



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 09:06 PM EDT

PDB ID : 3AG2 / pdb_00003ag2
Title : Bovine Heart Cytochrome c Oxidase in the Carbon Monoxide-bound Fully Reduced State at 100 K
Authors : Muramoto, K.; Ohta, K.; Shinzawa-Itoh, K.; Kanda, K.; Taniguchi, M.; Nabekura, H.; Yamashita, E.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2010-03-19
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

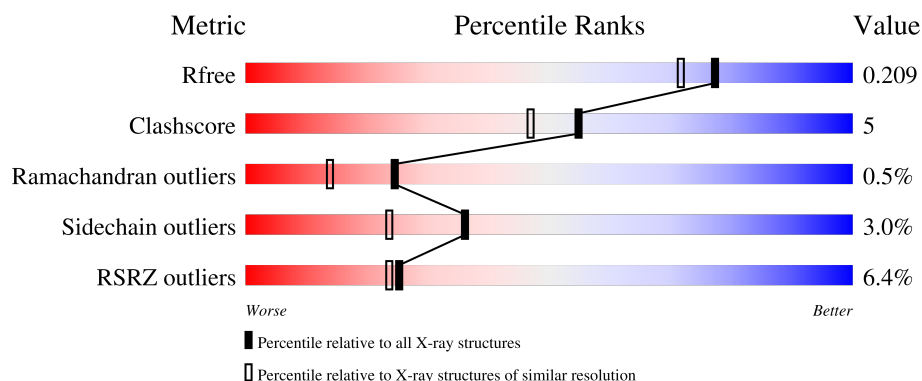
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



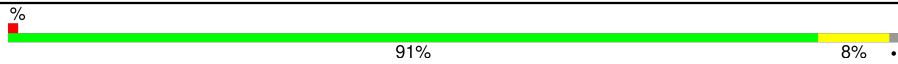
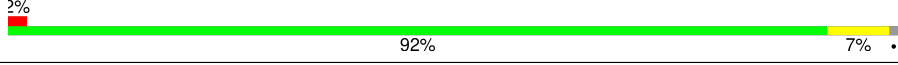
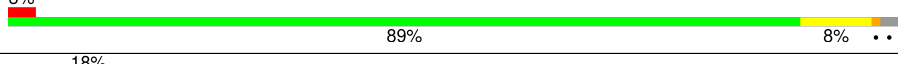
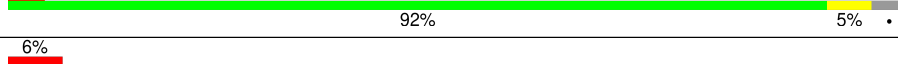
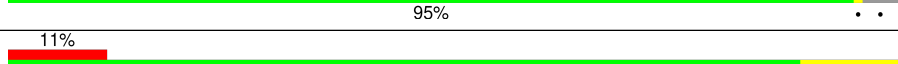
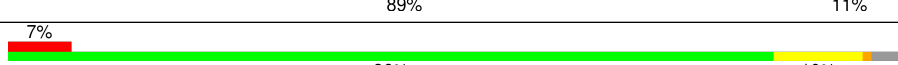
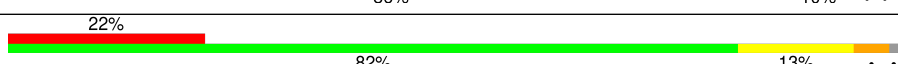
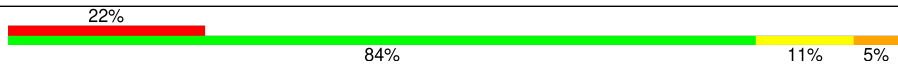
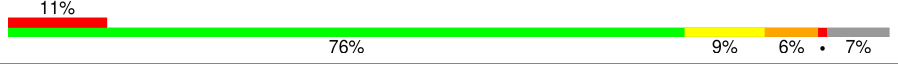
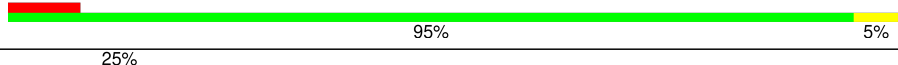
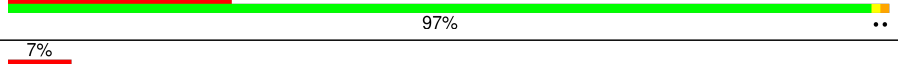
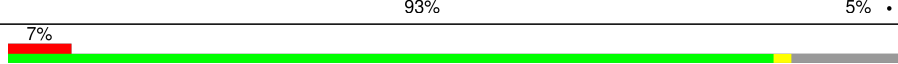
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	 92% 7% .
1	N	514	 86% 13% .
2	B	227	 85% 14% 6%
2	O	227	 81% 18% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	C	261	
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
21	EDO	A	619	-	-	X	-

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 33056 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	8	0
			4070	2715	631	687	37			
1	N	514	Total	C	N	O	S	0	10	0
			4074	2722	628	687	37			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	1	0
			1830	1191	281	340	18			
2	O	227	Total	C	N	O	S	0	2	0
			1834	1192	284	340	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	2	0
			2114	1413	336	353	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	1	0
			1203	785	196	218	4			
4	Q	141	Total	C	N	O	S	0	0	0
			1175	764	193	214	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	95	Total	C	N	O	S	0	1	0
			726	450	129	142	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	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, mitochondrial.

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

Continued on next page...

Continued from previous page...

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

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

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

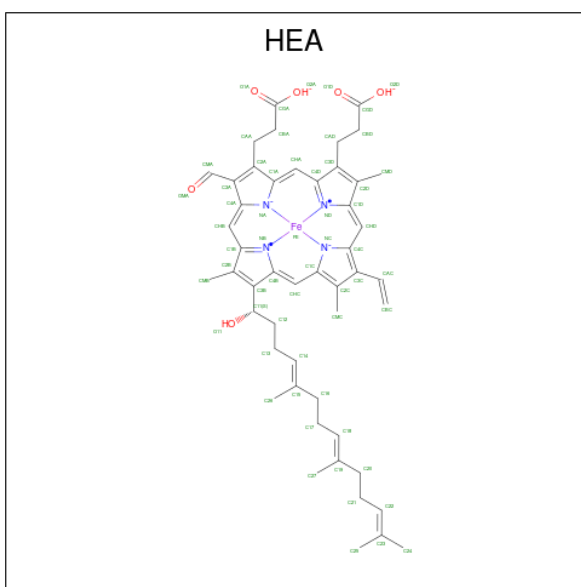
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

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

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

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

- Molecule 14 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 78	C 66	Fe 1	N 4	O 7	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 78	C 66	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

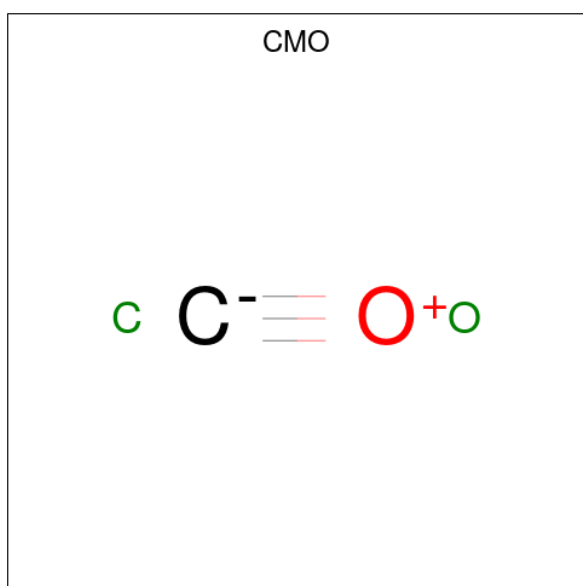
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (CCD ID: NA) (formula: Na).

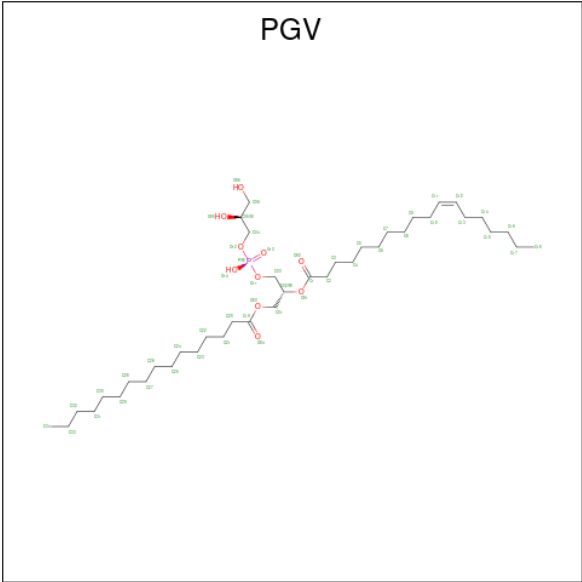
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



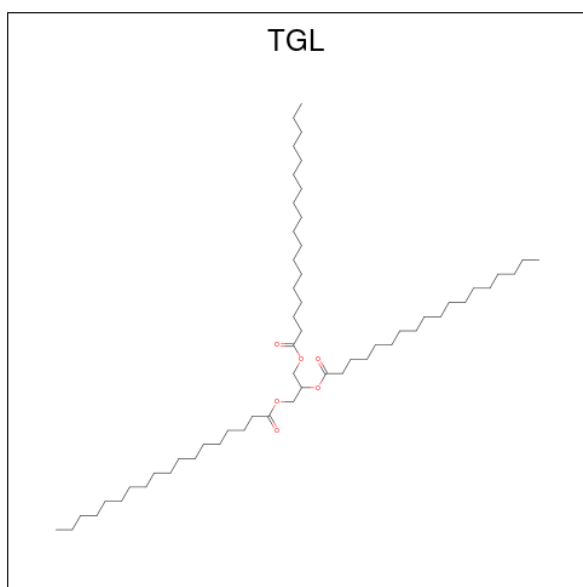
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	1
			4	2	2		
18	N	1	Total	C	O	0	1
			4	2	2		

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



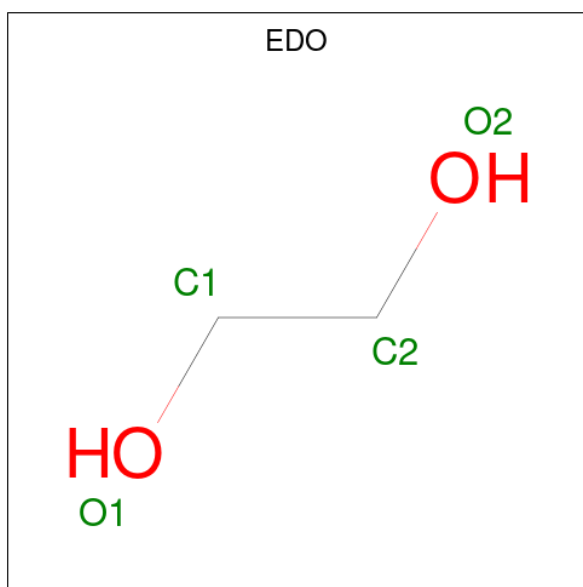
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			47	36	10	1		
19	C	1	Total	C	O	P	0	0
			49	38	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0
			47	38	8	1		
19	P	1	Total	C	O	P	0	0
			46	35	10	1		
19	Z	1	Total	C	O	P	0	0
			47	36	10	1		

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			59	53	6		
20	B	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			55	49	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	O	1	Total	C	O	0	0
			63	57	6		
20	Y	1	Total	C	O	0	0
			59	53	6		

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

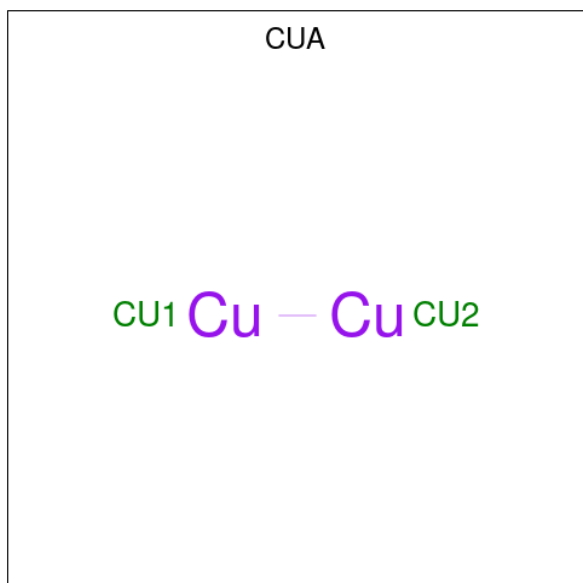
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	H	1	Total 4	C 2	O 2	0	0
21	I	1	Total 4	C 2	O 2	0	0
21	K	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 22 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



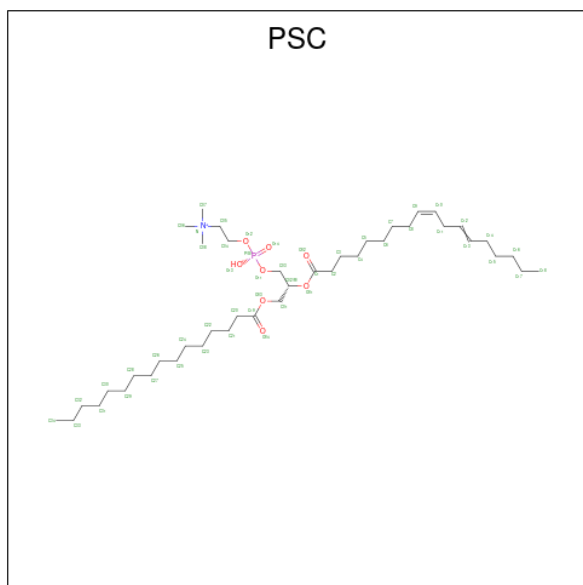
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0

Continued on next page...

Continued from previous page...

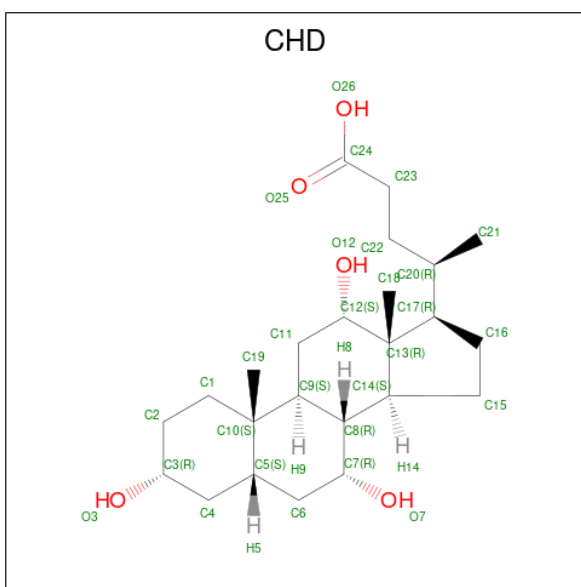
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	O	1	Total	Cu	0	0
			2	2		

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



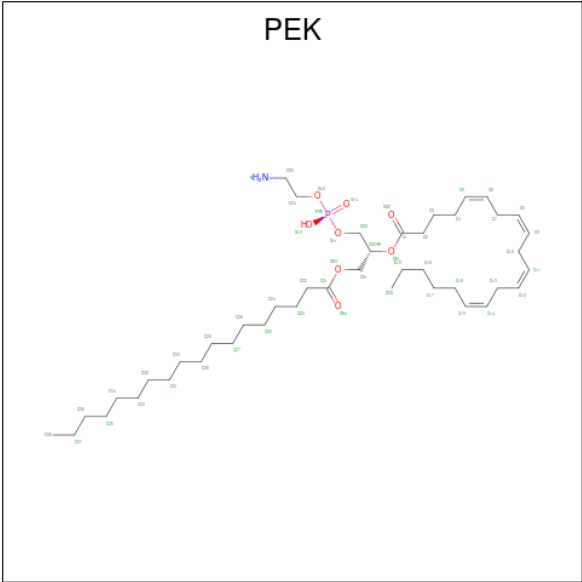
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
23	O	1	Total	C	N	O	P	0	0
			46	36	1	8	1		

- Molecule 24 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



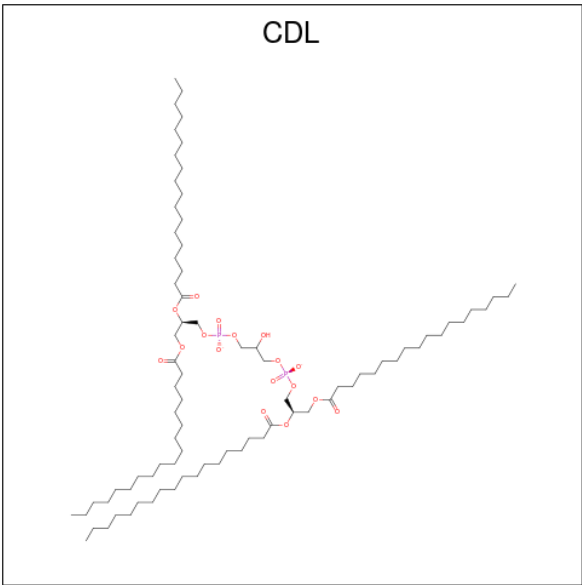
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total 29	C 24	O 5	0	0
24	C	1	Total 29	C 24	O 5	0	0
24	C	1	Total 29	C 24	O 5	0	0
24	C	1	Total 29	C 24	O 5	0	0
24	J	1	Total 29	C 24	O 5	0	0
24	O	1	Total 29	C 24	O 5	0	0
24	P	1	Total 29	C 24	O 5	0	0
24	P	1	Total 29	C 24	O 5	0	0
24	P	1	Total 29	C 24	O 5	0	0
24	Y	1	Total 28	C 23	O 5	0	0

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



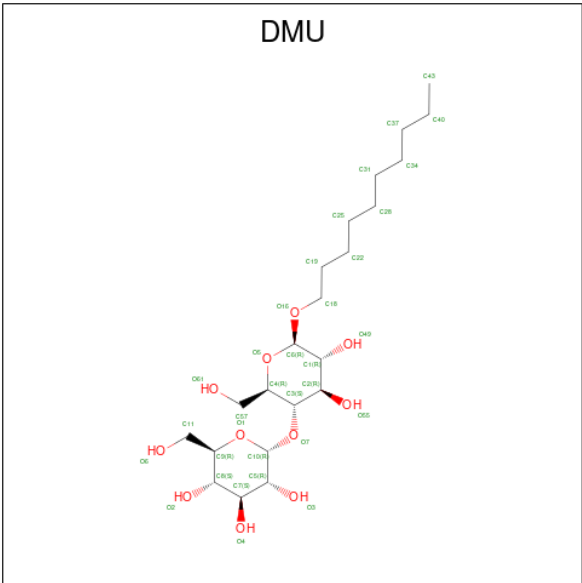
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			46	36	1	8	1		
25	G	1	Total	C	O	P		0	0
			50	41	8	1			
25	P	1	Total	C	O	P		0	0
			40	31	8	1			
25	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			82	63	17	2		
26	G	1	Total	C	O	P	0	0
			88	69	17	2		
26	P	1	Total	C	O	P	0	0
			91	73	16	2		
26	T	1	Total	C	O	P	0	0
			93	74	17	2		

- 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 33 22 11	0	0
27	C	1	Total C O 33 22 11	0	0
27	G	1	Total C O 33 22 11	0	0
27	L	1	Total C O 33 22 11	0	0
27	L	1	Total C O 33 22 11	0	0
27	M	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	P	1	Total C O 33 22 11	0	0
27	T	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0
27	Z	1	Total C O 33 22 11	0	0

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	222	Total O 222 222	0	0
29	B	157	Total O 157 157	0	0
29	C	122	Total O 122 122	0	0
29	D	99	Total O 99 99	0	1
29	E	69	Total O 69 69	0	0

Continued on next page...

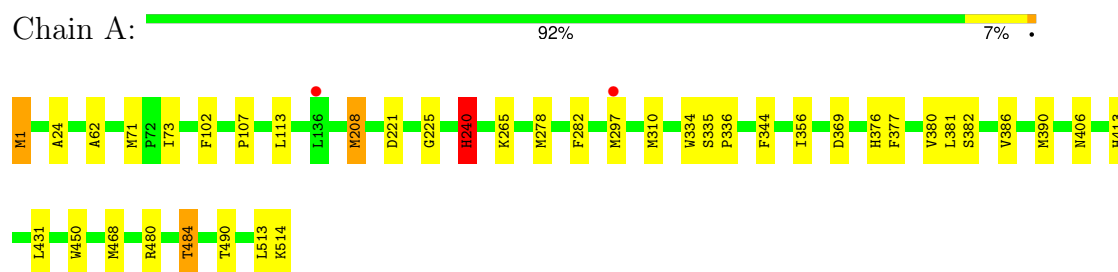
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	84	Total 84	O 84	0	1
29	G	42	Total 42	O 42	0	0
29	H	52	Total 52	O 52	0	0
29	I	32	Total 32	O 32	0	0
29	J	21	Total 21	O 21	0	0
29	K	21	Total 21	O 21	0	0
29	L	25	Total 25	O 25	0	0
29	M	24	Total 24	O 24	0	0
29	N	220	Total 220	O 220	0	0
29	O	121	Total 121	O 121	0	0
29	P	104	Total 104	O 104	0	0
29	Q	54	Total 54	O 54	0	0
29	R	47	Total 47	O 47	0	0
29	S	64	Total 64	O 64	0	0
29	T	54	Total 54	O 54	0	0
29	U	57	Total 57	O 57	0	0
29	V	22	Total 22	O 22	0	0
29	W	14	Total 14	O 14	0	0
29	X	17	Total 17	O 17	0	0
29	Y	12	Total 12	O 12	0	0
29	Z	9	Total 9	O 9	0	0

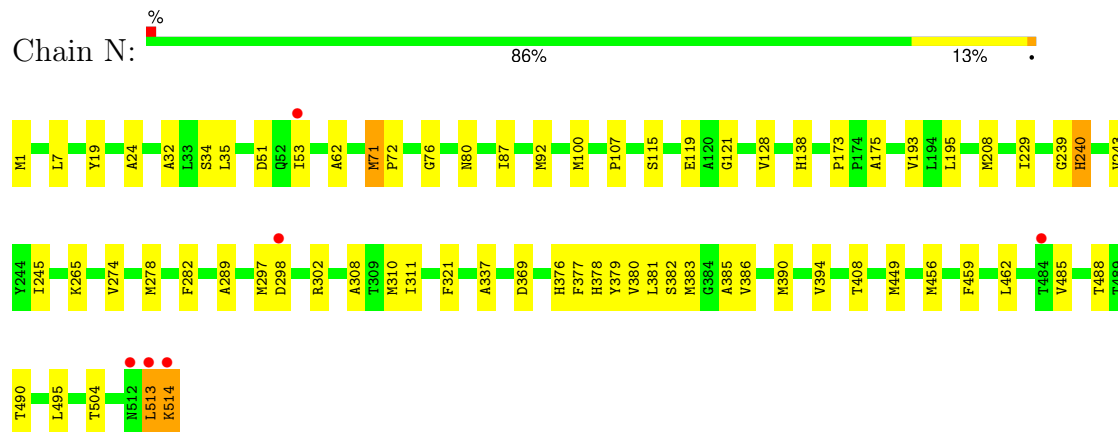
3 Residue-property plots

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

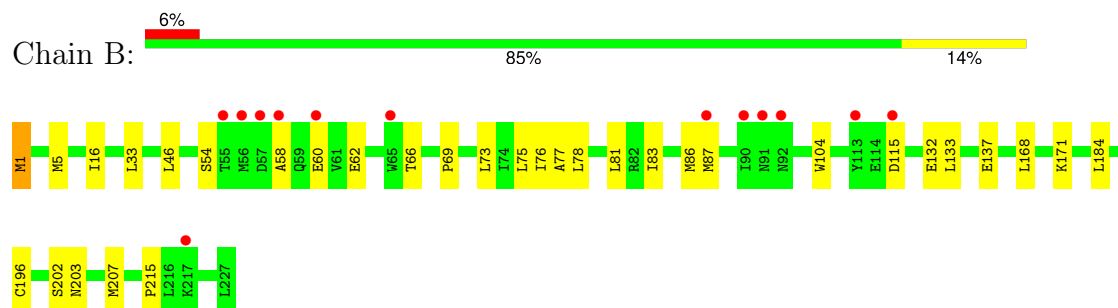
• Molecule 1: Cytochrome c oxidase subunit 1



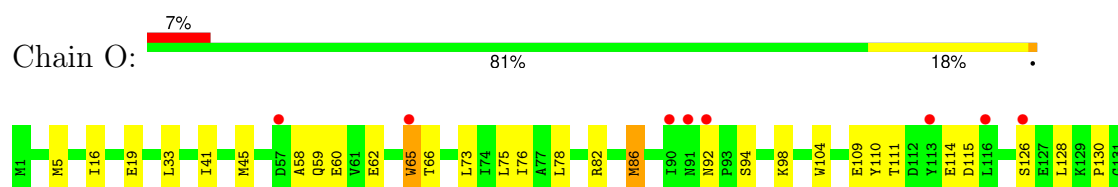
• Molecule 1: Cytochrome c oxidase subunit 1



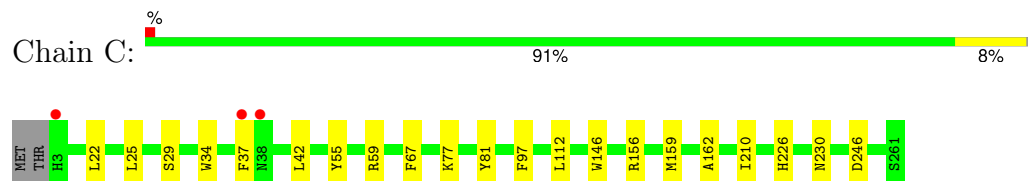
• Molecule 2: Cytochrome c oxidase subunit 2



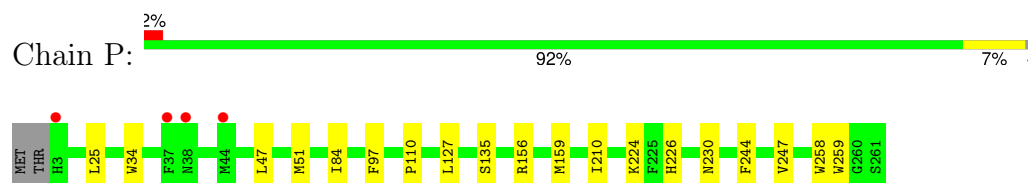
• Molecule 2: Cytochrome c oxidase subunit 2



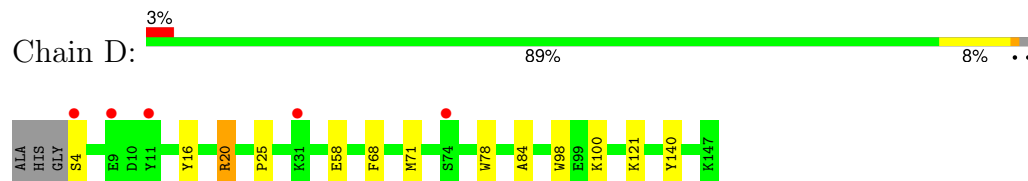
• Molecule 3: Cytochrome c oxidase subunit 3



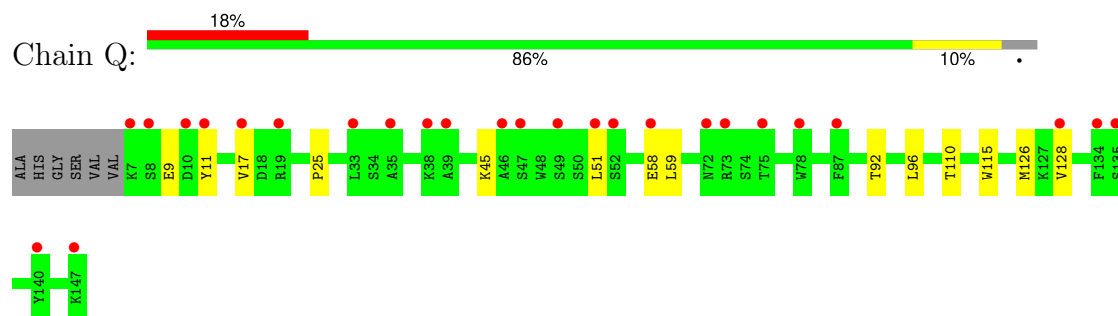
• Molecule 3: Cytochrome c oxidase subunit 3



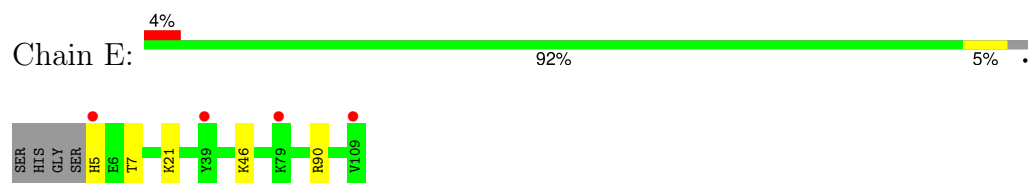
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



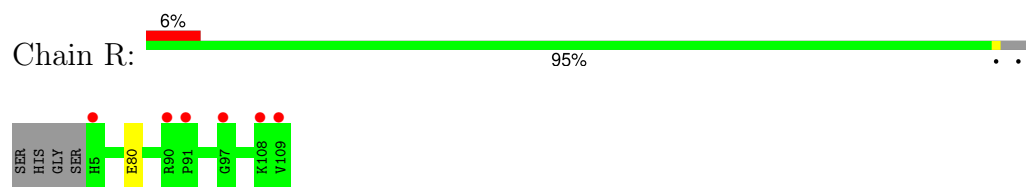
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



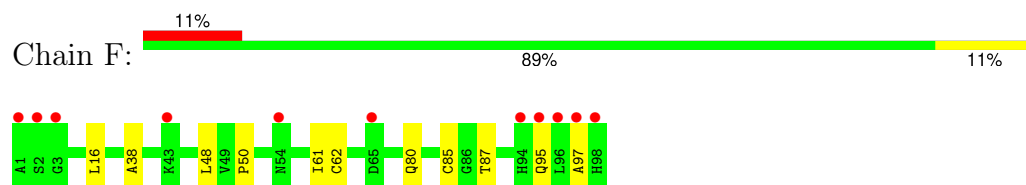
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



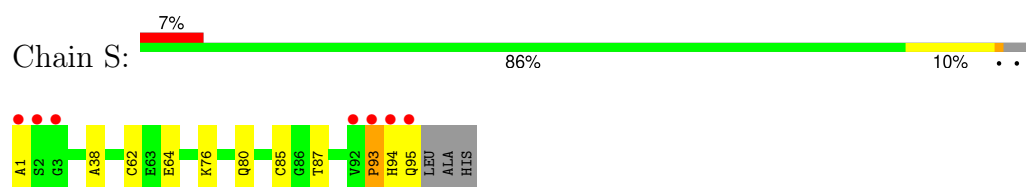
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



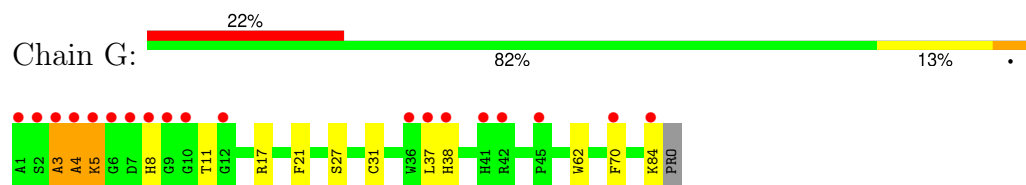
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



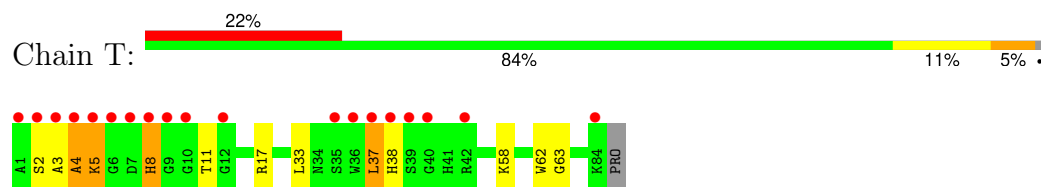
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



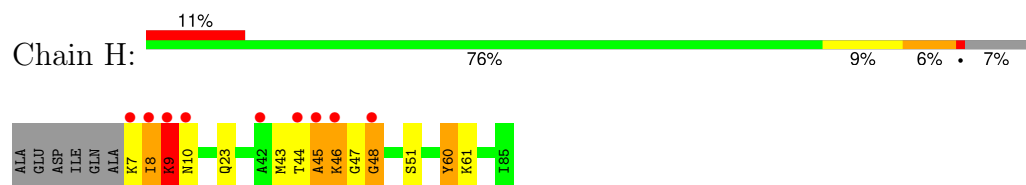
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



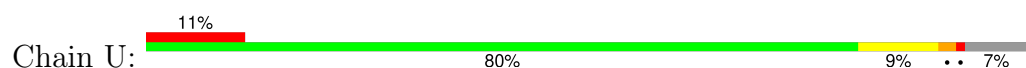
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



- Molecule 8: Cytochrome c oxidase subunit 6B1

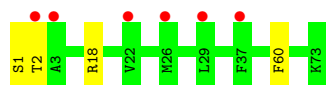


- Molecule 8: Cytochrome c oxidase subunit 6B1





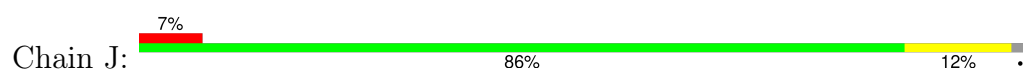
- Molecule 9: Cytochrome c oxidase subunit 6C



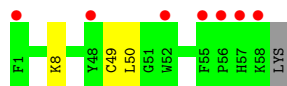
- Molecule 9: Cytochrome c oxidase subunit 6C



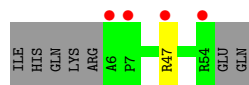
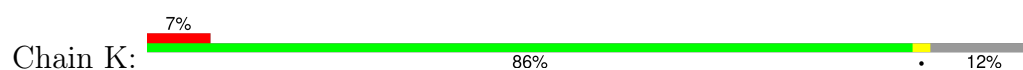
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



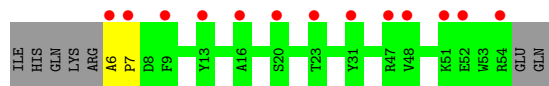
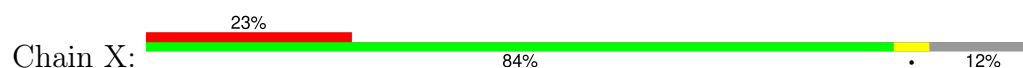
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



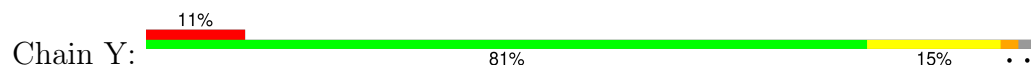
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



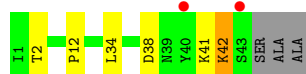
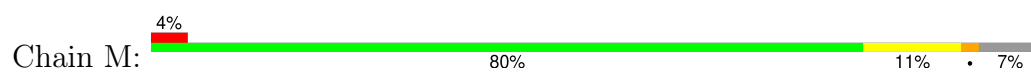
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



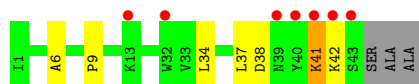
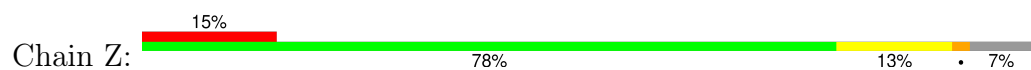
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	182.83Å 206.93Å 178.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.44 – 1.80 39.44 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.44-1.80) 99.5 (39.44-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.81Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.176 , 0.208 0.177 , 0.209	Depositor DCC
R_{free} test set	30375 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 68.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33056	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: CMO, CU, FME, CUA, PEK, TPO, NA, CHD, EDO, HEA, DMU, CDL, TGL, PGV, ZN, MG, SAC, PSC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.06	2/4222 (0.0%)	0.92	7/5765 (0.1%)
1	N	0.83	0/4234	0.82	4/5783 (0.1%)
2	B	0.90	0/1872	0.91	0/2550
2	O	0.74	1/1883 (0.1%)	0.84	1/2564 (0.0%)
3	C	0.82	0/2197	0.80	0/3005
3	P	0.75	0/2211	0.75	0/3024
4	D	0.80	0/1241	0.78	1/1674 (0.1%)
4	Q	0.52	0/1209	0.62	0/1630
5	E	0.73	0/871	0.72	0/1182
5	R	0.54	0/871	0.66	0/1182
6	F	0.83	0/765	0.94	2/1038 (0.2%)
6	S	0.71	0/747	0.84	2/1015 (0.2%)
7	G	0.65	0/690	0.75	0/937
7	T	0.63	0/690	0.76	0/937
8	H	0.74	0/682	0.80	0/921
8	U	0.62	0/682	0.74	2/921 (0.2%)
9	I	0.65	0/605	0.73	0/802
9	V	0.48	0/605	0.67	0/802
10	J	0.52	0/471	0.69	0/636
10	W	0.53	0/471	0.63	0/636
11	K	0.75	0/398	0.76	0/546
11	X	0.52	0/398	0.57	0/546
12	L	0.84	0/393	0.82	0/526
12	Y	0.59	0/393	0.69	0/526
13	M	0.82	0/345	0.78	0/470
13	Z	0.54	0/345	0.66	0/470
All	All	0.79	3/29491 (0.0%)	0.80	19/40088 (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
8	H	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	175	ILE	CA-C	-11.56	1.42	1.52
1	A	480	ARG	CD-NE	5.93	1.54	1.46
1	A	484	THR	CB-OG1	5.45	1.52	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	MET	CG-SD-CE	-8.46	82.28	100.90
6	S	93	PRO	CA-C-N	8.21	137.21	121.54
6	S	93	PRO	C-N-CA	8.21	137.21	121.54
6	F	97	ALA	CA-C-N	6.42	133.25	121.70
6	F	97	ALA	C-N-CA	6.42	133.25	121.70
1	A	240	HIS	CA-CB-CG	-6.16	107.64	113.80
1	N	240	HIS	CA-CB-CG	-5.75	108.05	113.80
1	A	376	HIS	CA-C-N	-5.70	111.16	121.14
1	A	376	HIS	C-N-CA	-5.70	111.16	121.14
4	D	20	ARG	NE-CZ-NH2	-5.56	114.20	119.20
1	N	71	MET	CG-SD-CE	-5.50	88.79	100.90
1	N	239	GLY	CA-C-N	-5.42	113.06	119.78
1	N	239	GLY	C-N-CA	-5.42	113.06	119.78
2	O	65	TRP	CA-CB-CG	5.37	123.81	113.60
1	A	278	MET	CG-SD-CE	-5.34	89.15	100.90
8	U	9	LYS	CA-C-N	5.28	131.20	121.70
8	U	9	LYS	C-N-CA	5.28	131.20	121.70
1	A	208	MET	CG-SD-CE	5.07	112.06	100.90
1	A	102	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4070	0	4039	34	0
1	N	4074	0	4057	52	0
2	B	1830	0	1838	21	0
2	O	1834	0	1839	23	0
3	C	2110	0	2027	20	0
3	P	2114	0	2028	17	0
4	D	1203	0	1192	9	0
4	Q	1175	0	1160	8	0
5	E	852	0	845	2	0
5	R	852	0	845	0	0
6	F	748	0	728	6	0
6	S	726	0	708	6	0
7	G	675	0	644	9	0
7	T	675	0	644	13	0
8	H	662	0	623	7	0
8	U	662	0	623	6	0
9	I	601	0	613	1	0
9	V	601	0	613	3	0
10	J	460	0	459	5	0
10	W	460	0	459	2	0
11	K	384	0	366	0	0
11	X	384	0	366	1	0
12	L	380	0	380	12	0
12	Y	380	0	380	8	0
13	M	335	0	352	4	0
13	Z	335	0	352	3	0
14	A	138	0	112	8	0
14	N	138	0	112	7	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	4	0	0	0	0
18	N	4	0	0	0	0
19	A	102	0	152	8	0
19	C	96	0	132	5	0
19	N	51	0	76	2	0
19	P	93	0	132	3	0
19	Z	47	0	65	1	0
20	A	59	0	95	3	0
20	B	63	0	110	1	0
20	D	55	0	88	3	0
20	N	63	0	110	2	0
20	O	63	0	110	2	0
20	Y	59	0	99	3	0
21	A	52	0	78	5	0
21	B	8	0	12	0	0
21	C	16	0	24	2	0
21	D	16	0	24	3	0
21	E	16	0	24	1	0
21	F	20	0	30	0	0
21	G	8	0	12	0	0
21	H	8	0	12	0	0
21	I	4	0	6	0	0
21	K	4	0	6	0	0
21	L	4	0	6	1	0
21	N	24	0	36	1	0
21	O	12	0	18	1	0
21	P	12	0	18	0	0
21	Q	8	0	12	1	0
21	R	8	0	12	0	0
21	S	24	0	36	0	0
21	T	8	0	12	0	0
21	U	4	0	6	0	0
21	V	8	0	12	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	50	0	71	3	0
23	O	46	0	62	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	B	29	0	39	0	0
24	C	87	0	117	3	0
24	J	29	0	39	2	0
24	O	29	0	39	2	0
24	P	87	0	117	10	0
24	Y	28	0	33	4	0
25	C	99	0	137	4	0
25	G	50	0	71	4	0
25	P	145	0	197	4	0
26	C	82	0	111	8	0
26	G	88	0	126	5	0
26	P	91	0	134	7	0
26	T	93	0	136	11	0
27	C	66	0	84	5	0
27	G	33	0	42	2	0
27	L	66	0	84	9	0
27	M	33	0	42	1	0
27	P	66	0	84	1	0
27	T	33	0	42	8	0
27	Z	66	0	84	2	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	222	0	0	6	0
29	B	157	0	0	1	0
29	C	122	0	0	1	0
29	D	99	0	0	3	0
29	E	69	0	0	1	0
29	F	84	0	0	1	0
29	G	42	0	0	0	0
29	H	52	0	0	0	0
29	I	32	0	0	0	0
29	J	21	0	0	0	0
29	K	21	0	0	1	0
29	L	25	0	0	0	0
29	M	24	0	0	0	0
29	N	220	0	0	0	0
29	O	121	0	0	1	0
29	P	104	0	0	1	0
29	Q	54	0	0	0	0
29	R	47	0	0	0	0
29	S	64	0	0	0	0
29	T	54	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	U	57	0	0	0	0
29	V	22	0	0	1	0
29	W	14	0	0	0	0
29	X	17	0	0	0	0
29	Y	12	0	0	0	0
29	Z	9	0	0	0	0
All	All	33056	0	31860	303	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:HD21	19:A:607:PGV:H21	1.45	0.80
7:T:37:LEU:HD23	26:T:102:CDL:H381	1.63	0.80
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.75
21:D:204:EDO:H11	29:D:320:HOH:O	1.87	0.75
7:T:63:GLY:HA2	27:T:101:DMU:H34	1.70	0.74
19:A:607:PGV:H221	19:A:607:PGV:H012	1.70	0.73
12:L:19:TRP:HE1	27:L:103:DMU:H40	1.53	0.73
12:Y:42:HIS:HB2	24:Y:102:CHD:H12	1.71	0.73
5:E:21:LYS:HE2	21:E:203:EDO:H11	1.71	0.73
21:O:305:EDO:H22	8:U:23:GLN:HG2	1.75	0.68
8:H:45:ALA:O	8:H:47:GLY:N	2.27	0.68
12:Y:42:HIS:HB2	24:Y:102:CHD:H212	1.75	0.67
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.75	0.67
1:A:310:MET:HE2	2:B:73:LEU:HD22	1.76	0.66
12:Y:24:MET:HE1	20:Y:101:TGL:H152	1.79	0.65
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.27	0.65
2:B:202:SER:C	2:B:203:ASN:HD22	2.05	0.65
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.61	0.65
8:H:45:ALA:C	8:H:47:GLY:H	2.06	0.64
1:N:175:ALA:HB1	1:N:513:LEU:HD13	1.80	0.63
12:L:26:THR:HG21	27:L:103:DMU:H21	1.81	0.62
12:L:2:HIS:CG	12:L:3:TYR:H	2.17	0.62
13:M:42:LYS:HG2	13:M:42:LYS:O	1.97	0.62
7:G:62:TRP:HB2	27:G:101:DMU:H36	1.83	0.61
3:C:226:HIS:CE1	26:C:306:CDL:HB31	2.36	0.61
7:T:5:LYS:NZ	29:T:202:HOH:O	2.33	0.61
3:C:226:HIS:HE1	26:C:306:CDL:HB31	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:62:TRP:HB3	27:T:101:DMU:H30	1.82	0.60
4:D:78:TRP:HB3	20:D:201:TGL:HB22	1.83	0.60
6:F:85:CYS:SG	6:F:87:THR:HG23	2.41	0.60
1:N:390:MET:O	1:N:394[A]:VAL:HG22	2.02	0.60
3:P:224:LYS:HD3	26:P:308:CDL:HB31	1.83	0.60
3:P:226:HIS:CE1	26:P:308:CDL:HB32	2.38	0.59
3:P:34:TRP:HE1	27:T:101:DMU:H29	1.68	0.59
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.84	0.59
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.85	0.59
3:C:67:PHE:HE2	26:C:306:CDL:HB21	1.67	0.59
2:O:58:ALA:O	2:O:62:GLU:HG3	2.04	0.58
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.85	0.58
1:N:297[B]:MET:HG2	1:N:302:ARG:HG3	1.85	0.58
20:O:303:TGL:HC22	29:V:220:HOH:O	2.04	0.57
19:C:305:PGV:H62	24:P:315:CHD:H20	1.86	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.86	0.57
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.86	0.57
19:A:607:PGV:H151	19:A:607:PGV:H322	1.85	0.56
27:T:101:DMU:H38	27:T:101:DMU:H28	1.51	0.56
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.86	0.56
1:A:310:MET:HE1	2:B:76:ILE:HB	1.88	0.56
3:C:67:PHE:CE2	26:C:306:CDL:HB21	2.41	0.56
27:T:101:DMU:O55	27:T:101:DMU:O3	2.14	0.56
7:G:31:CYS:SG	26:G:103:CDL:H551	2.46	0.56
1:N:378:HIS:O	1:N:382[B]:SER:HB2	2.06	0.56
7:G:27:SER:HB3	26:G:103:CDL:H562	1.89	0.55
2:B:83:ILE:O	2:B:87:MET:HG3	2.06	0.55
4:D:100:LYS:NZ	29:D:301:HOH:O	2.33	0.55
12:L:42:HIS:HB2	27:L:102:DMU:H6	1.87	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.54
3:P:226:HIS:HE1	26:P:308:CDL:HB32	1.70	0.54
26:G:103:CDL:H361	26:G:103:CDL:H141	1.89	0.54
3:P:247:VAL:HG12	25:P:301:PEK:H131	1.90	0.54
21:A:619:EDO:H21	29:A:735:HOH:O	2.08	0.54
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.89	0.54
1:A:382[B]:SER:O	1:A:386:VAL:HB	2.07	0.53
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.91	0.53
12:L:19:TRP:HE1	27:L:103:DMU:C11	2.20	0.53
3:C:246:ASP:HB2	29:C:494:HOH:O	2.09	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.91	0.52
2:O:19:GLU:OE2	2:O:82[A]:ARG:NH2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:HA	8:U:10:ASN:HB2	1.92	0.52
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.92	0.51
1:N:382[B]:SER:O	1:N:386:VAL:HB	2.09	0.51
14:A:601[B]:HEA:H122	29:A:741:HOH:O	2.10	0.51
24:Y:102:CHD:H12	24:Y:102:CHD:H212	1.91	0.51
19:C:305:PGV:H42	24:P:315:CHD:H183	1.93	0.51
1:A:390:MET:HE2	1:A:413:HIS:CE1	2.44	0.51
7:T:37:LEU:CD2	26:T:102:CDL:H381	2.37	0.51
4:D:140:TYR:CD1	21:D:204:EDO:H21	2.45	0.51
27:C:314:DMU:H11	10:J:49:CYS:HB3	1.91	0.51
2:B:81:LEU:HD12	26:T:102:CDL:H371	1.93	0.51
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.93	0.51
1:A:221:ASP:OD1	21:A:619:EDO:H11	2.11	0.51
10:J:55:PHE:HE1	27:L:102:DMU:H29	1.75	0.51
1:N:24:ALA:HB2	14:N:601[A]:HEA:H253	1.92	0.51
26:T:102:CDL:H732	26:T:102:CDL:H552	1.92	0.51
3:C:55:TYR:OH	26:C:306:CDL:OA3	2.23	0.50
3:P:259:TRP:O	24:P:315:CHD:O12	2.23	0.50
7:G:5:LYS:O	1:N:193:VAL:HG21	2.11	0.50
26:P:308:CDL:OB2	10:W:8:LYS:HE3	2.11	0.50
1:A:514:LYS:HE3	6:F:61:ILE:O	2.10	0.50
6:S:62:CYS:HB3	6:S:85:CYS:HB3	1.93	0.50
29:A:837:HOH:O	8:H:23:GLN:HG3	2.12	0.49
21:N:611:EDO:H12	4:Q:11:TYR:HB2	1.95	0.49
1:A:73:ILE:HD13	14:A:601[B]:HEA:H22	1.95	0.49
25:P:306:PEK:H042	7:T:17:ARG:HH22	1.78	0.49
7:T:38:HIS:NE2	26:T:102:CDL:C11	2.76	0.49
3:C:37:PHE:CE2	27:C:314:DMU:H13	2.48	0.49
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.94	0.49
14:A:602:HEA:H243	2:B:69:PRO:HB3	1.95	0.49
4:D:121:LYS:NZ	21:D:203:EDO:O2	2.46	0.48
2:O:41:ILE:O	2:O:45:MET:HG2	2.12	0.48
1:N:310:MET:HE1	2:O:76:ILE:HB	1.94	0.48
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.95	0.48
3:P:156:ARG:HE	24:P:309:CHD:C24	2.26	0.48
1:A:113:LEU:HB3	27:L:102:DMU:H23	1.94	0.48
20:A:609:TGL:HA62	12:L:25:MET:HG2	1.95	0.48
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.96	0.48
24:C:315:CHD:H181	19:P:302:PGV:H31	1.96	0.48
4:D:20:ARG:HG2	29:D:377:HOH:O	2.13	0.48
1:N:386:VAL:HG21	14:N:601[A]:HEA:H261	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:C:313:DMU:H2	27:C:314:DMU:H32	1.96	0.47
20:D:201:TGL:HA52	20:D:201:TGL:HB72	1.95	0.47
29:A:920:HOH:O	23:B:303:PSC:H52	2.13	0.47
1:N:381[B]:LEU:HB2	14:N:602:HEA:CAC	2.45	0.47
1:N:390:MET:O	1:N:394[B]:VAL:HG12	2.13	0.47
7:T:38:HIS:NE2	26:T:102:CDL:H112	2.28	0.47
12:L:41:ARG:HH12	27:L:102:DMU:H2	1.79	0.47
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.15	0.47
1:A:73:ILE:CD1	14:A:601[B]:HEA:H22	2.44	0.47
23:B:303:PSC:H31	23:B:303:PSC:H231	1.96	0.47
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.80	0.47
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.50	0.46
7:G:17:ARG:NH1	25:G:102:PEK:O13	2.48	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.15	0.46
1:N:308:ALA:HA	1:N:311:ILE:HD12	1.97	0.46
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.98	0.46
3:P:258:TRP:CD1	24:P:315:CHD:H161	2.50	0.46
3:C:59:ARG:HB2	26:C:306:CDL:H511	1.97	0.46
24:Y:102:CHD:H231	24:Y:102:CHD:H211	1.61	0.46
26:P:308:CDL:H521	26:P:308:CDL:HB62	1.98	0.46
24:C:315:CHD:H112	24:C:315:CHD:H12A	1.53	0.46
1:N:321:PHE:CD2	2:O:65:TRP:HB2	2.51	0.46
1:N:449:MET:SD	2:O:5:MET:HG2	2.56	0.46
2:O:82[A]:ARG:NH1	2:O:86:MET:HE1	2.31	0.46
5:E:46:LYS:NZ	29:E:302:HOH:O	2.48	0.46
3:C:37:PHE:CD2	27:C:314:DMU:H13	2.51	0.46
20:N:607:TGL:HC72	29:O:3080:HOH:O	2.16	0.46
24:P:315:CHD:H182	24:P:315:CHD:H8	1.64	0.46
6:S:95:GLN:OE1	6:S:95:GLN:N	2.48	0.46
25:G:102:PEK:H282	24:O:301:CHD:H11	1.99	0.45
24:P:309:CHD:H212	24:P:309:CHD:H12	1.98	0.45
1:A:310:MET:HE2	2:B:73:LEU:CD2	2.42	0.45
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.15	0.45
3:C:156:ARG:HE	24:C:307:CHD:C24	2.29	0.45
24:P:309:CHD:H232	24:P:309:CHD:H162	1.98	0.45
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.45
2:O:104:TRP:CD2	2:O:203:ASN:HB2	2.51	0.45
3:P:84:ILE:HG12	25:P:301:PEK:H32	1.99	0.45
7:T:62:TRP:CB	27:T:101:DMU:H30	2.46	0.45
1:A:1:FME:HE2	1:A:1:FME:HA	1.99	0.45
1:A:468:MET:HE1	14:A:601[B]:HEA:H271	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:607:PGV:H131	19:A:607:PGV:H302	1.99	0.45
26:G:103:CDL:HA62	26:G:103:CDL:H311	1.47	0.45
8:U:60:TYR:CD1	8:U:60:TYR:C	2.95	0.45
19:A:607:PGV:H02	29:K:207:HOH:O	2.16	0.45
24:J:101:CHD:H183	24:J:101:CHD:H20	1.85	0.45
1:N:119:GLU:O	12:Y:46:LYS:HE2	2.17	0.45
2:O:225:SER:C	2:O:227:LEU:H	2.25	0.45
25:G:102:PEK:H282	25:G:102:PEK:H252	1.74	0.45
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.52	0.45
1:N:337:ALA:HB2	1:N:394[B]:VAL:HG13	1.99	0.45
7:T:58:LYS:NZ	29:T:204:HOH:O	2.50	0.45
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.17	0.44
2:O:111:THR:HA	2:O:114:GLU:O	2.17	0.44
2:B:69:PRO:HG2	29:B:421:HOH:O	2.18	0.44
1:N:100:MET:HE1	19:N:608:PGV:H81	1.99	0.44
3:P:135:SER:HB3	26:T:102:CDL:H582	1.99	0.44
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.98	0.44
1:A:310:MET:HE3	1:A:356:ILE:HG23	1.99	0.44
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.52	0.44
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	2.00	0.44
27:P:313:DMU:H6	10:W:49:CYS:SG	2.57	0.44
1:N:381[B]:LEU:O	1:N:385:ALA:HB3	2.18	0.44
2:B:104:TRP:CD2	2:B:203:ASN:HB2	2.53	0.44
20:D:201:TGL:OG1	20:D:201:TGL:HB31	2.16	0.44
1:N:76:GLY:O	1:N:80:ASN:HB2	2.17	0.44
1:N:92:MET:HE3	1:N:92:MET:HB3	1.92	0.44
1:N:297[B]:MET:SD	1:N:302:ARG:HG2	2.57	0.44
27:C:313:DMU:H23	10:J:41:GLY:HA3	1.99	0.44
19:A:607:PGV:H012	19:A:607:PGV:H22	1.99	0.44
1:N:274:VAL:HG12	1:N:278:MET:HE2	2.00	0.44
2:O:227:LEU:HD23	2:O:227:LEU:HA	1.89	0.44
24:O:301:CHD:H212	24:O:301:CHD:H12	2.00	0.44
26:T:102:CDL:H111	26:T:102:CDL:H362	2.00	0.44
27:Z:103:DMU:H8	27:Z:103:DMU:H15	1.72	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.53	0.43
19:N:608:PGV:H42	19:N:608:PGV:H71	1.75	0.43
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.83	0.43
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.53	0.43
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.85	0.43
3:P:210:ILE:HG23	19:P:307:PGV:H91	2.00	0.43
1:A:113:LEU:HD12	20:A:609:TGL:H141	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.99	0.43
1:N:195:LEU:HD23	1:N:245:ILE:HD13	1.99	0.43
9:V:18:ARG:HG2	9:V:18:ARG:NH1	2.33	0.43
2:B:58:ALA:O	2:B:62:GLU:HG3	2.18	0.43
25:C:308:PEK:H051	7:T:8:HIS:NE2	2.33	0.43
13:M:41:LYS:O	13:M:42:LYS:HB3	2.18	0.43
1:N:376:HIS:CE1	1:N:380[B]:VAL:HG11	2.54	0.43
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.43
6:S:1:ALA:HB2	7:T:17:ARG:HH12	1.82	0.43
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.01	0.43
24:P:315:CHD:H211	24:P:315:CHD:H231	1.64	0.43
6:S:85:CYS:SG	6:S:87:THR:HG23	2.59	0.43
26:T:102:CDL:H521	26:T:102:CDL:H551	1.86	0.43
1:A:240:HIS:C	1:A:240:HIS:CD2	2.97	0.43
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.54	0.43
26:T:102:CDL:H332	26:T:102:CDL:HA62	2.00	0.43
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.63	0.43
14:A:601[A]:HEA:H271	14:A:601[A]:HEA:H211	1.74	0.43
3:C:55:TYR:CE1	26:C:306:CDL:H512	2.53	0.43
3:P:244:PHE:HA	25:P:301:PEK:H9	2.01	0.43
6:F:50:PRO:HG2	29:F:240:HOH:O	2.19	0.42
8:H:60:TYR:CD1	8:H:60:TYR:C	2.96	0.42
20:N:607:TGL:H192	20:N:607:TGL:H351	1.74	0.42
4:D:98:TRP:CE3	27:M:101:DMU:H12	2.54	0.42
1:A:335:SER:HB2	1:A:336:PRO:HD2	2.01	0.42
1:N:243:VAL:HB	14:N:602:HEA:CAC	2.49	0.42
21:A:619:EDO:C2	29:A:735:HOH:O	2.66	0.42
1:A:484:THR:HB	13:M:2:THR:OG1	2.20	0.42
21:C:312:EDO:H11	6:F:16:LEU:HD13	2.00	0.42
25:C:303:PEK:H161	25:C:303:PEK:H132	1.51	0.42
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.01	0.42
19:A:607:PGV:H231	13:M:12:PRO:HG3	2.02	0.42
12:L:41:ARG:NH2	27:L:102:DMU:O3	2.53	0.42
13:Z:42:LYS:HE2	13:Z:42:LYS:HB2	1.88	0.42
12:Y:13:PHE:HA	20:Y:101:TGL:HC22	2.01	0.42
24:J:101:CHD:H222	24:J:101:CHD:H162	1.49	0.42
12:L:22:LEU:HD23	27:L:103:DMU:H13	2.00	0.42
1:N:408:THR:HB	19:Z:101:PGV:H41	2.02	0.42
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.55	0.42
26:P:308:CDL:H182	26:P:308:CDL:H372	2.01	0.42
2:B:215:PRO:HD3	9:I:60:PHE:CD1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:210:ILE:HG23	19:C:304:PGV:H91	2.01	0.41
4:Q:59:LEU:HD23	4:Q:59:LEU:HA	1.82	0.41
1:N:310:MET:HE2	2:O:73:LEU:HD22	2.01	0.41
27:T:101:DMU:H26	27:T:101:DMU:H18	1.77	0.41
9:V:29:LEU:HA	9:V:29:LEU:HD12	1.81	0.41
2:B:5:MET:HE2	2:B:5:MET:HB3	1.83	0.41
23:B:303:PSC:H221	23:B:303:PSC:H251	1.87	0.41
19:C:305:PGV:H71	24:P:315:CHD:H20	2.02	0.41
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.02	0.41
11:X:6:ALA:HA	11:X:7:PRO:HD3	1.95	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.01	0.41
10:J:47:LEU:HA	10:J:47:LEU:HD23	1.86	0.41
1:N:51:ASP:OD2	2:O:206:PHE:HE2	2.03	0.41
1:N:87:ILE:O	1:N:173:PRO:HD3	2.19	0.41
19:C:305:PGV:H241	19:C:305:PGV:H272	1.85	0.41
1:N:115:SER:O	1:N:121:GLY:HA2	2.20	0.41
1:N:380[A]:VAL:HG21	14:N:602:HEA:C4C	2.50	0.41
20:A:609:TGL:H221	20:A:609:TGL:HA92	1.94	0.41
25:C:303:PEK:H041	7:G:70:PHE:HB2	2.03	0.41
8:H:43:MET:HE3	8:H:48:GLY:HA3	2.02	0.41
12:L:43:GLN:OE1	21:L:101:EDO:H12	2.21	0.41
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.03	0.41
8:H:7:LYS:C	8:H:9:LYS:H	2.27	0.41
8:H:46:LYS:H	8:H:46:LYS:HG2	1.72	0.41
2:O:134:ARG:HB2	4:Q:110:THR:HG21	2.03	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.03	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.99	0.41
2:B:77:ALA:O	2:B:81:LEU:HG	2.20	0.41
3:C:22:LEU:HD23	3:C:22:LEU:HA	1.92	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.41
12:L:2:HIS:CG	12:L:3:TYR:N	2.84	0.41
1:N:19:TYR:CD1	1:N:76:GLY:HA3	2.55	0.41
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.41
1:N:380[A]:VAL:HG21	14:N:602:HEA:C3C	2.51	0.41
3:P:34:TRP:NE1	27:T:101:DMU:H29	2.34	0.41
26:P:308:CDL:H852	26:P:308:CDL:H822	1.78	0.41
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.01	0.41
8:U:43:MET:HE3	8:U:48:GLY:HA3	2.03	0.41
13:Z:6:ALA:HB3	13:Z:9:PRO:HG3	2.02	0.41
19:A:607:PGV:H11	4:D:84:ALA:CB	2.51	0.41
3:C:81:TYR:HD1	25:C:308:PEK:H272	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.92	0.41
1:N:488:THR:HB	1:N:495:LEU:HD13	2.03	0.41
19:P:302:PGV:H331	29:P:504:HOH:O	2.19	0.41
8:U:7:LYS:HE2	8:U:7:LYS:HB3	1.74	0.41
12:Y:13:PHE:CZ	20:Y:101:TGL:HA72	2.56	0.41
26:C:306:CDL:H331	26:C:306:CDL:H141	2.03	0.40
7:G:3:ALA:O	7:G:4:ALA:HB2	2.21	0.40
2:O:160:LEU:HD22	2:O:175:ILE:HG12	2.03	0.40
26:T:102:CDL:H202	26:T:102:CDL:H531	2.01	0.40
1:N:107:PRO:HB3	3:P:25:LEU:HB2	2.04	0.40
21:Q:201:EDO:H11	21:Q:202:EDO:H22	2.03	0.40
20:B:302:TGL:H241	20:B:302:TGL:H211	1.82	0.40
7:G:21:PHE:CD1	25:G:102:PEK:H222	2.55	0.40
26:G:103:CDL:H381	26:G:103:CDL:H161	2.03	0.40
1:N:35:LEU:HD11	1:N:462:LEU:HB2	2.03	0.40
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	2.04	0.40
12:Y:23:ALA:HB2	27:Z:103:DMU:H17	2.03	0.40
21:A:619:EDO:O1	21:C:309:EDO:H12	2.21	0.40
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.52	0.40
3:C:29:SER:HB3	3:C:42:LEU:HD13	2.03	0.40
4:D:68:PHE:HA	4:D:71:MET:HE3	2.03	0.40
10:J:3:ASN:OD1	10:J:3:ASN:C	2.65	0.40
2:O:139:ASP:OD1	2:O:140:ASN:N	2.55	0.40
21:A:619:EDO:H22	29:A:887:HOH:O	2.21	0.40
3:C:34:TRP:HE1	27:G:101:DMU:H29	1.86	0.40
20:O:303:TGL:HA62	20:O:303:TGL:H112	2.03	0.40

There are no symmetry-related clashes.

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	521/514 (101%)	508 (98%)	13 (2%)	0	100	100
1	N	523/514 (102%)	514 (98%)	9 (2%)	0	100	100
2	B	226/227 (100%)	221 (98%)	5 (2%)	0	100	100
2	O	227/227 (100%)	218 (96%)	7 (3%)	2 (1%)	14	5
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	259/261 (99%)	254 (98%)	5 (2%)	0	100	100
4	D	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
4	Q	139/147 (95%)	133 (96%)	6 (4%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	93 (97%)	2 (2%)	1 (1%)	12	4
6	S	94/98 (96%)	89 (95%)	4 (4%)	1 (1%)	11	3
7	G	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	2	0
7	T	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	2	0
8	H	77/85 (91%)	69 (90%)	3 (4%)	5 (6%)	1	0
8	U	77/85 (91%)	74 (96%)	2 (3%)	1 (1%)	9	3
9	I	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
9	V	71/73 (97%)	69 (97%)	2 (3%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	4	1
All	All	3525/3614 (98%)	3415 (97%)	93 (3%)	17 (0%)	24	14

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
8	H	10	ASN
6	S	94	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	U	8	ILE
8	H	8	ILE
8	H	45	ALA
8	H	46	LYS
8	H	48	GLY
6	F	95	GLN
7	G	8	HIS
7	G	3	ALA
2	O	126	SER
7	T	4	ALA
7	T	8	HIS
7	T	3	ALA
13	Z	41	LYS
2	O	92	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	434/426 (102%)	432 (100%)	2 (0%)	81	80
1	N	436/426 (102%)	425 (98%)	11 (2%)	42	30
2	B	211/210 (100%)	202 (96%)	9 (4%)	26	13
2	O	212/210 (101%)	201 (95%)	11 (5%)	21	9
3	C	224/226 (99%)	221 (99%)	3 (1%)	61	54
3	P	226/226 (100%)	223 (99%)	3 (1%)	61	54
4	D	129/129 (100%)	127 (98%)	2 (2%)	55	47
4	Q	125/129 (97%)	121 (97%)	4 (3%)	34	22
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	21
5	R	92/95 (97%)	91 (99%)	1 (1%)	65	60
6	F	81/81 (100%)	79 (98%)	2 (2%)	42	30
6	S	80/81 (99%)	78 (98%)	2 (2%)	42	30
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	7
8	H	71/75 (95%)	65 (92%)	6 (8%)	10	3
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	4
9	I	57/57 (100%)	55 (96%)	2 (4%)	32	19
9	V	57/57 (100%)	56 (98%)	1 (2%)	51	43
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	15
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	38
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	28
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	3
12	Y	39/40 (98%)	36 (92%)	3 (8%)	12	3
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	3
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	3
All	All	3060/3082 (99%)	2969 (97%)	91 (3%)	36	24

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	MET
1	A	369	ASP
2	B	33	LEU
2	B	54	SER
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	115	ASP
2	B	171	LYS
3	C	77	LYS
3	C	159	MET
3	C	230	ASN
4	D	4	SER
4	D	58	GLU
5	E	5	HIS
5	E	7	THR
5	E	90	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	48	LEU
6	F	80	GLN
7	G	5	LYS
7	G	37	LEU
7	G	38	HIS
7	G	84	LYS
8	H	8	ILE
8	H	9	LYS
8	H	44	THR
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	18	ARG
10	J	27	THR
10	J	50	LEU
11	K	47	ARG
12	L	24	MET
12	L	26	THR
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	7	LEU
1	N	53	ILE
1	N	128	VAL
1	N	138	HIS
1	N	298[A]	ASP
1	N	298[B]	ASP
1	N	369	ASP
1	N	485	VAL
1	N	504	THR
1	N	513	LEU
1	N	514	LYS
2	O	16	ILE
2	O	33	LEU
2	O	59	GLN
2	O	60	GLU
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	86	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
3	P	127	LEU
3	P	159	MET
3	P	230	ASN
4	Q	9	GLU
4	Q	45	LYS
4	Q	51	LEU
4	Q	58	GLU
5	R	80	GLU
6	S	64	GLU
6	S	80	GLN
7	T	2	SER
7	T	5	LYS
7	T	33	LEU
7	T	37	LEU
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	29	LEU
10	W	50	LEU
12	Y	26	THR
12	Y	46	LYS
12	Y	47	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	512	ASN
2	B	140	ASN
3	C	50	ASN
3	C	76	GLN
4	D	119	GLN
6	F	54	ASN
1	N	4	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	422	ASN
2	O	10	GLN
2	O	91	ASN
2	O	203	ASN
3	P	3	HIS
3	P	50	ASN
3	P	76	GLN
4	Q	119	GLN
4	Q	143	ASN
5	R	78	HIS
7	T	34	ASN
8	U	23	GLN
8	U	28	ASN
8	U	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	1.35	1 (12%)	10,14,16	0.95	1 (10%)
2	FME	B	1	2	8,9,10	1.00	0	8,9,11	1.71	2 (25%)
9	SAC	I	1	9	7,8,9	0.92	0	7,9,11	1.26	1 (14%)
9	SAC	V	1	9	7,8,9	0.65	0	7,9,11	0.84	0
2	FME	O	1	2	8,9,10	0.63	0	8,9,11	1.07	0
1	FME	N	1	1	8,9,10	0.51	0	8,9,11	1.15	1 (12%)
7	TPO	T	11	7	8,10,11	1.38	1 (12%)	10,14,16	0.81	0
1	FME	A	1	1	8,9,10	0.78	0	8,9,11	1.33	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	2/7/8/10	-
9	SAC	V	1	9	-	4/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	5/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
1	FME	A	1	1	-	5/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-O1P	2.98	1.59	1.50
7	G	11	TPO	P-O1P	2.96	1.59	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.03	103.59	112.87
1	A	1	FME	O1-CN-N	-2.48	118.91	125.32
9	I	1	SAC	O-C-CA	-2.45	118.46	124.77
2	B	1	FME	O1-CN-N	-2.39	119.15	125.32
7	G	11	TPO	P-OG1-CB	-2.16	117.47	123.33
1	N	1	FME	O-C-CA	-2.08	119.41	124.77

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	O-C-CA-CB
7	G	11	TPO	CA-CB-OG1-P
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	N	1	FME	N-CA-CB-CG
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
9	V	1	SAC	C-CA-N-C1A
9	V	1	SAC	CB-CA-N-C1A
7	G	11	TPO	CB-OG1-P-O1P
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD
7	G	11	TPO	C-CA-CB-CG2
1	N	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-CG2
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	CB-CA-N-CN
7	T	11	TPO	CG2-CB-OG1-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	2	0
1	A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 10 are monoatomic - leaving 125 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	PEK	C	303	-	52,52,52	0.87	2 (3%)	55,57,57	1.63	7 (12%)
21	EDO	T	104	-	3,3,3	0.42	0	2,2,2	0.40	0
21	EDO	C	310	-	3,3,3	0.46	0	2,2,2	0.35	0
21	EDO	I	101	-	3,3,3	0.69	0	2,2,2	0.12	0
21	EDO	N	612	-	3,3,3	0.63	0	2,2,2	0.56	0
21	EDO	S	105	-	3,3,3	0.38	0	2,2,2	0.54	0
25	PEK	P	305	-	51,51,52	0.83	2 (3%)	54,56,57	1.46	6 (11%)
27	DMU	C	313	-	34,34,34	0.61	1 (2%)	45,45,45	1.30	6 (13%)
19	PGV	C	305	-	47,47,50	1.38	4 (8%)	47,51,56	1.54	4 (8%)
22	CUA	B	301	2	0,1,1	-	-	-	-	-
21	EDO	G	104	-	3,3,3	0.69	0	2,2,2	0.21	0
21	EDO	D	203	-	3,3,3	0.41	0	2,2,2	0.58	0
23	PSC	O	304	-	45,45,51	1.17	3 (6%)	48,50,59	1.27	3 (6%)
19	PGV	N	608	-	50,50,50	0.93	2 (4%)	53,56,56	1.37	5 (9%)
20	TGL	Y	101	-	58,58,62	1.25	3 (5%)	61,61,65	1.43	7 (11%)
26	CDL	T	102	-	92,92,99	1.47	12 (13%)	98,104,111	1.46	12 (12%)
27	DMU	P	313	-	34,34,34	0.46	0	45,45,45	1.51	8 (17%)
24	CHD	O	301	-	32,32,32	0.97	1 (3%)	51,51,51	1.42	4 (7%)
21	EDO	G	105	-	3,3,3	0.66	0	2,2,2	0.35	0
21	EDO	A	621	-	3,3,3	0.90	0	2,2,2	0.77	0
21	EDO	E	203	-	3,3,3	0.49	0	2,2,2	0.17	0
23	PSC	B	303	-	48,48,51	1.16	3 (6%)	51,54,59	1.05	2 (3%)
26	CDL	P	308	-	89,89,99	1.45	12 (13%)	95,99,111	1.66	14 (14%)
21	EDO	O	305	-	3,3,3	0.47	0	2,2,2	0.56	0
21	EDO	A	619	-	3,3,3	0.15	0	2,2,2	0.25	0
27	DMU	L	102	-	34,34,34	0.72	1 (2%)	45,45,45	1.29	4 (8%)
14	HEA	N	601[B]	-	67,67,67	1.74	17 (25%)	81,103,103	2.11	20 (24%)
21	EDO	A	620	-	3,3,3	0.58	0	2,2,2	0.82	0
21	EDO	N	613	-	3,3,3	0.48	0	2,2,2	0.38	0
21	EDO	N	614	-	3,3,3	0.48	0	2,2,2	0.22	0
21	EDO	N	610	-	3,3,3	0.61	0	2,2,2	0.45	0
21	EDO	D	205	-	3,3,3	0.62	0	2,2,2	0.18	0
21	EDO	P	311	-	3,3,3	0.75	0	2,2,2	0.49	0
27	DMU	L	103	-	34,34,34	0.76	1 (2%)	45,45,45	1.09	4 (8%)
21	EDO	V	102	-	3,3,3	0.57	0	2,2,2	0.15	0
21	EDO	P	312	-	3,3,3	0.68	0	2,2,2	0.21	0
21	EDO	T	103	-	3,3,3	0.53	0	2,2,2	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	C	304	-	46,46,50	0.84	1 (2%)	49,52,56	1.12	5 (10%)
21	EDO	E	204	-	3,3,3	0.48	0	2,2,2	0.35	0
25	PEK	P	306	-	52,52,52	1.04	2 (3%)	55,57,57	1.17	4 (7%)
21	EDO	O	306	-	3,3,3	0.51	0	2,2,2	0.07	0
21	EDO	B	305	-	3,3,3	0.64	0	2,2,2	0.67	0
25	PEK	P	301	-	39,39,52	1.13	2 (5%)	42,44,57	1.76	7 (16%)
21	EDO	D	202	-	3,3,3	0.50	0	2,2,2	0.19	0
27	DMU	Z	103	-	34,34,34	0.55	0	45,45,45	0.98	2 (4%)
24	CHD	C	315	-	32,32,32	0.82	1 (3%)	51,51,51	2.26	15 (29%)
27	DMU	T	101	-	34,34,34	0.57	0	45,45,45	2.44	11 (24%)
21	EDO	N	611	-	3,3,3	0.51	0	2,2,2	0.38	0
14	HEA	A	602	1	67,67,67	2.14	20 (29%)	81,103,103	2.38	33 (40%)
18	CMO	N	606[B]	15	0,1,1	-	-	-	-	-
27	DMU	Z	102	-	34,34,34	0.50	0	45,45,45	1.06	6 (13%)
19	PGV	A	607	-	50,50,50	0.97	2 (4%)	53,56,56	1.32	5 (9%)
18	CMO	A	606[B]	15	0,1,1	-	-	-	-	-
21	EDO	F	104	-	3,3,3	0.63	0	2,2,2	0.64	0
21	EDO	A	617	-	3,3,3	0.37	0	2,2,2	0.74	0
21	EDO	V	101	-	3,3,3	0.64	0	2,2,2	0.25	0
21	EDO	N	609	-	3,3,3	0.81	0	2,2,2	0.65	0
21	EDO	A	611	-	3,3,3	0.54	0	2,2,2	0.93	0
21	EDO	S	107	-	3,3,3	0.55	0	2,2,2	0.59	0
14	HEA	A	601[A]	-	67,67,67	1.98	22 (32%)	81,103,103	2.15	30 (37%)
21	EDO	O	307	-	3,3,3	0.76	0	2,2,2	0.19	0
21	EDO	L	101	-	3,3,3	0.90	0	2,2,2	0.28	0
14	HEA	N	602	1	67,67,67	1.82	22 (32%)	81,103,103	1.92	22 (27%)
21	EDO	A	612	-	3,3,3	0.91	0	2,2,2	0.64	0
21	EDO	S	102	-	3,3,3	0.75	0	2,2,2	0.79	0
21	EDO	E	202	-	3,3,3	0.62	0	2,2,2	0.24	0
14	HEA	N	601[A]	-	67,67,67	1.74	17 (25%)	81,103,103	2.02	25 (30%)
24	CHD	J	101	-	32,32,32	0.72	0	51,51,51	1.77	10 (19%)
21	EDO	H	102	-	3,3,3	0.44	0	2,2,2	0.42	0
19	PGV	Z	101	-	46,46,50	1.01	2 (4%)	49,52,56	1.40	6 (12%)
26	CDL	G	103	-	87,87,99	1.41	10 (11%)	93,99,111	1.30	6 (6%)
21	EDO	R	202	-	3,3,3	0.50	0	2,2,2	0.29	0
20	TGL	D	201	-	54,54,62	1.24	4 (7%)	57,57,65	1.16	7 (12%)
21	EDO	A	614	-	3,3,3	0.71	0	2,2,2	0.94	0
21	EDO	F	105	-	3,3,3	0.59	0	2,2,2	0.56	0
21	EDO	F	102	-	3,3,3	0.88	0	2,2,2	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	P	302	-	46,46,50	1.12	2 (4%)	49,51,56	1.75	7 (14%)
22	CUA	O	302	2	0,1,1	-	-	-		
24	CHD	P	315	-	32,32,32	0.85	0	51,51,51	2.47	20 (39%)
21	EDO	A	618	-	3,3,3	0.67	0	2,2,2	0.34	0
21	EDO	Q	202	-	3,3,3	0.33	0	2,2,2	0.27	0
21	EDO	Q	201	-	3,3,3	0.28	0	2,2,2	0.70	0
27	DMU	G	101	-	34,34,34	0.77	1 (2%)	45,45,45	2.25	12 (26%)
21	EDO	P	310	-	3,3,3	0.20	0	2,2,2	0.70	0
18	CMO	A	606[A]	-	0,1,1	-	-	-		
24	CHD	P	309	-	32,32,32	0.93	1 (3%)	51,51,51	2.00	18 (35%)
21	EDO	F	103	-	3,3,3	0.74	0	2,2,2	0.17	0
21	EDO	S	103	-	3,3,3	0.57	0	2,2,2	1.26	0
27	DMU	C	314	-	34,34,34	0.60	1 (2%)	45,45,45	1.00	1 (2%)
27	DMU	P	314	-	34,34,34	0.58	1 (2%)	45,45,45	1.12	4 (8%)
24	CHD	B	304	-	32,32,32	1.05	2 (6%)	51,51,51	1.64	13 (25%)
19	PGV	P	307	-	45,45,50	0.83	2 (4%)	48,51,56	1.13	3 (6%)
25	PEK	G	102	-	49,49,52	1.05	3 (6%)	52,54,57	1.40	5 (9%)
24	CHD	P	304	-	32,32,32	0.86	0	51,51,51	1.70	12 (23%)
21	EDO	F	106	-	3,3,3	0.54	0	2,2,2	0.45	0
21	EDO	C	311	-	3,3,3	0.47	0	2,2,2	0.28	0
19	PGV	A	608	-	50,50,50	1.09	5 (10%)	53,56,56	1.29	7 (13%)
21	EDO	K	101	-	3,3,3	0.64	0	2,2,2	0.35	0
21	EDO	U	101	-	3,3,3	0.44	0	2,2,2	0.61	0
21	EDO	A	615	-	3,3,3	0.64	0	2,2,2	0.19	0
24	CHD	Y	102	-	30,30,32	0.85	1 (3%)	45,47,51	2.30	15 (33%)
21	EDO	R	201	-	3,3,3	0.60	0	2,2,2	0.34	0
20	TGL	B	302	-	62,62,62	1.12	3 (4%)	65,65,65	1.23	3 (4%)
27	DMU	M	101	-	34,34,34	0.50	0	45,45,45	1.63	10 (22%)
20	TGL	O	303	-	62,62,62	1.09	3 (4%)	65,65,65	1.17	5 (7%)
20	TGL	A	609	-	57,57,62	1.18	3 (5%)	59,59,65	1.60	9 (15%)
25	PEK	C	308	-	45,45,52	1.07	2 (4%)	48,50,57	1.10	3 (6%)
21	EDO	C	309	-	3,3,3	0.65	0	2,2,2	0.32	0
21	EDO	D	204	-	3,3,3	0.49	0	2,2,2	0.34	0
21	EDO	S	104	-	3,3,3	0.66	0	2,2,2	0.16	0
21	EDO	H	101	-	3,3,3	0.47	0	2,2,2	0.18	0
20	TGL	N	607	-	62,62,62	1.06	3 (4%)	65,65,65	1.17	7 (10%)
21	EDO	A	613	-	3,3,3	0.60	0	2,2,2	0.08	0
26	CDL	C	306	-	81,81,99	1.37	9 (11%)	87,93,111	1.61	17 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CMO	N	606[A]	-	0,1,1	-	-	-		
21	EDO	A	610	-	3,3,3	1.04	0	2,2,2	0.54	0
21	EDO	A	622	-	3,3,3	0.44	0	2,2,2	0.29	0
14	HEA	A	601[B]	-	67,67,67	1.99	22 (32%)	81,103,103	2.30	32 (39%)
21	EDO	A	616	-	3,3,3	0.86	0	2,2,2	0.47	0
21	EDO	C	312	-	3,3,3	0.64	0	2,2,2	0.32	0
24	CHD	C	307	-	32,32,32	0.76	0	51,51,51	1.24	4 (7%)
21	EDO	B	306	-	3,3,3	0.52	0	2,2,2	0.20	0
21	EDO	S	106	-	3,3,3	0.58	0	2,2,2	0.28	0
24	CHD	C	301	-	32,32,32	1.36	4 (12%)	51,51,51	1.51	11 (21%)
21	EDO	E	201	-	3,3,3	0.41	0	2,2,2	0.53	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
25	PEK	C	303	-	-	20/56/56/56	-
21	EDO	T	104	-	-	0/1/1/1	-
21	EDO	C	310	-	-	0/1/1/1	-
21	EDO	I	101	-	-	1/1/1/1	-
21	EDO	N	612	-	-	0/1/1/1	-
21	EDO	S	105	-	-	1/1/1/1	-
25	PEK	P	305	-	-	9/55/55/56	-
27	DMU	C	313	-	-	4/19/59/59	0/2/2/2
19	PGV	C	305	-	-	18/49/49/55	-
21	EDO	G	104	-	-	1/1/1/1	-
21	EDO	D	203	-	-	0/1/1/1	-
23	PSC	O	304	-	-	14/49/49/55	-
19	PGV	N	608	-	-	11/55/55/55	-
20	TGL	Y	101	-	-	28/61/61/65	-
26	CDL	T	102	-	-	33/103/103/110	-
27	DMU	P	313	-	-	6/19/59/59	0/2/2/2
24	CHD	O	301	-	-	2/9/74/74	0/4/4/4
21	EDO	G	105	-	-	0/1/1/1	-
21	EDO	A	621	-	-	0/1/1/1	-
21	EDO	E	203	-	-	0/1/1/1	-
23	PSC	B	303	-	-	16/49/49/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	P	308	-	-	50/95/95/110	-
21	EDO	O	305	-	-	0/1/1/1	-
21	EDO	A	619	-	-	0/1/1/1	-
27	DMU	L	102	-	-	5/19/59/59	0/2/2/2
14	HEA	N	601[B]	-	-	5/36/76/76	-
21	EDO	A	620	-	-	1/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	N	614	-	-	1/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
21	EDO	D	205	-	-	0/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
27	DMU	L	103	-	-	10/19/59/59	0/2/2/2
21	EDO	V	102	-	-	0/1/1/1	-
21	EDO	P	312	-	-	1/1/1/1	-
21	EDO	T	103	-	-	0/1/1/1	-
19	PGV	C	304	-	-	8/51/51/55	-
21	EDO	E	204	-	-	0/1/1/1	-
25	PEK	P	306	-	-	25/56/56/56	-
21	EDO	O	306	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
25	PEK	P	301	-	-	17/41/41/56	-
21	EDO	D	202	-	-	1/1/1/1	-
27	DMU	Z	103	-	-	9/19/59/59	0/2/2/2
24	CHD	C	315	-	-	3/9/74/74	0/4/4/4
27	DMU	T	101	-	-	8/19/59/59	0/2/2/2
21	EDO	N	611	-	-	0/1/1/1	-
14	HEA	A	602	1	-	6/36/76/76	-
27	DMU	Z	102	-	-	5/19/59/59	0/2/2/2
19	PGV	A	607	-	-	32/55/55/55	-
21	EDO	V	101	-	-	1/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
21	EDO	A	617	-	-	0/1/1/1	-
21	EDO	N	609	-	-	0/1/1/1	-
21	EDO	A	611	-	-	1/1/1/1	-
21	EDO	S	107	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	9/36/76/76	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	L	101	-	-	1/1/1/1	-
14	HEA	N	602	1	-	5/36/76/76	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	7/36/76/76	-
24	CHD	J	101	-	-	8/9/74/74	0/4/4/4
21	EDO	H	102	-	-	0/1/1/1	-
19	PGV	Z	101	-	-	12/51/51/55	-
26	CDL	G	103	-	-	36/98/98/110	-
21	EDO	R	202	-	-	0/1/1/1	-
20	TGL	D	201	-	-	18/57/57/65	-
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
19	PGV	P	302	-	-	12/50/50/55	-
24	CHD	P	315	-	-	3/9/74/74	0/4/4/4
21	EDO	A	618	-	-	0/1/1/1	-
21	EDO	Q	202	-	-	0/1/1/1	-
21	EDO	Q	201	-	-	1/1/1/1	-
27	DMU	G	101	-	-	14/19/59/59	0/2/2/2
21	EDO	P	310	-	-	1/1/1/1	-
24	CHD	P	309	-	-	4/9/74/74	0/4/4/4
21	EDO	F	103	-	-	0/1/1/1	-
21	EDO	S	103	-	-	1/1/1/1	-
27	DMU	C	314	-	-	4/19/59/59	0/2/2/2
27	DMU	P	314	-	-	7/19/59/59	0/2/2/2
24	CHD	B	304	-	-	2/9/74/74	0/4/4/4
19	PGV	P	307	-	-	6/50/50/55	-
25	PEK	G	102	-	-	25/51/51/56	-
24	CHD	P	304	-	-	1/9/74/74	0/4/4/4
21	EDO	F	106	-	-	0/1/1/1	-
21	EDO	C	311	-	-	0/1/1/1	-
19	PGV	A	608	-	-	6/55/55/55	-
21	EDO	K	101	-	-	0/1/1/1	-
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	A	615	-	-	0/1/1/1	-
24	CHD	Y	102	-	-	2/12/67/74	0/3/3/4
21	EDO	R	201	-	-	0/1/1/1	-
20	TGL	B	302	-	-	20/65/65/65	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DMU	M	101	-	-	5/19/59/59	0/2/2/2
20	TGL	O	303	-	-	27/65/65/65	-
20	TGL	A	609	-	-	28/57/57/65	-
25	PEK	C	308	-	-	16/49/49/56	-
21	EDO	C	309	-	-	0/1/1/1	-
21	EDO	D	204	-	-	1/1/1/1	-
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	H	101	-	-	0/1/1/1	-
20	TGL	N	607	-	-	22/65/65/65	-
21	EDO	A	613	-	-	1/1/1/1	-
26	CDL	C	306	-	-	46/92/92/110	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	A	622	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	6/36/76/76	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	C	312	-	-	0/1/1/1	-
24	CHD	C	307	-	-	4/9/74/74	0/4/4/4
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	S	106	-	-	1/1/1/1	-
24	CHD	C	301	-	-	1/9/74/74	0/4/4/4
21	EDO	E	201	-	-	1/1/1/1	-

All (237) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	305	PGV	O01-C1	5.84	1.45	1.33
20	Y	101	TGL	OG2-CB1	5.52	1.49	1.34
14	A	602	HEA	C4A-NA	-5.48	1.29	1.39
20	A	609	TGL	OG2-CB1	5.23	1.49	1.34
23	B	303	PSC	O01-C1	5.22	1.49	1.34
20	Y	101	TGL	OG3-CC1	5.21	1.48	1.33
20	D	201	TGL	OG2-CB1	5.18	1.48	1.34
20	B	302	TGL	OG1-CA1	4.98	1.47	1.33
14	A	601[A]	HEA	C4D-C3D	-4.95	1.36	1.45
14	A	601[B]	HEA	C4D-C3D	-4.95	1.36	1.45
26	T	102	CDL	OB8-CB7	4.93	1.47	1.33
14	A	602	HEA	CHD-C1D	4.89	1.48	1.38
19	P	302	PGV	O03-C19	4.88	1.47	1.33
14	N	602	HEA	CHB-C4A	4.84	1.47	1.38
25	P	301	PEK	O03-C21	4.83	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	201	TGL	OG1-CA1	4.77	1.47	1.33
20	B	302	TGL	OG2-CB1	4.77	1.47	1.34
14	N	601[A]	HEA	CHA-C1A	4.74	1.47	1.38
14	N	601[B]	HEA	CHA-C1A	4.74	1.47	1.38
20	O	303	TGL	OG2-CB1	4.71	1.47	1.34
19	C	305	PGV	O03-C19	4.70	1.47	1.33
25	C	308	PEK	O03-C21	4.66	1.46	1.33
19	P	302	PGV	O01-C1	4.65	1.47	1.34
23	O	304	PSC	O01-C1	4.64	1.47	1.34
20	Y	101	TGL	OG1-CA1	4.63	1.46	1.33
14	A	602	HEA	FE-NC	4.62	2.10	1.95
26	P	308	CDL	OA8-CA7	4.60	1.46	1.33
26	P	308	CDL	OB8-CB7	4.58	1.46	1.33
20	N	607	TGL	OG1-CA1	4.57	1.46	1.33
19	Z	101	PGV	O03-C19	4.55	1.46	1.33
26	C	306	CDL	OA8-CA7	4.54	1.46	1.33
20	O	303	TGL	OG1-CA1	4.52	1.46	1.33
26	G	103	CDL	OB8-CB7	4.51	1.46	1.33
26	G	103	CDL	OA6-CA5	4.51	1.47	1.34
26	C	306	CDL	OA6-CA5	4.49	1.47	1.34
25	G	102	PEK	O03-C21	4.48	1.46	1.33
19	A	607	PGV	O01-C1	4.48	1.46	1.34
20	O	303	TGL	OG3-CC1	4.48	1.46	1.33
25	P	306	PEK	O03-C21	4.48	1.46	1.33
20	N	607	TGL	OG2-CB1	4.47	1.46	1.34
26	T	102	CDL	OA8-CA7	4.43	1.46	1.33
25	P	306	PEK	O01-C1	4.42	1.46	1.34
20	A	609	TGL	OG1-CA1	4.41	1.46	1.33
20	B	302	TGL	OG3-CC1	4.40	1.46	1.33
26	G	103	CDL	OA8-CA7	4.37	1.46	1.33
14	A	602	HEA	CHB-C4A	4.36	1.46	1.38
25	C	308	PEK	O01-C1	4.35	1.46	1.34
25	G	102	PEK	O01-C1	4.33	1.46	1.34
26	C	306	CDL	OB8-CB7	4.29	1.45	1.33
14	A	602	HEA	FE-NA	4.29	2.09	1.95
26	T	102	CDL	OA6-CA5	4.27	1.46	1.34
14	A	602	HEA	C4D-C3D	-4.21	1.37	1.45
23	O	304	PSC	O03-C19	4.19	1.45	1.33
26	P	308	CDL	OB6-CB5	4.19	1.46	1.34
20	N	607	TGL	OG3-CC1	4.16	1.45	1.33
26	G	103	CDL	OB6-CB5	4.14	1.46	1.34
14	A	601[A]	HEA	CMC-C2C	4.13	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	601[B]	HEA	CMC-C2C	4.13	1.59	1.50
14	A	602	HEA	CHC-C4B	4.10	1.46	1.38
19	A	607	PGV	O03-C19	4.07	1.45	1.33
14	N	602	HEA	CHA-C1A	4.06	1.46	1.38
26	P	308	CDL	OA6-CA5	4.02	1.45	1.34
26	T	102	CDL	OB6-CB5	3.98	1.45	1.34
14	A	601[A]	HEA	CBD-CGD	3.98	1.59	1.50
14	A	601[B]	HEA	CBD-CGD	3.98	1.59	1.50
25	P	301	PEK	O01-C1	3.96	1.45	1.34
14	A	601[A]	HEA	CHD-C1D	3.94	1.46	1.38
14	A	601[B]	HEA	CHD-C1D	3.94	1.46	1.38
20	A	609	TGL	OG3-CC1	3.93	1.52	1.33
23	B	303	PSC	C13-C12	3.90	1.53	1.31
19	N	608	PGV	O03-C19	3.90	1.44	1.33
19	A	608	PGV	O03-C19	3.90	1.44	1.33
26	T	102	CDL	C59-C58	-3.90	1.32	1.51
26	G	103	CDL	C59-C58	-3.86	1.32	1.51
26	T	102	CDL	C42-C41	-3.78	1.33	1.51
26	G	103	CDL	C62-C61	-3.77	1.33	1.51
26	T	102	CDL	C19-C18	-3.76	1.33	1.51
26	T	102	CDL	C39-C38	-3.73	1.33	1.51
19	Z	101	PGV	O01-C1	3.73	1.44	1.34
23	O	304	PSC	C13-C12	3.70	1.52	1.31
26	C	306	CDL	OB6-CB5	3.70	1.44	1.34
26	P	308	CDL	C59-C58	-3.69	1.33	1.51
26	P	308	CDL	C79-C78	-3.69	1.33	1.51
25	C	303	PEK	O03-C21	3.68	1.44	1.33
14	N	601[A]	HEA	C4B-NB	-3.67	1.33	1.40
14	N	601[B]	HEA	C4B-NB	-3.67	1.33	1.40
26	P	308	CDL	C19-C18	-3.67	1.33	1.51
26	T	102	CDL	C82-C81	-3.65	1.33	1.51
26	T	102	CDL	C79-C78	-3.64	1.33	1.51
14	A	602	HEA	C4C-NC	-3.64	1.32	1.39
19	N	608	PGV	O01-C1	3.62	1.44	1.34
26	C	306	CDL	C42-C41	-3.61	1.33	1.51
26	C	306	CDL	C39-C38	-3.60	1.33	1.51
14	A	601[A]	HEA	CHB-C4A	3.59	1.45	1.38
14	A	601[B]	HEA	CHB-C4A	3.59	1.45	1.38
26	P	308	CDL	C22-C21	-3.59	1.33	1.51
26	T	102	CDL	C62-C61	-3.58	1.34	1.51
26	C	306	CDL	C79-C78	-3.56	1.34	1.51
26	C	306	CDL	C82-C81	-3.55	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	308	CDL	C82-C81	-3.54	1.34	1.51
26	P	308	CDL	C39-C38	-3.52	1.34	1.51
26	G	103	CDL	C42-C41	-3.47	1.34	1.51
26	G	103	CDL	C82-C81	-3.47	1.34	1.51
26	P	308	CDL	C42-C41	-3.43	1.34	1.51
25	C	303	PEK	O01-C1	3.42	1.43	1.34
20	D	201	TGL	OG3-CC1	3.42	1.43	1.33
26	G	103	CDL	C39-C38	-3.40	1.34	1.51
14	N	602	HEA	C1D-C2D	-3.38	1.37	1.44
14	N	601[A]	HEA	CHB-C4A	3.36	1.45	1.38
14	N	601[B]	HEA	CHB-C4A	3.36	1.45	1.38
19	C	305	PGV	C12-C11	3.36	1.50	1.31
14	A	601[A]	HEA	C4A-NA	-3.32	1.33	1.39
14	A	601[B]	HEA	C4A-NA	-3.32	1.33	1.39
26	G	103	CDL	C79-C78	-3.30	1.35	1.51
14	N	602	HEA	C4B-C3B	-3.27	1.39	1.44
23	B	303	PSC	O03-C19	3.26	1.45	1.33
19	A	608	PGV	O01-C1	3.25	1.43	1.34
14	N	601[A]	HEA	CHC-C4B	3.24	1.45	1.38
14	N	601[B]	HEA	CHC-C4B	3.24	1.45	1.38
25	P	305	PEK	O03-C21	3.21	1.42	1.33
27	G	101	DMU	O16-C6	3.17	1.45	1.40
24	C	301	CHD	O12-C12	3.17	1.48	1.43
14	A	601[A]	HEA	C4B-C3B	-3.12	1.39	1.44
14	A	601[B]	HEA	C4B-C3B	-3.12	1.39	1.44
25	P	305	PEK	O01-C1	3.06	1.42	1.34
26	C	306	CDL	C59-C58	-3.02	1.33	1.51
14	A	601[A]	HEA	FE-NA	3.00	2.05	1.95
14	A	601[B]	HEA	FE-NA	3.00	2.05	1.95
14	N	602	HEA	C4D-C3D	-2.96	1.40	1.45
14	A	602	HEA	CMC-C2C	2.96	1.56	1.50
19	P	307	PGV	O01-C1	2.93	1.42	1.34
14	A	601[A]	HEA	C1A-NA	-2.90	1.34	1.39
14	A	601[B]	HEA	C1A-NA	-2.90	1.34	1.39
14	N	602	HEA	FE-NA	2.90	2.04	1.95
14	A	601[A]	HEA	CHA-C4D	2.89	1.45	1.39
14	A	601[B]	HEA	CHA-C4D	2.89	1.45	1.39
14	N	601[A]	HEA	FE-NA	2.89	2.04	1.95
14	N	601[B]	HEA	FE-NA	2.89	2.04	1.95
14	N	602	HEA	C1B-C2B	-2.89	1.38	1.44
14	A	602	HEA	CHA-C1A	2.89	1.44	1.38
24	C	301	CHD	C11-C9	2.89	1.58	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602	HEA	CHA-C4D	2.89	1.45	1.39
19	C	305	PGV	C10-C11	-2.89	1.34	1.50
14	A	602	HEA	C1A-NA	-2.87	1.34	1.39
14	N	601[A]	HEA	C3A-C4A	-2.86	1.41	1.46
14	N	601[B]	HEA	C3A-C4A	-2.86	1.41	1.46
14	A	601[A]	HEA	CHB-C1B	2.85	1.45	1.39
14	A	601[B]	HEA	CHB-C1B	2.85	1.45	1.39
14	N	601[A]	HEA	FE-ND	2.84	2.03	1.94
14	N	601[B]	HEA	FE-ND	2.84	2.03	1.94
14	A	601[A]	HEA	CHA-C1A	2.83	1.43	1.38
14	A	601[B]	HEA	CHA-C1A	2.83	1.43	1.38
14	A	602	HEA	C11-C3B	2.82	1.54	1.51
27	L	103	DMU	O16-C6	2.81	1.44	1.40
14	A	601[A]	HEA	C3D-C2D	2.79	1.42	1.36
14	A	601[B]	HEA	C3D-C2D	2.79	1.42	1.36
14	N	601[A]	HEA	CHD-C1D	2.78	1.44	1.38
14	N	601[B]	HEA	CHD-C1D	2.78	1.44	1.38
14	A	602	HEA	CHD-C4C	2.76	1.45	1.39
14	A	602	HEA	C1D-C2D	-2.76	1.38	1.44
14	A	601[A]	HEA	C1D-C2D	-2.76	1.38	1.44
14	A	601[B]	HEA	C1D-C2D	-2.76	1.38	1.44
14	A	601[A]	HEA	C4C-NC	-2.74	1.34	1.39
14	A	601[B]	HEA	C4C-NC	-2.74	1.34	1.39
14	N	601[A]	HEA	C4A-NA	-2.72	1.34	1.39
14	N	601[B]	HEA	C4A-NA	-2.72	1.34	1.39
19	C	304	PGV	O03-C19	2.69	1.41	1.33
14	N	602	HEA	FE-ND	2.69	2.03	1.94
20	D	201	TGL	OB1-CB1	2.68	1.30	1.22
14	A	602	HEA	C4B-C3B	-2.64	1.40	1.44
14	N	602	HEA	C3A-C4A	-2.64	1.41	1.46
24	C	301	CHD	C4-C5	2.62	1.58	1.53
14	N	602	HEA	FE-NC	2.61	2.03	1.95
27	L	102	DMU	O16-C6	2.60	1.44	1.40
14	A	601[A]	HEA	CHC-C4B	2.60	1.43	1.38
14	A	601[B]	HEA	CHC-C4B	2.60	1.43	1.38
14	N	602	HEA	CHD-C4C	2.59	1.45	1.39
14	N	602	HEA	CHC-C1C	2.58	1.45	1.39
14	A	602	HEA	C1C-NC	-2.56	1.34	1.39
19	P	307	PGV	O03-C19	2.54	1.40	1.33
24	B	304	CHD	C13-C12	-2.54	1.50	1.54
14	N	602	HEA	C1A-C2A	-2.53	1.40	1.45
14	N	602	HEA	CHB-C1B	2.51	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	304	CHD	C11-C12	2.50	1.57	1.53
14	N	601[A]	HEA	C4B-C3B	-2.47	1.40	1.44
14	N	601[B]	HEA	C4B-C3B	-2.47	1.40	1.44
14	A	601[A]	HEA	O11-C11	2.46	1.48	1.42
14	A	602	HEA	FE-ND	2.45	2.02	1.94
19	A	608	PGV	O01-C02	-2.43	1.40	1.46
27	C	314	DMU	O16-C6	2.43	1.44	1.40
14	A	601[A]	HEA	CMB-C2B	2.42	1.55	1.50
14	A	601[B]	HEA	CMB-C2B	2.42	1.55	1.50
14	A	601[A]	HEA	CBA-CGA	2.41	1.56	1.50
14	A	601[B]	HEA	CBA-CGA	2.41	1.56	1.50
14	N	602	HEA	C4B-NB	-2.40	1.36	1.40
14	A	601[A]	HEA	CAD-C3D	2.39	1.57	1.51
14	A	601[B]	HEA	CAD-C3D	2.39	1.57	1.51
14	A	602	HEA	CMB-C2B	2.38	1.55	1.50
24	O	301	CHD	O7-C7	2.35	1.48	1.43
19	A	608	PGV	O03-C01	2.34	1.50	1.45
14	N	602	HEA	FE-NB	2.34	2.02	1.94
14	N	601[A]	HEA	CMD-C2D	2.32	1.55	1.50
14	N	601[B]	HEA	CMD-C2D	2.32	1.55	1.50
14	N	602	HEA	CHC-C4B	2.31	1.43	1.38
24	C	315	CHD	C10-C9	-2.31	1.52	1.56
14	N	601[A]	HEA	C1B-C2B	-2.29	1.39	1.44
14	N	601[B]	HEA	C1B-C2B	-2.29	1.39	1.44
24	C	301	CHD	C13-C12	-2.26	1.51	1.54
14	A	602	HEA	CHB-C1B	2.25	1.44	1.39
14	N	601[A]	HEA	C1C-NC	-2.23	1.35	1.39
14	N	601[B]	HEA	C1C-NC	-2.23	1.35	1.39
14	N	601[A]	HEA	C4C-NC	-2.22	1.35	1.39
14	N	601[B]	HEA	C4C-NC	-2.22	1.35	1.39
14	N	601[A]	HEA	CMC-C2C	2.21	1.55	1.50
14	N	601[B]	HEA	CMC-C2C	2.21	1.55	1.50
26	T	102	CDL	C22-C21	-2.21	1.34	1.50
24	P	309	CHD	C10-C9	-2.20	1.52	1.56
14	A	601[A]	HEA	FE-NB	2.19	2.01	1.94
14	A	601[B]	HEA	FE-NB	2.19	2.01	1.94
14	N	601[A]	HEA	CBD-CGD	2.13	1.55	1.50
14	N	601[B]	HEA	CBD-CGD	2.13	1.55	1.50
19	A	608	PGV	C20-C19	2.12	1.56	1.50
27	P	314	DMU	O16-C6	2.12	1.43	1.40
26	P	308	CDL	PA1-OA2	2.12	1.62	1.54
14	A	602	HEA	C12-C11	2.11	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	102	PEK	P-O12	2.09	1.62	1.54
14	A	601[B]	HEA	O11-C11	2.06	1.47	1.42
14	N	601[A]	HEA	FE-NC	2.06	2.01	1.95
14	N	601[B]	HEA	FE-NC	2.06	2.01	1.95
14	N	602	HEA	O11-C11	2.05	1.47	1.42
14	N	602	HEA	CMA-C3A	2.04	1.49	1.45
14	N	602	HEA	C4C-NC	-2.03	1.35	1.39
14	N	602	HEA	CHD-C1D	2.02	1.42	1.38
24	Y	102	CHD	C13-C14	-2.02	1.52	1.55
27	C	313	DMU	O16-C6	2.01	1.43	1.40
14	A	601[A]	HEA	CBC-CAC	2.01	1.40	1.30
14	A	601[B]	HEA	CBC-CAC	2.01	1.40	1.30

All (518) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601[B]	HEA	C13-C12-C11	-7.59	102.26	114.39
27	T	101	DMU	O4-C7-C5	-7.34	93.06	110.38
19	P	302	PGV	O01-C1-C2	7.24	127.14	111.48
25	P	301	PEK	O01-C1-C2	6.62	125.81	111.48
19	C	305	PGV	O01-C1-O02	-6.56	117.29	125.70
24	C	315	CHD	C5-C4-C3	-6.23	103.31	112.71
27	G	101	DMU	O4-C7-C5	-6.20	95.77	110.38
26	P	308	CDL	CA4-OA6-CA5	6.15	132.51	117.80
26	P	308	CDL	OB6-CB5-C51	6.00	124.45	111.48
24	C	315	CHD	C1-C10-C5	5.94	116.28	107.75
20	A	609	TGL	OG3-CC1-CC2	5.91	137.44	112.38
25	C	303	PEK	C2-C3-C4	5.90	126.25	113.35
14	N	601[A]	HEA	C13-C12-C11	-5.81	105.11	114.39
14	N	601[B]	HEA	C27-C19-C20	5.78	125.27	115.23
14	A	601[B]	HEA	C12-C11-C3B	5.77	121.14	112.12
20	B	302	TGL	OG2-CB1-CB2	5.69	123.78	111.48
24	P	315	CHD	C13-C14-C8	-5.63	107.58	114.72
27	T	101	DMU	O2-C8-C9	-5.62	95.48	109.32
14	A	601[A]	HEA	C3D-C4D-ND	5.59	115.75	110.35
14	A	601[B]	HEA	C3D-C4D-ND	5.59	115.75	110.35
20	O	303	TGL	OG2-CB1-CB2	5.55	123.49	111.48
24	P	315	CHD	C6-C5-C4	-5.53	104.90	111.23
27	T	101	DMU	O1-C10-C5	5.50	121.68	110.37
26	G	103	CDL	OA6-CA5-C11	5.49	123.36	111.48
14	A	602	HEA	C27-C19-C20	5.46	124.71	115.23
27	G	101	DMU	C18-O16-C6	5.42	122.93	113.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602	HEA	C27-C19-C20	5.40	124.59	115.23
14	N	602	HEA	C3C-C4C-NC	5.35	114.31	109.80
14	A	601[B]	HEA	C13-C12-C11	-5.34	105.86	114.39
24	J	101	CHD	C6-C5-C4	-5.29	105.18	111.23
14	N	602	HEA	CHB-C1B-NB	5.23	130.06	124.42
19	Z	101	PGV	O01-C1-C2	5.21	122.75	111.48
14	A	602	HEA	CHB-C4A-NA	5.20	130.12	124.45
19	C	305	PGV	O03-C19-C20	5.20	127.69	111.83
14	A	602	HEA	C2B-C1B-NB	5.10	115.80	109.90
19	P	302	PGV	O03-C19-C20	5.05	127.23	111.83
23	O	304	PSC	O01-C1-C2	5.03	122.36	111.48
20	Y	101	TGL	OG2-CB1-CB2	4.99	122.27	111.48
26	T	102	CDL	OA6-CA5-C11	4.99	122.27	111.48
25	G	102	PEK	O01-C1-C2	4.98	122.24	111.48
20	N	607	TGL	OG2-CB1-CB2	4.95	122.20	111.48
26	T	102	CDL	OB6-CB5-C51	4.94	122.17	111.48
26	P	308	CDL	OA6-CA4-CA3	4.94	126.06	108.34
24	Y	102	CHD	C5-C6-C7	4.93	120.26	114.40
26	C	306	CDL	CB4-OB6-CB5	-4.92	106.01	117.80
19	A	608	PGV	O03-C19-O04	-4.85	111.49	123.63
24	C	315	CHD	C22-C20-C17	-4.85	100.28	110.33
14	N	602	HEA	CHB-C1B-C2B	-4.85	117.38	125.03
24	C	315	CHD	C11-C9-C10	-4.84	108.79	113.70
24	Y	102	CHD	C6-C7-C8	4.83	116.77	111.50
14	N	601[A]	HEA	C3C-C2C-C1C	-4.81	101.50	107.17
14	N	601[B]	HEA	C3C-C2C-C1C	-4.81	101.50	107.17
24	J	101	CHD	C5-C6-C7	4.79	120.09	114.40
27	T	101	DMU	C10-O7-C3	-4.78	106.64	117.98
27	G	101	DMU	C10-O7-C3	-4.75	106.71	117.98
14	A	601[A]	HEA	CHA-C1A-NA	4.75	129.62	124.45
14	A	601[B]	HEA	CHA-C1A-NA	4.75	129.62	124.45
25	C	303	PEK	O01-C1-O02	-4.74	112.62	123.70
24	C	315	CHD	C21-C20-C17	4.73	119.98	112.88
24	Y	102	CHD	C13-C17-C20	-4.69	113.80	119.48
27	G	101	DMU	O7-C10-C5	4.69	119.62	108.09
14	N	601[A]	HEA	C2D-C1D-ND	4.66	115.19	109.84
14	N	601[B]	HEA	C2D-C1D-ND	4.66	115.19	109.84
14	A	602	HEA	CHD-C4C-NC	4.65	132.29	123.86
27	T	101	DMU	O1-C9-C8	4.63	118.05	109.70
24	Y	102	CHD	O12-C12-C11	4.63	118.54	109.12
26	P	308	CDL	OB8-CB7-C71	4.59	125.82	111.83
26	C	306	CDL	O1-C1-CA2	-4.54	94.01	109.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	315	CHD	C1-C2-C3	4.52	116.47	110.48
24	P	315	CHD	C11-C9-C10	-4.52	109.11	113.70
14	A	601[A]	HEA	C2B-C1B-NB	4.50	115.10	109.90
14	A	601[B]	HEA	C2B-C1B-NB	4.50	115.10	109.90
24	P	304	CHD	C22-C20-C17	-4.45	101.10	110.33
14	A	602	HEA	C4B-NB-C1B	-4.44	99.94	105.21
14	A	602	HEA	C3D-C4D-ND	4.44	114.64	110.35
24	P	309	CHD	C11-C9-C10	-4.36	109.28	113.70
20	A	609	TGL	OC1-CC1-CC2	-4.36	109.32	124.77
26	T	102	CDL	CA4-OA6-CA5	-4.36	107.36	117.80
14	N	601[B]	HEA	C12-C11-C3B	4.35	118.92	112.12
14	N	601[A]	HEA	C3D-C4D-ND	4.33	114.54	110.35
14	N	601[B]	HEA	C3D-C4D-ND	4.33	114.54	110.35
19	A	608	PGV	O03-C19-C20	4.32	124.99	111.83
20	A	609	TGL	OG2-CB1-CB2	4.31	120.81	111.48
14	A	602	HEA	C13-C12-C11	-4.30	107.52	114.39
27	G	101	DMU	O5-C6-O16	4.27	120.14	110.04
25	P	305	PEK	O03-C21-O04	-4.26	112.97	123.63
24	P	315	CHD	C9-C8-C7	4.24	117.19	111.86
14	A	602	HEA	C4C-CHD-C1D	-4.24	116.28	126.25
25	G	102	PEK	O03-C21-C22	4.23	124.73	111.83
24	Y	102	CHD	C17-C13-C14	4.21	104.33	100.11
26	G	103	CDL	OB6-CB5-C51	4.19	120.54	111.48
27	T	101	DMU	C7-C8-C9	4.18	117.82	110.23
26	C	306	CDL	OB6-CB5-C51	4.17	120.51	111.48
24	P	315	CHD	C17-C13-C14	4.14	104.27	100.11
20	Y	101	TGL	OG3-CC1-CC2	4.12	124.39	111.83
14	A	602	HEA	C1D-ND-C4D	-4.11	100.34	105.21
26	P	308	CDL	CB4-OB6-CB5	-4.10	107.98	117.80
19	Z	101	PGV	C02-O01-C1	-4.10	107.99	117.80
24	P	315	CHD	C10-C9-C8	4.09	116.40	111.84
14	N	601[A]	HEA	C2C-C1C-NC	4.09	116.69	110.14
14	N	601[B]	HEA	C2C-C1C-NC	4.09	116.69	110.14
24	P	309	CHD	C21-C20-C22	-4.06	104.05	110.34
19	A	607	PGV	O03-C19-C20	4.06	124.21	111.83
24	Y	102	CHD	C6-C5-C4	-4.02	105.72	111.71
27	T	101	DMU	C10-C5-C7	4.02	118.46	110.01
24	P	309	CHD	C15-C14-C13	4.00	107.42	103.54
14	A	601[A]	HEA	C4B-NB-C1B	-4.00	100.47	105.21
14	A	601[B]	HEA	C4B-NB-C1B	-4.00	100.47	105.21
24	P	315	CHD	C19-C10-C1	-3.99	101.96	108.31
19	N	608	PGV	O03-C19-C20	3.99	123.99	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	601[A]	HEA	C1D-ND-C4D	-3.99	100.49	105.21
14	A	601[B]	HEA	C1D-ND-C4D	-3.99	100.49	105.21
25	P	305	PEK	O03-C21-C22	3.97	123.95	111.83
26	G	103	CDL	CB4-OB6-CB5	-3.96	108.33	117.80
27	M	101	DMU	O7-C10-C5	3.95	117.80	108.09
27	T	101	DMU	C10-O1-C9	3.95	121.42	113.72
19	N	608	PGV	O03-C19-O04	-3.94	113.77	123.63
24	C	301	CHD	C22-C20-C17	-3.94	102.16	110.33
14	A	601[A]	HEA	O11-C11-C3B	-3.94	104.03	111.26
27	C	313	DMU	O1-C9-C11	3.94	116.20	106.44
26	C	306	CDL	OA6-CA5-C11	3.93	119.98	111.48
27	P	313	DMU	C10-O1-C9	3.92	121.38	113.72
24	Y	102	CHD	C13-C14-C8	-3.92	109.75	114.72
25	P	306	PEK	O03-C21-C22	3.91	123.77	111.83
24	P	315	CHD	C6-C5-C10	3.90	116.81	112.66
14	N	601[A]	HEA	C1D-ND-C4D	-3.83	100.67	105.21
14	N	601[B]	HEA	C1D-ND-C4D	-3.83	100.67	105.21
23	B	303	PSC	O01-C1-C2	3.80	119.70	111.48
24	C	315	CHD	C1-C10-C9	-3.79	105.45	111.34
14	A	601[A]	HEA	CAA-CBA-CGA	-3.78	103.63	113.67
14	A	601[B]	HEA	CAA-CBA-CGA	-3.78	103.63	113.67
27	G	101	DMU	C7-C8-C9	3.78	117.08	110.23
24	J	101	CHD	C6-C7-C8	3.77	115.62	111.50
24	P	315	CHD	O3-C3-C4	-3.77	102.34	109.84
24	O	301	CHD	C6-C5-C4	-3.76	106.93	111.23
14	A	601[B]	HEA	O11-C11-C3B	-3.75	104.37	111.26
19	A	607	PGV	C3-C2-C1	-3.75	99.95	113.69
14	N	602	HEA	C4A-CHB-C1B	-3.74	118.07	126.02
19	A	607	PGV	O03-C19-O04	-3.74	114.28	123.63
26	C	306	CDL	CA6-CA4-CA3	-3.70	103.15	111.78
14	A	602	HEA	CMB-C2B-C1B	3.69	130.81	125.03
14	N	601[A]	HEA	C3C-C4C-NC	3.68	112.90	109.80
14	N	601[B]	HEA	C3C-C4C-NC	3.68	112.90	109.80
26	T	102	CDL	CB4-OB6-CB5	-3.68	109.00	117.80
26	T	102	CDL	OA8-CA7-C31	3.67	123.03	111.83
14	A	602	HEA	O11-C11-C3B	-3.66	104.55	111.26
14	A	601[A]	HEA	O2A-CGA-CBA	3.65	125.53	114.00
14	A	601[B]	HEA	O2A-CGA-CBA	3.65	125.53	114.00
25	P	301	PEK	C02-O01-C1	-3.64	109.08	117.80
24	P	309	CHD	C13-C17-C20	-3.63	115.08	119.48
24	P	309	CHD	C16-C17-C20	3.61	117.64	112.18
24	P	304	CHD	C15-C14-C13	3.61	107.04	103.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	306	PEK	O01-C1-C2	3.61	119.28	111.48
14	A	602	HEA	C2D-C1D-ND	3.61	113.98	109.84
24	C	301	CHD	C15-C14-C13	3.60	107.03	103.54
24	P	315	CHD	C4-C3-C2	3.59	115.00	110.62
24	P	315	CHD	C1-C10-C5	3.58	112.89	107.75
14	A	602	HEA	C20-C19-C18	-3.56	113.17	121.17
27	P	314	DMU	C10-O1-C9	3.55	120.65	113.72
24	P	309	CHD	C13-C14-C8	-3.54	110.23	114.72
14	A	601[A]	HEA	CHA-C1A-C2A	-3.54	119.27	124.86
14	A	601[B]	HEA	CHA-C1A-C2A	-3.54	119.27	124.86
25	P	301	PEK	O03-C21-C22	3.52	122.57	111.83
24	P	304	CHD	C1-C10-C5	3.52	112.80	107.75
20	N	607	TGL	OG1-CA1-CA2	3.51	122.55	111.83
27	L	102	DMU	O1-C10-C5	3.50	117.56	110.37
20	B	302	TGL	OG1-CA1-CA2	3.50	122.51	111.83
27	L	102	DMU	C10-C5-C7	3.48	117.33	110.01
14	A	602	HEA	C3B-C4B-NB	3.48	113.84	109.84
14	A	601[A]	HEA	CAD-CBD-CGD	-3.47	104.46	113.67
14	A	601[B]	HEA	CAD-CBD-CGD	-3.47	104.46	113.67
27	P	313	DMU	O1-C10-C5	3.46	117.48	110.37
24	P	309	CHD	C1-C2-C3	3.46	115.06	110.48
24	B	304	CHD	C1-C10-C5	3.45	112.70	107.75
25	P	305	PEK	O01-C1-O02	-3.44	115.66	123.70
24	B	304	CHD	C17-C13-C12	3.43	120.76	117.67
26	P	308	CDL	OA8-CA7-C31	3.43	122.30	111.83
14	A	601[A]	HEA	C12-C11-C3B	3.43	117.48	112.12
19	P	302	PGV	O01-C1-O02	-3.42	115.70	123.70
24	Y	102	CHD	C21-C20-C22	-3.41	105.06	110.34
27	L	102	DMU	C10-O1-C9	3.40	120.36	113.72
25	P	305	PEK	O01-C1-C2	3.39	118.81	111.48
19	P	302	PGV	C21-C20-C19	-3.39	101.29	113.69
14	N	602	HEA	CBD-CAD-C3D	3.39	121.89	112.53
27	T	101	DMU	O7-C10-C5	3.38	116.42	108.09
24	O	301	CHD	C1-C2-C3	-3.38	106.00	110.48
24	P	304	CHD	C21-C20-C22	-3.38	105.11	110.34
24	Y	102	CHD	C10-C9-C8	-3.37	108.08	111.84
27	G	101	DMU	C8-C7-C5	3.37	116.74	110.83
14	A	602	HEA	O1A-CGA-CBA	-3.36	112.43	123.09
20	N	607	TGL	OG3-CC1-CC2	3.35	122.04	111.83
24	Y	102	CHD	C17-C13-C12	-3.33	114.67	117.67
27	G	101	DMU	O3-C5-C10	3.32	118.00	110.08
20	O	303	TGL	OG1-CA1-CA2	3.29	121.88	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	101	CHD	C14-C8-C7	3.27	116.19	111.85
24	J	101	CHD	C13-C17-C20	-3.26	115.54	119.48
24	C	307	CHD	C4-C5-C10	3.25	116.12	112.66
25	C	303	PEK	O01-C1-C2	3.25	118.52	111.48
26	C	306	CDL	OB8-CB7-C71	3.22	121.65	111.83
14	A	602	HEA	C3A-C2A-C1A	-3.22	104.00	107.05
14	A	602	HEA	C25-C23-C24	3.22	121.99	114.59
14	A	601[A]	HEA	C3A-C2A-C1A	-3.22	104.00	107.05
14	A	601[B]	HEA	C3A-C2A-C1A	-3.22	104.00	107.05
14	A	601[B]	HEA	C27-C19-C20	3.20	120.79	115.23
24	B	304	CHD	O12-C12-C13	-3.19	105.63	111.02
19	N	608	PGV	C03-C02-C01	-3.18	104.37	111.78
20	D	201	TGL	OG3-CG3-CG2	-3.18	99.23	108.40
14	A	601[A]	HEA	O1A-CGA-CBA	-3.18	113.01	123.09
14	A	601[B]	HEA	O1A-CGA-CBA	-3.18	113.01	123.09
20	D	201	TGL	OG1-CA1-CA2	3.17	121.50	111.83
19	P	307	PGV	O01-C1-O02	-3.17	116.30	123.70
14	A	601[A]	HEA	C13-C12-C11	-3.17	109.33	114.39
27	P	313	DMU	C10-O7-C3	-3.15	110.51	117.98
14	A	602	HEA	CAA-C2A-C1A	3.15	131.26	124.85
25	G	102	PEK	C02-O01-C1	-3.14	110.29	117.80
25	C	308	PEK	O01-C1-C2	3.12	118.22	111.48
25	P	306	PEK	O03-C21-O04	-3.08	115.93	123.63
23	B	303	PSC	C03-C02-C01	-3.07	104.62	111.78
24	P	309	CHD	C14-C8-C9	-3.07	105.46	109.75
27	P	314	DMU	O7-C3-C4	3.07	117.53	109.48
19	P	302	PGV	O03-C19-O04	-3.06	115.97	123.63
14	N	601[A]	HEA	O11-C11-C3B	-3.06	105.65	111.26
14	A	601[A]	HEA	C3B-C4B-NB	3.05	113.34	109.84
14	A	601[B]	HEA	C3B-C4B-NB	3.05	113.34	109.84
19	Z	101	PGV	O03-C19-C20	3.04	121.10	111.83
19	C	305	PGV	O03-C19-O04	-3.04	116.03	123.63
19	A	607	PGV	O01-C1-C2	3.04	118.05	111.48
25	G	102	PEK	O03-C21-O04	-3.03	116.06	123.63
27	T	101	DMU	O3-C5-C10	3.00	117.23	110.08
24	C	315	CHD	C11-C12-C13	-3.00	108.21	111.26
24	C	301	CHD	C6-C5-C4	-2.99	107.81	111.23
14	N	602	HEA	C4C-CHD-C1D	-2.97	119.25	126.25
24	B	304	CHD	C15-C14-C8	-2.97	114.29	118.36
14	N	601[A]	HEA	C26-C15-C16	2.93	120.32	115.23
26	C	306	CDL	OB2-PB2-OB3	2.92	120.53	108.94
14	A	601[B]	HEA	C25-C23-C24	2.92	121.32	114.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	101	DMU	C10-O7-C3	-2.91	111.07	117.98
27	M	101	DMU	O16-C18-C19	-2.91	99.48	109.37
24	C	315	CHD	C13-C14-C8	-2.90	111.04	114.72
24	B	304	CHD	C2-C1-C10	-2.90	107.85	112.74
24	B	304	CHD	C6-C5-C4	-2.89	107.92	111.23
27	M	101	DMU	O1-C10-C5	-2.89	104.44	110.37
24	J	101	CHD	C6-C5-C10	2.88	115.73	112.66
25	C	308	PEK	O03-C21-C22	2.88	120.62	111.83
24	C	315	CHD	O3-C3-C4	2.87	115.56	109.84
14	A	602	HEA	C4A-CHB-C1B	-2.87	119.92	126.02
25	C	303	PEK	O03-C21-C22	2.87	120.58	111.83
19	P	302	PGV	C01-O03-C19	2.87	127.59	117.12
27	P	313	DMU	O1-C9-C11	2.85	113.51	106.44
14	A	602	HEA	CMB-C2B-C3B	-2.85	124.76	130.28
14	A	601[A]	HEA	C4C-CHD-C1D	-2.85	119.55	126.25
14	A	601[B]	HEA	C4C-CHD-C1D	-2.85	119.55	126.25
24	P	309	CHD	C21-C20-C17	2.85	117.16	112.88
24	P	315	CHD	C2-C1-C10	2.85	117.54	112.74
14	A	601[A]	HEA	CHB-C1B-NB	-2.84	121.37	124.42
14	A	601[B]	HEA	CHB-C1B-NB	-2.84	121.37	124.42
14	N	601[A]	HEA	CAA-CBA-CGA	-2.84	106.14	113.67
14	N	601[B]	HEA	CAA-CBA-CGA	-2.84	106.14	113.67
24	C	301	CHD	C23-C22-C20	-2.83	109.17	114.46
14	N	601[B]	HEA	C27-C19-C18	-2.83	116.37	123.63
25	P	301	PEK	O01-C1-O02	-2.82	117.10	123.70
14	N	601[A]	HEA	C27-C19-C20	2.82	120.13	115.23
14	N	602	HEA	C20-C19-C18	-2.82	114.85	121.17
24	P	304	CHD	C18-C13-C12	2.80	111.86	109.06
20	A	609	TGL	OG3-CG3-CG2	2.78	116.42	108.40
26	C	306	CDL	PA1-OA2-CA2	-2.78	105.43	121.35
25	C	303	PEK	C3-C2-C1	-2.77	103.53	113.69
14	A	602	HEA	CBD-CAD-C3D	2.76	120.17	112.53
26	P	308	CDL	OB8-CB7-OB9	-2.74	116.77	123.63
20	N	607	TGL	OG2-CB1-OB1	-2.73	117.31	123.70
27	G	101	DMU	C6-C1-C2	-2.73	104.26	110.01
14	N	601[A]	HEA	C4C-NC-C1C	-2.73	101.37	105.82
14	N	601[B]	HEA	C4C-NC-C1C	-2.73	101.37	105.82
27	P	313	DMU	C7-C8-C9	2.73	115.18	110.23
14	N	601[A]	HEA	C1B-C2B-C3B	-2.72	103.64	106.80
14	N	601[B]	HEA	C1B-C2B-C3B	-2.72	103.64	106.80
24	C	307	CHD	C6-C5-C4	-2.72	108.12	111.23
27	M	101	DMU	O5-C4-C57	2.71	113.17	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	101	TGL	CG3-CG2-CG1	-2.70	105.48	111.78
27	C	313	DMU	C10-O1-C9	2.70	118.99	113.72
14	A	602	HEA	C4A-NA-C1A	2.70	110.22	105.82
19	N	608	PGV	O01-C1-O02	-2.69	117.42	123.70
19	C	304	PGV	O03-C19-C20	2.69	120.03	111.83
14	N	601[A]	HEA	C13-C14-C15	-2.68	121.49	127.62
20	A	609	TGL	CG3-CG2-CG1	-2.68	105.54	111.78
27	Z	103	DMU	O1-C10-C5	2.68	115.87	110.37
26	P	308	CDL	OA8-CA7-OA9	-2.67	116.94	123.63
27	M	101	DMU	C31-C28-C25	-2.67	100.86	114.37
26	C	306	CDL	CA4-OA6-CA5	-2.66	111.43	117.80
14	N	602	HEA	C2D-C1D-ND	2.65	112.89	109.84
20	A	609	TGL	OG1-CA1-CA2	2.65	119.91	111.83
24	Y	102	CHD	C11-C12-C13	-2.65	108.57	111.26
24	P	309	CHD	C19-C10-C9	-2.64	107.62	111.18
25	P	301	PEK	O13-P-O14	2.64	121.14	110.83
27	P	313	DMU	O1-C9-C8	2.64	114.46	109.70
14	N	601[A]	HEA	O2A-CGA-CBA	2.64	122.34	114.00
14	N	601[B]	HEA	O2A-CGA-CBA	2.64	122.34	114.00
24	P	315	CHD	O7-C7-C8	2.64	115.56	109.52
26	C	306	CDL	OA8-CA7-C31	2.63	119.86	111.83
25	P	301	PEK	C2-C3-C4	-2.62	107.63	113.35
14	A	601[A]	HEA	C2D-C1D-ND	2.62	112.85	109.84
14	A	601[B]	HEA	C2D-C1D-ND	2.62	112.85	109.84
24	C	301	CHD	C16-C17-C20	-2.61	108.23	112.18
26	C	306	CDL	OB6-CB5-OB7	-2.61	117.61	123.70
14	A	601[A]	HEA	C4D-C3D-C2D	-2.60	103.10	106.89
14	A	601[B]	HEA	C4D-C3D-C2D	-2.60	103.10	106.89
25	C	303	PEK	C24-C23-C22	-2.60	103.57	113.13
26	C	306	CDL	OB8-CB7-OB9	-2.59	117.14	123.63
19	C	304	PGV	C21-C20-C19	-2.59	104.20	113.69
14	N	601[A]	HEA	C17-C18-C19	-2.59	121.69	127.62
27	T	101	DMU	O16-C6-C1	2.59	112.21	108.27
19	Z	101	PGV	O03-C01-C02	2.59	115.86	108.40
20	Y	101	TGL	OG3-CC1-OC1	-2.58	117.16	123.63
14	A	601[A]	HEA	CHA-C4D-ND	-2.58	121.64	124.42
14	A	601[B]	HEA	CHA-C4D-ND	-2.58	121.64	124.42
14	N	601[A]	HEA	CHD-C1D-C2D	-2.58	119.62	126.95
14	N	601[B]	HEA	CHD-C1D-C2D	-2.58	119.62	126.95
24	P	309	CHD	C1-C10-C5	2.58	111.45	107.75
24	B	304	CHD	C19-C10-C1	-2.58	104.20	108.31
24	C	315	CHD	C6-C5-C10	2.58	115.40	112.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	102	CDL	OB6-CB5-OB7	-2.58	117.68	123.70
24	P	315	CHD	C6-C7-C8	-2.57	108.69	111.50
26	P	308	CDL	C80-C79-C78	2.57	127.37	114.37
14	A	601[A]	HEA	CHD-C4C-NC	2.57	128.52	123.86
14	A	601[B]	HEA	CHD-C4C-NC	2.57	128.52	123.86
14	N	601[A]	HEA	C21-C22-C23	-2.57	119.08	127.64
14	A	602	HEA	C26-C15-C16	2.57	119.69	115.23
20	N	607	TGL	OG1-CA1-OA1	-2.56	117.22	123.63
24	Y	102	CHD	C16-C17-C20	2.56	116.05	112.18
24	O	301	CHD	C13-C17-C20	-2.55	116.39	119.48
25	C	308	PEK	C2-C3-C4	2.55	118.92	113.35
20	D	201	TGL	CB4-CB3-CB2	-2.55	103.77	113.13
14	A	602	HEA	CHA-C4D-C3D	-2.55	121.06	124.77
20	A	609	TGL	OG1-CG1-CG2	2.54	115.73	108.40
14	N	602	HEA	CMD-C2D-C1D	2.54	129.00	125.03
14	N	602	HEA	C3B-C4B-NB	2.53	112.75	109.84
14	A	602	HEA	CMD-C2D-C1D	2.53	128.99	125.03
26	C	306	CDL	C81-C80-C79	-2.53	101.57	114.37
14	N	601[A]	HEA	O2D-CGD-CBD	2.53	122.00	114.00
14	N	601[B]	HEA	O2D-CGD-CBD	2.53	122.00	114.00
24	C	315	CHD	C15-C14-C13	2.53	105.99	103.54
14	A	601[B]	HEA	C20-C19-C18	-2.53	115.49	121.17
14	N	602	HEA	O2D-CGD-O1D	2.53	129.83	123.33
19	P	307	PGV	O03-C19-O04	-2.52	117.34	123.63
26	T	102	CDL	OA8-CA7-OA9	-2.51	117.35	123.63
14	N	602	HEA	C4C-NC-C1C	-2.51	101.73	105.82
14	A	601[A]	HEA	C3C-C2C-C1C	-2.51	104.21	107.17
14	A	601[B]	HEA	C3C-C2C-C1C	-2.51	104.21	107.17
24	B	304	CHD	C5-C4-C3	-2.51	108.92	112.71
27	Z	102	DMU	O1-C9-C8	2.49	114.19	109.70
24	P	315	CHD	C4-C5-C10	-2.49	110.01	112.66
14	N	601[A]	HEA	C21-C20-C19	-2.48	104.98	113.19
19	P	307	PGV	O01-C1-C2	2.48	116.84	111.48
20	D	201	TGL	CG2-OG2-CB1	2.48	123.72	117.80
27	C	313	DMU	C1-C2-C3	2.48	115.30	109.68
24	P	304	CHD	C16-C15-C14	-2.48	100.30	105.14
20	Y	101	TGL	OG3-CG3-CG2	2.47	115.53	108.40
24	P	309	CHD	C15-C16-C17	2.47	109.98	105.14
19	C	304	PGV	O14-P-O13	2.47	123.94	112.44
27	M	101	DMU	O3-C5-C7	2.47	116.19	110.38
14	A	602	HEA	CAD-C3D-C4D	2.46	128.98	124.70
24	B	304	CHD	C16-C17-C13	2.46	105.92	103.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	601[A]	HEA	OMA-CMA-C3A	-2.46	120.08	125.62
14	N	601[B]	HEA	OMA-CMA-C3A	-2.46	120.08	125.62
27	L	103	DMU	C6-C1-C2	2.45	115.16	110.01
20	N	607	TGL	CG2-OG2-CB1	-2.44	111.94	117.80
23	O	304	PSC	C03-C02-C01	-2.43	106.12	111.78
27	C	313	DMU	C7-C8-C9	2.43	114.63	110.23
19	C	305	PGV	C21-C20-C19	-2.43	104.80	113.69
26	G	103	CDL	OA6-CA5-OA7	-2.42	118.05	123.70
24	P	304	CHD	C19-C10-C1	-2.42	104.46	108.31
24	J	101	CHD	C1-C10-C5	2.41	111.20	107.75
25	C	303	PEK	C3-C4-C5	-2.41	99.12	112.60
27	L	102	DMU	C6-O5-C4	2.41	118.42	113.72
20	Y	101	TGL	OG1-CA1-CA2	2.40	119.16	111.83
26	T	102	CDL	C19-C18-C17	-2.40	102.23	114.37
27	C	313	DMU	O1-C10-C5	2.40	115.30	110.37
14	A	601[A]	HEA	C21-C22-C23	-2.39	119.66	127.64
19	A	608	PGV	C21-C20-C19	-2.39	104.93	113.69
20	N	607	TGL	OG3-CC1-OC1	-2.39	117.65	123.63
24	C	307	CHD	C19-C10-C9	-2.38	107.98	111.18
24	C	301	CHD	C15-C16-C17	2.38	109.80	105.14
14	A	602	HEA	CHD-C4C-C3C	-2.38	117.06	127.37
24	Y	102	CHD	C19-C10-C1	-2.37	104.47	107.70
25	P	301	PEK	C03-C02-C01	-2.37	106.26	111.78
14	A	601[A]	HEA	CHC-C4B-NB	-2.37	121.44	124.37
14	A	601[B]	HEA	CHC-C4B-NB	-2.37	121.44	124.37
14	N	602	HEA	CHC-C1C-C2C	-2.37	120.56	127.43
19	C	304	PGV	O03-C19-O04	-2.37	117.71	123.63
24	J	101	CHD	C17-C13-C14	2.36	102.48	100.11
27	M	101	DMU	C6-O5-C4	-2.36	109.11	113.72
20	D	201	TGL	OG1-CA1-OA1	-2.36	117.72	123.63
20	O	303	TGL	CG3-OG3-CC1	2.36	125.73	117.12
27	M	101	DMU	O49-C1-C2	-2.36	104.82	110.38
14	N	602	HEA	C4C-C3C-C2C	-2.35	104.38	107.30
20	A	609	TGL	CG2-OG2-CB1	2.35	123.42	117.80
24	Y	102	CHD	C11-C9-C8	2.35	114.37	110.89
24	O	301	CHD	C11-C12-C13	2.34	113.65	111.26
14	A	601[A]	HEA	C21-C20-C19	-2.34	105.44	113.19
20	B	302	TGL	OG3-CC1-CC2	2.33	118.95	111.83
26	P	308	CDL	C53-C52-C51	-2.33	104.57	113.13
27	P	313	DMU	O55-C2-C3	2.33	115.91	109.94
24	J	101	CHD	C11-C9-C10	-2.32	111.35	113.70
19	Z	101	PGV	O01-C1-O02	-2.32	118.29	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	301	CHD	C16-C15-C14	-2.30	100.64	105.14
24	P	309	CHD	C22-C23-C24	-2.30	106.36	112.49
14	N	602	HEA	C2B-C1B-NB	2.29	112.55	109.90
24	B	304	CHD	C11-C9-C10	-2.29	111.38	113.70
24	C	307	CHD	C17-C13-C14	2.29	102.41	100.11
24	C	301	CHD	C5-C4-C3	-2.29	109.26	112.71
14	A	602	HEA	CHB-C4A-C3A	-2.28	121.36	125.21
26	C	306	CDL	C77-C76-C75	-2.28	102.84	114.37
14	A	601[A]	HEA	CBD-CAD-C3D	-2.28	106.23	112.53
14	A	601[B]	HEA	CBD-CAD-C3D	-2.28	106.23	112.53
19	A	607	PGV	O14-P-O13	2.28	123.03	112.44
24	P	304	CHD	C5-C6-C7	2.27	117.10	114.40
14	A	601[A]	HEA	C16-C15-C14	-2.27	116.07	121.17
20	O	303	TGL	OG2-CB1-OB1	-2.27	118.41	123.70
14	A	601[A]	HEA	C20-C19-C18	-2.26	116.09	121.17
25	P	305	PEK	C32-C31-C30	-2.26	102.94	114.37
27	G	101	DMU	O7-C3-C4	2.26	115.40	109.48
14	A	602	HEA	O2A-CGA-CBA	2.26	121.13	114.00
26	T	102	CDL	OA6-CA5-OA7	-2.25	118.43	123.70
20	D	201	TGL	OG2-CB1-OB1	2.25	128.96	123.70
14	A	602	HEA	O1D-CGD-CBD	-2.25	115.96	123.09
14	A	601[B]	HEA	C16-C15-C14	2.25	126.21	121.17
24	C	315	CHD	C21-C20-C22	2.25	113.81	110.34
19	P	302	PGV	O14-P-O13	2.25	122.89	112.44
27	P	314	DMU	O1-C10-C5	2.24	114.97	110.37
27	Z	102	DMU	C31-C28-C25	-2.24	103.04	114.37
14	A	601[A]	HEA	C26-C15-C16	2.24	119.11	115.23
19	C	304	PGV	O01-C1-C2	2.23	116.31	111.48
24	P	309	CHD	O25-C24-C23	-2.23	116.01	123.09
26	T	102	CDL	C20-C19-C18	2.23	125.63	114.37
24	P	315	CHD	C15-C14-C13	2.23	105.70	103.54
24	P	304	CHD	O7-C7-C8	2.22	114.61	109.52
27	L	103	DMU	C10-O7-C3	-2.22	112.71	117.98
20	D	201	TGL	OG3-CC1-OC1	-2.22	118.07	123.63
24	P	315	CHD	C18-C13-C17	-2.22	107.73	111.20
27	C	313	DMU	C6-C1-C2	2.22	114.67	110.01
14	N	602	HEA	CHD-C1D-C2D	-2.21	120.66	126.95
25	G	102	PEK	O13-P-O14	2.21	119.44	110.83
27	P	313	DMU	C1-C2-C3	-2.21	104.67	109.68
27	Z	102	DMU	O16-C6-C1	2.21	111.62	108.27
23	O	304	PSC	C3-C2-C1	-2.20	105.62	113.69
26	C	306	CDL	OA6-CA4-CA3	2.20	116.24	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	103	DMU	O7-C3-C2	2.19	112.80	107.23
14	A	601[B]	HEA	C21-C22-C23	-2.19	120.33	127.64
26	P	308	CDL	OB8-CB6-CB4	2.19	114.71	108.40
24	P	304	CHD	O26-C24-O25	-2.18	117.72	123.33
14	A	602	HEA	CAD-CBD-CGD	-2.18	107.88	113.67
14	N	601[A]	HEA	C12-C11-C3B	2.18	115.52	112.12
24	C	301	CHD	C1-C2-C3	-2.17	107.61	110.48
19	A	608	PGV	C9-C10-C11	-2.17	100.45	112.60
27	M	101	DMU	C8-C7-C5	-2.17	107.02	110.83
26	C	306	CDL	OA4-PA1-OA5	2.17	117.38	107.57
24	P	309	CHD	C17-C13-C14	2.16	102.28	100.11
20	O	303	TGL	OG1-CA1-OA1	-2.16	118.22	123.63
27	P	314	DMU	O1-C9-C8	2.16	113.59	109.70
14	A	602	HEA	C1B-C2B-C3B	-2.15	104.30	106.80
26	G	103	CDL	CB6-OB8-CB7	2.15	124.97	117.12
24	P	309	CHD	C4-C3-C2	2.15	113.24	110.62
14	N	601[A]	HEA	C2B-C1B-NB	2.15	112.39	109.90
14	N	601[B]	HEA	C2B-C1B-NB	2.15	112.39	109.90
14	N	601[A]	HEA	CHA-C4D-ND	-2.15	122.11	124.42
14	N	601[B]	HEA	CHA-C4D-ND	-2.15	122.11	124.42
19	A	608	PGV	O01-C1-C2	2.15	116.12	111.48
20	Y	101	TGL	CG2-OG2-CB1	2.15	122.93	117.80
27	L	103	DMU	O5-C6-C1	2.14	114.77	110.37
14	A	601[A]	HEA	C2C-C1C-NC	2.14	113.57	110.14
14	A	601[B]	HEA	C2C-C1C-NC	2.14	113.57	110.14
27	Z	103	DMU	C10-O7-C3	-2.14	112.91	117.98
24	P	315	CHD	O12-C12-C13	-2.13	107.42	111.02
27	G	101	DMU	O3-C5-C7	2.12	115.38	110.38
14	N	602	HEA	C1C-CHC-C4B	-2.12	121.26	126.25
14	A	602	HEA	CHB-C1B-C2B	-2.12	121.68	125.03
26	T	102	CDL	CB6-OB8-CB7	2.12	124.87	117.12
24	B	304	CHD	C18-C13-C14	2.12	114.53	111.20
19	A	608	PGV	O01-C1-O02	-2.12	118.75	123.70
27	Z	102	DMU	C7-C8-C9	2.11	114.06	110.23
14	N	602	HEA	O2A-CGA-CBA	2.11	120.66	114.00
14	N	602	HEA	OMA-CMA-C3A	-2.11	120.86	125.62
26	P	308	CDL	OA4-PA1-OA3	2.10	119.03	110.83
14	N	601[A]	HEA	CMC-C2C-C3C	2.10	131.50	126.55
14	N	601[B]	HEA	CMC-C2C-C3C	2.10	131.50	126.55
14	A	601[B]	HEA	C26-C15-C14	-2.10	118.23	123.63
24	C	301	CHD	C17-C13-C12	-2.10	115.78	117.67
20	A	609	TGL	CA5-CA4-CA3	-2.10	103.76	114.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	315	CHD	C14-C13-C12	2.09	109.33	107.42
24	C	315	CHD	C1-C2-C3	-2.09	107.71	110.48
24	J	101	CHD	C15-C14-C8	2.09	121.22	118.36
25	P	306	PEK	C01-O03-C21	2.08	124.74	117.12
26	G	103	CDL	OB6-CB5-OB7	-2.08	118.85	123.70
24	P	304	CHD	C18-C13-C17	-2.07	107.96	111.20
14	N	602	HEA	C3A-C2A-C1A	-2.07	105.09	107.05
14	N	602	HEA	C2C-C1C-NC	2.06	113.45	110.14
24	C	315	CHD	C11-C9-C8	2.06	113.94	110.89
26	P	308	CDL	C21-C20-C19	-2.06	103.96	114.37
25	P	305	PEK	C4-C5-C6	-2.05	109.47	124.83
26	P	308	CDL	OB6-CB5-OB7	-2.05	118.92	123.70
27	Z	102	DMU	O7-C10-C5	2.05	113.12	108.09
26	C	306	CDL	CB2-C1-CA2	-2.04	106.78	112.65
19	N	608	PGV	C7-C6-C5	-2.04	104.08	114.37
24	P	304	CHD	C19-C10-C9	2.03	113.91	111.18
24	B	304	CHD	C18-C13-C17	-2.03	108.02	111.20
19	Z	101	PGV	O03-C19-O04	-2.03	118.56	123.63
27	Z	102	DMU	C1-C2-C3	2.02	114.27	109.68
26	T	102	CDL	C33-C32-C31	-2.02	105.70	113.13
24	P	309	CHD	C17-C13-C12	-2.02	115.85	117.67
24	P	315	CHD	C18-C13-C14	-2.02	108.04	111.20
24	C	301	CHD	O12-C12-C13	-2.02	107.61	111.02
27	G	101	DMU	C1-C2-C3	-2.02	105.11	109.68
24	Y	102	CHD	O25-C24-C23	-2.01	116.71	123.09
24	P	309	CHD	C14-C8-C7	-2.01	109.19	111.85
27	C	314	DMU	C10-O1-C9	-2.01	109.80	113.72
19	A	608	PGV	C03-C02-C01	-2.00	107.11	111.78
14	A	601[B]	HEA	C17-C16-C15	-2.00	106.55	113.19
24	B	304	CHD	C15-C14-C13	2.00	105.48	103.54

There are no chirality outliers.

All (721) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	A	601[B]	HEA	C2A-C3A-CMA-OMA
14	N	601[A]	HEA	C2A-C3A-CMA-OMA
14	N	601[B]	HEA	C2A-C3A-CMA-OMA
19	A	607	PGV	C03-O11-P-O12
19	A	607	PGV	C03-O11-P-O13
19	A	607	PGV	C04-O12-P-O11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	A	607	PGV	C04-O12-P-O14
19	A	607	PGV	O12-C04-C05-C06
19	A	607	PGV	O02-C1-O01-C02
19	A	607	PGV	O04-C19-O03-C01
19	C	305	PGV	C03-O11-P-O12
19	C	305	PGV	C03-O11-P-O13
19	C	305	PGV	O02-C1-O01-C02
19	C	305	PGV	O04-C19-O03-C01
19	C	305	PGV	C20-C19-O03-C01
19	Z	101	PGV	O04-C19-O03-C01
19	Z	101	PGV	C20-C19-O03-C01
20	A	609	TGL	OB1-CB1-OG2-CG2
20	D	201	TGL	CB2-CB1-OG2-CG2
20	Y	101	TGL	OB1-CB1-OG2-CG2
23	B	303	PSC	C04-O12-P-O11
23	B	303	PSC	C04-O12-P-O13
23	B	303	PSC	O02-C1-O01-C02
23	B	303	PSC	C2-C1-O01-C02
23	O	304	PSC	C04-O12-P-O11
23	O	304	PSC	C04-O12-P-O13
23	O	304	PSC	O12-C04-C05-N
23	O	304	PSC	C2-C1-O01-C02
25	C	303	PEK	O12-C04-C05-N
25	C	308	PEK	O04-C21-O03-C01
25	C	308	PEK	C22-C21-O03-C01
25	G	102	PEK	C03-O11-P-O12
25	G	102	PEK	C03-O11-P-O13
25	G	102	PEK	O04-C21-O03-C01
25	G	102	PEK	C22-C21-O03-C01
25	P	301	PEK	O04-C21-O03-C01
25	P	301	PEK	C22-C21-O03-C01
25	P	305	PEK	O12-C04-C05-N
25	P	306	PEK	C03-O11-P-O13
25	P	306	PEK	O12-C04-C05-N
25	P	306	PEK	O04-C21-O03-C01
25	P	306	PEK	C22-C21-O03-C01
25	P	306	PEK	C11-C12-C13-C14
26	C	306	CDL	CA3-OA5-PA1-OA2
26	C	306	CDL	OA7-CA5-OA6-CA4
26	C	306	CDL	C11-CA5-OA6-CA4
26	C	306	CDL	CB2-OB2-PB2-OB3
26	C	306	CDL	CB2-OB2-PB2-OB5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	306	CDL	CB3-OB5-PB2-OB2
26	G	103	CDL	CA2-OA2-PA1-OA5
26	G	103	CDL	CA3-OA5-PA1-OA2
26	G	103	CDL	CA3-OA5-PA1-OA3
26	G	103	CDL	OA9-CA7-OA8-CA6
26	G	103	CDL	C31-CA7-OA8-CA6
26	G	103	CDL	CB2-OB2-PB2-OB3
26	G	103	CDL	CB2-OB2-PB2-OB5
26	G	103	CDL	CB3-OB5-PB2-OB2
26	G	103	CDL	CB3-OB5-PB2-OB3
26	P	308	CDL	CA3-OA5-PA1-OA2
26	P	308	CDL	CA3-OA5-PA1-OA4
26	P	308	CDL	OA6-CA4-CA6-OA8
26	P	308	CDL	CB2-OB2-PB2-OB3
26	P	308	CDL	C51-CB5-OB6-CB4
26	T	102	CDL	CA2-OA2-PA1-OA3
26	T	102	CDL	CA3-OA5-PA1-OA3
26	T	102	CDL	OA9-CA7-OA8-CA6
26	T	102	CDL	C31-CA7-OA8-CA6
26	T	102	CDL	CB3-OB5-PB2-OB3
27	G	101	DMU	O5-C6-O16-C18
27	Z	103	DMU	C1-C6-O16-C18
27	Z	103	DMU	O5-C6-O16-C18
19	P	302	PGV	O04-C19-O03-C01
19	P	302	PGV	C20-C19-O03-C01
24	J	101	CHD	C13-C17-C20-C21
20	D	201	TGL	OB1-CB1-OG2-CG2
23	O	304	PSC	O02-C1-O01-C02
26	P	308	CDL	OB7-CB5-OB6-CB4
19	A	607	PGV	C20-C19-O03-C01
26	P	308	CDL	C31-CA7-OA8-CA6
27	P	314	DMU	C4-C3-O7-C10
19	A	607	PGV	C2-C1-O01-C02
20	A	609	TGL	CB2-CB1-OG2-CG2
20	Y	101	TGL	CB2-CB1-OG2-CG2
24	P	315	CHD	C21-C20-C22-C23
24	Y	102	CHD	C21-C20-C22-C23
24	J	101	CHD	C16-C17-C20-C21
24	J	101	CHD	C13-C17-C20-C22
14	N	601[A]	HEA	C27-C19-C20-C21
14	N	601[A]	HEA	C18-C19-C20-C21
27	Z	103	DMU	O5-C4-C57-O61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	G	102	PEK	C10-C11-C12-C13
27	L	103	DMU	O1-C10-O7-C3
24	J	101	CHD	C16-C17-C20-C22
19	A	607	PGV	O12-C04-C05-O05
20	Y	101	TGL	CA2-CA1-OG1-CG1
26	P	308	CDL	OA9-CA7-OA8-CA6
24	P	309	CHD	C21-C20-C22-C23
24	P	315	CHD	C17-C20-C22-C23
27	Z	103	DMU	C3-C4-C57-O61
20	Y	101	TGL	OA1-CA1-OG1-CG1
27	T	101	DMU	O5-C4-C57-O61
24	C	307	CHD	C21-C20-C22-C23
26	T	102	CDL	C57-C58-C59-C60
27	L	102	DMU	O5-C6-O16-C18
27	M	101	DMU	O5-C6-O16-C18
27	P	313	DMU	O5-C6-O16-C18
27	T	101	DMU	O6-C11-C9-O1
27	L	103	DMU	O5-C4-C57-O61
24	C	307	CHD	C17-C20-C22-C23
27	G	101	DMU	C5-C10-O7-C3
23	B	303	PSC	C11-C12-C13-C14
25	P	301	PEK	C7-C8-C9-C10
25	P	301	PEK	C13-C14-C15-C16
25	P	305	PEK	C4-C5-C6-C7
25	P	306	PEK	C4-C5-C6-C7
27	G	101	DMU	O5-C4-C57-O61
26	G	103	CDL	C80-C81-C82-C83
26	P	308	CDL	C17-C18-C19-C20
20	O	303	TGL	CA4-CA5-CA6-CA7
24	P	309	CHD	C17-C20-C22-C23
27	G	101	DMU	C3-C4-C57-O61
27	L	102	DMU	C1-C6-O16-C18
27	P	313	DMU	C1-C6-O16-C18
19	Z	101	PGV	C19-C20-C21-C22
27	G	101	DMU	O1-C10-O7-C3
26	T	102	CDL	OB6-CB4-CB6-OB8
25	C	303	PEK	C4-C5-C6-C7
25	C	308	PEK	C4-C5-C6-C7
25	P	306	PEK	C7-C8-C9-C10
25	P	306	PEK	C10-C11-C12-C13
25	P	306	PEK	C13-C14-C15-C16
25	G	102	PEK	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	609	TGL	CA1-CA2-CA3-CA4
20	Y	101	TGL	CB1-CB2-CB3-CB4
27	P	314	DMU	O16-C18-C19-C22
26	P	308	CDL	CB2-OB2-PB2-OB5
24	P	309	CHD	C20-C22-C23-C24
27	C	314	DMU	O16-C18-C19-C22
20	B	302	TGL	CB1-CB2-CB3-CB4
20	O	303	TGL	CA1-CA2-CA3-CA4
26	C	306	CDL	CB7-C71-C72-C73
26	T	102	CDL	C52-C53-C54-C55
27	T	101	DMU	C3-C4-C57-O61
26	P	308	CDL	C82-C83-C84-C85
26	C	306	CDL	CA7-C31-C32-C33
26	T	102	CDL	CA7-C31-C32-C33
20	Y	101	TGL	CC2-CC1-OG3-CG3
27	T	101	DMU	C5-C10-O7-C3
20	D	201	TGL	CC4-CC5-CC6-CC7
24	C	315	CHD	C13-C17-C20-C21
23	O	304	PSC	C11-C10-C9-C8
25	P	305	PEK	C13-C14-C15-C16
27	L	103	DMU	O16-C18-C19-C22
24	P	315	CHD	C20-C22-C23-C24
19	C	305	PGV	C04-C05-C06-O06
26	P	308	CDL	CA3-CA4-OA6-CA5
27	T	101	DMU	O5-C6-O16-C18
20	O	303	TGL	CB2-CB1-OG2-CG2
25	P	301	PEK	C2-C1-O01-C02
20	N	607	TGL	C19-C33-C34-C35
20	N	607	TGL	CC6-CC7-CC8-CC9
27	Z	102	DMU	C28-C31-C34-C37
26	P	308	CDL	C31-C32-C33-C34
25	G	102	PEK	C7-C8-C9-C10
25	P	305	PEK	C10-C11-C12-C13
20	B	302	TGL	C20-C21-C22-C23
26	G	103	CDL	C60-C61-C62-C63
26	P	308	CDL	C57-C58-C59-C60
26	C	306	CDL	C42-C43-C44-C45
20	A	609	TGL	C21-C20-CA9-CA8
27	G	101	DMU	C28-C31-C34-C37
26	C	306	CDL	OA9-CA7-OA8-CA6
20	B	302	TGL	CA5-CA6-CA7-CA8
26	P	308	CDL	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	609	TGL	C10-C11-C12-C13
20	O	303	TGL	CA5-CA6-CA7-CA8
19	P	307	PGV	C10-C11-C12-C13
20	B	302	TGL	CC2-CC1-OG3-CG3
26	C	306	CDL	C31-CA7-OA8-CA6
19	A	607	PGV	C13-C14-C15-C16
20	D	201	TGL	C21-C20-CA9-CA8
26	T	102	CDL	C53-C54-C55-C56
27	T	101	DMU	C28-C31-C34-C37
20	O	303	TGL	CC7-CC8-CC9-C15
20	O	303	TGL	C15-C16-C17-C18
26	P	308	CDL	C21-C22-C23-C24
26	P	308	CDL	C36-C37-C38-C39
26	T	102	CDL	C77-C78-C79-C80
20	Y	101	TGL	OC1-CC1-OG3-CG3
27	C	314	DMU	C18-C19-C22-C25
23	B	303	PSC	C4-C5-C6-C7
20	B	302	TGL	CB2-CB1-OG2-CG2
25	G	102	PEK	C2-C1-O01-C02
19	A	608	PGV	C10-C11-C12-C13
19	Z	101	PGV	C10-C11-C12-C13
25	G	102	PEK	C13-C14-C15-C16
20	N	607	TGL	C23-C24-C25-C26
20	Y	101	TGL	C11-C12-C13-C14
25	C	303	PEK	C21-C22-C23-C24
20	A	609	TGL	CA5-CA6-CA7-CA8
20	Y	101	TGL	C21-C22-C23-C24
26	P	308	CDL	C35-C36-C37-C38
20	O	303	TGL	OB1-CB1-OG2-CG2
25	P	301	PEK	O02-C1-O01-C02
20	D	201	TGL	CB2-CB3-CB4-CB5
20	Y	101	TGL	CA9-C20-C21-C22
25	P	305	PEK	C23-C24-C25-C26
20	N	607	TGL	C21-C20-CA9-CA8
26	P	308	CDL	C20-C21-C22-C23
19	N	608	PGV	C29-C30-C31-C32
27	Z	102	DMU	C22-C25-C28-C31
27	G	101	DMU	C1-C6-O16-C18
20	Y	101	TGL	C13-C14-C29-C30
20	N	607	TGL	CB2-CB1-OG2-CG2
26	C	306	CDL	C51-CB5-OB6-CB4
20	N	607	TGL	OB1-CB1-OG2-CG2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	306	CDL	OB7-CB5-OB6-CB4
20	D	201	TGL	CC6-CC7-CC8-CC9
20	Y	101	TGL	CC1-CC2-CC3-CC4
26	C	306	CDL	C79-C80-C81-C82
14	A	601[A]	HEA	C27-C19-C20-C21
27	G	101	DMU	C18-C19-C22-C25
26	P	308	CDL	C43-C44-C45-C46
20	D	201	TGL	C16-C17-C18-C19
23	O	304	PSC	C23-C24-C25-C26
26	G	103	CDL	C51-CB5-OB6-CB4
26	T	102	CDL	C11-CA5-OA6-CA4
20	A	609	TGL	C24-C25-C26-C27
20	O	303	TGL	C12-C13-C14-C29
19	A	607	PGV	C19-C20-C21-C22
20	N	607	TGL	C20-C21-C22-C23
26	P	308	CDL	C76-C77-C78-C79
26	T	102	CDL	C42-C43-C44-C45
27	L	103	DMU	C3-C4-C57-O61
19	A	607	PGV	C14-C15-C16-C17
27	C	313	DMU	C22-C25-C28-C31
20	N	607	TGL	CC7-CC8-CC9-C15
26	C	306	CDL	C39-C40-C41-C42
19	N	608	PGV	C23-C24-C25-C26
26	C	306	CDL	C40-C41-C42-C43
20	B	302	TGL	CB6-CB7-CB8-CB9
26	C	306	CDL	C37-C38-C39-C40
26	T	102	CDL	C16-C17-C18-C19
26	C	306	CDL	C11-C12-C13-C14
25	G	102	PEK	O02-C1-O01-C02
19	A	607	PGV	C7-C8-C9-C10
25	G	102	PEK	C24-C25-C26-C27
27	P	314	DMU	C19-C22-C25-C28
26	C	306	CDL	C36-C37-C38-C39
27	Z	103	DMU	O16-C18-C19-C22
20	B	302	TGL	OC1-CC1-OG3-CG3
25	G	102	PEK	C27-C28-C29-C30
20	N	607	TGL	CA9-C20-C21-C22
19	A	607	PGV	C3-C4-C5-C6
19	A	607	PGV	C29-C30-C31-C32
20	A	609	TGL	C21-C22-C23-C24
20	N	607	TGL	CB9-C10-C11-C12
20	O	303	TGL	C20-C21-C22-C23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	T	102	CDL	C15-C16-C17-C18
26	T	102	CDL	C37-C38-C39-C40
26	T	102	CDL	OB5-CB3-CB4-CB6
19	Z	101	PGV	O02-C1-O01-C02
26	G	103	CDL	OB7-CB5-OB6-CB4
26	T	102	CDL	OA7-CA5-OA6-CA4
25	P	306	PEK	C25-C26-C27-C28
19	A	607	PGV	C21-C22-C23-C24
27	T	101	DMU	C34-C37-C40-C43
25	P	306	PEK	C26-C27-C28-C29
19	Z	101	PGV	C2-C1-O01-C02
20	Y	101	TGL	CA4-CA5-CA6-CA7
19	Z	101	PGV	C2-C3-C4-C5
27	P	313	DMU	O6-C11-C9-C8
20	A	609	TGL	CA2-CA1-OG1-CG1
25	C	303	PEK	C16-C17-C18-C19
20	B	302	TGL	OB1-CB1-OG2-CG2
25	C	303	PEK	C7-C8-C9-C10
27	L	103	DMU	O6-C11-C9-O1
26	C	306	CDL	CA3-CA4-CA6-OA8
26	C	306	CDL	CB3-CB4-CB6-OB8
26	T	102	CDL	CB3-CB4-CB6-OB8
19	Z	101	PGV	C20-C21-C22-C23
19	C	305	PGV	C12-C13-C14-C15
20	O	303	TGL	C16-C17-C18-C19
25	P	305	PEK	C22-C23-C24-C25
26	P	308	CDL	C22-C23-C24-C25
27	G	101	DMU	C25-C28-C31-C34
21	A	610	EDO	O1-C1-C2-O2
21	A	611	EDO	O1-C1-C2-O2
21	D	204	EDO	O1-C1-C2-O2
21	S	106	EDO	O1-C1-C2-O2
21	U	101	EDO	O1-C1-C2-O2
25	P	301	PEK	C22-C23-C24-C25
26	G	103	CDL	C34-C35-C36-C37
19	N	608	PGV	C7-C8-C9-C10
26	T	102	CDL	C14-C15-C16-C17
27	Z	102	DMU	C25-C28-C31-C34
27	L	102	DMU	O6-C11-C9-O1
20	A	609	TGL	OA1-CA1-OG1-CG1
25	G	102	PEK	C03-O11-P-O14
26	P	308	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	O	303	TGL	C10-C11-C12-C13
27	C	314	DMU	O6-C11-C9-O1
20	N	607	TGL	C11-C10-CB9-CB8
26	P	308	CDL	C73-C74-C75-C76
19	C	305	PGV	C19-C20-C21-C22
20	B	302	TGL	CC7-CC8-CC9-C15
20	Y	101	TGL	C24-C25-C26-C27
19	A	607	PGV	C11-C10-C9-C8
19	A	607	PGV	C12-C13-C14-C15
25	C	303	PEK	C22-C23-C24-C25
14	A	602	HEA	C2A-C3A-CMA-OMA
25	C	303	PEK	C10-C11-C12-C13
25	C	303	PEK	C13-C14-C15-C16
25	P	301	PEK	C4-C5-C6-C7
19	C	304	PGV	C28-C29-C30-C31
19	C	305	PGV	C6-C7-C8-C9
27	Z	103	DMU	C19-C22-C25-C28
27	Z	102	DMU	O16-C18-C19-C22
26	P	308	CDL	C77-C78-C79-C80
20	Y	101	TGL	C25-C26-C27-C28
27	G	101	DMU	C19-C22-C25-C28
20	A	609	TGL	OG1-CG1-CG2-OG2
20	O	303	TGL	OG2-CG2-CG3-OG3
19	C	304	PGV	C20-C21-C22-C23
20	A	609	TGL	CC7-CC8-CC9-C15
20	O	303	TGL	C17-C18-C19-C33
20	D	201	TGL	CB9-C10-C11-C12
20	Y	101	TGL	C16-C17-C18-C19
20	A	609	TGL	CC4-CC5-CC6-CC7
24	J	101	CHD	C17-C20-C22-C23
27	G	101	DMU	C22-C25-C28-C31
20	N	607	TGL	C12-C13-C14-C29
26	C	306	CDL	C82-C83-C84-C85
19	P	302	PGV	C10-C11-C12-C13
27	P	313	DMU	C19-C18-O16-C6
27	M	101	DMU	C19-C22-C25-C28
25	C	303	PEK	O03-C21-C22-C23
19	A	607	PGV	C24-C25-C26-C27
19	C	305	PGV	C4-C5-C6-C7
27	Z	102	DMU	C34-C37-C40-C43
20	A	609	TGL	CB3-CB4-CB5-CB6
27	P	314	DMU	C1-C6-O16-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	N	607	TGL	CC1-CC2-CC3-CC4
26	P	308	CDL	CA5-C11-C12-C13
23	B	303	PSC	C01-C02-C03-O11
25	G	102	PEK	C01-C02-C03-O11
26	P	308	CDL	C40-C41-C42-C43
24	Y	102	CHD	C17-C20-C22-C23
19	Z	101	PGV	O12-C04-C05-O05
19	C	305	PGV	C3-C4-C5-C6
20	A	609	TGL	C29-C30-C31-C32
20	A	609	TGL	C11-C12-C13-C14
26	G	103	CDL	C81-C82-C83-C84
26	P	308	CDL	C24-C25-C26-C27
19	A	607	PGV	C6-C7-C8-C9
19	P	307	PGV	C1-C2-C3-C4
19	N	608	PGV	C31-C32-C33-C34
25	P	306	PEK	O03-C01-C02-C03
26	G	103	CDL	CA3-CA4-CA6-OA8
26	P	308	CDL	CB3-CB4-CB6-OB8
26	T	102	CDL	CA3-CA4-CA6-OA8
26	P	308	CDL	C84-C85-C86-C87
25	P	306	PEK	C29-C30-C31-C32
20	O	303	TGL	CC9-C15-C16-C17
19	N	608	PGV	C26-C27-C28-C29
27	M	101	DMU	C34-C37-C40-C43
23	O	304	PSC	C28-C29-C30-C31
23	B	303	PSC	O01-C02-C03-O11
20	D	201	TGL	C23-C24-C25-C26
27	L	103	DMU	C19-C22-C25-C28
19	A	608	PGV	C19-C20-C21-C22
27	L	103	DMU	C34-C37-C40-C43
20	O	303	TGL	CB6-CB7-CB8-CB9
20	B	302	TGL	OG1-CG1-CG2-OG2
20	O	303	TGL	OG1-CG1-CG2-OG2
20	Y	101	TGL	OG2-CG2-CG3-OG3
25	P	306	PEK	O03-C01-C02-O01
26	C	306	CDL	OA6-CA4-CA6-OA8
26	C	306	CDL	OB6-CB4-CB6-OB8
26	G	103	CDL	OA6-CA4-CA6-OA8
26	P	308	CDL	OB6-CB4-CB6-OB8
26	T	102	CDL	OA6-CA4-CA6-OA8
19	A	607	PGV	C4-C5-C6-C7
23	B	303	PSC	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	303	PSC	C10-C11-C12-C13
23	O	304	PSC	C9-C10-C11-C12
23	O	304	PSC	C10-C11-C12-C13
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	308	PEK	C5-C6-C7-C8
25	C	308	PEK	C11-C10-C9-C8
25	C	308	PEK	C9-C10-C11-C12
25	C	308	PEK	C11-C12-C13-C14
25	C	308	PEK	C12-C13-C14-C15
25	G	102	PEK	C5-C6-C7-C8
25	G	102	PEK	C6-C7-C8-C9
25	G	102	PEK	C11-C10-C9-C8
25	G	102	PEK	C9-C10-C11-C12
25	G	102	PEK	C11-C12-C13-C14
25	G	102	PEK	C12-C13-C14-C15
25	P	301	PEK	C5-C6-C7-C8
25	P	301	PEK	C6-C7-C8-C9
25	P	301	PEK	C11-C10-C9-C8
25	P	301	PEK	C9-C10-C11-C12
25	P	301	PEK	C11-C12-C13-C14
25	P	301	PEK	C12-C13-C14-C15
25	P	305	PEK	C12-C13-C14-C15
25	P	306	PEK	C5-C6-C7-C8
25	P	306	PEK	C6-C7-C8-C9
25	P	306	PEK	C11-C10-C9-C8
25	P	306	PEK	C9-C10-C11-C12
25	P	306	PEK	C12-C13-C14-C15
24	C	315	CHD	C16-C17-C20-C22
19	N	608	PGV	C5-C6-C7-C8
20	B	302	TGL	CC5-CC6-CC7-CC8
19	A	608	PGV	C29-C30-C31-C32
20	O	303	TGL	C13-C14-C29-C30
26	G	103	CDL	C57-C58-C59-C60
26	P	308	CDL	C58-C59-C60-C61
26	T	102	CDL	C60-C61-C62-C63
25	P	306	PEK	C33-C34-C35-C36
26	C	306	CDL	C31-C32-C33-C34
27	M	101	DMU	C25-C28-C31-C34
19	Z	101	PGV	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	D	201	TGL	CA4-CA5-CA6-CA7
19	C	304	PGV	C11-C12-C13-C14
20	N	607	TGL	CC2-CC1-OG3-CG3
26	T	102	CDL	C71-CB7-OB8-CB6
27	P	313	DMU	C22-C25-C28-C31
27	Z	103	DMU	C18-C19-C22-C25
24	J	101	CHD	C21-C20-C22-C23
19	C	305	PGV	C01-C02-C03-O11
26	C	306	CDL	OA5-CA3-CA4-CA6
26	C	306	CDL	OB5-CB3-CB4-CB6
26	P	308	CDL	OA5-CA3-CA4-CA6
19	C	304	PGV	C02-C03-O11-P
19	A	607	PGV	C25-C26-C27-C28
25	C	308	PEK	C2-C1-O01-C02
26	G	103	CDL	C37-C38-C39-C40
26	C	306	CDL	C52-C53-C54-C55
26	T	102	CDL	OB9-CB7-OB8-CB6
20	O	303	TGL	C21-C22-C23-C24
20	Y	101	TGL	CB2-CB3-CB4-CB5
26	G	103	CDL	C55-C56-C57-C58
25	C	308	PEK	O02-C1-O01-C02
26	C	306	CDL	OB5-CB3-CB4-OB6
26	T	102	CDL	OB5-CB3-CB4-OB6
20	O	303	TGL	CG1-CG2-CG3-OG3
20	Y	101	TGL	CG1-CG2-CG3-OG3
23	O	304	PSC	C19-C20-C21-C22
26	G	103	CDL	C52-C53-C54-C55
26	G	103	CDL	C11-C12-C13-C14
14	A	601[A]	HEA	C18-C19-C20-C21
20	B	302	TGL	C13-C14-C29-C30
20	Y	101	TGL	C10-C11-C12-C13
21	I	101	EDO	O1-C1-C2-O2
20	A	609	TGL	C11-C10-CB9-CB8
20	A	609	TGL	OG2-CG2-CG3-OG3
20	D	201	TGL	CA9-C20-C21-C22
19	N	608	PGV	C24-C25-C26-C27
26	P	308	CDL	C74-C75-C76-C77
26	G	103	CDL	C39-C40-C41-C42
19	A	607	PGV	C26-C27-C28-C29
19	P	302	PGV	C2-C1-O01-C02
20	A	609	TGL	CB6-CB7-CB8-CB9
27	C	313	DMU	C19-C22-C25-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	A	609	TGL	C15-C16-C17-C18
23	B	303	PSC	O12-C04-C05-N
26	C	306	CDL	C43-C44-C45-C46
24	C	315	CHD	C16-C17-C20-C21
19	C	305	PGV	C13-C14-C15-C16
20	B	302	TGL	CA3-CA4-CA5-CA6
26	P	308	CDL	C34-C35-C36-C37
26	C	306	CDL	C44-C45-C46-C47
20	B	302	TGL	C21-C22-C23-C24
26	C	306	CDL	C81-C82-C83-C84
19	P	307	PGV	C11-C10-C9-C8
19	P	302	PGV	C29-C30-C31-C32
26	P	308	CDL	C23-C24-C25-C26
19	P	302	PGV	O02-C1-O01-C02
20	Y	101	TGL	C21-C20-CA9-CA8
26	P	308	CDL	C72-C73-C74-C75
27	C	313	DMU	O5-C4-C57-O61
26	P	308	CDL	CA4-CA3-OA5-PA1
27	L	103	DMU	C2-C3-O7-C10
26	C	306	CDL	OA5-CA3-CA4-OA6
20	N	607	TGL	CC2-CC3-CC4-CC5
14	A	601[A]	HEA	C4A-C3A-CMA-OMA
14	A	601[B]	HEA	C4A-C3A-CMA-OMA
14	A	602	HEA	C4A-C3A-CMA-OMA
14	N	601[A]	HEA	C4A-C3A-CMA-OMA
14	N	601[B]	HEA	C4A-C3A-CMA-OMA
20	A	609	TGL	CA4-CA5-CA6-CA7
19	P	302	PGV	O03-C01-C02-C03
20	A	609	TGL	CG1-CG2-CG3-OG3
27	G	101	DMU	C31-C34-C37-C40
20	A	609	TGL	CA3-CA4-CA5-CA6
20	Y	101	TGL	CB3-CB4-CB5-CB6
23	B	303	PSC	C12-C13-C14-C15
25	G	102	PEK	C3-C4-C5-C6
25	G	102	PEK	C14-C15-C16-C17
27	P	314	DMU	O5-C6-O16-C18
21	A	620	EDO	O1-C1-C2-O2
26	P	308	CDL	C79-C80-C81-C82
20	N	607	TGL	OC1-CC1-OG3-CG3
19	C	304	PGV	C7-C8-C9-C10
19	A	607	PGV	C03-O11-P-O14
19	A	607	PGV	C04-O12-P-O13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
19	C	305	PGV	C03-O11-P-O14
19	P	302	PGV	C03-O11-P-O12
26	C	306	CDL	CA3-OA5-PA1-OA3
26	C	306	CDL	CB2-OB2-PB2-OB4
26	G	103	CDL	CA2-OA2-PA1-OA3
26	G	103	CDL	CB2-OB2-PB2-OB4
26	G	103	CDL	CB3-OB5-PB2-OB4
20	D	201	TGL	C15-C16-C17-C18
19	P	307	PGV	C02-C03-O11-P
26	C	306	CDL	CA4-CA3-OA5-PA1
26	G	103	CDL	C1-CB2-OB2-PB2
27	G	101	DMU	O6-C11-C9-C8
26	P	308	CDL	C80-C81-C82-C83
19	A	607	PGV	C03-C02-O01-C1
26	C	306	CDL	C41-C42-C43-C44
20	D	201	TGL	CA5-CA6-CA7-CA8
19	C	305	PGV	C11-C12-C13-C14
26	G	103	CDL	CA7-C31-C32-C33
20	O	303	TGL	C23-C24-C25-C26
19	C	305	PGV	O01-C02-C03-O11
20	D	201	TGL	OG3-CC1-CC2-CC3
26	G	103	CDL	C31-C32-C33-C34
26	T	102	CDL	C54-C55-C56-C57
26	P	308	CDL	C52-C51-CB5-OB6
27	L	103	DMU	C22-C25-C28-C31
26	P	308	CDL	CB2-OB2-PB2-OB4
20	A	609	TGL	OG1-CG1-CG2-CG3
23	O	304	PSC	C12-C13-C14-C15
21	E	202	EDO	O1-C1-C2-O2
20	A	609	TGL	C20-C21-C22-C23
19	C	304	PGV	C30-C31-C32-C33
27	Z	103	DMU	C31-C34-C37-C40
27	G	101	DMU	C19-C18-O16-C6
27	M	101	DMU	C19-C18-O16-C6
20	B	302	TGL	C11-C10-CB9-CB8
20	Y	101	TGL	CA2-CA3-CA4-CA5
23	O	304	PSC	C7-C8-C9-C10
25	P	306	PEK	C3-C4-C5-C6
19	C	305	PGV	C9-C10-C11-C12
26	G	103	CDL	OB9-CB7-OB8-CB6
25	G	102	PEK	C34-C35-C36-C37
26	G	103	CDL	OB6-CB4-CB6-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	N	607	TGL	CA3-CA4-CA5-CA6
26	G	103	CDL	C77-C78-C79-C80
20	O	303	TGL	CC4-CC5-CC6-CC7
27	L	103	DMU	C4-C3-O7-C10
24	O	301	CHD	C22-C23-C24-O26
20	B	302	TGL	OG1-CG1-CG2-CG3
26	P	308	CDL	CA3-CA4-CA6-OA8
20	Y	101	TGL	CA5-CA6-CA7-CA8
21	P	310	EDO	O1-C1-C2-O2
21	V	101	EDO	O1-C1-C2-O2
27	Z	103	DMU	C28-C31-C34-C37
24	B	304	CHD	C22-C23-C24-O25
25	C	303	PEK	O04-C21-C22-C23
26	T	102	CDL	OA5-CA3-CA4-OA6
19	C	305	PGV	C24-C25-C26-C27
24	O	301	CHD	C22-C23-C24-O25
19	A	608	PGV	C11-C12-C13-C14
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
24	J	101	CHD	C22-C23-C24-O25
19	C	304	PGV	C29-C30-C31-C32
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	CAD-CBD-CGD-O1D
14	A	602	HEA	CAD-CBD-CGD-O2D
19	P	302	PGV	O03-C01-C02-O01
14	N	602	HEA	CAA-CBA-CGA-O1A
24	B	304	CHD	C22-C23-C24-O26
27	C	313	DMU	C25-C28-C31-C34
27	L	102	DMU	C31-C34-C37-C40
25	C	303	PEK	C5-C6-C7-C8
25	C	308	PEK	C6-C7-C8-C9
25	P	305	PEK	C9-C10-C11-C12
26	G	103	CDL	C13-C14-C15-C16
26	C	306	CDL	O1-C1-CA2-OA2
20	Y	101	TGL	C12-C13-C14-C29
26	G	103	CDL	C63-C64-C65-C66
14	A	602	HEA	CAA-CBA-CGA-O1A
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
26	C	306	CDL	C78-C79-C80-C81
20	O	303	TGL	C16-C15-CC9-CC8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	602	HEA	CAA-CBA-CGA-O2A
19	Z	101	PGV	C21-C22-C23-C24
14	A	602	HEA	CAA-CBA-CGA-O2A
25	C	303	PEK	C29-C30-C31-C32
24	J	101	CHD	C22-C23-C24-O26
25	G	102	PEK	O01-C02-C03-O11
26	P	308	CDL	OA5-CA3-CA4-OA6
14	N	602	HEA	C26-C15-C16-C17
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
19	A	608	PGV	O03-C19-C20-C21
21	P	311	EDO	O1-C1-C2-O2
21	S	103	EDO	O1-C1-C2-O2
21	S	105	EDO	O1-C1-C2-O2
23	B	303	PSC	C7-C8-C9-C10
25	P	306	PEK	C14-C15-C16-C17
19	A	607	PGV	O03-C19-C20-C21
25	C	308	PEK	C7-C8-C9-C10
25	P	305	PEK	C7-C8-C9-C10
23	B	303	PSC	C04-C05-N-C06
20	D	201	TGL	CC1-CC2-CC3-CC4
20	O	303	TGL	CA2-CA3-CA4-CA5
19	P	307	PGV	C9-C10-C11-C12
26	P	308	CDL	C37-C38-C39-C40
20	D	201	TGL	CA3-CA4-CA5-CA6
25	P	301	PEK	C25-C26-C27-C28
24	P	309	CHD	C22-C23-C24-O26
26	T	102	CDL	C79-C80-C81-C82
14	N	602	HEA	CAD-CBD-CGD-O2D
24	C	301	CHD	C22-C23-C24-O25
25	P	301	PEK	C03-O11-P-O13
19	C	304	PGV	C24-C25-C26-C27
26	P	308	CDL	CA7-C31-C32-C33
19	N	608	PGV	C9-C10-C11-C12
27	P	314	DMU	C2-C3-O7-C10
19	P	302	PGV	C04-O12-P-O13
19	A	607	PGV	C11-C12-C13-C14
25	C	308	PEK	C3-C4-C5-C6
26	G	103	CDL	C56-C57-C58-C59
27	C	314	DMU	C28-C31-C34-C37
24	C	307	CHD	C22-C23-C24-O25
24	P	304	CHD	C22-C23-C24-O25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	C	307	CHD	C20-C22-C23-C24
27	P	313	DMU	C18-C19-C22-C25
20	N	607	TGL	CA1-CA2-CA3-CA4
19	P	302	PGV	C5-C6-C7-C8
19	A	608	PGV	C9-C10-C11-C12
19	Z	101	PGV	C11-C12-C13-C14
26	G	103	CDL	C71-CB7-OB8-CB6
20	N	607	TGL	CB3-CB4-CB5-CB6
20	O	303	TGL	C22-C23-C24-C25
19	N	608	PGV	C30-C31-C32-C33
20	D	201	TGL	C17-C18-C19-C33
14	N	602	HEA	CAD-CBD-CGD-O1D
20	N	607	TGL	OG3-CC1-CC2-CC3
27	T	101	DMU	O6-C11-C9-C8
25	C	303	PEK	C32-C33-C34-C35
21	D	202	EDO	O1-C1-C2-O2
21	E	201	EDO	O1-C1-C2-O2
21	G	104	EDO	O1-C1-C2-O2
21	L	101	EDO	O1-C1-C2-O2
21	N	614	EDO	O1-C1-C2-O2
21	P	312	EDO	O1-C1-C2-O2
19	A	607	PGV	C9-C10-C11-C12
19	N	608	PGV	C11-C12-C13-C14
19	P	302	PGV	C9-C10-C11-C12
26	C	306	CDL	C12-C11-CA5-OA6
23	O	304	PSC	C21-C22-C23-C24
20	N	607	TGL	CA6-CA7-CA8-CA9
26	P	308	CDL	C12-C11-CA5-OA6
26	T	102	CDL	C34-C35-C36-C37
20	O	303	TGL	CB1-CB2-CB3-CB4
25	P	301	PEK	C3-C4-C5-C6
25	C	308	PEK	C23-C24-C25-C26
20	B	302	TGL	CA7-CA8-CA9-C20
20	A	609	TGL	CA9-C20-C21-C22
20	Y	101	TGL	C23-C24-C25-C26
26	C	306	CDL	C34-C35-C36-C37
26	P	308	CDL	C18-C19-C20-C21
19	A	607	PGV	O01-C1-C2-C3
26	C	306	CDL	C32-C31-CA7-OA8
25	C	308	PEK	C24-C25-C26-C27
26	P	308	CDL	C78-C79-C80-C81
25	P	306	PEK	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	Y	101	TGL	OG3-CC1-CC2-CC3
19	P	307	PGV	C7-C8-C9-C10
20	A	609	TGL	C25-C26-C27-C28
20	O	303	TGL	OG3-CC1-CC2-CC3
27	P	314	DMU	C22-C25-C28-C31
26	P	308	CDL	C12-C13-C14-C15
21	A	613	EDO	O1-C1-C2-O2
26	T	102	CDL	C13-C14-C15-C16
25	G	102	PEK	C01-C02-O01-C1
25	P	306	PEK	C01-C02-O01-C1
26	T	102	CDL	C32-C31-CA7-OA8
20	Y	101	TGL	CB6-CB7-CB8-CB9
20	A	609	TGL	CC5-CC6-CC7-CC8
20	N	607	TGL	C16-C15-CC9-CC8
20	B	302	TGL	C25-C26-C27-C28
26	C	306	CDL	C57-C58-C59-C60
20	D	201	TGL	OG2-CB1-CB2-CB3
23	B	303	PSC	C04-C05-N-C08
19	A	607	PGV	O02-C1-C2-C3
26	C	306	CDL	C32-C31-CA7-OA9
25	C	303	PEK	O02-C1-C2-C3
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A
26	T	102	CDL	C32-C31-CA7-OA9
26	C	306	CDL	C12-C11-CA5-OA7
27	L	102	DMU	C34-C37-C40-C43
20	B	302	TGL	C14-C29-C30-C31
14	A	601[A]	HEA	C12-C13-C14-C15
23	B	303	PSC	C04-C05-N-C07
19	N	608	PGV	O03-C19-C20-C21
20	O	303	TGL	OC1-CC1-CC2-CC3
25	C	308	PEK	O03-C21-C22-C23
25	P	306	PEK	C23-C24-C25-C26
21	Q	201	EDO	O1-C1-C2-O2
25	C	303	PEK	O01-C1-C2-C3
20	B	302	TGL	C11-C12-C13-C14
25	C	303	PEK	C2-C1-O01-C02
26	C	306	CDL	C53-C54-C55-C56
14	A	601[A]	HEA	CAA-CBA-CGA-O1A
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
14	A	601[B]	HEA	CAA-CBA-CGA-O1A
14	A	601[B]	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

55 monomers are involved in 152 short contacts:

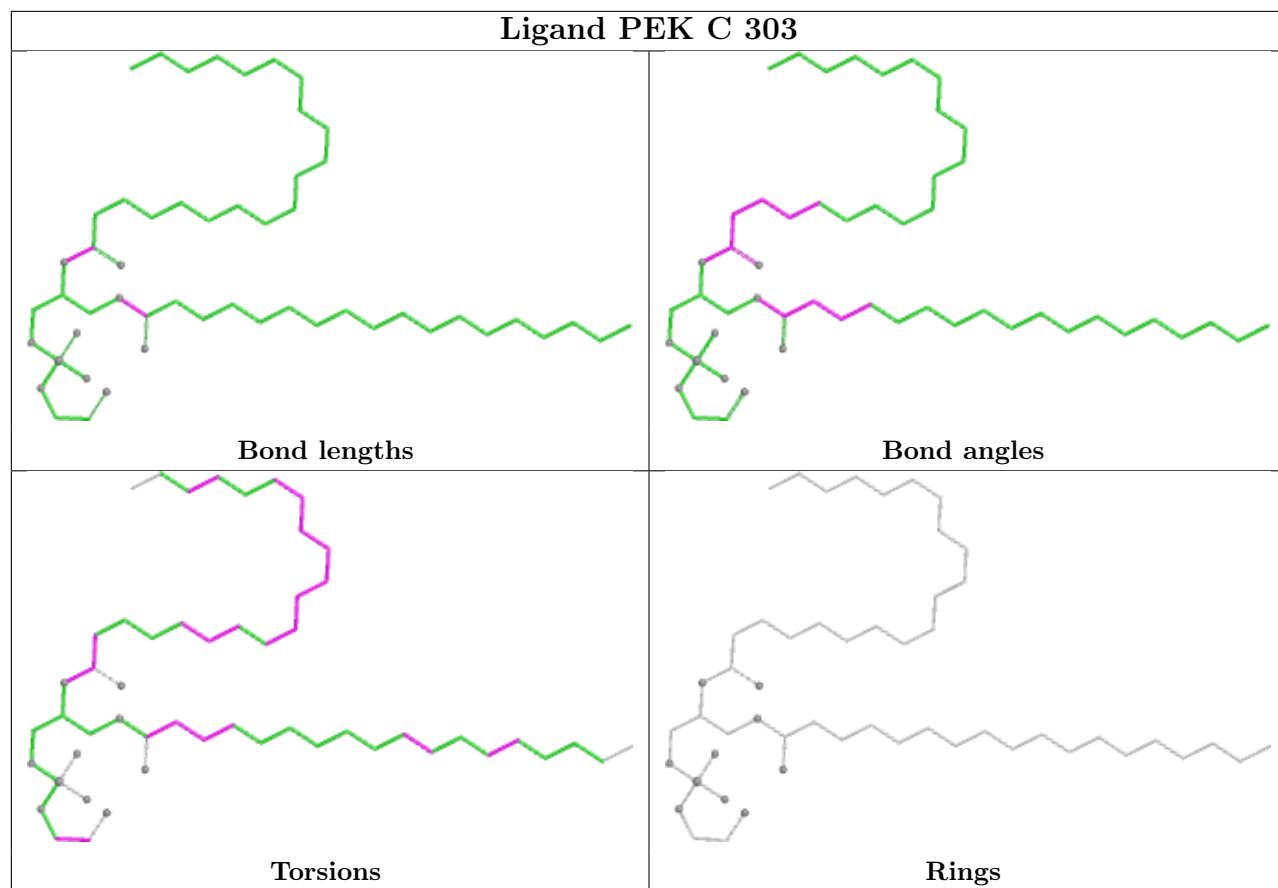
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	303	PEK	2	0
27	C	313	DMU	2	0
19	C	305	PGV	4	0
21	D	203	EDO	1	0
19	N	608	PGV	2	0
20	Y	101	TGL	3	0
26	T	102	CDL	11	0
27	P	313	DMU	1	0
24	O	301	CHD	2	0
21	E	203	EDO	1	0
23	B	303	PSC	3	0
26	P	308	CDL	7	0
21	O	305	EDO	1	0
21	A	619	EDO	5	0
27	L	102	DMU	5	0
27	L	103	DMU	4	0
19	C	304	PGV	1	0
25	P	306	PEK	1	0
25	P	301	PEK	3	0
27	Z	103	DMU	2	0
24	C	315	CHD	2	0
27	T	101	DMU	8	0
21	N	611	EDO	1	0
14	A	602	HEA	2	0
19	A	607	PGV	8	0
14	A	601[A]	HEA	2	0
21	L	101	EDO	1	0
14	N	602	HEA	4	0
14	N	601[A]	HEA	3	0
24	J	101	CHD	2	0
19	Z	101	PGV	1	0
26	G	103	CDL	5	0
20	D	201	TGL	3	0
19	P	302	PGV	2	0
24	P	315	CHD	7	0
21	Q	202	EDO	1	0
21	Q	201	EDO	1	0
27	G	101	DMU	2	0
24	P	309	CHD	3	0
27	C	314	DMU	4	0

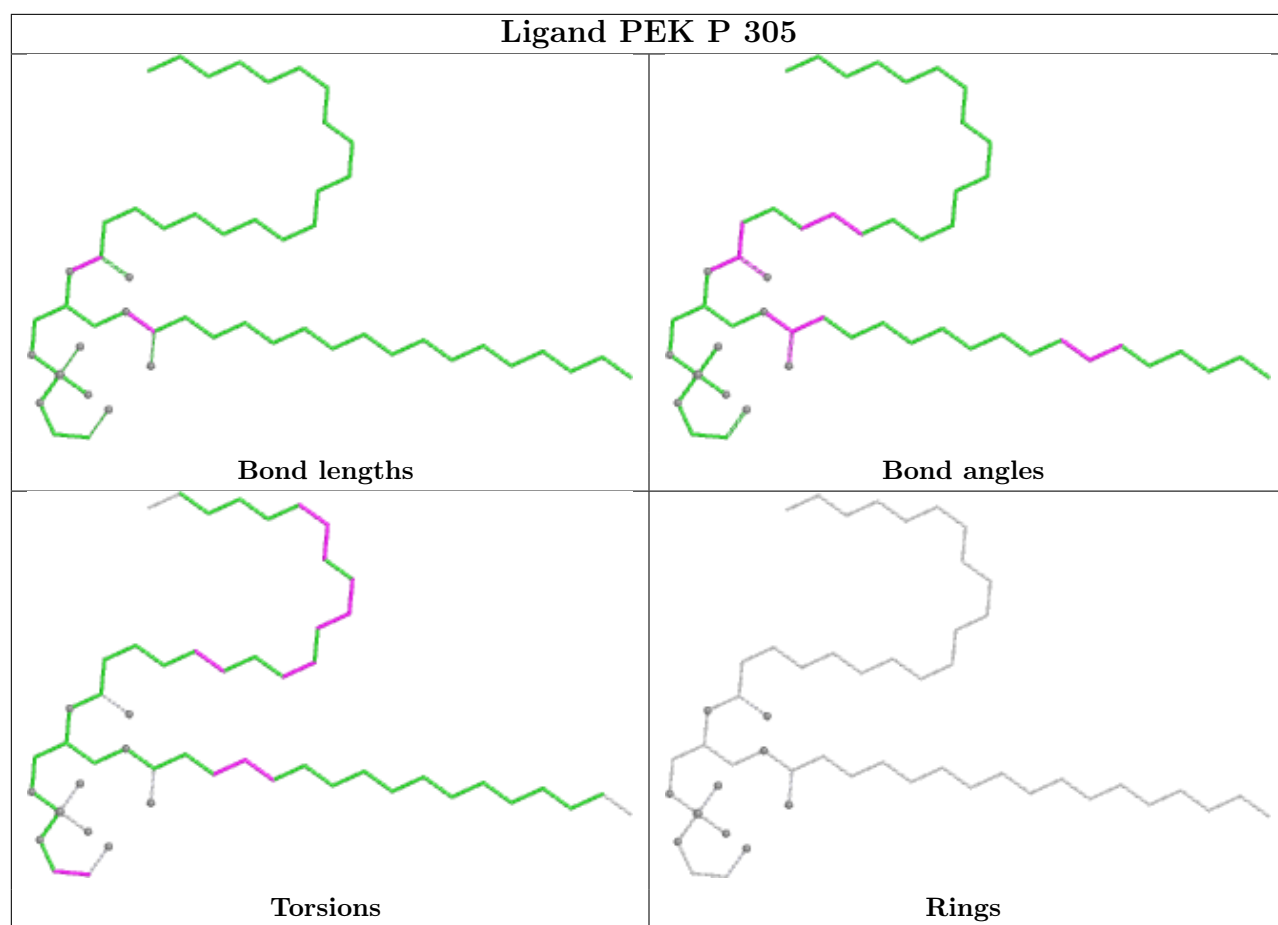
Continued on next page...

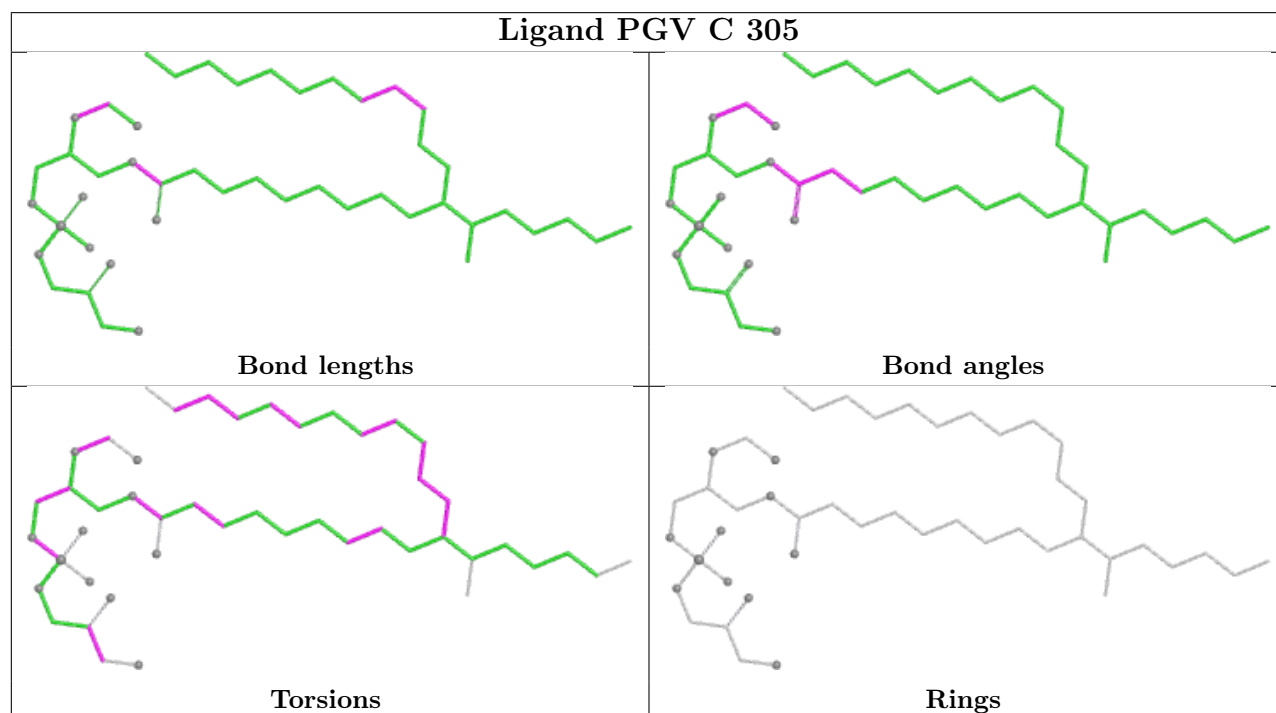
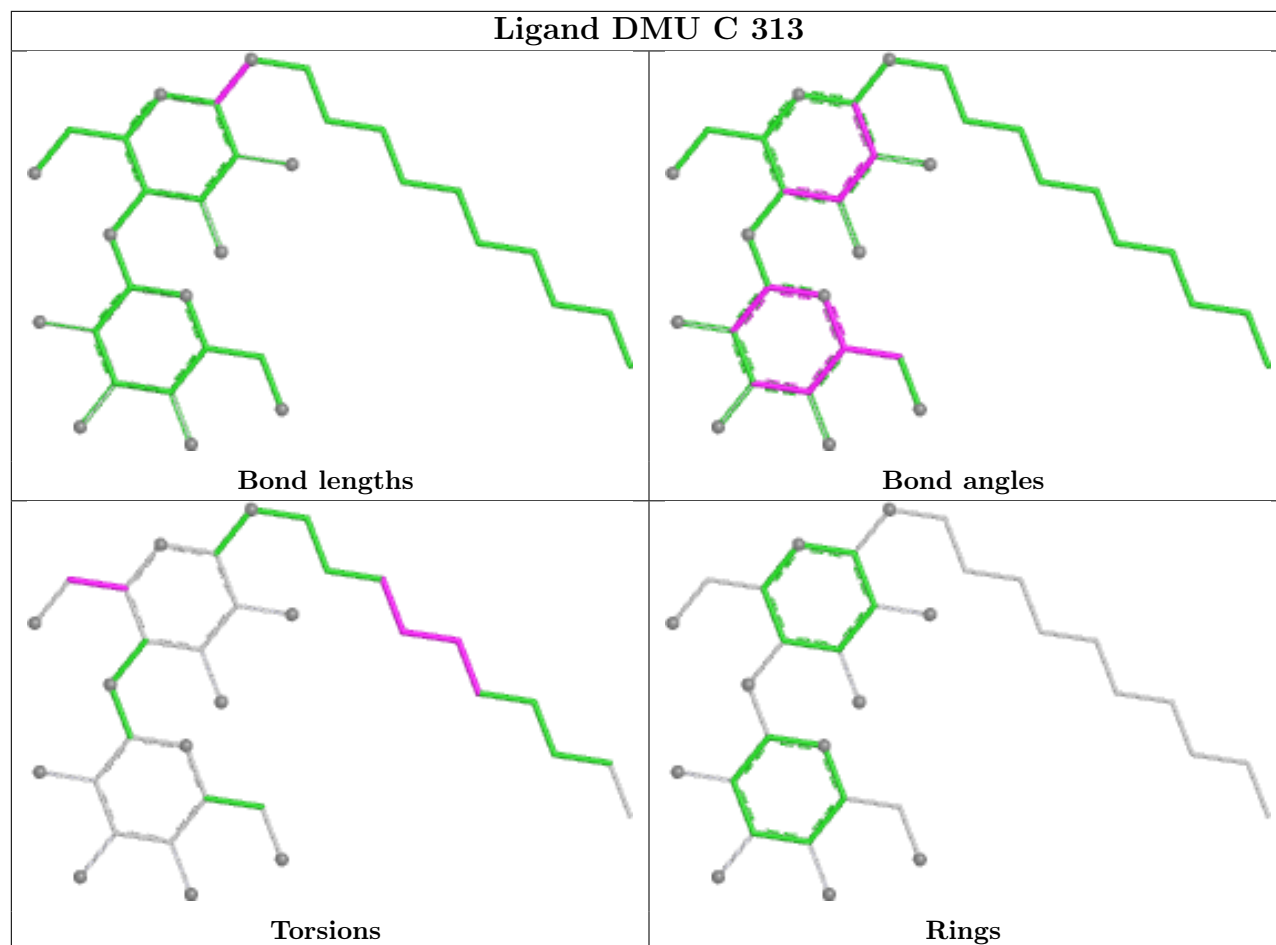
Continued from previous page...

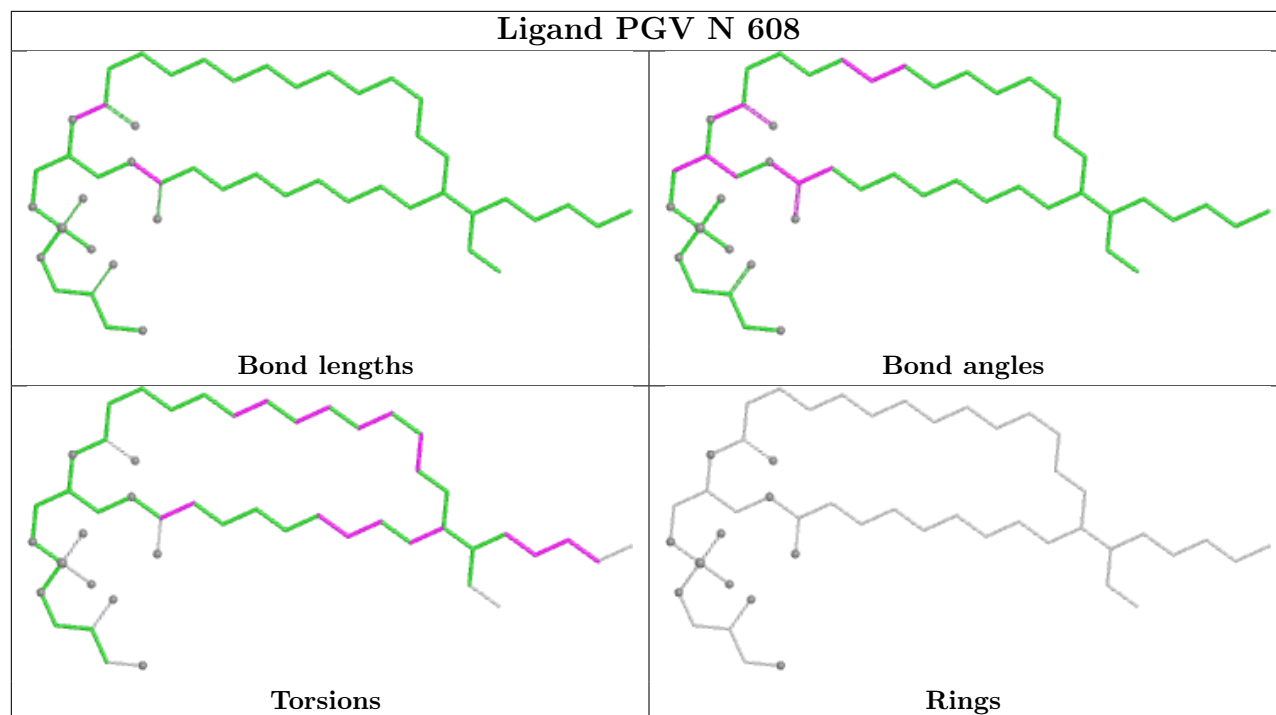
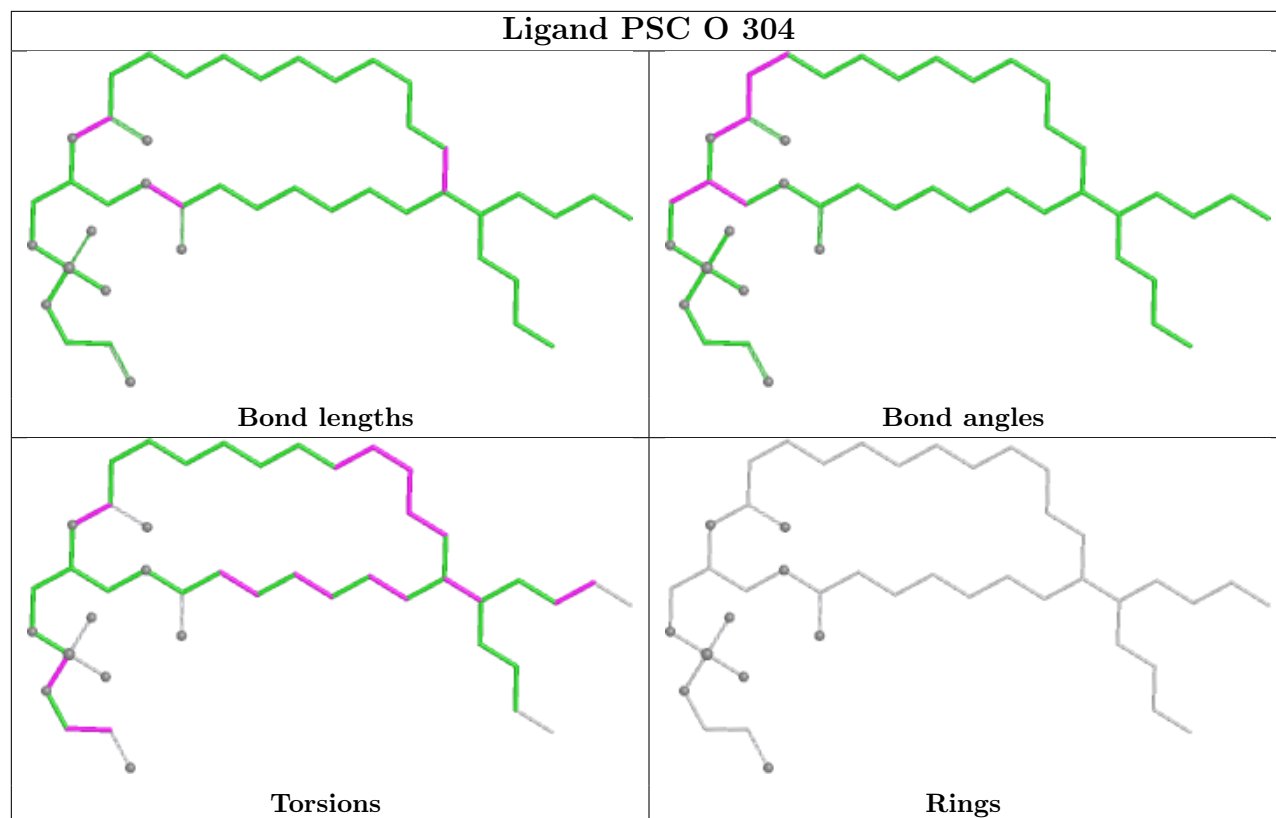
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	307	PGV	1	0
25	G	102	PEK	4	0
24	Y	102	CHD	4	0
20	B	302	TGL	1	0
27	M	101	DMU	1	0
20	O	303	TGL	2	0
20	A	609	TGL	3	0
25	C	308	PEK	2	0
21	C	309	EDO	1	0
21	D	204	EDO	2	0
20	N	607	TGL	2	0
26	C	306	CDL	8	0
14	A	601[B]	HEA	4	0
21	C	312	EDO	1	0
24	C	307	CHD	1	0

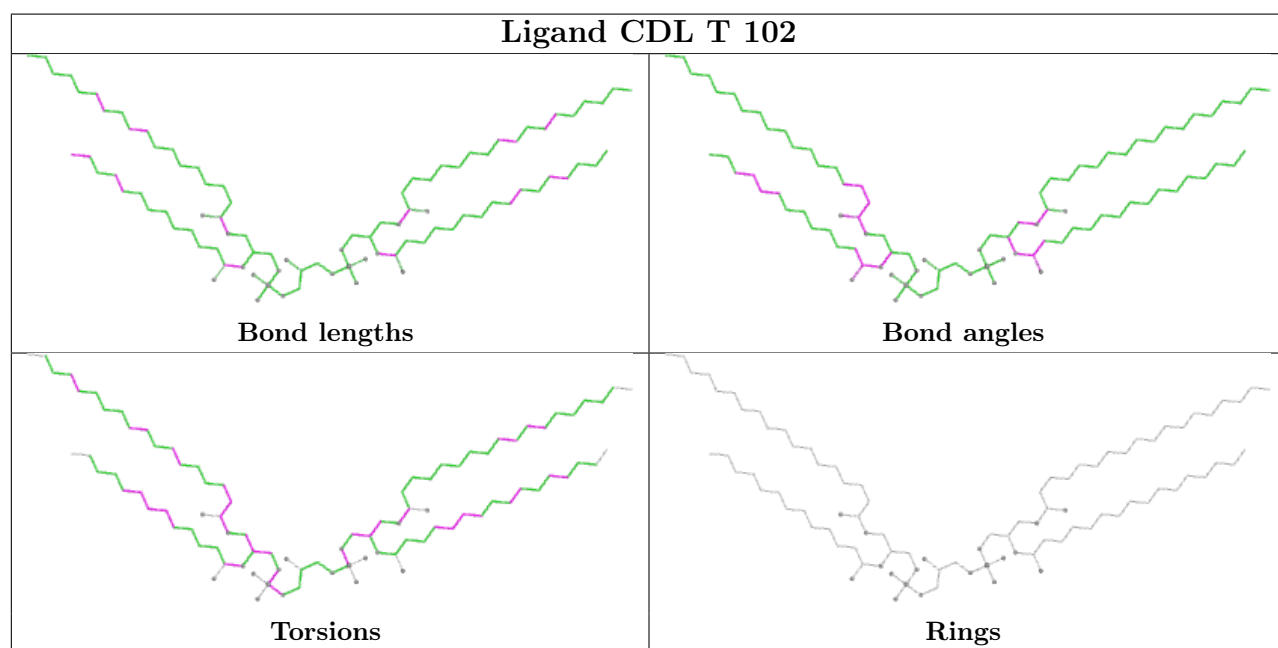
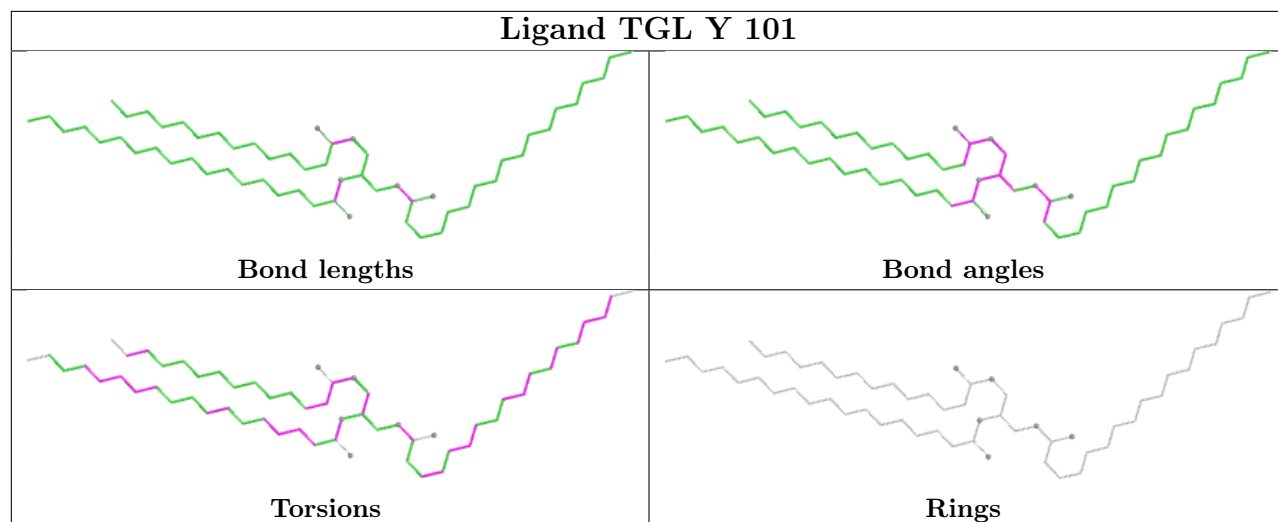
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

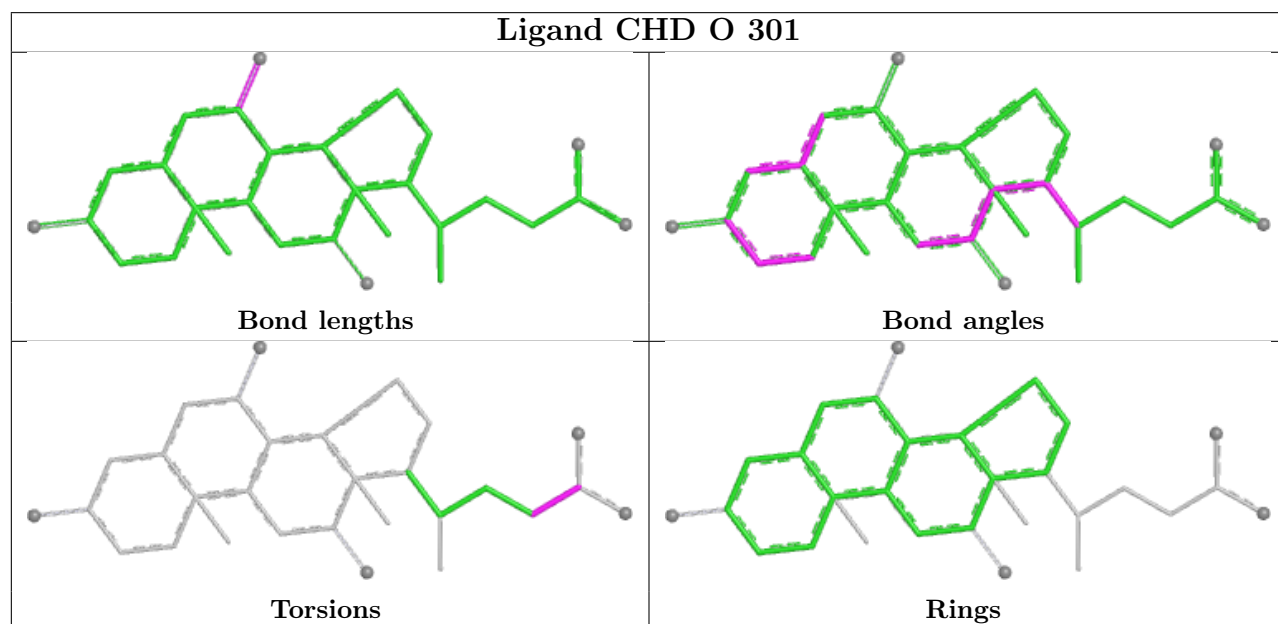
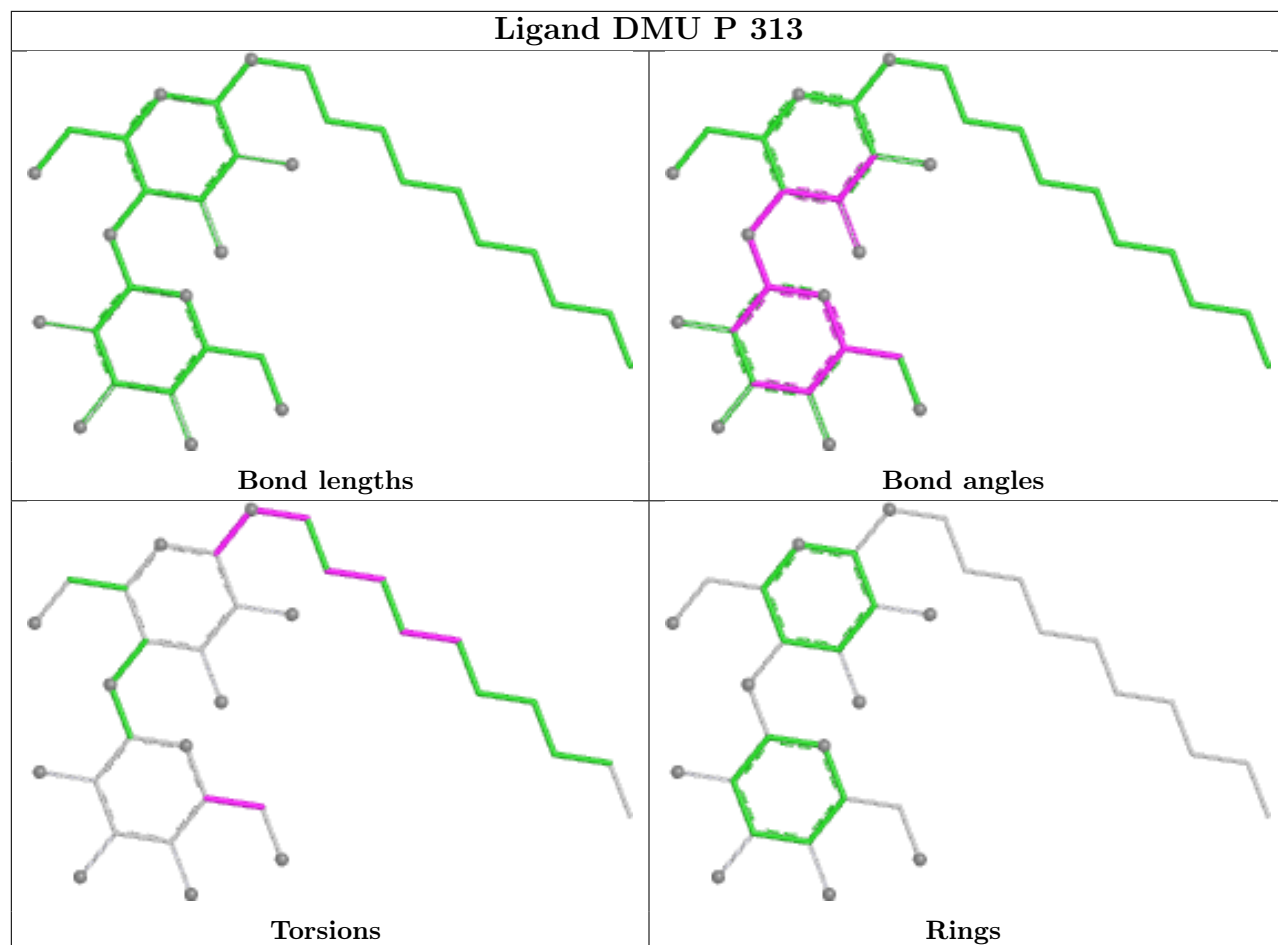


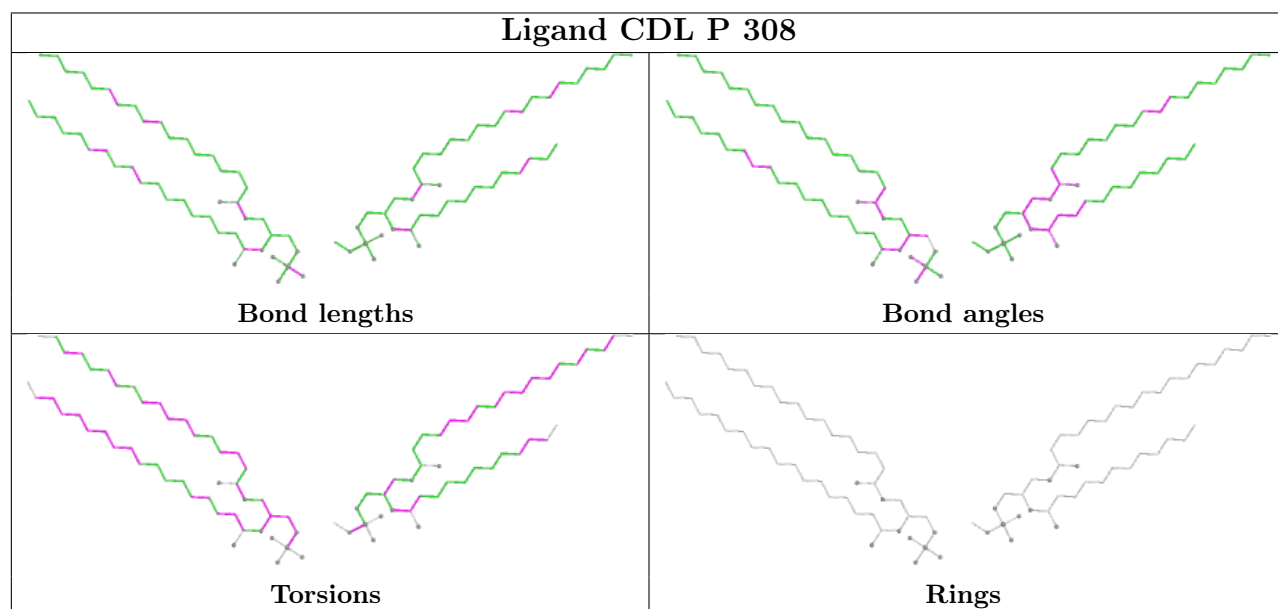
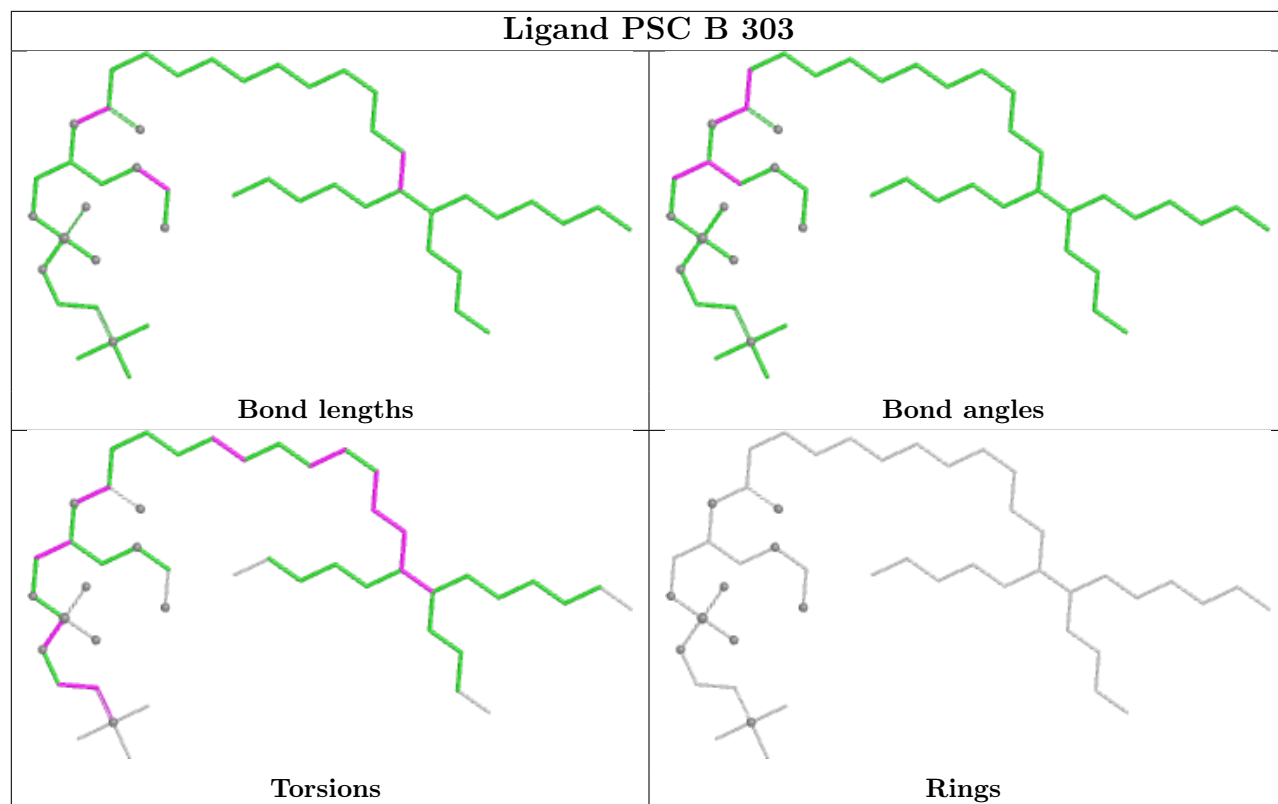


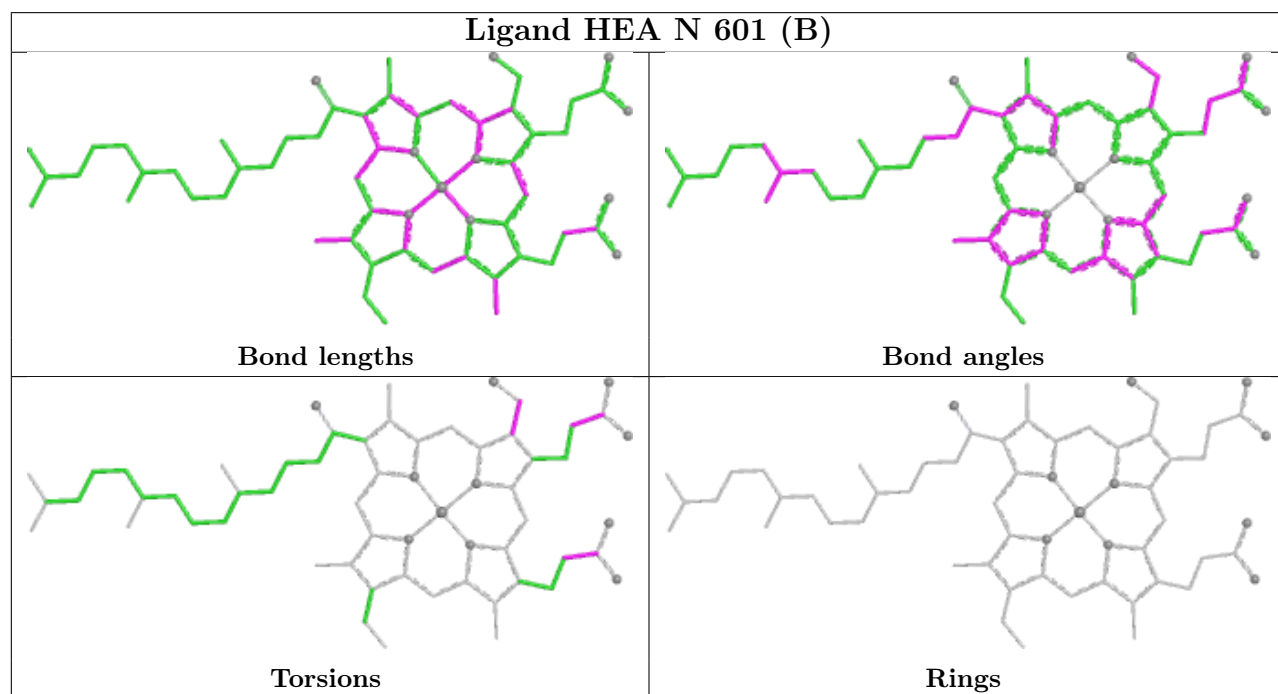
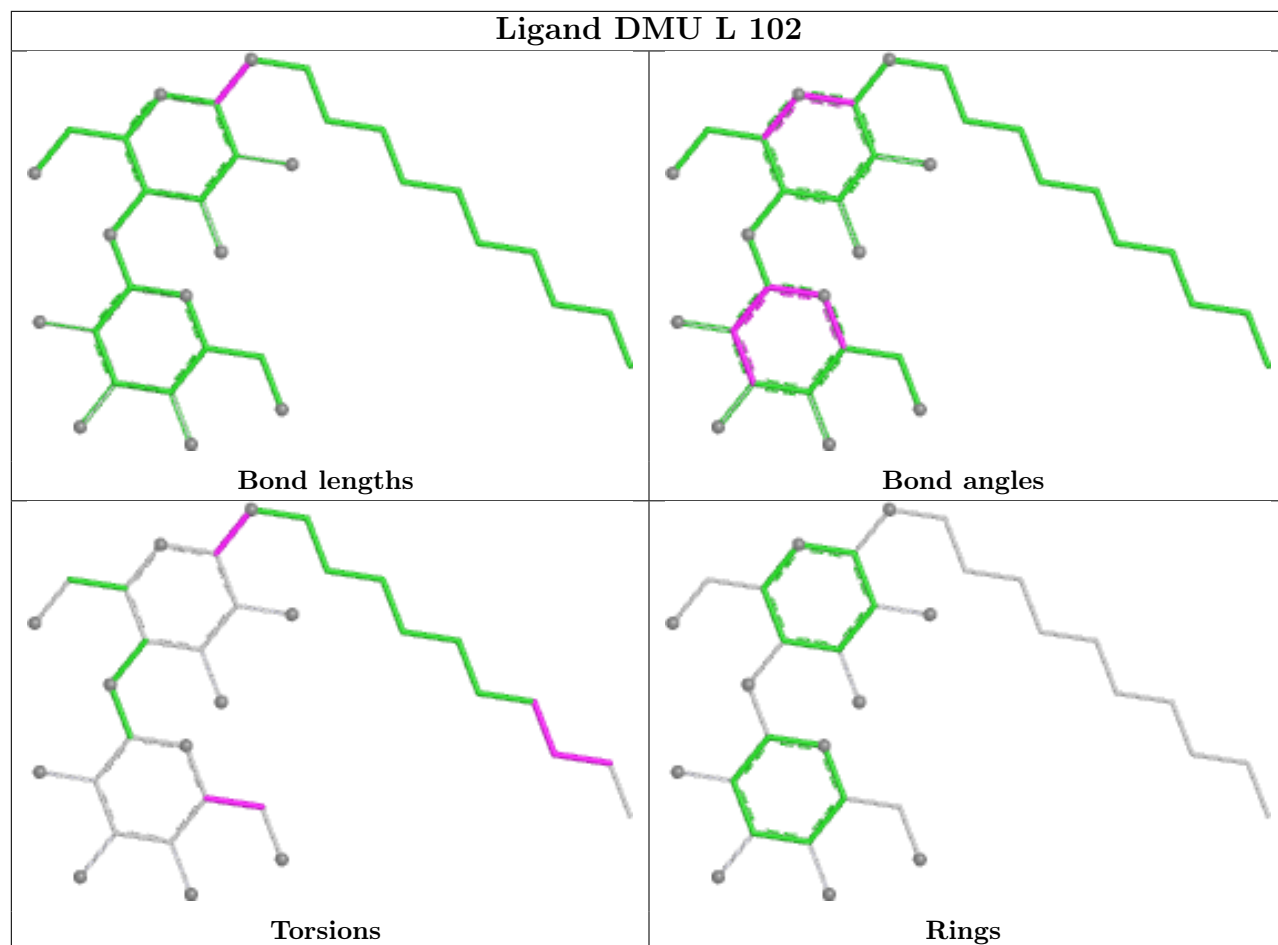


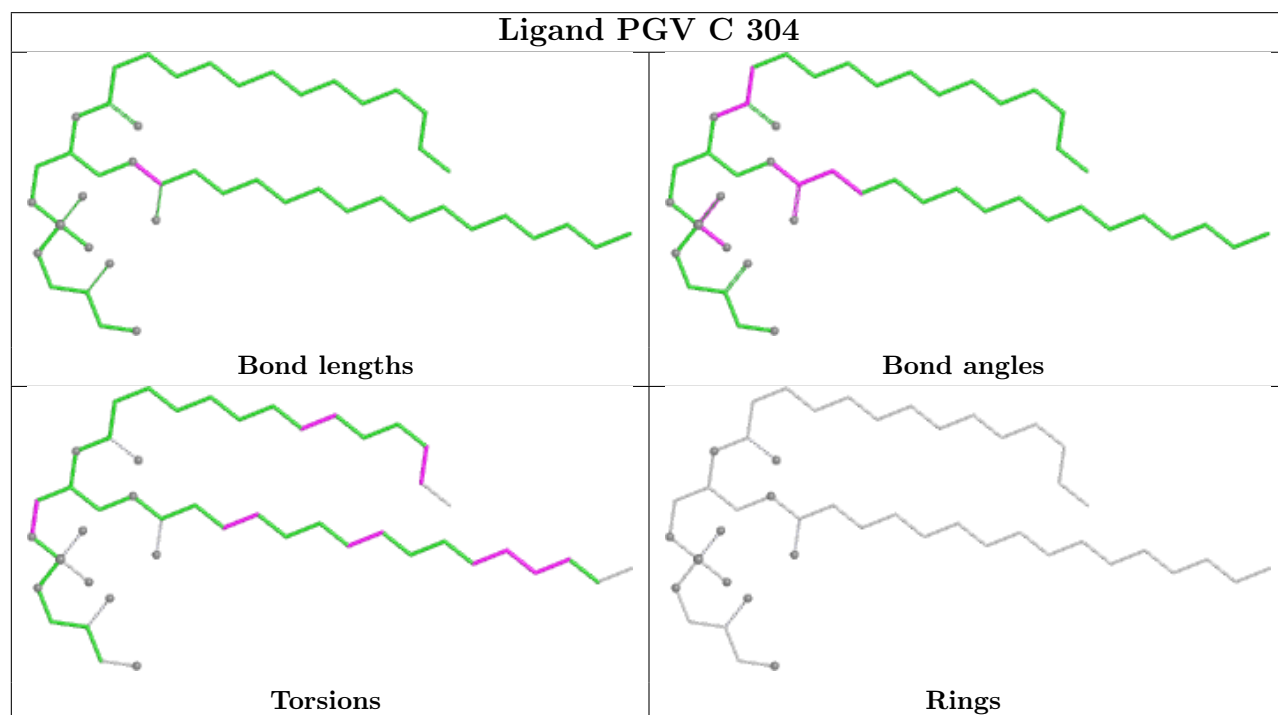
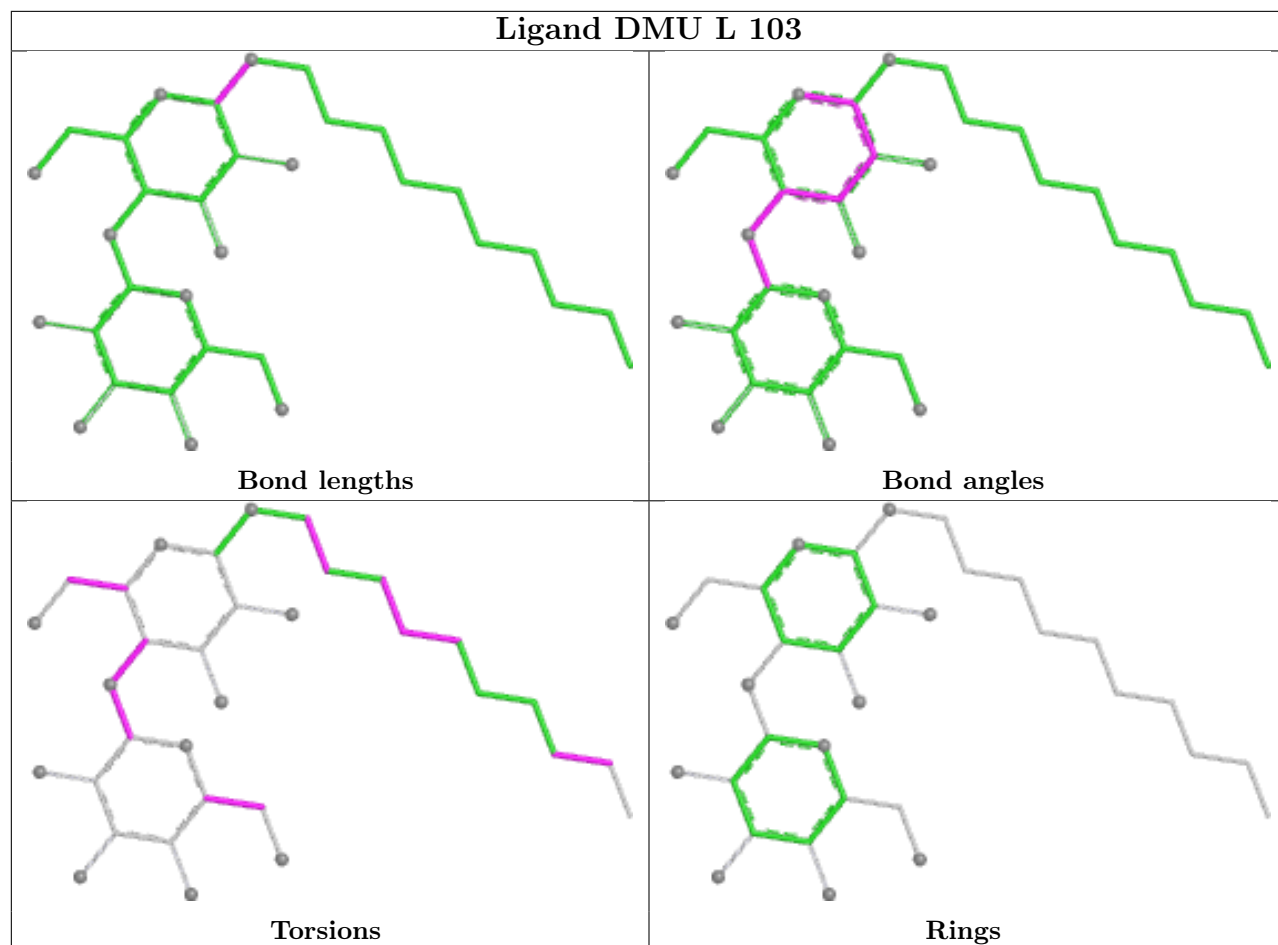


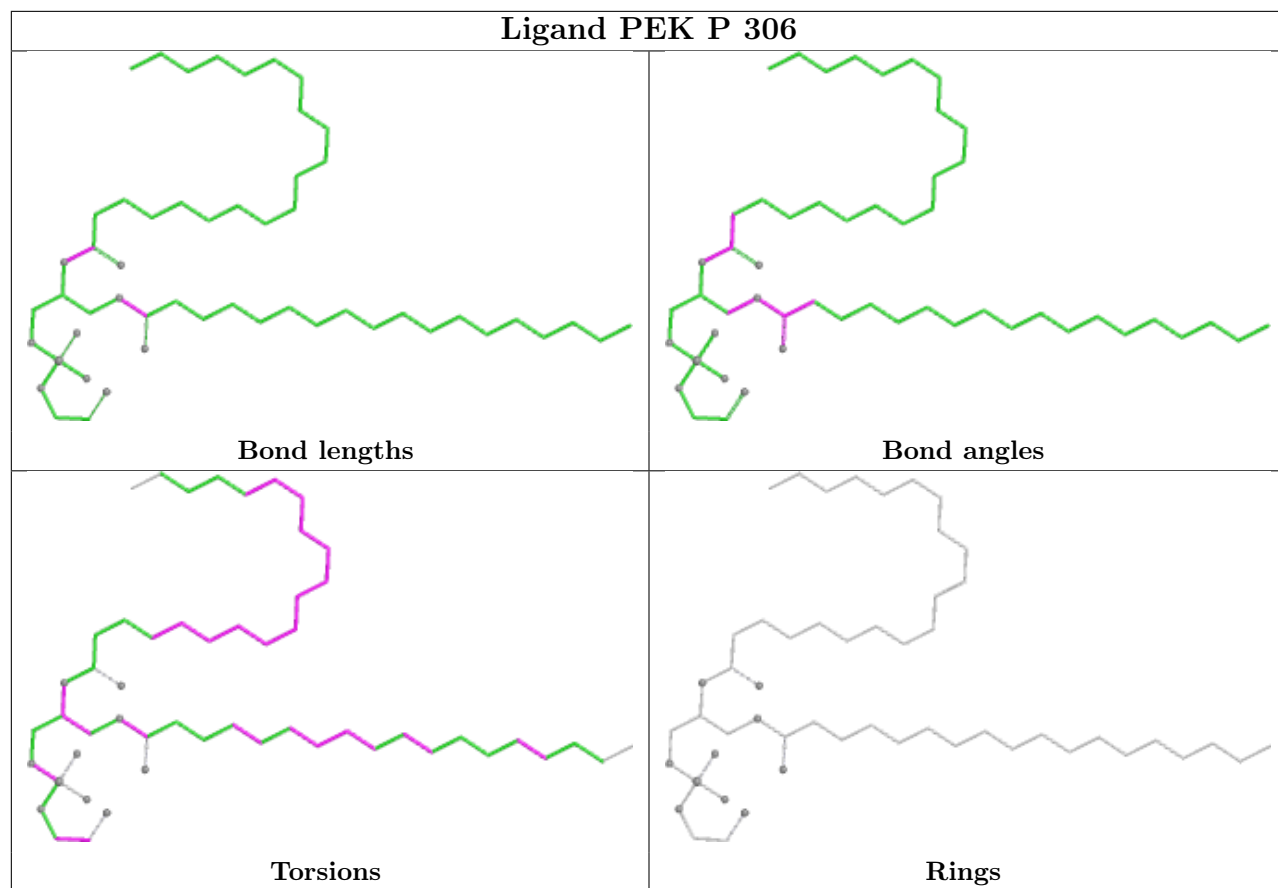


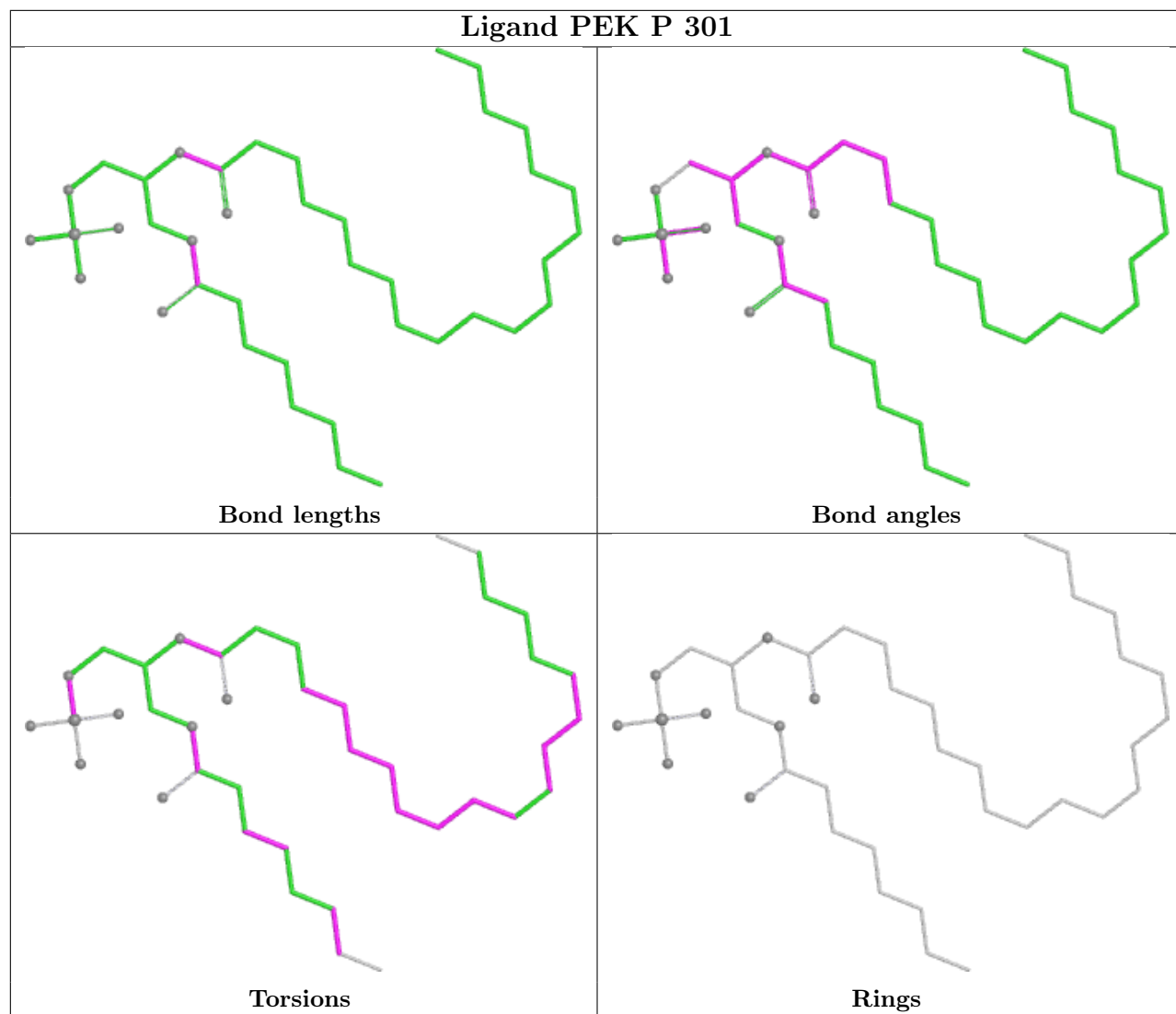


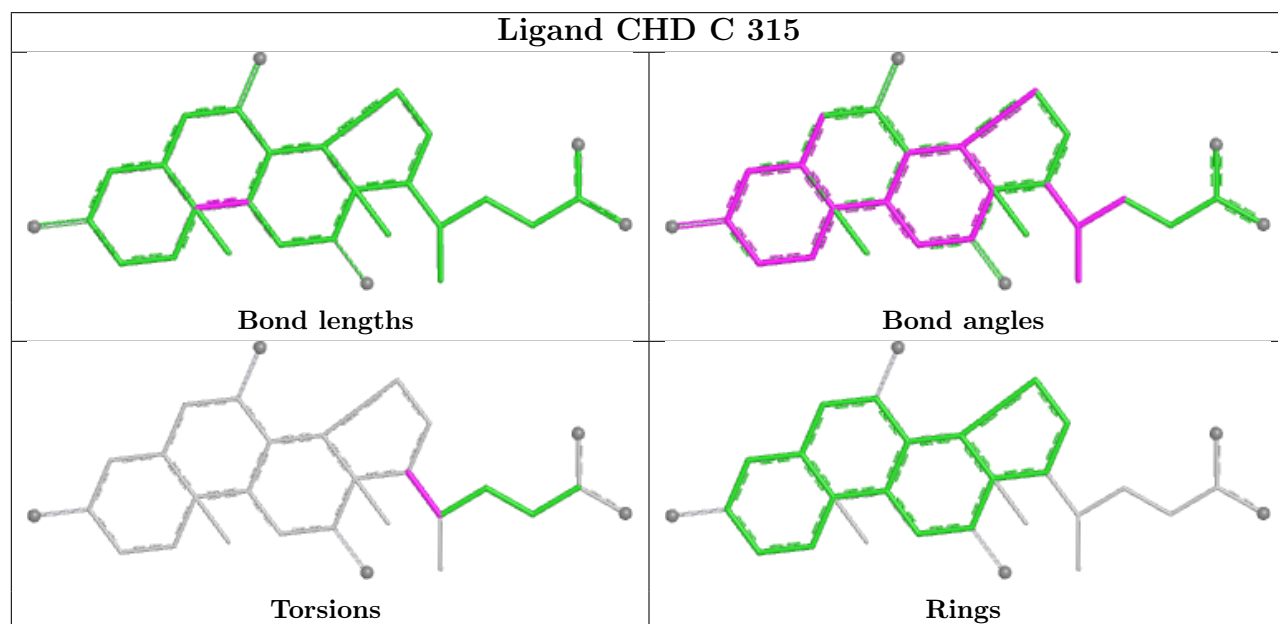
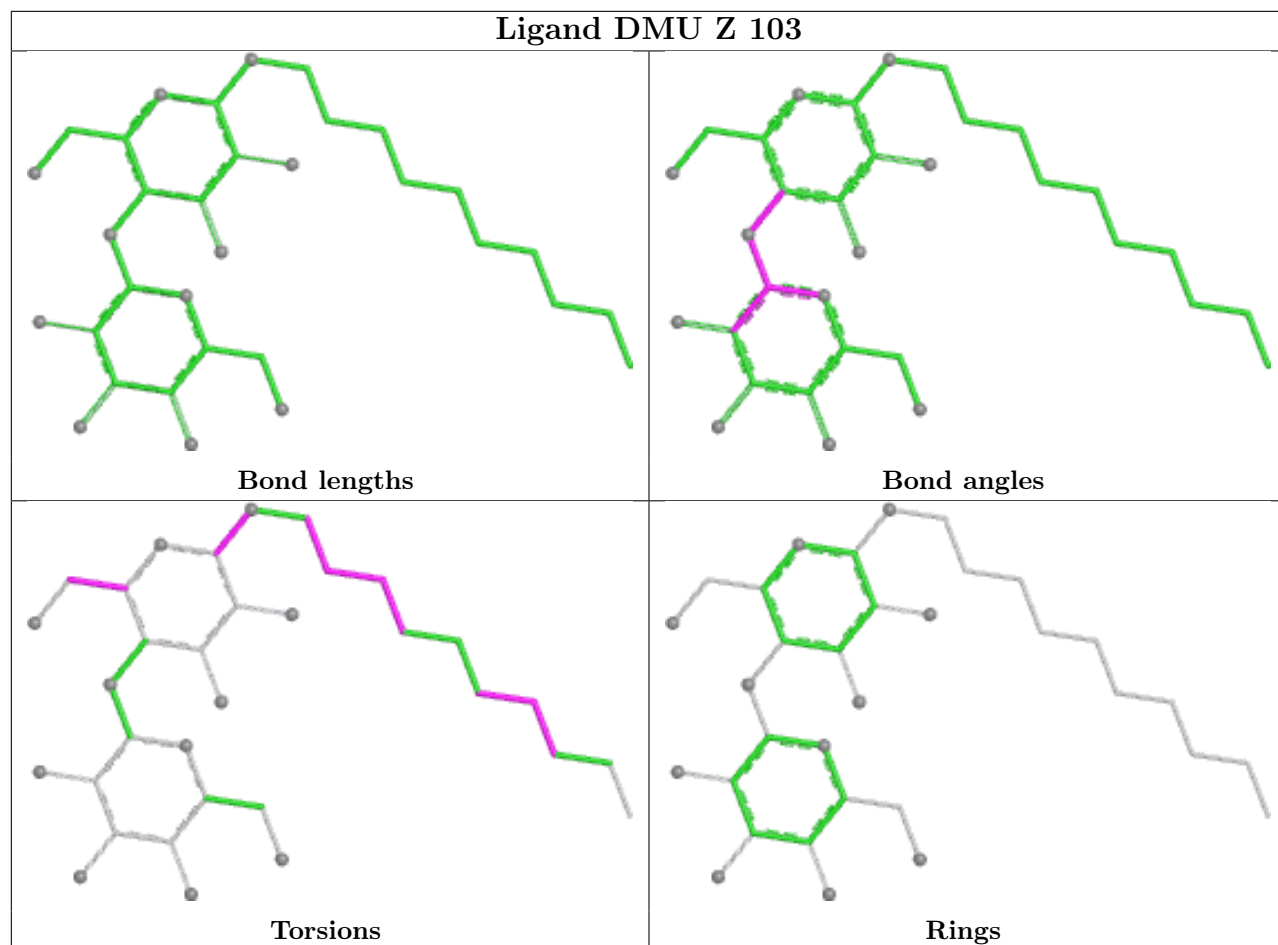


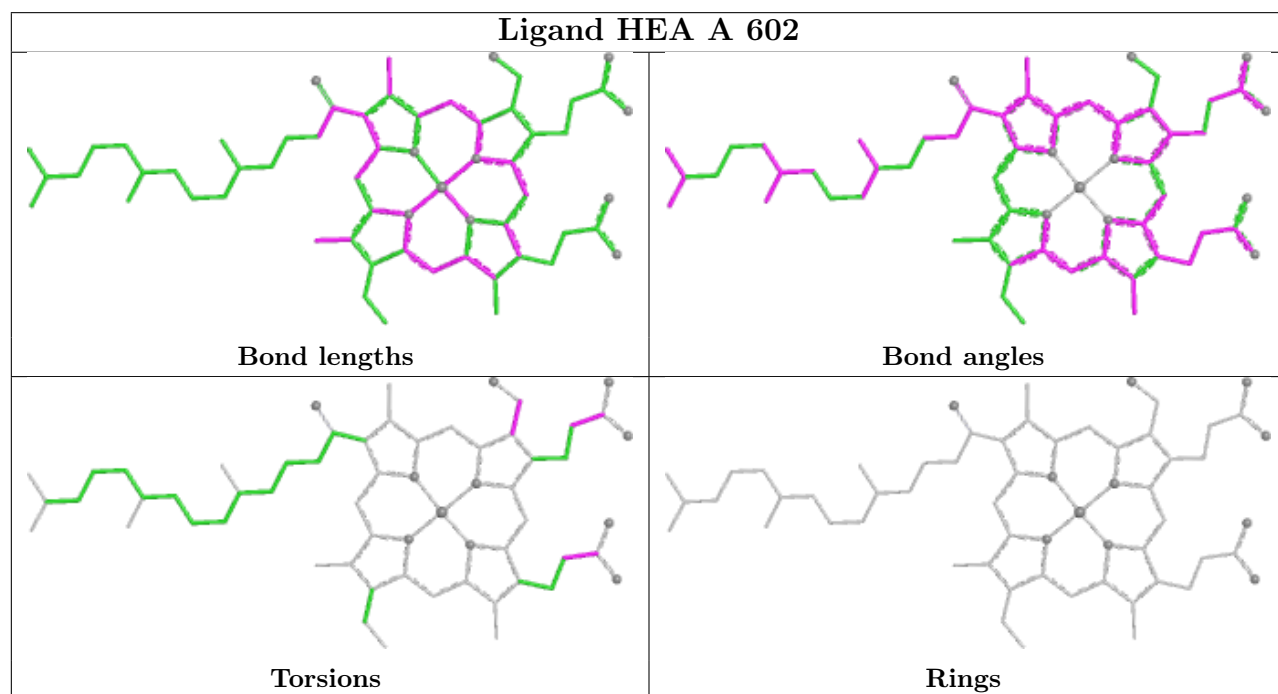
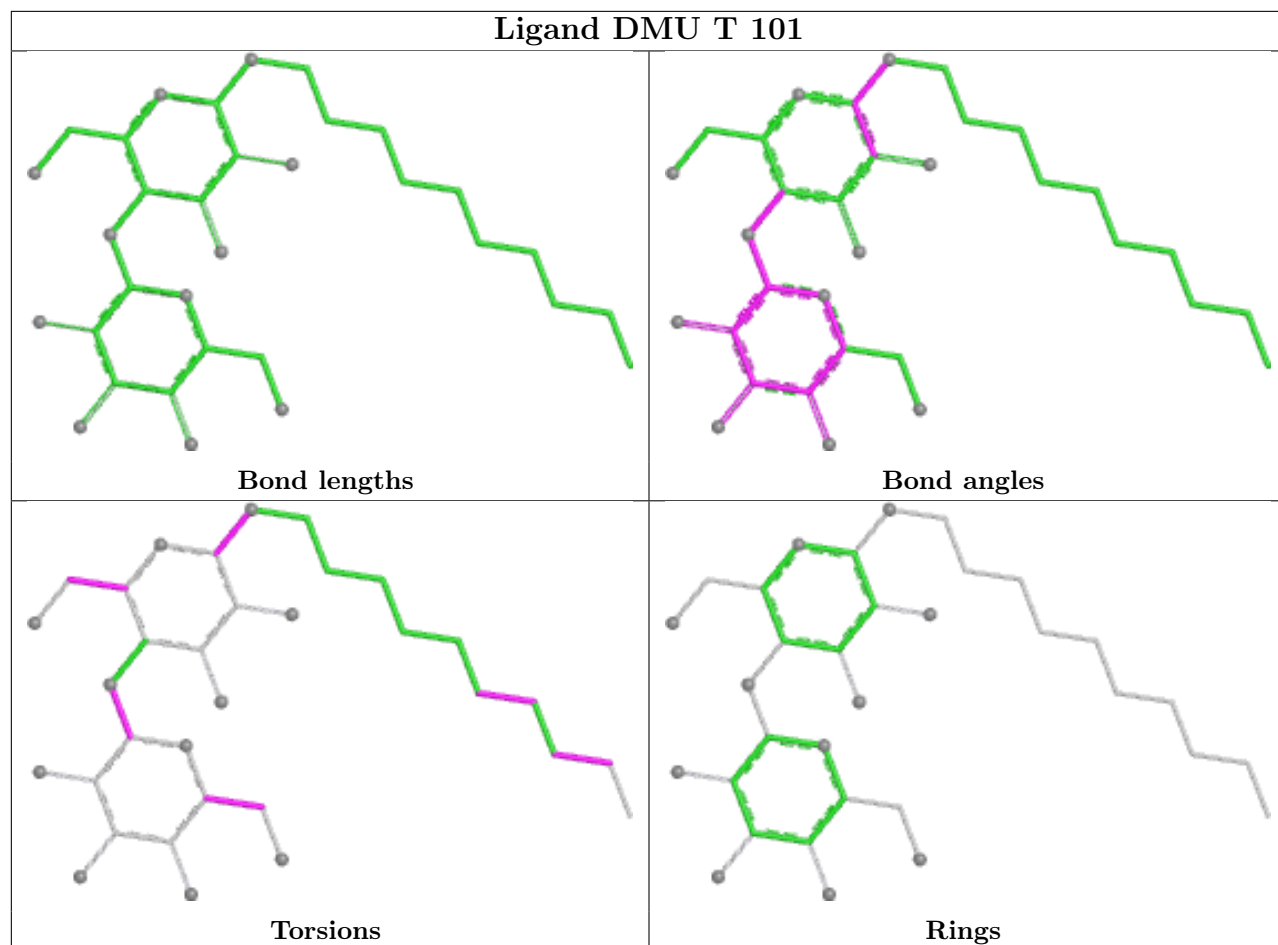


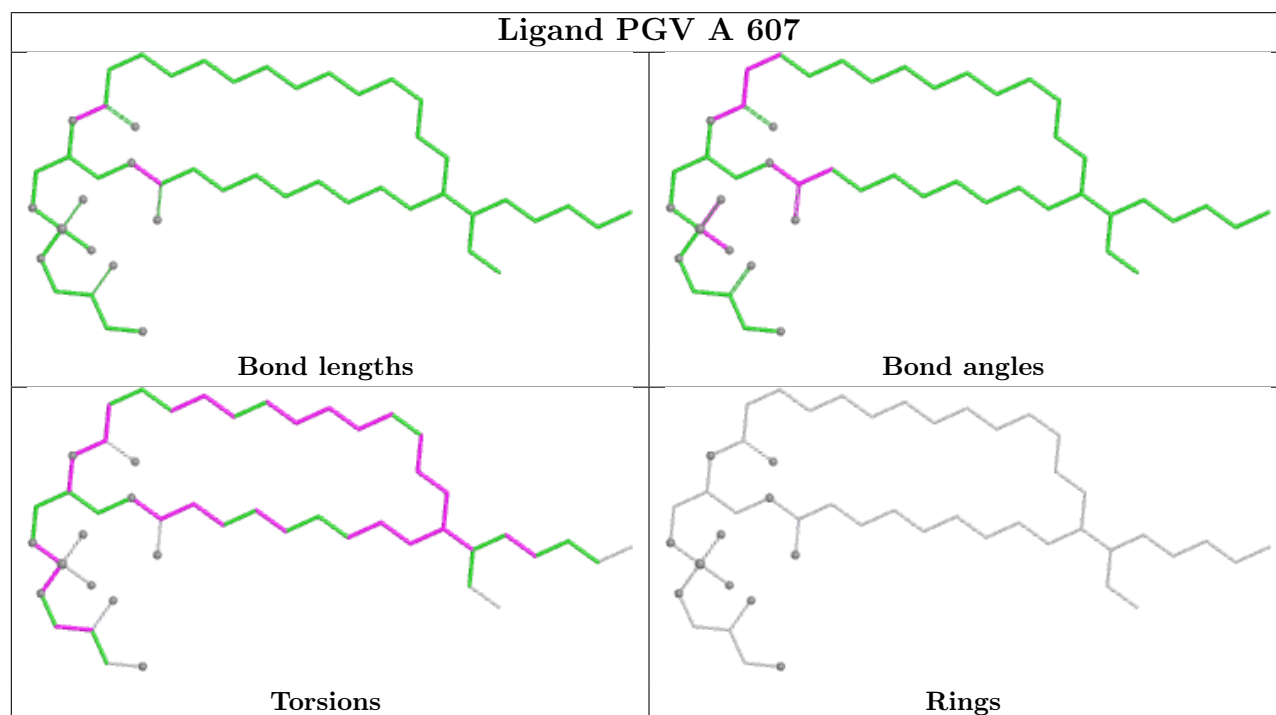
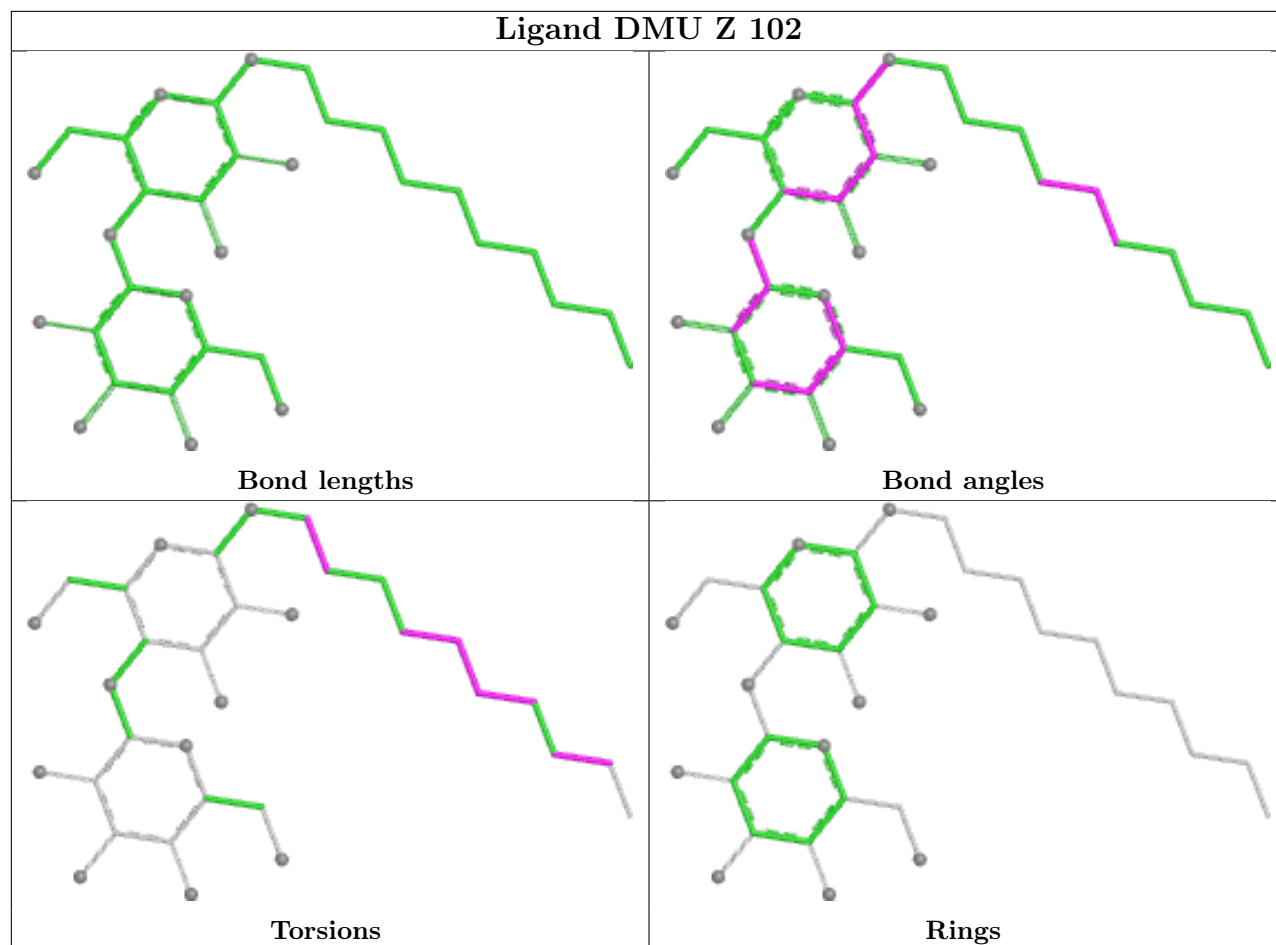


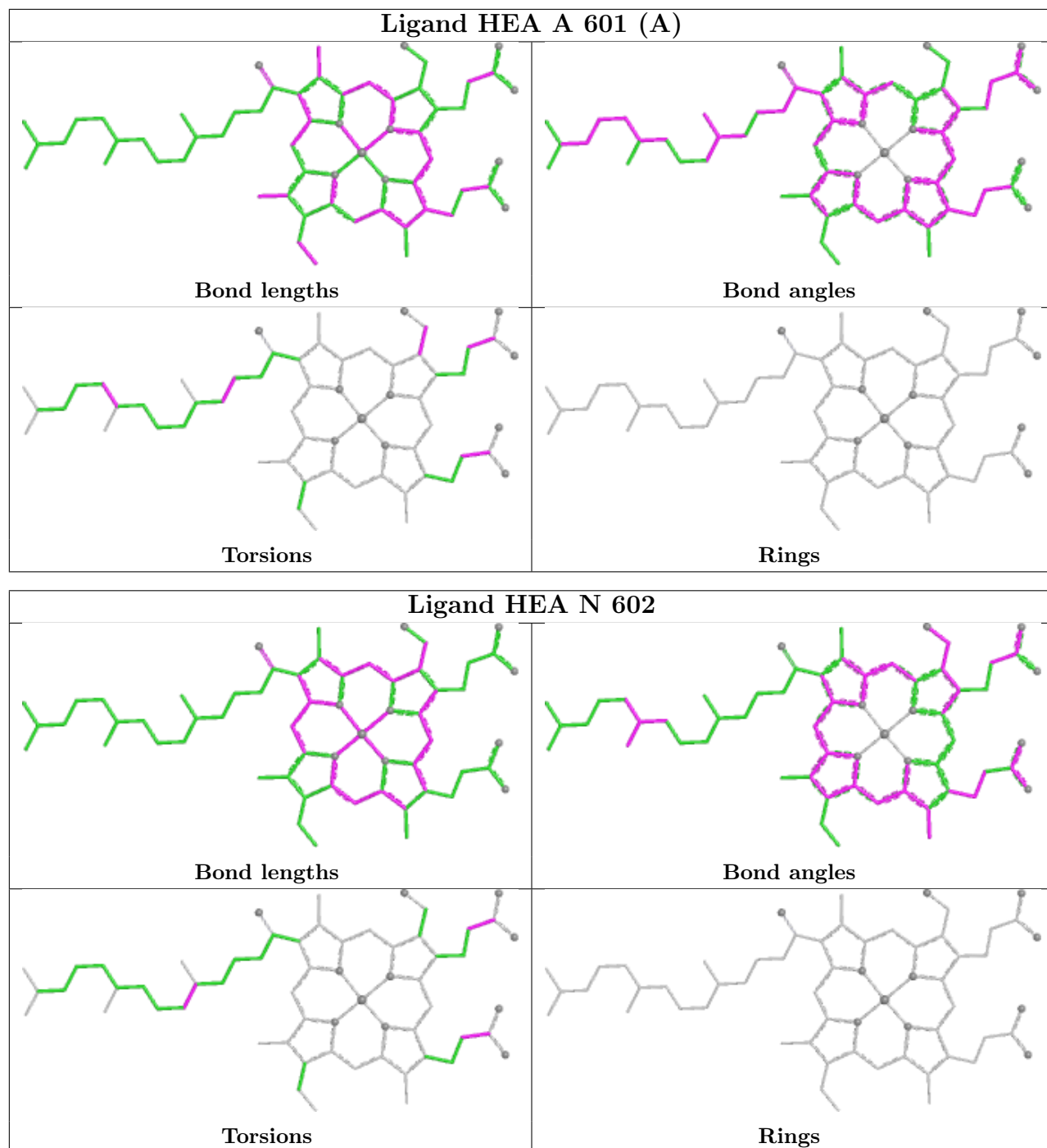


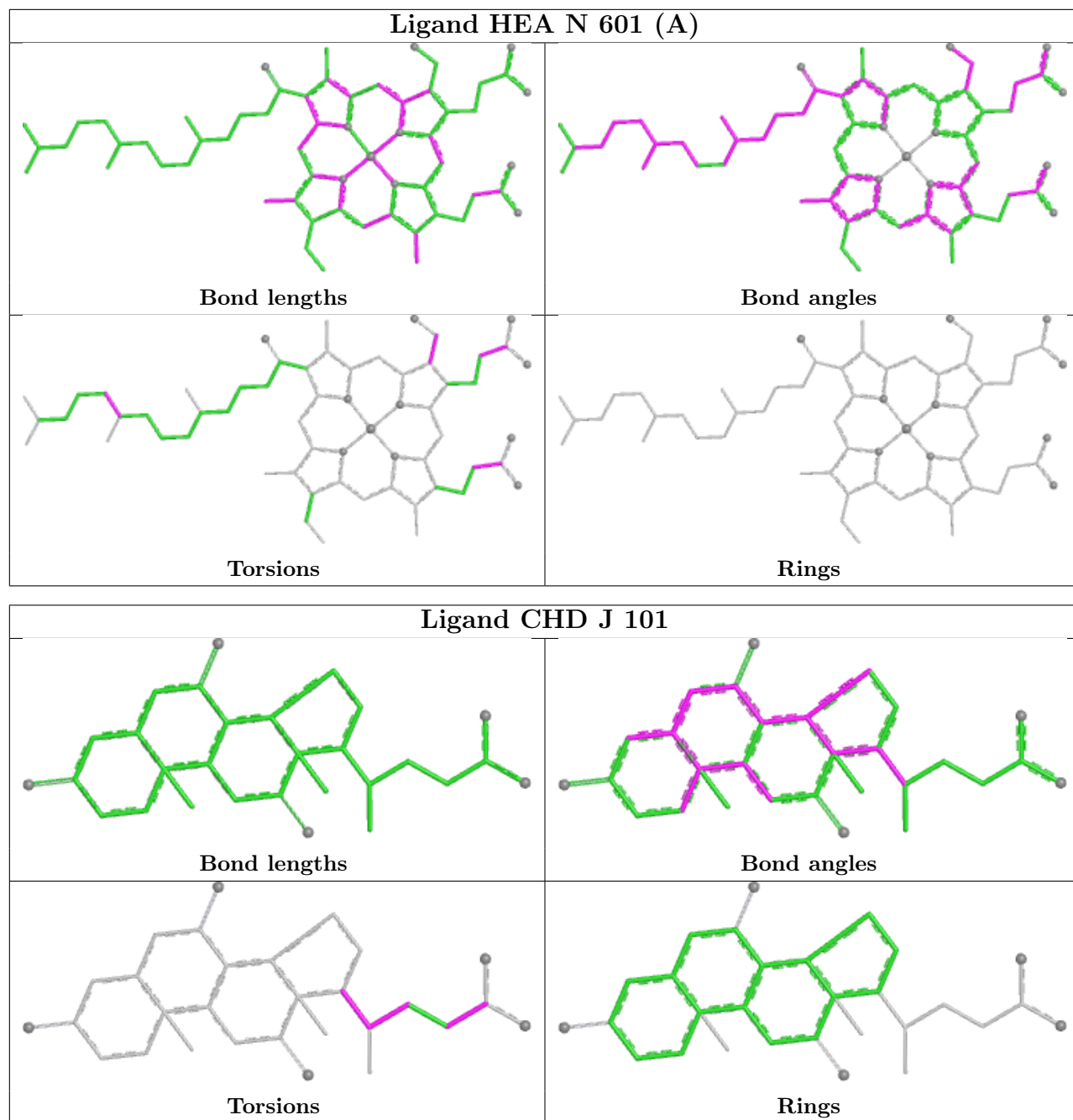


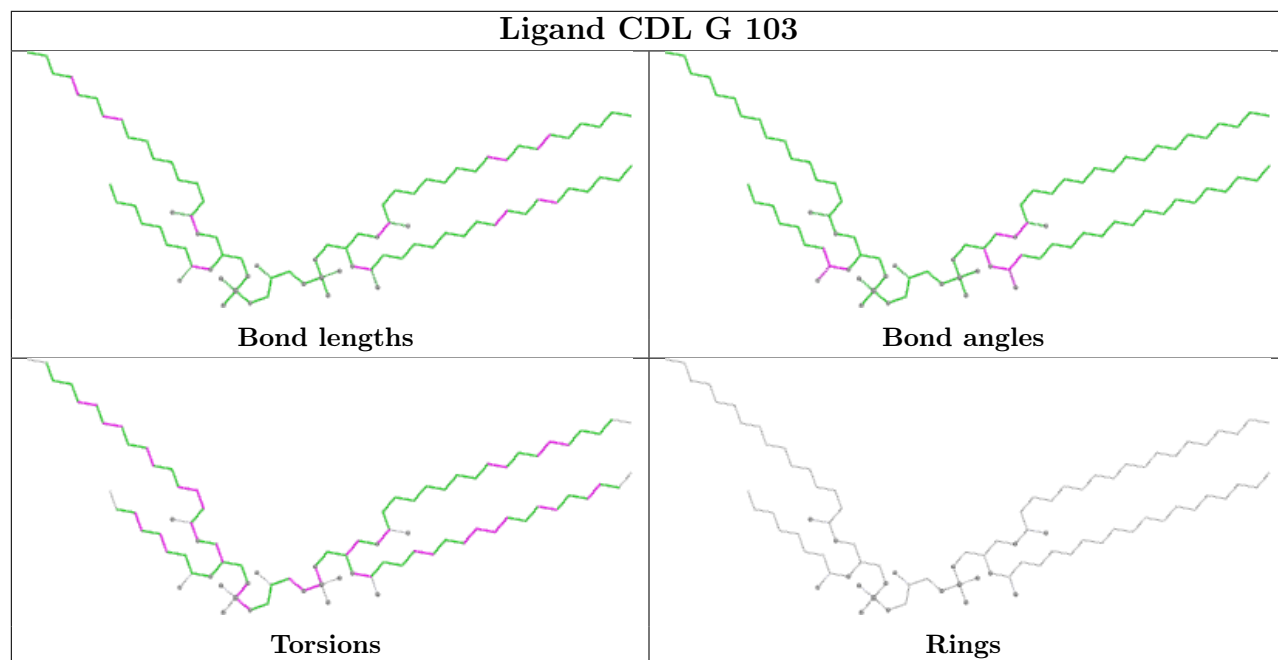
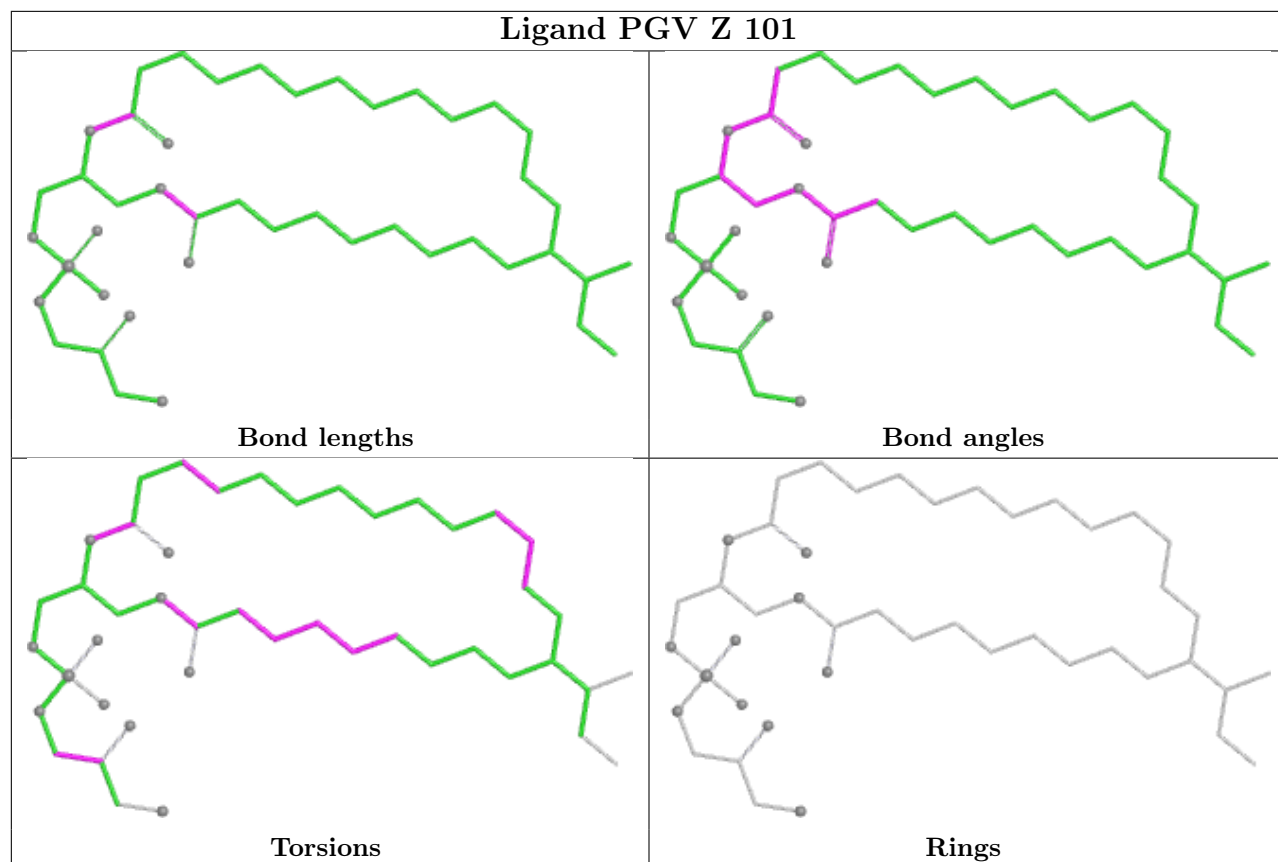


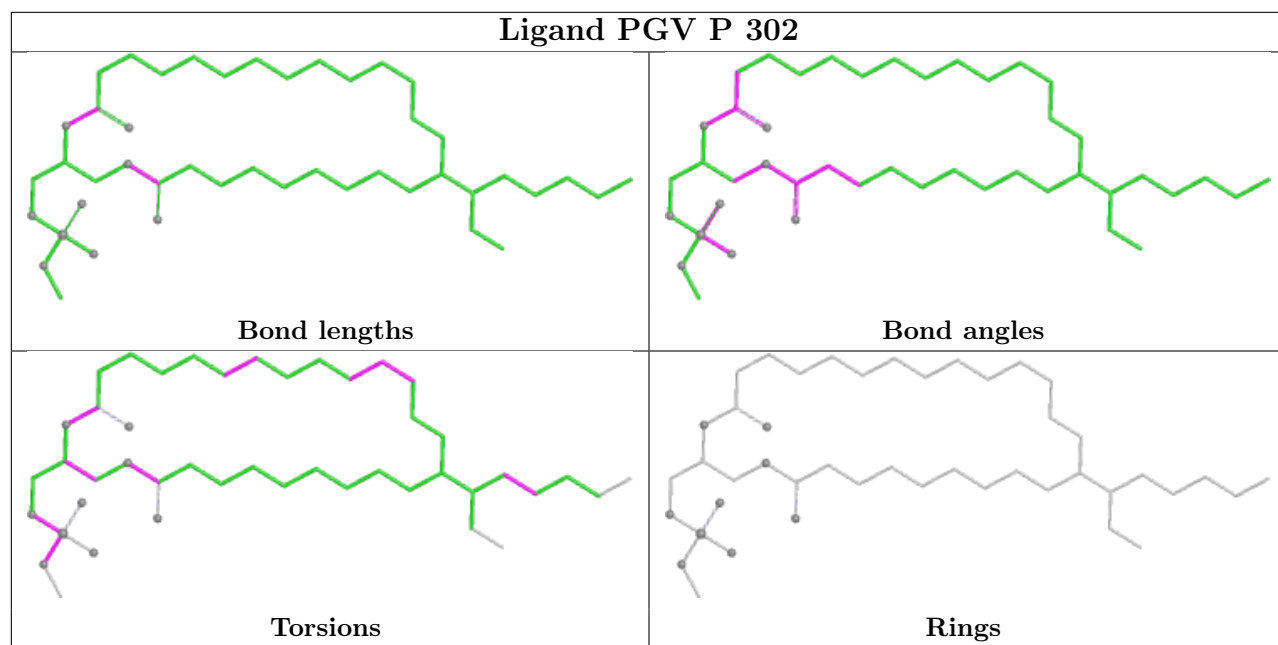
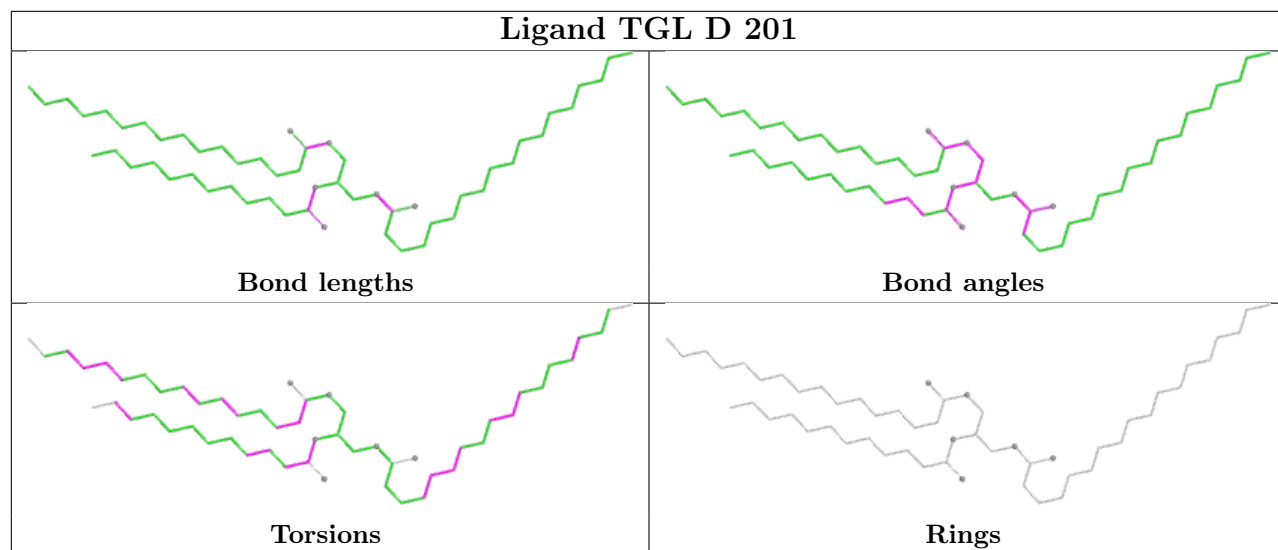


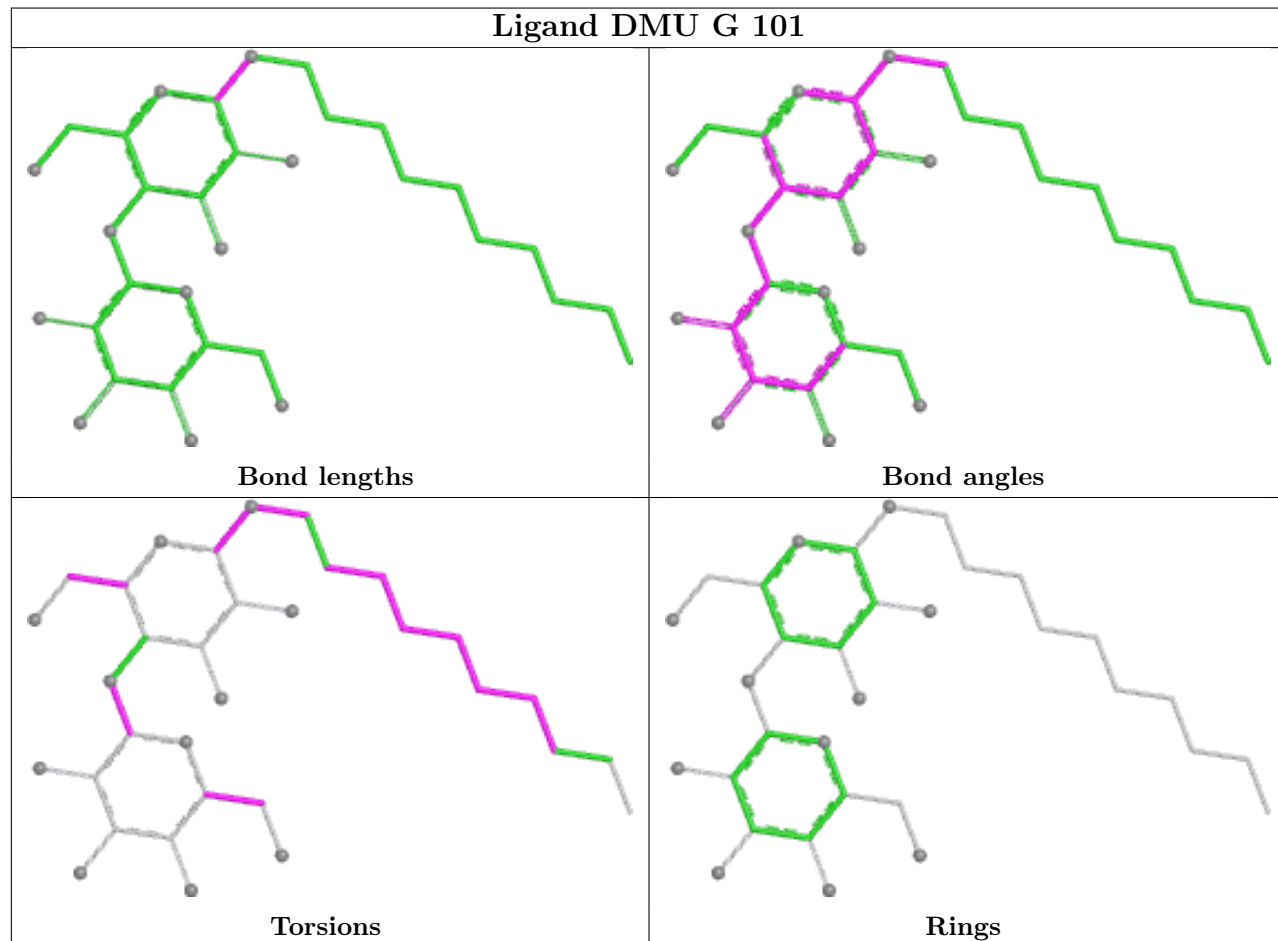
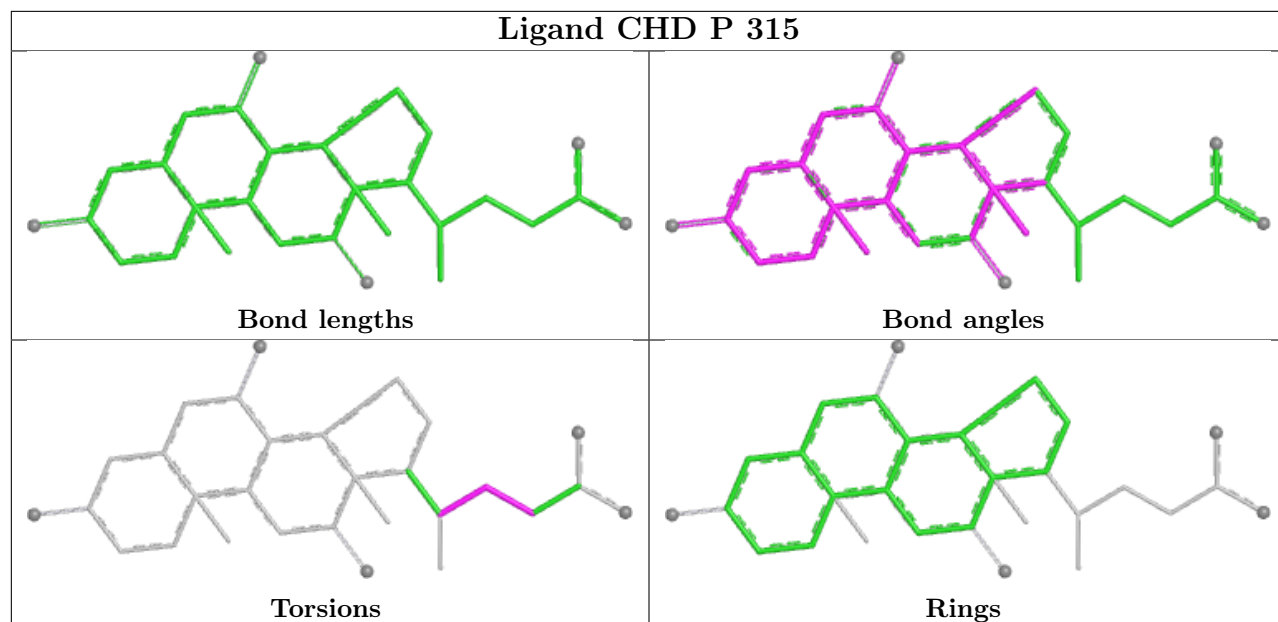


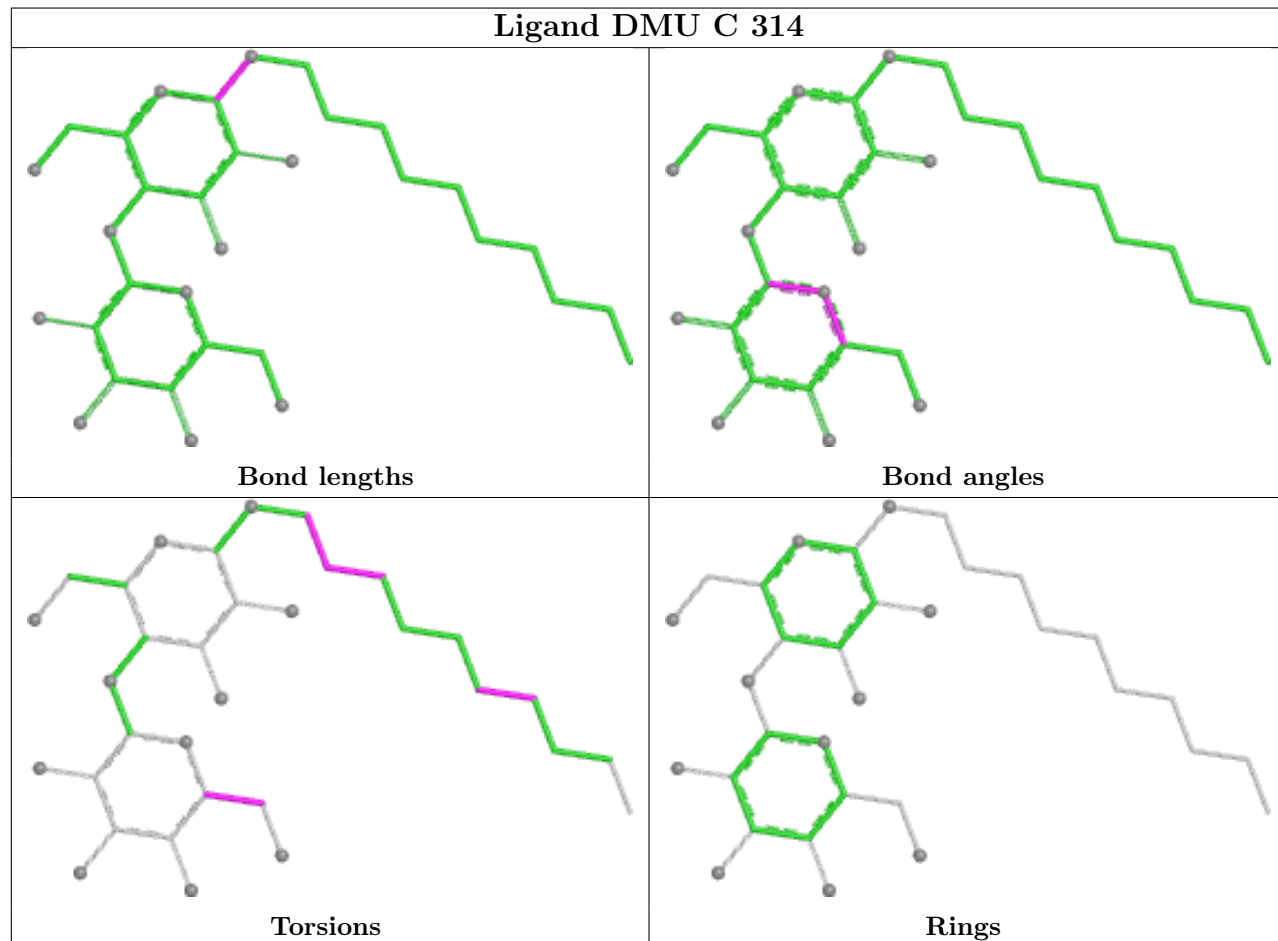
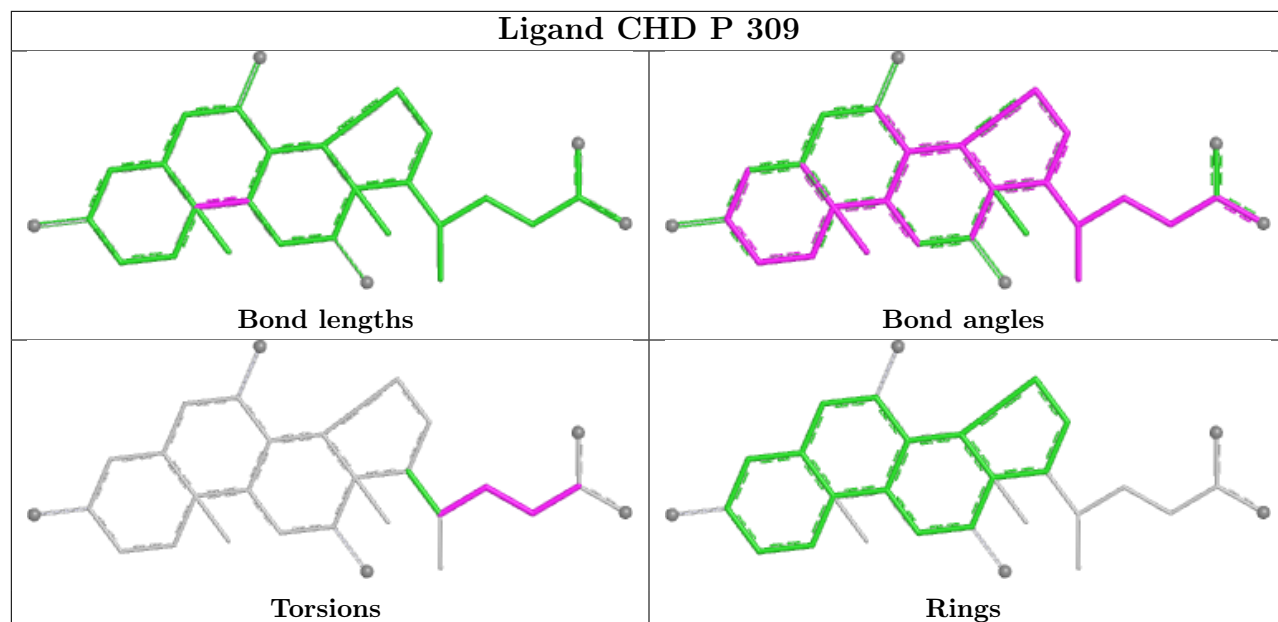


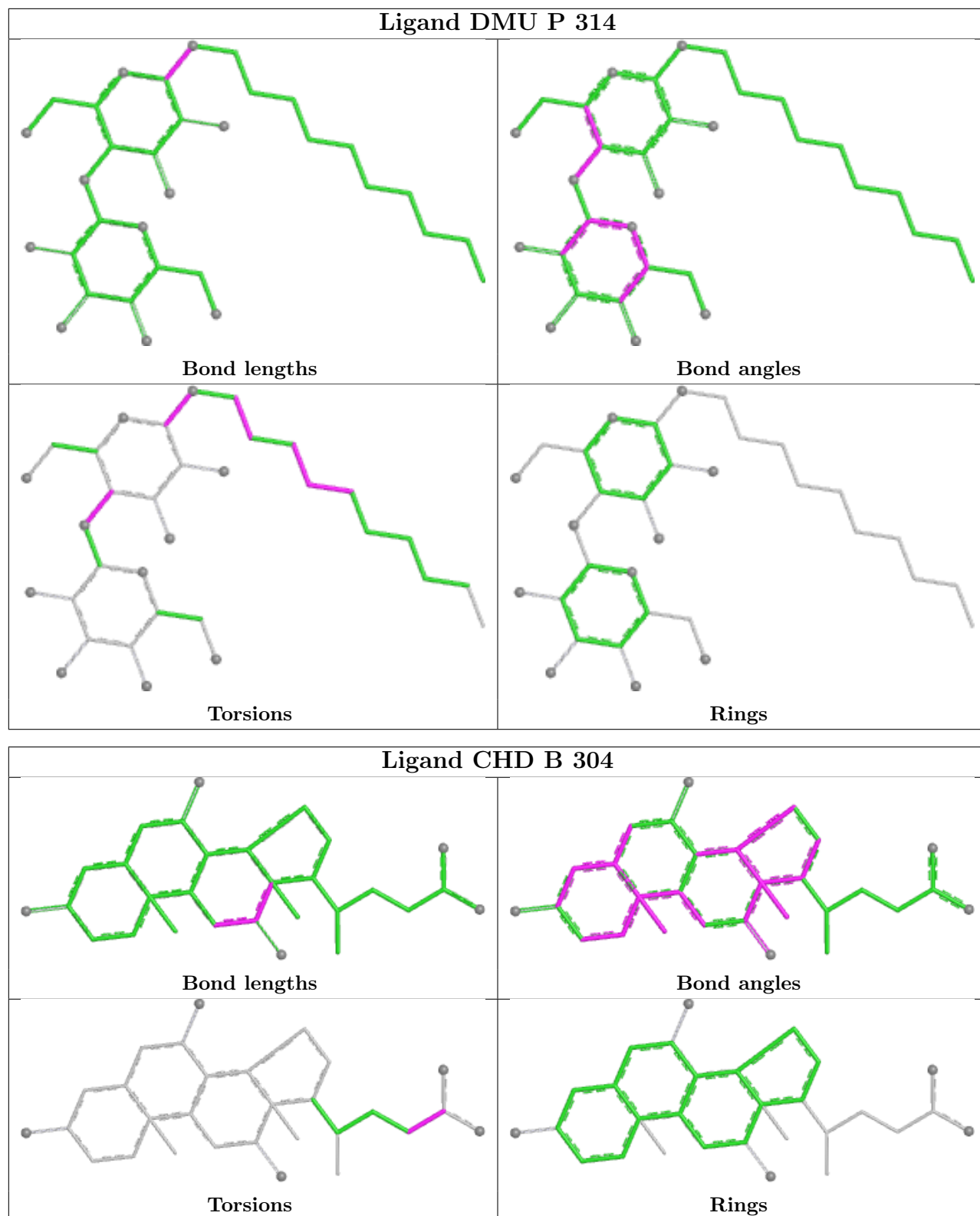


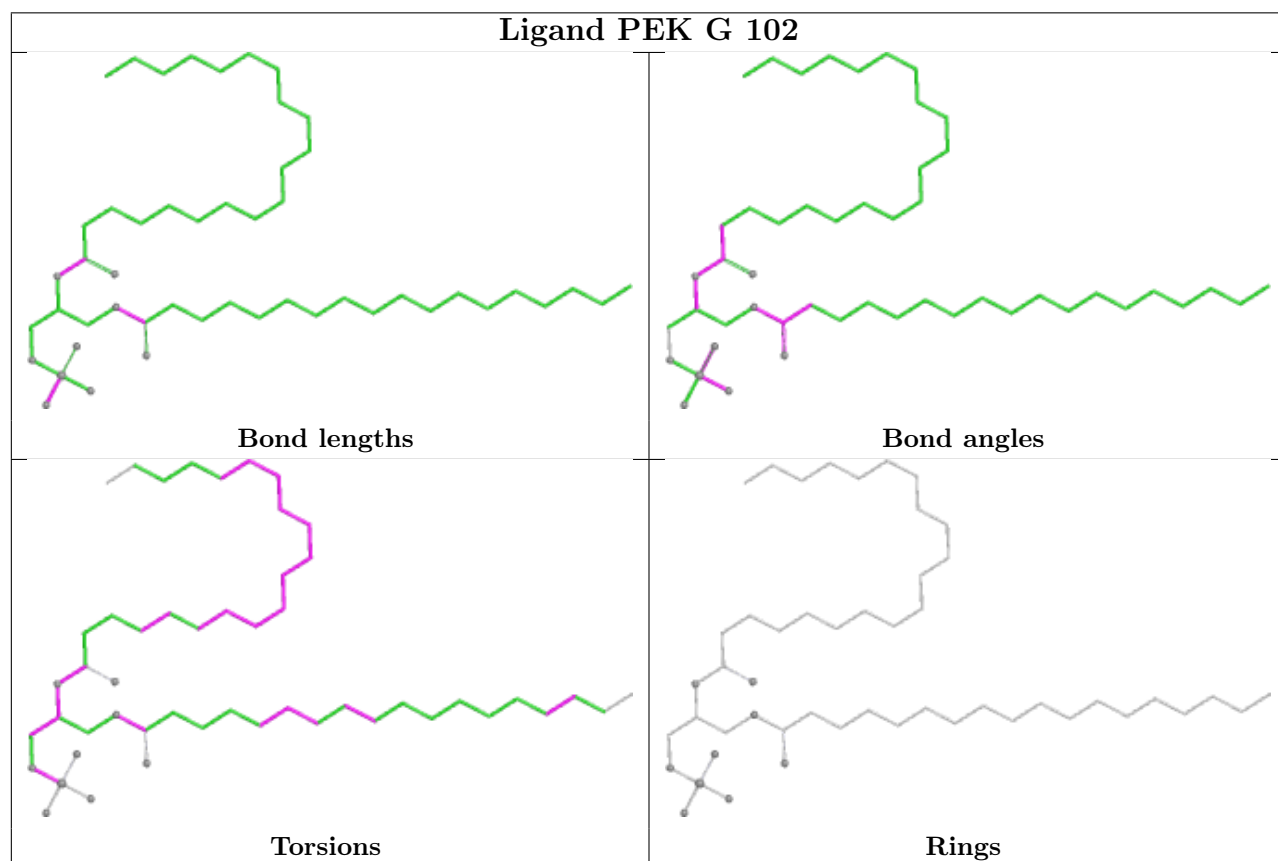
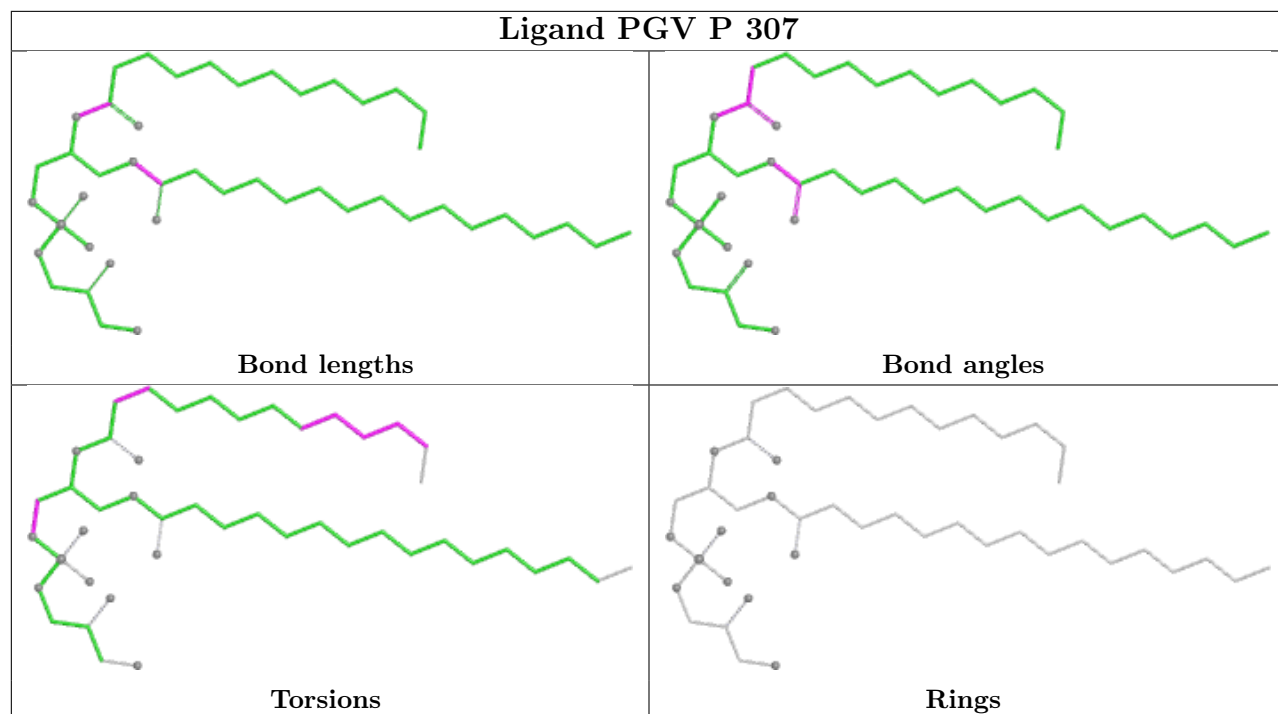


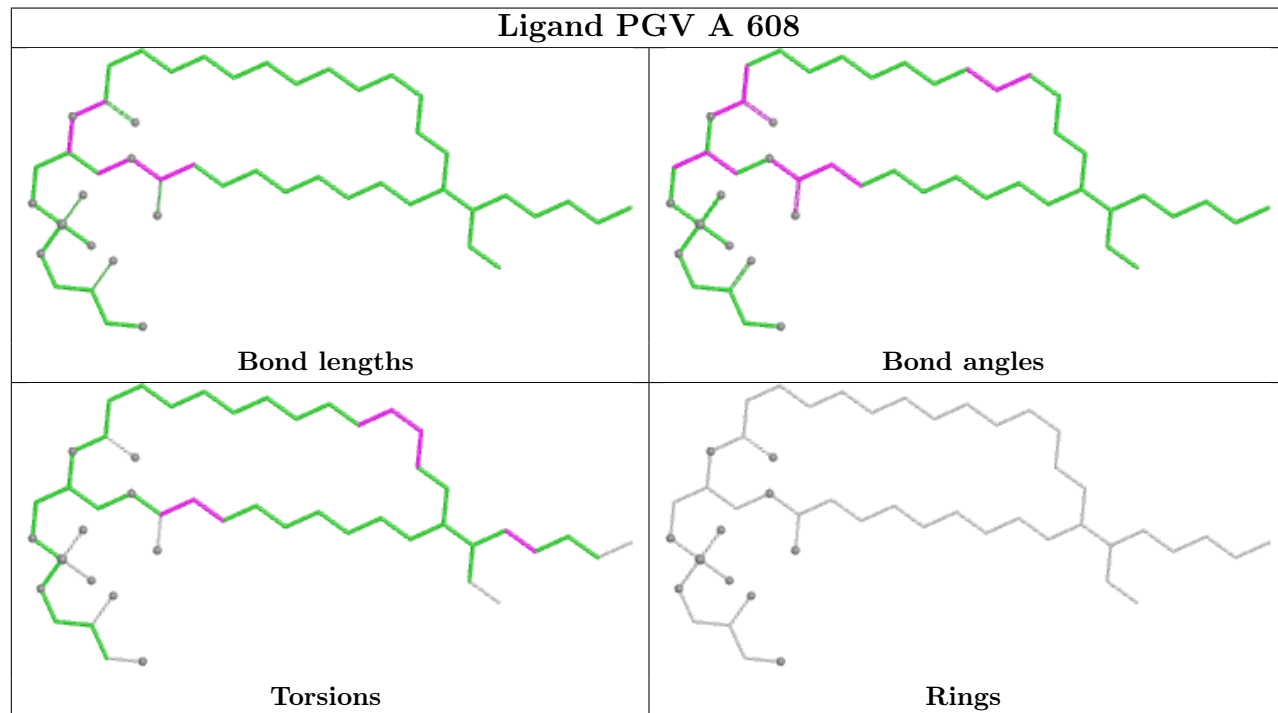
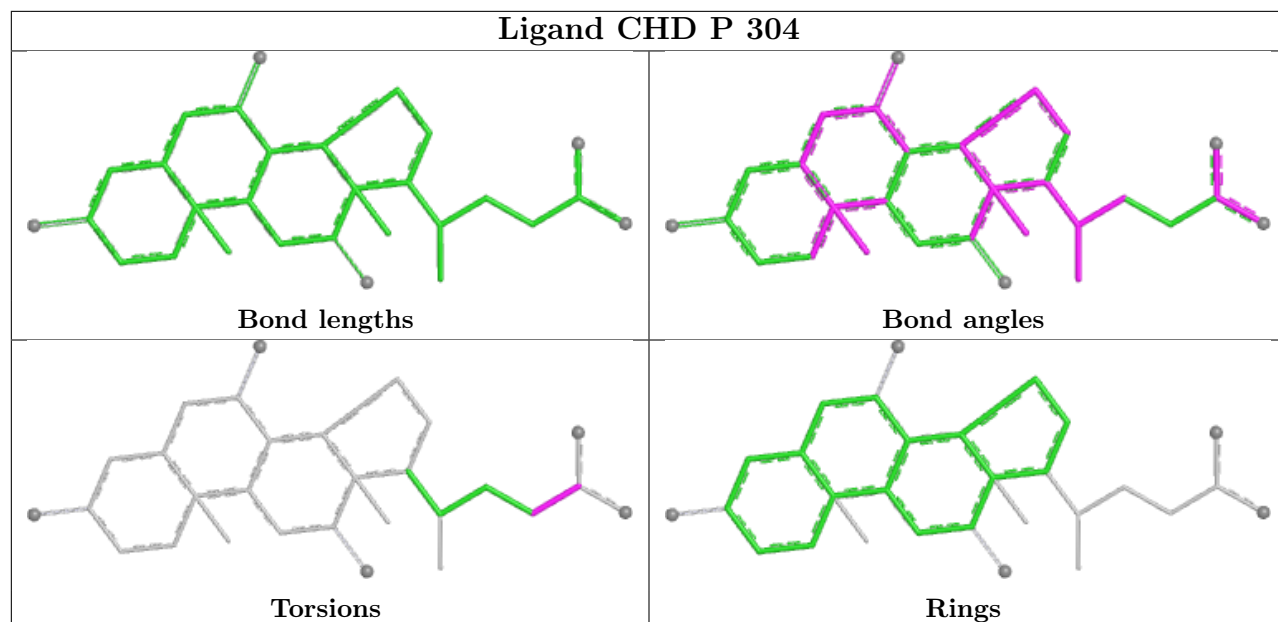


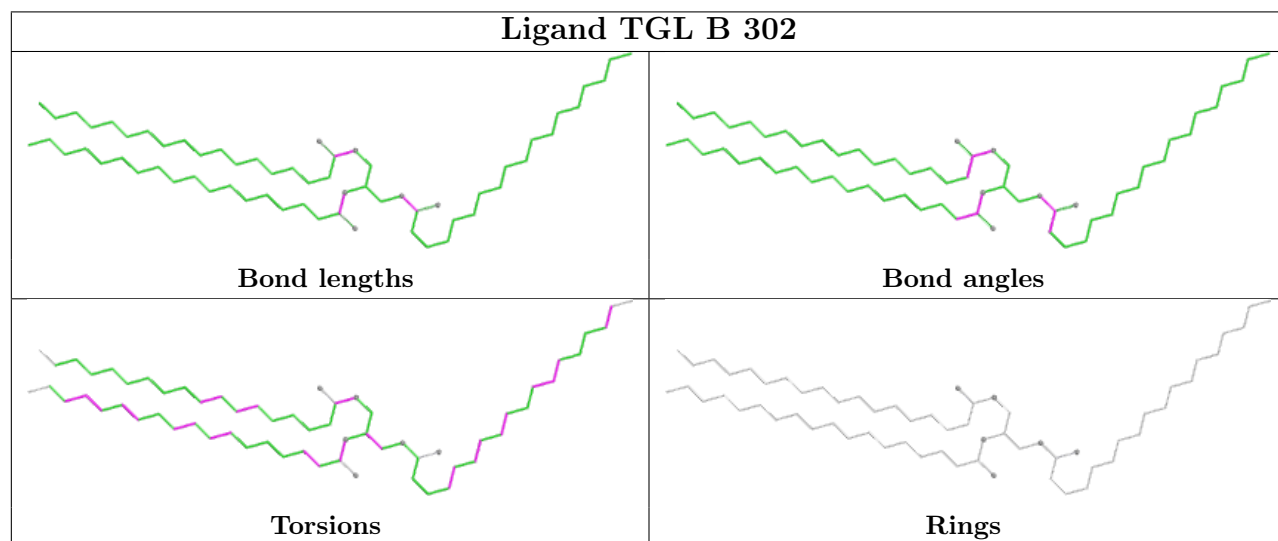
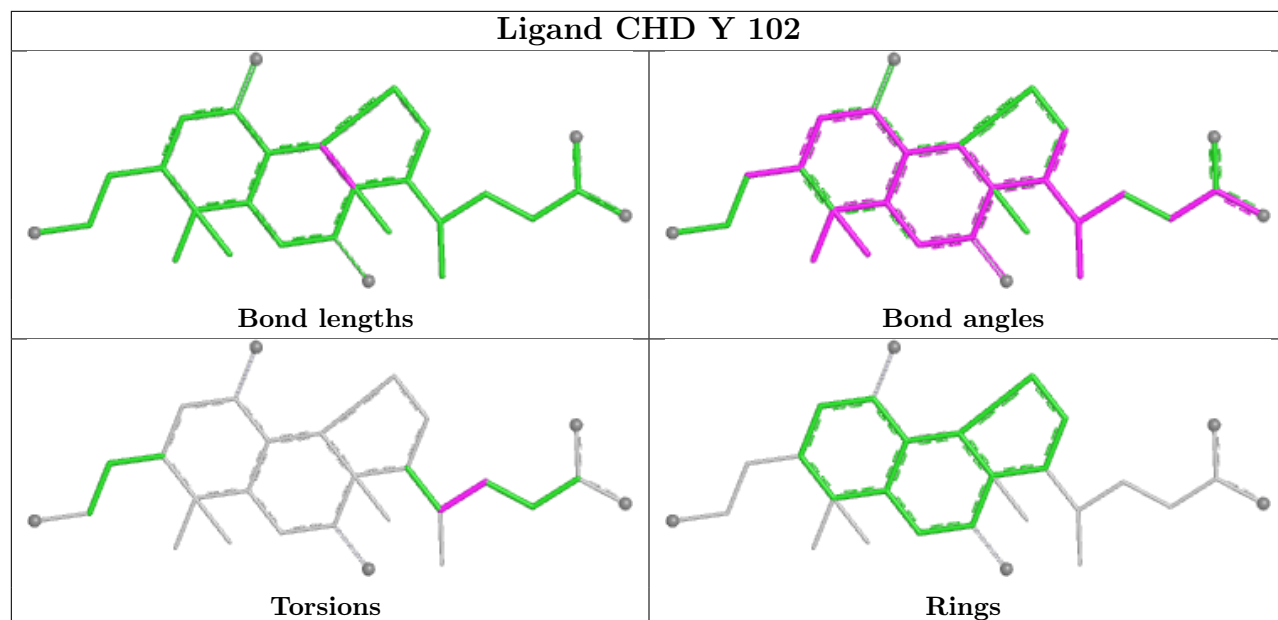


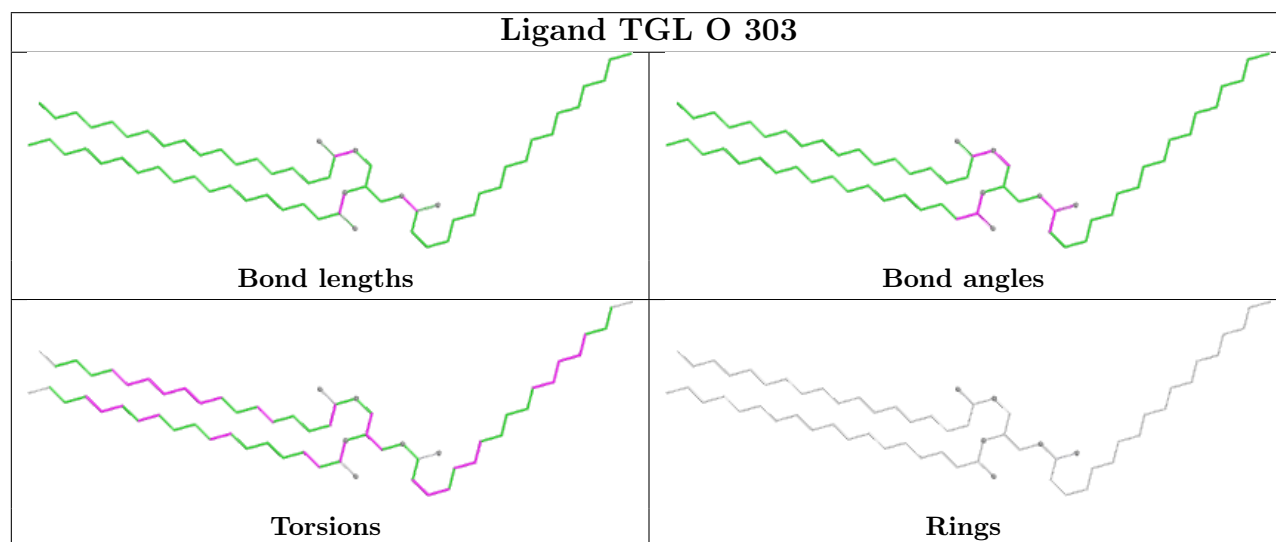
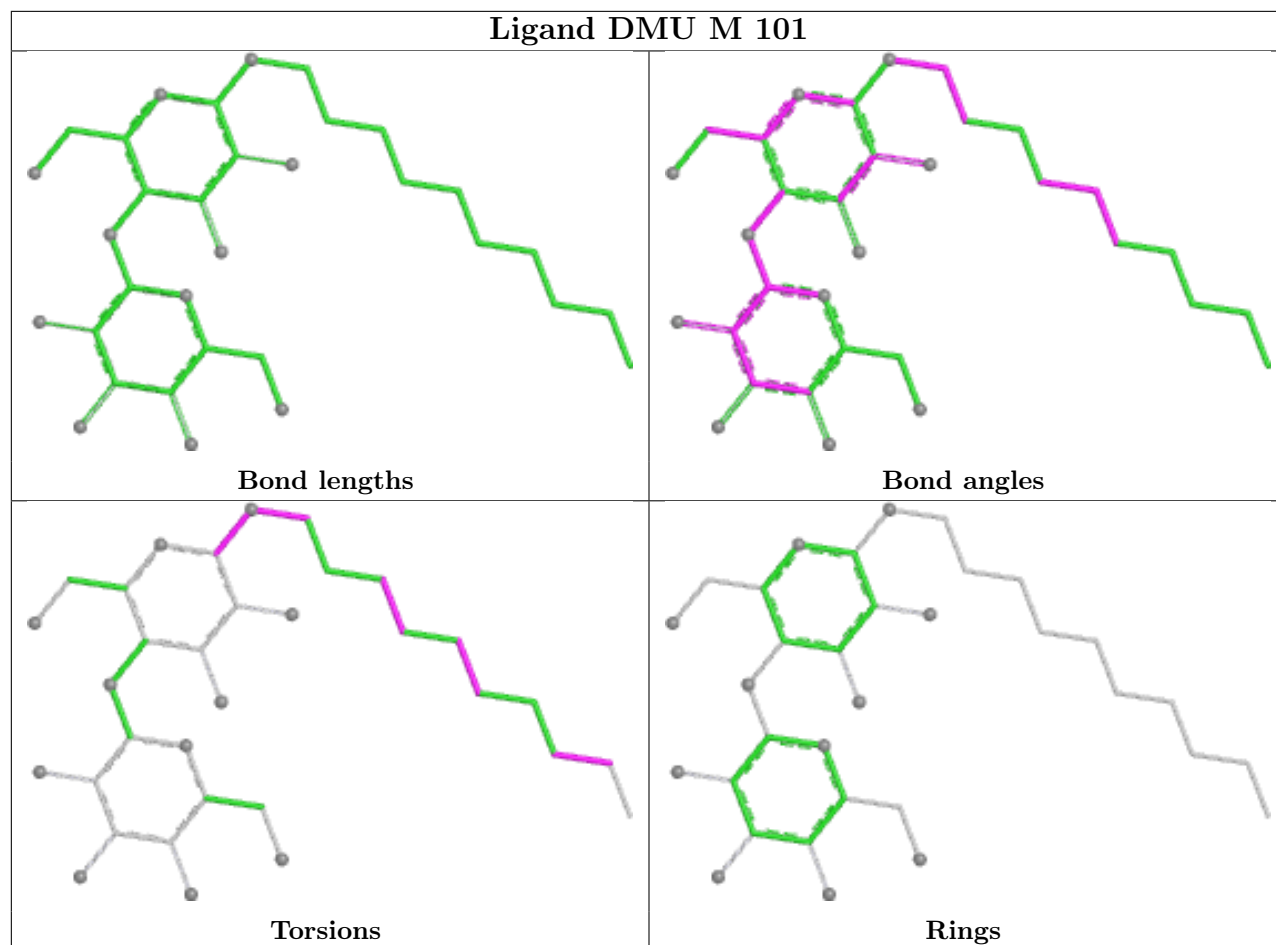


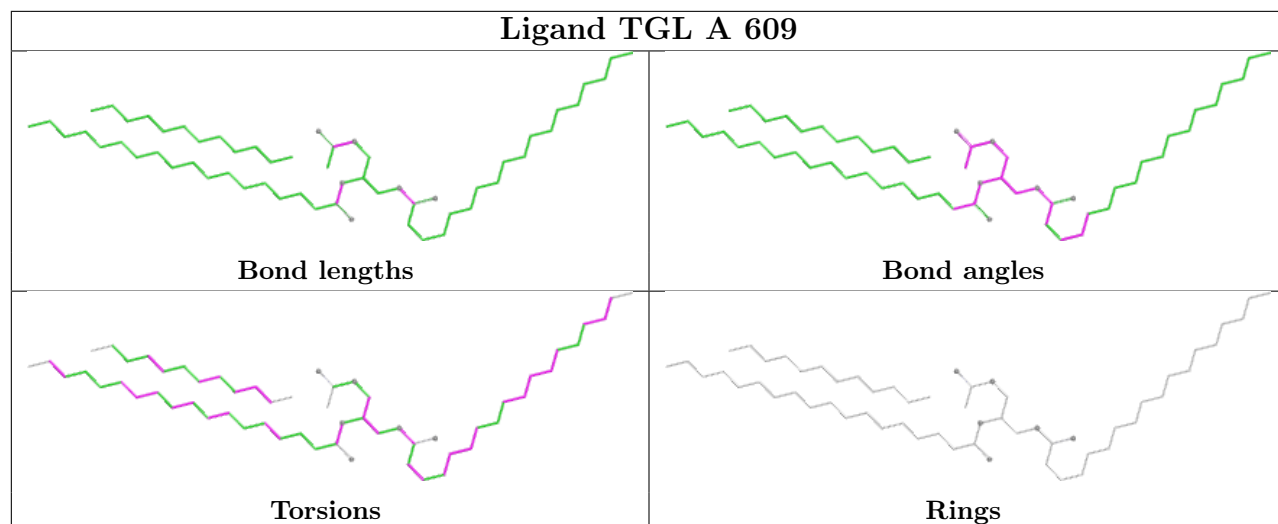


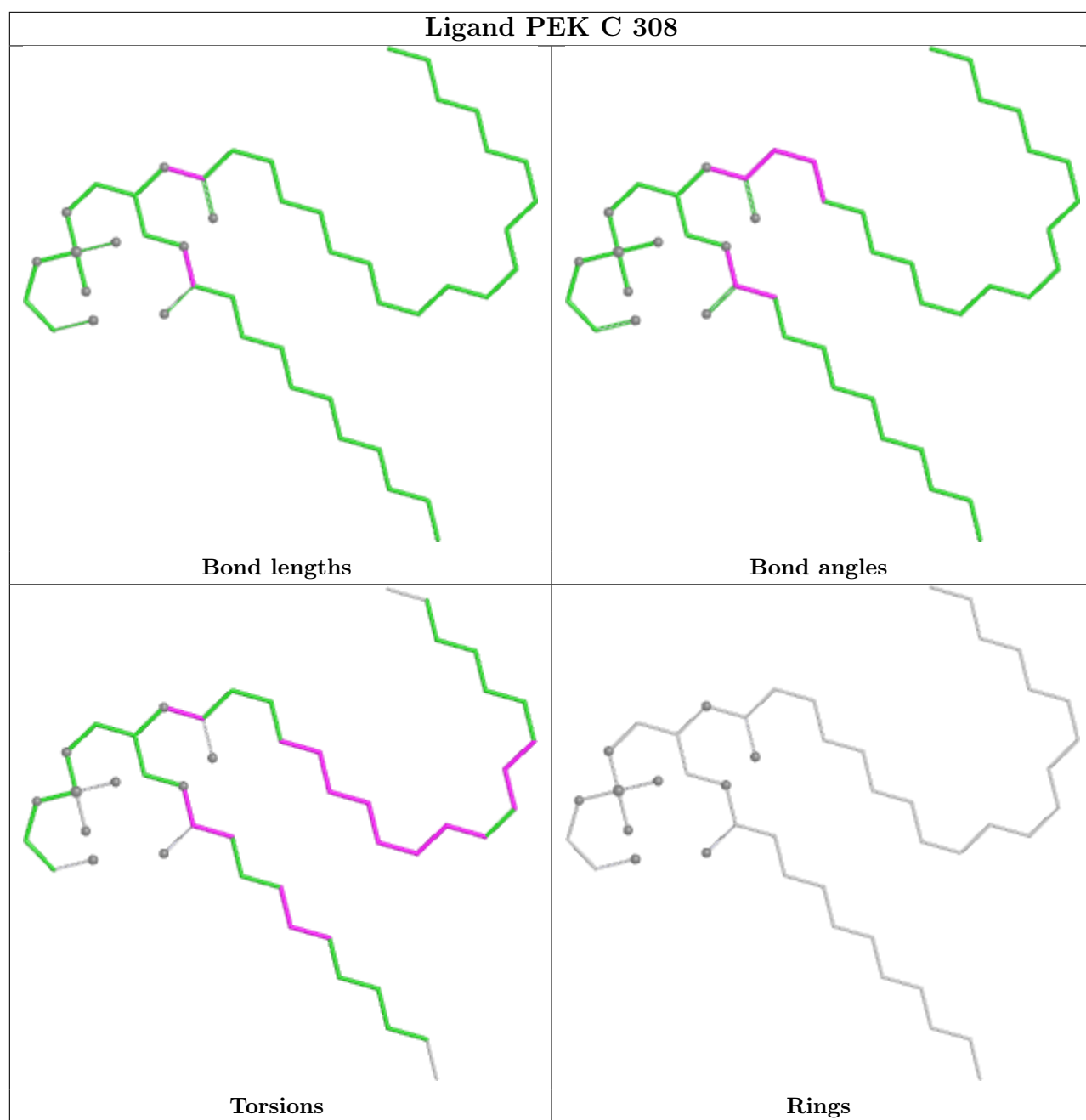


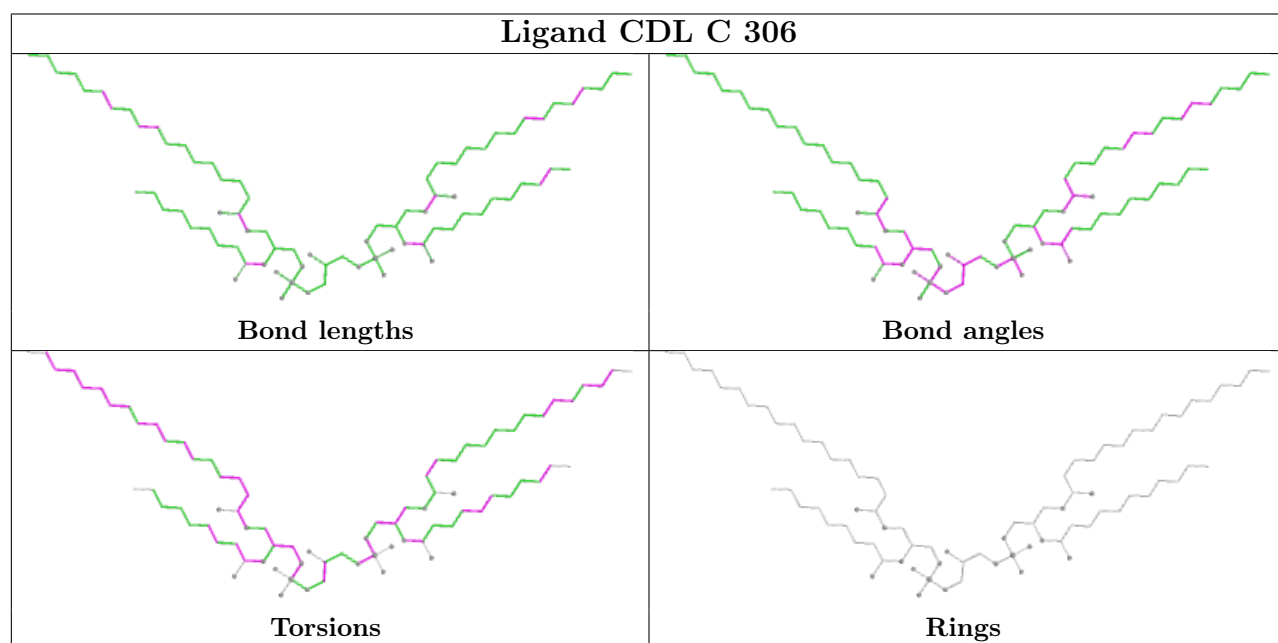
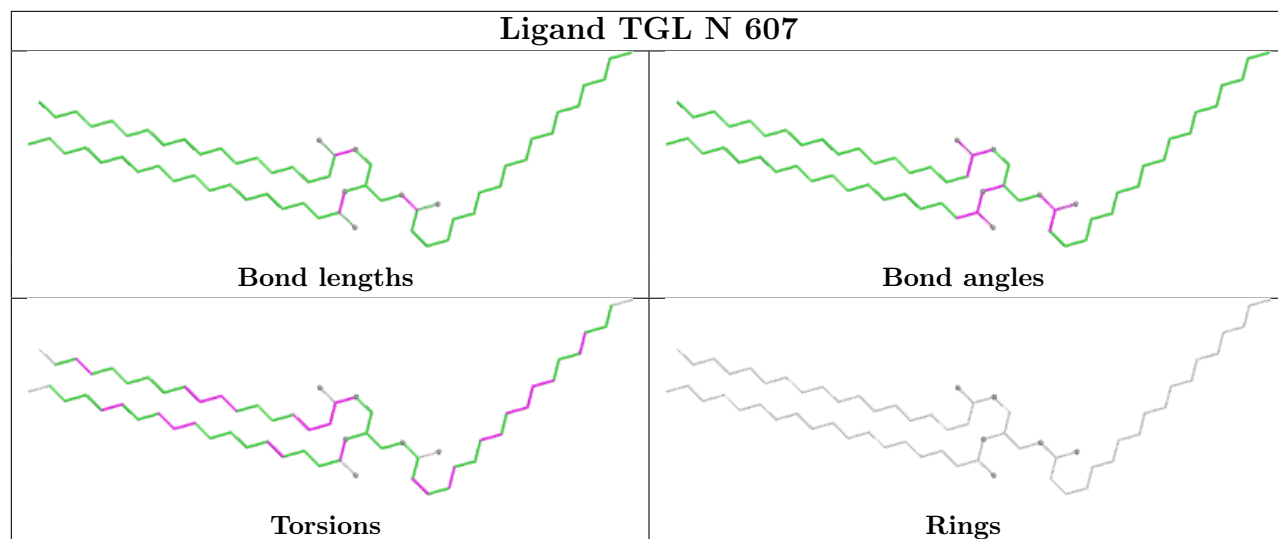


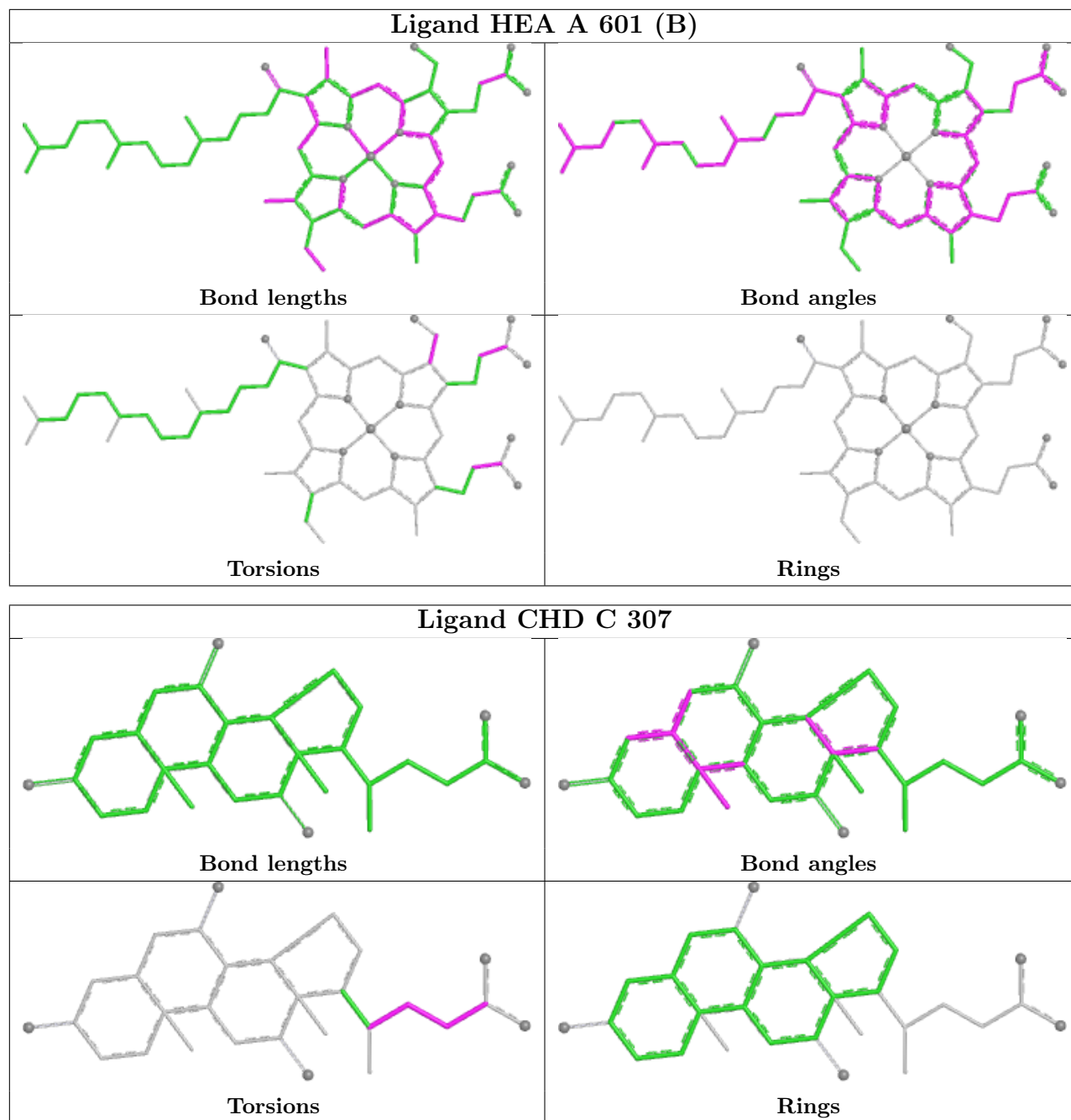


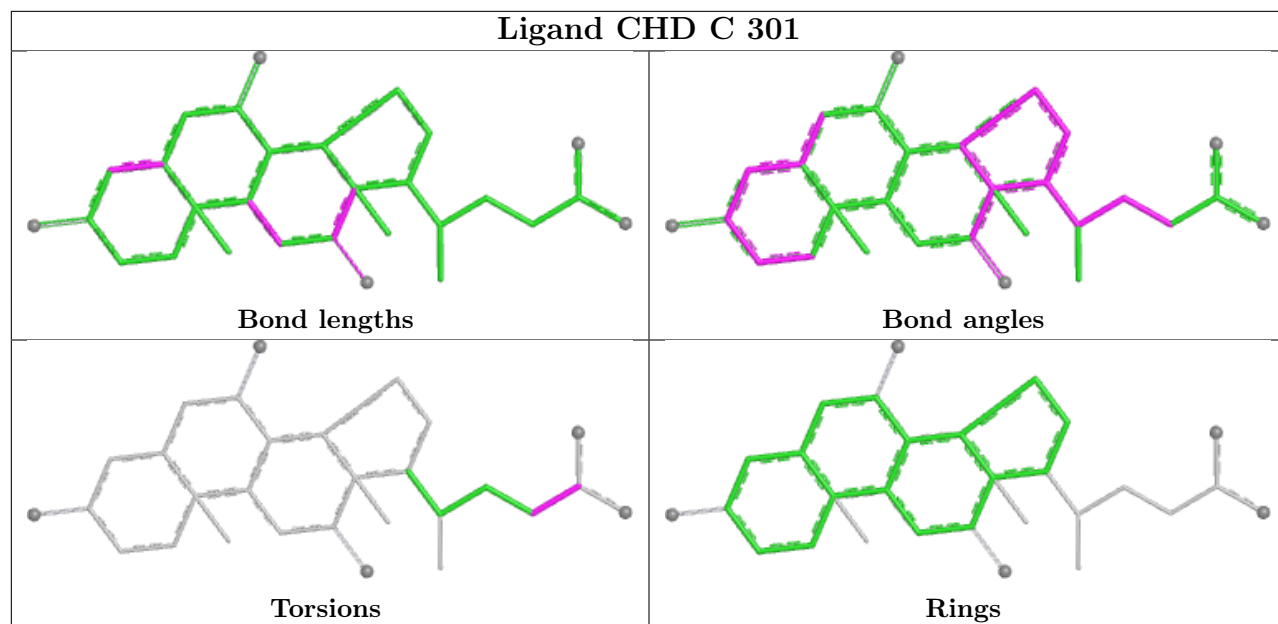












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.60	2 (0%) 88 89	12, 28, 38, 87	8 (1%)
1	N	513/514 (99%)	-0.37	6 (1%) 76 77	16, 35, 49, 99	10 (1%)
2	B	226/227 (99%)	-0.09	13 (5%) 29 27	24, 35, 74, 120	1 (0%)
2	O	226/227 (99%)	0.35	16 (7%) 22 20	30, 45, 96, 173	2 (0%)
3	C	259/261 (99%)	-0.33	3 (1%) 76 77	25, 33, 54, 113	0
3	P	259/261 (99%)	-0.28	4 (1%) 72 72	22, 35, 54, 130	2 (0%)
4	D	144/147 (97%)	0.15	5 (3%) 47 47	20, 41, 74, 120	1 (0%)
4	Q	141/147 (95%)	1.27	26 (18%) 3 2	41, 61, 112, 228	0
5	E	105/109 (96%)	0.26	4 (3%) 44 44	36, 45, 88, 160	0
5	R	105/109 (96%)	0.64	6 (5%) 29 28	40, 56, 98, 174	0
6	F	98/98 (100%)	0.36	11 (11%) 10 8	27, 42, 151, 193	0
6	S	95/98 (96%)	0.49	7 (7%) 20 19	32, 44, 97, 198	1 (1%)
7	G	83/85 (97%)	1.01	19 (22%) 2 1	31, 42, 160, 182	0
7	T	83/85 (97%)	0.97	19 (22%) 2 1	28, 45, 139, 207	0
8	H	79/85 (92%)	0.55	9 (11%) 10 8	31, 43, 133, 161	0
8	U	79/85 (92%)	0.70	9 (11%) 10 8	38, 48, 144, 170	0
9	I	72/73 (98%)	0.65	6 (8%) 17 15	35, 52, 92, 157	0
9	V	72/73 (98%)	1.22	18 (25%) 2 1	43, 67, 111, 166	0
10	J	58/59 (98%)	0.36	4 (6%) 23 21	35, 46, 100, 140	0
10	W	58/59 (98%)	0.56	7 (12%) 8 7	38, 50, 113, 173	0
11	K	49/56 (87%)	0.40	4 (8%) 17 15	34, 42, 78, 119	0
11	X	49/56 (87%)	1.18	13 (26%) 1 1	49, 62, 124, 139	0
12	L	46/47 (97%)	0.01	3 (6%) 25 23	27, 34, 66, 116	0
12	Y	46/47 (97%)	0.51	5 (10%) 10 9	38, 45, 100, 138	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.12	2 (4%) 36 35	31, 35, 98, 161	0
13	Z	43/46 (93%)	0.82	7 (16%) 4 3	43, 51, 120, 241	0
All	All	3544/3614 (98%)	0.11	228 (6%) 25 24	12, 39, 96, 241	25 (0%)

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	3	ALA	7.9
7	T	36	TRP	7.8
6	F	96	LEU	7.0
2	O	113	TYR	6.9
8	H	8	ILE	6.9
7	T	3	ALA	6.7
7	G	6	GLY	6.7
7	T	2	SER	6.7
7	G	4	ALA	6.6
6	F	97	ALA	6.5
10	J	1	PHE	6.5
7	G	5	LYS	6.4
5	R	109	VAL	6.3
7	G	36	TRP	6.3
6	S	93	PRO	6.1
9	I	2	THR	6.0
6	S	1	ALA	6.0
6	F	98	HIS	6.0
4	D	4	SER	5.9
6	S	94	HIS	5.8
7	G	2	SER	5.8
7	T	1	ALA	5.8
7	G	9	GLY	5.7
8	H	45	ALA	5.7
7	G	7	ASP	5.7
6	S	95	GLN	5.6
8	U	8	ILE	5.5
13	Z	43	SER	5.5
6	F	1	ALA	5.4
2	O	226	MET	5.2
8	H	46	LYS	5.2
6	S	3	GLY	5.1
6	F	3	GLY	5.1
10	W	48	TYR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	1	ALA	4.9
2	O	227	LEU	4.9
13	M	43	SER	4.9
7	T	40	GLY	4.8
10	W	1	PHE	4.8
9	V	37	PHE	4.6
9	V	3	ALA	4.6
2	B	113	TYR	4.6
13	Z	40	TYR	4.5
3	P	3	HIS	4.4
8	U	47	GLY	4.3
11	K	6	ALA	4.3
7	T	6	GLY	4.3
7	T	8	HIS	4.3
7	G	10	GLY	4.2
7	T	9	GLY	4.2
8	H	48	GLY	4.2
12	L	2	HIS	4.2
7	T	5	LYS	4.2
4	Q	7	LYS	4.2
8	U	45	ALA	4.1
6	F	2	SER	4.1
4	Q	39	ALA	4.1
8	H	44	THR	4.0
9	I	37	PHE	4.0
8	U	46	LYS	4.0
12	Y	47	LYS	4.0
5	E	109	VAL	3.9
1	N	513	LEU	3.8
12	Y	2	HIS	3.8
7	T	39	SER	3.8
11	X	47	ARG	3.8
9	I	3	ALA	3.8
7	T	7	ASP	3.7
1	N	484	THR	3.7
7	T	10	GLY	3.7
11	X	23	THR	3.7
4	Q	35	ALA	3.7
6	S	2	SER	3.7
4	Q	72	ASN	3.6
5	E	5	HIS	3.6
4	Q	51	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	140	TYR	3.5
3	C	3	HIS	3.5
4	Q	8	SER	3.5
4	Q	46	ALA	3.5
7	G	8	HIS	3.5
12	Y	20	ARG	3.5
9	V	36	LYS	3.5
8	H	9	LYS	3.4
2	B	57	ASP	3.4
8	H	10	ASN	3.4
9	V	25	PHE	3.4
11	K	54	ARG	3.4
2	B	55	THR	3.4
11	X	52	GLU	3.3
10	J	56	PRO	3.3
6	S	92	VAL	3.3
10	J	48	TYR	3.2
2	O	224	ALA	3.2
7	T	4	ALA	3.2
4	Q	33	LEU	3.2
2	O	225	SER	3.2
2	O	65	TRP	3.2
5	R	108	LYS	3.2
8	U	9	LYS	3.2
7	G	37	LEU	3.1
11	K	47	ARG	3.1
9	V	70	GLN	3.1
1	A	297	MET	3.1
9	V	26	MET	3.1
9	V	67	GLY	3.0
2	O	126	SER	3.0
10	J	58	LYS	3.0
2	O	90	ILE	3.0
2	O	116	LEU	3.0
4	Q	78	TRP	3.0
9	V	2	THR	3.0
4	Q	19	ARG	3.0
12	L	20	ARG	3.0
11	X	20	SER	2.9
5	R	5	HIS	2.9
7	G	41	HIS	2.9
7	G	42	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	T	12	GLY	2.9
9	I	22	VAL	2.8
12	L	47	LYS	2.8
13	Z	42	LYS	2.8
11	X	6	ALA	2.8
11	X	9	PHE	2.8
9	I	29	LEU	2.8
9	V	15	ARG	2.8
13	M	40	TYR	2.8
7	T	38	HIS	2.8
13	Z	32	TRP	2.8
13	Z	41	LYS	2.8
3	C	38	ASN	2.7
2	B	60	GLU	2.7
2	O	222	TRP	2.7
10	W	58	LYS	2.7
2	B	87	MET	2.7
4	Q	10	ASP	2.7
4	Q	52	SER	2.7
5	R	90	ARG	2.7
3	P	38	ASN	2.7
7	G	38	HIS	2.7
2	O	223	SER	2.7
4	Q	135	SER	2.7
2	O	57	ASP	2.6
4	D	11	TYR	2.6
7	G	70	PHE	2.6
4	D	9	GLU	2.6
3	P	37	PHE	2.6
4	Q	87	PHE	2.6
6	F	94	HIS	2.6
11	X	16	ALA	2.6
2	B	65	TRP	2.6
9	V	72	ALA	2.6
6	F	54	ASN	2.6
5	E	39	TYR	2.5
11	X	54	ARG	2.5
6	F	95	GLN	2.5
7	T	84	LYS	2.5
8	H	7	LYS	2.5
11	X	51	LYS	2.5
13	Z	39	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	183	THR	2.5
6	F	65	ASP	2.5
5	R	97	GLY	2.5
2	B	56	MET	2.5
2	B	58	ALA	2.5
4	D	31	LYS	2.4
4	Q	38	LYS	2.4
8	U	7	LYS	2.4
2	B	115	ASP	2.4
9	V	69	PHE	2.4
11	K	7	PRO	2.4
7	G	12	GLY	2.4
1	N	514	LYS	2.4
4	Q	147	LYS	2.4
13	Z	13	LYS	2.4
11	X	13	TYR	2.3
4	Q	58	GLU	2.3
12	Y	4	GLU	2.3
9	V	29	LEU	2.3
8	U	10	ASN	2.3
11	X	48	VAL	2.3
10	W	52	TRP	2.3
9	I	26	MET	2.3
11	X	7	PRO	2.3
2	B	92	ASN	2.3
2	O	91	ASN	2.3
9	V	44	LYS	2.3
4	Q	134	PHE	2.2
7	T	35	SER	2.2
4	Q	17	VAL	2.2
7	T	37	LEU	2.2
3	C	37	PHE	2.2
2	O	217	LYS	2.2
7	G	84	LYS	2.2
8	U	52	VAL	2.2
12	Y	16	GLU	2.2
4	D	74	SER	2.2
1	N	53	ILE	2.2
3	P	44	MET	2.2
9	V	65	LYS	2.2
8	U	44	THR	2.2
2	O	92	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	90	ILE	2.1
4	Q	49	SER	2.1
1	A	136	LEU	2.1
9	V	73	LYS	2.1
10	W	56	PRO	2.1
4	Q	128	VAL	2.1
9	V	30	GLY	2.1
2	B	217	LYS	2.1
10	W	57	HIS	2.1
8	H	42	ALA	2.1
1	N	298[A]	ASP	2.1
4	Q	73	ARG	2.1
7	T	42	ARG	2.1
5	R	91	PRO	2.1
10	W	55	PHE	2.0
4	Q	47	SER	2.0
11	X	31	TYR	2.0
2	B	91	ASN	2.0
7	G	45	PRO	2.0
5	E	79	LYS	2.0
6	F	43	LYS	2.0
9	V	19	PHE	2.0
4	Q	75	THR	2.0
1	N	512	ASN	2.0
4	Q	11	TYR	2.0
9	V	64	ARG	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	-0.04	0.20	183,230,258,263	0
9	SAC	I	1	9/10	0.64	0.18	113,138,176,201	0
7	TPO	T	11	11/12	0.70	0.28	113,188,264,274	0
7	TPO	G	11	11/12	0.70	0.28	133,196,252,264	0
1	FME	N	1	10/11	0.92	0.12	41,59,101,103	0
1	FME	A	1	10/11	0.93	0.11	41,54,85,120	0
2	FME	O	1	10/11	0.97	0.09	34,43,53,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FME	B	1	10/11	0.98	0.08	31,35,41,111	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CHD	Y	102	28/29	0.60	0.28	69,133,187,220	0
24	CHD	J	101	29/29	0.68	0.21	73,152,246,260	0
21	EDO	D	205	4/4	0.71	0.27	52,77,109,114	0
24	CHD	C	315	29/29	0.71	0.28	47,113,216,236	0
24	CHD	P	315	29/29	0.74	0.23	54,105,213,227	0
27	DMU	Z	103	33/33	0.74	0.17	57,104,162,167	0
27	DMU	P	314	33/33	0.75	0.16	58,119,191,241	0
21	EDO	O	307	4/4	0.76	0.20	48,65,75,87	0
27	DMU	C	313	33/33	0.77	0.14	54,104,173,187	0
21	EDO	A	611	4/4	0.78	0.27	47,48,75,86	0
21	EDO	S	103	4/4	0.78	0.32	46,50,91,138	0
25	PEK	P	301	40/53	0.78	0.21	49,80,243,289	0
19	PGV	P	302	47/51	0.79	0.24	43,83,176,216	0
25	PEK	C	308	46/53	0.79	0.24	49,88,237,256	0
27	DMU	T	101	33/33	0.80	0.18	57,117,233,237	0
27	DMU	L	103	33/33	0.81	0.18	49,89,213,237	0
21	EDO	V	102	4/4	0.81	0.18	71,87,100,102	0
20	TGL	A	609	59/63	0.81	0.24	37,62,180,255	0
27	DMU	G	101	33/33	0.81	0.17	59,100,205,249	0
20	TGL	B	302	63/63	0.82	0.20	41,71,128,147	0
21	EDO	F	104	4/4	0.82	0.32	54,54,65,140	0
19	PGV	Z	101	47/51	0.82	0.20	40,91,183,222	0
21	EDO	R	202	4/4	0.82	0.21	68,76,116,136	0
25	PEK	P	306	53/53	0.82	0.22	40,84,194,289	0
26	CDL	G	103	88/100	0.82	0.26	54,100,223,283	0
23	PSC	O	304	46/52	0.83	0.24	40,92,231,329	0
25	PEK	G	102	50/53	0.83	0.22	45,87,241,290	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CHD	P	309	29/29	0.83	0.17	67,120,177,198	0
27	DMU	P	313	33/33	0.83	0.19	49,111,196,214	0
24	CHD	C	307	29/29	0.83	0.18	59,124,188,226	0
23	PSC	B	303	50/52	0.83	0.21	44,106,211,318	0
26	CDL	T	102	93/100	0.83	0.25	46,97,196,240	0
21	EDO	A	619	4/4	0.84	0.26	61,62,69,166	0
21	EDO	C	311	4/4	0.84	0.15	50,57,70,84	0
19	PGV	C	305	49/51	0.84	0.24	48,81,199,279	0
21	EDO	A	616	4/4	0.84	0.27	52,53,57,101	0
27	DMU	L	102	33/33	0.84	0.16	52,105,200,217	0
20	TGL	O	303	63/63	0.85	0.20	49,78,150,203	0
21	EDO	I	101	4/4	0.85	0.17	57,65,72,90	0
21	EDO	L	101	4/4	0.85	0.18	49,52,61,84	0
21	EDO	N	614	4/4	0.85	0.14	63,65,69,78	0
20	TGL	N	607	63/63	0.85	0.21	52,77,148,175	0
21	EDO	A	613	4/4	0.86	0.20	50,61,72,78	0
19	PGV	A	607	51/51	0.86	0.21	31,78,182,264	0
26	CDL	P	308	91/100	0.86	0.22	41,88,197,256	0
20	TGL	D	201	55/63	0.87	0.21	37,71,132,200	0
21	EDO	H	101	4/4	0.87	0.22	47,78,84,105	0
21	EDO	S	106	4/4	0.87	0.17	53,60,63,90	0
21	EDO	U	101	4/4	0.87	0.25	51,62,106,158	0
21	EDO	O	305	4/4	0.88	0.15	52,70,74,80	0
21	EDO	D	202	4/4	0.88	0.21	49,59,98,118	0
21	EDO	H	102	4/4	0.88	0.19	29,64,86,98	0
21	EDO	A	620	4/4	0.88	0.18	47,67,67,76	0
20	TGL	Y	101	59/63	0.88	0.21	45,71,181,274	0
21	EDO	G	104	4/4	0.88	0.20	44,54,67,104	0
21	EDO	S	107	4/4	0.89	0.17	42,54,82,89	0
21	EDO	F	106	4/4	0.89	0.21	42,67,70,120	0
21	EDO	K	101	4/4	0.89	0.19	48,60,62,117	0
26	CDL	C	306	82/100	0.89	0.20	40,90,223,304	0
21	EDO	A	610	4/4	0.89	0.23	40,60,63,93	0
21	EDO	Q	202	4/4	0.90	0.16	49,60,63,68	0
21	EDO	E	201	4/4	0.90	0.14	58,66,74,78	0
27	DMU	C	314	33/33	0.90	0.14	42,84,148,224	0
21	EDO	P	311	4/4	0.90	0.15	55,58,63,74	0
27	DMU	Z	102	33/33	0.90	0.12	46,66,102,181	0
21	EDO	V	101	4/4	0.90	0.16	51,67,83,115	0
21	EDO	T	104	4/4	0.91	0.15	47,54,63,77	0
21	EDO	R	201	4/4	0.91	0.19	60,73,75,85	0
21	EDO	A	621	4/4	0.91	0.20	30,57,83,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	C	312	4/4	0.91	0.19	45,70,88,158	0
21	EDO	P	312	4/4	0.91	0.14	48,56,59,68	0
21	EDO	B	306	4/4	0.91	0.14	44,49,50,81	0
27	DMU	M	101	33/33	0.92	0.10	34,53,80,98	0
21	EDO	A	618	4/4	0.92	0.16	41,42,68,71	0
21	EDO	E	204	4/4	0.92	0.17	56,56,71,75	0
21	EDO	D	204	4/4	0.93	0.14	46,64,73,79	0
21	EDO	A	622	4/4	0.93	0.19	46,64,67,125	0
21	EDO	E	202	4/4	0.94	0.09	46,46,47,55	0
21	EDO	A	615	4/4	0.94	0.10	36,49,50,62	0
21	EDO	A	614	4/4	0.94	0.13	34,35,43,58	0
21	EDO	O	306	4/4	0.94	0.13	47,63,68,72	0
21	EDO	S	105	4/4	0.95	0.11	48,54,66,74	0
21	EDO	Q	201	4/4	0.95	0.10	41,48,52,80	0
21	EDO	N	611	4/4	0.95	0.14	48,54,55,77	0
25	PEK	C	303	53/53	0.95	0.14	32,49,123,160	0
21	EDO	N	613	4/4	0.95	0.11	49,58,66,68	0
21	EDO	D	203	4/4	0.95	0.10	43,50,54,82	0
21	EDO	N	610	4/4	0.95	0.13	38,56,57,101	0
25	PEK	P	305	52/53	0.95	0.14	32,52,124,204	0
21	EDO	F	103	4/4	0.96	0.09	40,42,55,61	0
21	EDO	S	104	4/4	0.96	0.10	47,47,55,58	0
21	EDO	P	310	4/4	0.96	0.12	35,40,51,54	0
19	PGV	N	608	51/51	0.96	0.10	26,41,69,88	0
21	EDO	N	612	4/4	0.96	0.07	27,34,36,39	0
24	CHD	P	304	29/29	0.96	0.07	28,36,42,47	0
21	EDO	F	105	4/4	0.96	0.10	38,45,48,57	0
21	EDO	C	309	4/4	0.96	0.09	37,43,45,46	0
21	EDO	C	310	4/4	0.96	0.10	38,47,50,59	0
21	EDO	N	609	4/4	0.96	0.16	35,38,46,58	0
21	EDO	A	617	4/4	0.97	0.12	44,48,55,110	0
19	PGV	A	608	51/51	0.97	0.10	24,37,69,99	0
19	PGV	P	307	46/51	0.97	0.09	27,40,63,76	0
21	EDO	S	102	4/4	0.97	0.10	34,34,35,37	0
19	PGV	C	304	47/51	0.97	0.10	27,38,66,94	0
17	NA	N	605	1/1	0.97	0.12	41,41,41,41	0
17	NA	C	302	1/1	0.97	0.05	42,42,42,42	0
24	CHD	C	301	29/29	0.97	0.06	27,32,39,40	0
21	EDO	B	305	4/4	0.97	0.08	27,29,29,35	0
21	EDO	G	105	4/4	0.98	0.06	36,39,45,47	0
24	CHD	O	301	29/29	0.98	0.06	24,34,46,48	0
21	EDO	A	612	4/4	0.98	0.07	27,29,30,33	0

Continued on next page...

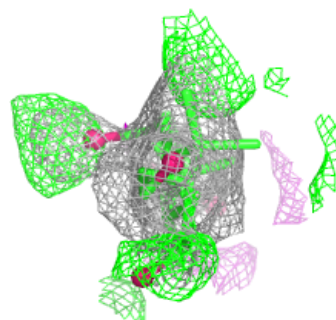
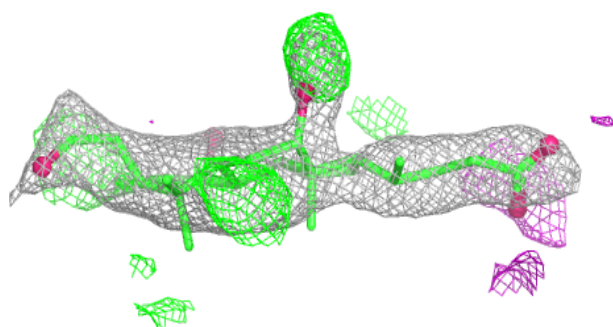
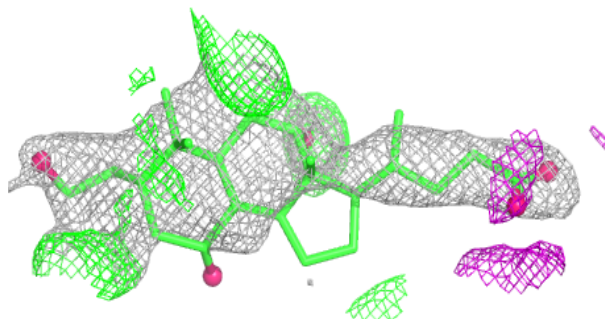
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	CMO	N	606[A]	2/2	0.98	0.12	21,21,21,22	2
18	CMO	N	606[B]	2/2	0.98	0.12	15,15,15,29	2
24	CHD	B	304	29/29	0.98	0.04	25,32,43,49	0
21	EDO	T	103	4/4	0.98	0.07	37,39,43,57	0
21	EDO	E	203	4/4	0.98	0.06	41,46,49,50	0
17	NA	P	303	1/1	0.98	0.08	38,38,38,38	0
21	EDO	F	102	4/4	0.99	0.06	29,29,31,39	0
18	CMO	A	606[B]	2/2	0.99	0.10	10,10,10,16	2
14	HEA	N	601[A]	60/60	0.99	0.07	16,33,62,79	18
14	HEA	N	601[B]	60/60	0.99	0.07	27,33,47,59	18
14	HEA	N	602	60/60	0.99	0.05	21,30,38,42	0
16	MG	A	604	1/1	0.99	0.06	21,21,21,21	0
16	MG	N	604	1/1	0.99	0.08	24,24,24,24	0
17	NA	A	605	1/1	0.99	0.06	32,32,32,32	0
14	HEA	A	601[A]	60/60	0.99	0.05	14,23,53,77	18
14	HEA	A	601[B]	60/60	0.99	0.05	19,23,35,50	18
14	HEA	A	602	60/60	0.99	0.05	17,24,33,40	0
18	CMO	A	606[A]	2/2	0.99	0.10	18,18,18,26	2
28	ZN	S	101	1/1	0.99	0.02	40,40,40,40	0
22	CUA	B	301	2/2	1.00	0.01	25,25,25,26	0
22	CUA	O	302	2/2	1.00	0.04	32,32,32,32	0
15	CU	A	603	1/1	1.00	0.01	25,25,25,25	0
28	ZN	F	101	1/1	1.00	0.03	32,32,32,32	0
15	CU	N	603	1/1	1.00	0.01	28,28,28,28	0

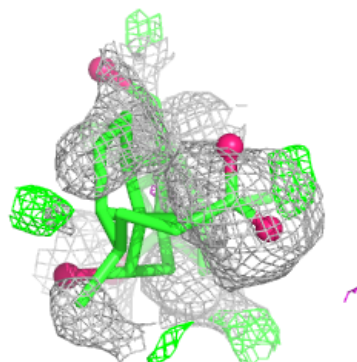
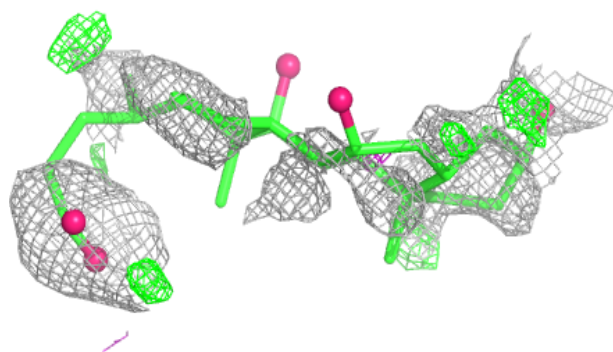
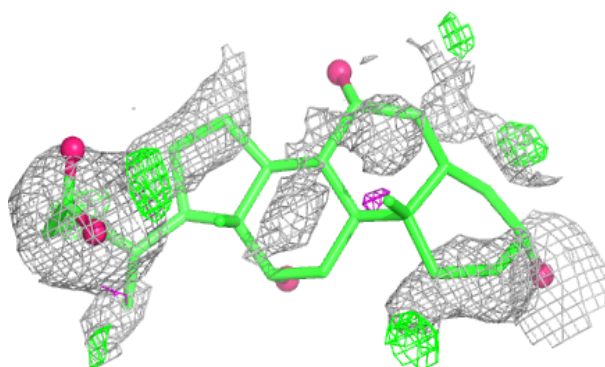
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CHD Y 102:

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

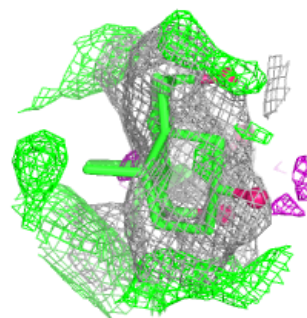
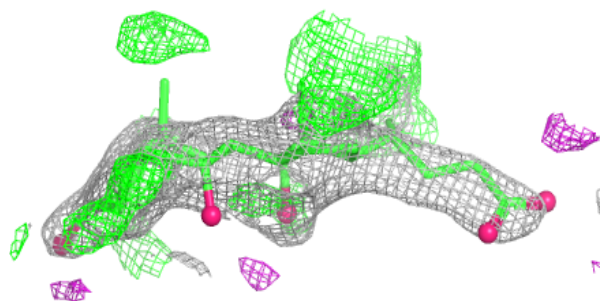
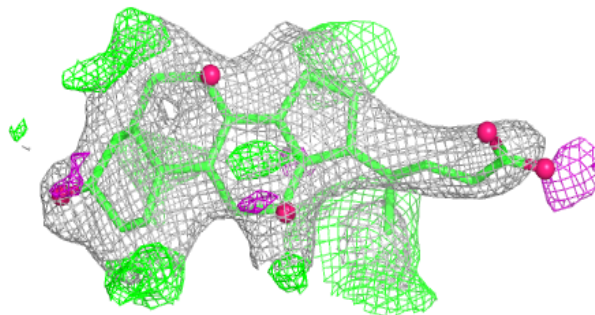
**Electron density around CHD J 101:**

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

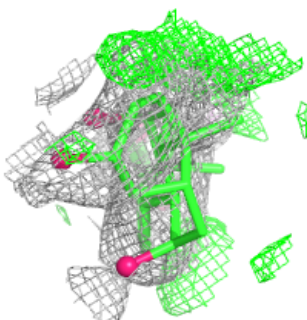
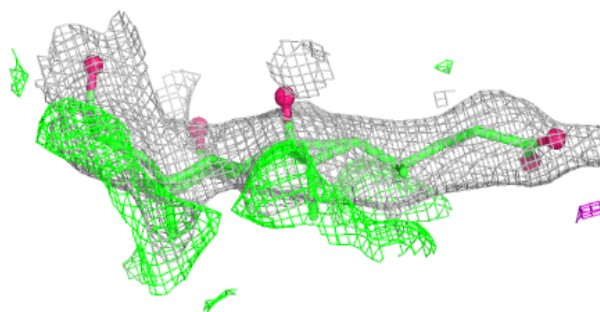
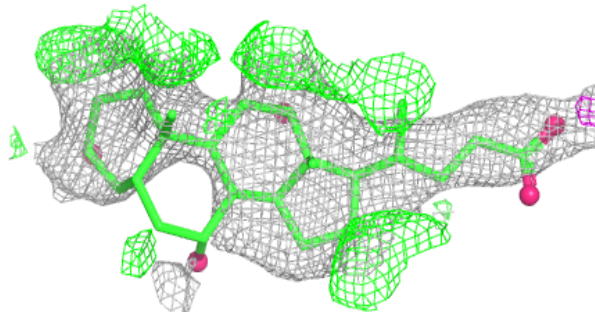


Electron density around CHD C 315:

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

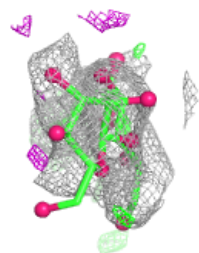
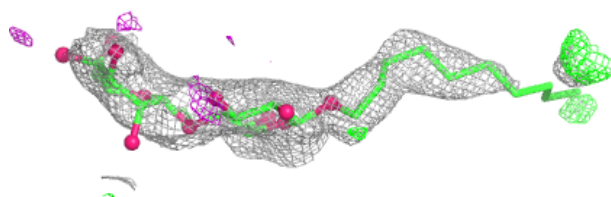
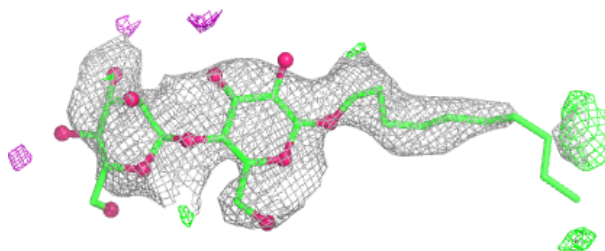
**Electron density around CHD P 315:**

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

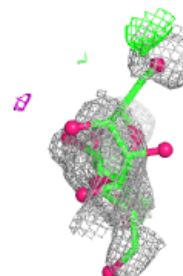
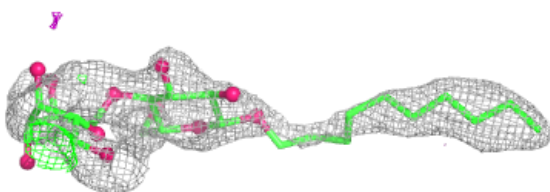
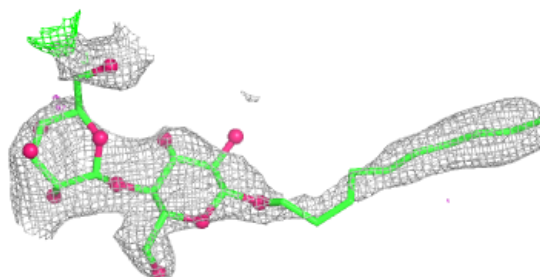


Electron density around DMU Z 103:

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

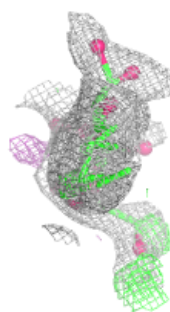
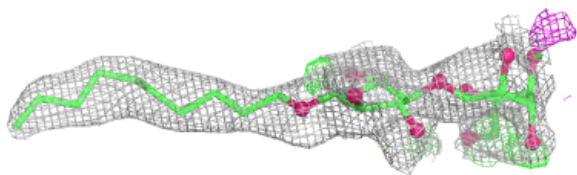
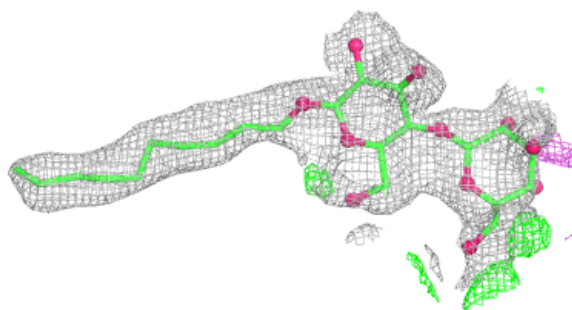
**Electron density around DMU P 314:**

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

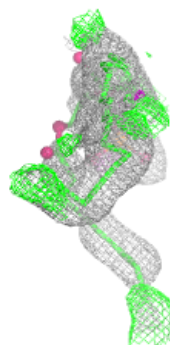
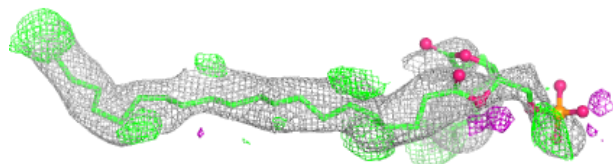
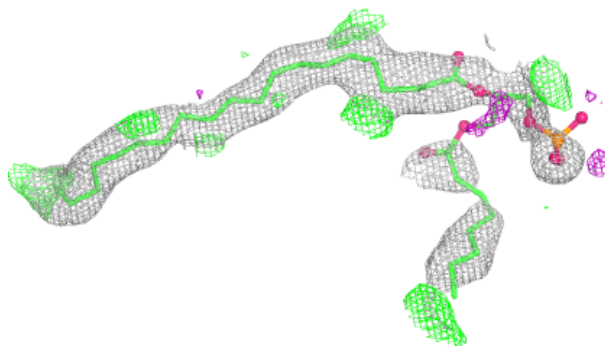


Electron density around DMU C 313:

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

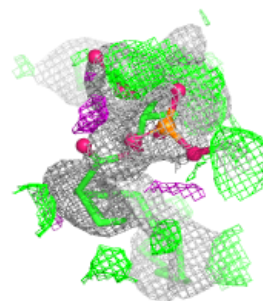
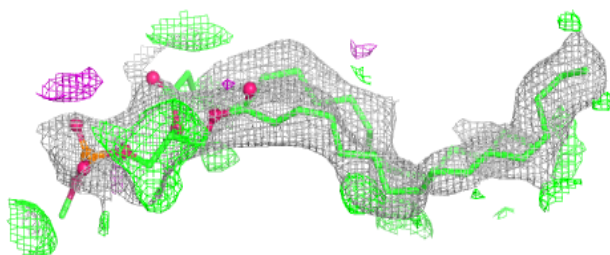
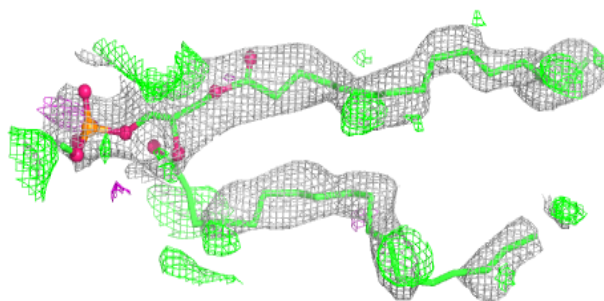
**Electron density around PEK P 301:**

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

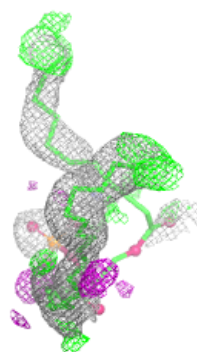
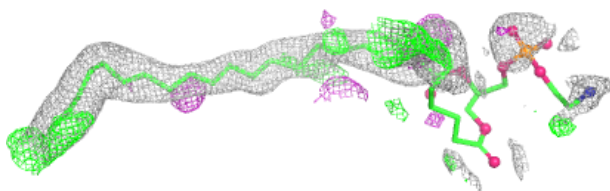
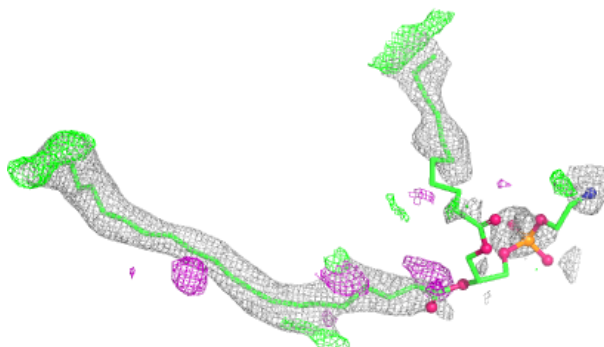


Electron density around PGV P 302:

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

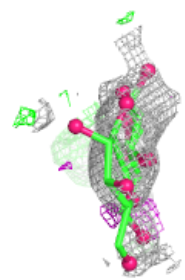
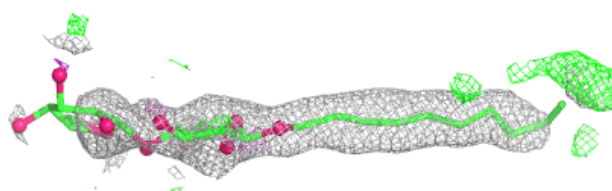
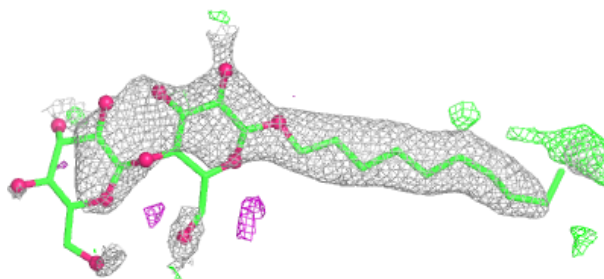
**Electron density around PEK C 308:**

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

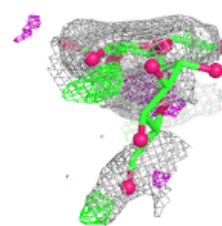
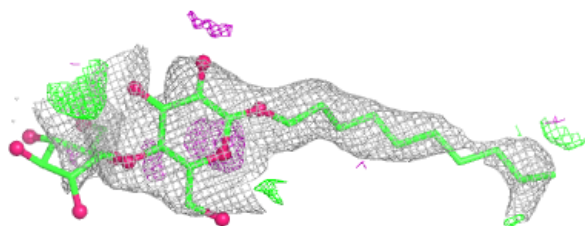
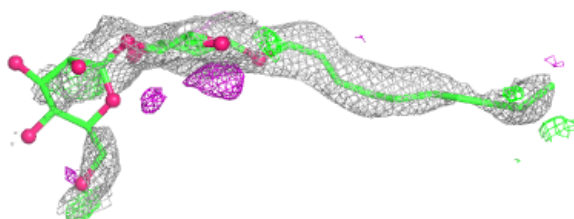


Electron density around DMU T 101:

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

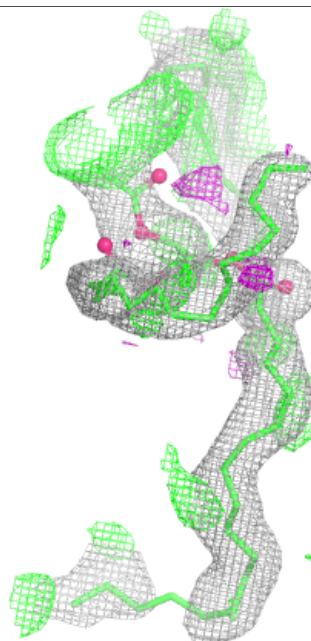
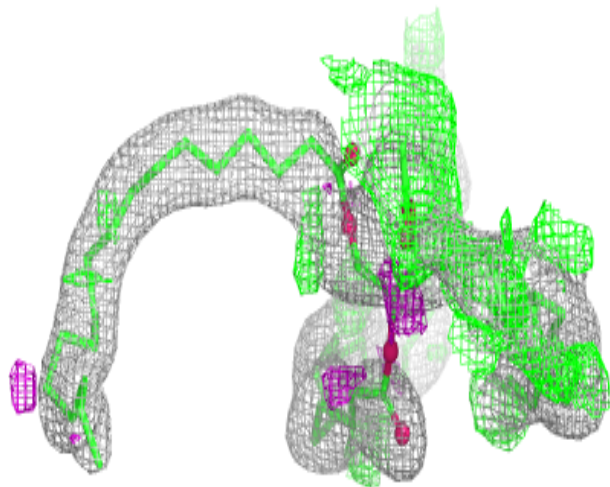
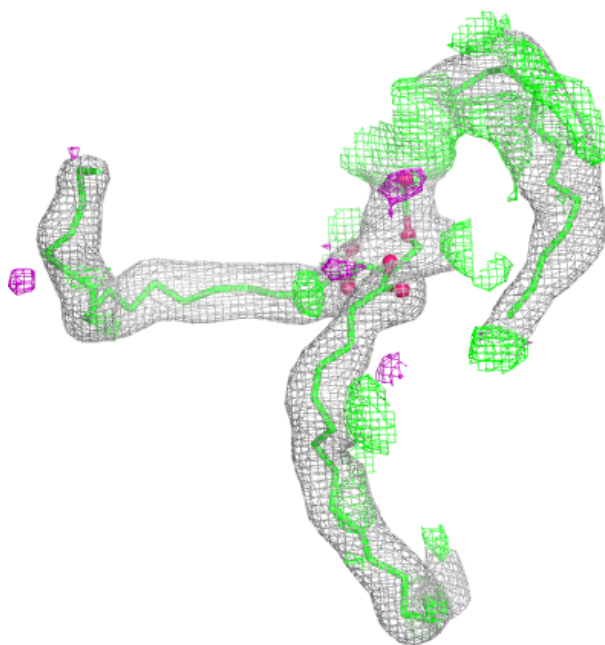
**Electron density around DMU L 103:**

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



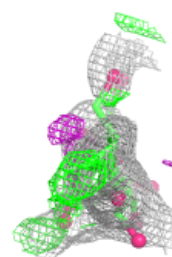
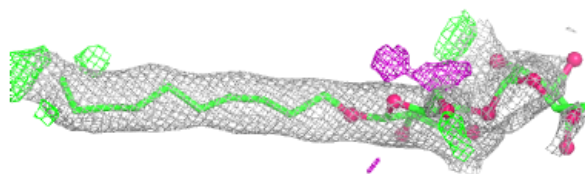
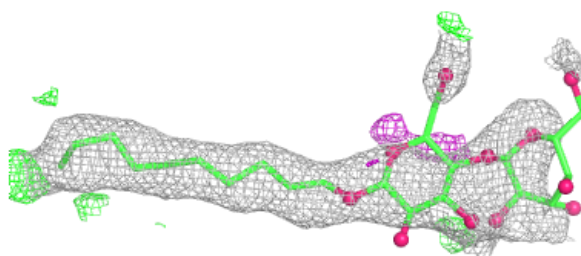
Electron density around TGL A 609:

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

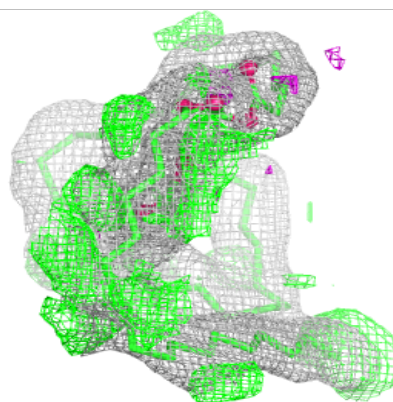
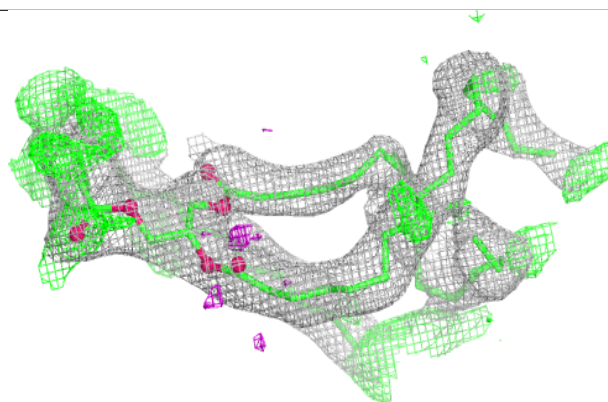
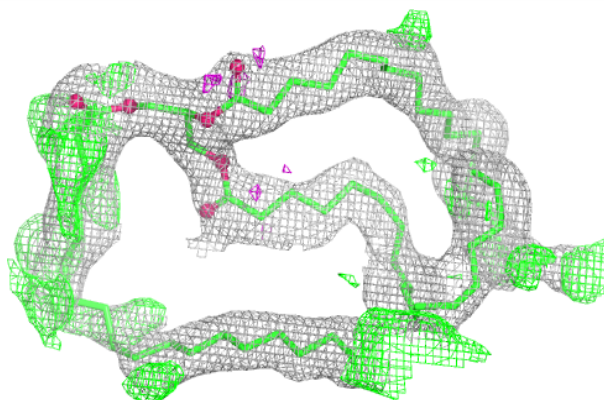


Electron density around DMU G 101:

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

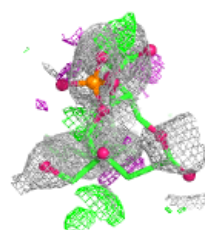
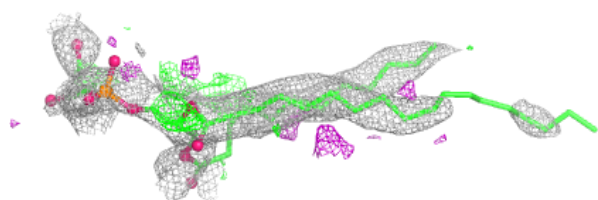
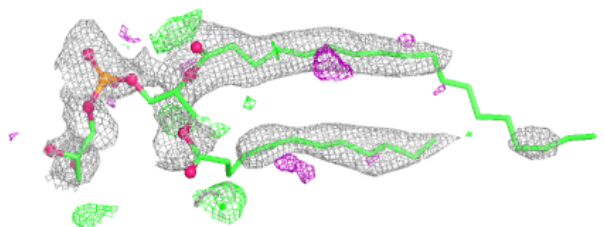
**Electron density around TGL B 302:**

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

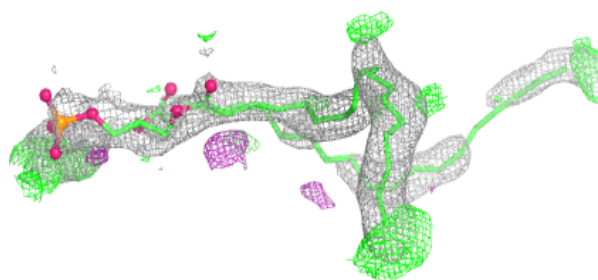
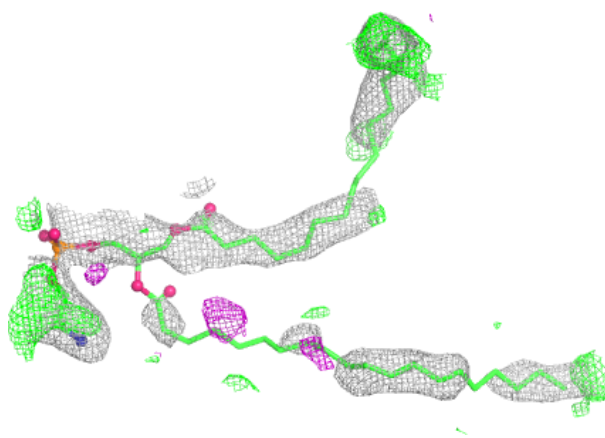


Electron density around PGV Z 101:

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

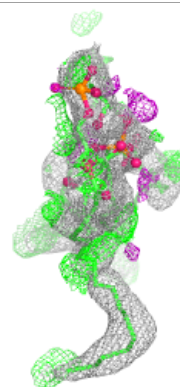
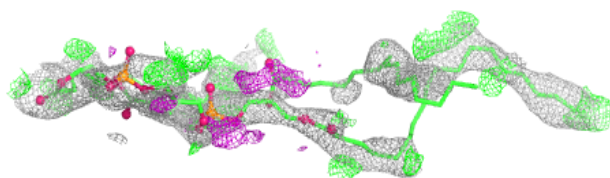
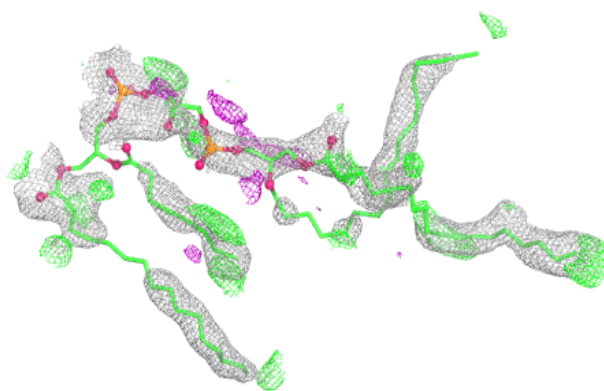
**Electron density around PEK P 306:**

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

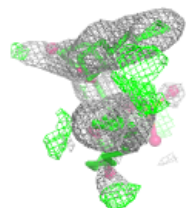
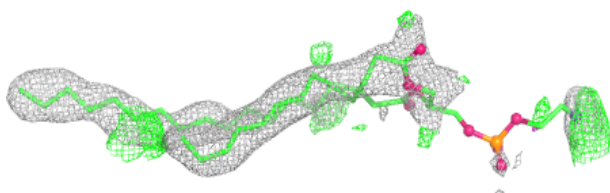
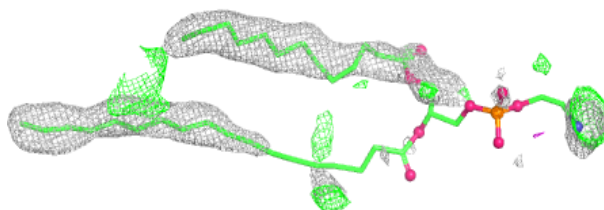


Electron density around CDL G 103:

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

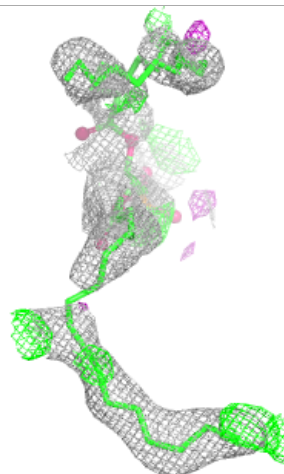
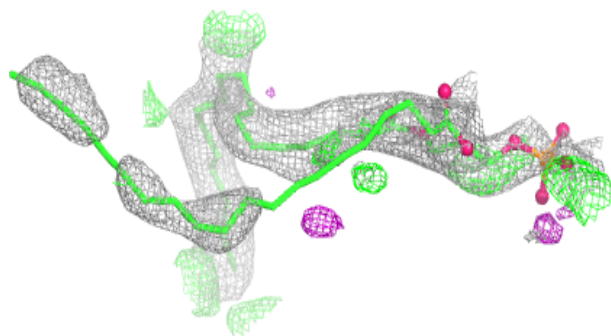
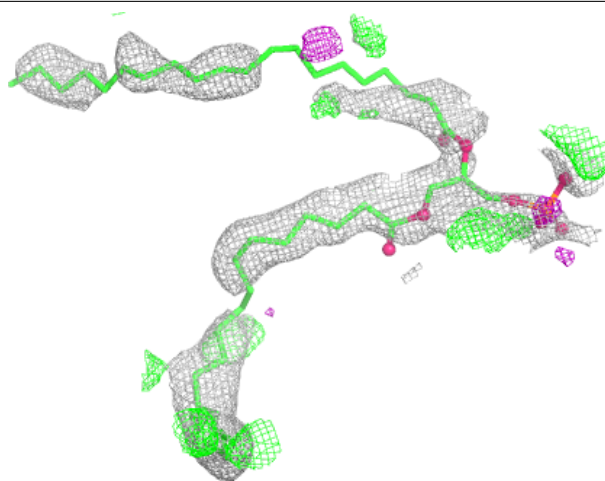
**Electron density around PSC O 304:**

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



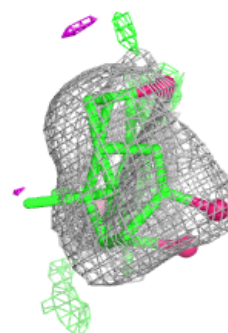
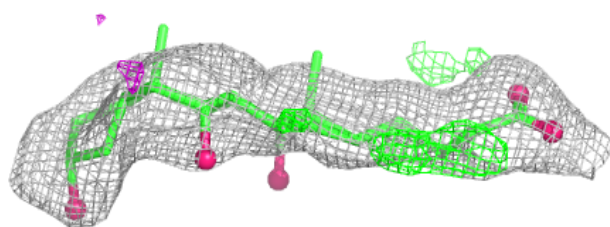
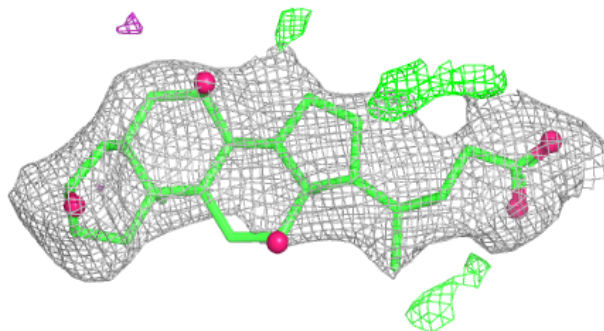
Electron density around PEK G 102:

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

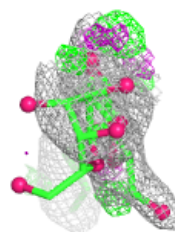
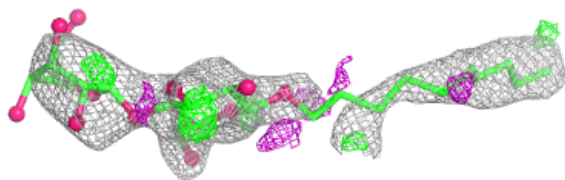
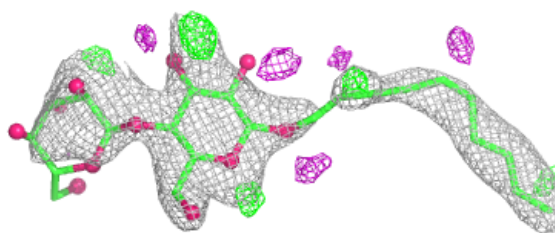


Electron density around CHD P 309:

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

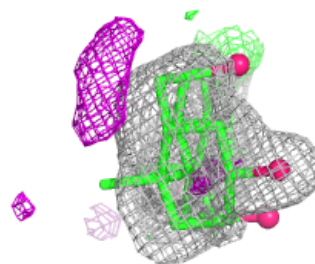
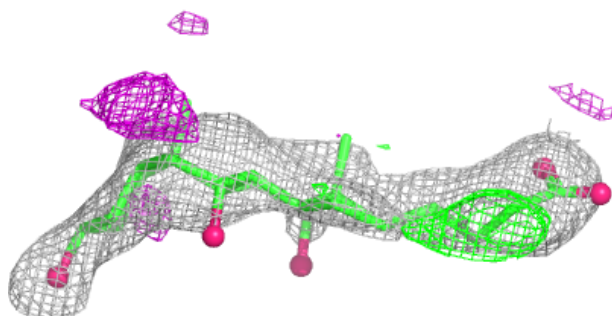
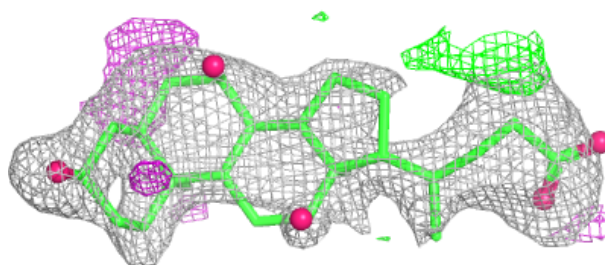
**Electron density around DMU P 313:**

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

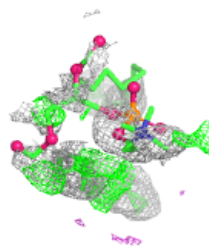
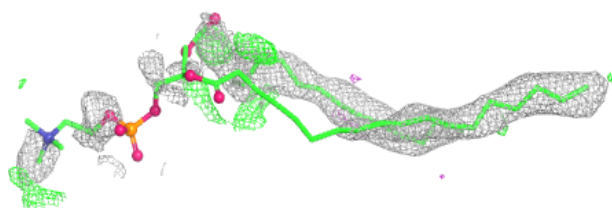
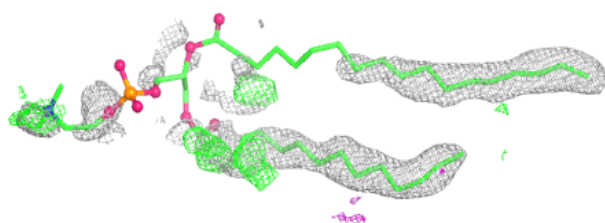


Electron density around CHD C 307:

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

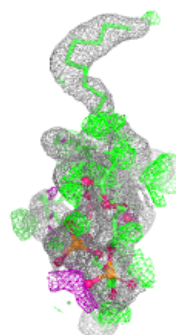
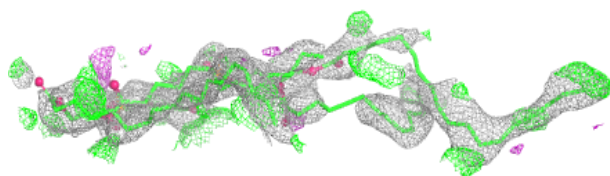
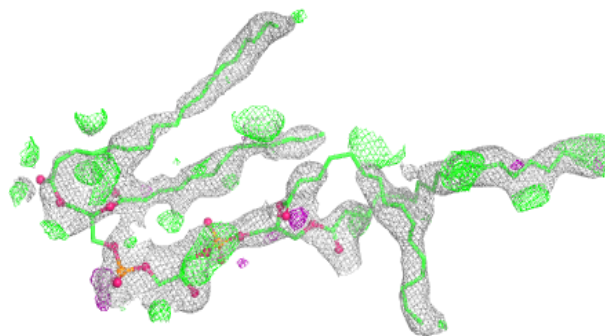
**Electron density around PSC B 303:**

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

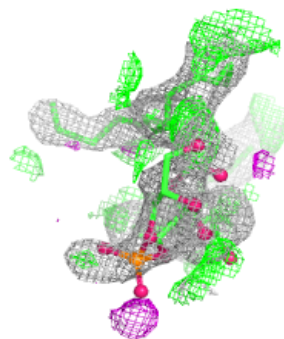
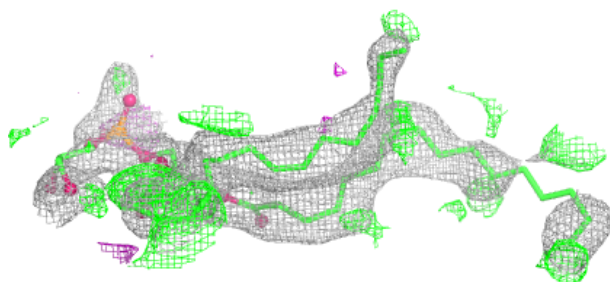
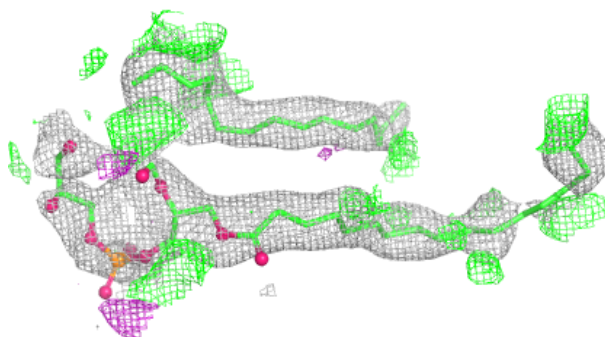


Electron density around CDL T 102:

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

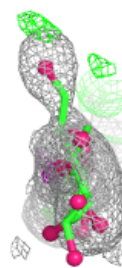
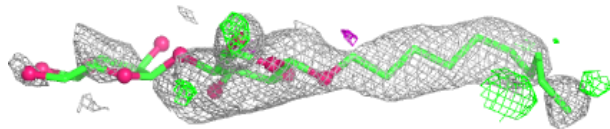
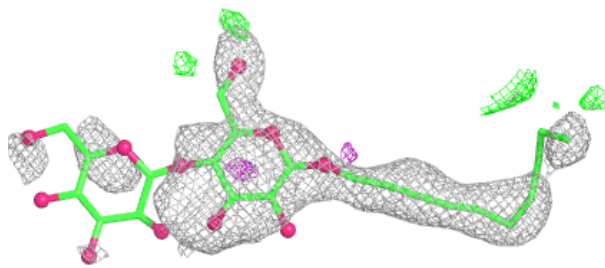
**Electron density around PGV C 305:**

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

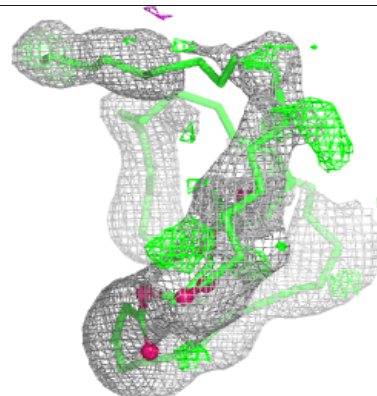
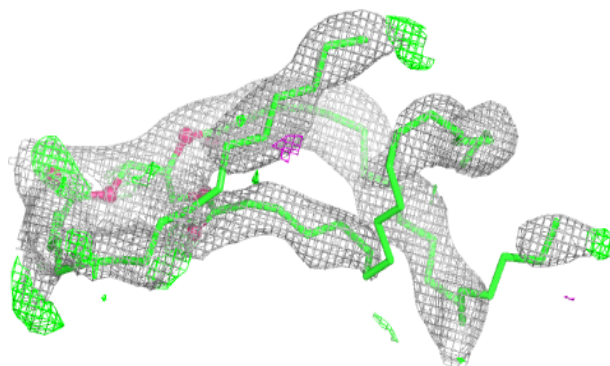
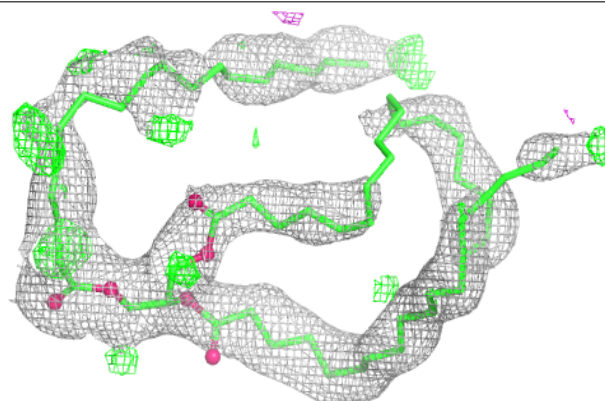


Electron density around DMU L 102:

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

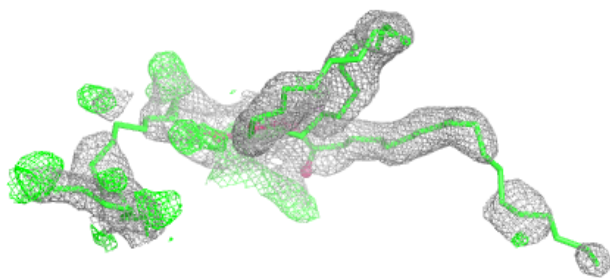
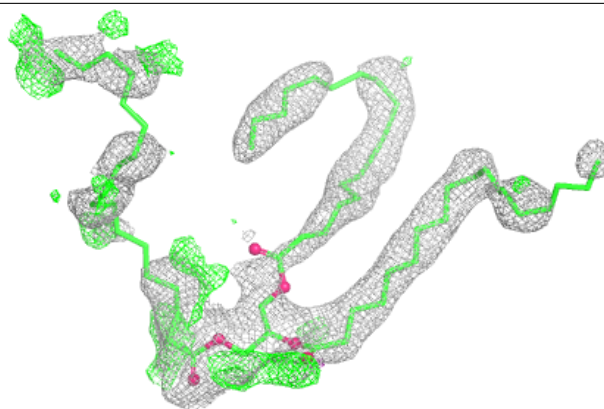
**Electron density around TGL O 303:**

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

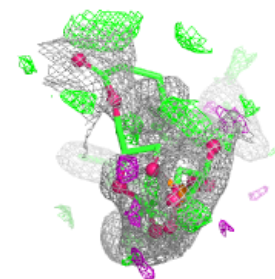
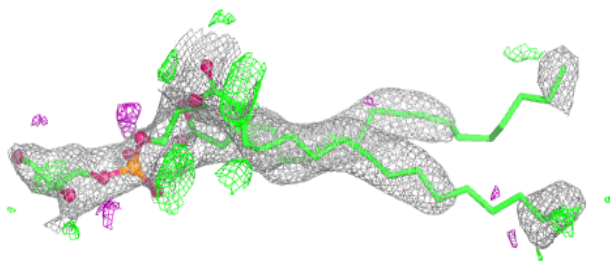
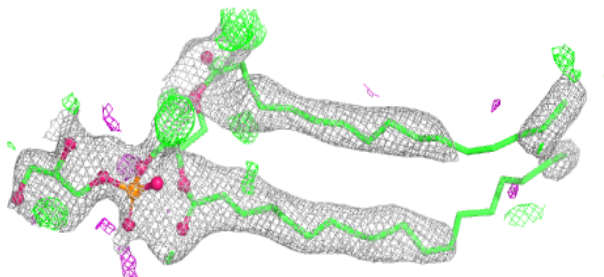


Electron density around TGL N 607:

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

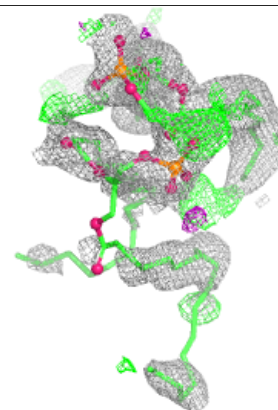
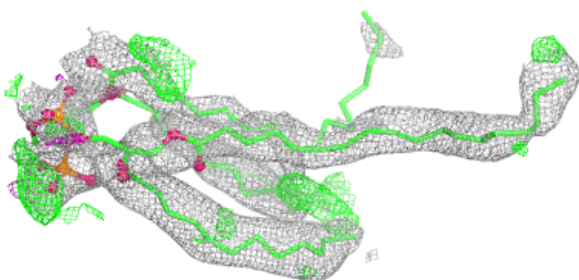
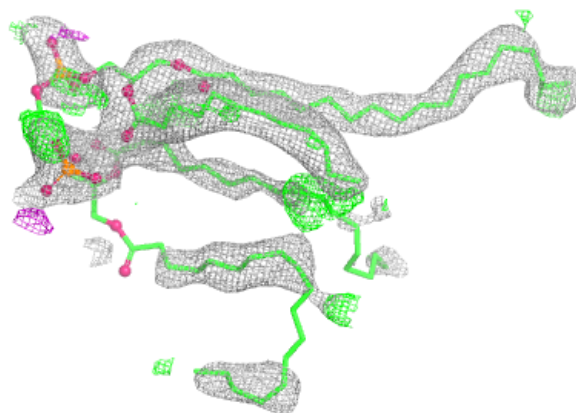
**Electron density around PGV A 607:**

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



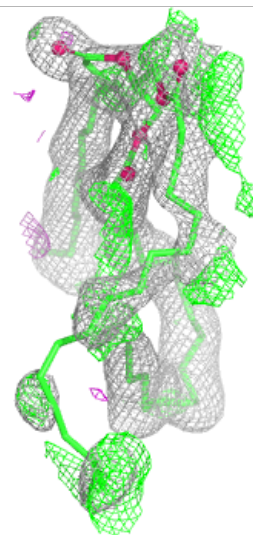
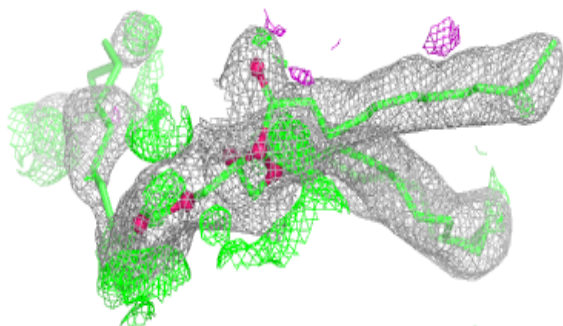
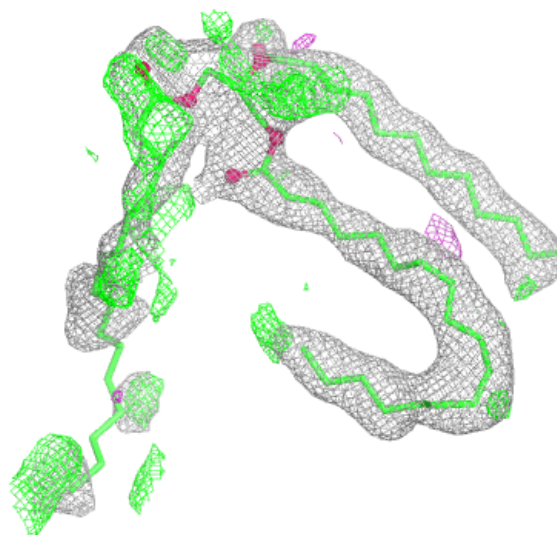
Electron density around CDL P 308:

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



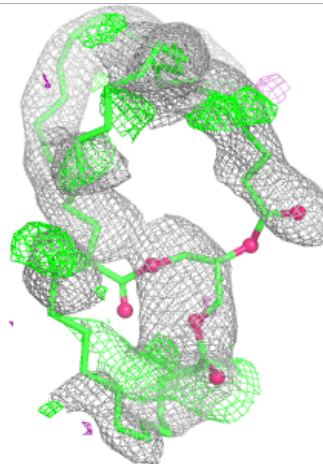
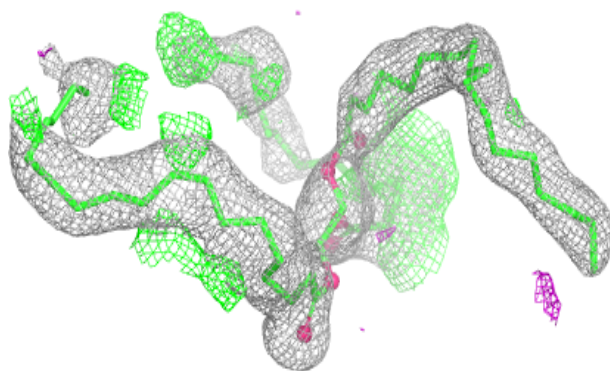
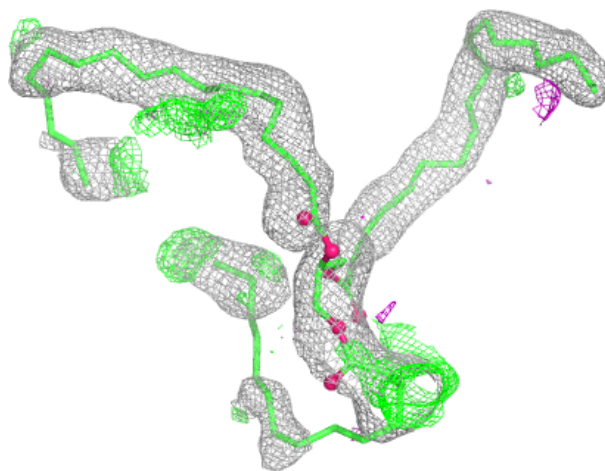
Electron density around TGL D 201:

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



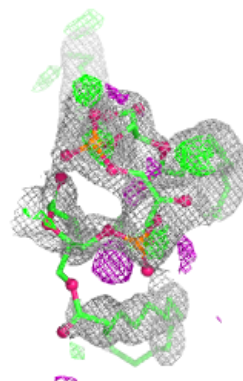
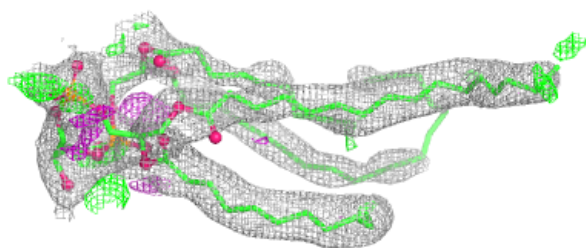
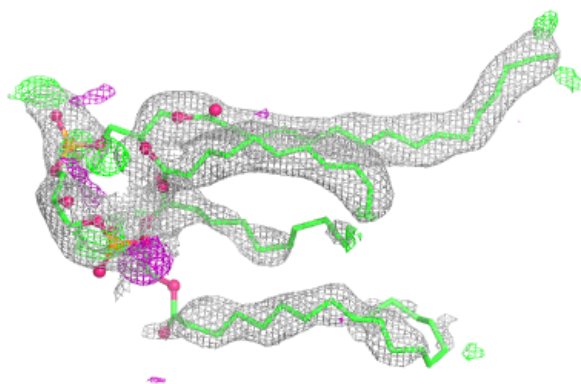
Electron density around TGL Y 101:

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

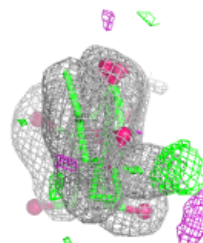
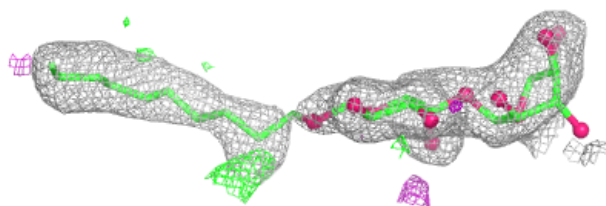
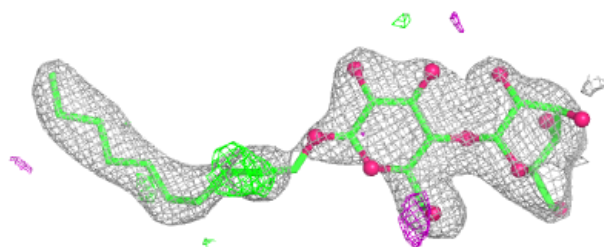


Electron density around CDL C 306:

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

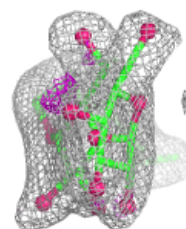
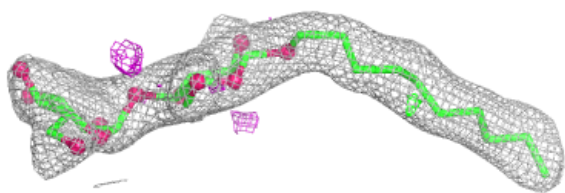
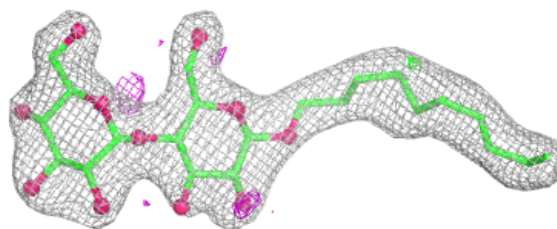
**Electron density around DMU C 314:**

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

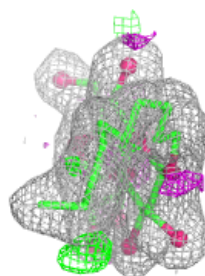
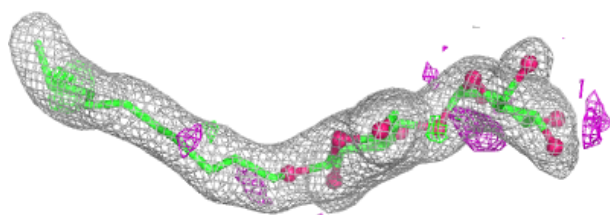
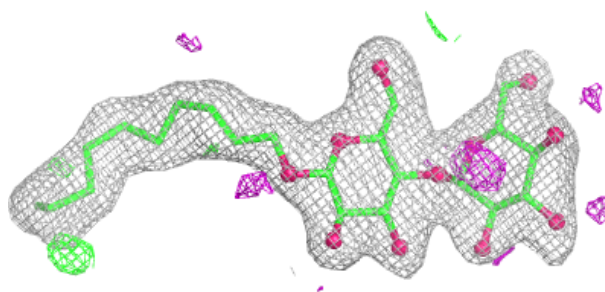


Electron density around DMU Z 102:

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

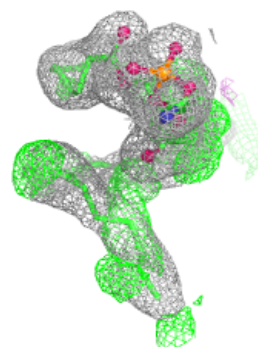
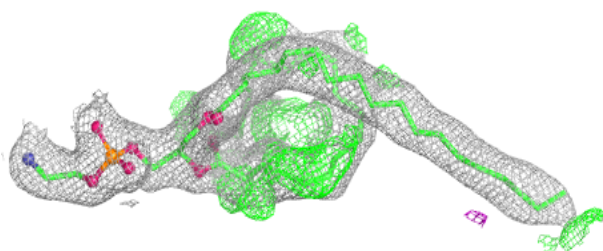
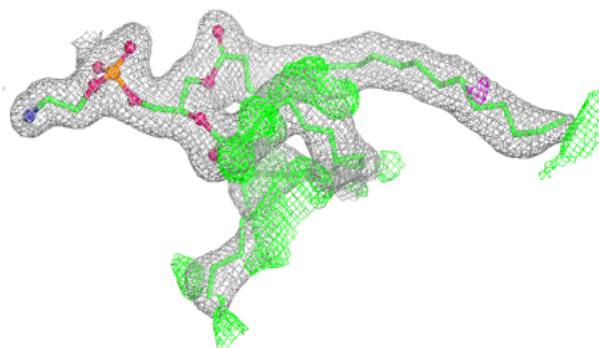
**Electron density around DMU M 101:**

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

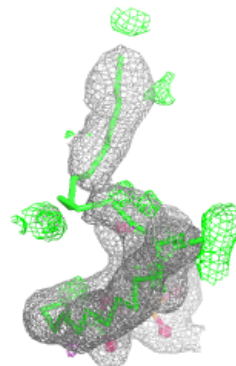
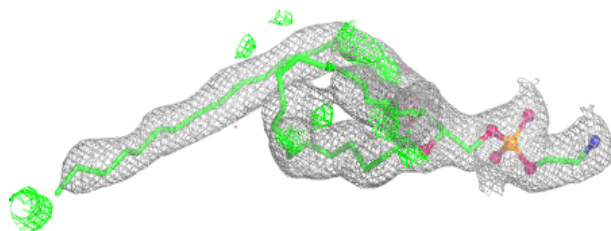
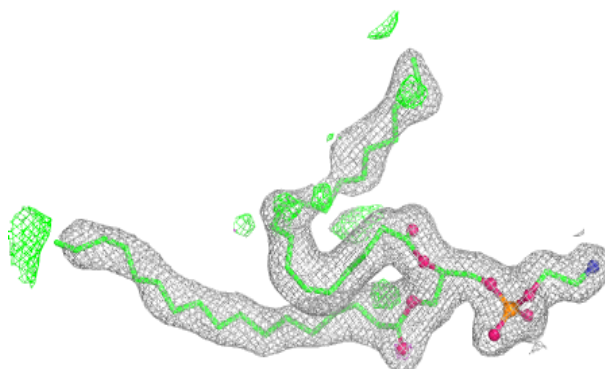


Electron density around PEK C 303:

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

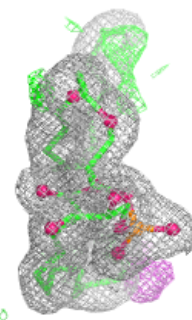
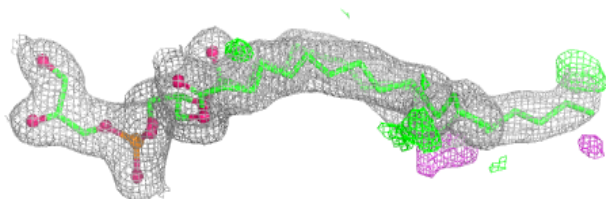
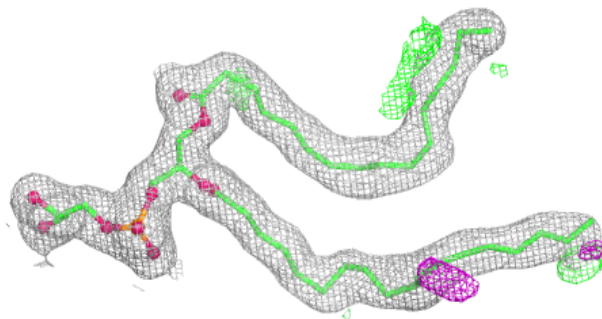
**Electron density around PEK P 305:**

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

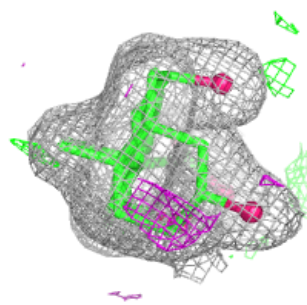
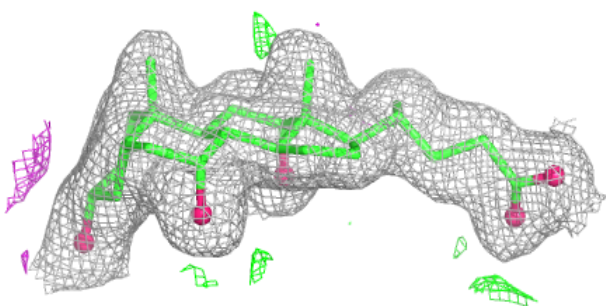
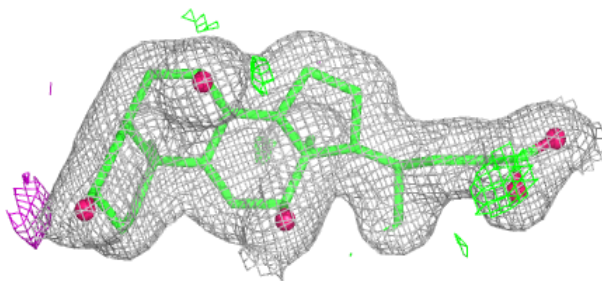


Electron density around PGV N 608:

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

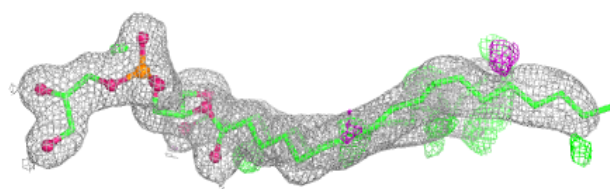
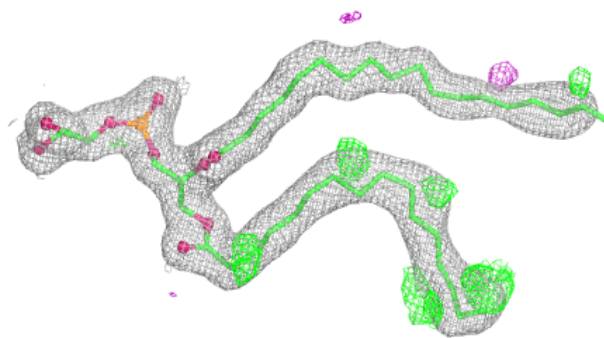
**Electron density around CHD P 304:**

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

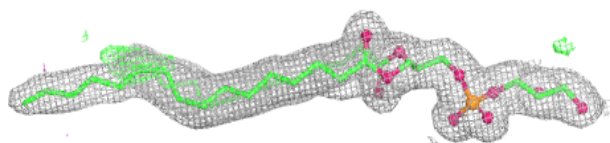
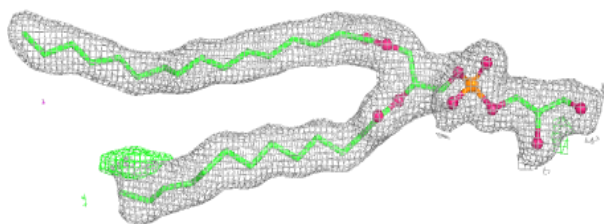


Electron density around PGV A 608:

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

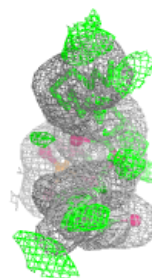
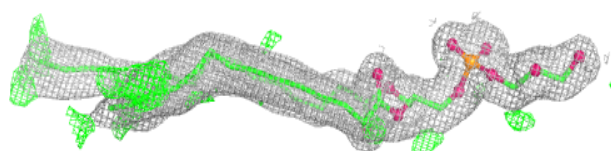
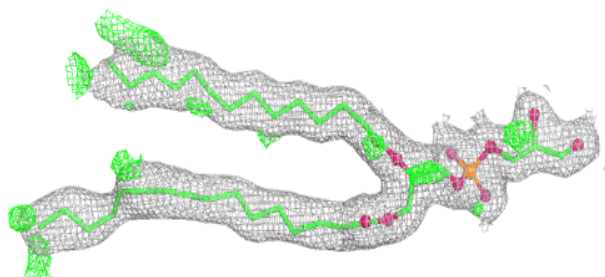
**Electron density around PGV P 307:**

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

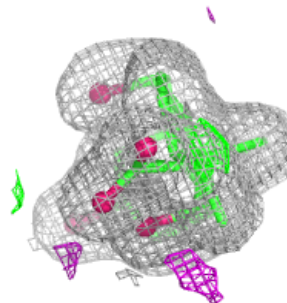
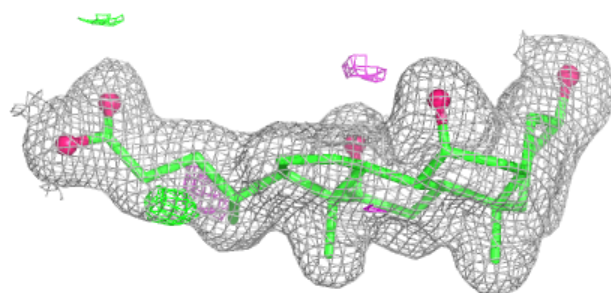
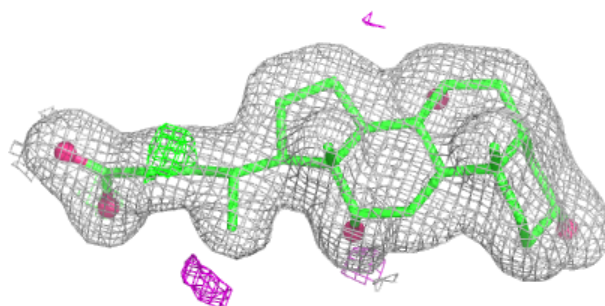


Electron density around PGV C 304:

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

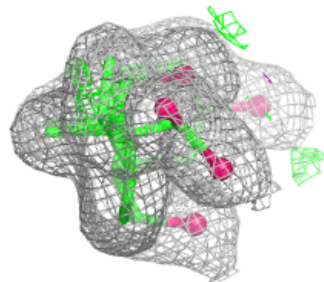
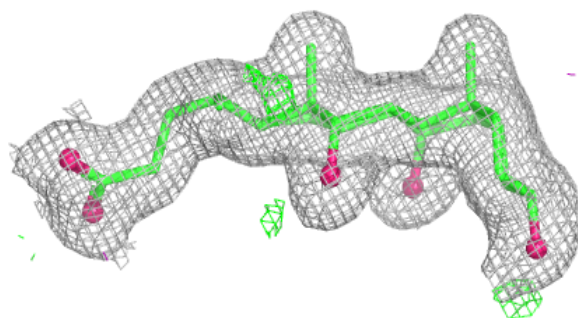
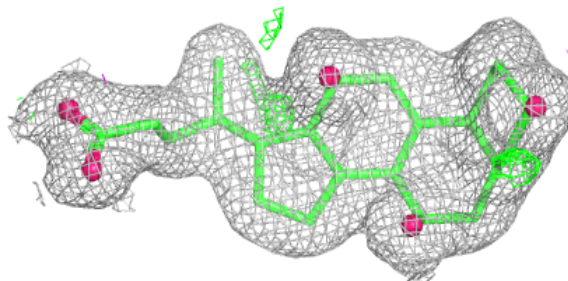
**Electron density around CHD C 301:**

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

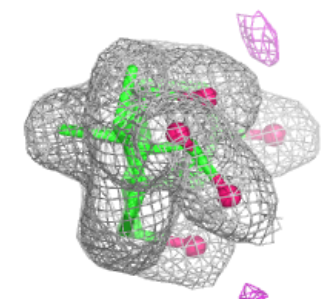
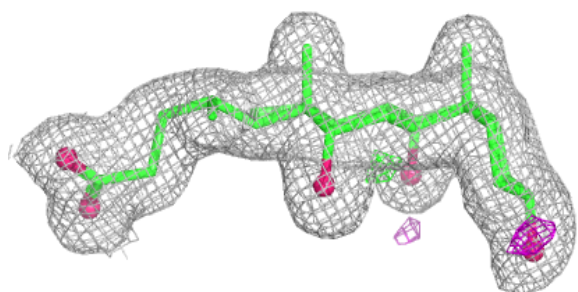
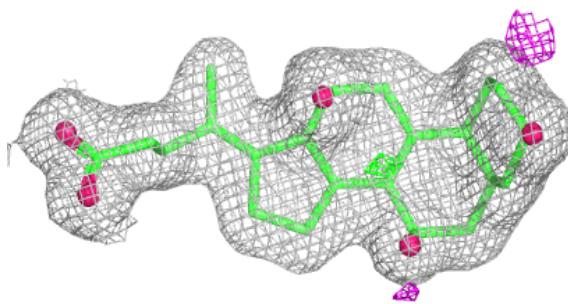


Electron density around CHD O 301:

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

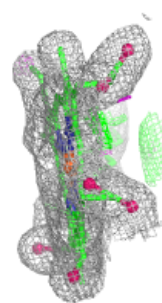
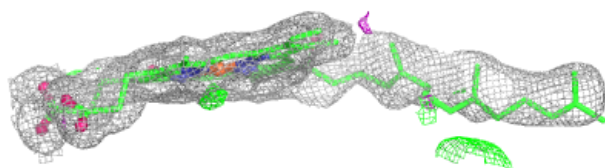
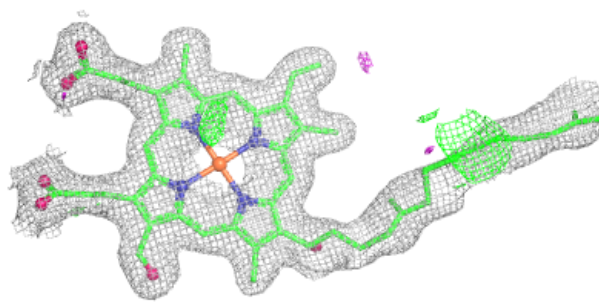
**Electron density around CHD B 304:**

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

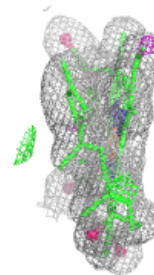
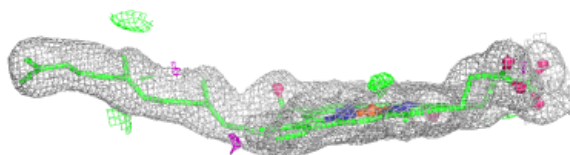
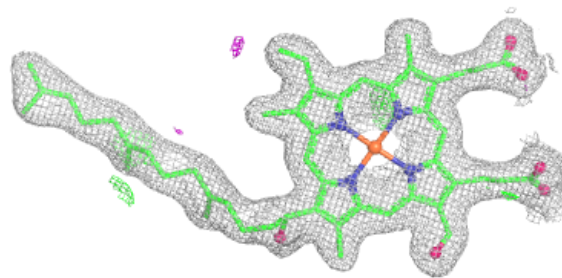


Electron density around HEA N 601 (A):

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

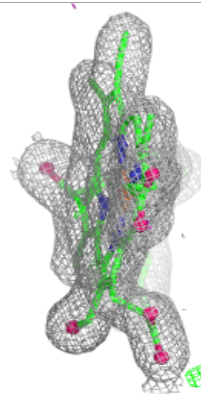
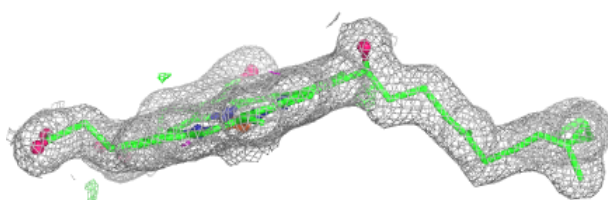
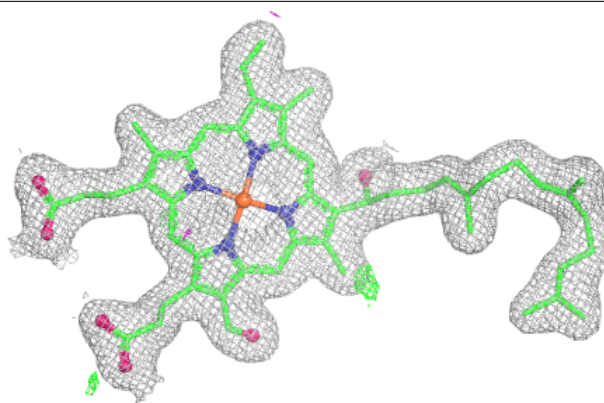
**Electron density around HEA N 601 (B):**

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

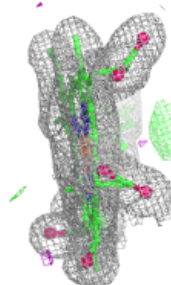
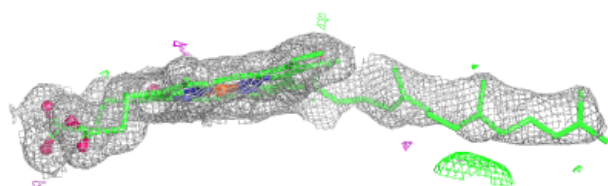
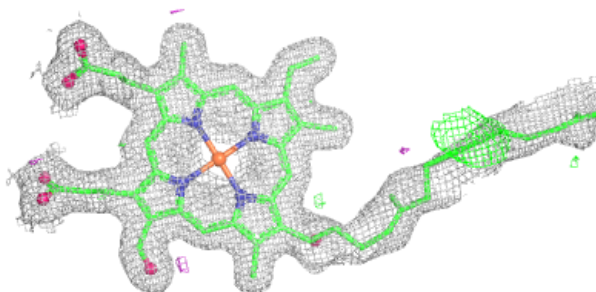


Electron density around HEA N 602:

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

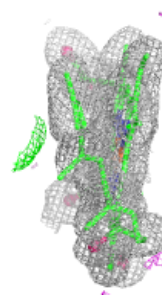
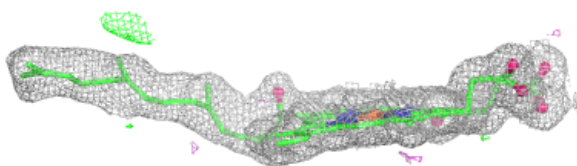
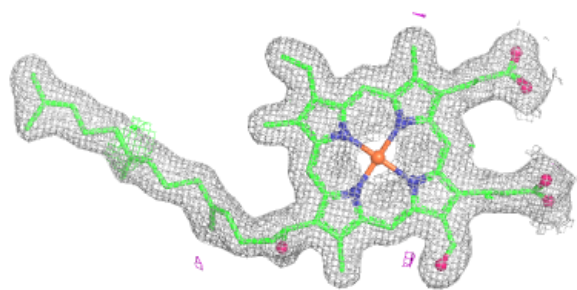
**Electron density around HEA A 601 (A):**

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

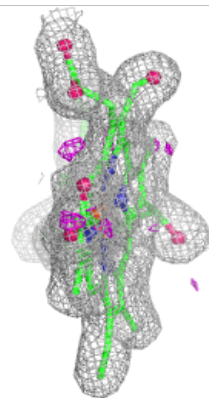
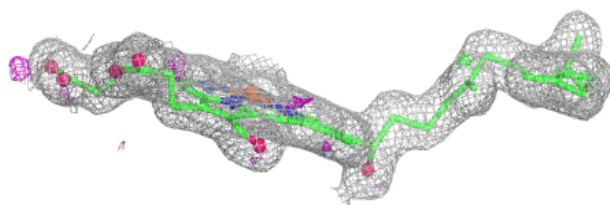
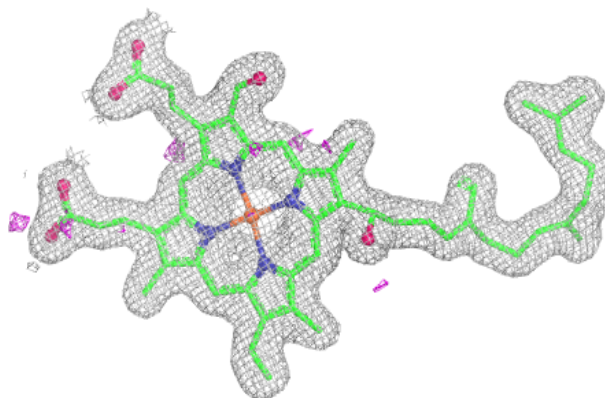


Electron density around HEA A 601 (B):

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

**Electron density around HEA A 602:**

$2mF_o-DF_c$ (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.