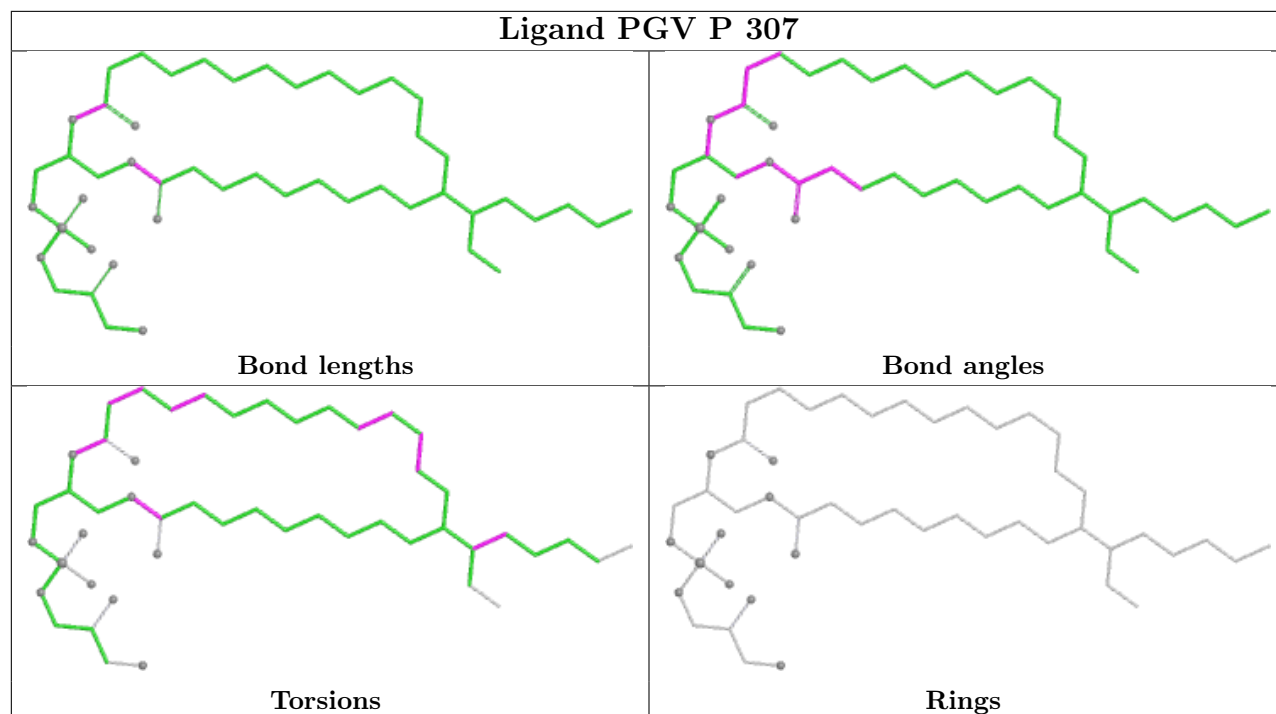












5.7 Other polymers [i](#)

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 i

6.1 Protein, DNA and RNA chains i

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%)	-0.34	5 (0%) 79 82	10, 23, 29, 74	30 (5%)
1	N	513/514 (99%)	-0.27	5 (0%) 79 82	11, 25, 33, 69	28 (5%)
2	B	226/227 (99%)	0.29	16 (7%) 22 24	20, 29, 46, 108	11 (4%)
2	O	226/227 (99%)	0.29	14 (6%) 26 29	18, 34, 62, 118	10 (4%)
3	C	259/261 (99%)	0.02	6 (2%) 61 65	17, 26, 38, 84	9 (3%)
3	P	259/261 (99%)	0.19	6 (2%) 61 65	17, 27, 39, 108	11 (4%)
4	D	144/147 (97%)	0.19	6 (4%) 40 45	18, 32, 50, 86	5 (3%)
4	Q	144/147 (97%)	1.04	17 (11%) 9 9	28, 44, 89, 254	3 (2%)
5	E	105/109 (96%)	0.17	5 (4%) 35 39	26, 31, 57, 134	0
5	R	105/109 (96%)	0.37	4 (3%) 44 48	26, 38, 64, 127	0
6	F	94/98 (95%)	0.48	6 (6%) 25 27	22, 32, 61, 160	3 (3%)
6	S	94/98 (95%)	0.52	8 (8%) 16 17	22, 31, 58, 169	3 (3%)
7	G	83/85 (97%)	1.80	22 (26%) 1 1	25, 33, 142, 185	0
7	T	83/85 (97%)	1.77	22 (26%) 1 1	24, 36, 125, 185	1 (1%)
8	H	79/85 (92%)	1.02	14 (17%) 4 3	26, 35, 117, 150	0
8	U	79/85 (92%)	1.06	14 (17%) 4 3	30, 40, 135, 187	0
9	I	72/73 (98%)	1.01	16 (22%) 2 2	28, 42, 71, 85	0
9	V	72/73 (98%)	1.38	23 (31%) 1 1	28, 49, 81, 147	0
10	J	58/59 (98%)	0.95	7 (12%) 8 8	26, 36, 78, 150	0
10	W	58/59 (98%)	0.67	6 (10%) 12 12	27, 37, 80, 213	0
11	K	49/56 (87%)	0.68	3 (6%) 27 29	28, 36, 50, 82	0
11	X	49/56 (87%)	1.04	7 (14%) 6 5	35, 44, 76, 96	0
12	L	46/47 (97%)	0.16	2 (4%) 40 44	24, 28, 44, 108	2 (4%)
12	Y	46/47 (97%)	0.40	4 (8%) 16 17	27, 33, 63, 135	4 (8%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.46	5 (11%) 9 9	24, 29, 69, 120	0
13	Z	43/46 (93%)	0.93	7 (16%) 4 4	31, 37, 96, 250	0
All	All	3542/3614 (98%)	0.31	250 (7%) 22 24	10, 30, 66, 254	120 (3%)

All (250) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	ALA	14.8
7	G	3	ALA	13.7
7	G	4	ALA	13.7
6	F	1	ALA	12.6
7	T	3	ALA	12.3
7	G	6	GLY	11.8
4	Q	6	VAL	11.7
6	S	94	HIS	11.0
6	S	1	ALA	10.9
7	T	36	TRP	10.9
7	G	36	TRP	10.7
7	G	8	HIS	9.9
8	U	8	ILE	9.6
7	T	7[A]	ASP	9.5
7	G	5	LYS	8.5
7	T	2	SER	8.4
8	H	8	ILE	8.2
4	Q	5	VAL	8.2
4	D	4	SER	8.2
7	T	5	LYS	8.1
6	S	3	GLY	8.0
7	G	7	ASP	8.0
2	B	90	ILE	7.9
7	T	4	ALA	7.8
4	Q	8	SER	7.8
7	T	6	GLY	7.7
10	J	55	PHE	7.4
7	T	9	GLY	7.3
7	T	8	HIS	7.3
7	G	2	SER	7.3
3	P	3	HIS	7.1
2	O	227	LEU	7.0
7	G	10	GLY	7.0
8	U	48	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
9	V	2	THR	6.8
6	F	3	GLY	6.8
8	U	47	GLY	6.5
2	O	113	TYR	6.3
8	H	46	LYS	6.1
6	F	2	SER	6.0
12	L	2[A]	HIS	6.0
8	U	46	LYS	6.0
2	O	90	ILE	5.9
7	G	9	GLY	5.9
11	X	6	ALA	5.8
6	S	93	PRO	5.7
6	S	2	SER	5.7
10	J	1	PHE	5.7
10	J	58	LYS	5.6
10	W	58	LYS	5.5
7	G	41	HIS	5.5
8	H	48	GLY	5.2
13	Z	43	SER	5.2
6	F	94	HIS	5.2
7	G	1	ALA	5.2
2	B	91	ASN	5.0
9	I	29	LEU	4.9
9	V	3	ALA	4.8
8	H	47	GLY	4.7
1	A	514	LYS	4.6
4	Q	7	LYS	4.6
13	Z	42	LYS	4.6
8	U	45	ALA	4.5
9	V	37	PHE	4.5
8	H	9	LYS	4.5
5	R	109	VAL	4.4
8	H	45	ALA	4.4
11	K	6	ALA	4.4
13	Z	40	TYR	4.4
13	M	43	SER	4.4
8	H	44	THR	4.3
2	O	91	ASN	4.3
8	U	9	LYS	4.3
4	Q	9	GLU	4.3
7	T	10	GLY	4.3
8	H	42	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
4	Q	31	LYS	4.2
12	L	47	LYS	4.2
4	Q	4	SER	4.2
7	T	12	GLY	4.2
12	Y	2[A]	HIS	4.2
8	H	10	ASN	4.1
7	T	84	LYS	4.1
10	W	57	HIS	4.1
4	Q	10	ASP	4.1
8	H	7	LYS	4.1
9	I	25	PHE	4.0
7	T	39	SER	3.9
3	P	33	MET	3.9
9	I	32	ALA	3.9
13	Z	41	LYS	3.9
7	G	37	LEU	3.8
7	T	40	GLY	3.8
9	V	34	PHE	3.8
3	C	3	HIS	3.8
2	B	61	VAL	3.8
5	R	80	GLU	3.8
2	B	113	TYR	3.8
11	K	54	ARG	3.7
13	M	42	LYS	3.6
7	T	38	HIS	3.6
8	U	44	THR	3.6
2	B	57	ASP	3.6
2	B	60[A]	GLU	3.6
7	G	84	LYS	3.6
10	W	1	PHE	3.6
8	U	10	ASN	3.6
12	Y	16	GLU	3.6
3	P	37	PHE	3.5
4	Q	51	LEU	3.5
4	Q	72	ASN	3.5
9	I	2	THR	3.5
7	T	42	ARG	3.5
5	E	5	HIS	3.5
2	B	92	ASN	3.4
9	I	37	PHE	3.4
4	D	5	VAL	3.4
9	V	36	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
10	J	56	PRO	3.4
11	X	52	GLU	3.4
7	T	35	SER	3.4
3	C	37	PHE	3.4
13	Z	32	TRP	3.4
7	G	12	GLY	3.4
2	B	87[A]	MET	3.4
12	Y	47	LYS	3.3
7	T	33	LEU	3.3
1	N	514	LYS	3.3
10	J	52	TRP	3.3
9	V	33	THR	3.3
11	X	47	ARG	3.3
4	Q	35	ALA	3.2
11	X	7	PRO	3.2
9	I	34	PHE	3.2
8	U	55	TRP	3.2
11	K	47	ARG	3.2
2	B	58	ALA	3.2
7	G	38	HIS	3.2
1	A	513	LEU	3.1
2	B	59	GLN	3.1
8	U	42	ALA	3.1
2	O	59	GLN	3.1
2	B	82	ARG	3.1
8	U	50	VAL	3.1
9	I	36	LYS	3.0
1	N	483	LEU	3.0
1	N	513	LEU	3.0
10	J	27	THR	3.0
9	I	73	LYS	3.0
4	D	31	LYS	3.0
9	V	30	GLY	3.0
10	W	56	PRO	3.0
9	V	44	LYS	2.9
7	G	42	ARG	2.9
4	D	9	GLU	2.9
5	E	109	VAL	2.9
13	M	40	TYR	2.9
7	T	37	LEU	2.9
3	C	33	MET	2.8
8	U	7	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
5	E	7	THR	2.8
2	O	221	LYS	2.8
5	R	5	HIS	2.8
10	J	57	HIS	2.8
2	O	89	GLU	2.8
2	B	130	PRO	2.8
9	V	8	GLN	2.7
9	V	73	LYS	2.7
2	O	116	LEU	2.7
3	C	38	ASN	2.7
13	M	38	ASP	2.7
9	I	15	ARG	2.6
2	O	226	MET	2.6
9	I	30	GLY	2.6
2	B	115[A]	ASP	2.6
13	Z	39	ASN	2.6
7	G	40	GLY	2.6
9	V	29	LEU	2.6
4	Q	17[A]	VAL	2.6
8	U	52	VAL	2.6
5	R	108	LYS	2.6
12	Y	26	THR	2.5
11	X	54	ARG	2.5
2	O	114	GLU	2.5
7	G	39	SER	2.5
2	B	37	LEU	2.5
6	S	37	LYS	2.5
8	H	50	VAL	2.5
7	G	43	GLU	2.5
4	Q	33	LEU	2.4
6	F	64	GLU	2.4
9	I	31	PHE	2.4
6	F	65	ASP	2.4
8	H	55	TRP	2.4
9	V	64	ARG	2.4
4	Q	73	ARG	2.3
9	V	10	ARG	2.3
10	W	27	THR	2.3
9	V	65	LYS	2.3
9	V	57	MET	2.3
3	C	258	TRP	2.3
2	O	92	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	45	PRO	2.3
9	I	35	TYR	2.3
6	S	64	GLU	2.3
9	V	15	ARG	2.3
8	H	43	MET	2.3
9	I	22	VAL	2.3
7	T	41	HIS	2.2
9	V	38	ALA	2.2
9	I	18	ARG	2.2
13	M	39	ASN	2.2
7	G	33	LEU	2.2
2	B	16	ILE	2.2
4	Q	53	ILE	2.2
9	I	21	ILE	2.2
9	V	22	VAL	2.2
9	V	61	GLU	2.2
11	X	12	LYS	2.2
1	A	113[A]	LEU	2.2
9	V	26	MET	2.2
9	V	27	VAL	2.2
4	Q	36	SER	2.2
2	B	33[A]	LEU	2.2
2	O	32[A]	PHE	2.2
9	V	25	PHE	2.2
8	H	49	ASP	2.1
13	Z	38	ASP	2.1
9	I	39	VAL	2.1
3	P	44[A]	MET	2.1
1	A	486[A]	ASP	2.1
4	D	8	SER	2.1
5	E	39	TYR	2.1
3	P	38	ASN	2.1
1	A	297[A]	MET	2.1
5	E	9	GLU	2.1
2	O	68[A]	LEU	2.1
3	C	41	THR	2.1
2	O	58	ALA	2.0
11	X	16	ALA	2.0
6	S	65	ASP	2.0
1	N	361	SER	2.0
8	U	84	LYS	2.0
3	P	258	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
10	W	52	TRP	2.0
4	Q	19[A]	ARG	2.0
7	T	74	ARG	2.0
9	V	18	ARG	2.0
1	N	366[A]	VAL	2.0
4	D	147	LYS	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
9	SAC	V	1	9/10	0.24	0.23	179,194,204,205	0
7	TPO	T	11	11/12	0.41	0.35	140,173,213,214	0
7	TPO	G	11	11/12	0.45	0.29	130,158,180,180	0
9	SAC	I	1	9/10	0.55	0.27	124,152,158,159	0
1	FME	A	1	10/11	0.93	0.11	35,41,68,72	0
1	FME	N	1	10/11	0.94	0.12	35,41,68,69	0
2	FME	B	1	10/11	0.96	0.09	27,29,34,51	0
2	FME	O	1	10/11	0.97	0.09	34,36,41,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	D	206	4/4	0.60	0.48	167,169,170,172	0
20	EDO	B	314	4/4	0.62	0.42	167,168,169,169	0
23	CHD	C	311	29/29	0.63	0.37	104,140,160,162	0
27	DMU	V	102	33/33	0.66	0.23	71,155,170,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
23	CHD	P	310	29/29	0.67	0.35	92,136,146,150	0
23	CHD	Y	104	29/29	0.68	0.28	94,123,130,131	0
20	EDO	W	104	4/4	0.68	0.46	80,83,86,86	0
27	DMU	P	324	33/33	0.69	0.25	56,122,149,154	0
20	EDO	S	105	4/4	0.69	0.29	84,88,90,91	0
20	EDO	N	623	4/4	0.70	0.36	90,91,93,94	0
27	DMU	G	108	33/33	0.70	0.23	61,124,156,158	0
20	EDO	A	623	4/4	0.71	0.27	51,66,75,81	0
20	EDO	N	619	4/4	0.72	0.36	85,86,89,89	0
27	DMU	M	106	33/33	0.72	0.21	59,101,127,131	0
27	DMU	Z	102	33/33	0.72	0.24	75,102,117,127	0
14	PGV	P	307	51/51	0.73	0.30	65,96,161,165	0
20	EDO	D	202	4/4	0.73	0.40	83,91,98,99	0
25	PEK	P	305	53/53	0.73	0.33	39,89,206,231	0
26	CDL	P	308	100/100	0.73	0.33	43,112,160,168	0
20	EDO	P	316	4/4	0.73	0.32	53,58,65,66	0
20	EDO	R	205	4/4	0.73	0.26	68,73,75,76	0
14	PGV	C	307	51/51	0.73	0.31	51,91,167,179	0
20	EDO	L	104	4/4	0.73	0.18	58,59,60,60	0
20	EDO	N	618	4/4	0.73	0.25	41,41,44,47	0
27	DMU	C	319	33/33	0.74	0.21	50,98,119,120	0
23	CHD	P	311	29/29	0.74	0.24	80,96,107,109	0
20	EDO	D	205	4/4	0.74	0.25	60,62,71,74	0
25	PEK	C	303	53/53	0.74	0.26	46,134,181,186	0
20	EDO	C	313	4/4	0.74	0.34	56,66,73,73	0
20	EDO	B	309	4/4	0.74	0.42	98,99,99,100	0
20	EDO	S	111	4/4	0.75	0.24	49,52,60,60	0
20	EDO	P	319	4/4	0.75	0.29	47,54,56,58	0
21	TGL	L	101	63/63	0.75	0.29	30,76,115,139	0
20	EDO	P	320	4/4	0.75	0.31	85,85,87,88	0
20	EDO	S	108	4/4	0.75	0.25	43,53,63,69	0
26	CDL	T	101	100/100	0.75	0.30	58,102,162,185	0
20	EDO	K	102	4/4	0.76	0.33	97,97,98,99	0
20	EDO	B	307	4/4	0.76	0.25	60,61,66,67	0
29	PO4	U	102	5/5	0.76	0.23	157,157,158,159	0
20	EDO	B	312	4/4	0.77	0.28	59,63,64,66	0
20	EDO	O	305	4/4	0.77	0.42	89,94,97,99	0
21	TGL	N	608	63/63	0.77	0.24	52,73,109,113	0
21	TGL	Q	201	63/63	0.77	0.26	53,80,101,104	0
25	PEK	P	303	53/53	0.77	0.26	47,94,170,176	0
23	CHD	C	309	29/29	0.77	0.21	68,78,95,97	0
26	CDL	G	101	100/100	0.77	0.29	55,112,187,207	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	PGV	N	601	51/51	0.77	0.26	45,87,144,151	0
20	EDO	U	101	4/4	0.78	0.24	67,70,71,72	0
20	EDO	W	103	4/4	0.78	0.20	47,49,56,57	0
25	PEK	C	305	53/53	0.78	0.26	47,79,141,144	0
20	EDO	P	321	4/4	0.78	0.22	53,61,65,68	0
22	PSC	O	301	52/52	0.78	0.31	35,100,221,227	0
20	EDO	N	617	4/4	0.79	0.25	61,65,70,71	0
20	EDO	J	102	4/4	0.79	0.36	111,111,113,114	0
20	EDO	P	322	4/4	0.79	0.19	57,58,58,60	0
21	TGL	Y	101	63/63	0.79	0.26	42,68,122,141	0
20	EDO	A	614	4/4	0.79	0.36	108,110,111,113	0
14	PGV	A	601	51/51	0.79	0.30	32,79,182,190	0
20	EDO	N	630	4/4	0.79	0.49	94,94,94,97	0
20	EDO	M	103	4/4	0.79	0.27	91,92,94,96	0
20	EDO	P	315	4/4	0.79	0.28	32,50,59,60	0
20	EDO	M	104	4/4	0.79	0.25	57,58,58,66	0
20	EDO	N	616	4/4	0.79	0.17	61,62,63,65	0
21	TGL	B	301	63/63	0.79	0.24	45,67,109,115	0
23	CHD	J	101	29/29	0.80	0.24	101,111,135,139	0
22	PSC	B	302	52/52	0.80	0.31	44,121,206,217	0
20	EDO	N	612	4/4	0.80	0.24	42,50,50,54	0
26	CDL	C	308	100/100	0.80	0.27	41,94,151,153	0
23	CHD	W	101	29/29	0.80	0.22	97,102,131,133	0
20	EDO	D	203	4/4	0.80	0.30	85,87,90,91	0
20	EDO	O	307	4/4	0.80	0.26	85,87,88,89	0
20	EDO	S	110	4/4	0.81	0.16	51,53,58,58	0
20	EDO	G	104	4/4	0.81	0.39	107,109,111,112	0
21	TGL	D	201	63/63	0.81	0.24	36,71,99,104	0
20	EDO	A	622	4/4	0.81	0.20	63,65,67,67	0
27	DMU	C	310	33/33	0.81	0.20	48,101,111,113	0
20	EDO	M	105	4/4	0.81	0.23	35,47,53,56	0
20	EDO	J	103	4/4	0.82	0.19	57,61,65,72	0
20	EDO	G	107	4/4	0.82	0.18	35,50,57,58	0
20	EDO	B	311	4/4	0.82	0.23	79,80,81,82	0
27	DMU	P	309	33/33	0.83	0.19	46,101,136,137	0
27	DMU	P	323	33/33	0.83	0.15	51,88,98,100	0
20	EDO	R	203	4/4	0.83	0.28	60,64,66,68	0
20	EDO	O	306	4/4	0.84	0.30	73,80,80,82	0
20	EDO	Y	103	4/4	0.84	0.21	57,57,61,63	0
20	EDO	N	627	4/4	0.84	0.20	64,65,67,70	0
20	EDO	B	310	4/4	0.84	0.34	89,94,97,99	0
18	NA	C	302	1/1	0.84	0.33	809,809,809,809	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	A	624	4/4	0.85	0.13	58,59,60,64	0
20	EDO	A	625	4/4	0.85	0.16	50,54,60,61	0
20	EDO	T	103	4/4	0.85	0.16	40,46,48,51	0
20	EDO	H	101	4/4	0.85	0.22	56,57,62,63	0
20	EDO	P	314	4/4	0.85	0.20	49,50,55,55	0
20	EDO	A	621	4/4	0.85	0.22	40,47,52,55	0
20	EDO	C	316	4/4	0.85	0.19	31,39,40,41	0
20	EDO	F	105	4/4	0.85	0.22	65,68,73,75	0
20	EDO	G	105	4/4	0.86	0.26	74,75,75,77	0
20	EDO	Y	102	4/4	0.86	0.13	59,59,61,65	0
20	EDO	C	318	4/4	0.86	0.16	39,53,59,60	0
20	EDO	V	101	4/4	0.86	0.21	60,65,68,71	0
20	EDO	W	102	4/4	0.86	0.20	58,59,62,67	0
20	EDO	Q	202	4/4	0.86	0.19	65,67,71,77	0
20	EDO	D	204[A]	4/4	0.87	0.17	46,55,59,64	1
20	EDO	Q	203	4/4	0.87	0.17	47,58,58,61	0
20	EDO	P	318	4/4	0.87	0.14	38,42,46,46	0
20	EDO	N	629	4/4	0.87	0.40	110,114,115,115	0
20	EDO	P	313	4/4	0.87	0.15	60,62,63,63	0
20	EDO	C	317	4/4	0.87	0.22	75,78,78,79	0
29	PO4	H	104	5/5	0.87	0.14	90,91,95,96	0
20	EDO	A	617	4/4	0.87	0.25	52,56,61,62	0
20	EDO	R	204	4/4	0.88	0.18	68,68,69,70	0
20	EDO	N	625	4/4	0.88	0.22	54,56,58,59	0
20	EDO	L	105	4/4	0.88	0.15	53,55,57,59	0
20	EDO	S	106	4/4	0.88	0.18	40,51,51,56	0
27	DMU	Z	101	33/33	0.88	0.12	37,45,63,69	0
20	EDO	N	628	4/4	0.88	0.17	33,42,47,50	0
20	EDO	R	202	4/4	0.88	0.18	60,61,61,67	0
20	EDO	B	305	4/4	0.88	0.19	50,52,54,54	0
20	EDO	E	202	4/4	0.89	0.18	53,54,56,60	0
20	EDO	B	308	4/4	0.89	0.14	46,50,51,52	0
20	EDO	L	103	4/4	0.89	0.13	56,58,59,64	0
20	EDO	F	107	4/4	0.89	0.14	43,45,57,66	0
20	EDO	D	207	4/4	0.89	0.14	44,44,49,54	0
20	EDO	M	102	4/4	0.90	0.14	61,67,68,69	0
20	EDO	S	112	4/4	0.90	0.15	39,43,45,46	0
20	EDO	S	107	4/4	0.90	0.16	56,62,64,66	0
20	EDO	N	621	4/4	0.90	0.15	47,49,49,50	0
20	EDO	C	314	4/4	0.90	0.17	54,57,62,63	0
20	EDO	N	626	4/4	0.91	0.15	59,60,63,65	0
20	EDO	C	315	4/4	0.91	0.15	29,34,42,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	EDO	H	102	4/4	0.91	0.14	50,50,54,55	0
20	EDO	G	103	4/4	0.91	0.17	45,49,51,54	0
20	EDO	B	313	4/4	0.91	0.14	39,44,47,48	0
20	EDO	F	103	4/4	0.91	0.15	38,52,57,58	0
20	EDO	L	102	4/4	0.91	0.16	68,70,71,73	0
20	EDO	A	626	4/4	0.91	0.16	30,36,48,52	0
27	DMU	M	101	33/33	0.91	0.10	34,40,57,62	0
20	EDO	A	609	4/4	0.92	0.17	32,46,54,57	0
20	EDO	F	104	4/4	0.92	0.13	32,37,37,42	0
20	EDO	N	615	4/4	0.92	0.14	55,57,57,61	0
20	EDO	A	615	4/4	0.93	0.17	36,41,50,51	0
20	EDO	N	624	4/4	0.93	0.14	29,40,56,67	0
20	EDO	A	613	4/4	0.93	0.14	37,40,48,50	0
20	EDO	H	103	4/4	0.93	0.18	34,38,43,45	0
20	EDO	A	619	4/4	0.93	0.13	33,35,47,48	0
20	EDO	A	620	4/4	0.93	0.12	37,40,42,47	0
20	EDO	S	109	4/4	0.93	0.12	28,39,46,47	0
20	EDO	A	612	4/4	0.93	0.14	39,41,42,42	0
20	EDO	A	627	4/4	0.93	0.15	27,31,37,41	0
18	NA	P	302	1/1	0.94	0.30	17,17,17,17	1
20	EDO	A	618	4/4	0.94	0.14	30,42,54,61	0
20	EDO	E	201	4/4	0.94	0.14	59,62,66,68	0
20	EDO	N	611	4/4	0.95	0.10	36,39,40,41	0
20	EDO	K	101	4/4	0.95	0.09	49,49,50,53	0
20	EDO	P	312	4/4	0.95	0.10	28,34,39,47	0
20	EDO	N	614	4/4	0.95	0.09	36,37,41,44	0
25	PEK	C	304	53/53	0.95	0.14	26,43,87,91	0
20	EDO	A	610	4/4	0.95	0.10	27,27,31,32	0
20	EDO	O	303	4/4	0.95	0.09	29,29,30,30	0
25	PEK	P	304	53/53	0.95	0.13	25,44,95,99	0
23	CHD	C	301	29/29	0.95	0.07	23,27,31,33	0
20	EDO	O	304	4/4	0.95	0.10	40,40,44,46	0
20	EDO	P	317	4/4	0.95	0.14	36,39,40,42	0
20	EDO	N	620	4/4	0.95	0.10	37,38,41,42	0
20	EDO	T	102	4/4	0.95	0.10	31,31,36,38	0
20	EDO	R	201	4/4	0.96	0.08	40,40,41,41	0
14	PGV	C	306	51/51	0.96	0.12	21,28,77,81	0
20	EDO	C	312	4/4	0.96	0.08	31,34,34,35	0
23	CHD	B	303	29/29	0.96	0.06	22,25,33,38	0
20	EDO	A	616	4/4	0.96	0.14	28,36,38,38	0
20	EDO	N	610	4/4	0.96	0.11	26,26,26,31	0
20	EDO	S	103	4/4	0.96	0.10	33,34,38,38	0

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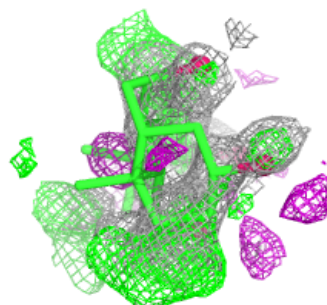
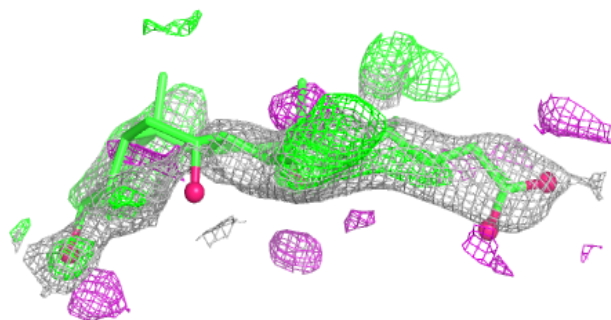
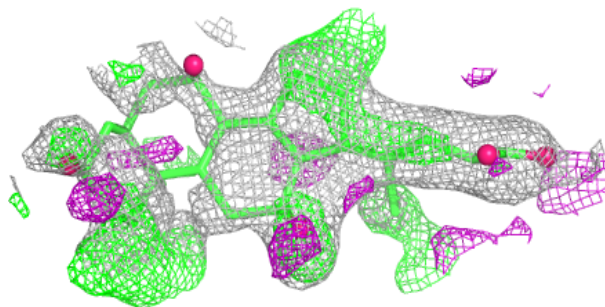
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	PGV	N	609	51/51	0.96	0.11	22,27,56,61	0
23	CHD	P	301	29/29	0.96	0.07	24,27,32,34	0
20	EDO	S	104	4/4	0.97	0.09	28,29,31,32	0
20	EDO	G	106	4/4	0.97	0.07	28,30,34,36	0
23	CHD	G	102	29/29	0.97	0.06	22,24,28,36	0
14	PGV	P	306	51/51	0.97	0.11	21,30,78,81	0
20	EDO	F	106	4/4	0.97	0.09	29,31,32,35	0
20	EDO	N	622	4/4	0.97	0.12	30,36,38,39	0
14	PGV	A	608	51/51	0.97	0.10	21,26,56,58	0
20	EDO	N	613	4/4	0.97	0.06	22,26,27,30	0
19	CMO	N	607[A]	2/2	0.98	0.13	19,19,19,19	2
19	CMO	N	607[B]	2/2	0.98	0.13	18,18,18,19	2
20	EDO	S	102	4/4	0.98	0.06	22,23,23,23	0
20	EDO	E	203	4/4	0.98	0.06	36,39,40,41	0
20	EDO	B	306	4/4	0.98	0.06	23,23,26,30	0
15	HEA	A	603	60/60	0.98	0.06	18,20,27,30	0
17	MG	A	605	1/1	0.98	0.03	22,22,22,22	0
20	EDO	A	611	4/4	0.98	0.07	21,23,24,27	0
24	CUA	O	302	2/2	0.99	0.04	25,25,25,25	0
15	HEA	A	602[C]	43/60	0.99	0.06	18,20,22,25	1
20	EDO	F	102	4/4	0.99	0.05	22,23,23,25	0
15	HEA	A	602[A]	60/60	0.99	0.06	18,21,28,29	18
19	CMO	A	607[A]	2/2	0.99	0.12	16,16,16,16	2
19	CMO	A	607[B]	2/2	0.99	0.12	16,16,16,16	2
15	HEA	N	602[A]	60/60	0.99	0.06	21,25,30,32	18
15	HEA	N	602[B]	60/60	0.99	0.06	21,25,30,32	18
15	HEA	N	602[C]	43/60	0.99	0.06	21,24,26,27	1
15	HEA	N	603	60/60	0.99	0.05	19,23,28,30	0
28	ZN	F	101	1/1	0.99	0.02	27,27,27,27	0
15	HEA	A	602[B]	60/60	0.99	0.06	18,21,28,30	18
17	MG	N	605	1/1	0.99	0.06	26,26,26,26	0
18	NA	N	606	1/1	1.00	0.02	31,31,31,31	0
16	CU	N	604	1/1	1.00	0.02	23,23,23,23	0
18	NA	A	606	1/1	1.00	0.05	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.02	27,27,27,27	0
16	CU	A	604	1/1	1.00	0.02	20,20,20,20	0
24	CUA	B	304	2/2	1.00	0.02	21,21,21,21	0

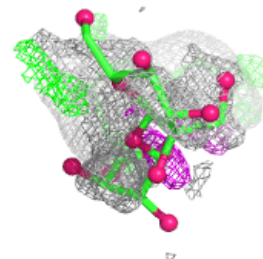
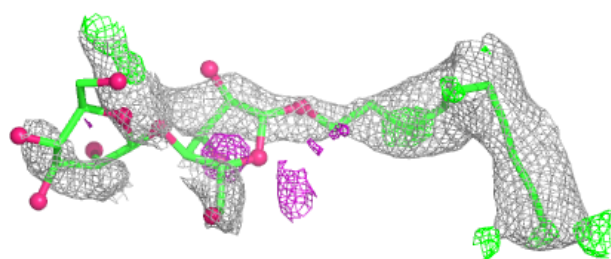
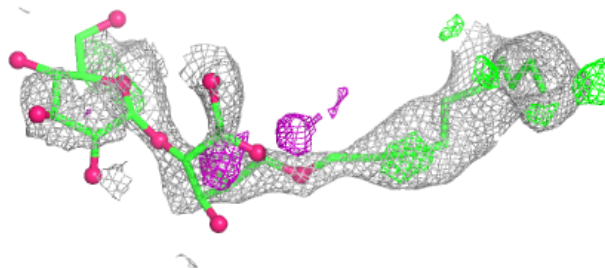
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD 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)

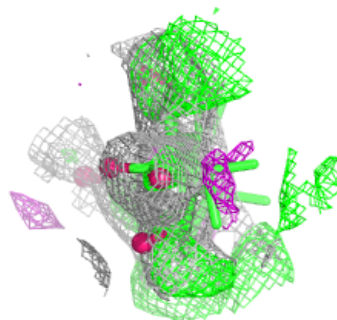
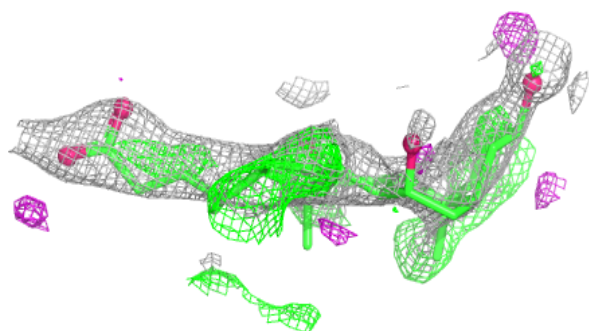
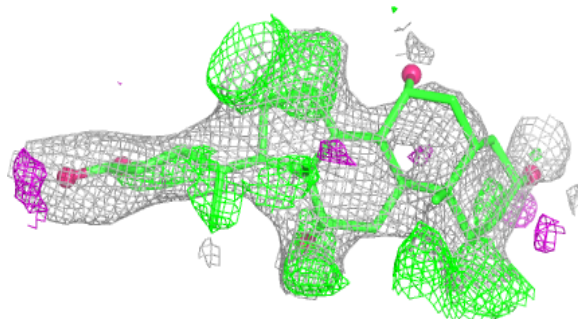
**Electron density around DMU V 102:**

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

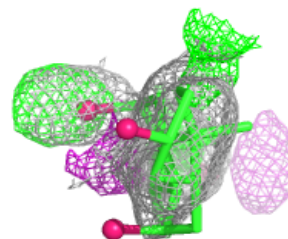
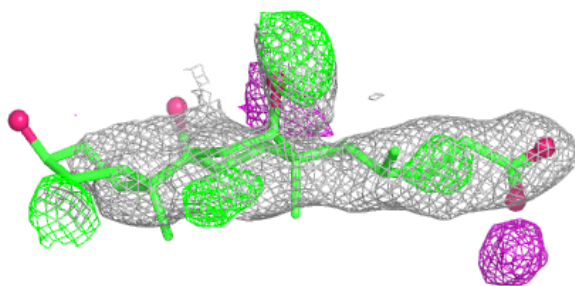
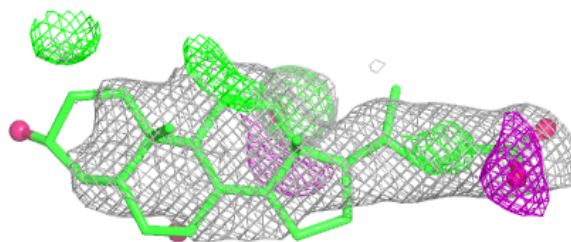


Electron density around CHD P 310:

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

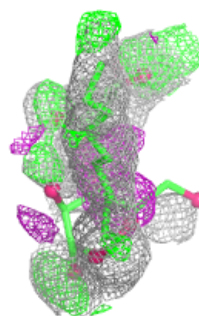
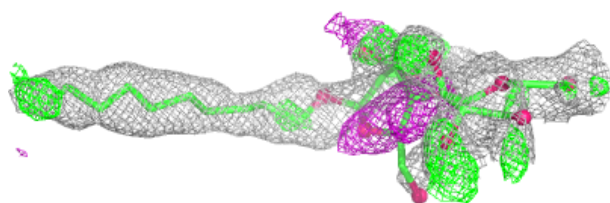
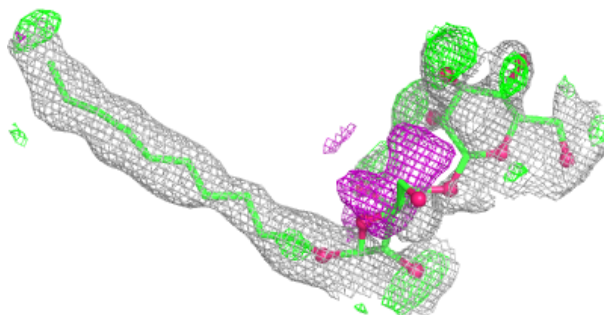
**Electron density around CHD Y 104:**

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

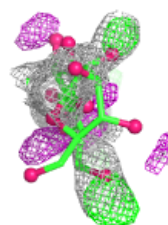
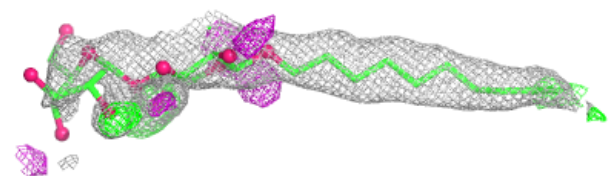
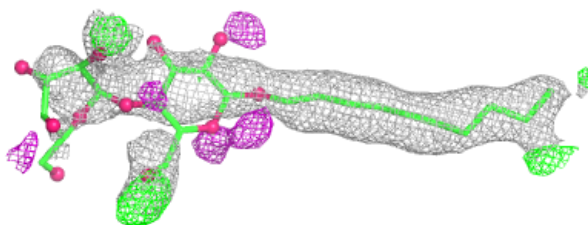


Electron density around DMU P 324:

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

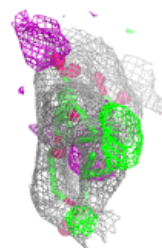
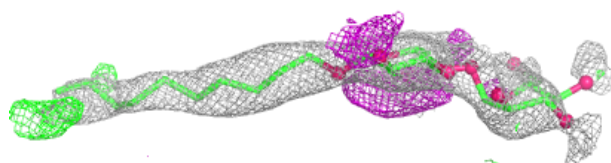
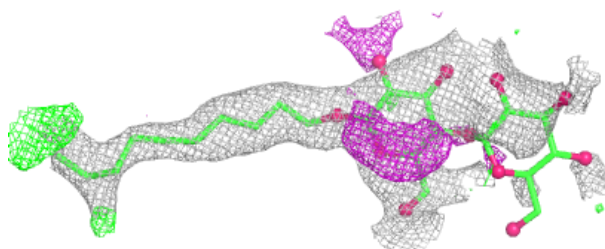
**Electron density around DMU G 108:**

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

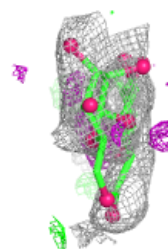
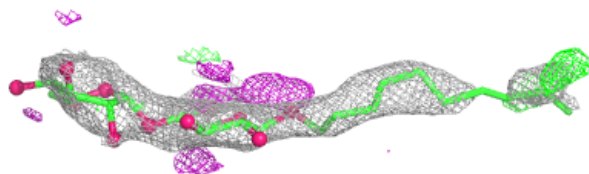
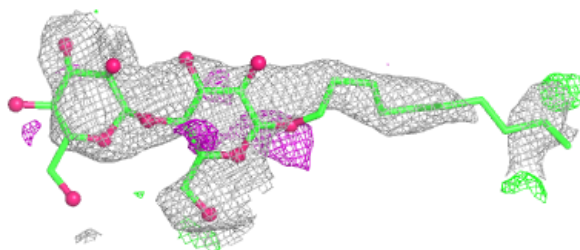


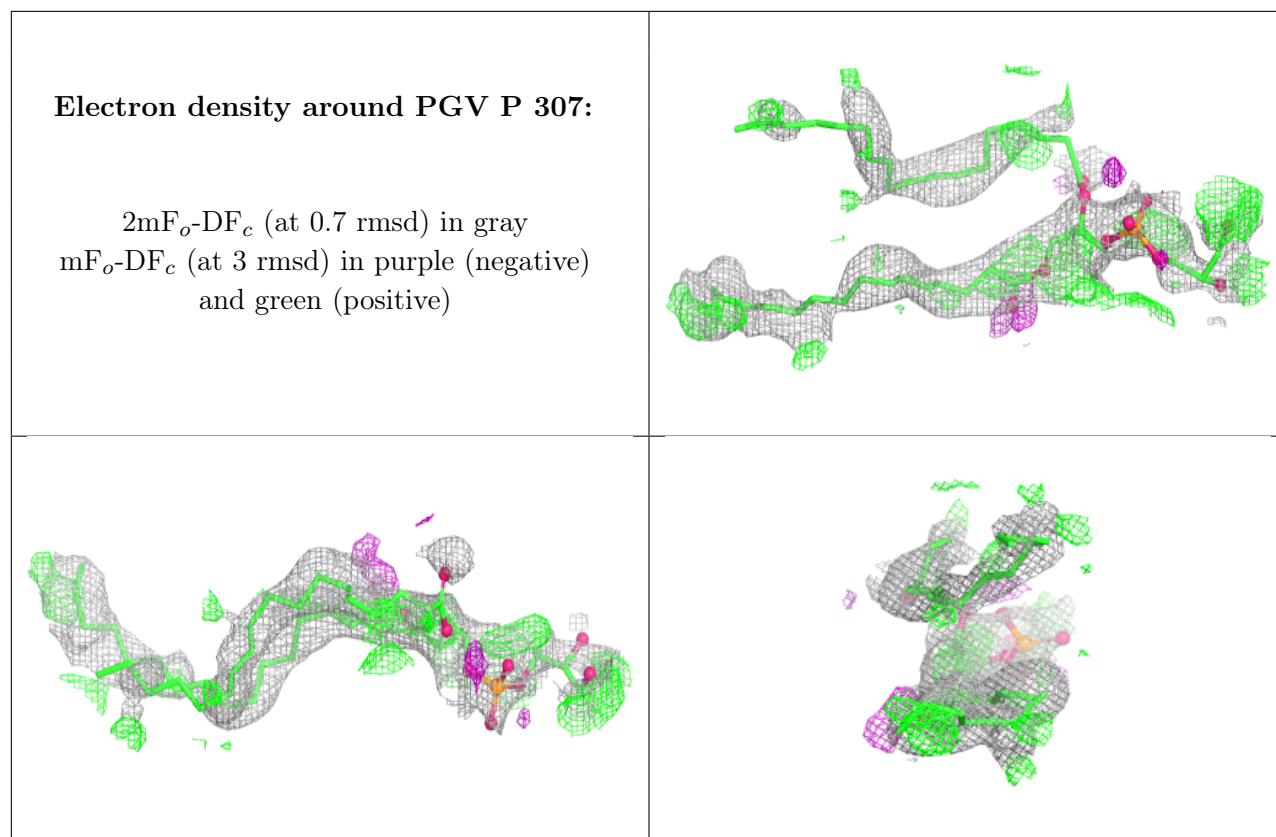
Electron density around DMU M 106:

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

**Electron density around DMU Z 102:**

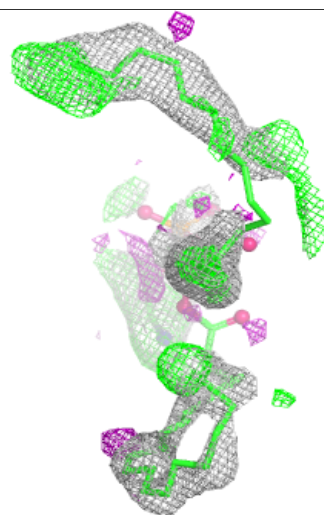
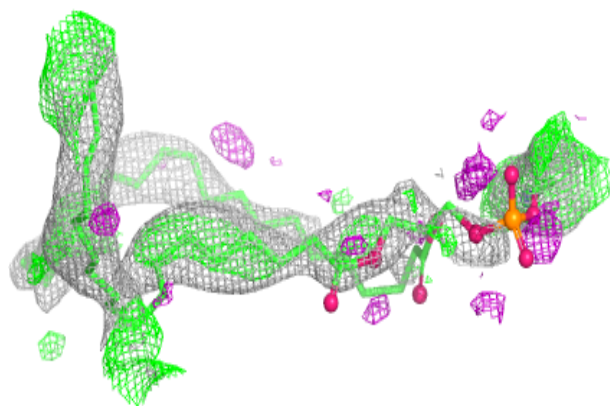
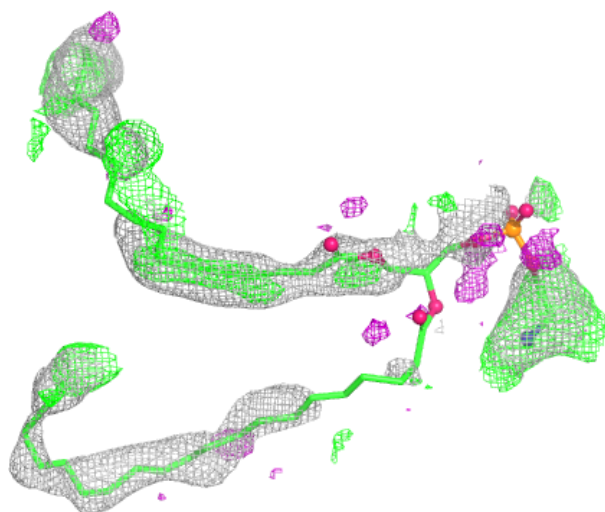
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





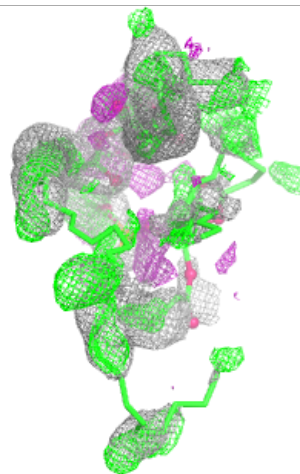
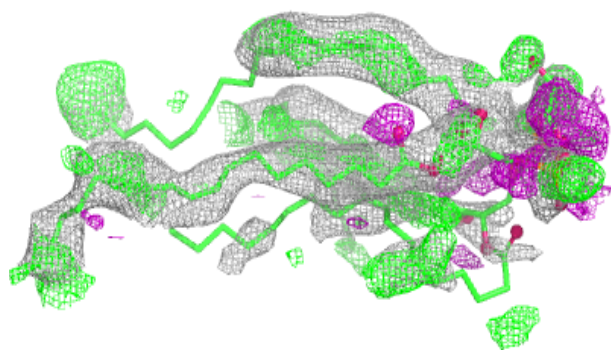
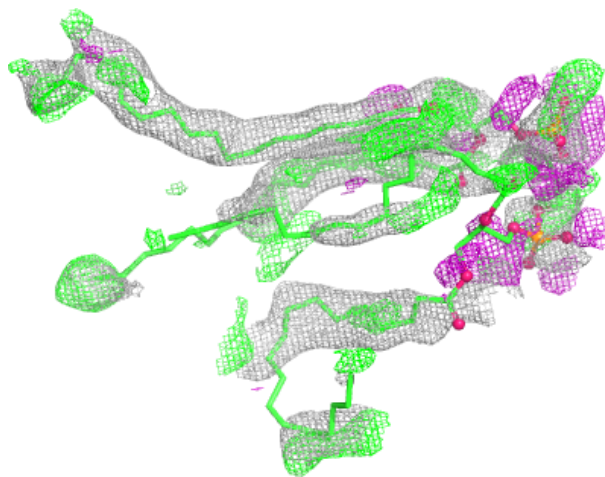
Electron density around PEK P 305:

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



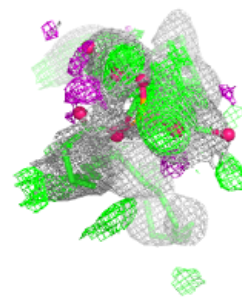
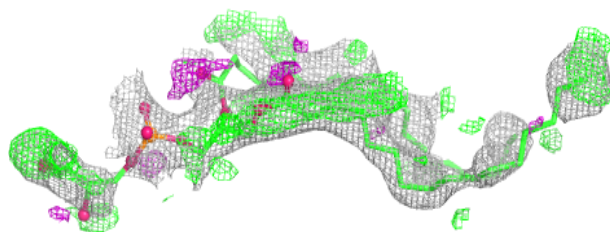
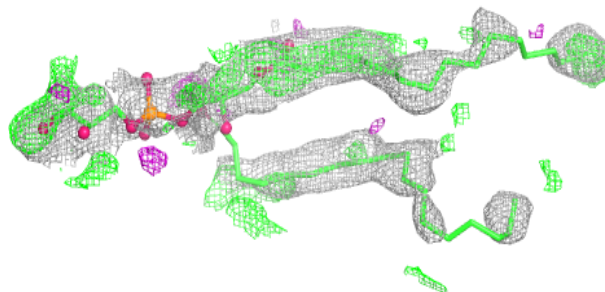
Electron density around CDL P 308:

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

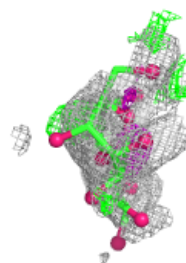
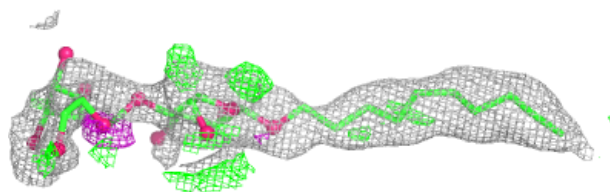
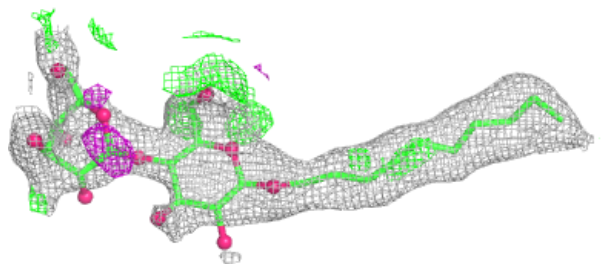


Electron density around PGV C 307:

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

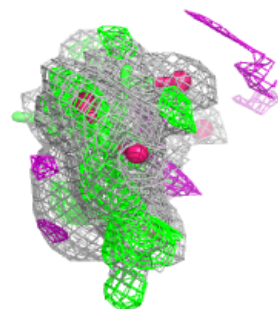
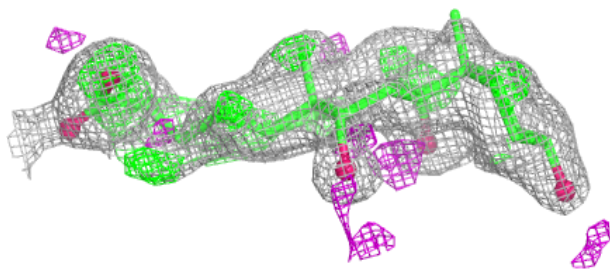
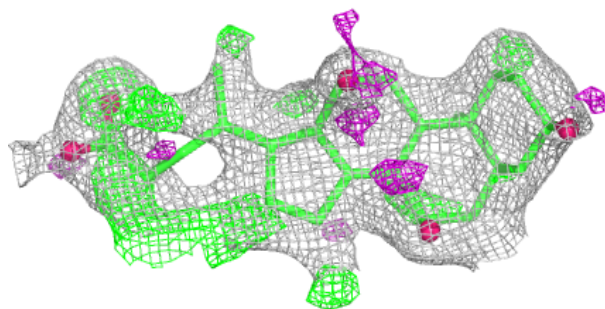
**Electron density around DMU C 319:**

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

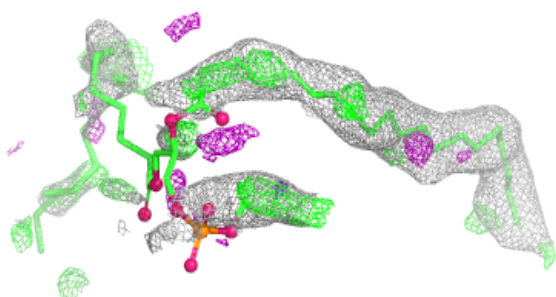
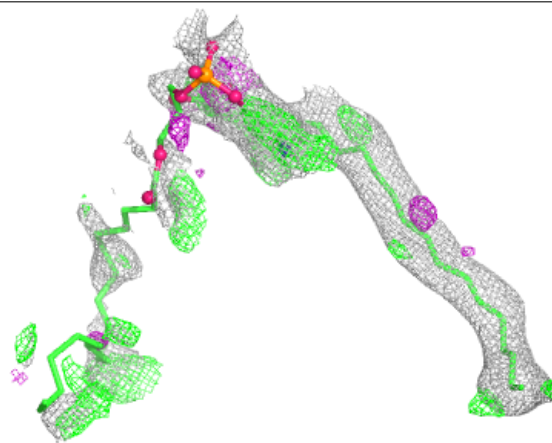


Electron density around CHD P 311:

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

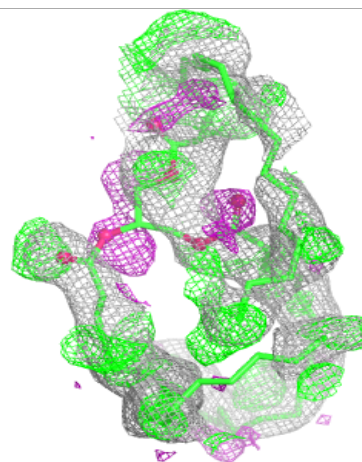
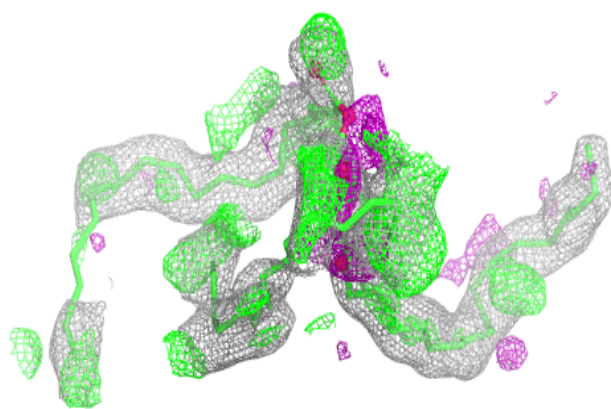
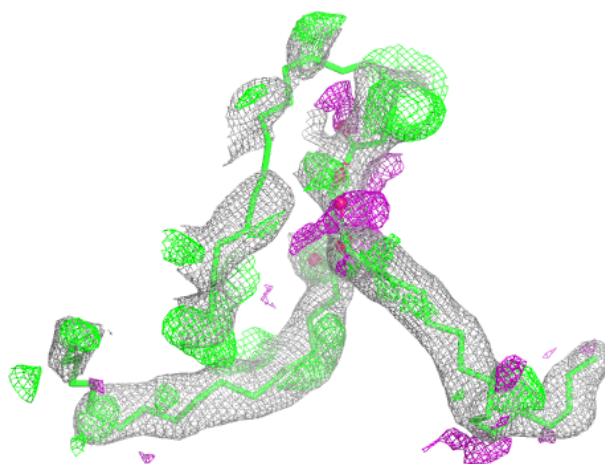
**Electron density around PEK C 303:**

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



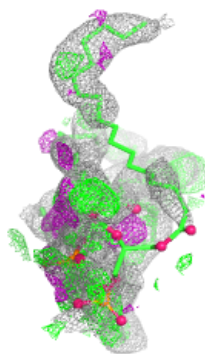
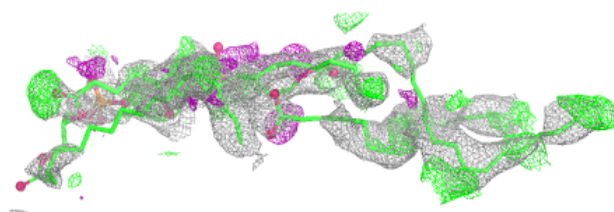
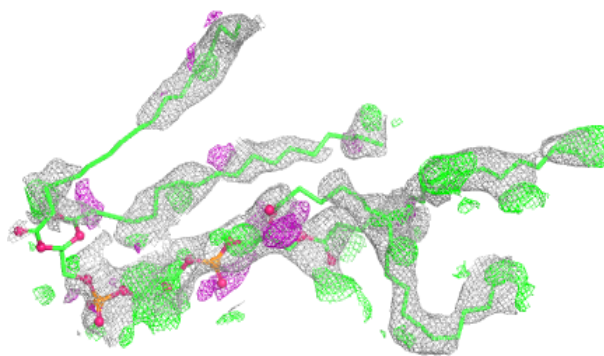
Electron density around TGL L 101:

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

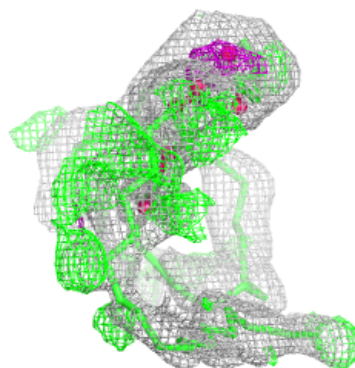
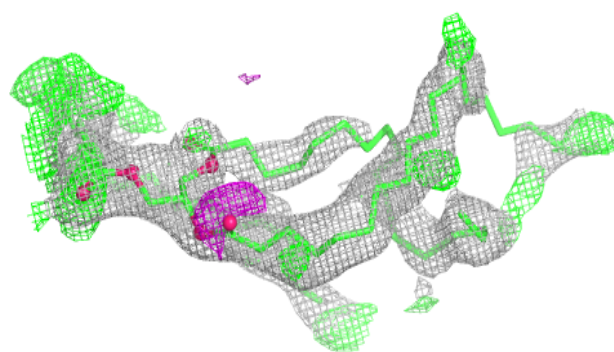
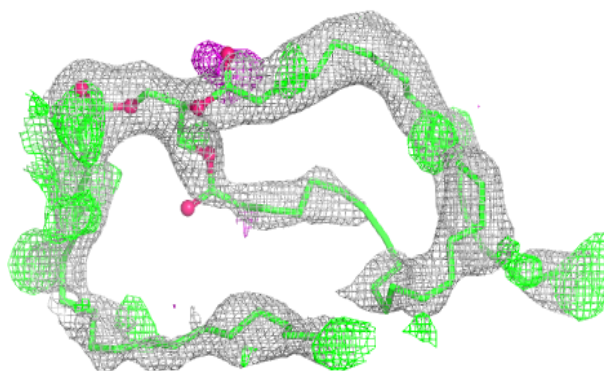


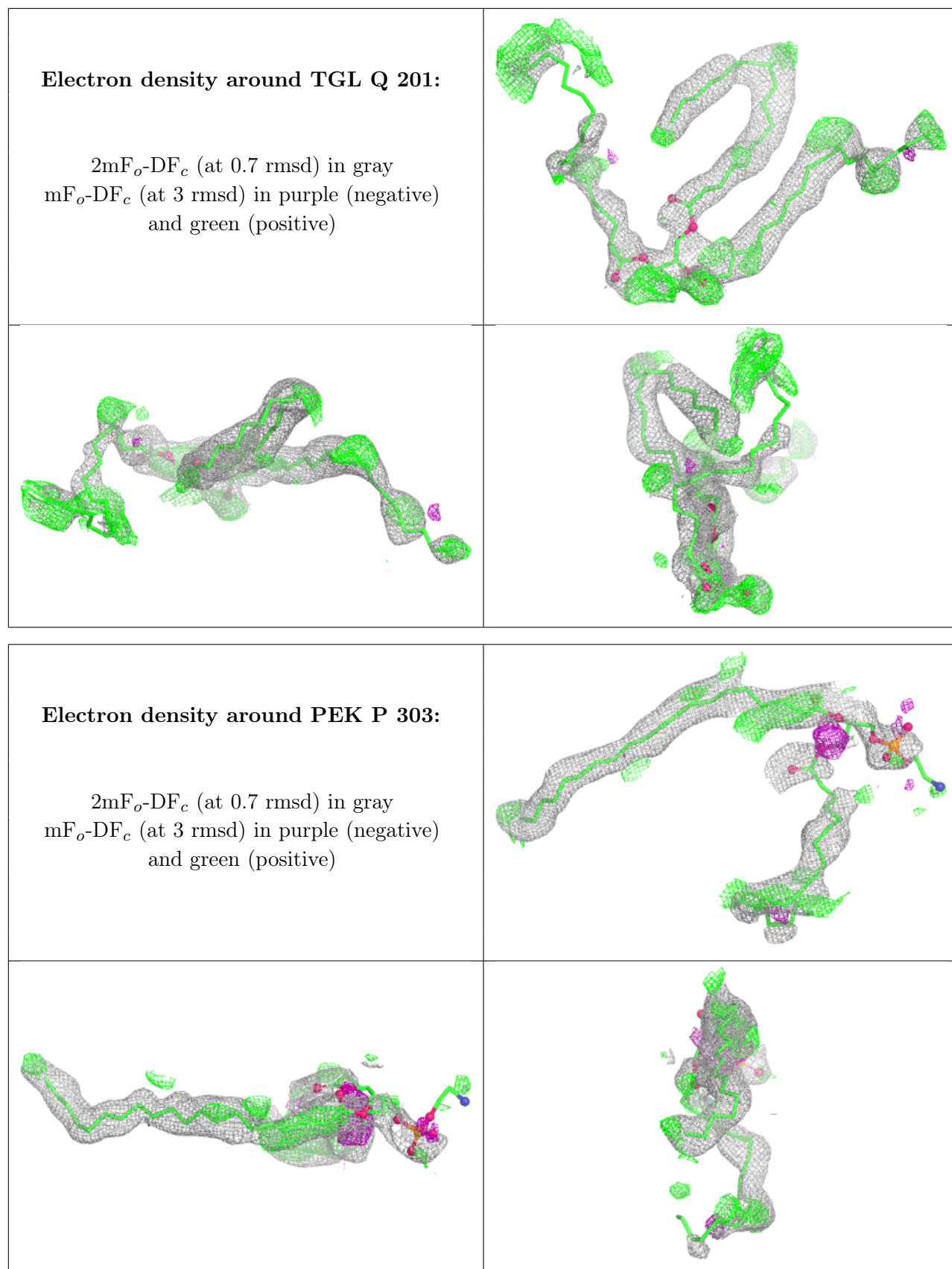
Electron density around CDL T 101:

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

**Electron density around TGL N 608:**

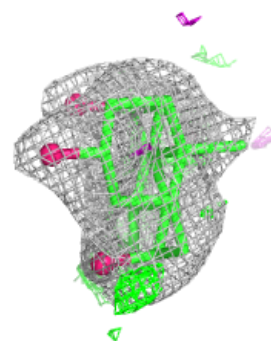
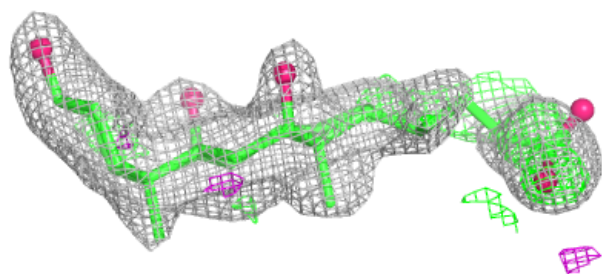
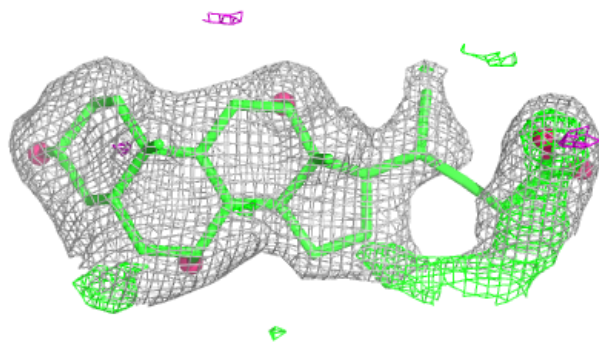
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



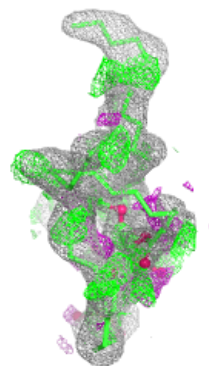
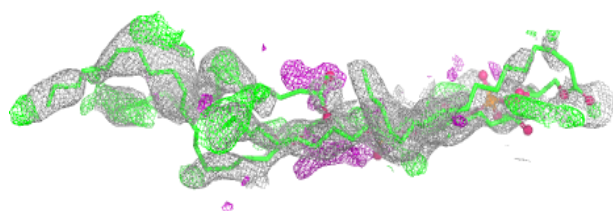
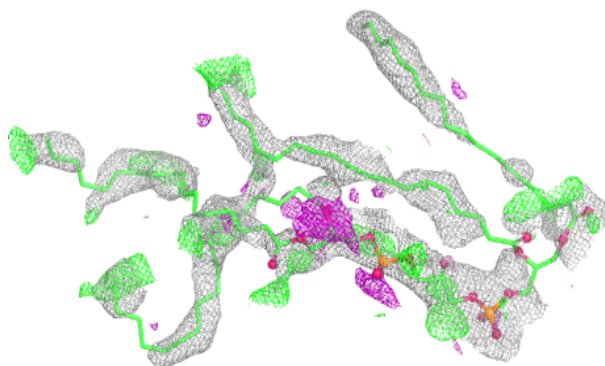


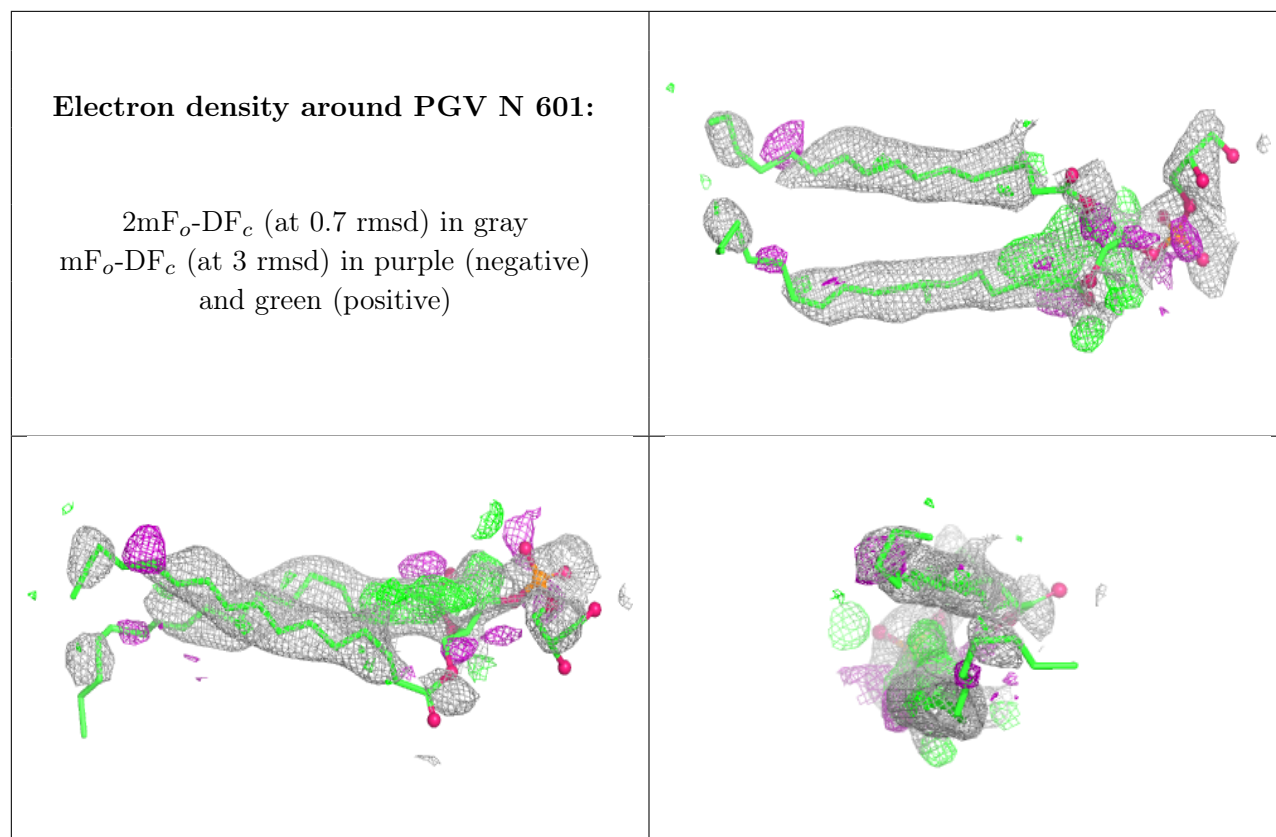
Electron density around CHD C 309:

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

**Electron density around CDL G 101:**

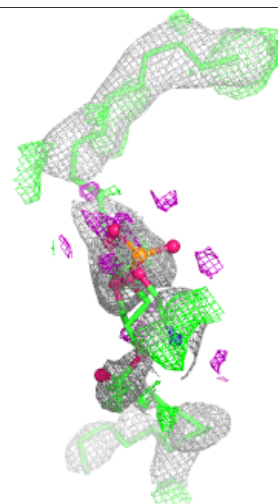
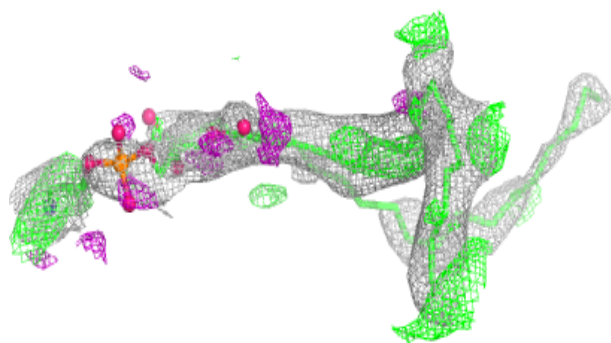
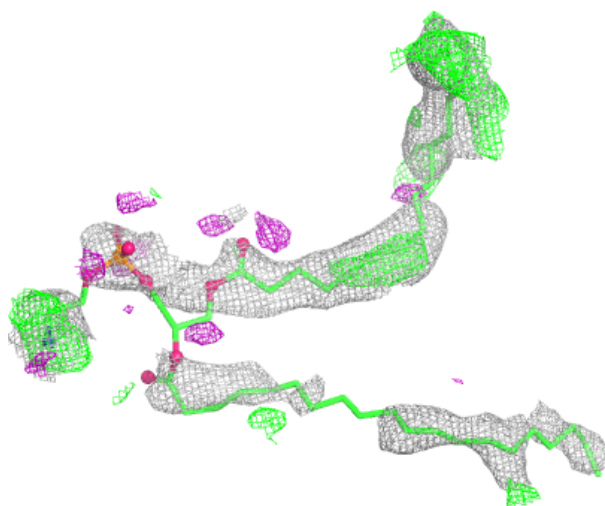
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





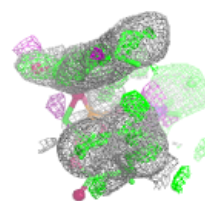
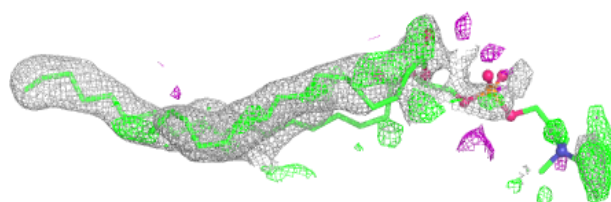
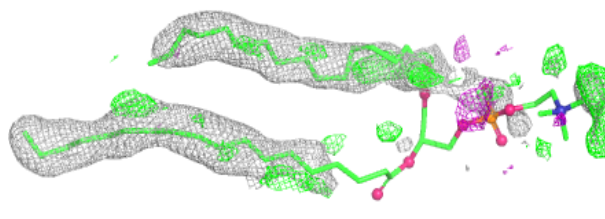
Electron density around PEK C 305:

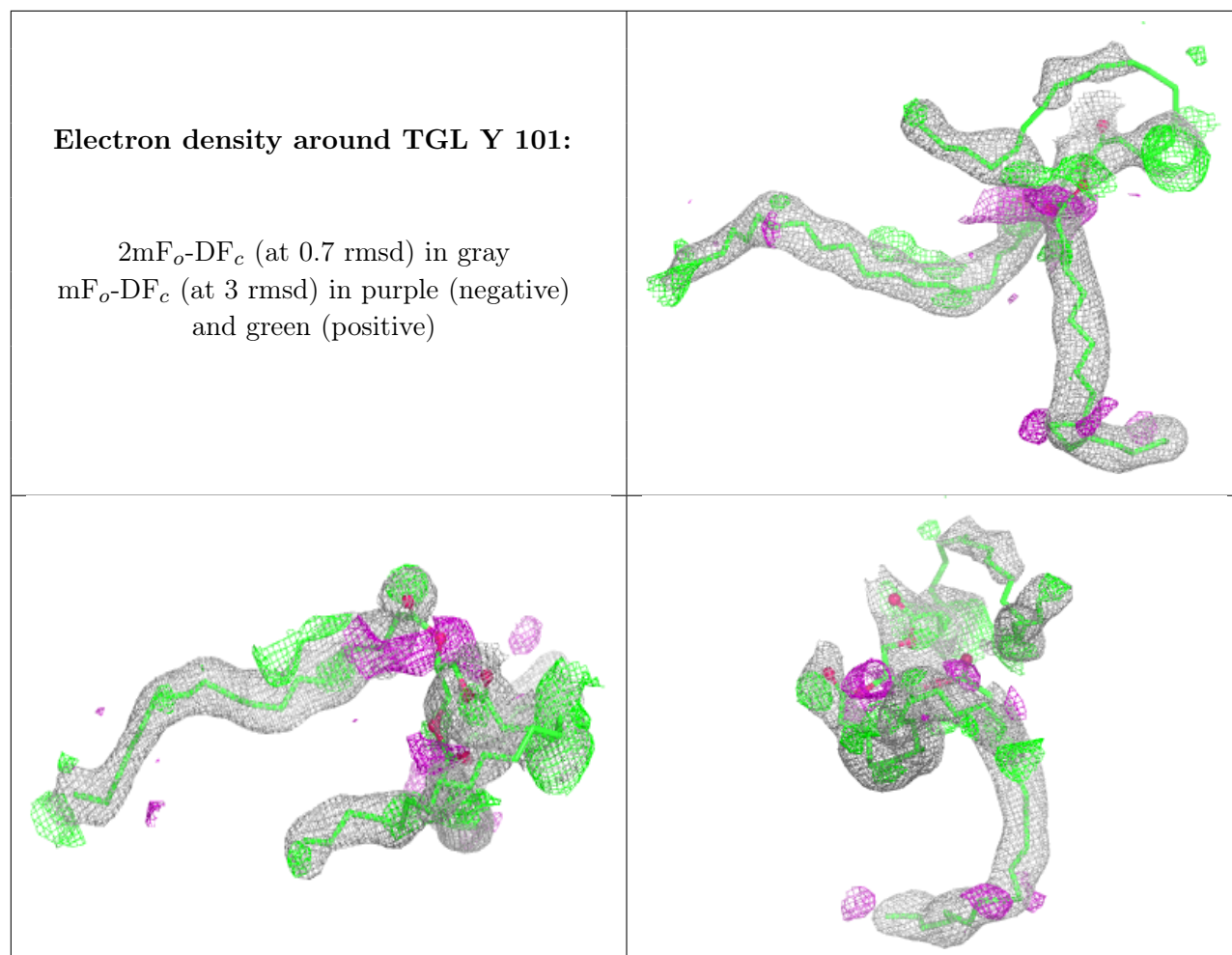
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PSC O 301:

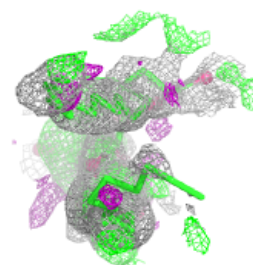
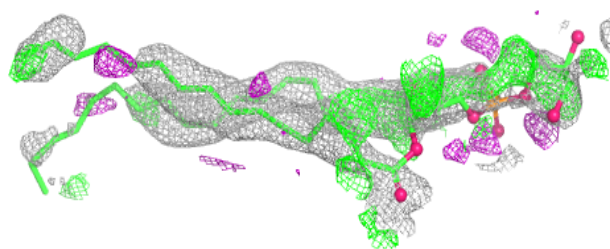
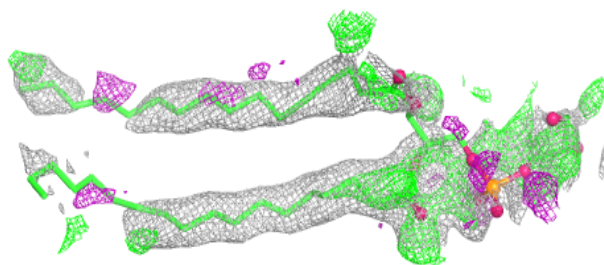
$2mF_o-DF_c$ (at 0.7 rnsd) in gray
 mF_o-DF_c (at 3 rnsd) in purple (negative)
and green (positive)



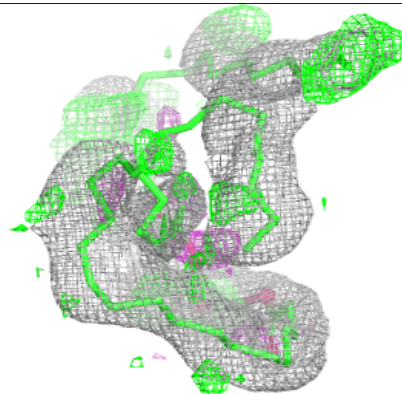
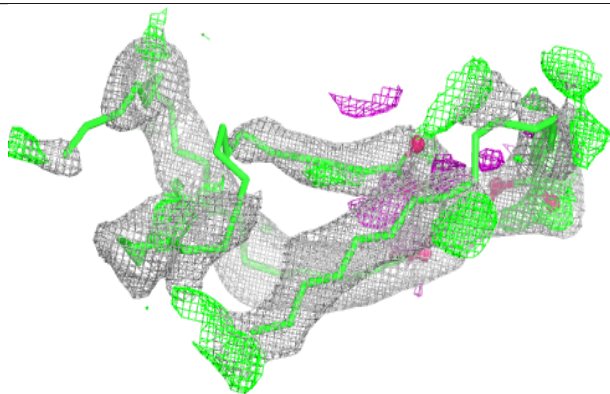
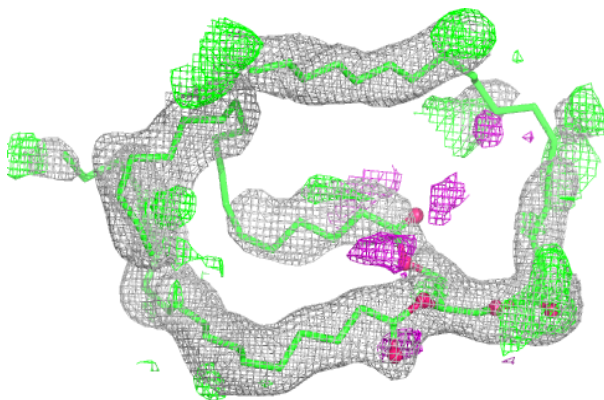


Electron density around PGV A 601:

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

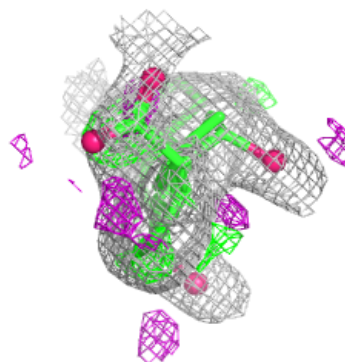
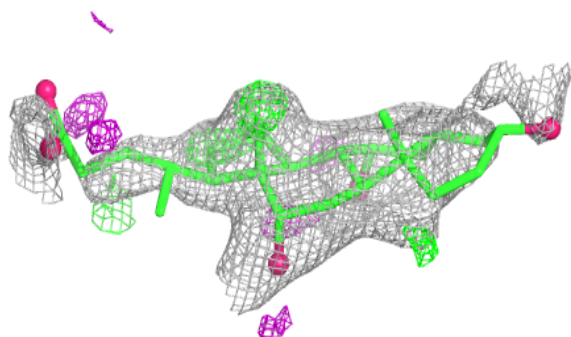
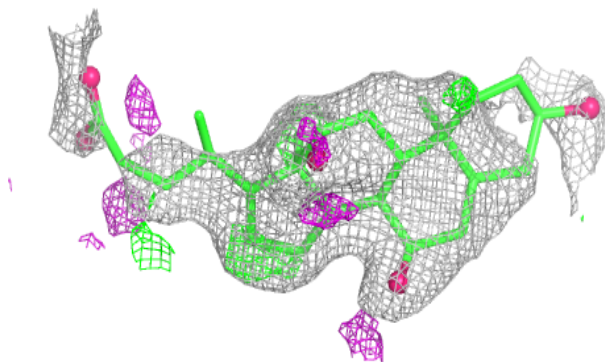
**Electron density around TGL B 301:**

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

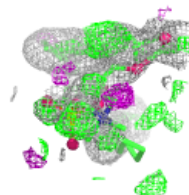
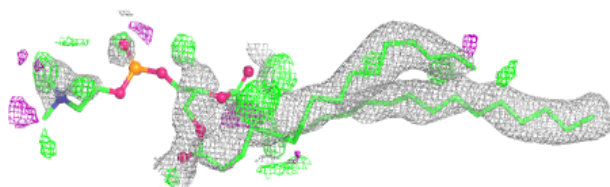
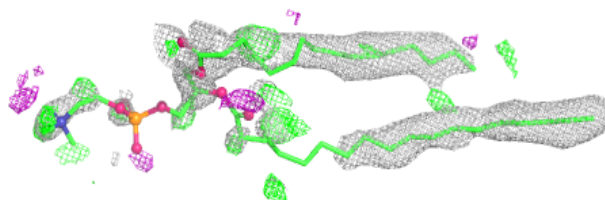


Electron density around CHD J 101:

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

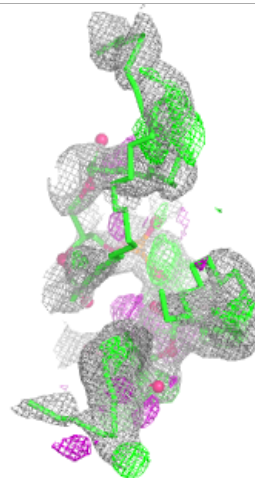
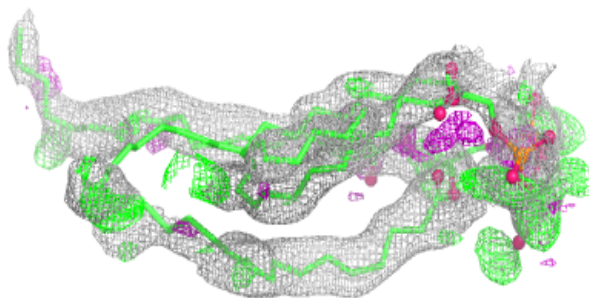
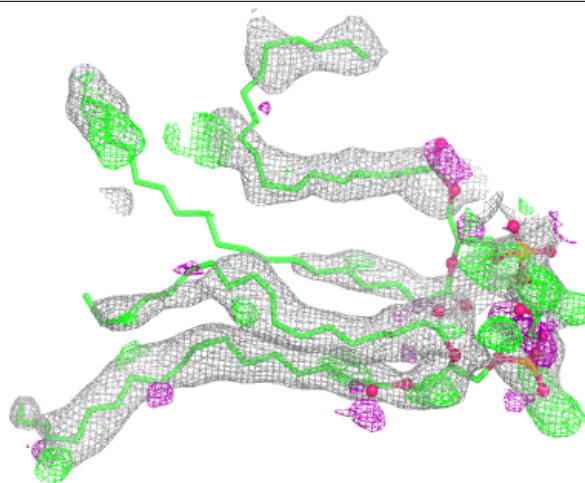
**Electron density around PSC B 302:**

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



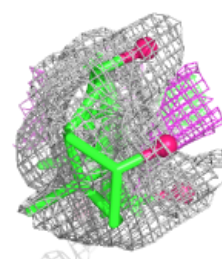
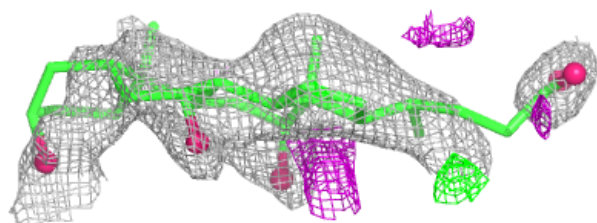
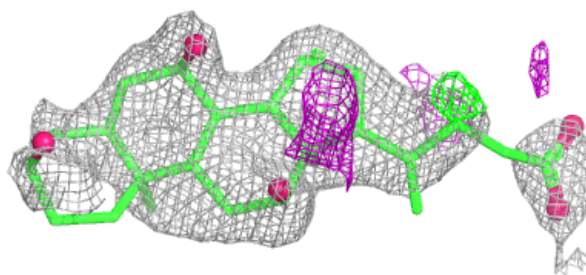
Electron density around CDL C 308:

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

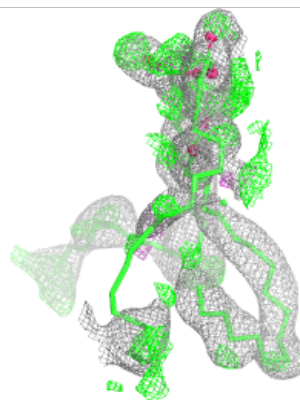
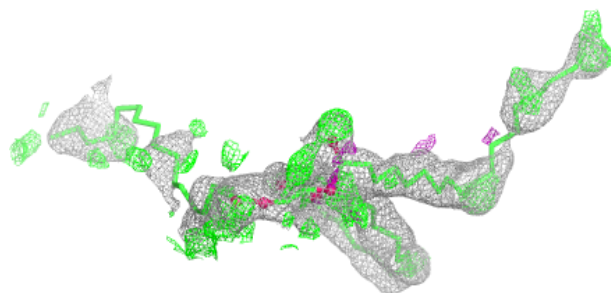
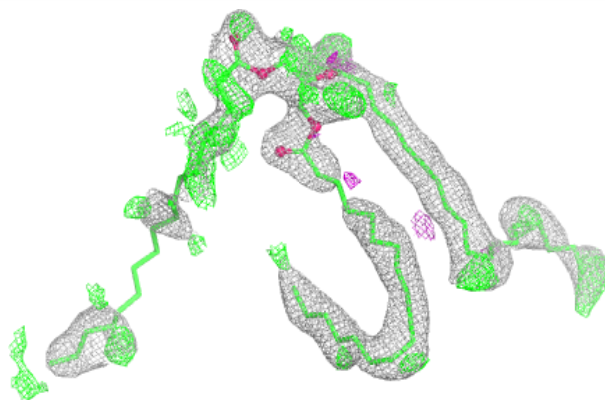


Electron density around CHD W 101:

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

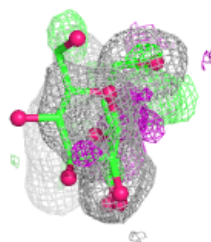
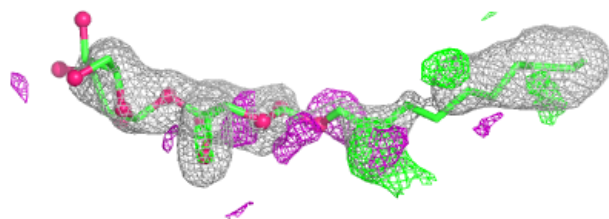
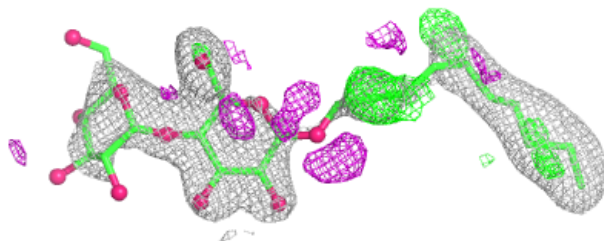
**Electron density around TGL D 201:**

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

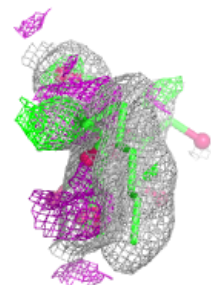
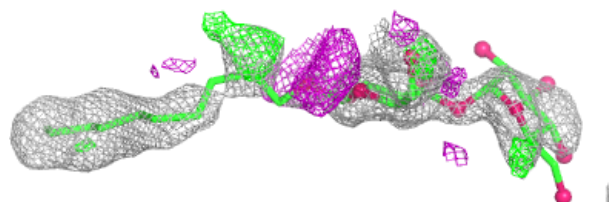
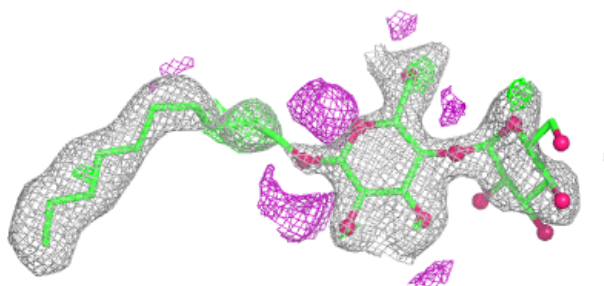


Electron density around DMU C 310:

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

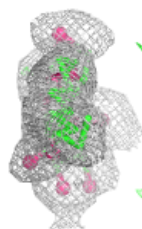
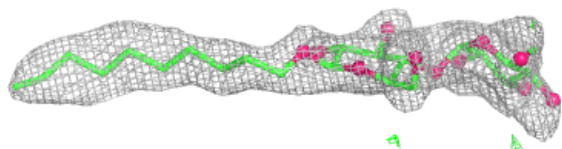
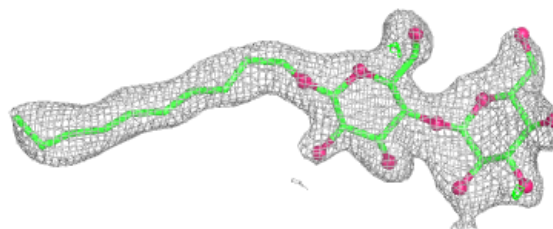
**Electron density around DMU P 309:**

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

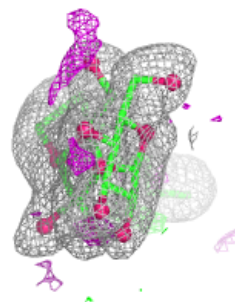
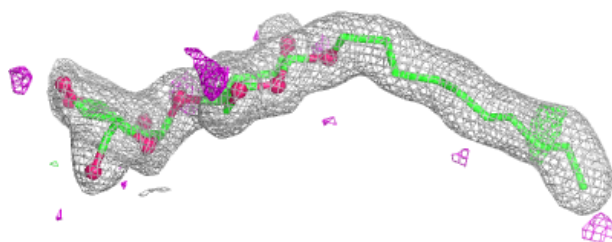
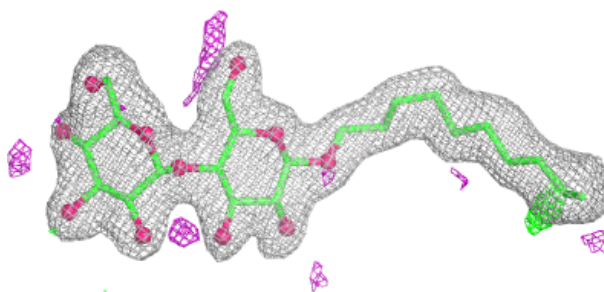


Electron density around DMU P 323:

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

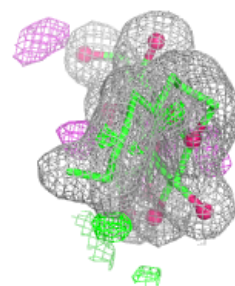
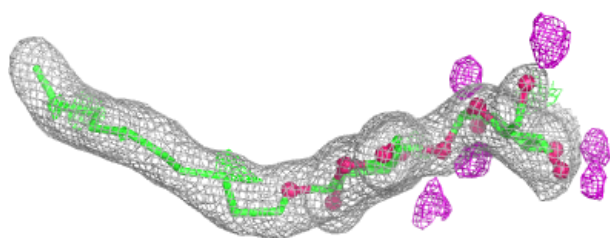
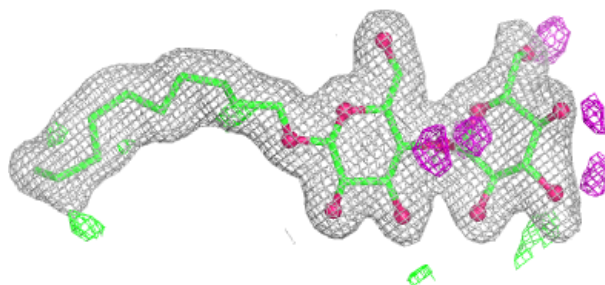
**Electron density around DMU Z 101:**

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

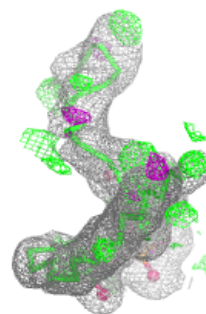
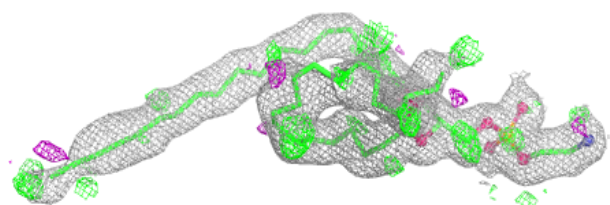
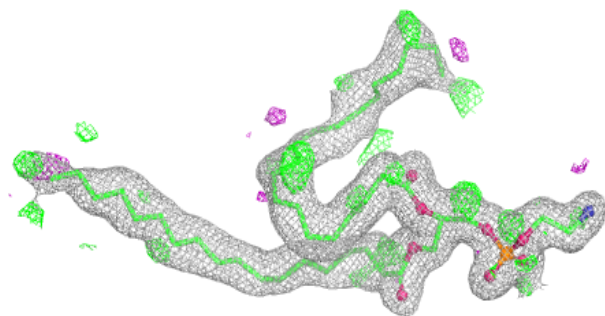


Electron density around DMU M 101:

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

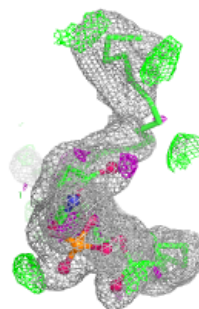
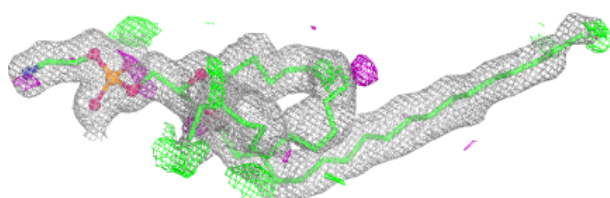
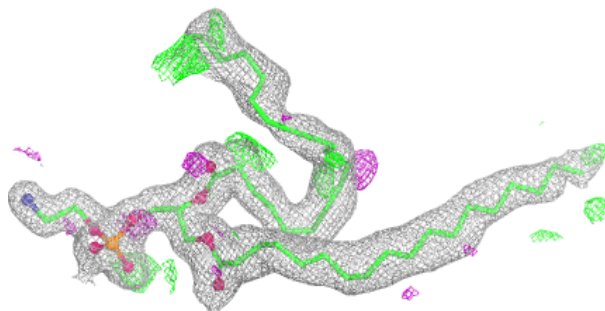
**Electron density around PEK C 304:**

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

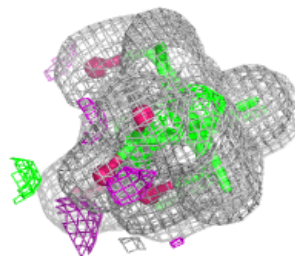
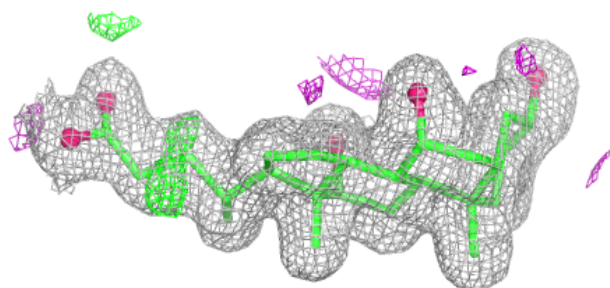
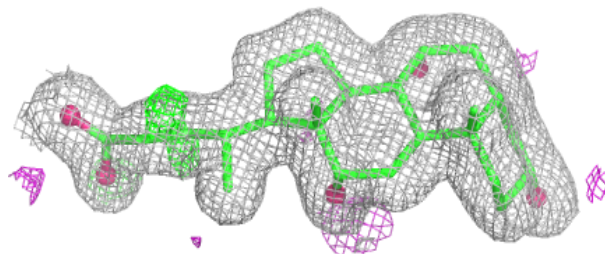


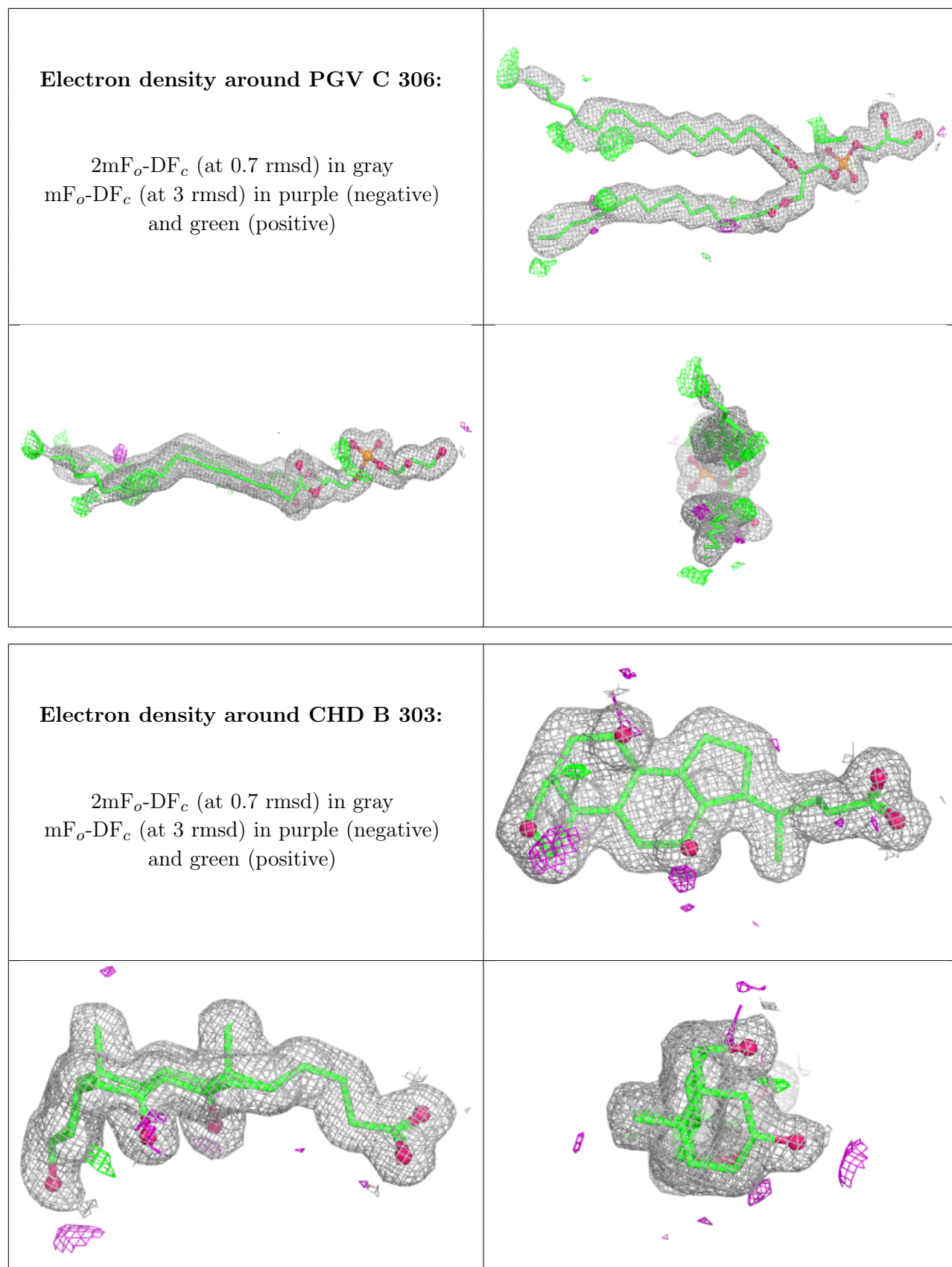
Electron density around PEK P 304:

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

**Electron density around CHD C 301:**

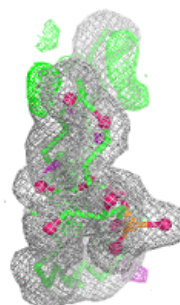
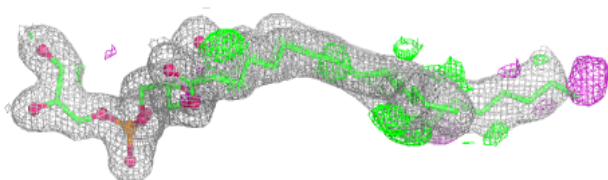
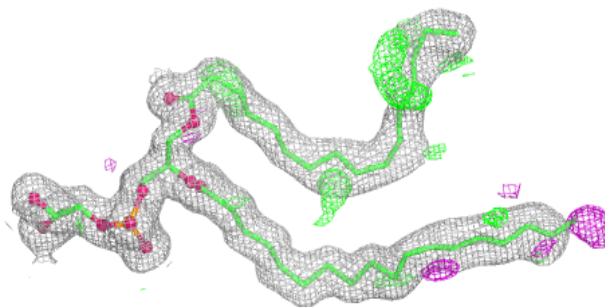
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



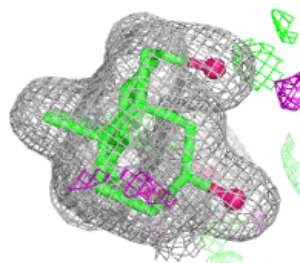
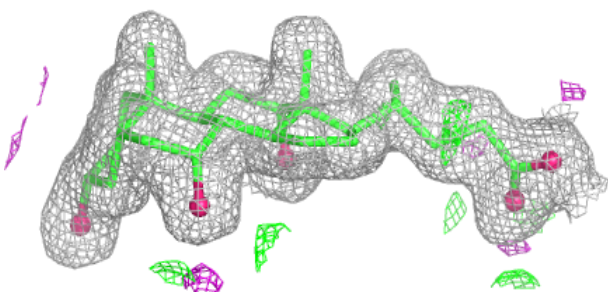
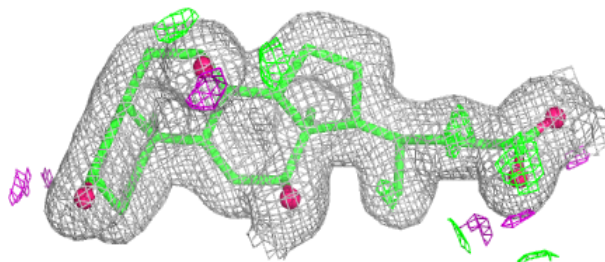


Electron density around PGV N 609:

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

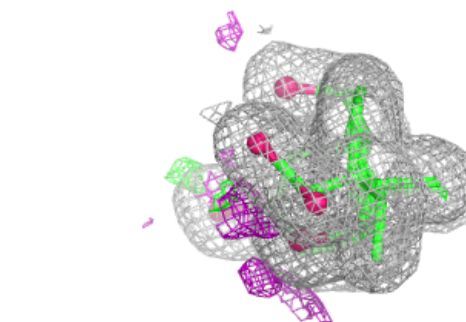
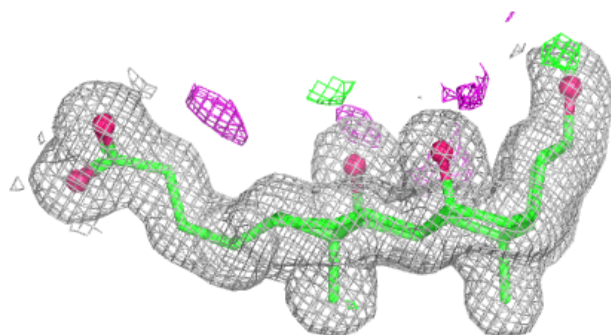
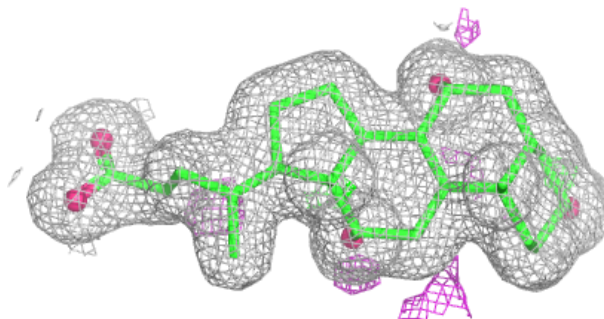
**Electron density around CHD P 301:**

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

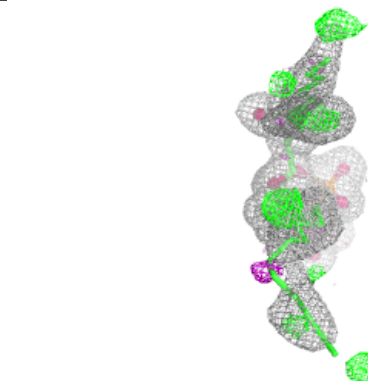
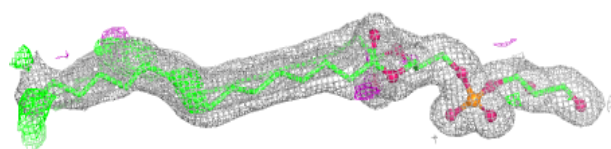
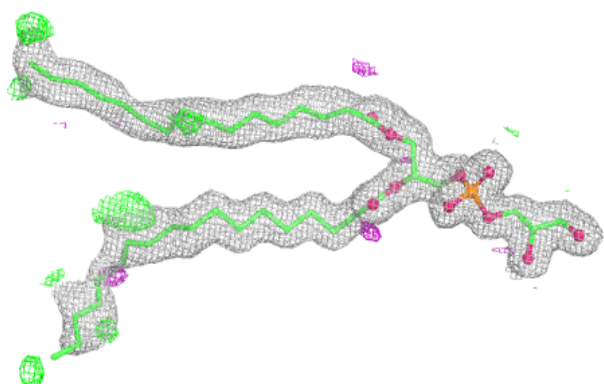


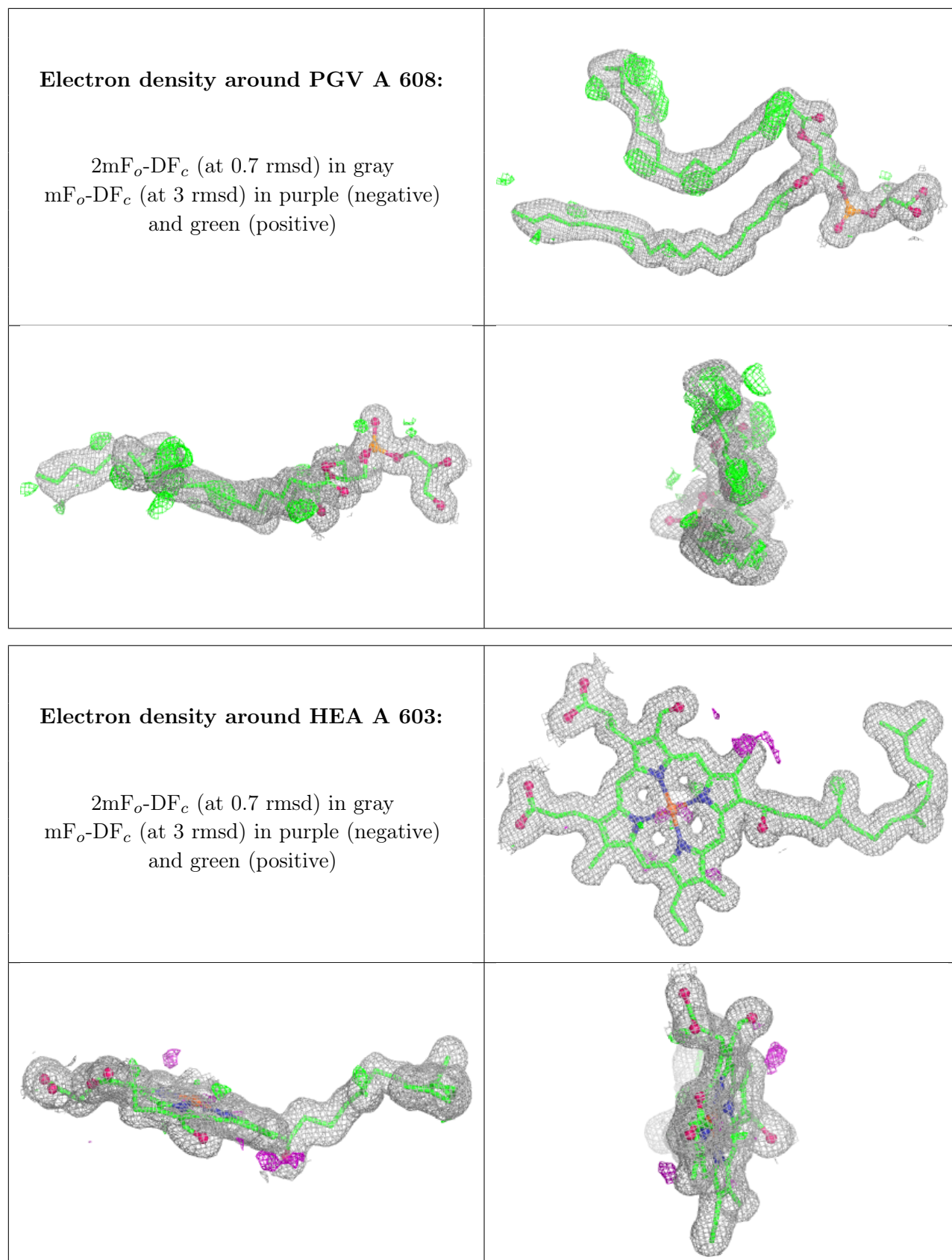
Electron density around CHD G 102:

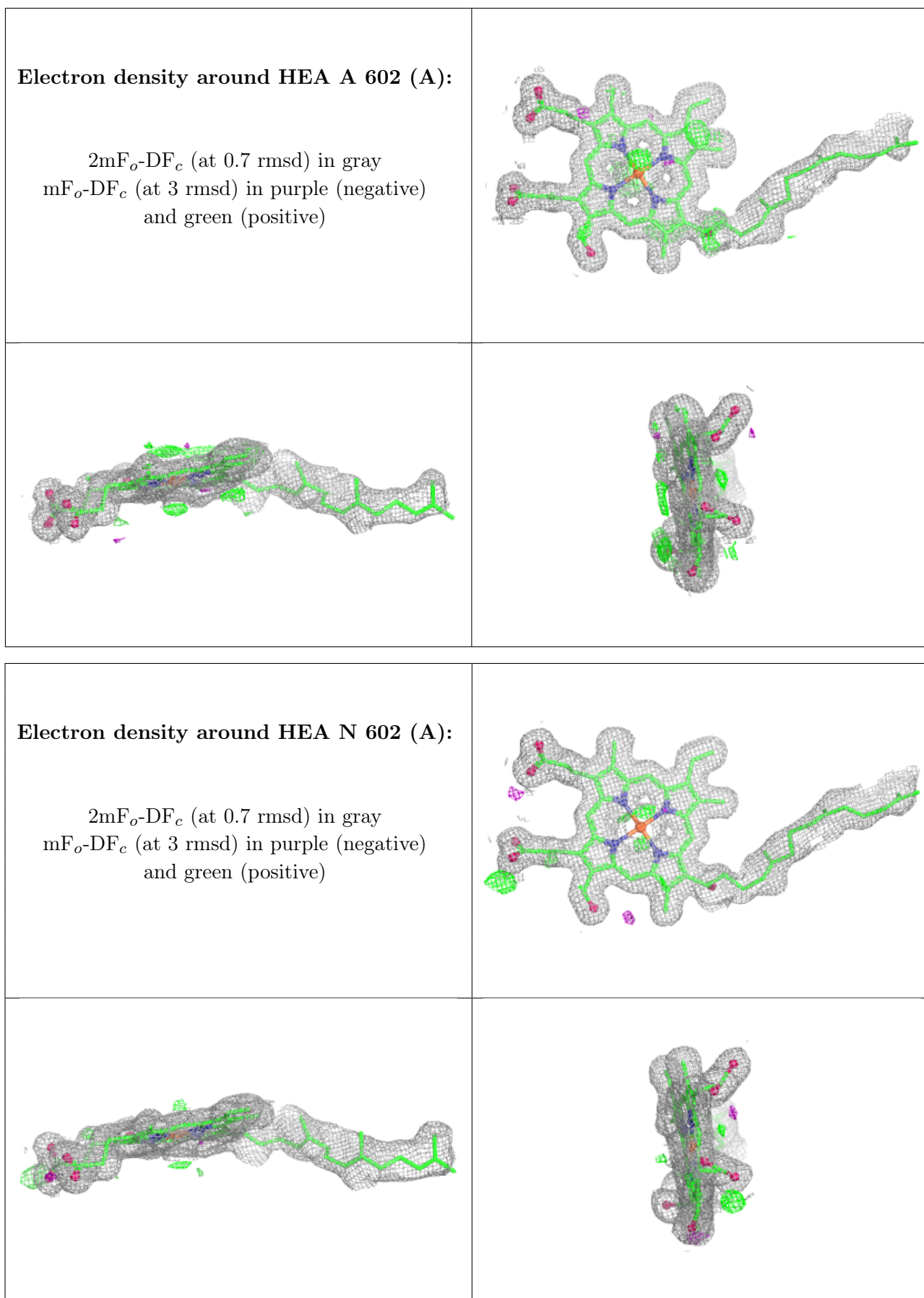
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PGV P 306:**

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

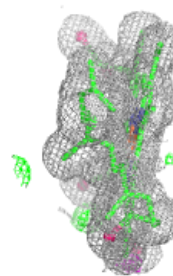
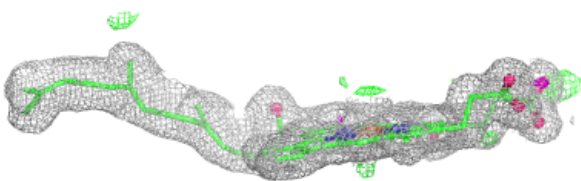
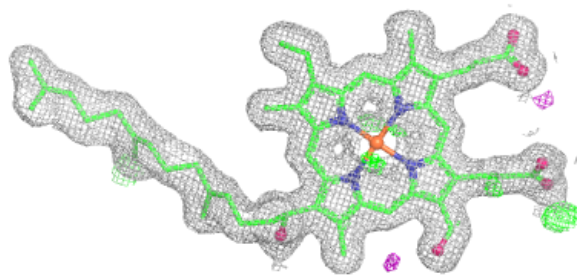




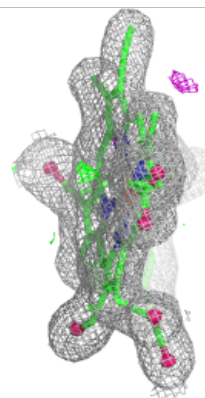
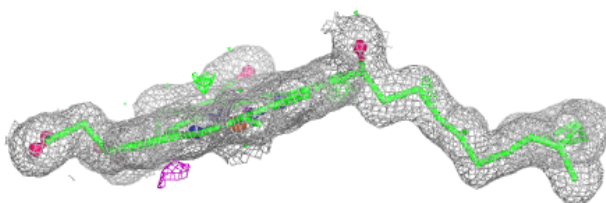
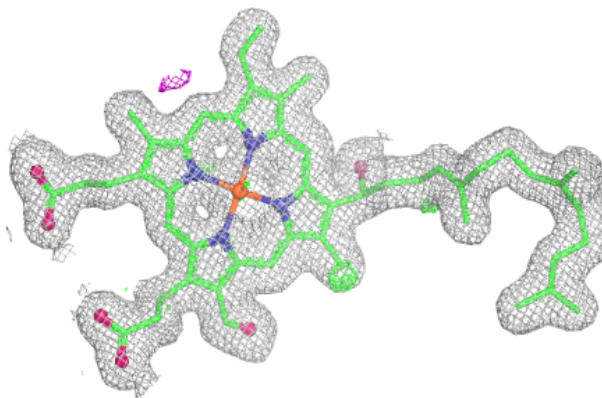


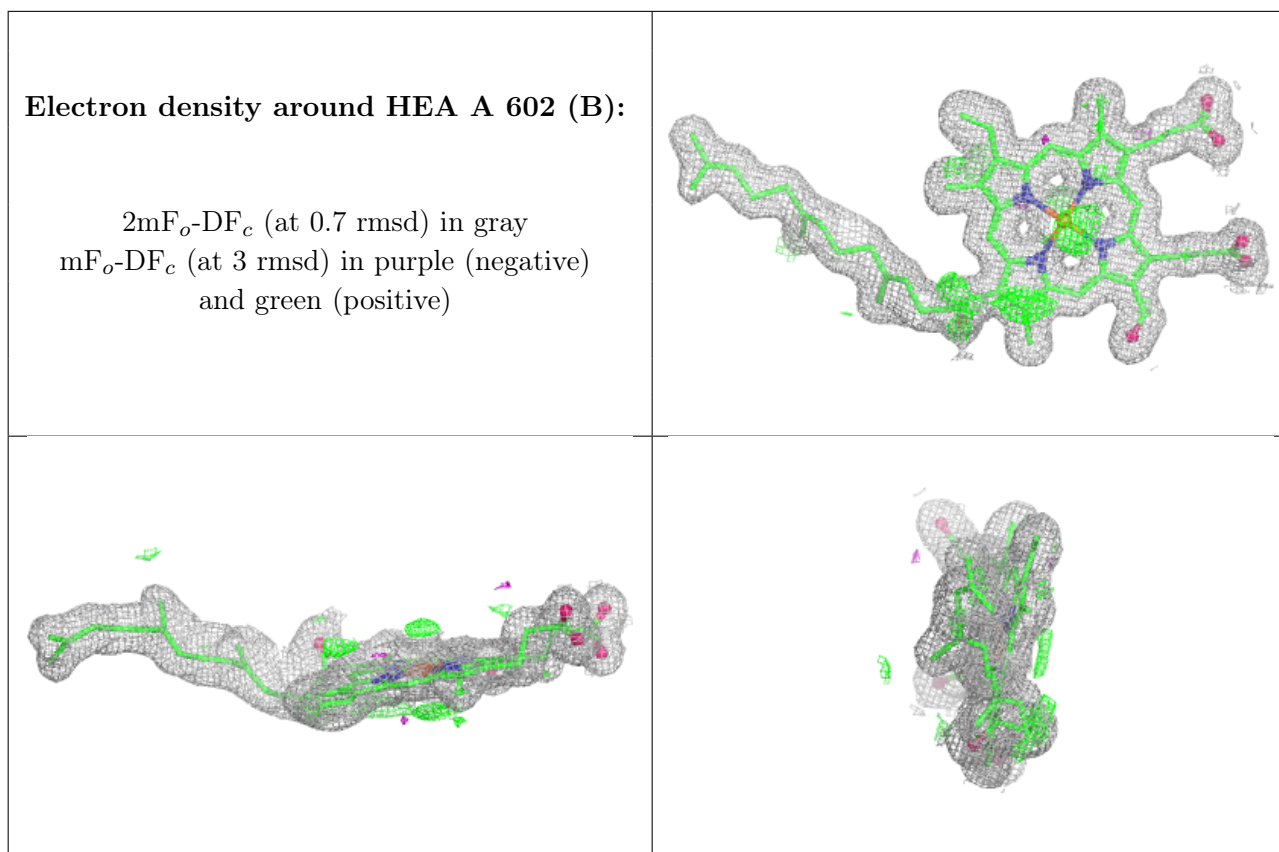
Electron density around HEA N 602 (B):

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

**Electron density around HEA N 603:**

$2mF_o-DF_c$ (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.