



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:02 PM JST

PDB ID : 7CP5 / pdb_00007cp5
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of E at 1.76 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-08-06
Resolution : 1.76 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:

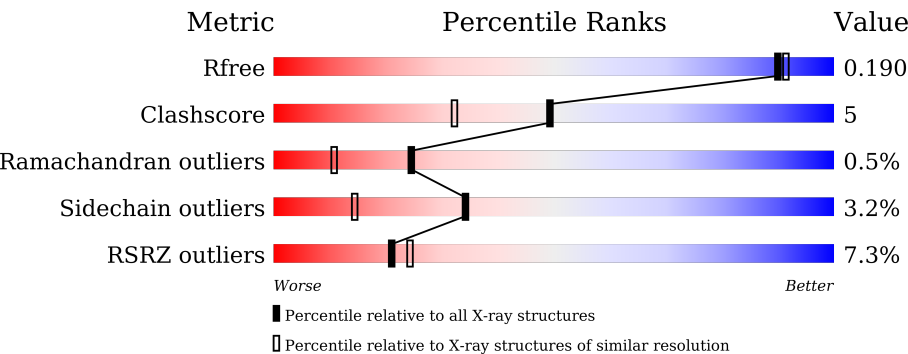
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	6% 90%9% .
1	N	514	91%9%
2	B	227	6% 84%15%
2	O	227	7% 78%20% .
3	C	259	2% 92%8%
3	P	259	3% 87%13%

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

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34258 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	31	0
			4190	2796	644	711	39			
1	N	514	Total	C	N	O	S	0	35	0
			4213	2816	642	713	42			

- 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	7	0
			1862	1214	281	347	20			
2	O	227	Total	C	N	O	S	0	11	0
			1882	1229	287	345	21			

- 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	12	0
			2167	1451	341	360	15			
3	P	259	Total	C	N	O	S	0	12	0
			2161	1448	341	357	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	3	0
			1211	790	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1199	781	196	218	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	1	0
			860	549	147	162	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	94	Total	C	N	O	S	0	5	0
			736	458	128	144	6			
6	S	94	Total	C	N	O	S	0	0	0
			716	444	127	140	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	S	0	4	0
			692	448	129	114	1			
7	T	84	Total	C	N	O	S	0	0	0
			672	431	129	111	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	1	0
			667	420	122	120	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	1	0
			604	391	107	102	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	1	0
			464	299	78	84	3			

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	3	0
			395	260	65	68	2			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

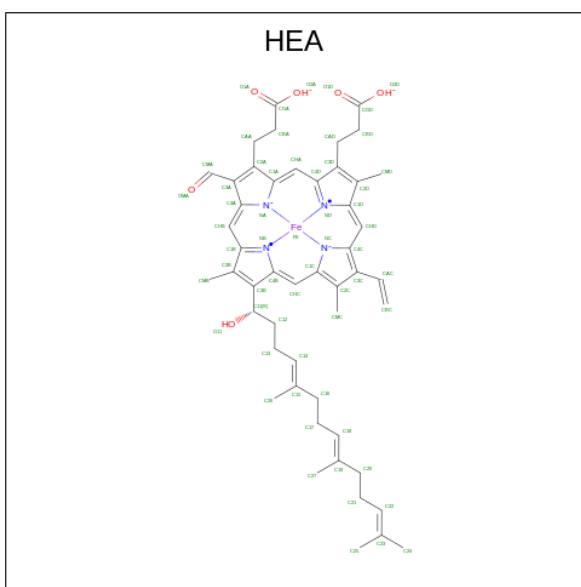
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	1	0
			384	258	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
			336	223	53	60			
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		

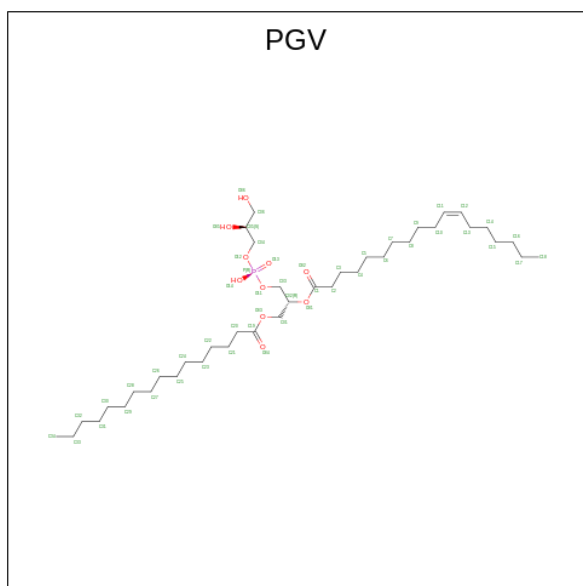
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0
17	P	1	Total Na 1 1	0	0

- Molecule 18 is (1R)-2-{{[[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



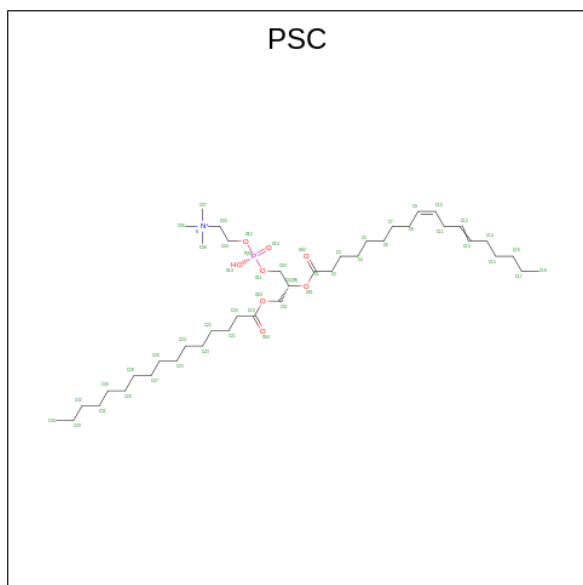
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O 22 21 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 48 37 10 1	0	0
18	C	1	Total C O 28 26 2	0	0
18	G	1	Total C O 32 30 2	0	0
18	N	1	Total C 24 24	0	0
18	N	1	Total C O P 51 40 10 1	0	0

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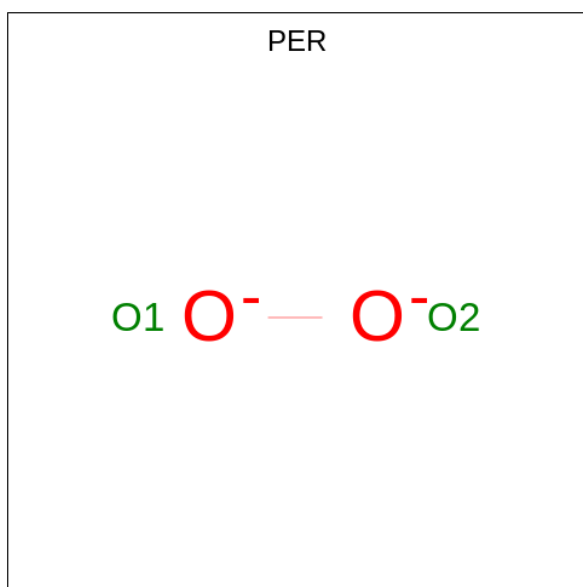
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 19 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).



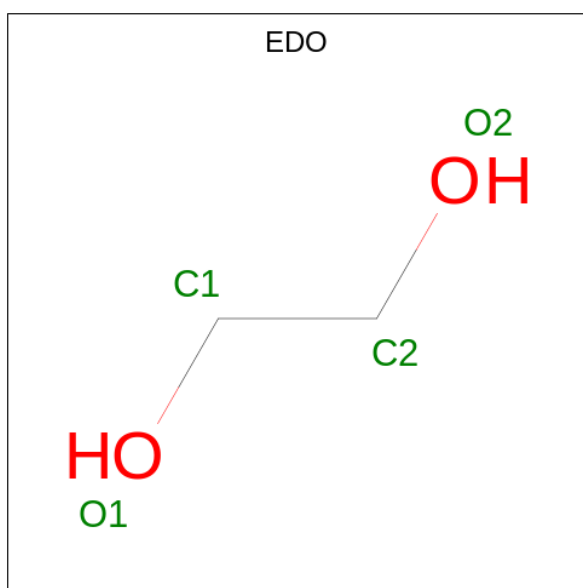
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	C	0	0
			27	27		
19	O	1	Total	C	O	0
			30	28	2	

- Molecule 20 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



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

- Molecule 21 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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		

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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	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	J	1	Total 4	C 2	O 2	0	0
21	J	1	Total 4	C 2	O 2	0	0
21	L	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0

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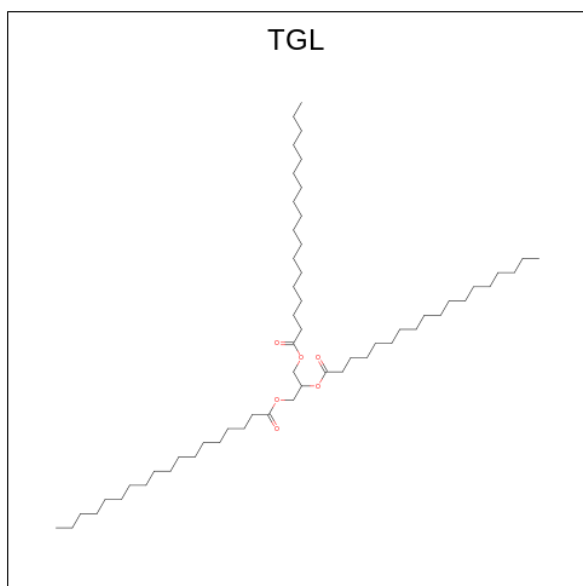
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4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

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

- Molecule 22 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



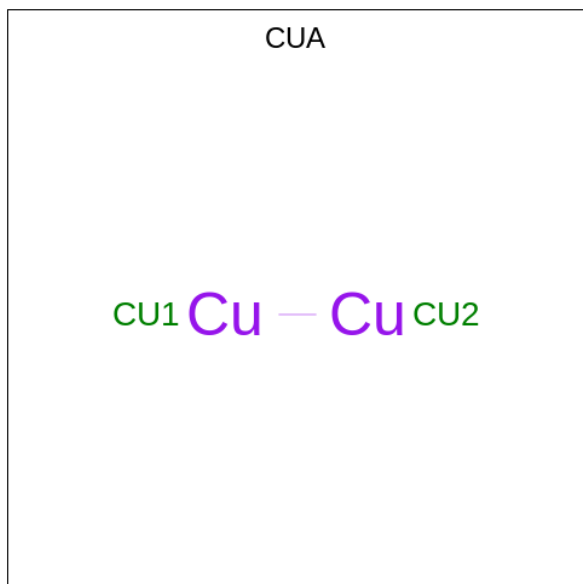
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 49 43 6	0	0
22	D	1	Total C O 57 51 6	0	0
22	L	1	Total C O 56 52 4	0	0
22	N	1	Total C O 63 57 6	0	0
22	N	1	Total C 48 48	0	0

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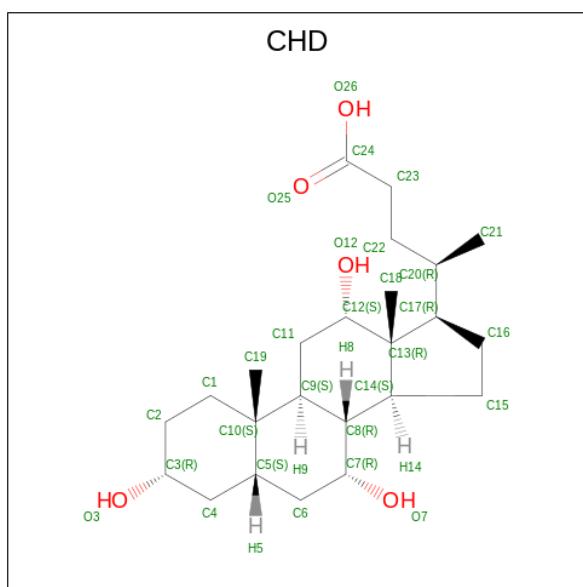
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total	C	O	0	0
			44	39	5		

- Molecule 23 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



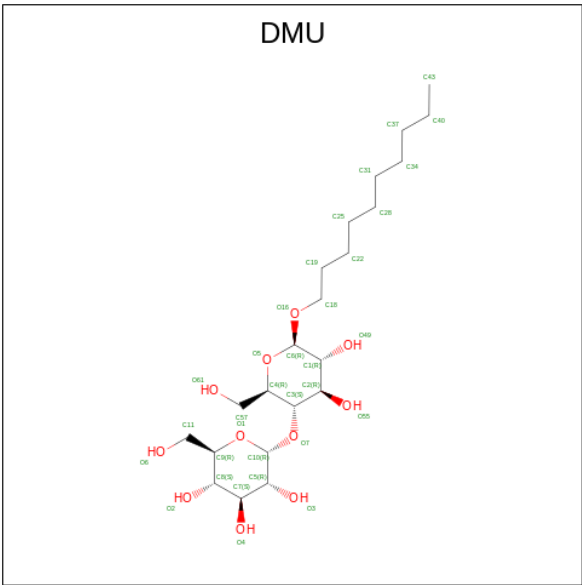
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	B	1	Total	Cu	0	0
			2	2		
23	O	1	Total	Cu	0	0
			2	2		

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



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

- Molecule 25 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



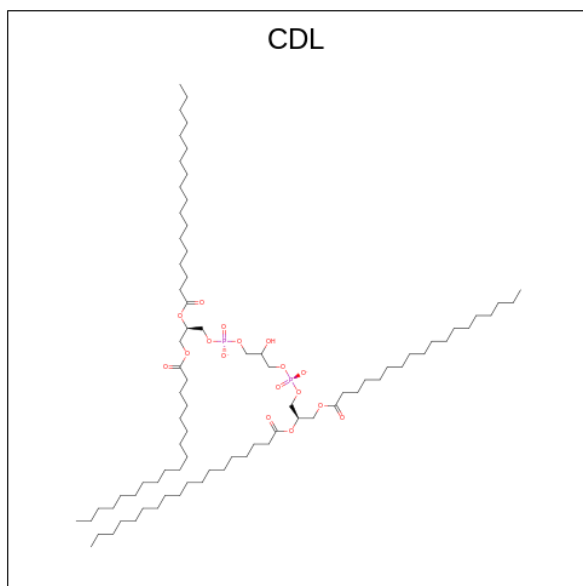
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	C	1	Total	C	O	0	0
			13	11	2		
25	C	1	Total	C	O	0	0
			21	16	5		
25	D	1	Total	C	O	0	0
			11	10	1		
25	D	1	Total	C	O	0	0
			11	10	1		
25	J	1	Total	C	O	0	0
			11	10	1		
25	K	1	Total	C		0	0
			9	9			
25	K	1	Total	C		0	0
			10	10			
25	K	1	Total	C	O	0	0
			11	10	1		
25	K	1	Total	C		0	0
			9	9			
25	K	1	Total	C		0	0
			9	9			
25	K	1	Total	C		0	0
			10	10			
25	L	1	Total	C	O	0	0
			21	16	5		
25	M	1	Total	C	O	0	0
			33	22	11		
25	O	1	Total	C	O	0	0
			11	10	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	P	1	Total C O 13 11 2	0	0
25	P	1	Total C O 11 10 1	0	0
25	Q	1	Total C 10 10	0	0
25	W	1	Total C O 11 10 1	0	0
25	X	1	Total C O 11 10 1	0	0
25	X	1	Total C 10 10	0	0
25	X	1	Total C 9 9	0	0
25	X	1	Total C 10 10	0	0
25	Z	1	Total C O 33 22 11	0	0

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



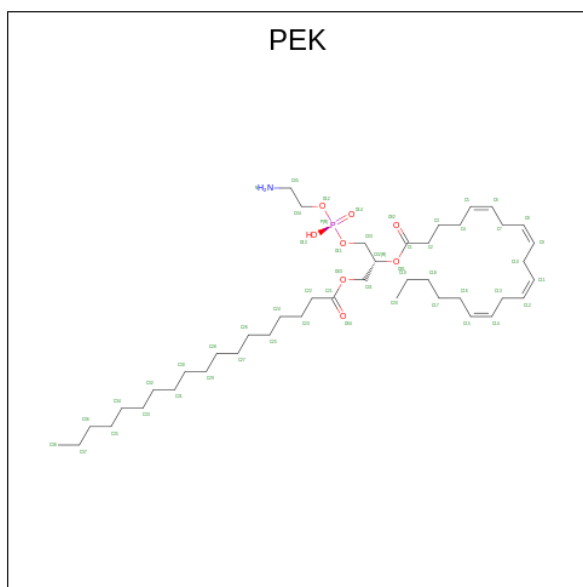
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O 58 56 2	0	0
26	N	1	Total C O 55 54 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	P	1	Total	C	O	0	0
			61	58	3		
26	T	1	Total	C	O	0	0
			57	54	3		

- Molecule 27 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).

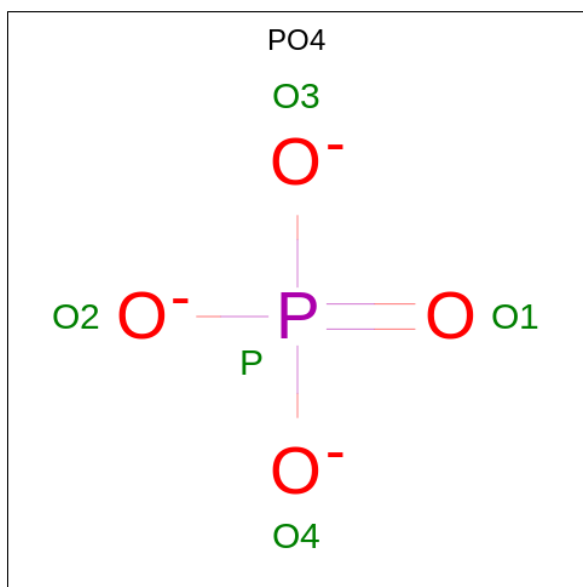


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	C	1	Total	C			0	0
			25	25				
27	C	1	Total	C	N	O	0	0
			53	43	1	8		
27	C	1	Total	C			0	0
			36	36				
27	P	1	Total	C			0	0
			20	20				
27	P	1	Total	C	N	O	0	0
			53	43	1	8		
27	P	1	Total	C			0	0
			34	34				

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

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

- Molecule 29 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	273	Total	O	0	14
			273	273		
30	B	223	Total	O	0	2
			223	223		
30	C	142	Total	O	0	2
			142	142		
30	D	213	Total	O	0	0
			213	213		
30	E	160	Total	O	0	0
			160	160		
30	F	162	Total	O	0	3
			162	162		

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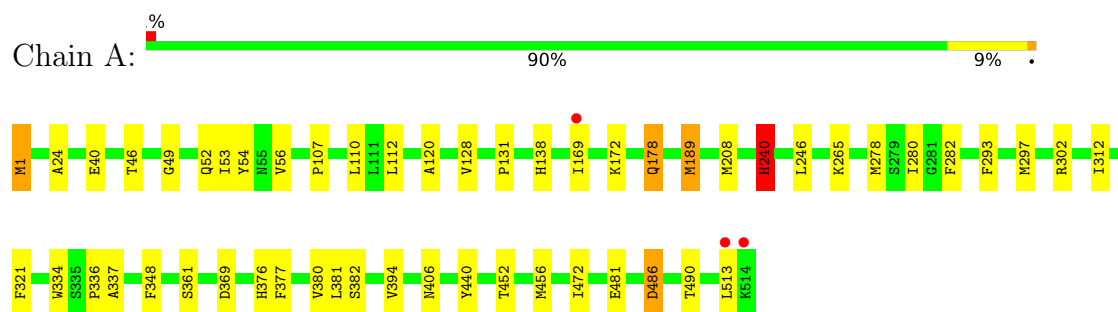
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	G	89	Total 89	O 89	0	0
30	H	94	Total 94	O 94	0	0
30	I	70	Total 70	O 70	0	0
30	J	58	Total 58	O 58	0	0
30	K	44	Total 44	O 44	0	0
30	L	38	Total 38	O 38	0	1
30	M	39	Total 39	O 39	0	0
30	N	273	Total 273	O 273	0	12
30	O	205	Total 205	O 205	0	2
30	P	147	Total 147	O 147	0	0
30	Q	114	Total 114	O 114	0	0
30	R	117	Total 117	O 117	0	0
30	S	141	Total 141	O 141	0	0
30	T	66	Total 66	O 66	0	0
30	U	94	Total 94	O 94	0	0
30	V	72	Total 72	O 72	0	0
30	W	43	Total 43	O 43	0	0
30	X	31	Total 31	O 31	0	0
30	Y	31	Total 31	O 31	0	0
30	Z	29	Total 29	O 29	0	0

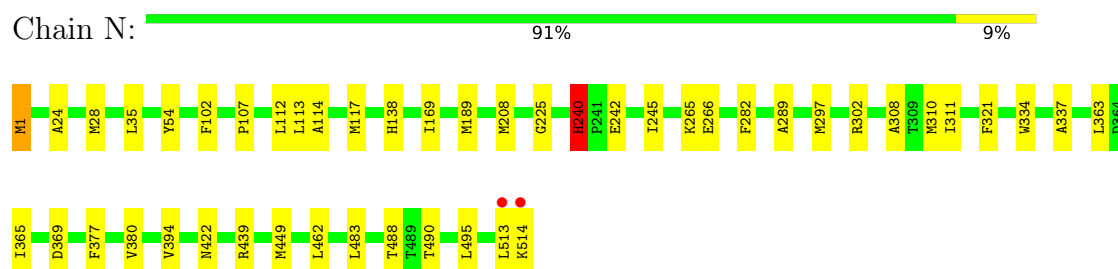
3 Residue-property plots

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.

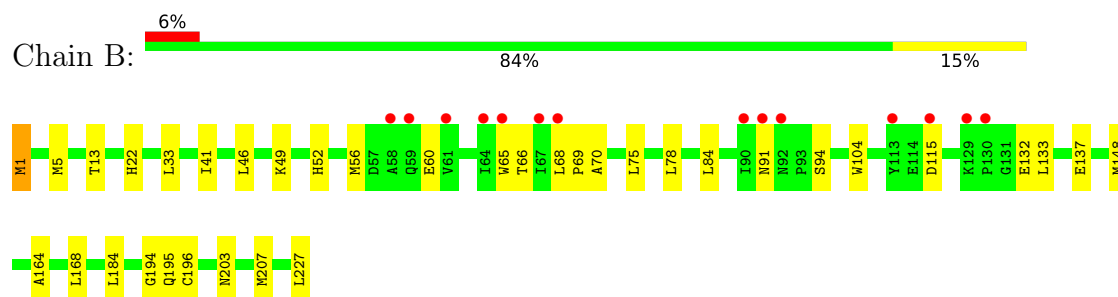
• Molecule 1: Cytochrome c oxidase subunit 1



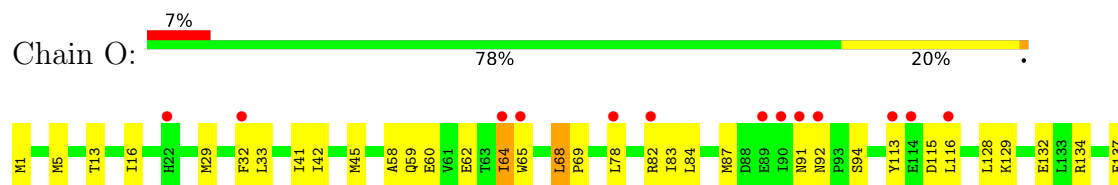
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

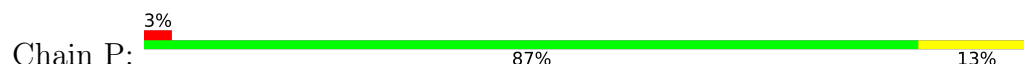




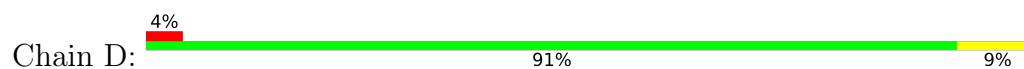
- Molecule 3: Cytochrome c oxidase subunit 3



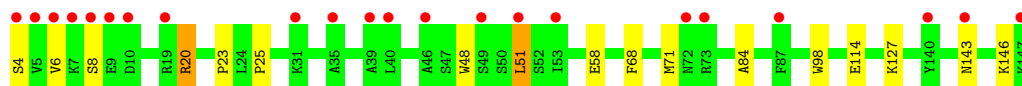
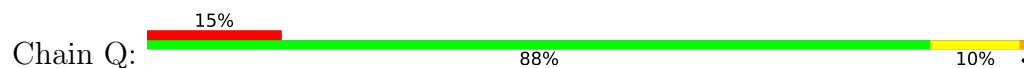
- Molecule 3: Cytochrome c oxidase subunit 3



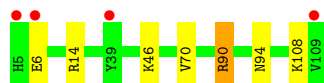
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



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



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

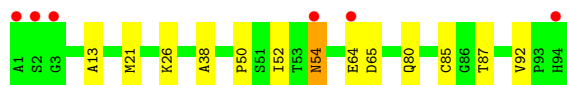
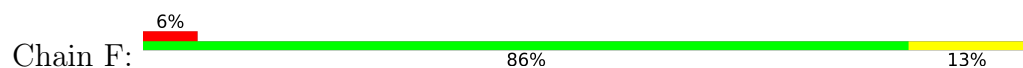


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

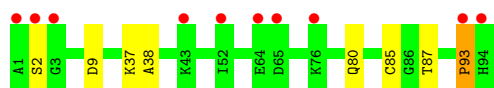




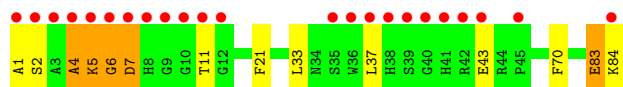
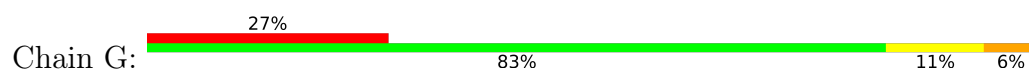
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



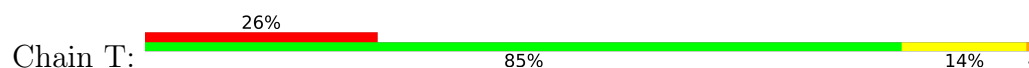
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



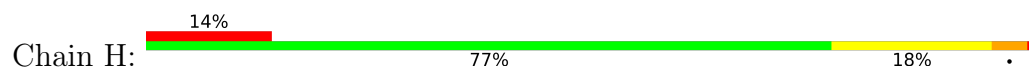
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



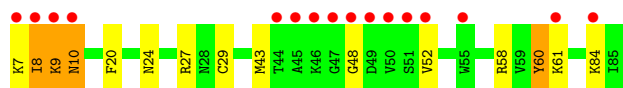
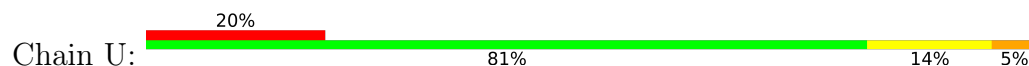
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



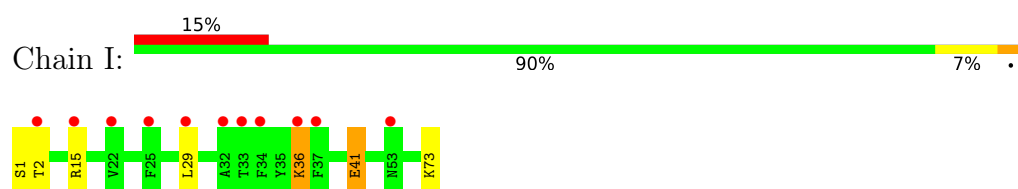
- Molecule 8: Cytochrome c oxidase subunit 6B1



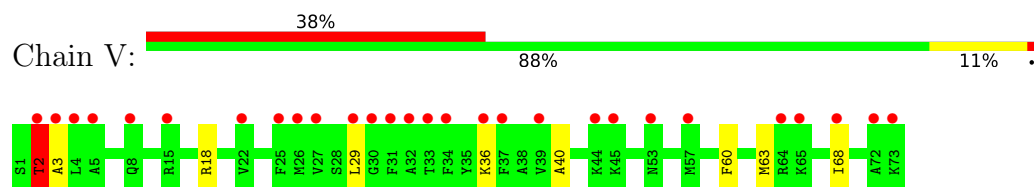
- Molecule 8: Cytochrome c oxidase subunit 6B1



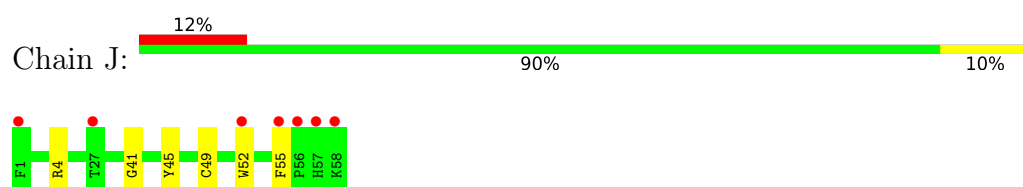
- Molecule 9: Cytochrome c oxidase subunit 6C



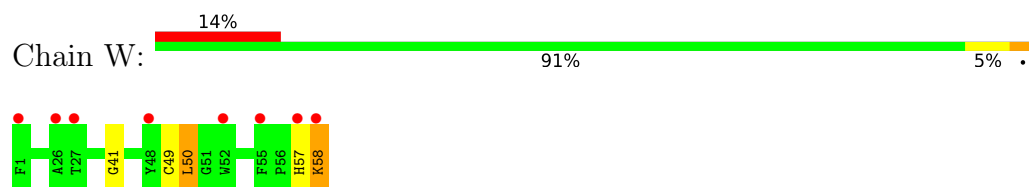
- Molecule 9: Cytochrome c oxidase subunit 6C



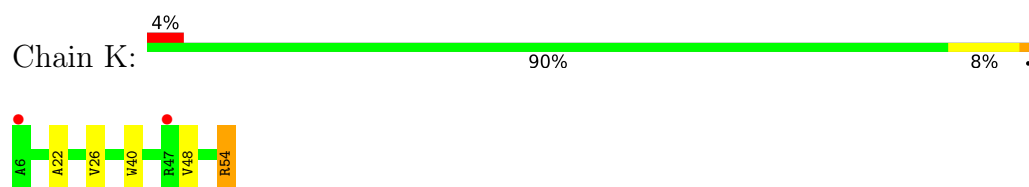
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



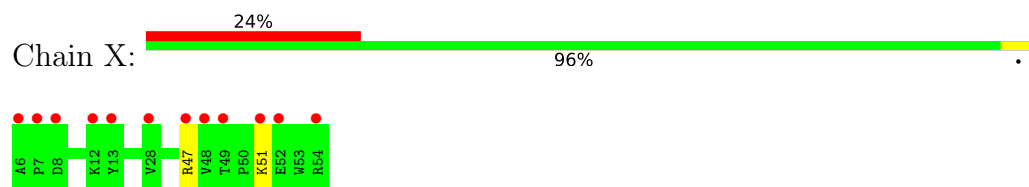
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



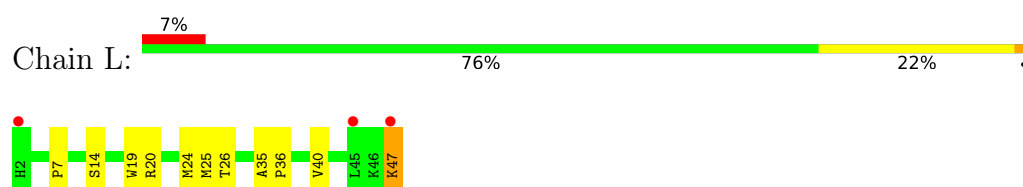
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



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

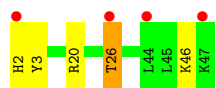


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

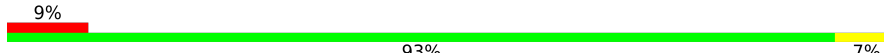


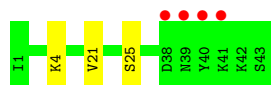
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  9% 89% 9%



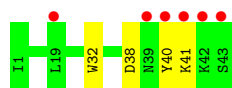
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  9% 93% 7%



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

Chain Z:  14% 91% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.59Å 203.22Å 177.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.76 39.91 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.76) 99.8 (39.91-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 1.76Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.160 , 0.189 0.162 , 0.190	Depositor DCC
R_{free} test set	32242 reflections (2.54%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.782	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34258	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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: SAC, EDO, NA, CU, PEK, PGV, ZN, CDL, CUA, PER, DMU, HEA, CHD, TGL, PO4, MG, FME, 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	0.87	1/4411 (0.0%)	0.88	6/6016 (0.1%)
1	N	0.78	1/4434 (0.0%)	0.84	3/6051 (0.0%)
2	B	0.79	0/1920	0.92	0/2613
2	O	0.71	0/1966	0.84	1/2675 (0.0%)
3	C	0.73	0/2296	0.73	0/3136
3	P	0.71	0/2295	0.75	0/3134
4	D	0.75	0/1259	0.79	0/1698
4	Q	0.54	0/1236	0.66	0/1668
5	E	0.71	0/871	0.72	0/1182
5	R	0.59	0/882	0.69	0/1196
6	F	0.74	0/771	0.81	0/1047
6	S	0.73	0/732	0.81	0/993
7	G	0.68	0/734	0.86	1/997 (0.1%)
7	T	0.63	0/699	0.82	0/950
8	H	0.70	0/690	0.82	1/932 (0.1%)
8	U	0.63	0/682	0.73	0/921
9	I	0.62	0/614	0.70	0/814
9	V	0.53	0/605	0.69	0/802
10	J	0.55	0/478	0.67	0/644
10	W	0.50	0/472	0.71	0/636
11	K	0.66	0/420	0.70	0/576
11	X	0.53	0/399	0.61	0/546
12	L	0.79	0/401	0.83	0/537
12	Y	0.67	0/393	0.74	0/526
13	M	0.74	0/346	0.76	0/470
13	Z	0.55	0/345	0.71	0/470
All	All	0.73	2/30351 (0.0%)	0.80	12/41230 (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
6	S	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	MET	CG-SD	-5.93	1.66	1.80
1	N	310	MET	SD-CE	-5.19	1.66	1.79

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	MET	CG-SD-CE	-7.85	83.64	100.90
1	N	240	HIS	CA-CB-CG	-6.96	106.84	113.80
1	A	189	MET	CG-SD-CE	-6.81	85.93	100.90
1	A	240	HIS	CA-CB-CG	-6.43	107.37	113.80
1	A	376	HIS	CA-C-N	-5.36	111.77	121.14
1	A	376	HIS	C-N-CA	-5.36	111.77	121.14
8	H	75	ARG	CA-CB-CG	-5.30	103.51	114.10
1	N	310	MET	CG-SD-CE	-5.28	89.28	100.90
7	G	6	GLY	N-CA-C	5.21	125.54	113.18
1	A	278	MET	CA-CB-CG	-5.17	103.76	114.10
2	O	192	TYR	CA-CB-CG	-5.14	104.65	113.90
1	N	102	PHE	CA-CB-CG	-5.03	108.77	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
6	S	93	PRO	Peptide

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	4190	0	4166	51	0
1	N	4213	0	4222	44	0
2	B	1862	0	1881	26	0
2	O	1882	0	1903	32	0
3	C	2167	0	2104	16	0
3	P	2161	0	2106	29	0
4	D	1211	0	1202	14	0
4	Q	1199	0	1192	11	0
5	E	852	0	845	6	0
5	R	860	0	858	3	0
6	F	736	0	726	12	0
6	S	716	0	697	6	0
7	G	692	0	672	7	0
7	T	672	0	645	4	0
8	H	667	0	629	9	0
8	U	662	0	623	9	0
9	I	604	0	611	3	0
9	V	601	0	613	4	0
10	J	464	0	464	6	0
10	W	461	0	459	4	0
11	K	395	0	389	7	0
11	X	385	0	366	1	0
12	L	384	0	391	14	0
12	Y	380	0	380	2	0
13	M	336	0	352	4	0
13	Z	335	0	352	2	0
14	A	138	0	111	6	0
14	N	138	0	111	5	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	22	0	33	2	0
18	C	127	0	181	6	0
18	G	32	0	51	2	0
18	N	75	0	114	4	0
18	P	51	0	76	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	27	0	48	4	0
19	O	30	0	47	4	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	A	40	0	60	2	0
21	B	16	0	24	0	0
21	C	36	0	54	1	0
21	D	12	0	18	0	0
21	E	12	0	18	0	0
21	F	20	0	29	0	0
21	G	8	0	12	0	0
21	J	8	0	12	1	0
21	L	4	0	6	0	0
21	N	36	0	54	0	0
21	O	12	0	18	3	0
21	P	32	0	48	1	0
21	Q	4	0	6	0	0
21	S	20	0	30	1	0
21	T	12	0	18	0	0
21	W	4	0	6	1	0
21	Y	8	0	12	0	0
22	B	49	0	77	1	0
22	D	57	0	95	9	0
22	L	56	0	94	9	0
22	N	155	0	275	14	0
23	B	2	0	0	0	0
23	O	2	0	0	0	0
24	B	29	0	39	0	0
24	C	29	0	39	0	0
24	G	29	0	39	1	0
24	L	29	0	39	4	0
24	P	29	0	39	0	0
24	Y	29	0	39	1	0
25	C	34	0	51	5	0
25	D	22	0	40	2	0
25	J	11	0	21	2	0
25	K	58	0	110	4	0
25	L	21	0	30	1	0
25	M	33	0	42	2	0
25	O	11	0	21	1	0
25	P	24	0	42	6	0
25	Q	10	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	11	0	21	1	0
25	X	40	0	74	0	0
25	Z	33	0	42	1	0
26	C	58	0	100	6	0
26	N	55	0	101	3	0
26	P	61	0	104	4	0
26	T	57	0	88	7	0
27	C	114	0	173	8	0
27	P	107	0	163	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	H	5	0	0	0	0
29	U	5	0	0	0	0
30	A	273	0	0	2	0
30	B	223	0	0	1	0
30	C	142	0	0	1	0
30	D	213	0	0	1	0
30	E	160	0	0	3	0
30	F	162	0	0	4	0
30	G	89	0	0	0	0
30	H	94	0	0	1	0
30	I	70	0	0	2	0
30	J	58	0	0	3	0
30	K	44	0	0	1	0
30	L	38	0	0	1	0
30	M	39	0	0	0	0
30	N	273	0	0	4	0
30	O	205	0	0	4	0
30	P	147	0	0	0	0
30	Q	114	0	0	2	0
30	R	117	0	0	0	0
30	S	141	0	0	3	0
30	T	66	0	0	0	0
30	U	94	0	0	0	0
30	V	72	0	0	1	0
30	W	43	0	0	1	0
30	X	31	0	0	0	0
30	Y	31	0	0	0	0
30	Z	29	0	0	2	0
All	All	34258	0	32062	342	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 (342) 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)
20:N:610[A]:PER:O2	20:N:610[A]:PER:O1	1.54	1.25
20:A:608[A]:PER:O2	20:A:608[A]:PER:O1	1.55	1.25
1:N:311[A]:ILE:HG22	26:N:601:CDL:H441	1.58	0.85
3:P:224[B]:LYS:HE2	26:P:304:CDL:H131	1.62	0.82
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.47	0.79
12:L:20:ARG:HH21	22:L:103:TGL:HC32	1.47	0.79
12:L:20:ARG:HH22	22:L:103:TGL:HC72	1.49	0.78
19:A:607:PSC:H242	2:B:56:MET:HB3	1.65	0.77
3:P:62:ILE:HD12	26:P:304:CDL:H522	1.65	0.77
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.67	0.76
21:O:305:EDO:H21	8:U:24:ASN:HD21	1.49	0.75
3:C:213:THR:HG23	26:C:305:CDL:H771	1.69	0.74
3:P:33[A]:MET:HG2	25:P:309:DMU:H12	1.70	0.73
3:P:59:ARG:HG3	26:P:304:CDL:H512	1.71	0.72
2:B:94:SER:HB2	2:B:148[B]:MET:HE3	1.72	0.71
10:W:41:GLY:HA3	25:W:101:DMU:H23	1.71	0.71
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.31	0.70
6:F:54[A]:ASN:ND2	30:F:201:HOH:O	2.24	0.70
7:G:1:ALA:HB2	18:G:102:PGV:H342	1.74	0.70
1:N:169:ILE:HG13	1:N:189[B]:MET:HE1	1.73	0.69
1:A:302[B]:ARG:NH1	30:A:701:HOH:O	2.25	0.68
11:K:22:ALA:O	11:K:26[B]:VAL:HG22	1.93	0.68
6:S:85:CYS:SG	6:S:87:THR:HG23	2.34	0.68
3:P:33[A]:MET:SD	25:P:309:DMU:H8	2.34	0.67
1:A:321[A]:PHE:CD2	2:B:65:TRP:HB2	2.29	0.66
3:P:33[A]:MET:HE2	3:P:42:LEU:HB2	1.76	0.65
8:U:7:LYS:O	8:U:9:LYS:N	2.26	0.65
3:P:33[B]:MET:HE2	3:P:42:LEU:HB2	1.78	0.64
25:P:309:DMU:H11	10:W:49:CYS:HB3	1.79	0.64
25:K:104:DMU:H20	25:K:106:DMU:H11	1.79	0.64
25:C:310:DMU:H11	10:J:49:CYS:HB3	1.78	0.63
27:C:307:PEK:H101	27:C:307:PEK:H42	1.79	0.63
12:L:14:SER:H	22:L:103:TGL:HC31	1.63	0.63
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.81	0.63
1:N:113:LEU:HB2	22:N:612:TGL:H301	1.80	0.62
9:I:36:LYS:O	9:I:41:GLU:HB2	1.99	0.62
1:N:289:ALA:HB1	1:N:297[C]:MET:HE1	1.81	0.62
3:P:213:THR:HG23	26:P:304:CDL:H772	1.82	0.62
22:N:609:TGL:H312	22:N:609:TGL:H201	1.81	0.62
27:P:306:PEK:H101	27:P:306:PEK:H42	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:4:SER:HB2	30:D:363:HOH:O	1.99	0.62
12:L:20:ARG:NH2	22:L:103:TGL:HC52	2.16	0.61
3:P:33[A]:MET:HG2	25:P:309:DMU:C25	2.30	0.61
24:L:102:CHD:H232	13:M:21:VAL:HG21	1.83	0.60
26:T:101:CDL:H602	26:T:101:CDL:H782	1.83	0.60
3:C:51[A]:MET:SD	26:C:305:CDL:H622	2.42	0.60
19:A:607:PSC:H222	2:B:52:HIS:HE1	1.68	0.58
6:F:92[A]:VAL:HG21	30:F:345:HOH:O	2.03	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.85	0.57
4:D:78:TRP:CA	22:D:202:TGL:HB32	2.35	0.57
3:C:165:ILE:HG12	27:C:309:PEK:H9	1.87	0.57
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.57
1:N:112:LEU:HD23	1:N:112:LEU:C	2.30	0.57
22:N:611:TGL:HA32	22:N:611:TGL:HB51	1.87	0.57
1:N:24:ALA:HB2	14:N:602[A]:HEA:H253	1.87	0.56
22:N:611:TGL:H232	2:O:42:ILE:HG21	1.86	0.56
4:Q:98:TRP:HB2	25:Q:201:DMU:H18	1.86	0.56
9:V:63:MET:HB3	9:V:68:ILE:HG12	1.88	0.56
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.56
10:W:57:HIS:O	10:W:58:LYS:HB3	2.05	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.56
30:C:408:HOH:O	6:F:52:ILE:HD11	2.06	0.56
8:H:43:MET:HE1	8:U:43:MET:HE1	1.87	0.56
1:N:113:LEU:HB2	22:N:612:TGL:H322	1.87	0.55
3:P:33[B]:MET:SD	25:P:309:DMU:H8	2.46	0.55
3:P:168:THR:HG22	27:P:308:PEK:H14	1.87	0.55
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.37	0.55
1:A:334:TRP:HZ3	22:D:202:TGL:HA72	1.72	0.55
1:N:35[A]:LEU:HD11	1:N:462:LEU:HB2	1.88	0.55
30:N:918:HOH:O	4:Q:20:ARG:HG2	2.07	0.55
1:N:297[C]:MET:SD	1:N:302:ARG:HG2	2.47	0.55
26:T:101:CDL:H601	26:T:101:CDL:H762	1.88	0.54
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.37	0.54
2:O:129:LYS:NZ	30:O:403:HOH:O	2.41	0.54
2:B:22:HIS:HB3	30:I:154:HOH:O	2.07	0.54
26:T:101:CDL:H752	26:T:101:CDL:H212	1.89	0.54
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.89	0.54
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.07	0.54
22:D:202:TGL:HA41	22:D:202:TGL:HB52	1.89	0.53
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.90	0.53
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:49:ASP:O	8:H:52:VAL:HG22	2.09	0.53
4:D:94:LEU:HB3	25:D:201:DMU:H18	1.91	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.91	0.53
30:A:732:HOH:O	12:L:7:PRO:HG3	2.09	0.53
7:G:83[B]:GLU:HB3	7:G:84:LYS:HG2	1.90	0.52
1:A:40:GLU:HG2	1:A:54[B]:TYR:CD1	2.44	0.52
10:J:55:PHE:HE1	25:L:101:DMU:H29	1.73	0.52
2:O:64[A]:ILE:HD11	19:O:303:PSC:H141	1.91	0.52
4:D:78:TRP:HA	22:D:202:TGL:HB32	1.91	0.52
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.39	0.52
10:J:4:ARG:NH1	30:J:202:HOH:O	2.43	0.52
5:R:80:GLU:OE1	5:R:80:GLU:N	2.43	0.52
2:O:60[A]:GLU:OE2	30:O:401:HOH:O	2.19	0.52
1:A:302[B]:ARG:HE	2:B:84:LEU:HD11	1.75	0.52
1:A:486[B]:ASP:OD2	4:D:19[B]:ARG:HD3	2.10	0.52
12:L:47:LYS:HA	12:L:47:LYS:HE3	1.92	0.51
4:D:78:TRP:HB3	22:D:202:TGL:HB32	1.92	0.51
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.92	0.51
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.10	0.51
2:B:164:ALA:O	2:B:194:GLY:HA3	2.10	0.51
3:P:178:ALA:HB2	27:P:306:PEK:H202	1.92	0.51
1:A:334:TRP:CZ3	22:D:202:TGL:HA52	2.46	0.51
1:N:334:TRP:CE3	22:N:611:TGL:HA31	2.46	0.51
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.93	0.51
11:K:26[B]:VAL:HG23	30:K:223:HOH:O	2.10	0.51
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.92	0.50
26:C:305:CDL:H642	18:C:308:PGV:H12	1.94	0.50
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.46	0.50
12:L:26:THR:HG23	13:M:25:SER:HB3	1.92	0.50
25:K:102:DMU:H18	25:K:105:DMU:H13	1.94	0.50
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.92	0.50
7:G:83[A]:GLU:HB2	7:G:84:LYS:HG2	1.94	0.50
1:A:348:PHE:CE1	1:A:380[B]:VAL:HG22	2.47	0.49
4:D:19[B]:ARG:HH11	4:D:21:ASP:CG	2.20	0.49
22:N:611:TGL:HA92	22:N:611:TGL:H231	1.92	0.49
1:N:514:LYS:HG2	6:S:38:ALA:CB	2.42	0.49
3:P:165:ILE:HG12	27:P:308:PEK:H11	1.95	0.49
12:L:24:MET:HG3	30:L:221:HOH:O	2.11	0.49
3:C:210:ILE:HG12	18:C:308:PGV:H132	1.94	0.49
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.95	0.49
3:P:80[A]:ARG:HG2	3:P:240:TRP:HH2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD13	1:A:381[B]:LEU:HD11	1.95	0.49
1:A:472:ILE:HG21	22:L:103:TGL:HA91	1.95	0.49
3:C:99:TRP:CZ3	18:C:311:PGV:H271	2.48	0.49
13:Z:41:LYS:HE2	30:Z:201:HOH:O	2.12	0.49
12:L:25:MET:HG2	22:L:103:TGL:HA62	1.95	0.49
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.47	0.48
30:N:790:HOH:O	21:O:305:EDO:H11	2.12	0.48
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.95	0.48
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.48
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.95	0.48
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.95	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.48
2:O:84:LEU:HA	2:O:87:MET:HE2	1.95	0.48
8:U:43:MET:HE3	8:U:48:GLY:HA3	1.95	0.48
12:L:26:THR:HG23	13:M:25:SER:CB	2.43	0.48
5:E:90:ARG:HD2	30:E:402:HOH:O	2.13	0.48
26:T:101:CDL:H762	26:T:101:CDL:C60	2.43	0.48
4:D:78:TRP:CB	22:D:202:TGL:HB32	2.44	0.48
22:N:609:TGL:H222	22:N:609:TGL:H271	1.95	0.48
14:N:603:HEA:H243	2:O:69:PRO:HB3	1.94	0.48
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.49	0.48
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.40	0.48
22:L:103:TGL:HA92	22:L:103:TGL:H221	1.68	0.48
1:A:302[B]:ARG:CZ	1:A:361[B]:SER:OG	2.62	0.47
5:E:94:ASN:HB3	30:E:427:HOH:O	2.14	0.47
6:F:50:PRO:HG2	30:F:277:HOH:O	2.15	0.47
4:Q:146:LYS:NZ	30:Q:302:HOH:O	2.46	0.47
5:E:46:LYS:NZ	30:E:301:HOH:O	2.28	0.47
26:T:101:CDL:H212	26:T:101:CDL:H732	1.96	0.47
26:C:305:CDL:H851	26:C:305:CDL:H822	1.50	0.47
8:U:9:LYS:HB3	8:U:10:ASN:H	1.48	0.47
1:A:321[A]:PHE:HB3	2:B:65:TRP:CE3	2.49	0.47
22:B:301:TGL:H142	22:B:301:TGL:H112	1.33	0.47
8:H:45:ALA:O	8:H:47:GLY:N	2.47	0.47
1:N:297[C]:MET:CG	1:N:302:ARG:HG3	2.45	0.47
2:O:68:LEU:HD23	19:O:303:PSC:H171	1.97	0.47
1:A:131:PRO:HB3	21:A:613:EDO:H12	1.97	0.47
25:D:201:DMU:H26	25:M:101:DMU:H8	1.97	0.47
1:N:1:FME:HE2	12:Y:3:TYR:CE1	2.50	0.46
9:V:36:LYS:HD2	9:V:40:ALA:HB3	1.96	0.46
3:C:90[B]:GLU:OE2	18:C:301:PGV:H321	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:608:PGV:H183	27:P:306:PEK:H342	1.96	0.46
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.77	0.46
3:C:58:TRP:HB2	26:C:305:CDL:H551	1.97	0.46
1:N:242:GLU:HA	1:N:245:ILE:HD12	1.96	0.46
1:N:514:LYS:HD2	30:S:270:HOH:O	2.16	0.46
18:N:607:PGV:H11	4:Q:84:ALA:CB	2.45	0.46
22:N:609:TGL:HC42	22:N:609:TGL:H152	1.97	0.46
2:O:13:THR:HB	2:O:168:LEU:HD23	1.96	0.46
4:Q:4:SER:N	30:Q:304:HOH:O	2.47	0.46
3:P:47:LEU:O	3:P:51[B]:MET:HG2	2.16	0.46
1:A:240:HIS:CD2	1:A:240:HIS:C	2.94	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
2:B:70:ALA:HB1	26:T:101:CDL:H441	1.98	0.46
18:G:102:PGV:H71	18:G:102:PGV:H42	1.60	0.46
8:H:9:LYS:HD2	8:H:11:TYR:HB2	1.98	0.46
19:A:607:PSC:H231	19:A:607:PSC:H262	1.75	0.45
6:S:87:THR:HG22	30:S:333:HOH:O	2.16	0.45
4:D:98:TRP:CE2	25:M:101:DMU:H11	2.51	0.45
11:K:26[A]:VAL:HG13	25:K:101:DMU:H11	1.98	0.45
24:Y:101:CHD:H112	24:Y:101:CHD:H12A	1.51	0.45
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.52	0.45
3:P:210:ILE:HG23	18:P:307:PGV:H91	1.99	0.45
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.99	0.45
1:A:452:THR:HG22	1:A:456:MET:HE3	1.98	0.45
21:J:103:EDO:H12	30:J:215:HOH:O	2.15	0.45
3:P:257:TYR:O	3:P:261:SER:HB3	2.16	0.45
19:A:607:PSC:H342	2:B:41:ILE:HD13	1.99	0.45
21:C:320:EDO:H21	30:J:204:HOH:O	2.16	0.45
1:N:514:LYS:HG2	6:S:38:ALA:HB2	1.98	0.45
22:N:611:TGL:H231	22:N:611:TGL:CA9	2.47	0.45
1:A:321[A]:PHE:CE2	2:B:65:TRP:HB2	2.52	0.45
5:E:6:GLU:OE1	5:E:14:ARG:NH2	2.46	0.45
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.98	0.44
1:N:488:THR:HB	1:N:495:LEU:HD13	1.99	0.44
3:P:80[A]:ARG:HG2	3:P:240:TRP:CH2	2.51	0.44
22:D:202:TGL:OG3	22:D:202:TGL:HC42	2.18	0.44
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.99	0.44
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.66	0.44
2:O:29[B]:MET:HE1	25:O:302:DMU:H13	2.00	0.44
1:A:112:LEU:C	1:A:112:LEU:HD23	2.42	0.44
22:L:103:TGL:CC1	22:L:103:TGL:HC61	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:92[A]:VAL:HG23	30:F:205:HOH:O	2.17	0.44
2:B:1:FME:HE1	2:B:133:LEU:HD22	1.99	0.44
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.99	0.44
25:P:303:DMU:H25	25:P:303:DMU:H18	1.63	0.44
2:B:60[A]:GLU:H	2:B:60[A]:GLU:CD	2.24	0.44
10:J:41:GLY:HA3	25:J:101:DMU:H23	2.00	0.44
22:N:609:TGL:HB32	22:N:609:TGL:HB61	1.88	0.43
3:P:33[B]:MET:HG2	3:P:39:SER:HB3	2.00	0.43
26:N:601:CDL:H582	26:N:601:CDL:H771	2.00	0.43
1:A:46:THR:HG22	1:A:49[B]:GLY:H	1.82	0.43
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.99	0.43
1:A:481:GLU:HB2	13:M:4:LYS:HD2	2.00	0.43
2:O:83:ILE:O	2:O:87:MET:HG3	2.18	0.43
8:U:60:TYR:CD1	8:U:60:TYR:C	2.96	0.43
1:A:406:ASN:ND2	18:A:606:PGV:H22	2.26	0.43
3:C:54[B]:MET:HE1	18:C:308:PGV:H142	1.99	0.43
10:J:45:TYR:OH	25:J:101:DMU:H7	2.18	0.43
1:A:169:ILE:HD11	1:A:189:MET:HE1	2.00	0.43
8:H:31:GLN:NE2	30:H:201:HOH:O	2.37	0.43
11:K:54:ARG:HE	11:K:54:ARG:HB3	1.54	0.43
3:P:116:TRP:HA	3:P:117:PRO:C	2.43	0.43
2:O:82[C]:ARG:HD3	30:O:402:HOH:O	2.17	0.43
9:V:2:THR:HB	9:V:3:ALA:H	1.63	0.43
27:C:307:PEK:H041	7:G:70[B]:PHE:HB2	2.00	0.43
3:P:22:LEU:O	3:P:26:LEU:HG	2.18	0.43
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.01	0.43
1:N:365:ILE:HD11	30:N:708:HOH:O	2.19	0.43
3:C:33:MET:HE3	25:C:310:DMU:O16	2.19	0.43
1:A:293:PHE:O	1:A:302[B]:ARG:NH1	2.52	0.43
1:N:266:GLU:OE1	21:S:106:EDO:H11	2.18	0.43
1:N:308:ALA:O	1:N:311[A]:ILE:HG12	2.19	0.43
2:B:227:LEU:HD21	30:B:501:HOH:O	2.19	0.42
24:L:102:CHD:H183	24:L:102:CHD:H212	2.01	0.42
3:C:99:TRP:CE2	18:C:311:PGV:H232	2.55	0.42
25:C:303:DMU:H23	27:C:307:PEK:H282	2.01	0.42
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.01	0.42
5:R:6:GLU:HB2	5:R:10:GLU:HB2	2.00	0.42
18:N:608:PGV:H343	27:P:306:PEK:C37	2.49	0.42
1:A:120:ALA:HB2	21:A:615:EDO:H12	2.01	0.42
2:B:13:THR:HB	2:B:168:LEU:HD23	2.02	0.42
2:B:132:GLU:HB3	2:B:137:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:449:MET:SD	2:O:5:MET:HG2	2.59	0.42
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.54	0.42
18:P:307:PGV:H131	18:P:307:PGV:H101	1.66	0.42
12:Y:26:THR:HA	30:Z:211:HOH:O	2.19	0.42
1:A:110:LEU:HD21	25:C:310:DMU:H24	2.01	0.42
3:P:168:THR:HG21	27:P:308:PEK:H12	2.00	0.42
2:B:5:MET:HB3	2:B:5:MET:HE2	1.85	0.42
6:F:64:GLU:O	6:F:65:ASP:HB2	2.20	0.42
9:I:36:LYS:HE2	9:I:36:LYS:HB2	1.68	0.42
24:L:102:CHD:H8	24:L:102:CHD:H182	1.84	0.42
19:O:303:PSC:H302	19:O:303:PSC:H111	2.02	0.42
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.73	0.42
1:A:336:PRO:HB2	1:A:394[B]:VAL:HG11	2.01	0.42
2:B:49:LYS:HE3	22:D:202:TGL:HC71	2.02	0.42
4:D:19[B]:ARG:NE	4:D:21:ASP:OD1	2.47	0.42
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.01	0.42
1:A:302[A]:ARG:HH11	1:A:302[A]:ARG:HD2	1.61	0.42
27:C:307:PEK:H221	27:C:307:PEK:H251	1.82	0.42
8:H:45:ALA:C	8:H:47:GLY:H	2.27	0.42
1:N:240:HIS:CD2	1:N:240:HIS:C	2.98	0.42
6:S:9:ASP:OD2	30:S:201:HOH:O	2.22	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.41
2:O:58:ALA:O	2:O:62:GLU:HG3	2.21	0.41
2:B:1:FME:HE1	2:B:133:LEU:CD2	2.50	0.41
3:C:59:ARG:HA	26:C:305:CDL:H512	2.02	0.41
1:N:114:ALA:HA	10:W:50:LEU:HD21	2.02	0.41
14:A:602:HEA:H243	2:B:69:PRO:HB3	2.03	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.41
1:N:321:PHE:HB3	2:O:65[A]:TRP:CE3	2.54	0.41
2:O:218:TYR:HB3	30:O:436:HOH:O	2.20	0.41
19:O:303:PSC:H262	19:O:303:PSC:H291	1.76	0.41
7:T:84:LYS:HE2	7:T:84:LYS:HB2	1.88	0.41
1:A:302[B]:ARG:HH21	2:B:84:LEU:CD1	2.33	0.41
1:N:28:MET:CE	14:N:602[C]:HEA:H271	2.50	0.41
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.55	0.41
26:T:101:CDL:OB6	26:T:101:CDL:H151	2.20	0.41
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.19	0.41
1:N:35[B]:LEU:HD22	1:N:462:LEU:HD22	2.02	0.41
1:N:117[B]:MET:HE3	1:N:117[B]:MET:HB3	1.99	0.41
2:O:5:MET:HB3	2:O:5:MET:HE2	1.75	0.41
3:P:219:PHE:CE2	3:P:223[A]:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:308:PEK:H222	7:T:21:PHE:CG	2.55	0.41
1:A:280:ILE:HG23	1:A:312[A]:ILE:HD11	2.02	0.41
14:A:601[A]:HEA:H211	14:A:601[A]:HEA:H271	1.85	0.41
5:E:6:GLU:H	5:E:6:GLU:HG2	1.55	0.41
1:N:54[A]:TYR:HB2	30:N:756[A]:HOH:O	2.19	0.41
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.21	0.41
1:A:1:FME:HE2	1:A:1:FME:HA	2.02	0.41
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.56	0.41
9:I:73:LYS:HE2	30:I:163:HOH:O	2.20	0.41
8:H:46:LYS:HG2	8:U:52:VAL:HA	2.01	0.41
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.94	0.41
3:C:161[A]:GLN:NE2	27:C:309:PEK:H41	2.36	0.41
25:C:310:DMU:H4	10:J:52:TRP:CZ2	2.56	0.41
24:G:101:CHD:H212	24:G:101:CHD:H12	2.02	0.41
12:L:19:TRP:CD2	24:L:102:CHD:O12	2.74	0.41
1:N:380[A]:VAL:HG21	14:N:603:HEA:C3C	2.51	0.41
1:N:422:ASN:HB3	22:N:609:TGL:H221	2.03	0.41
22:N:609:TGL:HB72	2:O:32[A]:PHE:CE2	2.56	0.41
5:R:43:PRO:HB2	5:R:48:ILE:HD11	2.03	0.41
27:C:309:PEK:H221	7:G:21:PHE:CD1	2.56	0.41
21:W:102:EDO:H12	30:W:204:HOH:O	2.21	0.41
4:Q:114:GLU:CD	11:X:51:LYS:HE2	2.46	0.40
4:Q:127:LYS:HD2	30:V:153:HOH:O	2.21	0.40
8:U:20:PHE:HE1	8:U:27:ARG:HG2	1.85	0.40
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.18	0.40
18:N:608:PGV:H343	27:P:306:PEK:H381	2.03	0.40
2:O:206:PHE:CE1	21:O:306:EDO:H21	2.55	0.40
11:K:40:TRP:CD2	25:K:103:DMU:H14	2.57	0.40
3:P:117:PRO:HA	3:P:118:PRO:HD3	1.94	0.40
4:Q:68:PHE:HA	4:Q:71:MET:HE3	2.02	0.40
14:A:601[C]:HEA:H212	14:A:601[C]:HEA:H271	1.86	0.40
3:C:117:PRO:HA	3:C:118:PRO:HD3	1.98	0.40
27:C:309:PEK:C37	26:N:601:CDL:H273	2.52	0.40
4:D:120:THR:HG21	11:K:48[B]:VAL:CG1	2.52	0.40
5:E:108:LYS:HE2	5:E:108:LYS:HB2	1.85	0.40
3:P:149:HIS:NE2	21:P:310:EDO:H12	2.36	0.40
12:L:20:ARG:HH22	22:L:103:TGL:HC52	1.82	0.40
1:N:35[B]:LEU:HD23	25:Z:101:DMU:H24	2.04	0.40
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	2.01	0.40
22:N:612:TGL:H222	22:N:612:TGL:HA91	1.71	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	545/514 (106%)	530 (97%)	15 (3%)	0	100	100
1	N	550/514 (107%)	538 (98%)	12 (2%)	0	100	100
2	B	232/227 (102%)	227 (98%)	5 (2%)	0	100	100
2	O	236/227 (104%)	229 (97%)	6 (2%)	1 (0%)	30	15
3	C	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
3	P	269/259 (104%)	264 (98%)	5 (2%)	0	100	100
4	D	145/144 (101%)	142 (98%)	3 (2%)	0	100	100
4	Q	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
5	E	103/105 (98%)	103 (100%)	0	0	100	100
5	R	104/105 (99%)	103 (99%)	1 (1%)	0	100	100
6	F	97/94 (103%)	95 (98%)	2 (2%)	0	100	100
6	S	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
7	G	86/84 (102%)	77 (90%)	4 (5%)	5 (6%)	1	0
7	T	82/84 (98%)	72 (88%)	5 (6%)	5 (6%)	1	0
8	H	78/79 (99%)	70 (90%)	5 (6%)	3 (4%)	2	0
8	U	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	9	2
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	2 (3%)	1 (1%)	9	2
10	J	57/58 (98%)	56 (98%)	1 (2%)	0	100	100
10	W	56/58 (97%)	56 (100%)	0	0	100	100
11	K	50/49 (102%)	48 (96%)	2 (4%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	45/46 (98%)	43 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
All	All	3632/3550 (102%)	3525 (97%)	91 (2%)	16 (0%)	24	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	37	LEU
7	T	4	ALA
7	T	5	LYS
8	U	8	ILE
8	H	46	LYS
7	T	3	ALA
7	G	5	LYS
7	T	7	ASP
8	H	45	ALA
9	V	2	THR
7	T	6	GLY
8	H	48	GLY
2	O	92	ASN
7	G	6	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	456/426 (107%)	447 (98%)	9 (2%)	48	29
1	N	460/426 (108%)	457 (99%)	3 (1%)	76	67
2	B	217/210 (103%)	209 (96%)	8 (4%)	30	11
2	O	221/210 (105%)	207 (94%)	14 (6%)	16	3
3	C	236/224 (105%)	232 (98%)	4 (2%)	53	36
3	P	236/224 (105%)	233 (99%)	3 (1%)	61	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	131/128 (102%)	129 (98%)	2 (2%)	57	41
4	Q	129/128 (101%)	124 (96%)	5 (4%)	28	9
5	E	92/92 (100%)	90 (98%)	2 (2%)	45	26
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	79 (95%)	4 (5%)	23	6
6	S	78/78 (100%)	74 (95%)	4 (5%)	21	5
7	G	72/68 (106%)	63 (88%)	9 (12%)	4	0
7	T	68/68 (100%)	62 (91%)	6 (9%)	9	1
8	H	72/71 (101%)	65 (90%)	7 (10%)	8	1
8	U	71/71 (100%)	64 (90%)	7 (10%)	7	1
9	I	58/57 (102%)	53 (91%)	5 (9%)	10	1
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	5
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	27	8
11	K	42/39 (108%)	41 (98%)	1 (2%)	43	23
11	X	39/39 (100%)	38 (97%)	1 (3%)	40	20
12	L	40/39 (103%)	39 (98%)	1 (2%)	42	22
12	Y	39/39 (100%)	35 (90%)	4 (10%)	7	0
13	M	37/37 (100%)	37 (100%)	0	100	100
13	Z	37/37 (100%)	36 (97%)	1 (3%)	39	19
All	All	3163/3036 (104%)	3058 (97%)	105 (3%)	34	13

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	138	HIS
1	A	178	GLN
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER
1	A	382[C]	SER
1	A	486[A]	ASP
1	A	486[B]	ASP
2	B	33	LEU

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Mol	Chain	Res	Type
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP
3	C	40	MET
3	C	76	GLN
3	C	159	MET
3	C	230	ASN
4	D	74	SER
4	D	147	LYS
5	E	70	VAL
5	E	90	ARG
6	F	26	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80	GLN
7	G	2	SER
7	G	5	LYS
7	G	7	ASP
7	G	11	THR
7	G	33[A]	LEU
7	G	33[B]	LEU
7	G	43	GLU
7	G	83[A]	GLU
7	G	83[B]	GLU
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	46	LYS
8	H	51	SER
8	H	60	TYR
8	H	61	LYS
9	I	2	THR
9	I	15	ARG
9	I	29	LEU
9	I	36	LYS
9	I	41	GLU
11	K	54	ARG
12	L	47	LYS

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Mol	Chain	Res	Type
1	N	138	HIS
1	N	363	LEU
1	N	369	ASP
2	O	33	LEU
2	O	59	GLN
2	O	64[A]	ILE
2	O	64[B]	ILE
2	O	68	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	115	ASP
2	O	158	ASP
2	O	223	SER
2	O	225	SER
2	O	226	MET
2	O	227	LEU
3	P	76	GLN
3	P	159	MET
3	P	230	ASN
4	Q	8	SER
4	Q	20	ARG
4	Q	51	LEU
4	Q	58	GLU
4	Q	143	ASN
6	S	2	SER
6	S	37	LYS
6	S	80	GLN
6	S	93	PRO
7	T	2	SER
7	T	11	THR
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
8	U	8	ILE
8	U	9	LYS
8	U	10	ASN
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS

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Mol	Chain	Res	Type
9	V	2	THR
9	V	18	ARG
9	V	29	LEU
10	W	50	LEU
10	W	58	LYS
11	X	47	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
12	Y	46	LYS
13	Z	38	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	178	GLN
1	A	422	ASN
2	B	140	ASN
2	B	181	GLN
4	D	29	HIS
4	D	76	ASN
4	D	119	GLN
6	F	94	HIS
8	H	31	GLN
9	I	53	ASN
1	N	80	ASN
1	N	98	ASN
1	N	170	ASN
1	N	422	ASN
2	O	10	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
8	U	12	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	1.01	1 (12%)	7,9,11	1.86	2 (28%)
2	FME	O	1	2	8,9,10	0.80	0	7,9,11	1.54	2 (28%)
9	SAC	I	1	9	7,8,9	0.68	0	8,9,11	1.42	1 (12%)
9	SAC	V	1	9	7,8,9	0.61	0	8,9,11	0.90	0
1	FME	N	1	1	8,9,10	0.56	0	7,9,11	1.47	1 (14%)
1	FME	A	1	1	8,9,10	0.47	0	7,9,11	1.26	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	0/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	2/7/8/10	-
9	SAC	V	1	9	-	4/7/8/10	-
1	FME	N	1	1	-	3/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CG-SD	-2.03	1.70	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-3.36	103.62	112.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CG-CB-CA	-2.67	105.52	112.95
1	N	1	FME	O-C-CA	-2.67	117.79	124.78
9	I	1	SAC	CA-N-C1A	-2.58	118.38	123.15
2	B	1	FME	C-CA-N	-2.46	105.29	109.73
2	O	1	FME	O1-CN-N	-2.27	119.30	125.27
1	A	1	FME	C-CA-N	2.12	113.55	109.73

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	N-CA-CB-OG
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	N-CA-CB-OG
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 150 ligands modelled in this entry, 10 are monoatomic - leaving 140 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	$\# Z > 2$
21	EDO	P	313	-	3,3,3	0.80	0	2,2,2	0.15	0
21	EDO	C	314	-	3,3,3	0.84	0	2,2,2	0.40	0
21	EDO	P	315	-	3,3,3	0.40	0	2,2,2	1.15	0
22	TGL	B	301	-	47,47,62	1.16	3 (6%)	50,50,65	1.47	5 (10%)
21	EDO	N	617	-	3,3,3	0.51	0	2,2,2	0.36	0
18	PGV	A	606	-	20,20,50	0.51	0	18,18,56	0.78	0
25	DMU	W	101	-	10,10,34	0.38	0	9,9,45	0.54	0
22	TGL	N	611	-	45,45,62	0.36	0	42,42,65	0.44	0
29	PO4	H	101	-	4,4,4	0.77	0	6,6,6	0.66	0
25	DMU	O	302	-	10,10,34	0.20	0	9,9,45	0.72	0
18	PGV	C	308	-	47,47,50	0.84	1 (2%)	50,53,56	0.93	3 (6%)
21	EDO	A	618	-	3,3,3	0.70	0	2,2,2	0.78	0
25	DMU	X	103	-	8,8,34	0.40	0	7,7,45	0.53	0
25	DMU	P	309	-	10,10,34	0.33	0	9,9,45	0.55	0
14	HEA	A	602	1,20,30	66,67,67	1.79	20 (30%)	78,103,103	1.98	21 (26%)
25	DMU	C	303	-	12,12,34	0.54	0	10,11,45	0.35	0
18	PGV	C	301	-	50,50,50	0.94	4 (8%)	53,56,56	1.21	4 (7%)
21	EDO	C	319	-	3,3,3	0.60	0	2,2,2	0.16	0
21	EDO	P	316	-	3,3,3	0.58	0	2,2,2	0.42	0
21	EDO	Y	102	-	3,3,3	0.46	0	2,2,2	0.21	0
21	EDO	N	621	-	3,3,3	0.56	0	2,2,2	0.09	0
21	EDO	N	616	-	3,3,3	0.47	0	2,2,2	0.50	0
18	PGV	C	311	-	26,26,50	1.17	1 (3%)	25,25,56	2.06	5 (20%)
21	EDO	B	306	-	3,3,3	0.82	0	2,2,2	0.33	0
21	EDO	B	305	-	3,3,3	0.41	0	2,2,2	0.78	0
29	PO4	U	101	-	4,4,4	1.14	0	6,6,6	0.76	0
21	EDO	N	615	-	3,3,3	0.58	0	2,2,2	0.12	0
25	DMU	P	303	-	11,11,34	0.43	0	10,10,45	0.37	0
25	DMU	J	101	-	10,10,34	0.36	0	9,9,45	0.39	0
25	DMU	K	103	-	10,10,34	0.40	0	9,9,45	0.48	0
21	EDO	F	104	-	3,3,3	0.58	0	2,2,2	0.68	0
27	PEK	P	306	-	52,52,52	0.75	2 (3%)	55,57,57	1.09	4 (7%)
14	HEA	N	602[A]	-	66,67,67	1.64	15 (22%)	78,103,103	1.87	24 (30%)
24	CHD	G	101	-	32,32,32	0.90	0	51,51,51	1.30	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	PGV	G	102	-	30,30,50	0.98	1 (3%)	28,29,56	1.48	3 (10%)
21	EDO	S	106	-	3,3,3	0.43	0	2,2,2	0.79	0
14	HEA	N	602[C]	-	66,58,67	3.25	15 (22%)	78,91,103	3.55	29 (37%)
24	CHD	P	301	-	32,32,32	0.78	0	51,51,51	1.52	8 (15%)
19	PSC	A	607	-	25,25,51	0.81	1 (4%)	22,23,59	0.93	0
21	EDO	W	102	-	3,3,3	0.34	0	2,2,2	0.24	0
24	CHD	Y	101	-	32,32,32	0.77	0	51,51,51	2.34	18 (35%)
21	EDO	T	102	-	3,3,3	0.65	0	2,2,2	0.77	0
25	DMU	C	310	-	21,21,34	0.88	1 (4%)	24,25,45	1.35	3 (12%)
21	EDO	S	104	-	3,3,3	0.50	0	2,2,2	0.23	0
21	EDO	P	314	-	3,3,3	0.44	0	2,2,2	0.87	0
25	DMU	K	106	-	9,9,34	0.28	0	8,8,45	0.32	0
26	CDL	P	304	-	57,57,99	1.22	7 (12%)	54,54,111	1.05	4 (7%)
20	PER	N	610[A]	14,15	1,1,1	1.17	0	-		
26	CDL	N	601	-	51,51,99	1.20	8 (15%)	47,47,111	0.88	1 (2%)
27	PEK	C	306	-	23,23,52	0.39	0	21,21,57	0.42	0
21	EDO	S	102	-	3,3,3	0.80	0	2,2,2	0.74	0
21	EDO	F	106	-	3,3,3	0.68	0	2,2,2	0.76	0
18	PGV	N	607	-	22,22,50	0.36	0	20,20,56	0.52	0
21	EDO	A	612	-	3,3,3	0.79	0	2,2,2	0.67	0
21	EDO	P	311	-	3,3,3	0.46	0	2,2,2	0.31	0
26	CDL	C	305	-	54,54,99	1.04	5 (9%)	50,50,111	1.12	5 (10%)
21	EDO	A	617	-	3,3,3	0.62	0	2,2,2	0.13	0
25	DMU	L	101	-	21,21,34	0.66	1 (4%)	24,25,45	2.46	6 (25%)
21	EDO	F	103	6	3,3,3	0.63	0	2,2,2	0.17	0
25	DMU	K	105	-	8,8,34	0.24	0	7,7,45	0.61	0
21	EDO	C	313	-	3,3,3	0.70	0	2,2,2	0.61	0
27	PEK	C	309	-	34,34,52	0.35	0	32,32,57	0.62	0
21	EDO	B	304	-	3,3,3	0.63	0	2,2,2	0.34	0
21	EDO	G	103	-	3,3,3	0.62	0	2,2,2	0.55	0
19	PSC	O	303	-	28,28,51	1.15	2 (7%)	27,27,59	1.08	3 (11%)
21	EDO	Q	202	-	3,3,3	0.46	0	2,2,2	0.64	0
22	TGL	N	612	-	43,43,62	1.18	2 (4%)	45,45,65	1.60	8 (17%)
22	TGL	N	609	-	62,62,62	1.13	3 (4%)	65,65,65	1.07	4 (6%)
21	EDO	N	618	-	3,3,3	0.50	0	2,2,2	0.36	0
21	EDO	D	206	-	3,3,3	0.56	0	2,2,2	0.13	0
18	PGV	P	307	-	50,50,50	0.69	2 (4%)	53,56,56	1.09	5 (9%)
21	EDO	O	304	-	3,3,3	0.66	0	2,2,2	0.30	0
25	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.03	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	C	312	-	3,3,3	0.47	0	2,2,2	0.14	0
21	EDO	C	320	-	3,3,3	0.68	0	2,2,2	0.53	0
21	EDO	D	204	-	3,3,3	0.57	0	2,2,2	0.13	0
27	PEK	P	308	-	32,32,52	0.43	0	29,30,57	0.57	0
27	PEK	C	307	-	52,52,52	0.84	2 (3%)	55,57,57	1.07	3 (5%)
21	EDO	C	315	-	3,3,3	0.39	0	2,2,2	1.06	0
24	CHD	C	304	-	32,32,32	0.90	1 (3%)	51,51,51	1.52	7 (13%)
21	EDO	A	609	-	3,3,3	0.57	0	2,2,2	0.60	0
21	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.28	0
21	EDO	P	317	-	3,3,3	0.55	0	2,2,2	0.17	0
21	EDO	F	105	-	3,3,3	0.58	0	2,2,2	0.36	0
22	TGL	D	202	-	56,56,62	1.17	3 (5%)	59,59,65	1.13	5 (8%)
25	DMU	M	101	-	34,34,34	0.57	0	45,45,45	1.28	4 (8%)
21	EDO	O	305	-	3,3,3	0.56	0	2,2,2	0.13	0
21	EDO	C	318	-	3,3,3	0.56	0	2,2,2	0.49	0
21	EDO	T	104	-	3,3,3	0.72	0	2,2,2	0.41	0
25	DMU	X	102	-	9,9,34	0.39	0	8,8,45	0.37	0
27	PEK	P	305	-	19,19,52	0.30	0	18,18,57	0.57	0
21	EDO	F	102	-	3,3,3	0.98	0	2,2,2	0.54	0
21	EDO	Y	103	-	3,3,3	0.50	0	2,2,2	0.71	0
21	EDO	E	203	-	3,3,3	0.57	0	2,2,2	0.27	0
25	DMU	K	104	-	8,8,34	0.53	0	7,7,45	0.25	0
24	CHD	B	303	-	32,32,32	0.96	1 (3%)	51,51,51	1.59	10 (19%)
21	EDO	A	611	-	3,3,3	0.81	0	2,2,2	0.53	0
21	EDO	S	105	-	3,3,3	0.78	0	2,2,2	0.53	0
21	EDO	N	619	-	3,3,3	0.74	0	2,2,2	0.18	0
25	DMU	K	101	-	8,8,34	0.28	0	7,7,45	0.59	0
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.35	0
25	DMU	D	203	-	9,9,34	0.36	0	8,8,45	0.55	0
25	DMU	K	102	-	9,9,34	0.27	0	8,8,45	0.46	0
18	PGV	N	608	-	50,50,50	0.90	4 (8%)	53,56,56	1.24	5 (9%)
21	EDO	T	103	-	3,3,3	0.49	0	2,2,2	0.34	0
25	DMU	X	104	-	9,9,34	0.46	0	8,8,45	0.18	0
24	CHD	L	102	-	32,32,32	0.75	0	51,51,51	2.79	20 (39%)
21	EDO	J	103	-	3,3,3	0.34	0	2,2,2	0.58	0
25	DMU	X	101	-	9,9,34	0.41	0	8,8,45	0.44	0
20	PER	A	608[A]	14,15	1,1,1	1.21	0	-	-	-
21	EDO	O	306	-	3,3,3	0.49	0	2,2,2	0.09	0
23	CUA	B	302	2	0,1,1	-	-	-	-	-
14	HEA	N	603	1,20,30	66,67,67	1.75	21 (31%)	78,103,103	1.73	18 (23%)
25	DMU	D	201	-	10,10,34	0.33	0	9,9,45	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	EDO	P	312	-	3,3,3	0.58	0	2,2,2	0.28	0
22	TGL	L	103	-	53,53,62	0.74	1 (1%)	51,51,65	1.08	3 (5%)
21	EDO	B	307	-	3,3,3	0.64	0	2,2,2	0.25	0
21	EDO	A	614	-	3,3,3	0.48	0	2,2,2	0.48	0
21	EDO	A	615	-	3,3,3	0.76	0	2,2,2	0.25	0
21	EDO	C	317	-	3,3,3	0.62	0	2,2,2	0.18	0
21	EDO	P	310	-	3,3,3	0.61	0	2,2,2	0.15	0
21	EDO	N	620	-	3,3,3	0.76	0	2,2,2	0.34	0
26	CDL	T	101	-	52,53,99	1.34	8 (15%)	49,51,111	1.21	4 (8%)
14	HEA	A	601[A]	-	66,67,67	1.77	19 (28%)	78,103,103	2.28	33 (42%)
21	EDO	C	316	-	3,3,3	0.40	0	2,2,2	0.36	0
25	DMU	Q	201	-	9,9,34	0.45	0	8,8,45	0.22	0
21	EDO	A	616	-	3,3,3	0.47	0	2,2,2	0.42	0
21	EDO	D	205	-	3,3,3	0.67	0	2,2,2	0.24	0
21	EDO	E	202	-	3,3,3	0.43	0	2,2,2	0.32	0
21	EDO	L	104	-	3,3,3	0.53	0	2,2,2	0.76	0
14	HEA	A	601[C]	-	66,58,67	1.82	20 (30%)	78,91,103	3.16	34 (43%)
23	CUA	O	301	2	0,1,1	-	-	-	-	-
21	EDO	G	104	-	3,3,3	0.62	0	2,2,2	0.16	0
21	EDO	E	201	-	3,3,3	0.54	0	2,2,2	0.38	0
21	EDO	N	613	-	3,3,3	0.81	0	2,2,2	0.75	0
21	EDO	A	613	-	3,3,3	0.51	0	2,2,2	0.26	0
21	EDO	S	103	-	3,3,3	0.63	0	2,2,2	0.06	0
21	EDO	J	102	-	3,3,3	0.53	0	2,2,2	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	P	313	-	-	0/1/1/1	-
21	EDO	C	314	-	-	0/1/1/1	-
21	EDO	P	315	-	-	1/1/1/1	-
22	TGL	B	301	-	-	29/50/50/65	-
21	EDO	N	617	-	-	0/1/1/1	-
18	PGV	A	606	-	-	3/15/16/55	-
25	DMU	W	101	-	-	1/8/8/59	-
22	TGL	N	611	-	-	20/39/39/65	-
25	DMU	O	302	-	-	3/8/8/59	-
18	PGV	C	308	-	-	10/52/52/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	618	-	-	0/1/1/1	-
25	DMU	X	103	-	-	1/6/6/59	-
25	DMU	P	309	-	-	2/8/8/59	-
14	HEA	A	602	1,20,30	-	5/36/76/76	-
25	DMU	C	303	-	-	2/9/10/59	-
18	PGV	C	301	-	-	8/55/55/55	-
21	EDO	C	319	-	-	0/1/1/1	-
21	EDO	P	316	-	-	0/1/1/1	-
21	EDO	Y	102	-	-	0/1/1/1	-
21	EDO	N	621	-	-	0/1/1/1	-
21	EDO	N	616	-	-	0/1/1/1	-
18	PGV	C	311	-	-	10/23/23/55	-
21	EDO	B	306	-	-	0/1/1/1	-
21	EDO	B	305	-	-	0/1/1/1	-
21	EDO	N	615	-	-	0/1/1/1	-
25	DMU	P	303	-	-	4/9/9/59	-
25	DMU	J	101	-	-	6/8/8/59	-
25	DMU	K	103	-	-	6/8/8/59	-
21	EDO	F	104	-	-	0/1/1/1	-
27	PEK	P	306	-	-	14/56/56/56	-
14	HEA	N	602[A]	-	-	5/36/76/76	-
24	CHD	G	101	-	-	2/9/74/74	0/4/4/4
18	PGV	G	102	-	-	7/27/27/55	-
21	EDO	S	106	-	-	0/1/1/1	-
14	HEA	N	602[C]	-	-	13/36/60/76	-
24	CHD	P	301	-	-	1/9/74/74	0/4/4/4
19	PSC	A	607	-	-	10/21/21/55	-
21	EDO	W	102	-	-	1/1/1/1	-
24	CHD	Y	101	-	-	4/9/74/74	0/4/4/4
21	EDO	T	102	-	-	0/1/1/1	-
25	DMU	C	310	-	-	5/13/29/59	0/1/1/2
21	EDO	S	104	-	-	0/1/1/1	-
21	EDO	P	314	-	-	0/1/1/1	-
25	DMU	K	106	-	-	3/7/7/59	-
26	CDL	P	304	-	-	17/49/50/110	-
26	CDL	N	601	-	-	17/42/43/110	-
27	PEK	C	306	-	-	9/19/19/56	-
21	EDO	S	102	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	F	106	-	-	0/1/1/1	-
18	PGV	N	607	-	-	5/18/18/55	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	P	311	-	-	1/1/1/1	-
26	CDL	C	305	-	-	14/45/46/110	-
21	EDO	A	617	-	-	0/1/1/1	-
25	DMU	L	101	-	-	4/13/29/59	0/1/1/2
21	EDO	F	103	6	-	0/1/1/1	-
25	DMU	K	105	-	-	4/6/6/59	-
21	EDO	C	313	-	-	0/1/1/1	-
27	PEK	C	309	-	-	15/30/30/56	-
21	EDO	B	304	-	-	0/1/1/1	-
21	EDO	G	103	-	-	0/1/1/1	-
19	PSC	O	303	-	-	9/24/24/55	-
21	EDO	Q	202	-	-	0/1/1/1	-
22	TGL	N	612	-	-	26/45/45/65	-
22	TGL	N	609	-	-	34/65/65/65	-
21	EDO	N	618	-	-	0/1/1/1	-
21	EDO	D	206	-	-	0/1/1/1	-
18	PGV	P	307	-	-	6/55/55/55	-
21	EDO	O	304	-	-	0/1/1/1	-
25	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
21	EDO	C	312	-	-	0/1/1/1	-
21	EDO	C	320	-	-	1/1/1/1	-
21	EDO	D	204	-	-	0/1/1/1	-
27	PEK	P	308	-	-	12/28/28/56	-
27	PEK	C	307	-	-	15/56/56/56	-
21	EDO	C	315	-	-	0/1/1/1	-
24	CHD	C	304	-	-	2/9/74/74	0/4/4/4
21	EDO	A	609	-	-	0/1/1/1	-
21	EDO	A	610	-	-	1/1/1/1	-
21	EDO	P	317	-	-	0/1/1/1	-
21	EDO	F	105	-	-	0/1/1/1	-
22	TGL	D	202	-	-	32/59/59/65	-
25	DMU	M	101	-	-	3/19/59/59	0/2/2/2
21	EDO	O	305	-	-	1/1/1/1	-
21	EDO	C	318	-	-	0/1/1/1	-
21	EDO	T	104	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DMU	X	102	-	-	2/7/7/59	-
27	PEK	P	305	-	-	10/17/17/56	-
21	EDO	F	102	-	-	0/1/1/1	-
21	EDO	Y	103	-	-	1/1/1/1	-
21	EDO	E	203	-	-	1/1/1/1	-
25	DMU	K	104	-	-	2/6/6/59	-
24	CHD	B	303	-	-	2/9/74/74	0/4/4/4
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
21	EDO	N	619	-	-	1/1/1/1	-
25	DMU	K	101	-	-	0/6/6/59	-
21	EDO	N	614	-	-	0/1/1/1	-
25	DMU	D	203	-	-	2/7/7/59	-
25	DMU	K	102	-	-	3/7/7/59	-
18	PGV	N	608	-	-	9/55/55/55	-
21	EDO	T	103	-	-	0/1/1/1	-
25	DMU	X	104	-	-	0/7/7/59	-
24	CHD	L	102	-	-	6/9/74/74	0/4/4/4
21	EDO	J	103	-	-	1/1/1/1	-
25	DMU	X	101	-	-	0/7/7/59	-
21	EDO	O	306	-	-	0/1/1/1	-
14	HEA	N	603	1,20,30	-	6/36/76/76	-
25	DMU	D	201	-	-	3/8/8/59	-
21	EDO	P	312	-	-	0/1/1/1	-
22	TGL	L	103	-	-	24/47/48/65	-
21	EDO	B	307	-	-	0/1/1/1	-
21	EDO	A	614	-	-	1/1/1/1	-
21	EDO	A	615	-	-	1/1/1/1	-
21	EDO	C	317	-	-	0/1/1/1	-
21	EDO	P	310	-	-	1/1/1/1	-
21	EDO	N	620	-	-	0/1/1/1	-
26	CDL	T	101	-	-	21/47/47/110	-
14	HEA	A	601[A]	-	-	7/36/76/76	-
21	EDO	C	316	-	-	0/1/1/1	-
25	DMU	Q	201	-	-	4/7/7/59	-
21	EDO	A	616	-	-	0/1/1/1	-
21	EDO	D	205	-	-	1/1/1/1	-
21	EDO	E	202	-	-	1/1/1/1	-
21	EDO	L	104	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	HEA	A	601[C]	-	-	11/36/60/76	-
21	EDO	G	104	-	-	1/1/1/1	-
21	EDO	E	201	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	A	613	-	-	1/1/1/1	-
21	EDO	S	103	-	-	0/1/1/1	-
21	EDO	J	102	-	-	1/1/1/1	-

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[C]	HEA	C18-C19	22.89	1.87	1.33
22	N	612	TGL	OG2-CB1	5.58	1.50	1.34
18	C	311	PGV	O03-C19	5.52	1.49	1.33
22	N	609	TGL	OG2-CB1	5.12	1.48	1.34
22	D	202	TGL	OG1-CA1	4.92	1.47	1.33
18	G	102	PGV	O03-C19	4.81	1.48	1.33
26	T	101	CDL	OB8-CB7	4.79	1.47	1.33
22	N	609	TGL	OG3-CC1	4.70	1.47	1.33
22	B	301	TGL	OG1-CA1	4.59	1.46	1.33
19	O	303	PSC	O03-C19	4.56	1.46	1.30
26	P	304	CDL	OB8-CB7	4.52	1.47	1.33
22	N	609	TGL	OG1-CA1	4.52	1.46	1.33
22	L	103	TGL	OG1-CA1	4.44	1.47	1.33
22	D	202	TGL	OG3-CC1	4.37	1.46	1.33
22	N	612	TGL	OG1-CA1	4.35	1.46	1.33
22	B	301	TGL	OG3-CC1	4.18	1.45	1.33
14	A	601[A]	HEA	CHD-C1D	4.13	1.46	1.38
14	A	601[C]	HEA	CHD-C1D	4.13	1.46	1.38
22	D	202	TGL	OG2-CB1	4.00	1.45	1.34
22	B	301	TGL	OG2-CB1	3.95	1.45	1.34
14	A	601[C]	HEA	C18-C19	3.89	1.42	1.33
14	N	602[A]	HEA	CHA-C1A	3.83	1.45	1.38
14	N	602[C]	HEA	CHA-C1A	3.83	1.45	1.38
19	A	607	PSC	C13-C12	3.77	1.53	1.31
14	N	603	HEA	C3A-C4A	-3.74	1.39	1.46
19	O	303	PSC	C13-C12	3.70	1.53	1.31
18	C	301	PGV	O01-C1	3.58	1.44	1.34
27	P	306	PEK	O03-C21	3.56	1.43	1.33
14	N	602[A]	HEA	C4B-NB	-3.55	1.34	1.40
14	N	602[C]	HEA	C4B-NB	-3.55	1.34	1.40
14	A	602	HEA	C4D-C3D	-3.55	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	CHB-C4A	3.55	1.45	1.38
14	A	601[A]	HEA	C1A-C2A	-3.54	1.38	1.45
14	A	601[C]	HEA	C1A-C2A	-3.54	1.38	1.45
14	N	603	HEA	C4D-C3D	-3.53	1.39	1.45
27	C	307	PEK	O03-C21	3.45	1.43	1.33
26	C	305	CDL	C59-C58	-3.38	1.32	1.51
14	N	602[A]	HEA	C1D-ND	-3.35	1.34	1.40
14	N	602[C]	HEA	C1D-ND	-3.35	1.34	1.40
14	N	602[A]	HEA	C3A-C4A	-3.35	1.40	1.46
14	N	602[C]	HEA	C3A-C4A	-3.35	1.40	1.46
14	A	602	HEA	CMC-C2C	3.31	1.57	1.50
14	N	603	HEA	CHA-C1A	3.28	1.44	1.38
14	N	602[A]	HEA	CHC-C4B	3.27	1.45	1.38
14	N	602[C]	HEA	CHC-C4B	3.27	1.45	1.38
14	A	602	HEA	O11-C11	3.27	1.49	1.42
26	C	305	CDL	C82-C81	-3.27	1.33	1.51
26	P	304	CDL	C82-C81	-3.24	1.33	1.51
14	A	602	HEA	CHC-C4B	3.23	1.45	1.38
26	T	101	CDL	C79-C78	-3.20	1.33	1.51
18	N	608	PGV	O01-C1	3.19	1.43	1.34
26	P	304	CDL	C19-C18	-3.19	1.33	1.51
26	P	304	CDL	C39-C38	-3.19	1.33	1.51
27	C	307	PEK	O01-C1	3.17	1.43	1.34
26	N	601	CDL	C62-C61	-3.16	1.33	1.51
26	C	305	CDL	C62-C61	-3.16	1.33	1.51
26	N	601	CDL	C42-C41	-3.15	1.33	1.51
26	N	601	CDL	C82-C81	-3.15	1.33	1.51
14	A	602	HEA	C4A-NA	-3.14	1.33	1.39
14	N	603	HEA	C1D-ND	-3.14	1.34	1.40
26	T	101	CDL	C82-C81	-3.13	1.34	1.51
26	P	304	CDL	C59-C58	-3.13	1.34	1.51
26	P	304	CDL	C79-C78	-3.13	1.34	1.51
14	A	601[A]	HEA	CHB-C4A	3.11	1.44	1.38
14	A	601[C]	HEA	CHB-C4A	3.11	1.44	1.38
26	C	305	CDL	C79-C78	-3.10	1.34	1.51
14	A	601[A]	HEA	CHC-C4B	3.07	1.44	1.38
14	A	601[C]	HEA	CHC-C4B	3.07	1.44	1.38
26	N	601	CDL	C22-C21	-3.06	1.34	1.51
26	P	304	CDL	C42-C41	-3.05	1.34	1.51
14	N	602[A]	HEA	CHB-C4A	3.04	1.44	1.38
14	N	602[C]	HEA	CHB-C4A	3.04	1.44	1.38
26	N	601	CDL	C19-C18	-3.03	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	310	DMU	O16-C6	3.03	1.45	1.40
26	T	101	CDL	C62-C61	-3.02	1.34	1.51
14	N	603	HEA	CHC-C4B	3.01	1.44	1.38
26	T	101	CDL	C42-C41	-3.01	1.34	1.51
26	T	101	CDL	C19-C18	-2.98	1.34	1.51
18	C	308	PGV	O01-C1	2.97	1.42	1.34
26	N	601	CDL	C79-C78	-2.96	1.34	1.51
14	A	602	HEA	CHD-C1D	2.95	1.44	1.38
14	N	603	HEA	CHB-C4A	2.91	1.44	1.38
26	T	101	CDL	C22-C21	-2.89	1.35	1.51
14	A	601[A]	HEA	CBD-CGD	2.86	1.57	1.50
14	A	601[C]	HEA	CBD-CGD	2.86	1.57	1.50
14	A	601[A]	HEA	C1D-ND	-2.83	1.35	1.40
14	A	601[C]	HEA	C1D-ND	-2.83	1.35	1.40
14	A	602	HEA	C4C-NC	-2.83	1.34	1.39
18	N	608	PGV	O03-C19	2.81	1.41	1.33
14	N	603	HEA	CHB-C1B	2.78	1.45	1.39
14	A	601[A]	HEA	CHB-C1B	2.75	1.45	1.39
14	A	601[C]	HEA	CHB-C1B	2.75	1.45	1.39
14	A	601[A]	HEA	C1D-C2D	-2.72	1.39	1.44
14	A	601[C]	HEA	C1D-C2D	-2.72	1.39	1.44
14	N	603	HEA	C1A-C2A	-2.70	1.40	1.45
14	N	602[A]	HEA	C1D-C2D	-2.68	1.39	1.44
14	N	602[C]	HEA	C1D-C2D	-2.68	1.39	1.44
14	A	601[A]	HEA	CAD-C3D	2.68	1.58	1.51
14	A	601[C]	HEA	CAD-C3D	2.68	1.58	1.51
14	A	602	HEA	C4B-C3B	-2.66	1.40	1.44
14	A	601[A]	HEA	C3A-C4A	-2.66	1.41	1.46
14	A	601[C]	HEA	C3A-C4A	-2.66	1.41	1.46
14	N	603	HEA	C4B-C3B	-2.65	1.40	1.44
14	A	602	HEA	FE-ND	2.65	2.03	1.94
14	N	602[A]	HEA	C1A-C2A	-2.62	1.40	1.45
14	N	602[C]	HEA	C1A-C2A	-2.62	1.40	1.45
14	N	603	HEA	FE-NA	2.56	2.03	1.95
14	N	603	HEA	O11-C11	2.55	1.48	1.42
26	N	601	CDL	C58-C59	-2.54	1.33	1.51
14	A	601[A]	HEA	FE-NA	2.53	2.03	1.95
14	A	601[C]	HEA	FE-NA	2.53	2.03	1.95
26	C	305	CDL	C39-C38	-2.53	1.33	1.51
14	A	602	HEA	C1B-C2B	-2.53	1.39	1.44
14	A	601[A]	HEA	CHA-C4D	2.52	1.45	1.39
14	A	601[C]	HEA	CHA-C4D	2.52	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	601	CDL	C38-C39	-2.49	1.34	1.51
14	A	602	HEA	C1D-C2D	-2.47	1.39	1.44
14	A	601[A]	HEA	CHA-C1A	2.45	1.43	1.38
14	A	601[C]	HEA	CHA-C1A	2.45	1.43	1.38
14	A	602	HEA	FE-NA	2.45	2.03	1.95
14	A	601[A]	HEA	C4A-NA	-2.44	1.35	1.39
14	A	601[C]	HEA	C4A-NA	-2.44	1.35	1.39
18	N	608	PGV	O01-C02	-2.41	1.40	1.46
14	N	603	HEA	CHC-C1C	2.41	1.44	1.39
14	A	602	HEA	CHA-C1A	2.40	1.43	1.38
14	N	603	HEA	C4B-NB	-2.39	1.36	1.40
18	C	301	PGV	O01-C02	-2.38	1.40	1.46
14	A	602	HEA	FE-NC	2.33	2.03	1.95
14	N	603	HEA	FE-ND	2.33	2.02	1.94
26	T	101	CDL	C58-C59	-2.32	1.35	1.51
14	A	601[A]	HEA	CBA-CGA	2.32	1.56	1.50
14	A	601[C]	HEA	CBA-CGA	2.32	1.56	1.50
14	N	603	HEA	CBD-CGD	2.31	1.55	1.50
14	N	602[A]	HEA	CHC-C1C	2.30	1.44	1.39
14	N	602[C]	HEA	CHC-C1C	2.30	1.44	1.39
14	A	601[A]	HEA	FE-NB	2.28	2.01	1.94
14	A	601[C]	HEA	FE-NB	2.28	2.01	1.94
14	A	602	HEA	CHA-C4D	2.26	1.44	1.39
14	N	602[A]	HEA	FE-ND	2.24	2.01	1.94
14	N	602[C]	HEA	FE-ND	2.24	2.01	1.94
25	L	101	DMU	O16-C6	2.24	1.44	1.40
14	A	602	HEA	C18-C19	2.24	1.38	1.33
14	N	602[A]	HEA	O2D-CGD	-2.23	1.23	1.30
14	N	602[C]	HEA	O2D-CGD	-2.23	1.23	1.30
14	N	603	HEA	CBA-CGA	2.22	1.55	1.50
24	C	304	CHD	O25-C24	2.22	1.29	1.22
14	N	603	HEA	C1B-NB	-2.21	1.34	1.38
14	A	602	HEA	CHC-C1C	2.21	1.44	1.39
18	C	301	PGV	O03-C19	2.18	1.39	1.33
14	N	602[A]	HEA	CHD-C4C	2.16	1.44	1.39
14	N	602[C]	HEA	CHD-C4C	2.16	1.44	1.39
14	A	602	HEA	C1C-NC	-2.15	1.35	1.39
14	A	601[A]	HEA	C4D-C3D	-2.14	1.41	1.45
14	A	601[C]	HEA	C4D-C3D	-2.14	1.41	1.45
14	A	601[A]	HEA	CHC-C1C	2.14	1.44	1.39
14	A	601[C]	HEA	CHC-C1C	2.14	1.44	1.39
14	N	602[A]	HEA	O11-C11	2.14	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	602[A]	HEA	O1A-CGA	2.14	1.29	1.22
14	N	602[C]	HEA	O1A-CGA	2.14	1.29	1.22
24	B	303	CHD	O7-C7	2.12	1.47	1.43
14	A	601[A]	HEA	C1C-NC	-2.10	1.35	1.39
14	A	601[C]	HEA	C1C-NC	-2.10	1.35	1.39
18	C	301	PGV	C03-C02	2.10	1.57	1.50
14	N	603	HEA	CMC-C2C	2.09	1.55	1.50
14	N	603	HEA	C4A-NA	-2.09	1.35	1.39
14	N	602[A]	HEA	CHD-C1D	2.09	1.42	1.38
14	N	602[C]	HEA	CHD-C1D	2.09	1.42	1.38
27	P	306	PEK	O01-C1	2.06	1.40	1.34
14	N	603	HEA	CHD-C4C	2.05	1.44	1.39
14	A	602	HEA	C1A-C2A	-2.04	1.41	1.45
18	P	307	PGV	O01-C1	2.04	1.40	1.34
14	N	603	HEA	C1A-NA	-2.03	1.35	1.39
18	P	307	PGV	O03-C19	2.01	1.39	1.33
18	N	608	PGV	C03-C02	2.01	1.56	1.50

All (318) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[C]	HEA	C20-C19-C18	18.57	158.70	121.12
14	N	602[C]	HEA	C27-C19-C18	-17.43	78.95	123.68
14	A	601[C]	HEA	C20-C19-C18	13.27	147.98	121.12
14	A	601[C]	HEA	C27-C19-C18	-12.76	90.94	123.68
14	A	601[C]	HEA	C13-C12-C11	-9.41	100.21	114.35
24	L	102	CHD	C6-C5-C4	-8.48	101.43	111.19
14	N	602[C]	HEA	C13-C12-C11	-7.29	103.39	114.35
25	L	101	DMU	O16-C6-C1	7.20	119.54	108.30
24	L	102	CHD	C10-C9-C8	7.14	119.48	111.82
18	C	311	PGV	O03-C19-C20	6.85	133.42	111.91
22	B	301	TGL	OG2-CB1-CB2	6.38	125.25	111.50
14	A	601[A]	HEA	C26-C15-C16	6.32	125.90	115.27
22	N	612	TGL	OG2-CB1-CB2	6.01	124.46	111.50
24	Y	101	CHD	C14-C8-C7	5.98	119.74	111.81
24	C	304	CHD	C18-C13-C12	5.61	114.78	109.07
25	L	101	DMU	C6-O5-C4	-5.48	107.06	113.13
14	N	602[A]	HEA	C3D-C4D-ND	5.27	115.46	110.36
14	N	602[C]	HEA	C3D-C4D-ND	5.27	115.46	110.36
24	Y	101	CHD	C1-C10-C5	5.24	115.52	107.77
14	A	601[A]	HEA	C2B-C1B-NB	5.21	116.13	109.88
14	A	601[C]	HEA	C2B-C1B-NB	5.21	116.13	109.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L	102	CHD	C21-C20-C17	5.16	120.82	112.92
25	L	101	DMU	C18-O16-C6	5.16	122.39	113.84
18	C	311	PGV	C01-O03-C19	5.03	133.17	116.92
14	A	602	HEA	C27-C19-C20	5.02	123.71	115.27
24	L	102	CHD	C11-C9-C10	-4.99	108.58	113.73
24	Y	101	CHD	C21-C20-C17	4.78	120.23	112.92
24	L	102	CHD	C17-C13-C12	-4.72	113.36	117.67
14	A	602	HEA	CMB-C2B-C1B	4.70	132.20	125.04
14	A	601[A]	HEA	CAA-CBA-CGA	-4.49	103.94	113.60
14	A	601[C]	HEA	CAA-CBA-CGA	-4.49	103.94	113.60
14	N	603	HEA	CAD-CBD-CGD	-4.44	104.05	113.60
14	N	603	HEA	C3C-C4C-NC	4.44	112.98	110.25
18	G	102	PGV	O03-C19-C20	4.37	129.52	112.23
14	A	601[A]	HEA	C27-C19-C20	4.37	122.62	115.27
14	N	602[A]	HEA	C1D-ND-C4D	-4.31	100.62	105.07
14	N	602[C]	HEA	C1D-ND-C4D	-4.31	100.62	105.07
24	P	301	CHD	C21-C20-C22	-4.29	103.64	110.36
18	C	311	PGV	O03-C19-O04	-4.28	112.80	123.59
14	A	602	HEA	C2B-C1B-NB	4.27	114.99	109.88
14	A	602	HEA	CAD-CBD-CGD	-4.22	104.52	113.60
14	N	602[C]	HEA	C27-C19-C20	4.21	122.34	115.27
22	N	609	TGL	OG2-CB1-CB2	4.17	120.48	111.50
14	A	602	HEA	C26-C15-C16	4.16	122.28	115.27
24	Y	101	CHD	C19-C10-C1	-4.14	101.59	108.26
14	A	601[A]	HEA	O2A-CGA-CBA	4.13	127.29	114.03
14	A	601[C]	HEA	O2A-CGA-CBA	4.13	127.29	114.03
14	A	602	HEA	CHB-C4A-NA	4.12	128.90	124.44
14	N	602[A]	HEA	C3C-C4C-NC	4.10	112.77	110.25
14	N	602[C]	HEA	C3C-C4C-NC	4.10	112.77	110.25
14	A	601[A]	HEA	C2D-C1D-ND	4.08	114.67	109.84
14	A	601[C]	HEA	C2D-C1D-ND	4.08	114.67	109.84
24	L	102	CHD	C14-C8-C7	4.05	117.17	111.81
14	A	601[A]	HEA	C13-C12-C11	-4.03	108.29	114.35
24	L	102	CHD	C13-C17-C20	3.98	124.24	119.50
24	Y	101	CHD	C10-C9-C8	3.96	116.07	111.82
18	C	301	PGV	O03-C19-C20	3.95	124.29	111.91
25	M	101	DMU	C18-O16-C6	-3.91	107.36	113.84
22	B	301	TGL	OG1-CA1-CA2	3.90	121.60	111.38
24	L	102	CHD	C1-C10-C9	-3.89	105.24	111.35
14	N	602[A]	HEA	C2D-C1D-ND	3.87	114.42	109.84
14	N	602[C]	HEA	C2D-C1D-ND	3.87	114.42	109.84
24	B	303	CHD	C19-C10-C1	-3.86	102.04	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	301	PGV	O03-C19-O04	-3.86	113.85	123.59
14	N	602[A]	HEA	C13-C12-C11	-3.85	108.57	114.35
14	A	601[A]	HEA	CHA-C4D-C3D	-3.84	119.19	124.84
14	A	601[C]	HEA	CHA-C4D-C3D	-3.84	119.19	124.84
14	A	601[C]	HEA	C25-C23-C24	3.83	123.06	114.60
24	Y	101	CHD	C9-C11-C12	-3.82	109.26	114.30
24	Y	101	CHD	C4-C3-C2	-3.74	106.09	110.55
14	A	602	HEA	CMB-C2B-C3B	-3.72	123.24	130.34
14	A	602	HEA	C20-C19-C18	-3.68	113.66	121.12
14	A	601[A]	HEA	C4B-NB-C1B	-3.66	101.30	105.07
14	A	601[C]	HEA	C4B-NB-C1B	-3.66	101.30	105.07
26	T	101	CDL	OB6-CB5-C51	3.66	123.27	109.74
24	Y	101	CHD	C16-C17-C13	-3.64	99.98	103.55
24	P	301	CHD	O12-C12-C13	-3.62	104.91	111.03
14	A	601[A]	HEA	C16-C15-C14	-3.62	113.79	121.12
14	A	602	HEA	C3C-C4C-NC	3.62	112.47	110.25
24	L	102	CHD	C15-C14-C8	3.54	123.28	118.33
24	C	304	CHD	C1-C2-C3	-3.52	105.94	110.47
18	N	608	PGV	O03-C19-O04	-3.51	114.73	123.59
18	G	102	PGV	C01-O03-C19	3.48	127.58	116.11
24	L	102	CHD	C9-C10-C5	3.48	113.47	108.58
24	B	303	CHD	C11-C9-C10	-3.48	110.14	113.73
24	L	102	CHD	C18-C13-C14	-3.47	105.78	111.21
22	B	301	TGL	CB3-CB2-CB1	-3.45	101.07	113.62
25	M	101	DMU	C28-C25-C22	-3.45	96.94	114.42
14	N	603	HEA	C16-C15-C14	-3.44	114.15	121.12
24	B	303	CHD	C4-C5-C10	-3.43	109.01	112.66
25	C	310	DMU	O5-C4-C57	3.43	112.32	106.83
22	D	202	TGL	CG2-OG2-CB1	-3.42	109.38	117.79
14	N	603	HEA	C13-C12-C11	-3.39	109.26	114.35
18	G	102	PGV	O03-C19-O04	-3.38	112.54	123.14
22	D	202	TGL	OG3-CC1-OC1	-3.38	115.06	123.59
14	A	601[A]	HEA	O1A-CGA-CBA	-3.38	112.24	123.08
14	A	601[C]	HEA	O1A-CGA-CBA	-3.38	112.24	123.08
26	P	304	CDL	OB8-CB7-C71	3.36	125.52	112.23
22	N	612	TGL	OG1-CA1-CA2	3.33	122.37	111.91
14	A	601[A]	HEA	CHD-C4C-NC	3.33	129.97	123.85
14	A	601[C]	HEA	CHD-C4C-NC	3.33	129.97	123.85
22	D	202	TGL	OG3-CC1-CC2	3.32	122.31	111.91
24	Y	101	CHD	C21-C20-C22	-3.31	105.18	110.36
25	Z	101	DMU	O1-C9-C8	3.30	115.69	109.69
22	N	612	TGL	CG2-OG2-CB1	3.26	125.83	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	101	CHD	C15-C14-C8	3.25	122.88	118.33
22	L	103	TGL	OG3-CC1-CC2	3.25	124.23	109.94
14	N	602[A]	HEA	C26-C15-C16	3.23	120.71	115.27
14	N	603	HEA	CHB-C1B-C2B	-3.22	119.95	124.98
14	A	601[C]	HEA	C17-C18-C19	3.21	135.39	127.66
24	L	102	CHD	C11-C12-C13	3.14	114.47	111.24
14	A	601[C]	HEA	C26-C15-C16	3.13	120.53	115.27
24	L	102	CHD	C13-C14-C8	-3.09	110.80	114.74
24	L	102	CHD	C18-C13-C12	3.08	112.20	109.07
18	P	307	PGV	O01-C1-O02	-3.08	116.27	123.70
24	Y	101	CHD	C9-C8-C7	-3.08	108.20	111.88
24	Y	101	CHD	C2-C1-C10	3.07	118.05	112.78
14	A	601[A]	HEA	C4C-CHD-C1D	-3.07	119.06	126.34
14	A	601[C]	HEA	C4C-CHD-C1D	-3.07	119.06	126.34
24	Y	101	CHD	C14-C13-C12	3.07	110.26	107.40
14	A	601[A]	HEA	CHA-C4D-ND	3.06	127.75	124.42
14	A	601[C]	HEA	CHA-C4D-ND	3.06	127.75	124.42
24	L	102	CHD	C14-C8-C9	-3.06	105.51	109.71
14	A	602	HEA	C4A-CHB-C1B	-3.05	119.48	126.06
25	L	101	DMU	O5-C6-O16	3.05	117.19	109.97
14	A	602	HEA	C16-C15-C14	-3.04	114.97	121.12
25	L	101	DMU	O5-C4-C57	3.02	111.67	106.83
22	D	202	TGL	OG1-CA1-CA2	3.01	121.37	111.91
25	M	101	DMU	O16-C6-C1	3.00	112.99	108.30
14	N	603	HEA	CHB-C1B-NB	2.99	127.67	124.42
14	N	602[A]	HEA	OMA-CMA-C3A	-2.99	118.92	125.69
14	N	602[C]	HEA	OMA-CMA-C3A	-2.99	118.92	125.69
14	N	603	HEA	C27-C19-C20	2.98	120.28	115.27
14	N	602[A]	HEA	O2A-CGA-CBA	2.97	123.58	114.03
14	N	602[C]	HEA	O2A-CGA-CBA	2.97	123.58	114.03
18	N	608	PGV	O01-C1-O02	-2.96	116.54	123.70
24	B	303	CHD	C16-C17-C13	2.96	106.45	103.55
14	N	602[A]	HEA	C4D-C3D-C2D	-2.95	102.60	106.90
14	N	602[C]	HEA	C4D-C3D-C2D	-2.95	102.60	106.90
22	N	609	TGL	OG3-CC1-CC2	2.93	121.11	111.91
14	A	601[A]	HEA	C1A-CHA-C4D	-2.91	119.79	126.06
14	A	601[C]	HEA	C1A-CHA-C4D	-2.91	119.79	126.06
14	N	602[A]	HEA	CHA-C4D-C3D	-2.91	120.57	124.84
14	N	602[C]	HEA	CHA-C4D-C3D	-2.91	120.57	124.84
24	P	301	CHD	C22-C20-C17	-2.89	104.31	110.28
24	Y	101	CHD	C6-C5-C4	-2.87	107.89	111.19
14	A	601[A]	HEA	C20-C19-C18	-2.86	115.32	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	608	PGV	C9-C10-C11	-2.86	96.04	112.43
14	N	602[A]	HEA	C27-C19-C20	2.86	120.08	115.27
14	N	603	HEA	O2D-CGD-O1D	2.85	130.40	123.30
24	C	304	CHD	C22-C20-C17	-2.85	104.40	110.28
14	A	602	HEA	C4B-NB-C1B	-2.84	102.14	105.07
14	A	601[C]	HEA	C13-C14-C15	-2.83	120.84	127.66
14	N	603	HEA	C26-C15-C16	2.83	120.03	115.27
14	A	601[C]	HEA	C25-C23-C22	-2.79	114.58	122.65
14	A	601[A]	HEA	C3D-C4D-ND	2.79	113.05	110.36
14	A	601[C]	HEA	C3D-C4D-ND	2.79	113.05	110.36
14	N	602[C]	HEA	C26-C15-C16	2.77	119.94	115.27
24	L	102	CHD	C1-C2-C3	2.77	114.02	110.47
24	C	304	CHD	C6-C7-C8	-2.76	108.53	111.48
14	N	602[C]	HEA	C13-C14-C15	-2.76	121.02	127.66
14	N	603	HEA	O1A-CGA-CBA	-2.75	114.24	123.08
14	N	602[A]	HEA	C2B-C1B-NB	2.75	113.18	109.88
14	N	602[C]	HEA	C2B-C1B-NB	2.75	113.18	109.88
14	A	601[A]	HEA	O2D-CGD-O1D	2.75	130.15	123.30
14	A	601[C]	HEA	O2D-CGD-O1D	2.75	130.15	123.30
14	A	602	HEA	CHA-C4D-C3D	-2.75	120.80	124.84
22	N	612	TGL	OG2-CB1-OB1	-2.74	117.08	123.70
24	B	303	CHD	C13-C14-C8	-2.74	111.24	114.74
26	T	101	CDL	OB8-CB7-C71	2.73	120.47	111.91
18	C	301	PGV	O01-C1-C2	2.72	117.36	111.50
14	N	603	HEA	C4C-NC-C1C	-2.71	102.69	105.35
24	B	303	CHD	O3-C3-C4	-2.67	104.53	109.85
14	A	602	HEA	CHB-C4A-C3A	-2.67	120.69	125.26
24	G	101	CHD	C4-C5-C10	-2.65	109.85	112.66
26	C	305	CDL	C83-C82-C81	2.63	127.76	114.42
24	Y	101	CHD	C15-C14-C13	-2.62	100.99	103.55
24	B	303	CHD	C19-C10-C5	-2.61	105.93	110.36
24	Y	101	CHD	C11-C9-C10	-2.60	111.04	113.73
14	A	601[C]	HEA	O11-C11-C12	-2.60	102.16	109.42
24	B	303	CHD	C15-C14-C13	2.59	106.09	103.55
14	N	602[A]	HEA	CAA-CBA-CGA	-2.58	108.05	113.60
14	N	602[C]	HEA	CAA-CBA-CGA	-2.58	108.05	113.60
27	P	306	PEK	C8-C7-C6	-2.57	99.39	112.02
14	A	601[A]	HEA	C21-C20-C19	-2.57	104.54	112.98
14	N	602[A]	HEA	C2A-C1A-NA	2.55	112.81	110.32
14	N	602[C]	HEA	C2A-C1A-NA	2.55	112.81	110.32
27	P	306	PEK	C3-C2-C1	-2.55	104.34	113.62
18	C	311	PGV	O04-C19-C20	-2.55	113.77	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	301	CHD	C6-C7-C8	-2.55	108.76	111.48
24	P	301	CHD	C16-C17-C20	-2.55	108.20	112.15
14	N	602[A]	HEA	O1D-CGD-CBD	-2.54	114.93	123.08
14	N	602[C]	HEA	O1D-CGD-CBD	-2.54	114.93	123.08
24	G	101	CHD	C17-C13-C12	2.53	119.97	117.67
26	P	304	CDL	OB8-CB7-OB9	-2.53	115.22	123.14
14	N	603	HEA	C4A-CHB-C1B	-2.52	120.62	126.06
27	C	307	PEK	O03-C21-C22	2.52	119.82	111.91
18	N	608	PGV	O03-C19-C20	2.52	119.81	111.91
14	A	601[A]	HEA	C3B-C4B-NB	2.52	112.82	109.84
14	A	601[C]	HEA	C3B-C4B-NB	2.52	112.82	109.84
24	C	304	CHD	O12-C12-C13	-2.51	106.78	111.03
14	A	601[A]	HEA	C1D-ND-C4D	-2.51	102.48	105.07
14	A	601[C]	HEA	C1D-ND-C4D	-2.51	102.48	105.07
27	P	306	PEK	O11-P-O14	-2.51	99.25	109.07
24	P	301	CHD	C18-C13-C17	-2.50	107.30	111.21
14	A	602	HEA	CHB-C1B-C2B	-2.50	121.08	124.98
22	N	609	TGL	OG1-CA1-CA2	2.50	119.75	111.91
14	A	601[C]	HEA	C26-C15-C14	-2.50	117.28	123.68
25	C	310	DMU	O16-C18-C19	2.49	118.30	109.56
18	P	307	PGV	C03-C02-C01	-2.49	105.90	111.79
26	C	305	CDL	C80-C79-C78	2.49	127.06	114.42
18	C	308	PGV	C21-C20-C19	-2.49	104.58	113.62
14	N	602[A]	HEA	O1A-CGA-CBA	-2.48	115.10	123.08
14	N	602[C]	HEA	O1A-CGA-CBA	-2.48	115.10	123.08
18	P	307	PGV	O03-C19-O04	-2.48	117.33	123.59
26	T	101	CDL	C43-C42-C41	2.48	126.99	114.42
24	P	301	CHD	C11-C9-C10	-2.47	111.17	113.73
26	N	601	CDL	C19-C18-C17	2.47	126.94	114.42
14	N	602[A]	HEA	CHD-C1D-C2D	-2.46	119.91	126.73
14	N	602[C]	HEA	CHD-C1D-C2D	-2.46	119.91	126.73
26	C	305	CDL	C61-C60-C59	-2.45	101.97	114.42
14	A	602	HEA	C3D-C4D-ND	2.42	112.70	110.36
18	C	311	PGV	C21-C20-C19	-2.42	104.81	113.62
14	N	602[C]	HEA	C17-C18-C19	-2.41	121.85	127.66
22	N	612	TGL	OG1-CA1-OA1	-2.40	117.52	123.59
24	G	101	CHD	C1-C10-C5	2.40	111.32	107.77
22	L	103	TGL	CG1-OG1-CA1	2.37	123.93	116.11
22	N	612	TGL	OG1-CG1-CG2	2.37	115.34	108.43
14	N	602[A]	HEA	C4C-NC-C1C	-2.37	103.03	105.35
14	N	602[C]	HEA	C4C-NC-C1C	-2.37	103.03	105.35
18	N	608	PGV	C01-O03-C19	-2.36	108.37	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	603	HEA	CAD-C3D-C4D	2.36	128.78	124.66
14	N	602[C]	HEA	C25-C23-C24	2.36	119.81	114.60
14	N	602[A]	HEA	O2D-CGD-CBD	2.36	121.60	114.03
14	N	602[C]	HEA	O2D-CGD-CBD	2.36	121.60	114.03
24	G	101	CHD	C9-C10-C5	2.35	111.88	108.58
22	B	301	TGL	OG3-CC1-CC2	2.34	119.24	111.91
24	L	102	CHD	C5-C6-C7	2.33	117.04	114.46
14	A	601[A]	HEA	CHA-C1A-NA	2.32	126.95	124.44
14	A	601[C]	HEA	CHA-C1A-NA	2.32	126.95	124.44
14	A	601[A]	HEA	C3A-C2A-C1A	-2.32	104.86	107.08
14	A	601[C]	HEA	C3A-C2A-C1A	-2.32	104.86	107.08
14	N	602[A]	HEA	CAD-C3D-C2D	2.32	132.19	127.88
14	N	602[C]	HEA	CAD-C3D-C2D	2.32	132.19	127.88
14	N	602[A]	HEA	C3A-C2A-C1A	-2.31	104.87	107.08
14	N	602[C]	HEA	C3A-C2A-C1A	-2.31	104.87	107.08
14	A	601[A]	HEA	CHD-C1D-C2D	-2.31	120.33	126.73
14	A	601[C]	HEA	CHD-C1D-C2D	-2.31	120.33	126.73
14	A	602	HEA	C4C-CHD-C1D	-2.30	120.88	126.34
14	A	601[A]	HEA	CHB-C4A-NA	2.30	126.92	124.44
14	A	601[C]	HEA	CHB-C4A-NA	2.30	126.92	124.44
19	O	303	PSC	O03-C19-O04	-2.30	117.58	123.30
26	P	304	CDL	C54-C53-C52	-2.28	102.83	114.42
14	N	602[A]	HEA	CHB-C1B-C2B	-2.27	121.43	124.98
14	N	602[C]	HEA	CHB-C1B-C2B	-2.27	121.43	124.98
14	A	601[A]	HEA	O11-C11-C12	2.26	115.73	109.42
18	P	307	PGV	O03-C01-C02	-2.26	101.86	108.43
14	A	601[A]	HEA	CHA-C1A-C2A	-2.26	121.28	124.94
14	A	601[C]	HEA	CHA-C1A-C2A	-2.26	121.28	124.94
24	G	101	CHD	C19-C10-C1	-2.26	104.62	108.26
14	N	603	HEA	O1D-CGD-CBD	-2.25	115.85	123.08
14	A	601[A]	HEA	C1B-C2B-C3B	-2.25	104.11	106.80
14	A	601[C]	HEA	C1B-C2B-C3B	-2.25	104.11	106.80
26	P	304	CDL	C59-C58-C57	2.25	125.84	114.42
19	O	303	PSC	C14-C13-C12	-2.24	107.50	124.73
14	A	602	HEA	C13-C12-C11	-2.24	110.98	114.35
14	N	603	HEA	C3B-C4B-NB	2.23	112.49	109.84
27	C	307	PEK	C02-O01-C1	-2.23	112.31	117.79
14	N	603	HEA	C2D-C1D-ND	2.22	112.47	109.84
24	L	102	CHD	C4-C5-C10	2.21	115.00	112.66
26	C	305	CDL	OB8-CB7-C71	2.21	119.64	109.94
14	A	602	HEA	C4A-NA-C1A	2.20	107.51	105.35
22	B	301	TGL	OB1-CB1-CB2	-2.20	115.16	123.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C25-C23-C22	-2.19	116.32	122.65
27	P	306	PEK	O03-C21-C22	2.19	118.78	111.91
24	C	304	CHD	C18-C13-C14	-2.19	107.79	111.21
14	A	601[A]	HEA	C21-C22-C23	-2.18	120.30	127.75
27	C	307	PEK	C3-C2-C1	-2.17	105.73	113.62
22	N	609	TGL	CG3-CG2-CG1	-2.17	106.66	111.79
14	N	602[C]	HEA	C16-C17-C18	-2.16	104.80	111.88
14	A	601[A]	HEA	C25-C23-C22	-2.15	116.42	122.65
14	A	601[C]	HEA	C12-C13-C14	-2.15	106.57	112.23
25	Z	101	DMU	O1-C9-C11	2.13	111.74	106.44
18	C	308	PGV	O03-C19-O04	-2.13	118.22	123.59
14	A	601[A]	HEA	CHB-C1B-NB	-2.13	122.11	124.42
14	A	601[C]	HEA	CHB-C1B-NB	-2.13	122.11	124.42
24	Y	101	CHD	O7-C7-C8	2.13	114.18	109.43
14	A	602	HEA	CHA-C1A-NA	2.12	126.74	124.44
25	L	101	DMU	O16-C18-C19	-2.12	102.13	109.56
22	N	612	TGL	C26-C25-C24	-2.12	103.66	114.42
22	L	103	TGL	OG1-CA1-CA2	2.11	120.58	112.23
24	P	301	CHD	C1-C2-C3	-2.11	107.76	110.47
24	Y	101	CHD	C13-C17-C20	2.11	122.01	119.50
19	O	303	PSC	O03-C19-C20	2.10	120.76	114.03
25	M	101	DMU	O7-C10-C5	2.09	113.52	108.10
25	C	310	DMU	C22-C19-C18	-2.07	104.32	113.49
18	C	308	PGV	O12-P-O13	-2.07	100.98	109.07
14	N	603	HEA	CBD-CAD-C3D	2.07	118.38	112.63
24	L	102	CHD	C5-C4-C3	2.07	115.79	112.76
14	A	601[A]	HEA	CHB-C1B-C2B	-2.06	121.76	124.98
14	A	601[C]	HEA	CHB-C1B-C2B	-2.06	121.76	124.98
14	A	601[A]	HEA	C25-C23-C24	2.05	119.14	114.60
24	G	101	CHD	C13-C14-C8	-2.05	112.12	114.74
26	C	305	CDL	C52-C51-CB5	-2.05	105.14	114.26
26	T	101	CDL	OB8-CB6-CB4	2.05	114.29	108.38
24	B	303	CHD	C19-C10-C9	2.04	114.00	111.18
14	A	602	HEA	CMD-C2D-C1D	2.04	128.15	125.04
18	P	307	PGV	C22-C21-C20	-2.04	105.85	113.19
24	C	304	CHD	C5-C6-C7	2.04	116.71	114.46
22	N	612	TGL	CA7-CA6-CA5	-2.04	104.08	114.42
24	L	102	CHD	O25-C24-C23	-2.03	116.55	123.08
14	N	603	HEA	C2C-C1C-NC	2.02	113.16	110.08
24	G	101	CHD	O3-C3-C4	-2.02	105.83	109.85
18	C	301	PGV	O01-C02-C01	-2.02	101.10	108.40
22	D	202	TGL	CB3-CB2-CB1	2.01	120.92	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	CAA-C2A-C1A	2.00	128.67	124.89
14	N	602[C]	HEA	CAA-C2A-C1A	2.00	128.67	124.89
24	B	303	CHD	C1-C10-C5	2.00	110.73	107.77

There are no chirality outliers.

All (536) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	A	601[C]	HEA	C2A-C3A-CMA-OMA
14	A	601[C]	HEA	C11-C12-C13-C14
14	N	602[C]	HEA	O11-C11-C3B-C2B
14	N	602[C]	HEA	C14-C15-C16-C17
14	N	602[C]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C17-C18-C19-C20
18	A	606	PGV	C1-C2-C3-C4
18	C	311	PGV	O04-C19-O03-C01
18	C	311	PGV	C20-C19-O03-C01
18	G	102	PGV	O04-C19-O03-C01
18	G	102	PGV	C20-C19-O03-C01
18	G	102	PGV	C11-C12-C13-C14
19	A	607	PSC	C7-C8-C9-C10
19	O	303	PSC	C10-C11-C12-C13
22	D	202	TGL	OB1-CB1-OG2-CG2
22	N	612	TGL	OB1-CB1-OG2-CG2
22	N	612	TGL	OG2-CG2-CG3-OG3
26	C	305	CDL	CB5-C51-C52-C53
26	T	101	CDL	OB6-CB4-CB6-OB8
27	C	306	PEK	C4-C5-C6-C7
27	C	306	PEK	C7-C8-C9-C10
27	C	306	PEK	C11-C10-C9-C8
27	P	306	PEK	C11-C12-C13-C14
24	L	102	CHD	C16-C17-C20-C21
24	L	102	CHD	C13-C17-C20-C21
24	L	102	CHD	C16-C17-C20-C22
24	L	102	CHD	C13-C17-C20-C22
22	D	202	TGL	CB2-CB1-OG2-CG2
22	N	612	TGL	CB2-CB1-OG2-CG2
27	C	307	PEK	C7-C8-C9-C10
27	C	309	PEK	C4-C5-C6-C7
27	C	309	PEK	C13-C14-C15-C16
14	A	601[C]	HEA	C17-C18-C19-C27

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Mol	Chain	Res	Type	Atoms
14	N	602[C]	HEA	C17-C18-C19-C27
22	L	103	TGL	CA2-CA1-OG1-CG1
22	N	609	TGL	CA4-CA5-CA6-CA7
24	Y	101	CHD	C13-C17-C20-C21
22	D	202	TGL	CG2-CG1-OG1-CA1
22	N	612	TGL	CA2-CA1-OG1-CG1
22	B	301	TGL	C11-C12-C13-C14
25	Z	101	DMU	O6-C11-C9-O1
22	L	103	TGL	OA1-CA1-OG1-CG1
24	Y	101	CHD	C16-C17-C20-C22
22	L	103	TGL	CC1-CC2-CC3-CC4
22	N	612	TGL	OA1-CA1-OG1-CG1
22	N	609	TGL	CB9-C10-C11-C12
14	N	602[C]	HEA	C15-C16-C17-C18
26	N	601	CDL	C40-C41-C42-C43
26	P	304	CDL	C40-C41-C42-C43
18	C	311	PGV	O03-C01-C02-C03
22	N	609	TGL	CB3-CB4-CB5-CB6
22	N	609	TGL	C14-C29-C30-C31
25	Z	101	DMU	O6-C11-C9-C8
22	N	611	TGL	C20-C21-C22-C23
22	L	103	TGL	C23-C24-C25-C26
26	P	304	CDL	C82-C83-C84-C85
18	C	308	PGV	C10-C11-C12-C13
18	N	608	PGV	C10-C11-C12-C13
27	P	305	PEK	C4-C5-C6-C7
22	B	301	TGL	CB1-CB2-CB3-CB4
22	L	103	TGL	CA9-C20-C21-C22
25	C	303	DMU	O16-C18-C19-C22
25	C	310	DMU	O16-C18-C19-C22
26	N	601	CDL	C80-C81-C82-C83
27	P	306	PEK	C16-C17-C18-C19
22	D	202	TGL	C21-C22-C23-C24
24	L	102	CHD	C20-C22-C23-C24
25	Z	101	DMU	O16-C18-C19-C22
22	N	612	TGL	C12-C13-C14-C29
26	P	304	CDL	C57-C58-C59-C60
22	L	103	TGL	CB3-CB4-CB5-CB6
22	N	609	TGL	CC5-CC6-CC7-CC8
22	N	611	TGL	C21-C22-C23-C24
26	T	101	CDL	C58-C59-C60-C61
22	L	103	TGL	CA5-CA6-CA7-CA8

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Mol	Chain	Res	Type	Atoms
25	L	101	DMU	C28-C31-C34-C37
18	G	102	PGV	C28-C29-C30-C31
22	B	301	TGL	CC7-CC8-CC9-C15
25	K	105	DMU	C31-C34-C37-C40
27	P	308	PEK	C13-C14-C15-C16
22	D	202	TGL	CB3-CB4-CB5-CB6
22	N	612	TGL	C21-C22-C23-C24
22	N	609	TGL	CB4-CB5-CB6-CB7
25	L	101	DMU	C1-C6-O16-C18
18	C	308	PGV	C7-C8-C9-C10
18	N	607	PGV	C4-C5-C6-C7
22	L	103	TGL	C21-C22-C23-C24
22	N	612	TGL	CB4-CB5-CB6-CB7
22	B	301	TGL	CB9-C10-C11-C12
22	N	609	TGL	C13-C14-C29-C30
22	N	609	TGL	C24-C25-C26-C27
22	N	611	TGL	CC5-CC6-CC7-CC8
22	N	611	TGL	CC9-C15-C16-C17
22	N	612	TGL	CA2-CA3-CA4-CA5
22	N	612	TGL	CB3-CB4-CB5-CB6
25	K	102	DMU	C28-C31-C34-C37
25	K	103	DMU	C31-C34-C37-C40
25	M	101	DMU	C19-C22-C25-C28
25	Z	101	DMU	C22-C25-C28-C31
26	C	305	CDL	C52-C53-C54-C55
26	C	305	CDL	C58-C59-C60-C61
27	C	307	PEK	C28-C29-C30-C31
19	A	607	PSC	C27-C28-C29-C30
22	N	611	TGL	C11-C10-CB9-CB8
25	K	104	DMU	C25-C28-C31-C34
26	P	304	CDL	C81-C82-C83-C84
22	L	103	TGL	CB5-CB6-CB7-CB8
26	C	305	CDL	C62-C63-C64-C65
22	D	202	TGL	CC6-CC7-CC8-CC9
22	N	611	TGL	CA4-CA5-CA6-CA7
22	N	611	TGL	CB5-CB6-CB7-CB8
26	T	101	CDL	C79-C80-C81-C82
19	A	607	PSC	C23-C24-C25-C26
22	D	202	TGL	CC2-CC3-CC4-CC5
22	L	103	TGL	C11-C10-CB9-CB8
25	Z	101	DMU	C25-C28-C31-C34
22	B	301	TGL	C13-C14-C29-C30

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Mol	Chain	Res	Type	Atoms
22	B	301	TGL	C17-C18-C19-C33
22	D	202	TGL	C16-C17-C18-C19
22	N	612	TGL	CA3-CA4-CA5-CA6
18	C	311	PGV	C6-C7-C8-C9
25	K	104	DMU	C22-C25-C28-C31
26	T	101	CDL	C72-C73-C74-C75
26	T	101	CDL	C73-C74-C75-C76
27	C	309	PEK	C22-C23-C24-C25
22	D	202	TGL	C20-C21-C22-C23
22	N	609	TGL	C10-C11-C12-C13
25	L	101	DMU	C25-C28-C31-C34
18	C	308	PGV	C28-C29-C30-C31
25	C	303	DMU	C19-C22-C25-C28
22	L	103	TGL	C21-C20-CA9-CA8
22	B	301	TGL	OG1-CG1-CG2-CG3
19	A	607	PSC	C11-C10-C9-C8
22	L	103	TGL	CC4-CC5-CC6-CC7
22	B	301	TGL	CC5-CC6-CC7-CC8
27	C	307	PEK	C23-C24-C25-C26
22	D	202	TGL	CA9-C20-C21-C22
22	N	612	TGL	C22-C23-C24-C25
26	P	304	CDL	C12-C13-C14-C15
25	P	303	DMU	C31-C34-C37-C40
26	C	305	CDL	C80-C81-C82-C83
26	P	304	CDL	C73-C74-C75-C76
22	N	609	TGL	C21-C20-CA9-CA8
25	W	101	DMU	C18-C19-C22-C25
18	G	102	PGV	C7-C8-C9-C10
26	T	101	CDL	C42-C43-C44-C45
26	T	101	CDL	C74-C75-C76-C77
19	O	303	PSC	C5-C6-C7-C8
21	D	205	EDO	O1-C1-C2-O2
21	E	203	EDO	O1-C1-C2-O2
21	P	310	EDO	O1-C1-C2-O2
21	W	102	EDO	O1-C1-C2-O2
22	B	301	TGL	CB4-CB5-CB6-CB7
26	C	305	CDL	C63-C64-C65-C66
22	N	609	TGL	CB2-CB1-OG2-CG2
22	D	202	TGL	CC9-C15-C16-C17
26	N	601	CDL	C23-C24-C25-C26
26	P	304	CDL	C15-C16-C17-C18
22	N	612	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
24	Y	101	CHD	C16-C17-C20-C21
22	N	609	TGL	C11-C10-CB9-CB8
22	N	611	TGL	CA7-CA8-CA9-C20
25	P	303	DMU	C34-C37-C40-C43
22	N	609	TGL	OB1-CB1-OG2-CG2
22	D	202	TGL	CA2-CA1-OG1-CG1
22	N	609	TGL	CC2-CC1-OG3-CG3
22	N	609	TGL	CB7-CB8-CB9-C10
22	D	202	TGL	CB4-CB5-CB6-CB7
18	N	608	PGV	C25-C26-C27-C28
22	N	609	TGL	C20-C21-C22-C23
26	T	101	CDL	C60-C61-C62-C63
18	C	308	PGV	C19-C20-C21-C22
22	N	611	TGL	CA5-CA6-CA7-CA8
18	C	311	PGV	C23-C24-C25-C26
22	N	612	TGL	C21-C20-CA9-CA8
22	D	202	TGL	CA3-CA4-CA5-CA6
22	N	611	TGL	CB4-CB5-CB6-CB7
22	B	301	TGL	C16-C17-C18-C19
22	N	612	TGL	CB7-CB8-CB9-C10
22	B	301	TGL	OG1-CG1-CG2-OG2
22	N	611	TGL	C19-C33-C34-C35
27	P	306	PEK	C15-C16-C17-C18
22	L	103	TGL	CC6-CC7-CC8-CC9
26	P	304	CDL	C36-C37-C38-C39
18	C	301	PGV	C10-C11-C12-C13
25	J	101	DMU	C18-C19-C22-C25
26	P	304	CDL	C37-C38-C39-C40
25	O	302	DMU	C28-C31-C34-C37
22	N	612	TGL	C11-C12-C13-C14
25	K	106	DMU	C31-C34-C37-C40
25	X	102	DMU	C34-C37-C40-C43
26	T	101	CDL	C21-C22-C23-C24
27	P	308	PEK	C28-C29-C30-C31
19	A	607	PSC	C26-C27-C28-C29
18	A	606	PGV	C11-C10-C9-C8
18	P	307	PGV	C11-C10-C9-C8
22	L	103	TGL	C18-C19-C33-C34
22	D	202	TGL	CA7-CA8-CA9-C20
22	D	202	TGL	OA1-CA1-OG1-CG1
22	B	301	TGL	C12-C13-C14-C29
25	J	101	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
22	D	202	TGL	OG1-CG1-CG2-CG3
22	N	612	TGL	OG1-CG1-CG2-CG3
25	O	302	DMU	C25-C28-C31-C34
25	L	101	DMU	C34-C37-C40-C43
25	M	101	DMU	C22-C25-C28-C31
22	N	609	TGL	CB6-CB7-CB8-CB9
25	K	102	DMU	C18-C19-C22-C25
25	K	105	DMU	C34-C37-C40-C43
26	T	101	CDL	C57-C58-C59-C60
22	N	611	TGL	CC2-CC3-CC4-CC5
26	T	101	CDL	C22-C23-C24-C25
22	N	609	TGL	C15-C16-C17-C18
22	N	609	TGL	OC1-CC1-OG3-CG3
25	K	105	DMU	C22-C25-C28-C31
26	T	101	CDL	C82-C83-C84-C85
22	N	612	TGL	C24-C25-C26-C27
25	D	203	DMU	C25-C28-C31-C34
22	N	612	TGL	CA1-CA2-CA3-CA4
27	P	306	PEK	C17-C18-C19-C20
22	L	103	TGL	CC2-CC3-CC4-CC5
22	N	609	TGL	C16-C15-CC9-CC8
25	J	101	DMU	O16-C18-C19-C22
14	N	602[C]	HEA	C11-C12-C13-C14
22	L	103	TGL	C11-C12-C13-C14
26	T	101	CDL	C71-C72-C73-C74
22	B	301	TGL	CC2-CC1-OG3-CG3
27	P	306	PEK	C4-C5-C6-C7
27	P	306	PEK	C13-C14-C15-C16
25	J	101	DMU	C22-C25-C28-C31
21	P	315	EDO	O1-C1-C2-O2
25	K	106	DMU	C22-C25-C28-C31
26	N	601	CDL	C14-C15-C16-C17
25	O	302	DMU	C34-C37-C40-C43
22	B	301	TGL	OB1-CB1-OG2-CG2
22	N	609	TGL	C23-C24-C25-C26
18	N	607	PGV	C2-C3-C4-C5
26	N	601	CDL	C13-C14-C15-C16
27	P	308	PEK	C10-C11-C12-C13
26	T	101	CDL	C39-C40-C41-C42
18	C	301	PGV	C31-C32-C33-C34
18	G	102	PGV	C4-C5-C6-C7
25	Z	101	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
25	K	103	DMU	C34-C37-C40-C43
18	N	607	PGV	C11-C10-C9-C8
27	C	307	PEK	C17-C18-C19-C20
26	T	101	CDL	CB3-CB4-CB6-OB8
26	N	601	CDL	C58-C59-C60-C61
18	C	311	PGV	C10-C11-C12-C13
27	C	307	PEK	C10-C11-C12-C13
27	P	306	PEK	C7-C8-C9-C10
22	B	301	TGL	C15-C16-C17-C18
25	C	310	DMU	C18-C19-C22-C25
14	A	601[A]	HEA	C27-C19-C20-C21
22	B	301	TGL	CC2-CC3-CC4-CC5
22	B	301	TGL	C18-C19-C33-C34
22	N	609	TGL	CA2-CA3-CA4-CA5
22	N	612	TGL	CB2-CB3-CB4-CB5
25	K	103	DMU	C28-C31-C34-C37
14	A	602	HEA	C2A-C3A-CMA-OMA
14	N	602[A]	HEA	C2A-C3A-CMA-OMA
14	N	602[C]	HEA	C2A-C3A-CMA-OMA
14	N	603	HEA	C2A-C3A-CMA-OMA
19	A	607	PSC	C9-C10-C11-C12
19	A	607	PSC	C10-C11-C12-C13
19	O	303	PSC	C9-C10-C11-C12
27	C	306	PEK	C5-C6-C7-C8
27	C	306	PEK	C6-C7-C8-C9
27	C	306	PEK	C9-C10-C11-C12
27	C	306	PEK	C11-C12-C13-C14
27	C	306	PEK	C12-C13-C14-C15
27	C	307	PEK	C6-C7-C8-C9
27	C	307	PEK	C9-C10-C11-C12
27	C	307	PEK	C11-C12-C13-C14
27	C	307	PEK	C12-C13-C14-C15
27	C	309	PEK	C5-C6-C7-C8
27	C	309	PEK	C6-C7-C8-C9
27	C	309	PEK	C11-C10-C9-C8
27	C	309	PEK	C9-C10-C11-C12
27	C	309	PEK	C11-C12-C13-C14
27	C	309	PEK	C12-C13-C14-C15
27	P	305	PEK	C5-C6-C7-C8
27	P	305	PEK	C11-C10-C9-C8
27	P	305	PEK	C11-C12-C13-C14
27	P	305	PEK	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
27	P	306	PEK	C9-C10-C11-C12
27	P	308	PEK	C5-C6-C7-C8
27	P	308	PEK	C6-C7-C8-C9
27	P	308	PEK	C11-C10-C9-C8
27	P	308	PEK	C9-C10-C11-C12
27	P	308	PEK	C11-C12-C13-C14
25	K	103	DMU	C22-C25-C28-C31
26	P	304	CDL	C58-C59-C60-C61
22	N	612	TGL	CG1-CG2-CG3-OG3
25	C	310	DMU	C22-C25-C28-C31
22	B	301	TGL	C10-C11-C12-C13
22	N	611	TGL	CA9-C20-C21-C22
26	T	101	CDL	C16-C17-C18-C19
25	Q	201	DMU	C19-C22-C25-C28
21	C	320	EDO	O1-C1-C2-O2
21	J	103	EDO	O1-C1-C2-O2
22	B	301	TGL	CB2-CB1-OG2-CG2
25	D	201	DMU	C34-C37-C40-C43
26	T	101	CDL	C80-C81-C82-C83
22	D	202	TGL	CC7-CC8-CC9-C15
25	Q	201	DMU	C28-C31-C34-C37
27	P	308	PEK	C3-C4-C5-C6
27	P	308	PEK	C29-C30-C31-C32
18	N	607	PGV	C10-C11-C12-C13
25	K	106	DMU	C28-C31-C34-C37
26	N	601	CDL	C81-C82-C83-C84
22	N	609	TGL	CB5-CB6-CB7-CB8
24	Y	101	CHD	C13-C17-C20-C22
22	D	202	TGL	C19-C33-C34-C35
22	N	612	TGL	C11-C10-CB9-CB8
25	K	105	DMU	C28-C31-C34-C37
22	N	609	TGL	C29-C30-C31-C32
25	K	103	DMU	C19-C22-C25-C28
26	P	304	CDL	C77-C78-C79-C80
22	B	301	TGL	OC1-CC1-OG3-CG3
22	B	301	TGL	CC9-C15-C16-C17
22	B	301	TGL	CC4-CC5-CC6-CC7
18	C	311	PGV	C24-C25-C26-C27
26	N	601	CDL	C37-C38-C39-C40
26	N	601	CDL	C20-C21-C22-C23
25	P	309	DMU	C28-C31-C34-C37
26	N	601	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
27	C	307	PEK	C26-C27-C28-C29
18	C	308	PGV	C27-C28-C29-C30
25	C	310	DMU	C3-C4-C57-O61
25	P	303	DMU	C28-C31-C34-C37
22	N	609	TGL	C12-C13-C14-C29
22	N	611	TGL	C15-C16-C17-C18
18	C	308	PGV	C02-C03-O11-P
18	P	307	PGV	C02-C03-O11-P
26	N	601	CDL	C60-C61-C62-C63
14	A	601[C]	HEA	O11-C11-C3B-C2B
18	C	308	PGV	C1-C2-C3-C4
22	D	202	TGL	CA1-CA2-CA3-CA4
25	D	201	DMU	C22-C25-C28-C31
25	Q	201	DMU	C18-C19-C22-C25
14	A	601[A]	HEA	C4A-C3A-CMA-OMA
14	A	601[C]	HEA	C4A-C3A-CMA-OMA
14	N	603	HEA	C4A-C3A-CMA-OMA
22	D	202	TGL	OG1-CG1-CG2-OG2
22	D	202	TGL	CB7-CB8-CB9-C10
22	N	609	TGL	C17-C18-C19-C33
25	K	102	DMU	C34-C37-C40-C43
22	D	202	TGL	OG3-CC1-CC2-CC3
26	N	601	CDL	C57-C58-C59-C60
22	N	609	TGL	CC6-CC7-CC8-CC9
25	M	101	DMU	C25-C28-C31-C34
27	C	307	PEK	C4-C5-C6-C7
26	T	101	CDL	C18-C19-C20-C21
26	T	101	CDL	C41-C42-C43-C44
25	K	103	DMU	C18-C19-C22-C25
22	L	103	TGL	CC3-CC4-CC5-CC6
25	P	309	DMU	O16-C18-C19-C22
22	B	301	TGL	CC3-CC4-CC5-CC6
22	N	609	TGL	OG3-CC1-CC2-CC3
19	O	303	PSC	C26-C27-C28-C29
26	P	304	CDL	C44-C45-C46-C47
22	L	103	TGL	CC9-C15-C16-C17
26	N	601	CDL	C19-C20-C21-C22
21	A	610	EDO	O1-C1-C2-O2
21	A	615	EDO	O1-C1-C2-O2
21	L	104	EDO	O1-C1-C2-O2
21	N	619	EDO	O1-C1-C2-O2
21	T	104	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	L	103	TGL	OG1-CA1-CA2-CA3
25	D	203	DMU	C28-C31-C34-C37
19	A	607	PSC	C12-C13-C14-C15
27	C	309	PEK	C3-C4-C5-C6
22	N	612	TGL	OG1-CG1-CG2-OG2
18	N	608	PGV	C20-C21-C22-C23
22	D	202	TGL	CG1-CG2-CG3-OG3
22	N	612	TGL	CB6-CB7-CB8-CB9
25	J	101	DMU	C25-C28-C31-C34
26	N	601	CDL	C17-C18-C19-C20
25	J	101	DMU	C19-C22-C25-C28
19	O	303	PSC	C11-C10-C9-C8
18	C	301	PGV	C29-C30-C31-C32
22	L	103	TGL	CA3-CA4-CA5-CA6
26	N	601	CDL	C61-C62-C63-C64
27	C	307	PEK	C27-C28-C29-C30
26	P	304	CDL	C78-C79-C80-C81
27	C	307	PEK	O03-C21-C22-C23
18	P	307	PGV	C7-C8-C9-C10
22	D	202	TGL	CC5-CC6-CC7-CC8
27	C	306	PEK	C2-C3-C4-C5
24	G	101	CHD	C22-C23-C24-O26
24	L	102	CHD	C17-C20-C22-C23
25	Q	201	DMU	C31-C34-C37-C40
26	C	305	CDL	C78-C79-C80-C81
18	C	301	PGV	C11-C12-C13-C14
18	C	308	PGV	C11-C12-C13-C14
27	P	305	PEK	C3-C4-C5-C6
26	P	304	CDL	C72-C73-C74-C75
22	N	609	TGL	C16-C17-C18-C19
21	A	614	EDO	O1-C1-C2-O2
26	P	304	CDL	CB7-C71-C72-C73
26	C	305	CDL	C60-C61-C62-C63
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[C]	HEA	CAD-CBD-CGD-O1D
24	B	303	CHD	C22-C23-C24-O25
14	N	603	HEA	CAA-CBA-CGA-O1A
24	G	101	CHD	C22-C23-C24-O25
18	N	608	PGV	C29-C30-C31-C32
14	A	601[C]	HEA	C26-C15-C16-C17
25	X	103	DMU	C28-C31-C34-C37
18	C	301	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	C	308	PGV	C9-C10-C11-C12
18	N	607	PGV	C9-C10-C11-C12
27	C	307	PEK	C14-C15-C16-C17
14	N	603	HEA	CAA-CBA-CGA-O2A
22	B	301	TGL	OG1-CA1-CA2-CA3
22	L	103	TGL	CC7-CC8-CC9-C15
27	P	305	PEK	C6-C7-C8-C9
27	P	305	PEK	C9-C10-C11-C12
27	P	306	PEK	C6-C7-C8-C9
27	P	306	PEK	C12-C13-C14-C15
27	P	308	PEK	C12-C13-C14-C15
22	N	611	TGL	CC6-CC7-CC8-CC9
14	A	602	HEA	CAD-CBD-CGD-O2D
26	T	101	CDL	C77-C78-C79-C80
22	N	612	TGL	CB9-C10-C11-C12
22	B	301	TGL	C19-C33-C34-C35
24	B	303	CHD	C22-C23-C24-O26
27	P	306	PEK	C22-C23-C24-C25
22	D	202	TGL	C22-C23-C24-C25
27	P	305	PEK	C7-C8-C9-C10
14	N	602[C]	HEA	C19-C20-C21-C22
22	N	609	TGL	OA1-CA1-OG1-CG1
26	N	601	CDL	C16-C17-C18-C19
18	A	606	PGV	C9-C10-C11-C12
27	P	305	PEK	C14-C15-C16-C17
26	P	304	CDL	C41-C42-C43-C44
21	A	613	EDO	O1-C1-C2-O2
21	E	202	EDO	O1-C1-C2-O2
21	O	305	EDO	O1-C1-C2-O2
26	C	305	CDL	C61-C62-C63-C64
22	B	301	TGL	CB5-CB6-CB7-CB8
22	N	609	TGL	CA9-C20-C21-C22
26	C	305	CDL	C57-C58-C59-C60
27	C	309	PEK	C28-C29-C30-C31
22	D	202	TGL	CC1-CC2-CC3-CC4
22	N	609	TGL	C22-C23-C24-C25
18	C	301	PGV	O03-C19-C20-C21
22	D	202	TGL	CB9-C10-C11-C12
18	C	311	PGV	C9-C10-C11-C12
19	O	303	PSC	C12-C13-C14-C15
18	C	301	PGV	C26-C27-C28-C29
19	A	607	PSC	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	P	306	PEK	O12-C04-C05-N
27	C	309	PEK	C33-C34-C35-C36
14	N	603	HEA	CAD-CBD-CGD-O2D
22	B	301	TGL	OG2-CG2-CG3-OG3
26	N	601	CDL	C15-C16-C17-C18
22	D	202	TGL	CC3-CC4-CC5-CC6
14	A	602	HEA	CAD-CBD-CGD-O1D
22	N	609	TGL	CA2-CA1-OG1-CG1
18	C	311	PGV	C11-C12-C13-C14
18	N	608	PGV	C11-C12-C13-C14
27	P	308	PEK	C14-C15-C16-C17
18	N	608	PGV	O03-C19-C20-C21
14	A	602	HEA	CAA-CBA-CGA-O1A
14	A	601[A]	HEA	C18-C19-C20-C21
26	C	305	CDL	C13-C14-C15-C16
18	C	308	PGV	C20-C21-C22-C23
18	G	102	PGV	C9-C10-C11-C12
27	C	309	PEK	C14-C15-C16-C17
14	A	602	HEA	CAA-CBA-CGA-O2A
22	L	103	TGL	C33-C34-C35-C36
26	T	101	CDL	CB3-CB4-OB6-CB5
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
14	N	602[C]	HEA	CAD-CBD-CGD-O1D
26	C	305	CDL	C37-C38-C39-C40
18	P	307	PGV	C11-C12-C13-C14
14	A	601[C]	HEA	C12-C11-C3B-C2B
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[C]	HEA	CAD-CBD-CGD-O2D
27	C	307	PEK	C22-C23-C24-C25
14	N	603	HEA	CAD-CBD-CGD-O1D
22	L	103	TGL	C19-C33-C34-C35
25	C	310	DMU	C28-C31-C34-C37
25	D	201	DMU	C25-C28-C31-C34
21	G	104	EDO	O1-C1-C2-O2
21	J	102	EDO	O1-C1-C2-O2
21	P	311	EDO	O1-C1-C2-O2
21	Y	103	EDO	O1-C1-C2-O2
19	O	303	PSC	O03-C19-C20-C21
22	N	611	TGL	CB3-CB4-CB5-CB6
24	P	301	CHD	C22-C23-C24-O25
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
14	N	602[C]	HEA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	D	202	TGL	OG2-CG2-CG3-OG3
22	N	609	TGL	OG2-CG2-CG3-OG3
18	N	608	PGV	C27-C28-C29-C30
18	N	608	PGV	C9-C10-C11-C12
27	C	309	PEK	C25-C26-C27-C28
27	C	309	PEK	C23-C24-C25-C26
19	O	303	PSC	O04-C19-C20-C21
24	C	304	CHD	C22-C23-C24-O25
22	D	202	TGL	CB5-CB6-CB7-CB8
22	N	611	TGL	CC3-CC4-CC5-CC6
27	P	306	PEK	C14-C15-C16-C17
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
14	N	602[C]	HEA	CAA-CBA-CGA-O1A
26	C	305	CDL	C31-C32-C33-C34
22	N	611	TGL	C18-C19-C33-C34
18	C	301	PGV	C11-C10-C9-C8
18	P	307	PGV	C13-C14-C15-C16
22	L	103	TGL	CA1-CA2-CA3-CA4
22	N	611	TGL	C16-C15-CC9-CC8
27	P	306	PEK	C26-C27-C28-C29
18	N	608	PGV	O04-C19-C20-C21
19	O	303	PSC	C15-C16-C17-C18
25	P	303	DMU	C19-C18-O16-C6
19	A	607	PSC	C24-C25-C26-C27
24	C	304	CHD	C22-C23-C24-O26
22	N	612	TGL	OG1-CA1-CA2-CA3
22	B	301	TGL	C11-C10-CB9-CB8
25	X	102	DMU	C25-C28-C31-C34
22	N	611	TGL	CC4-CC5-CC6-CC7
18	P	307	PGV	C05-C04-O12-P
14	A	601[C]	HEA	C14-C15-C16-C17
22	D	202	TGL	OG1-CA1-CA2-CA3
22	B	301	TGL	C29-C30-C31-C32
26	C	305	CDL	C53-C54-C55-C56
14	A	601[A]	HEA	CAA-CBA-CGA-O1A
14	A	601[C]	HEA	CAA-CBA-CGA-O1A
18	C	311	PGV	C20-C21-C22-C23
26	P	304	CDL	C17-C18-C19-C20
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
14	N	602[C]	HEA	CAA-CBA-CGA-O2A

There are no ring outliers.

62 monomers are involved in 141 short contacts:

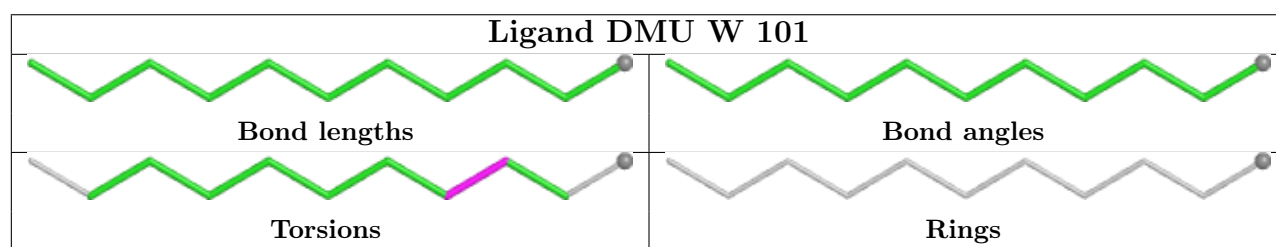
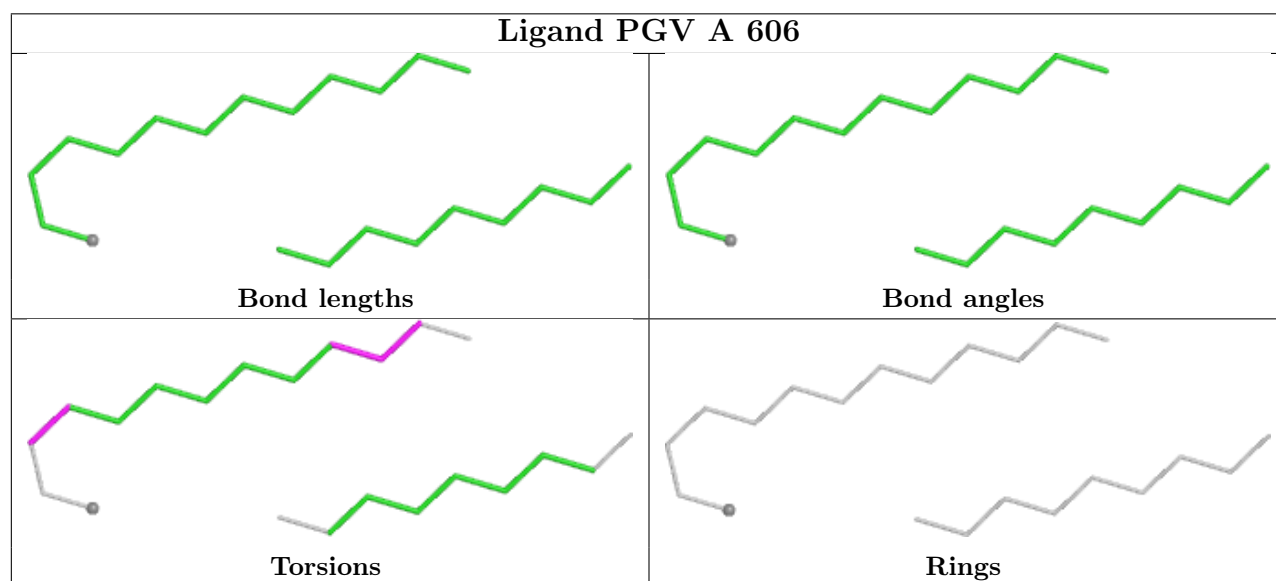
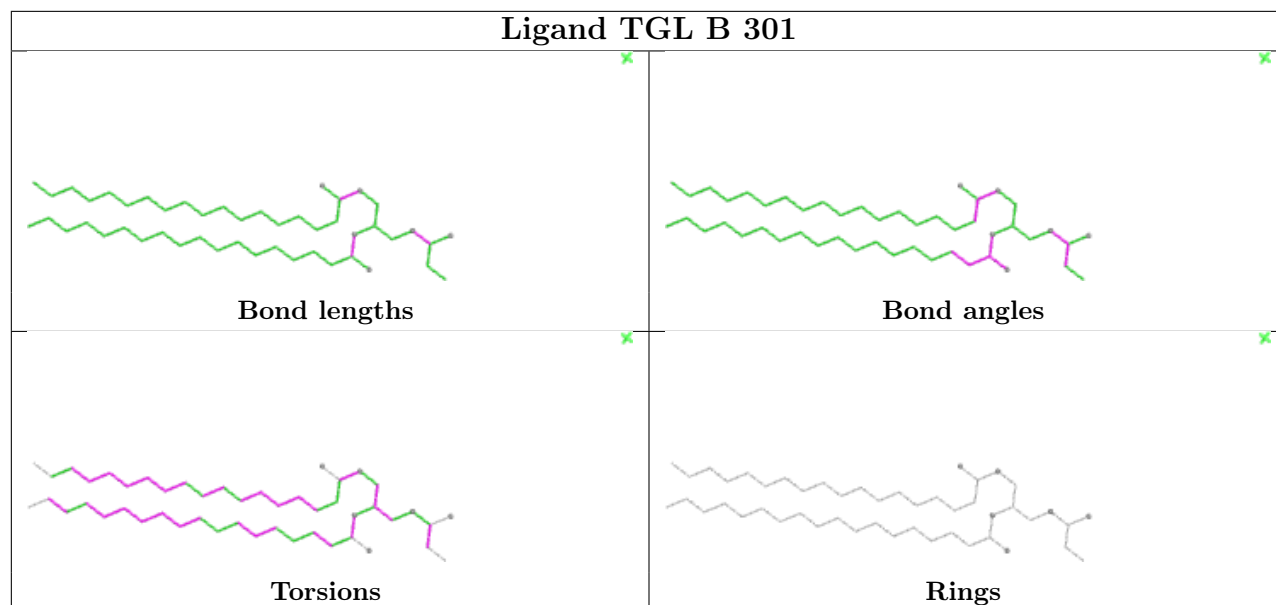
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	301	TGL	1	0
18	A	606	PGV	2	0
25	W	101	DMU	1	0
22	N	611	TGL	5	0
25	O	302	DMU	1	0
18	C	308	PGV	3	0
25	P	309	DMU	5	0
14	A	602	HEA	2	0
25	C	303	DMU	1	0
18	C	301	PGV	1	0
18	C	311	PGV	2	0
25	P	303	DMU	1	0
25	J	101	DMU	2	0
25	K	103	DMU	1	0
27	P	306	PEK	5	0
14	N	602[A]	HEA	2	0
24	G	101	CHD	1	0
18	G	102	PGV	2	0
21	S	106	EDO	1	0
14	N	602[C]	HEA	1	0
19	A	607	PSC	4	0
21	W	102	EDO	1	0
24	Y	101	CHD	1	0
25	C	310	DMU	4	0
25	K	106	DMU	1	0
26	P	304	CDL	4	0
20	N	610[A]	PER	1	0
26	N	601	CDL	3	0
18	N	607	PGV	1	0
26	C	305	CDL	6	0
25	L	101	DMU	1	0
25	K	105	DMU	1	0
27	C	309	PEK	4	0
19	O	303	PSC	4	0
22	N	612	TGL	3	0
22	N	609	TGL	6	0
18	P	307	PGV	2	0
25	Z	101	DMU	1	0
21	C	320	EDO	1	0
27	P	308	PEK	4	0
27	C	307	PEK	4	0
22	D	202	TGL	9	0

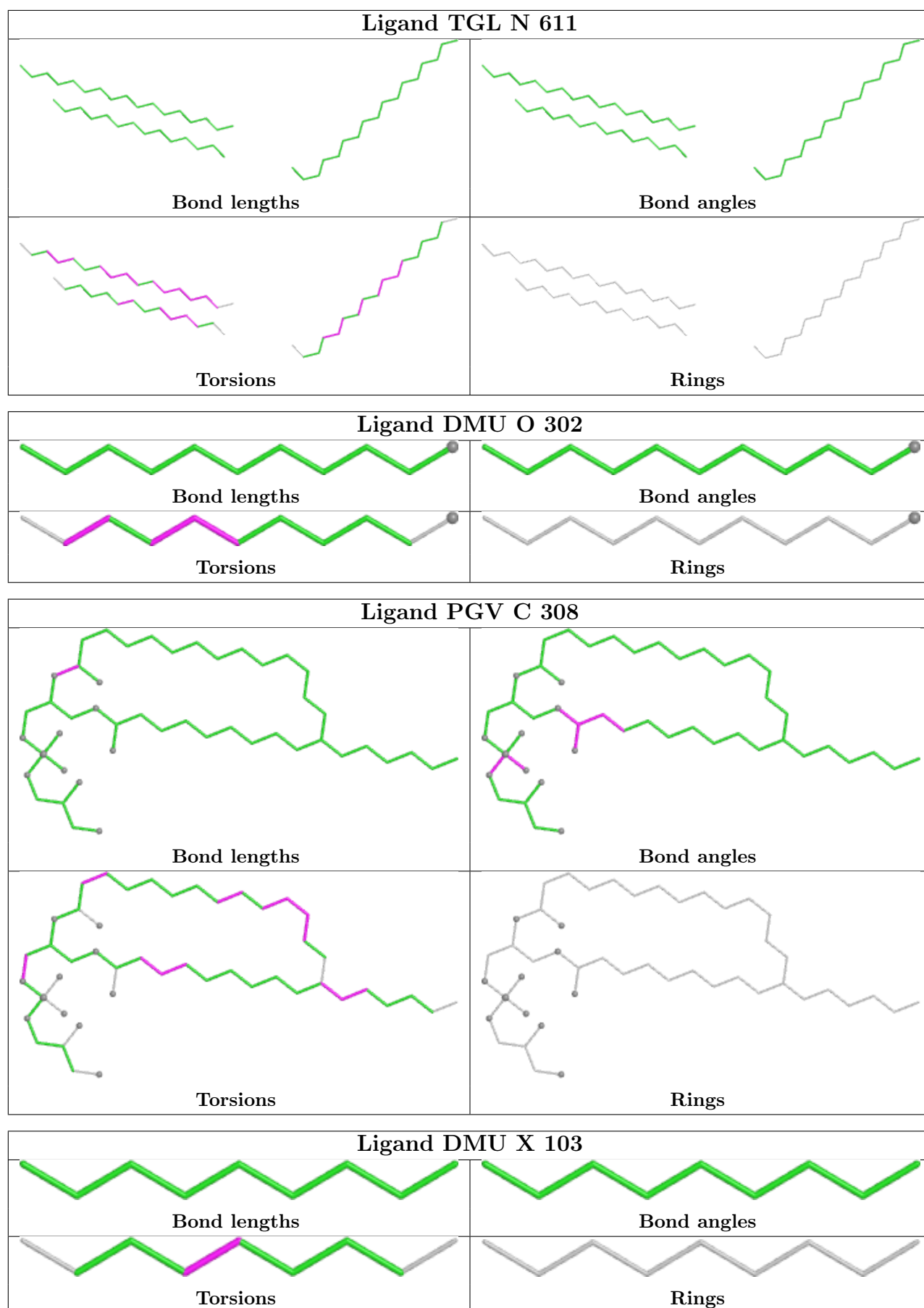
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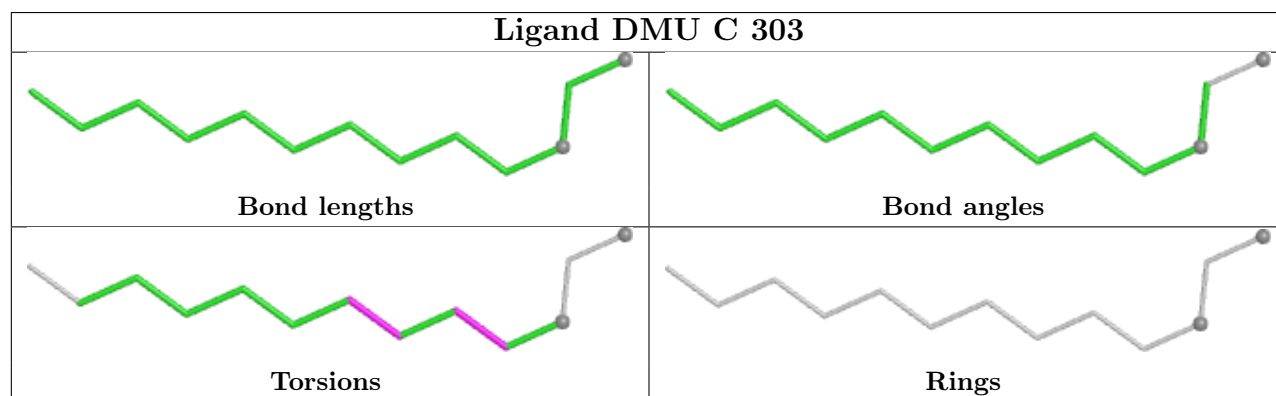
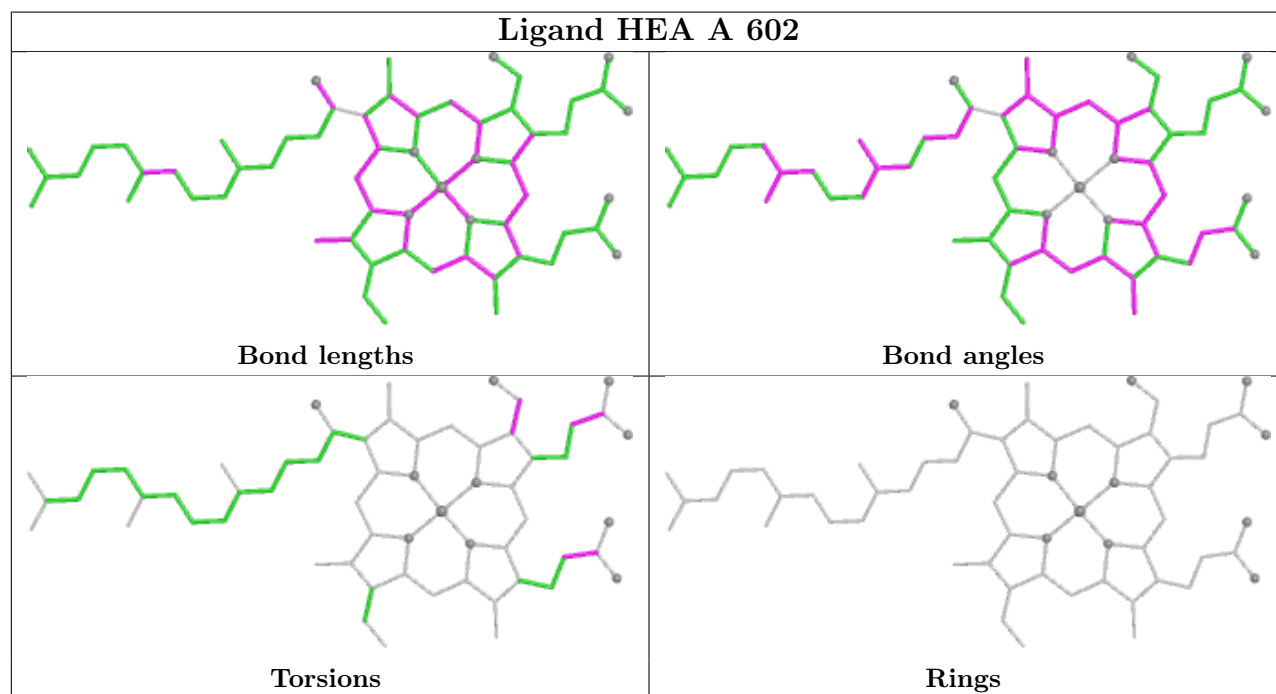
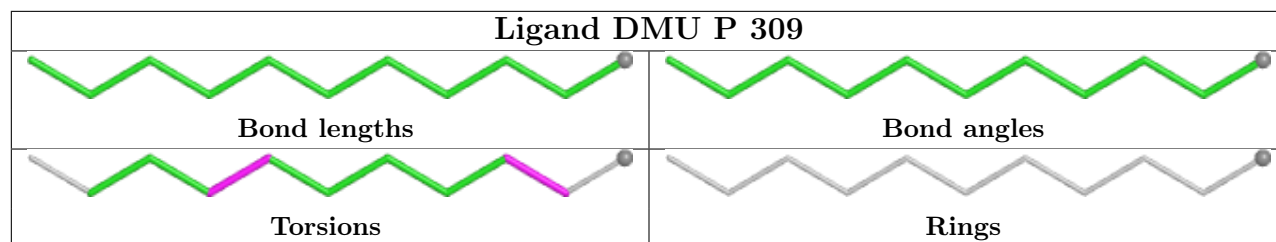
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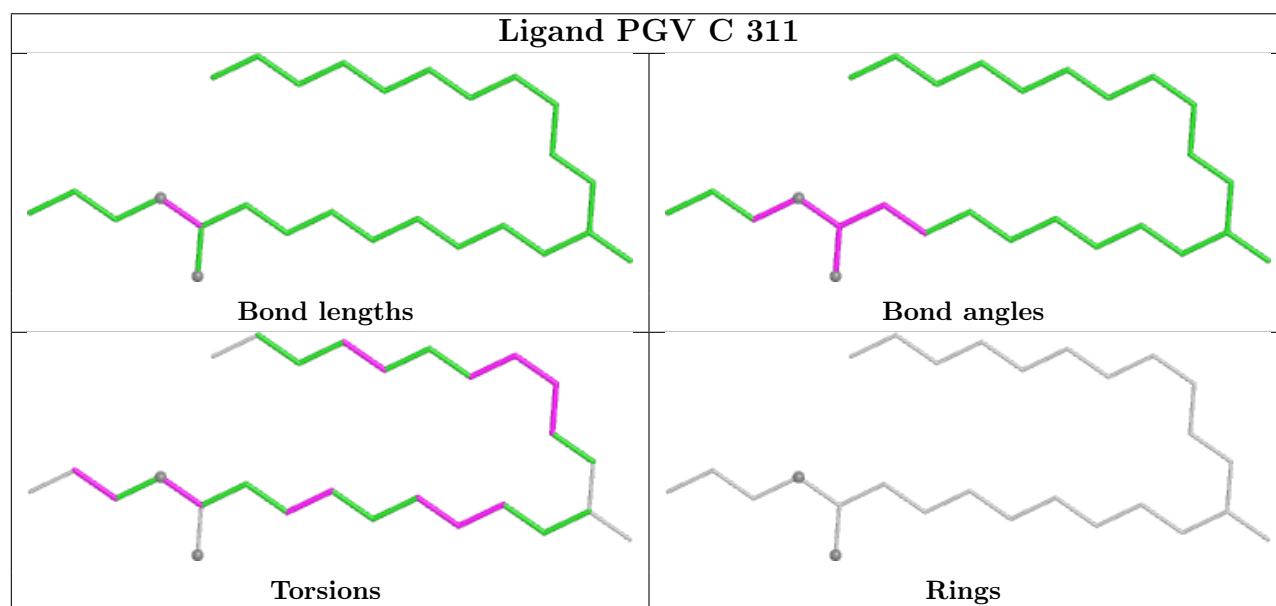
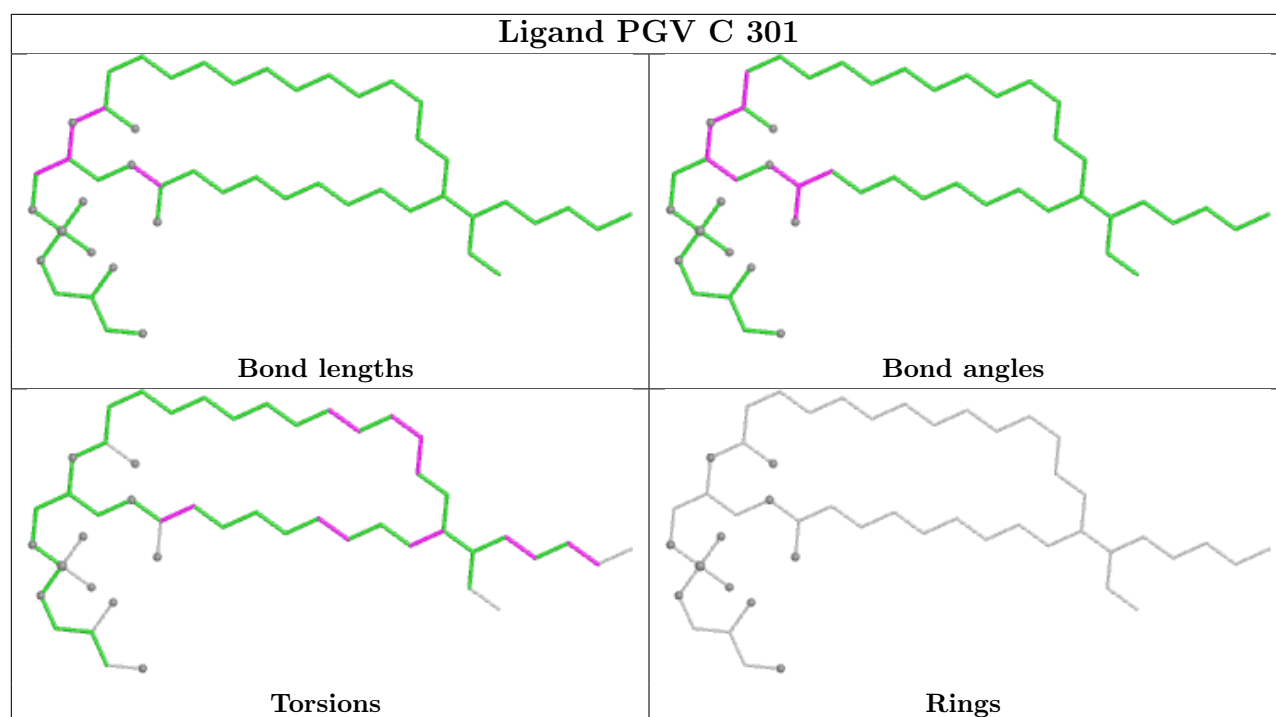
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	M	101	DMU	2	0
21	O	305	EDO	2	0
25	K	104	DMU	1	0
25	K	101	DMU	1	0
25	K	102	DMU	1	0
18	N	608	PGV	3	0
24	L	102	CHD	4	0
21	J	103	EDO	1	0
20	A	608[A]	PER	1	0
21	O	306	EDO	1	0
14	N	603	HEA	2	0
25	D	201	DMU	2	0
22	L	103	TGL	9	0
21	A	615	EDO	1	0
21	P	310	EDO	1	0
26	T	101	CDL	7	0
14	A	601[A]	HEA	2	0
25	Q	201	DMU	1	0
14	A	601[C]	HEA	1	0
21	A	613	EDO	1	0

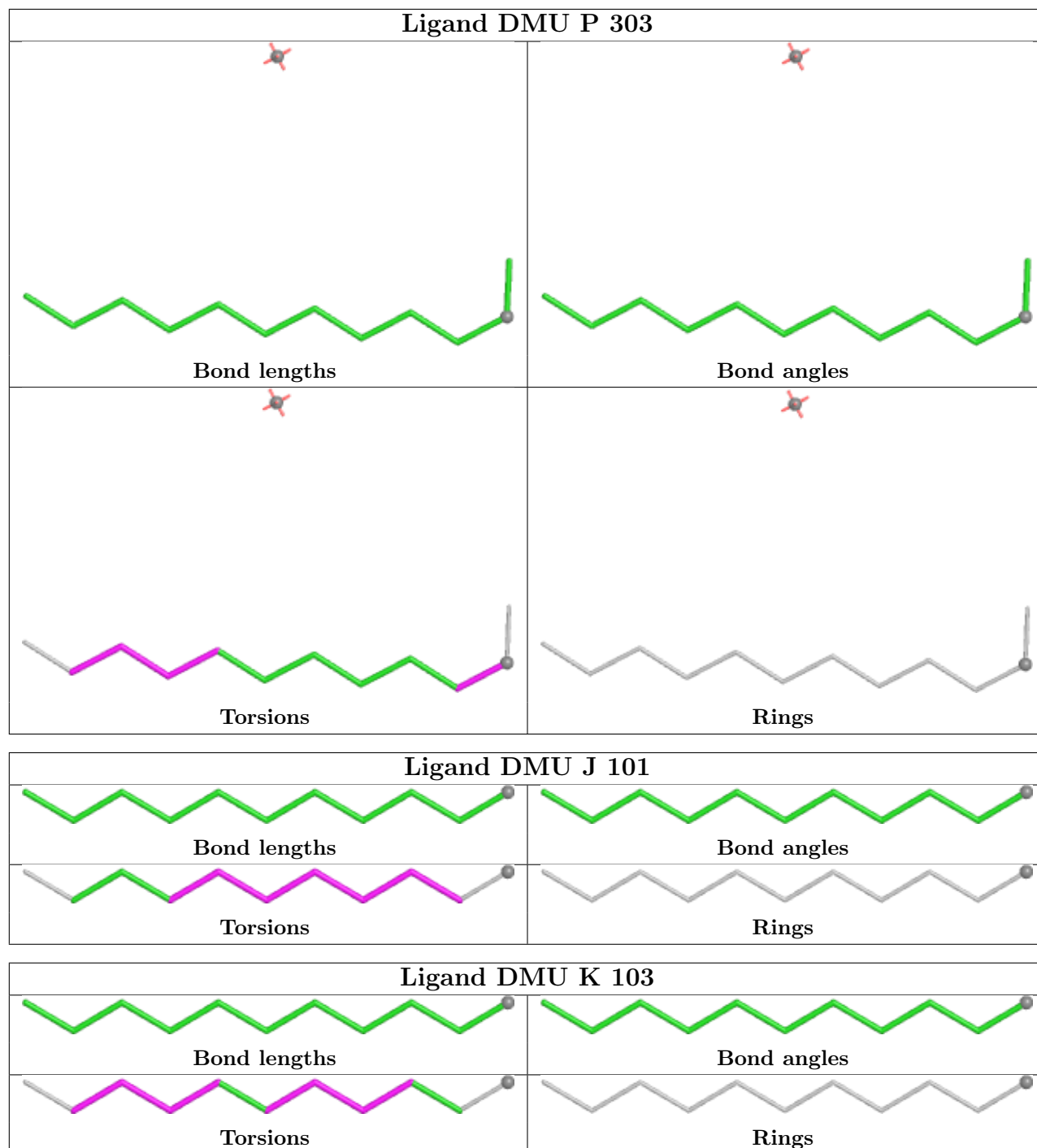
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

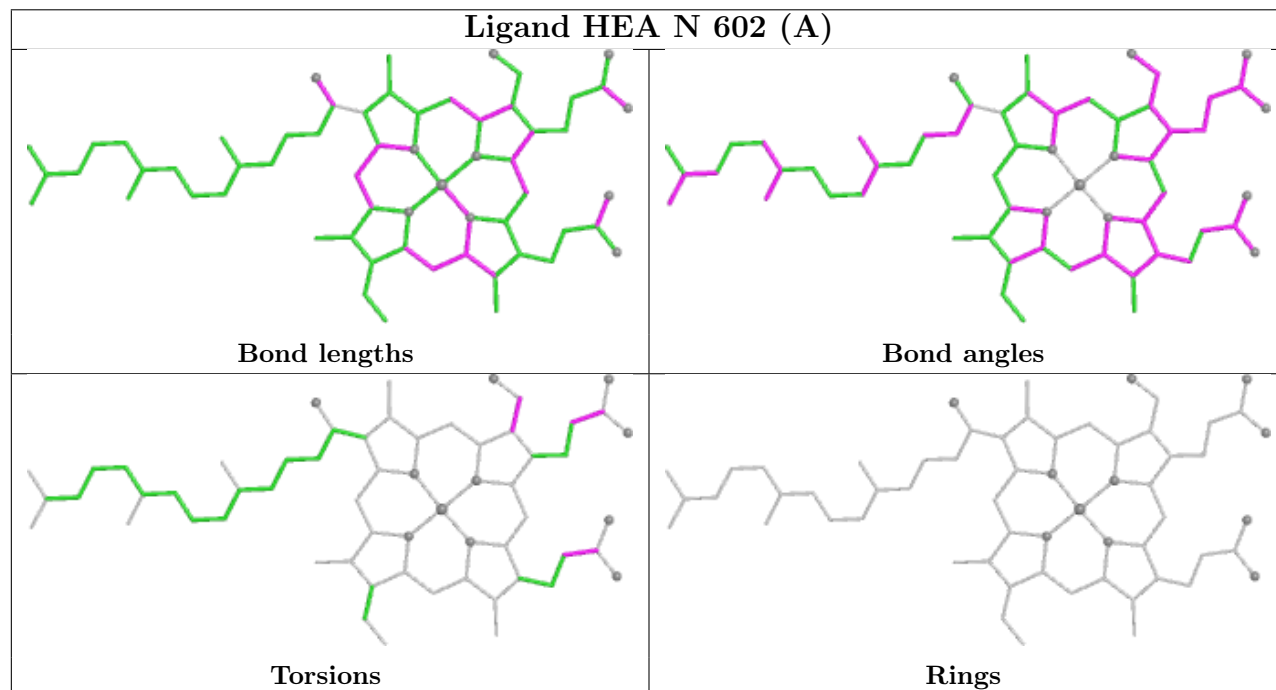
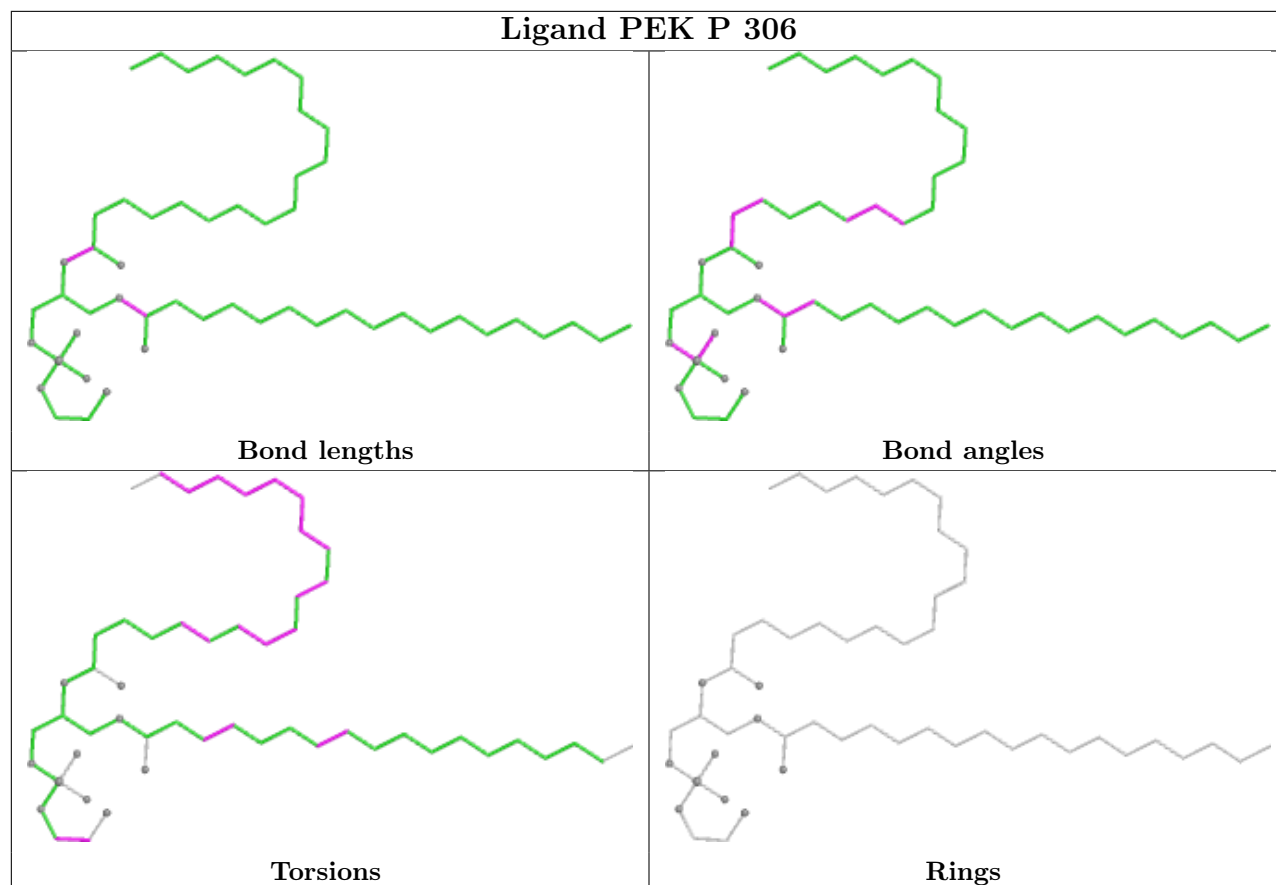


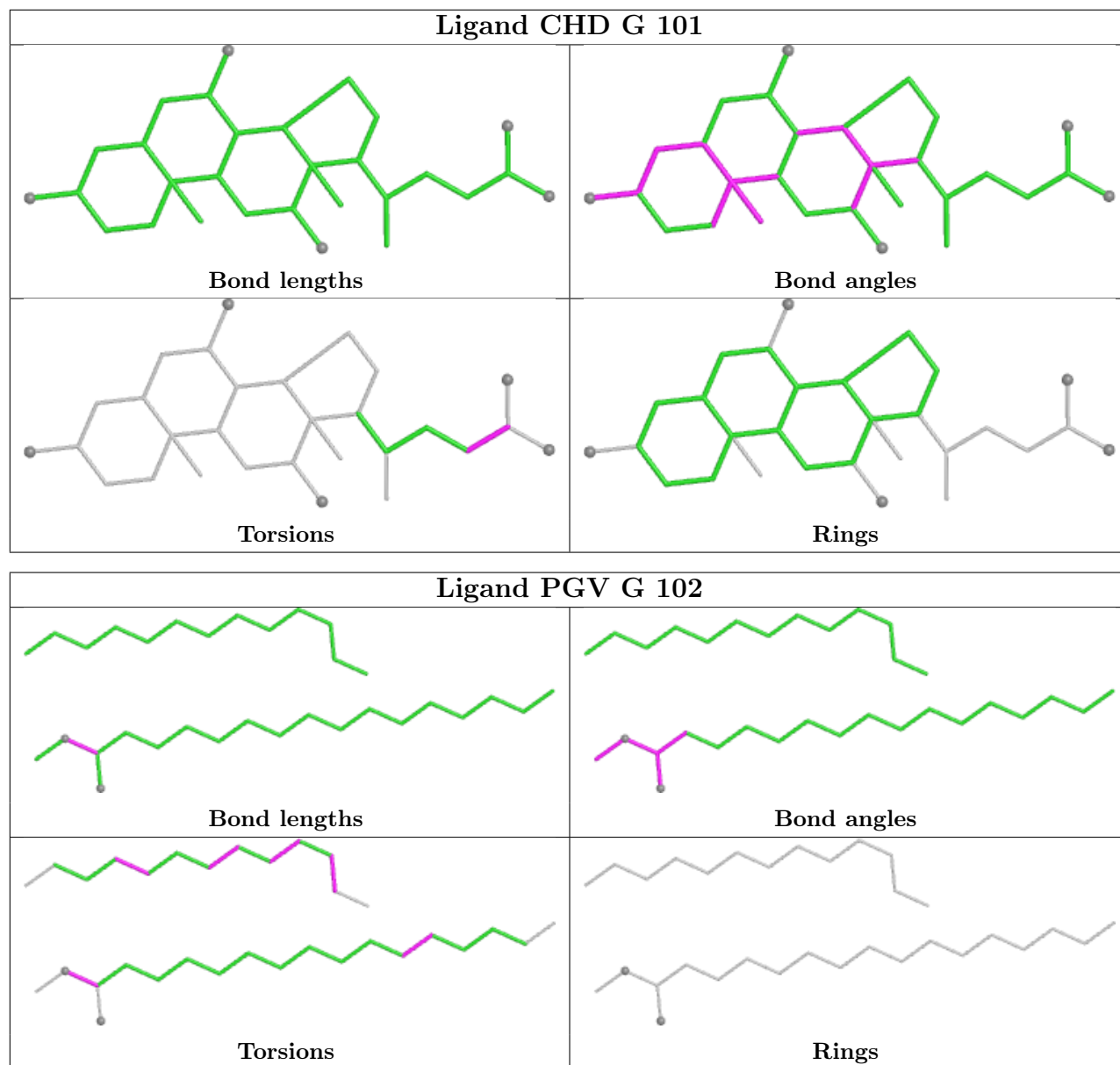


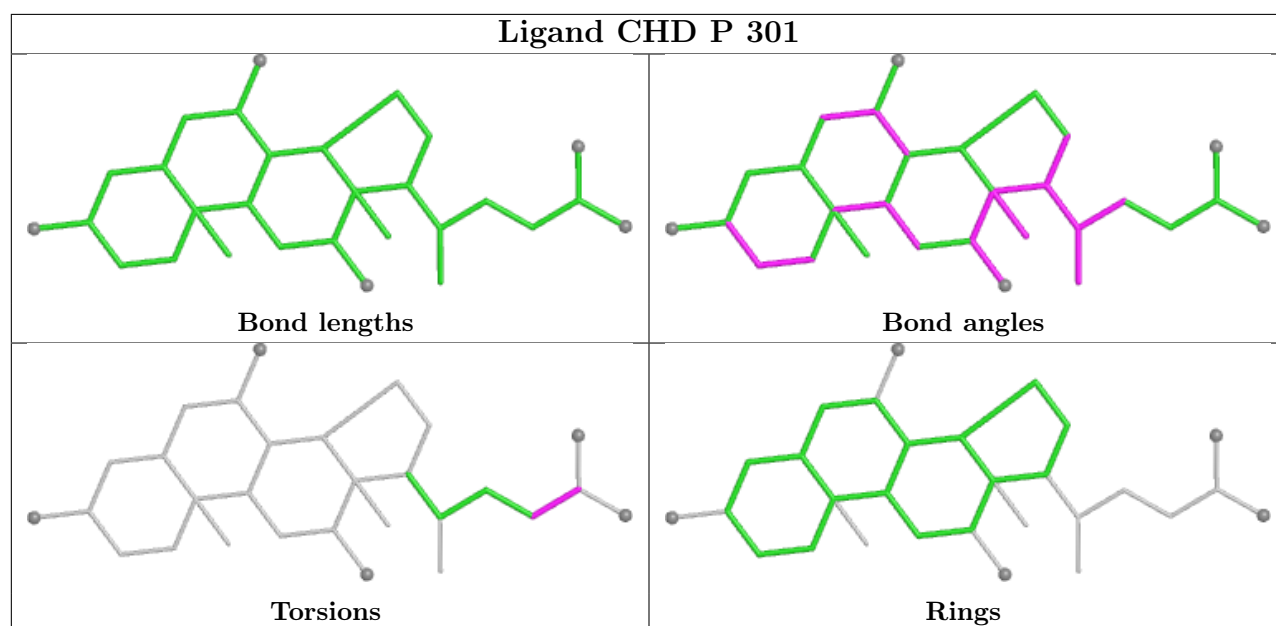
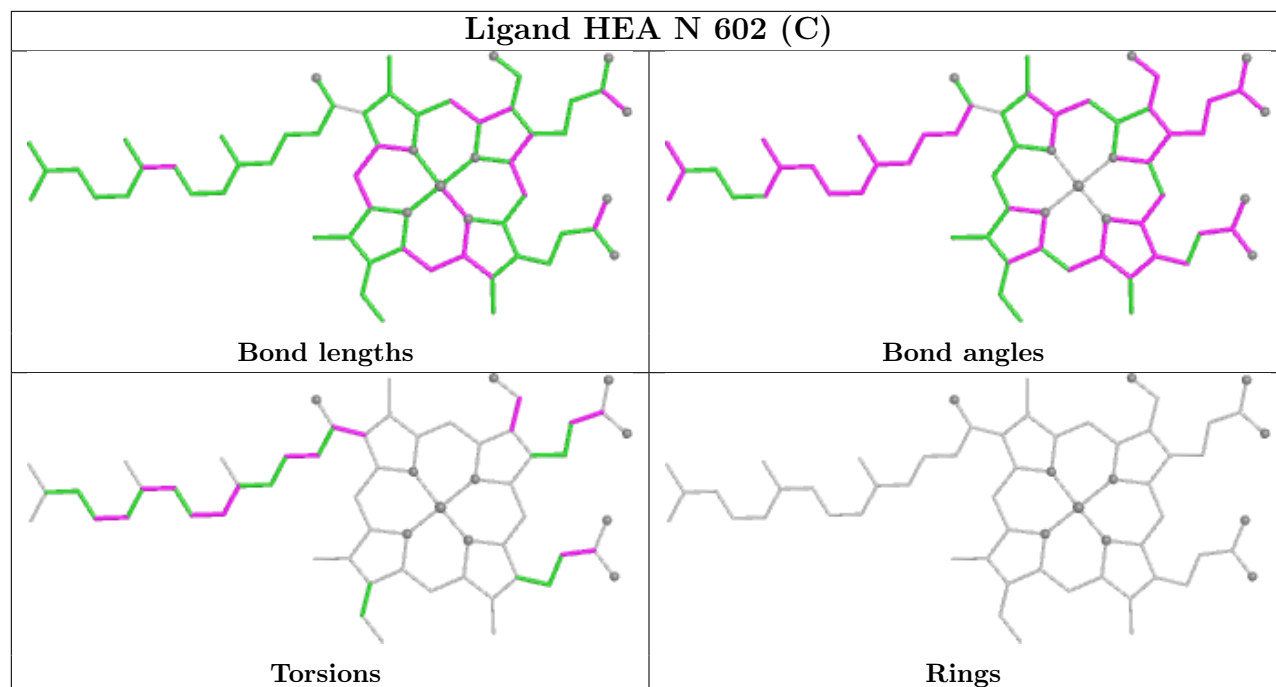


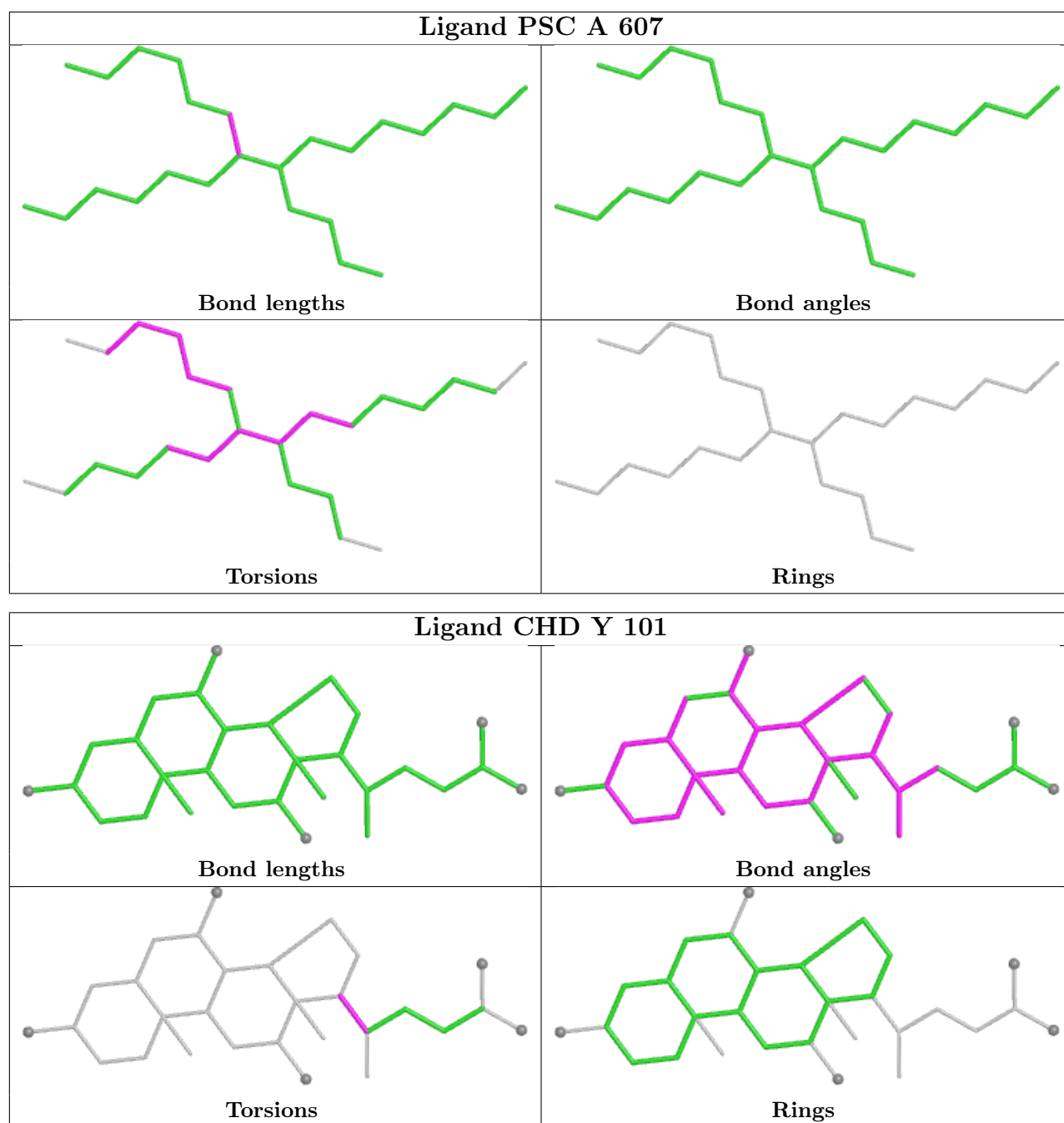


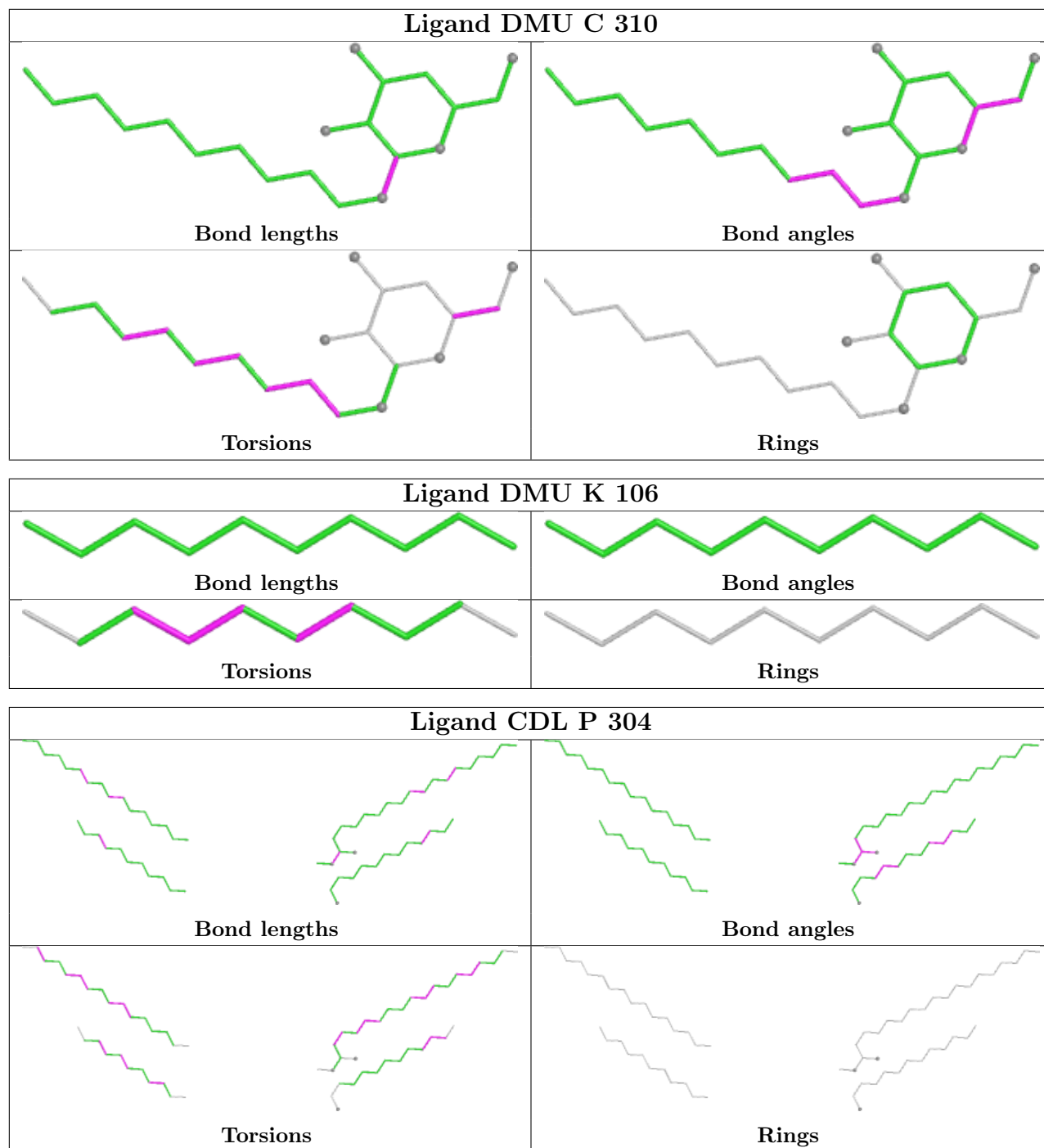


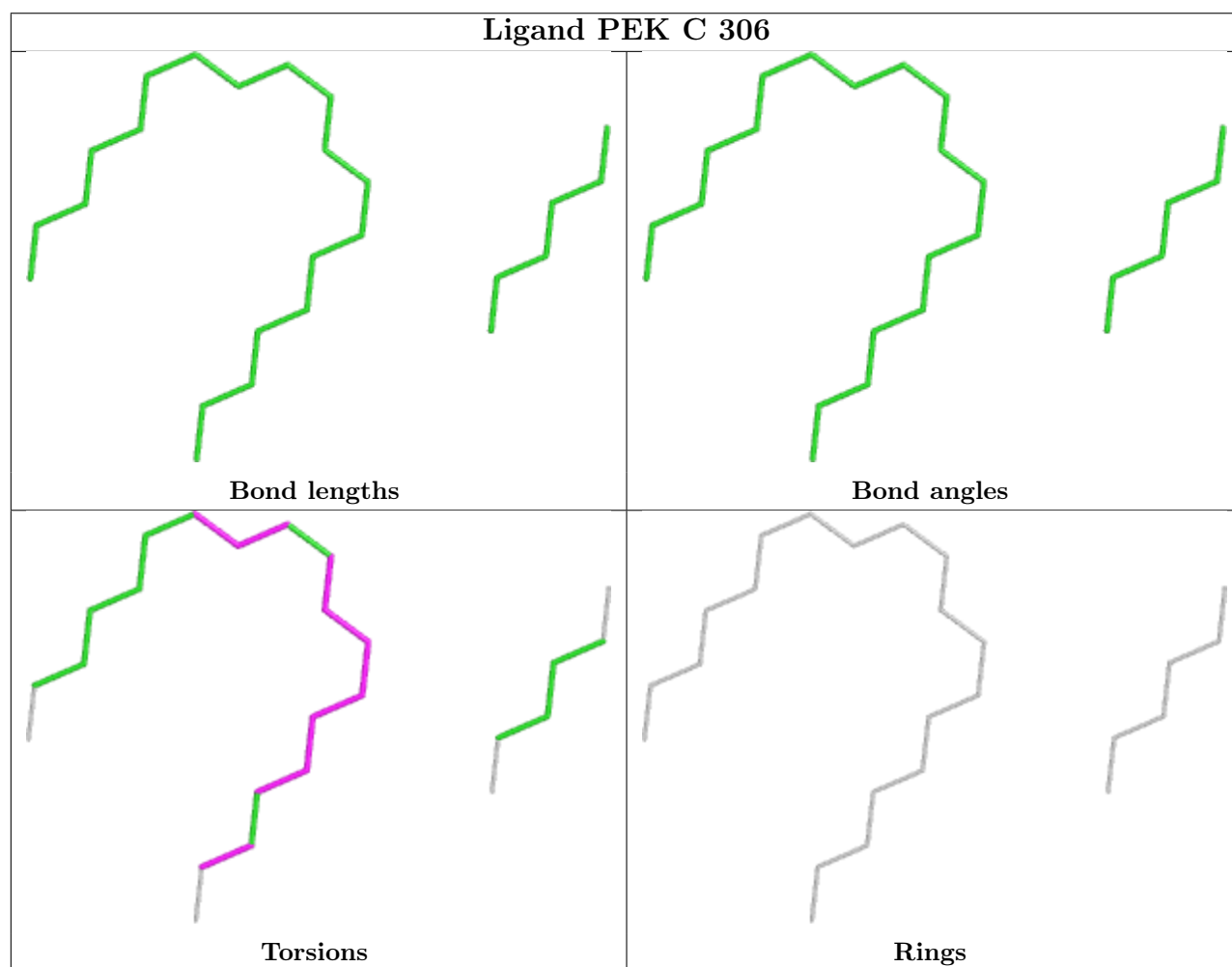
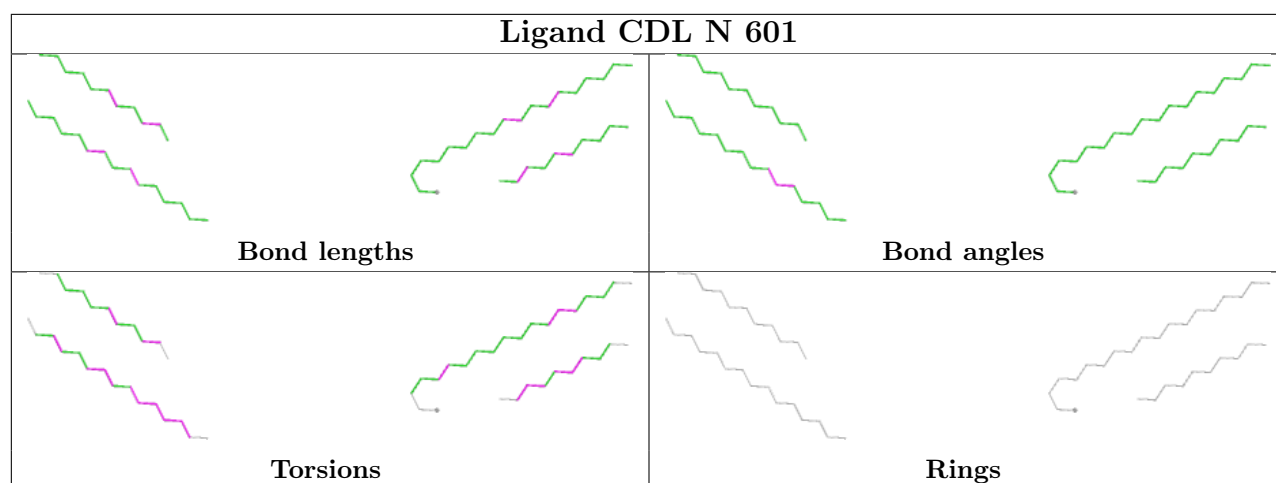


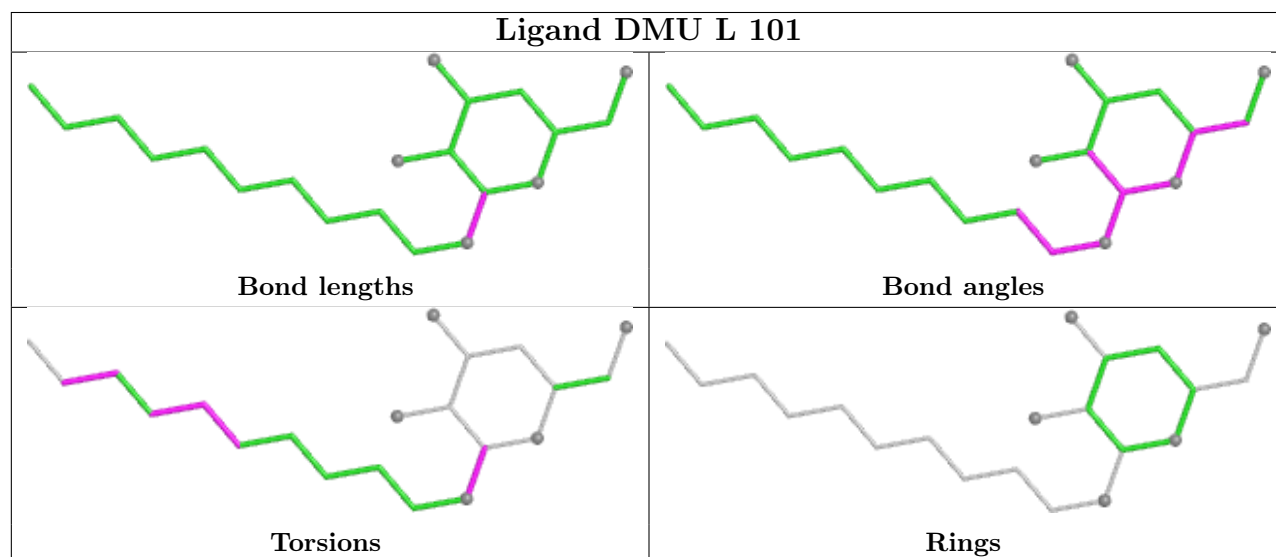
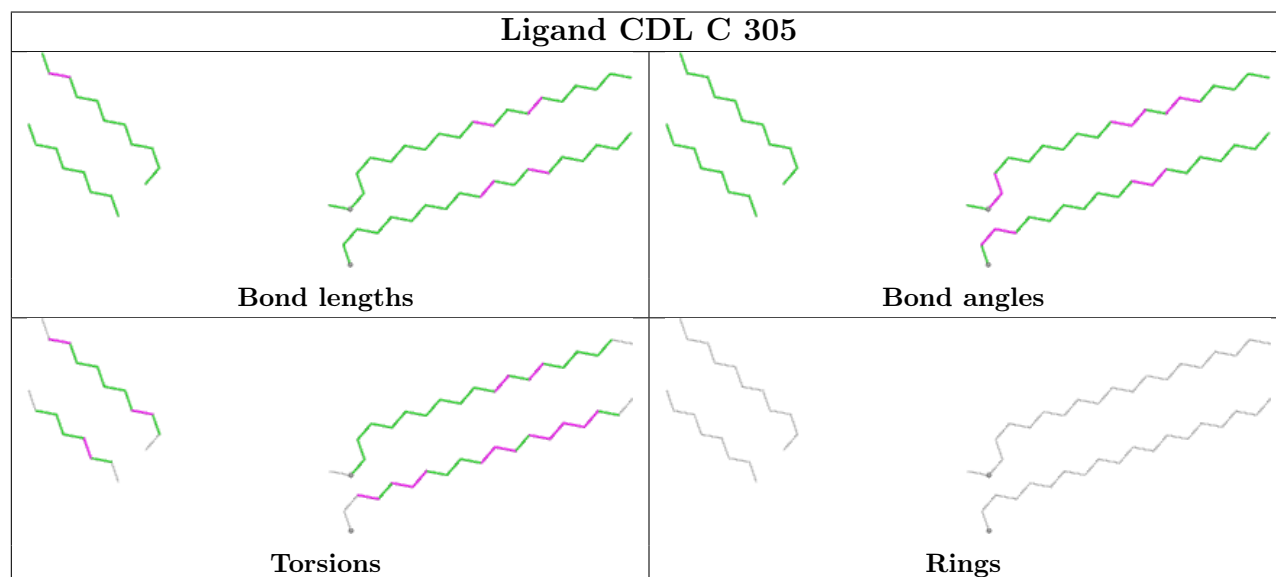
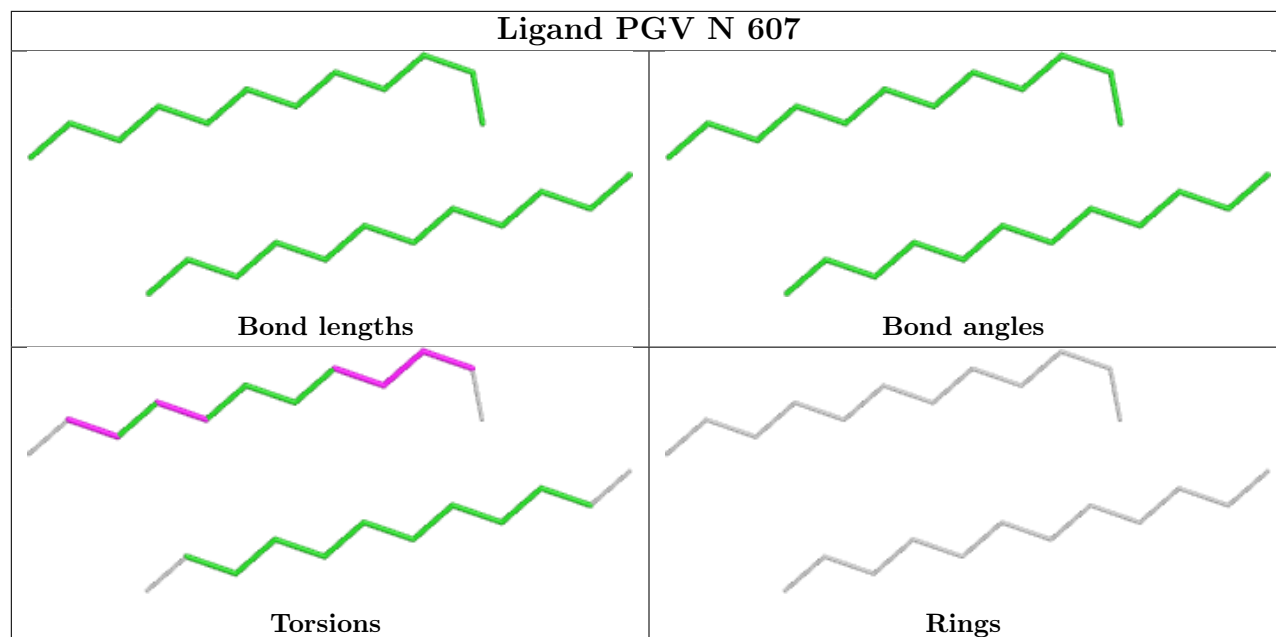


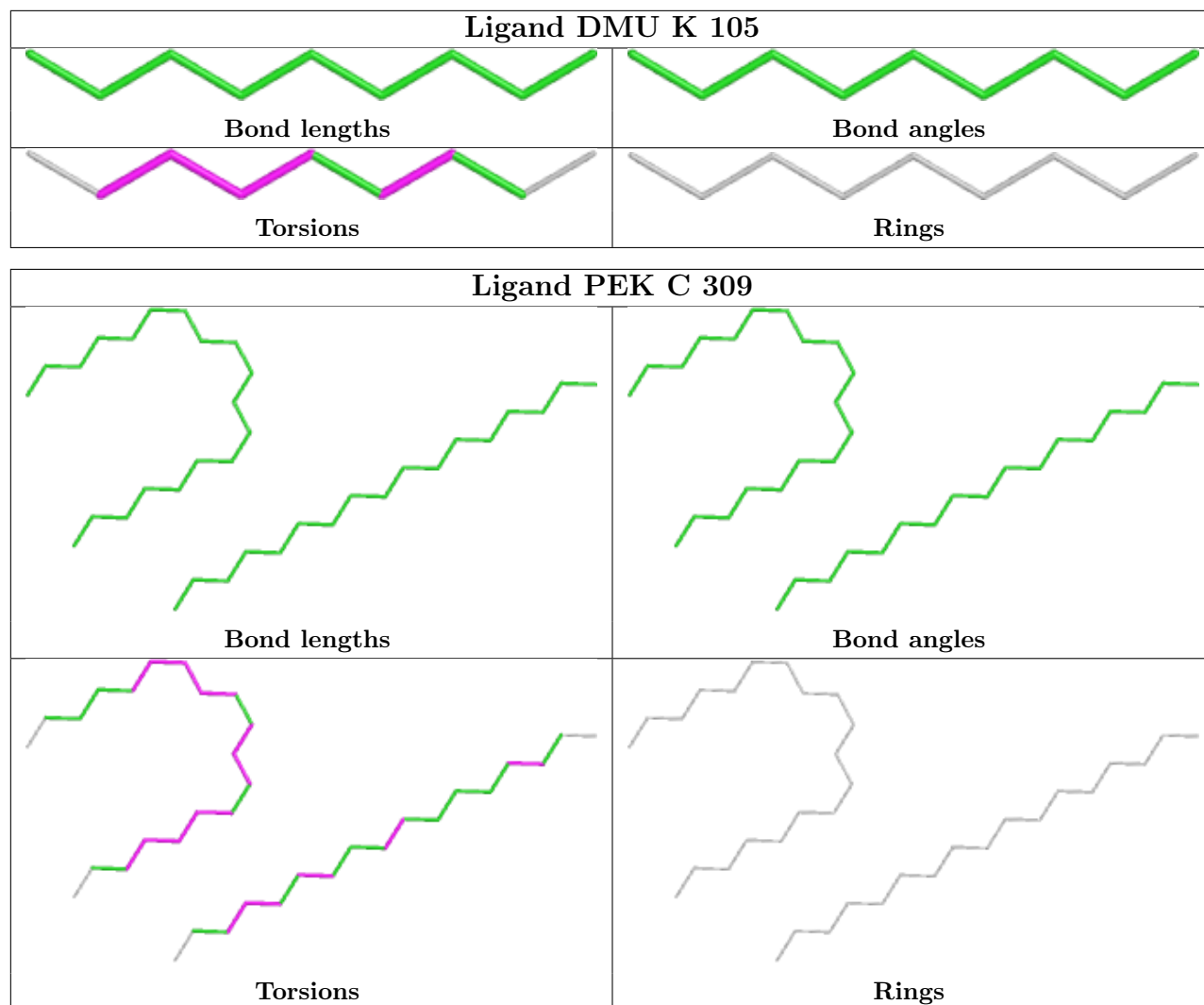


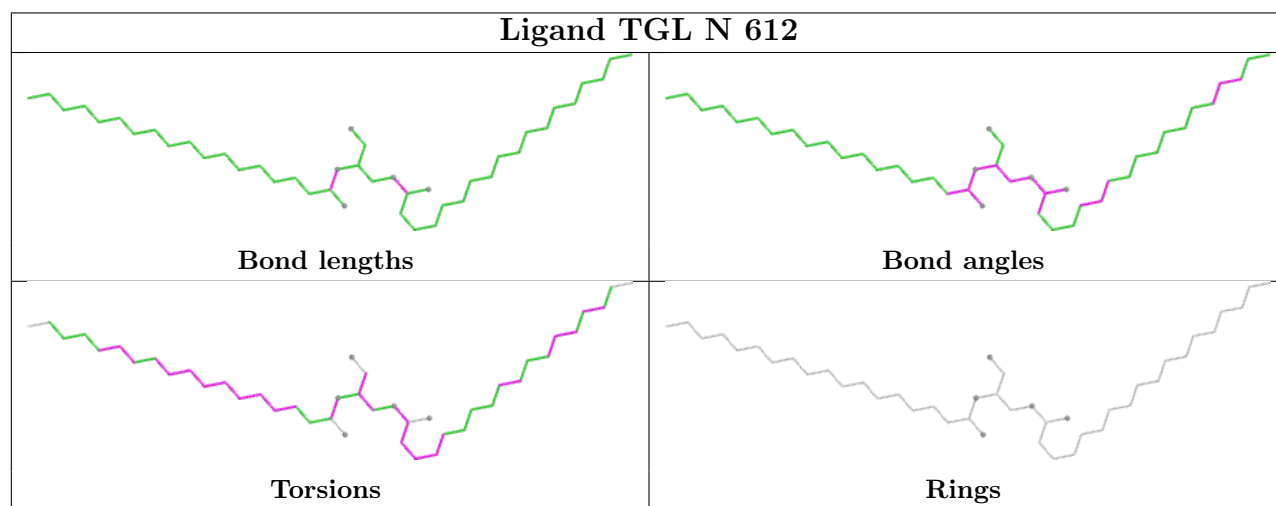
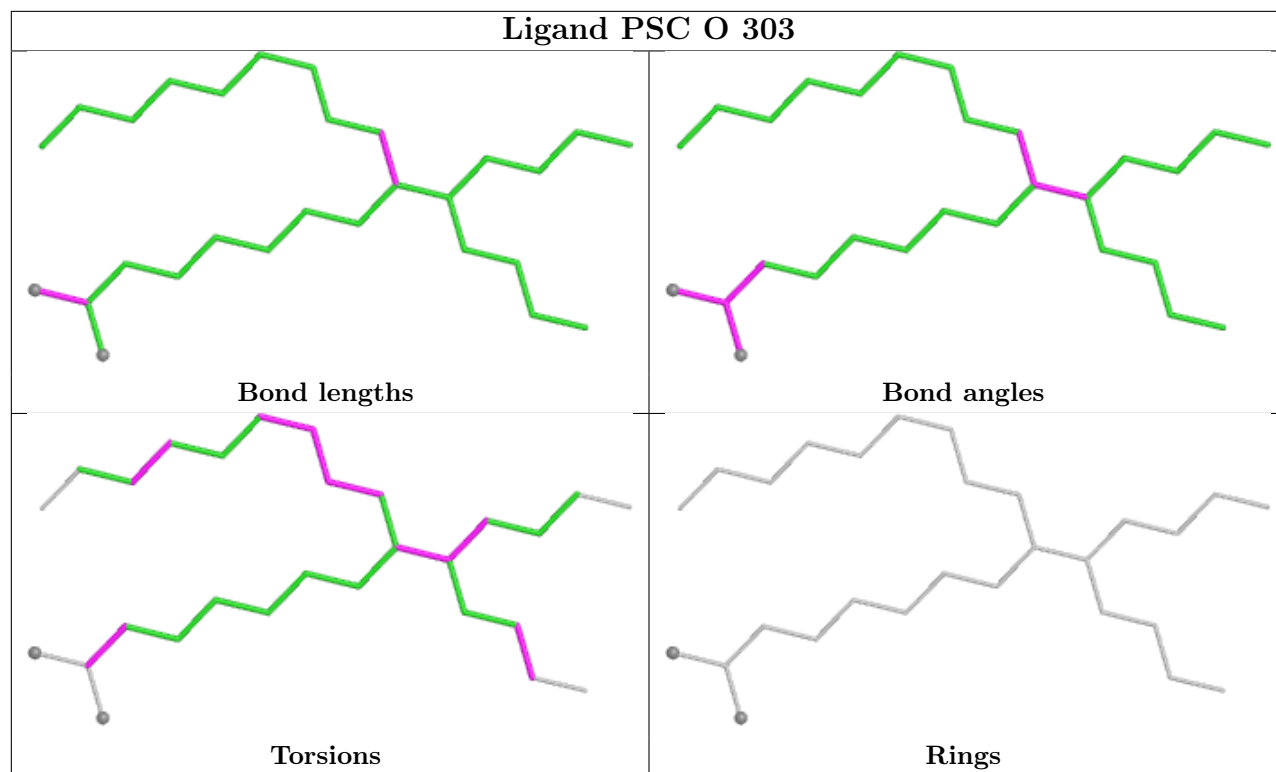


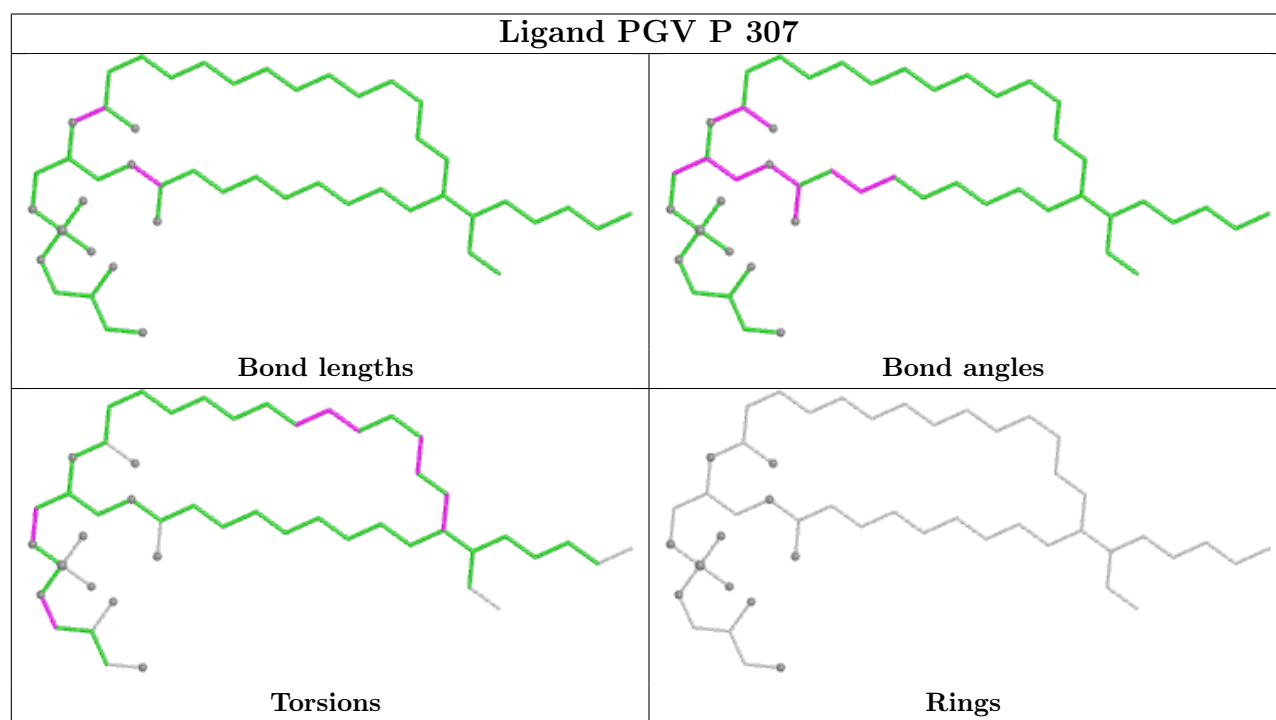
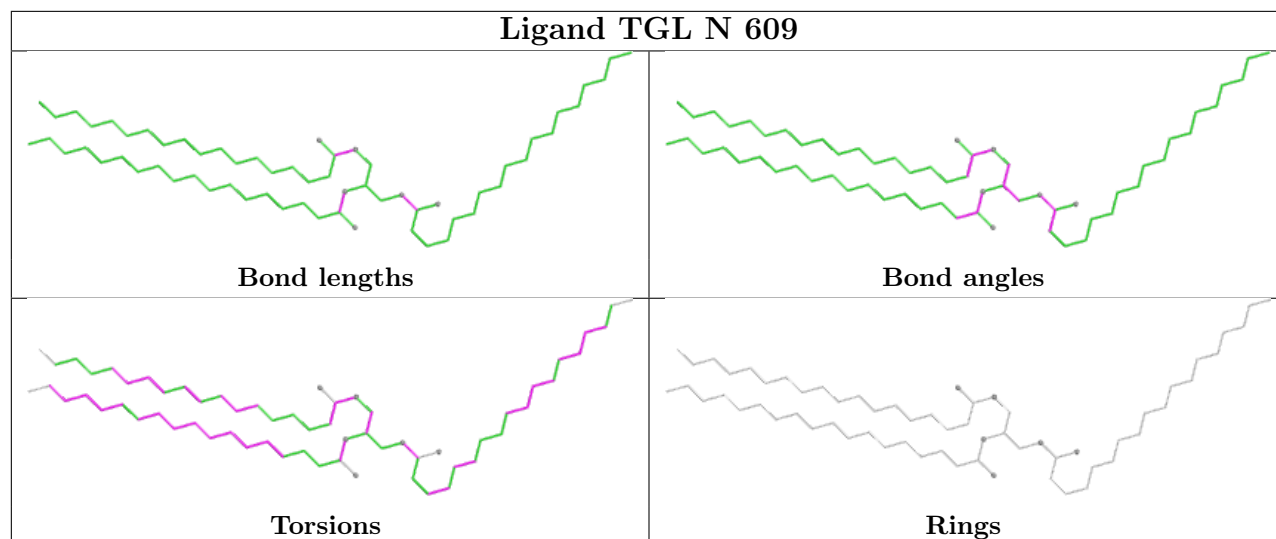


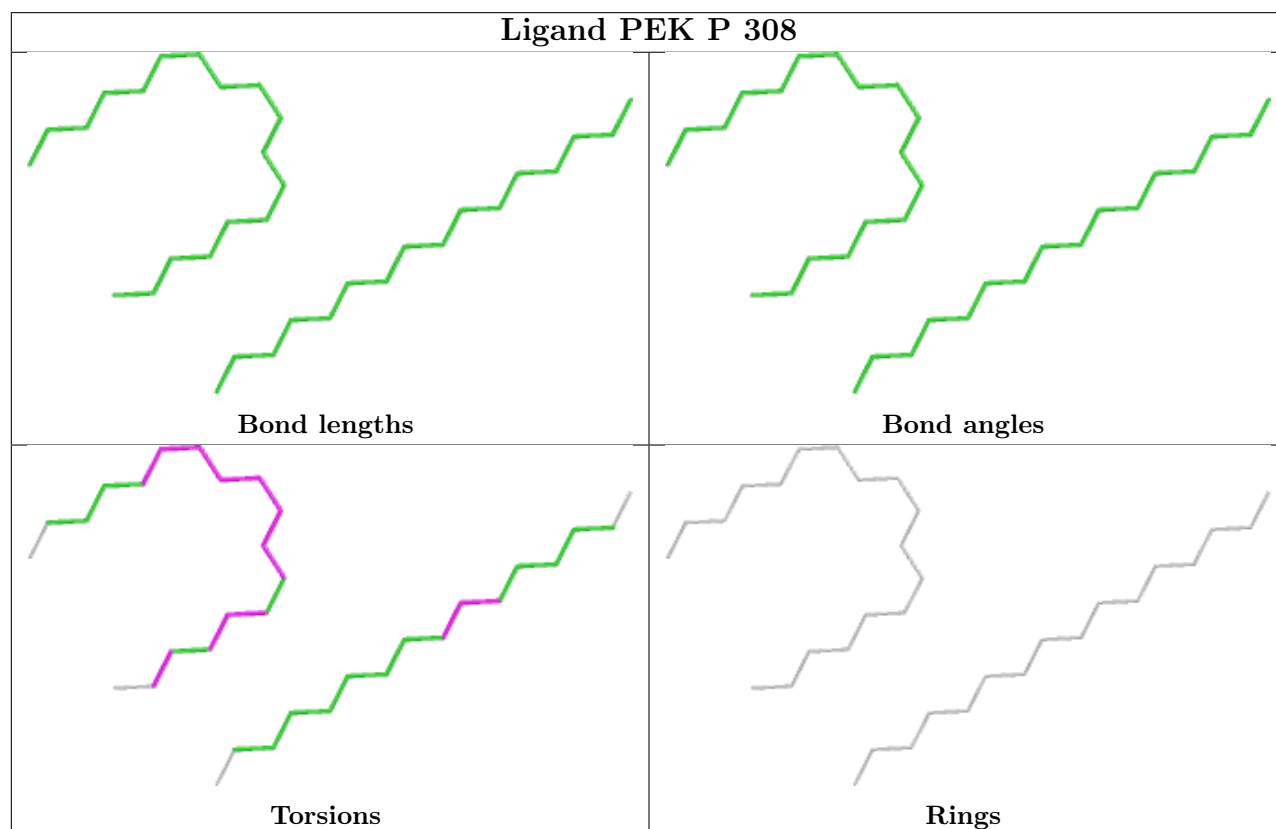
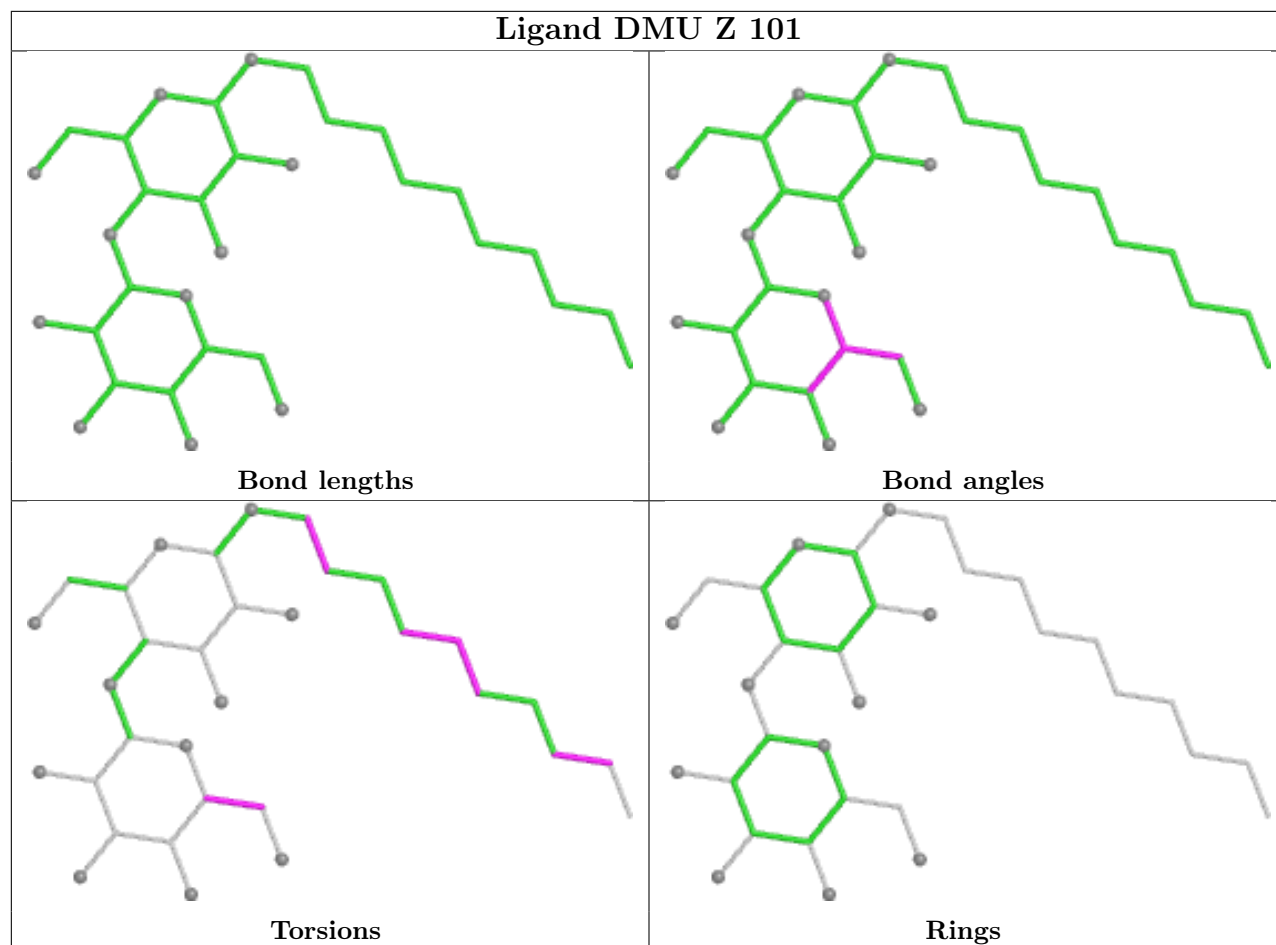




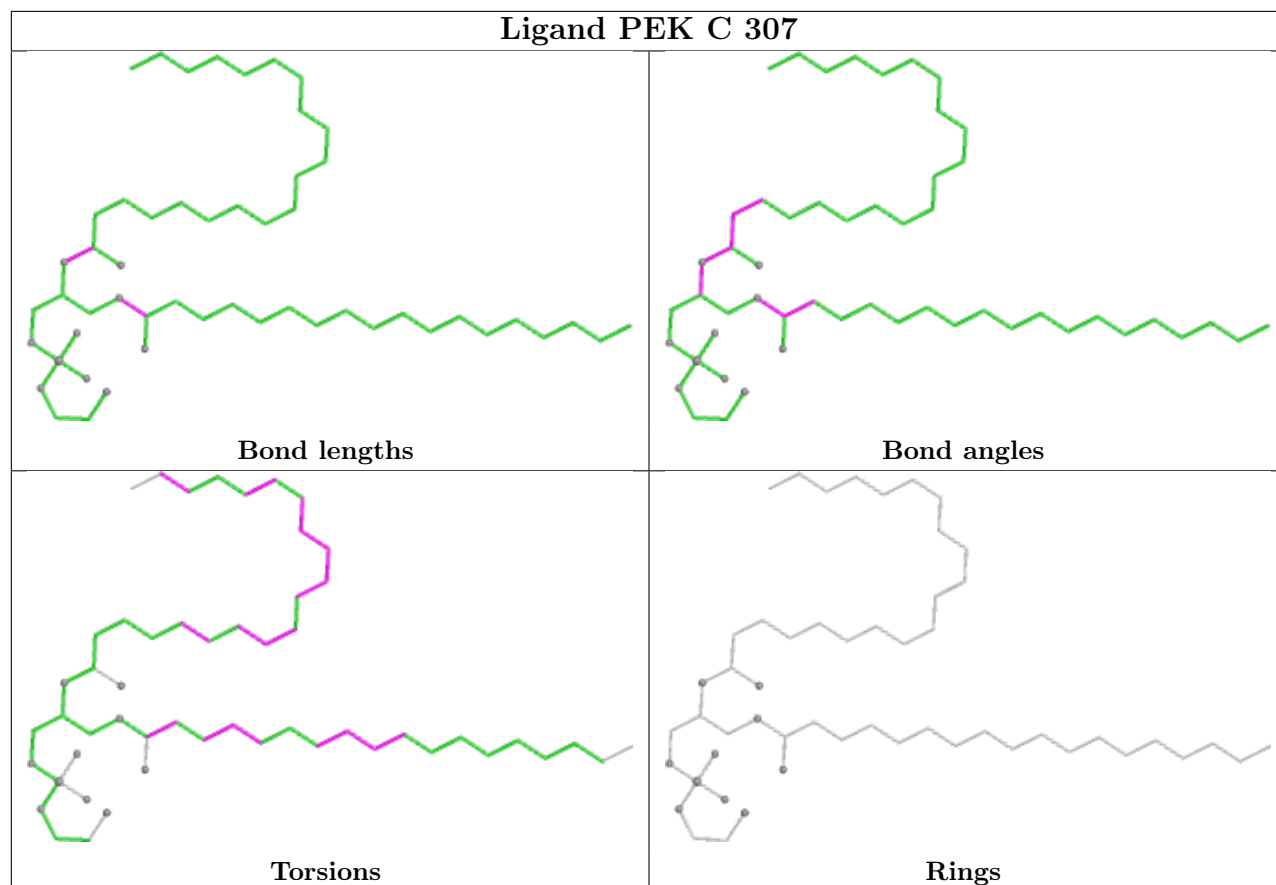




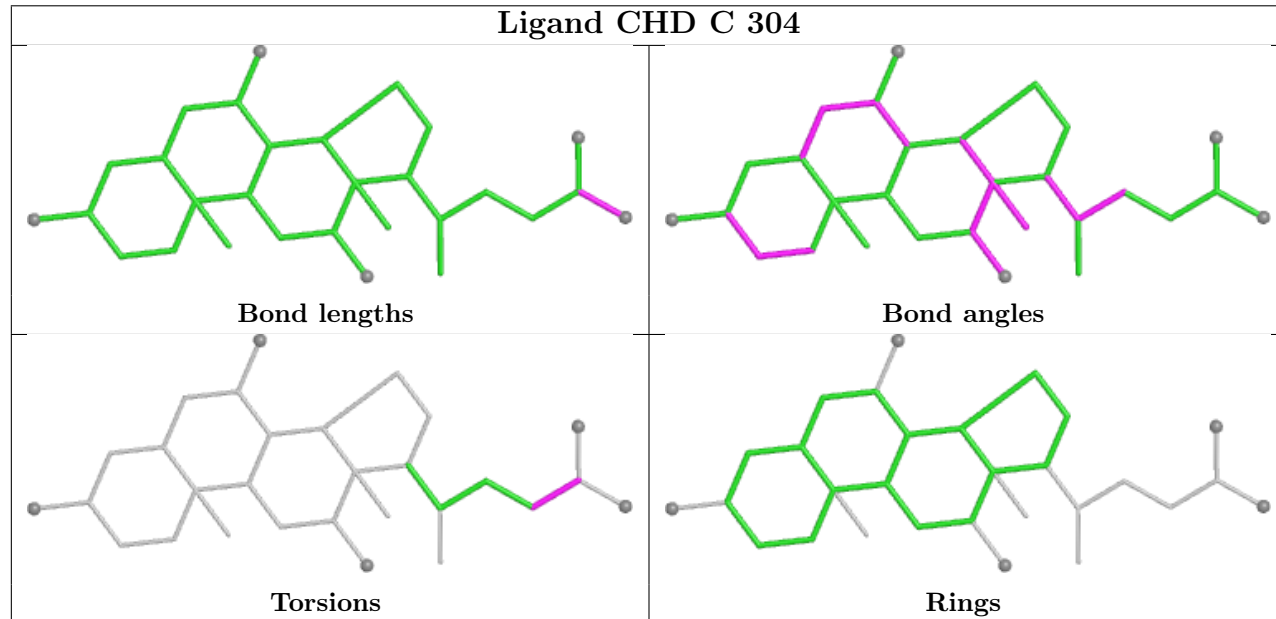


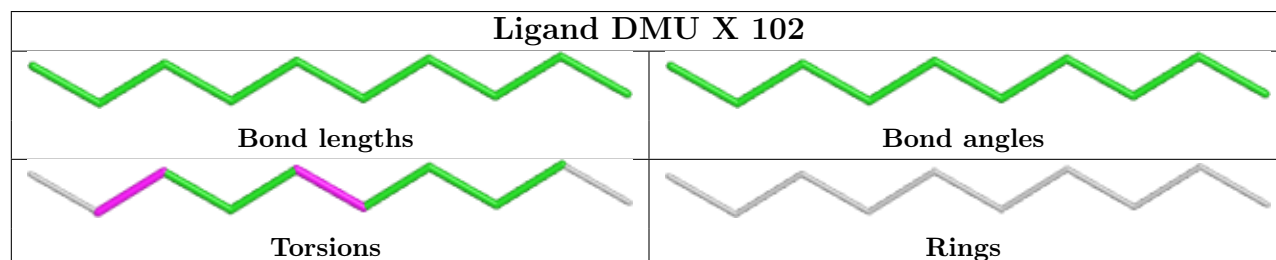
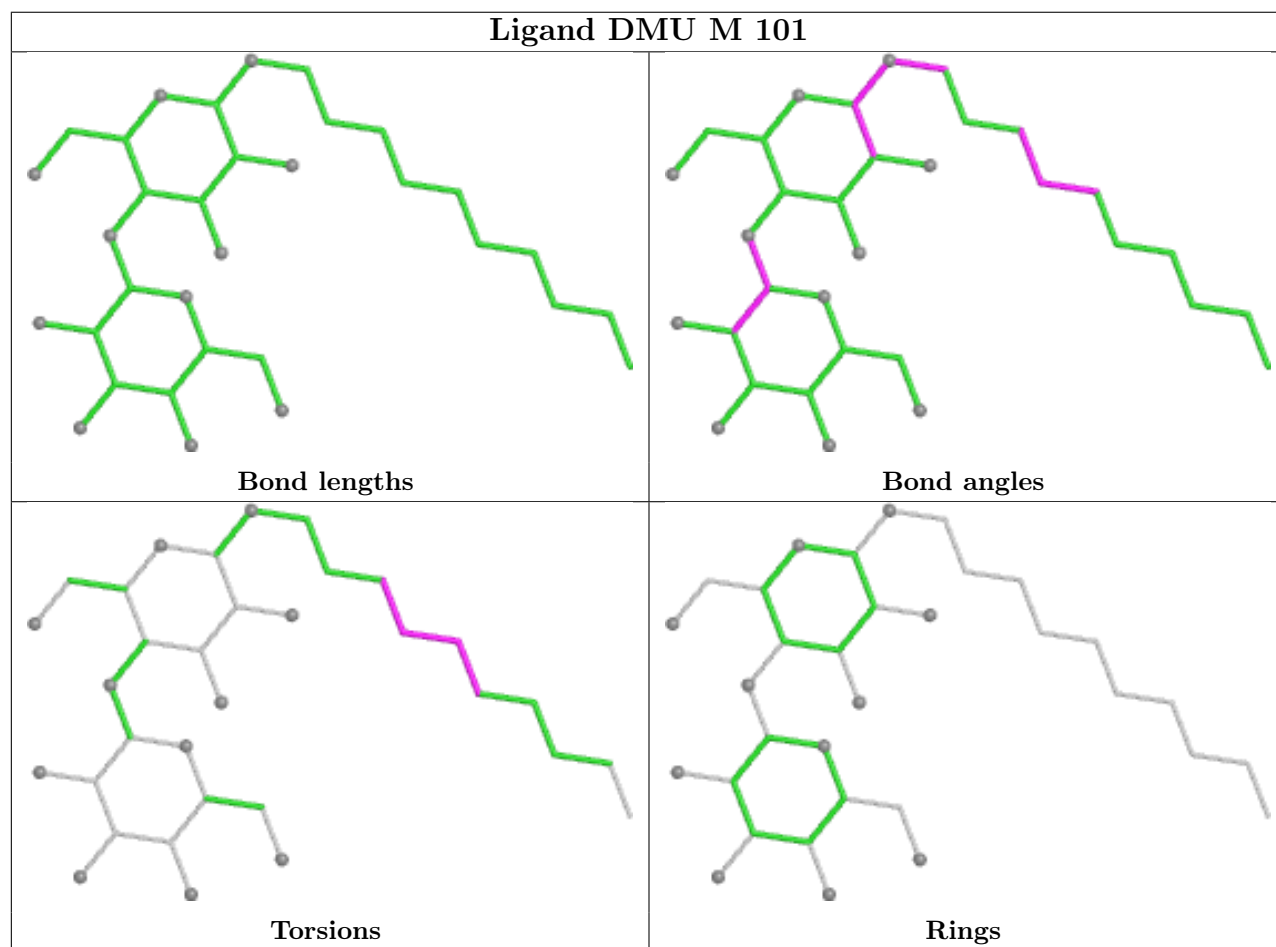
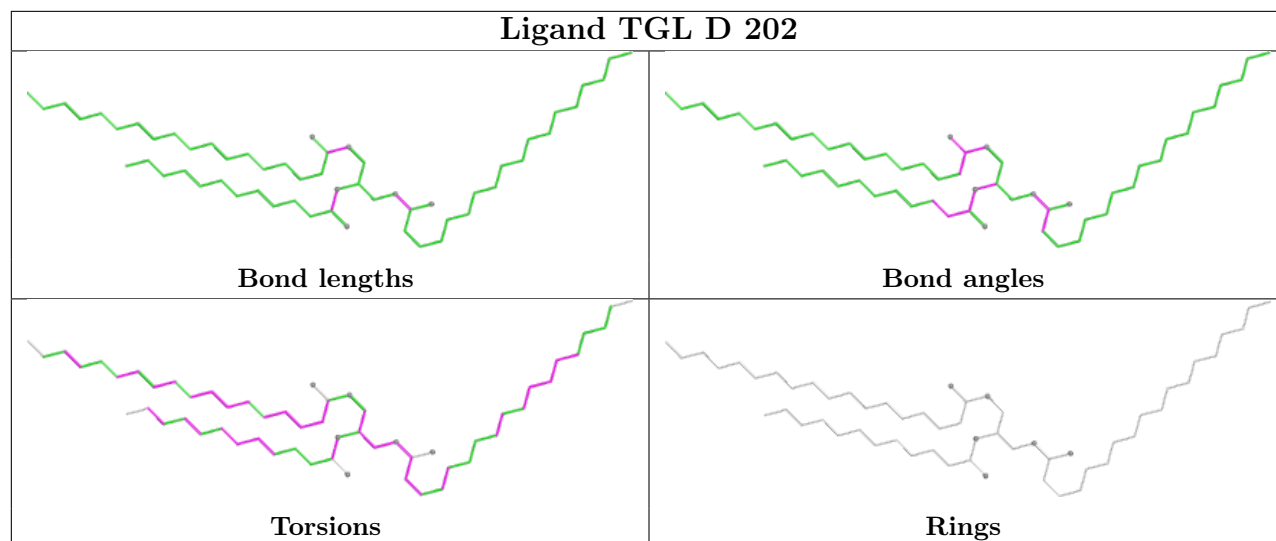


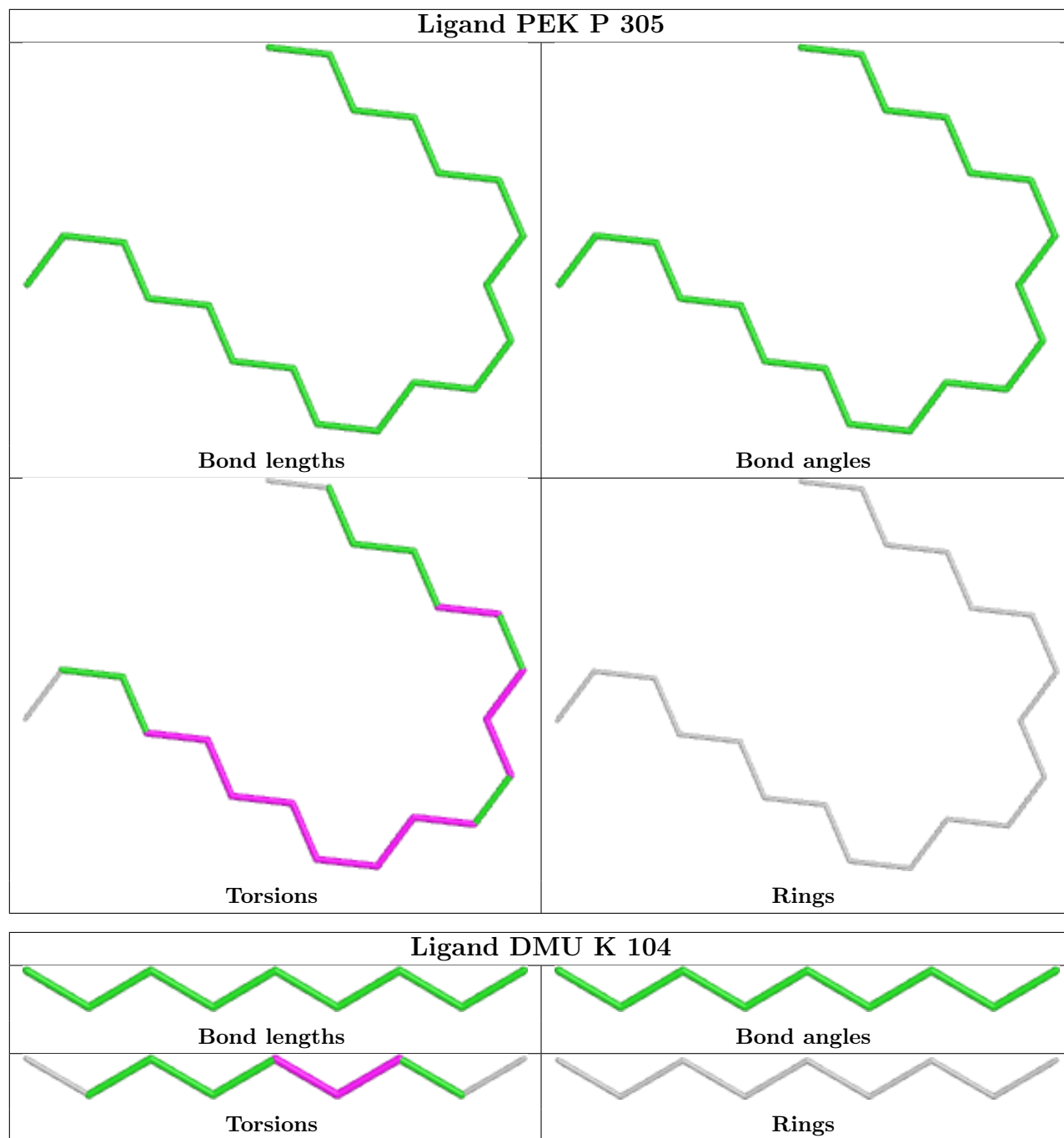
Ligand PEK C 307

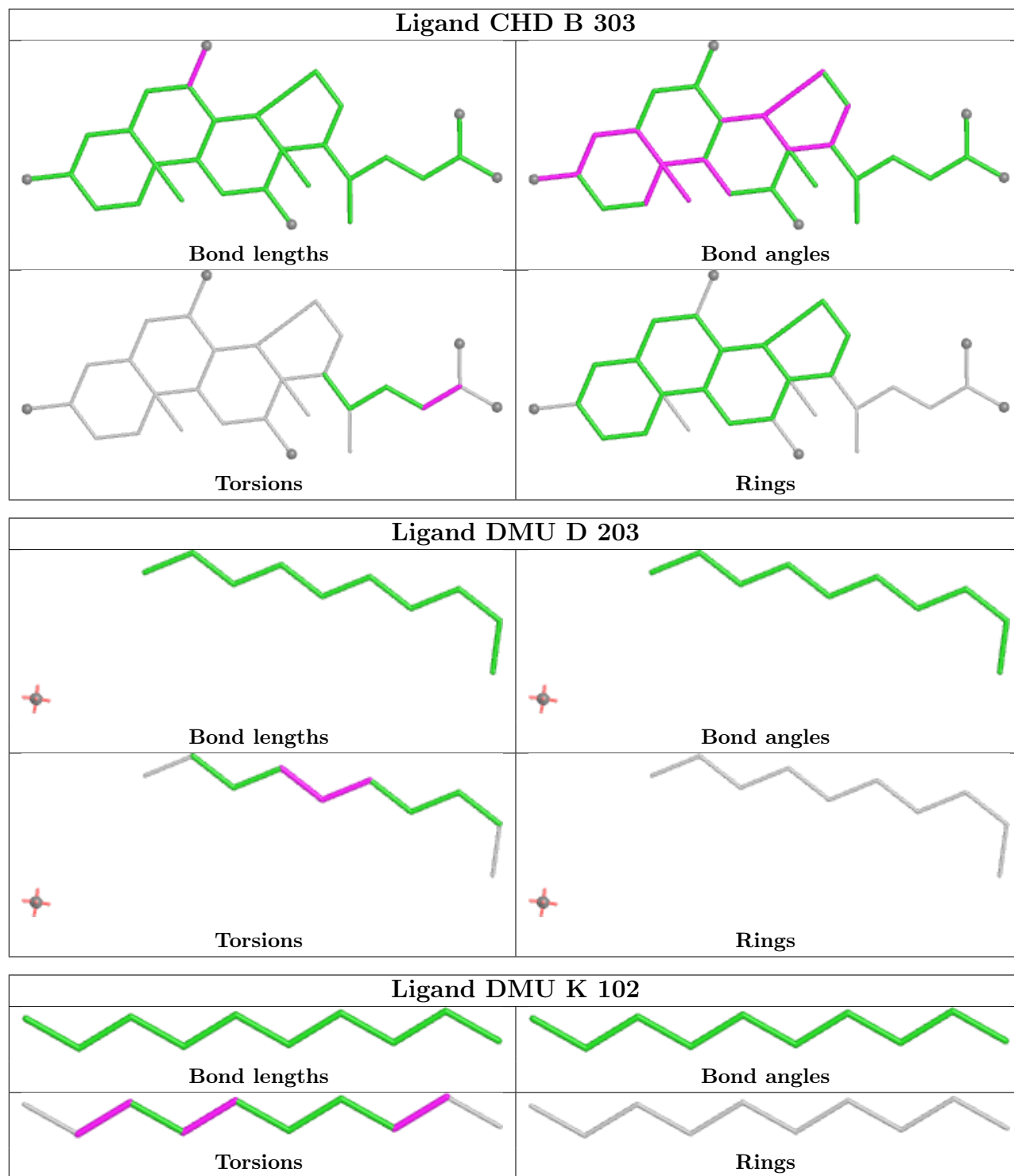


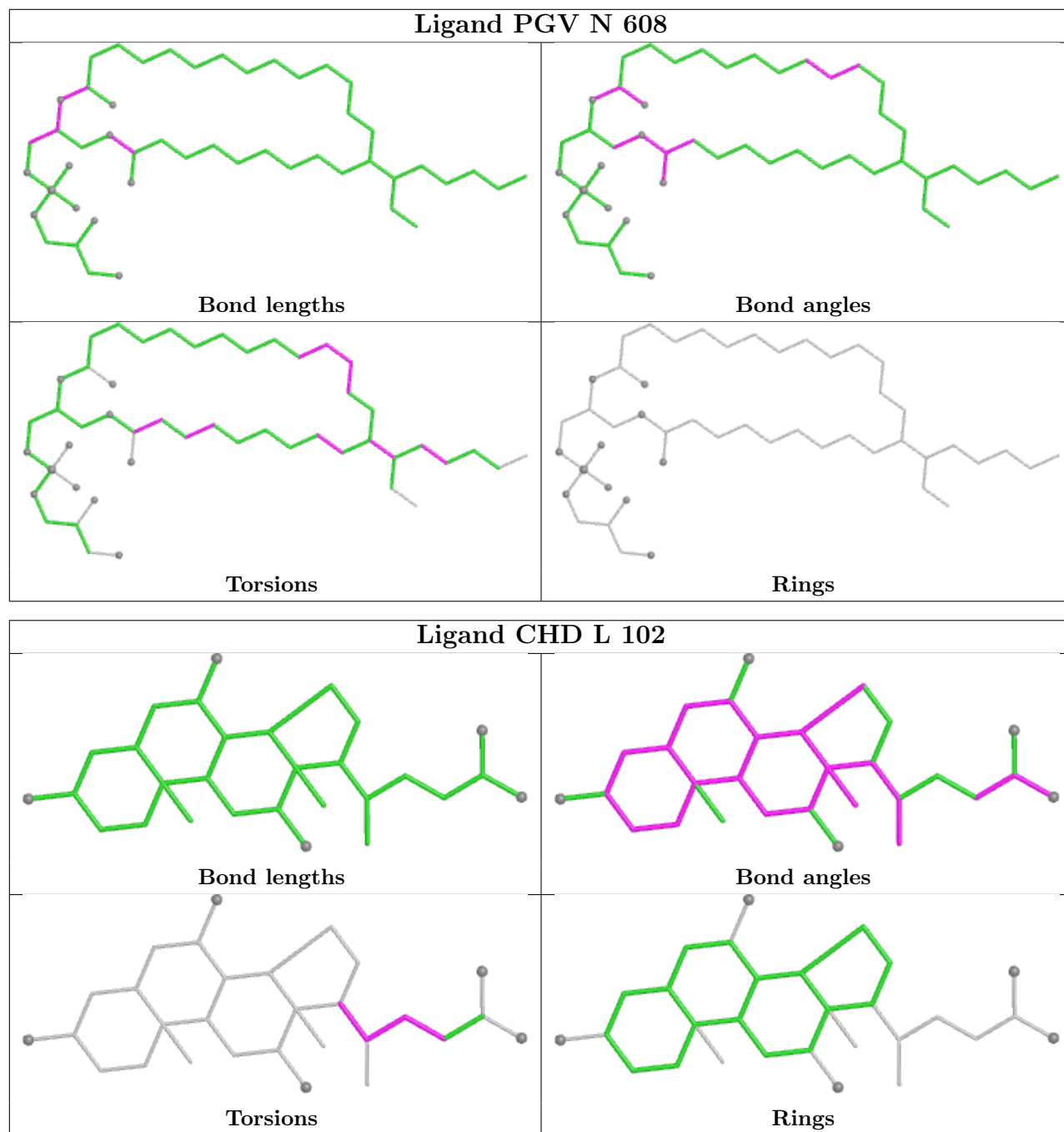
Ligand CHD C 304

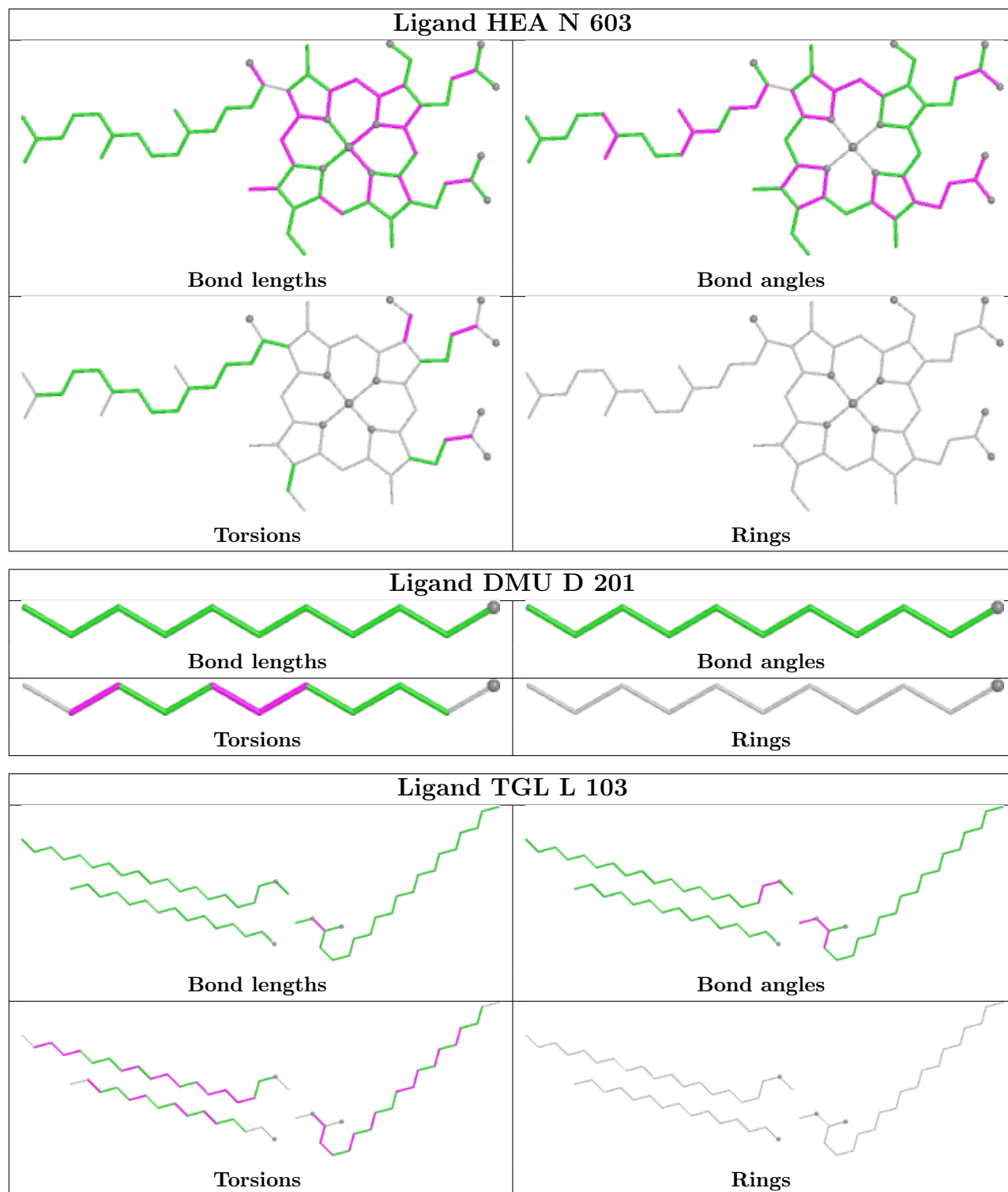


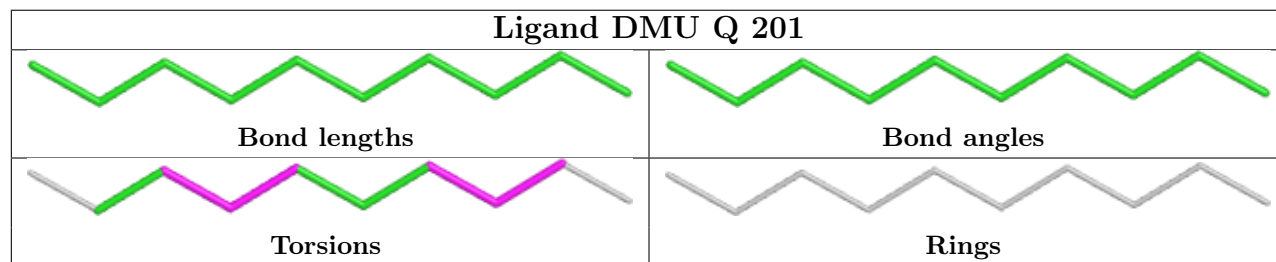
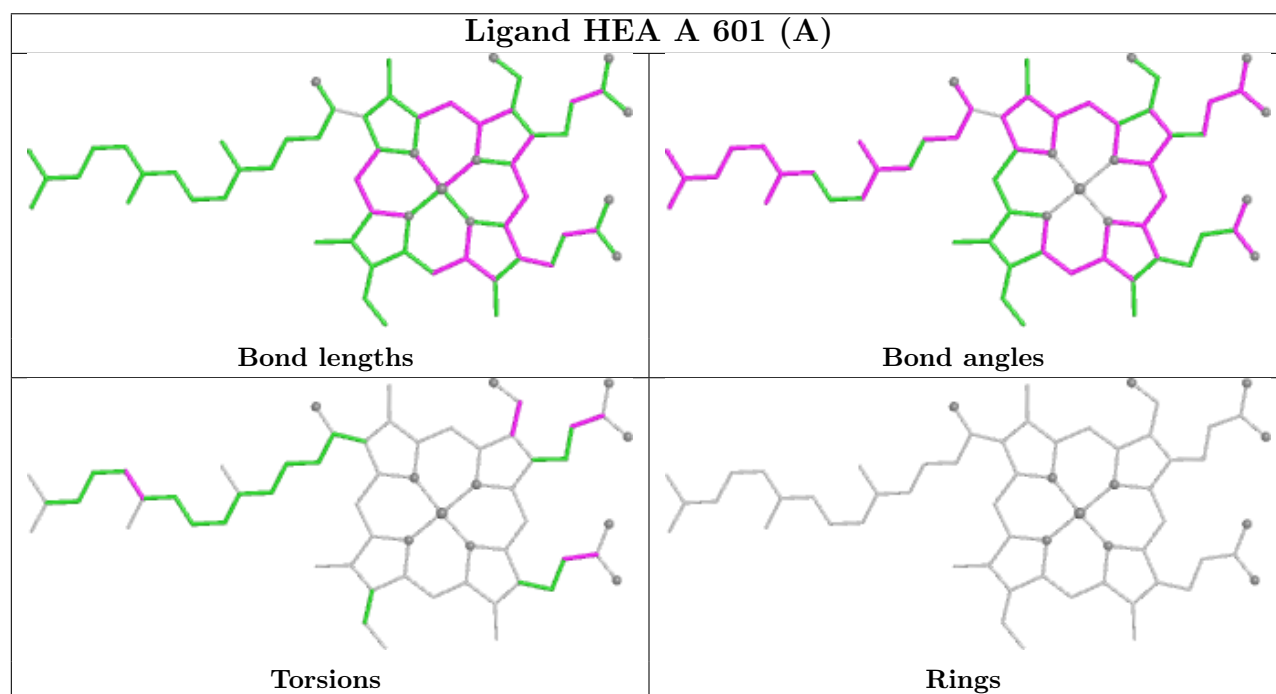
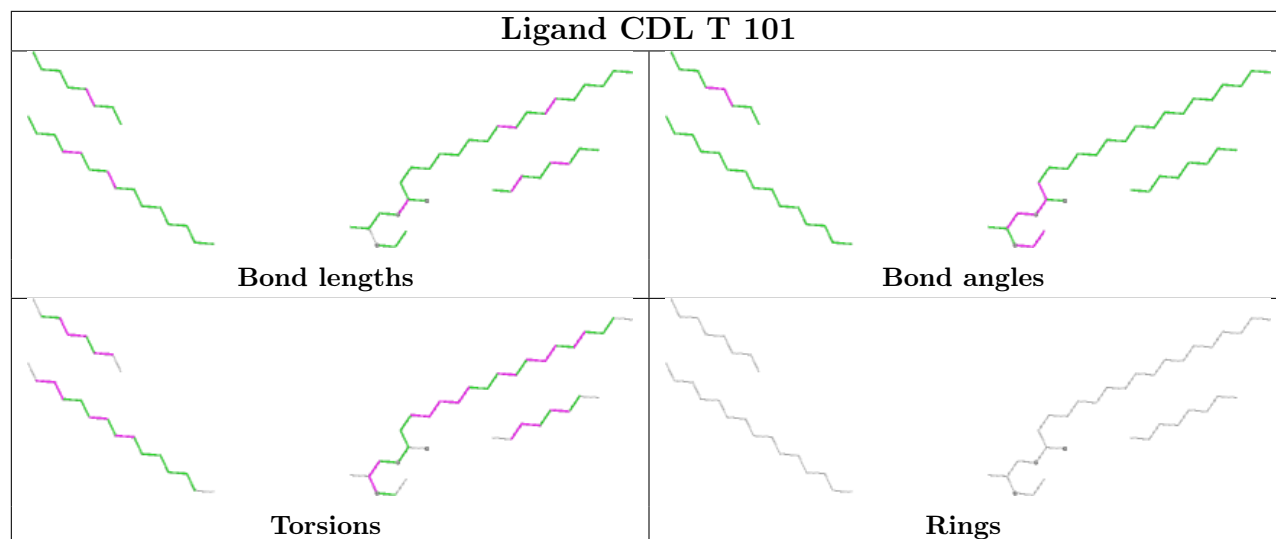


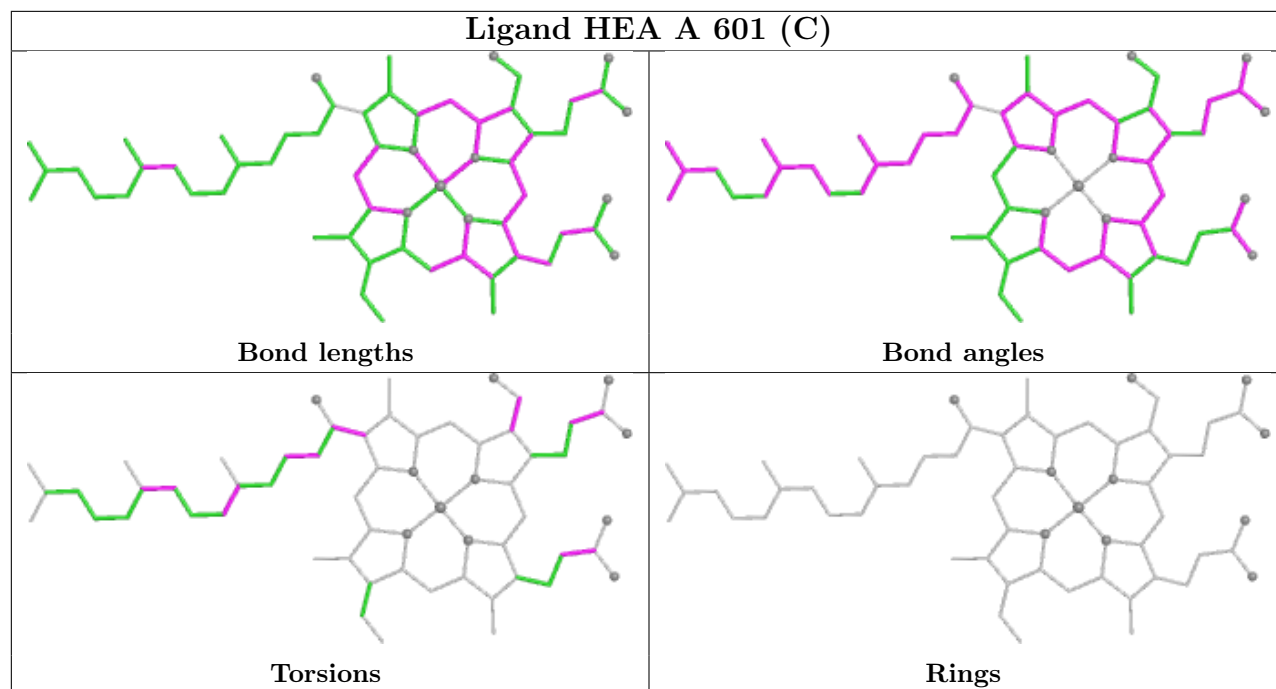












5.7 Other polymers [i](#)

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%)	-0.30	3 (0%) 85 89	10, 24, 31, 73	31 (6%)
1	N	513/514 (99%)	-0.19	2 (0%) 88 91	11, 26, 35, 89	35 (6%)
2	B	226/227 (99%)	0.24	14 (6%) 26 30	17, 30, 59, 105	7 (3%)
2	O	226/227 (99%)	0.45	15 (6%) 24 28	22, 34, 75, 148	11 (4%)
3	C	259/259 (100%)	-0.03	4 (1%) 72 78	15, 27, 41, 105	12 (4%)
3	P	259/259 (100%)	0.12	7 (2%) 56 62	15, 28, 42, 111	12 (4%)
4	D	144/144 (100%)	0.14	6 (4%) 40 46	19, 31, 57, 97	3 (2%)
4	Q	144/144 (100%)	1.27	22 (15%) 5 5	27, 46, 101, 215	1 (0%)
5	E	105/105 (100%)	0.17	4 (3%) 44 50	25, 32, 66, 157	0
5	R	105/105 (100%)	0.72	8 (7%) 20 23	28, 40, 78, 155	1 (0%)
6	F	94/94 (100%)	0.33	6 (6%) 25 29	19, 31, 66, 148	5 (5%)
6	S	94/94 (100%)	0.61	10 (10%) 11 13	23, 32, 73, 159	0
7	G	84/84 (100%)	1.47	23 (27%) 1 1	20, 36, 137, 156	4 (4%)
7	T	84/84 (100%)	1.54	22 (26%) 1 1	25, 38, 137, 184	0
8	H	79/79 (100%)	0.87	11 (13%) 6 7	26, 36, 116, 171	1 (1%)
8	U	79/79 (100%)	1.02	16 (20%) 3 3	30, 40, 117, 216	0
9	I	72/73 (98%)	0.97	11 (15%) 5 5	27, 45, 77, 103	1 (1%)
9	V	72/73 (98%)	1.58	28 (38%) 1 1	30, 52, 96, 146	0
10	J	58/58 (100%)	0.80	7 (12%) 8 10	27, 38, 93, 172	1 (1%)
10	W	58/58 (100%)	0.92	8 (13%) 6 7	29, 42, 92, 152	0
11	K	49/49 (100%)	0.55	2 (4%) 41 47	21, 37, 59, 79	3 (6%)
11	X	49/49 (100%)	1.43	12 (24%) 2 2	36, 48, 98, 113	0
12	L	46/46 (100%)	0.23	3 (6%) 25 29	23, 29, 57, 111	1 (2%)
12	Y	46/46 (100%)	0.60	4 (8%) 16 19	29, 36, 85, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.32	4 (9%) 14 17	25, 29, 95, 126	0
13	Z	43/43 (100%)	0.98	6 (13%) 6 7	32, 37, 110, 225	0
All	All	3544/3550 (99%)	0.34	258 (7%) 21 24	10, 30, 78, 225	129 (3%)

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	12.2
6	S	1	ALA	10.7
7	T	3	ALA	10.0
7	T	6	GLY	9.7
4	Q	5	VAL	9.3
7	T	7	ASP	8.4
7	G	3	ALA	8.3
4	Q	8	SER	8.2
7	G	6	GLY	8.1
7	G	8	HIS	8.0
7	G	7	ASP	8.0
6	F	1	ALA	7.7
3	P	3	HIS	7.7
6	F	2	SER	7.5
6	S	94	HIS	7.4
7	G	36	TRP	7.4
7	T	36	TRP	7.2
7	G	10	GLY	7.1
10	J	1	PHE	7.0
8	U	8	ILE	7.0
8	U	46	LYS	6.8
8	H	8	ILE	6.7
6	S	2	SER	6.6
2	O	91	ASN	6.1
7	T	5	LYS	6.1
7	T	9	GLY	6.1
7	G	9	GLY	6.0
4	Q	10	ASP	5.9
4	Q	9	GLU	5.9
7	T	8	HIS	5.9
4	Q	7	LYS	5.8
7	T	10	GLY	5.7
7	G	4	ALA	5.7
9	V	37	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
10	W	1	PHE	5.5
3	P	37	PHE	5.4
7	G	5	LYS	5.4
8	U	45	ALA	5.3
2	O	227	LEU	5.3
7	G	11	THR	5.3
7	T	2	SER	5.3
12	Y	2	HIS	5.3
8	H	46	LYS	5.2
7	T	1	ALA	5.2
9	I	37	PHE	5.1
6	F	3	GLY	5.0
7	T	11	THR	4.9
6	S	93	PRO	4.8
2	O	113	TYR	4.7
12	L	2	HIS	4.7
9	V	2	THR	4.7
4	D	4	SER	4.7
2	B	61	VAL	4.6
7	T	4	ALA	4.6
3	C	3	HIS	4.5
13	Z	42	LYS	4.5
9	I	2	THR	4.5
7	T	38	HIS	4.4
11	X	6	ALA	4.4
7	T	40	GLY	4.4
8	U	47	GLY	4.4
13	Z	43	SER	4.4
7	G	2	SER	4.3
8	H	47	GLY	4.3
9	I	29	LEU	4.3
7	G	38	HIS	4.2
1	A	514[A]	LYS	4.2
13	Z	40	TYR	4.2
10	J	57	HIS	4.2
11	X	7	PRO	4.2
4	Q	35	ALA	4.1
11	K	6	ALA	4.1
8	H	44	THR	4.1
13	M	40	TYR	4.1
6	S	3	GLY	4.0
4	Q	4	SER	4.0

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Mol	Chain	Res	Type	RSRZ
2	O	90	ILE	4.0
9	V	36	LYS	4.0
11	X	49	THR	3.9
7	G	84	LYS	3.9
2	B	90	ILE	3.9
8	U	9	LYS	3.8
2	O	82[B]	ARG	3.8
2	B	65	TRP	3.8
3	P	122	HIS	3.8
9	V	3	ALA	3.8
8	U	61	LYS	3.7
13	Z	41	LYS	3.7
7	G	1	ALA	3.7
5	E	5	HIS	3.7
13	Z	39	ASN	3.7
11	X	52	GLU	3.6
4	Q	51	LEU	3.6
2	B	91	ASN	3.6
2	B	129	LYS	3.6
8	U	7	LYS	3.5
12	L	47	LYS	3.5
10	J	58	LYS	3.5
7	T	12	GLY	3.5
8	U	48	GLY	3.5
7	G	42	ARG	3.5
8	H	10[A]	ASN	3.4
6	S	52	ILE	3.4
9	V	25	PHE	3.4
7	T	84	LYS	3.4
10	J	27	THR	3.3
5	R	109	VAL	3.3
9	V	65	LYS	3.3
4	Q	19	ARG	3.3
8	H	9	LYS	3.3
5	E	109	VAL	3.3
8	U	50	VAL	3.2
5	R	5	HIS	3.2
7	T	39	SER	3.2
11	X	54	ARG	3.2
2	O	92	ASN	3.2
8	U	84	LYS	3.2
10	W	58	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	87[A]	PHE	3.2
2	B	113	TYR	3.1
7	G	37	LEU	3.1
9	V	15	ARG	3.1
2	B	92	ASN	3.1
2	O	32[A]	PHE	3.1
4	Q	72	ASN	3.1
10	W	48	TYR	3.1
8	H	7	LYS	3.1
4	Q	73	ARG	3.0
11	X	47	ARG	3.0
7	T	37	LEU	3.0
6	S	64	GLU	3.0
9	I	32	ALA	3.0
9	V	29	LEU	3.0
6	F	64	GLU	3.0
8	U	10	ASN	2.9
10	J	56	PRO	2.9
11	X	12	LYS	2.9
10	W	27	THR	2.9
1	N	513	LEU	2.9
11	K	47	ARG	2.9
4	Q	143	ASN	2.9
4	D	5	VAL	2.9
8	U	52	VAL	2.9
4	Q	39	ALA	2.8
7	G	35	SER	2.8
11	X	48	VAL	2.8
5	R	96	LEU	2.8
12	Y	26	THR	2.8
7	T	70	PHE	2.7
9	V	34	PHE	2.7
8	H	50	VAL	2.7
10	W	57	HIS	2.7
4	Q	46	ALA	2.7
1	N	514	LYS	2.7
4	Q	87	PHE	2.7
9	I	25	PHE	2.7
7	T	42	ARG	2.7
10	J	55	PHE	2.7
10	W	52	TRP	2.7
4	D	143	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	64	ILE	2.7
9	V	5	ALA	2.7
9	I	34	PHE	2.6
5	R	79	LYS	2.6
9	I	53	ASN	2.6
9	V	73	LYS	2.6
3	C	258	TRP	2.6
8	U	55	TRP	2.6
7	G	45	PRO	2.6
7	G	40	GLY	2.6
8	U	44	THR	2.6
12	Y	44	LEU	2.6
2	O	22[A]	HIS	2.6
2	B	68	LEU	2.6
5	E	39	TYR	2.6
9	V	44	LYS	2.6
3	C	38	ASN	2.6
2	B	58	ALA	2.5
6	S	76	LYS	2.5
13	M	41	LYS	2.5
11	X	8	ASP	2.5
9	V	68	ILE	2.5
2	O	226	MET	2.5
10	W	26	ALA	2.5
5	R	85	VAL	2.5
8	H	84	LYS	2.5
9	I	22	VAL	2.5
9	V	64	ARG	2.5
5	R	90	ARG	2.4
9	I	15	ARG	2.4
7	G	41	HIS	2.4
10	J	52	TRP	2.4
5	E	6	GLU	2.4
8	H	48	GLY	2.4
3	P	258	TRP	2.4
8	U	49	ASP	2.4
5	R	80	GLU	2.4
4	Q	140	TYR	2.4
9	V	26	MET	2.4
6	F	54[A]	ASN	2.3
7	G	12	GLY	2.3
9	V	33	THR	2.3

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Mol	Chain	Res	Type	RSRZ
9	V	8	GLN	2.3
7	G	39	SER	2.3
7	G	43	GLU	2.3
2	B	59	GLN	2.3
3	C	37	PHE	2.3
3	P	38	ASN	2.3
13	M	39	ASN	2.3
9	I	36	LYS	2.3
1	A	513	LEU	2.3
2	O	114	GLU	2.3
4	D	31	LYS	2.3
5	R	108	LYS	2.3
3	P	33[A]	MET	2.3
4	Q	40	LEU	2.2
6	S	65	ASP	2.2
3	P	44[A]	MET	2.2
10	W	55	PHE	2.2
7	T	41	HIS	2.2
4	Q	147	LYS	2.2
7	T	33	LEU	2.2
9	V	30	GLY	2.2
4	Q	53	ILE	2.2
9	V	27	VAL	2.2
12	Y	47	LYS	2.2
2	O	116	LEU	2.2
6	F	94	HIS	2.2
4	Q	31	LYS	2.2
9	V	57	MET	2.1
2	O	89	GLU	2.1
8	H	45	ALA	2.1
2	O	78	LEU	2.1
9	V	4	LEU	2.1
6	S	43	LYS	2.1
9	V	45	LYS	2.1
9	V	53	ASN	2.1
9	V	31	PHE	2.1
9	V	72	ALA	2.1
11	X	28	VAL	2.1
11	X	51	LYS	2.1
12	L	45	LEU	2.1
13	Z	19	LEU	2.1
2	B	115[A]	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	67	ILE	2.1
9	V	39	VAL	2.1
13	M	38	ASP	2.1
2	O	65[A]	TRP	2.1
1	A	169	ILE	2.1
11	X	13	TYR	2.1
9	V	32	ALA	2.0
4	Q	49	SER	2.0
8	U	51	SER	2.0
9	I	33	THR	2.0
2	B	130	PRO	2.0
4	D	7	LYS	2.0
2	O	64[A]	ILE	2.0
9	V	22	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.30	0.21	113,156,190,197	0
9	SAC	I	1	9/10	0.58	0.27	112,134,180,200	0
1	FME	N	1	10/11	0.91	0.17	38,42,98,131	0
1	FME	A	1	10/11	0.95	0.09	35,49,83,103	0
2	FME	O	1	10/11	0.96	0.11	31,34,42,112	0
2	FME	B	1	10/11	0.96	0.13	27,28,38,142	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
25	DMU	X	102	10/33	0.58	0.32	62,71,99,116	0
25	DMU	D	203	11/33	0.69	0.25	52,74,124,137	0
25	DMU	K	105	9/33	0.71	0.22	72,75,92,107	0
24	CHD	Y	101	29/29	0.71	0.25	56,95,143,158	0
25	DMU	X	103	9/33	0.72	0.23	55,62,94,101	0
21	EDO	L	104	4/4	0.73	0.34	50,51,77,148	0
25	DMU	K	104	9/33	0.74	0.32	49,70,113,125	0
21	EDO	P	310	4/4	0.74	0.19	46,60,67,75	0
26	CDL	T	101	57/100	0.75	0.28	42,72,104,149	0
24	CHD	L	102	29/29	0.77	0.23	51,100,145,177	0
25	DMU	X	104	10/33	0.77	0.26	62,84,90,92	0
22	TGL	N	611	48/63	0.77	0.27	48,68,120,134	0
18	PGV	C	311	28/51	0.78	0.30	41,66,117,126	0
27	PEK	P	308	34/53	0.78	0.28	37,70,117,134	0
25	DMU	X	101	11/33	0.79	0.21	43,59,104,225	0
25	DMU	P	303	13/33	0.79	0.23	53,62,94,101	0
27	PEK	C	309	36/53	0.80	0.25	42,75,110,130	0
18	PGV	G	102	32/51	0.80	0.25	39,72,108,130	0
26	CDL	N	601	55/100	0.81	0.25	51,69,104,118	0
21	EDO	G	104	4/4	0.81	0.30	33,77,87,92	0
25	DMU	Q	201	10/33	0.81	0.25	52,62,68,111	0
22	TGL	B	301	49/63	0.81	0.22	38,61,98,147	0
21	EDO	P	317	4/4	0.82	0.17	57,90,97,106	0
22	TGL	N	609	63/63	0.82	0.23	40,72,117,154	0
25	DMU	K	106	10/33	0.83	0.25	52,65,91,120	0
25	DMU	L	101	21/33	0.83	0.18	42,81,114,129	0
27	PEK	C	306	25/53	0.83	0.24	41,57,96,119	0
25	DMU	C	303	13/33	0.83	0.20	53,63,88,92	0
27	PEK	P	305	20/53	0.83	0.21	47,56,95,96	0
22	TGL	D	202	57/63	0.83	0.23	32,65,134,156	0
21	EDO	S	104	4/4	0.84	0.20	40,56,58,88	0
25	DMU	K	102	10/33	0.84	0.21	46,69,87,103	0
18	PGV	N	607	24/51	0.84	0.27	41,53,106,166	0
26	CDL	P	304	61/100	0.85	0.25	37,69,128,196	0
25	DMU	O	302	11/33	0.85	0.19	54,58,104,111	0
22	TGL	L	103	56/63	0.85	0.22	28,56,121,139	0
21	EDO	A	615	4/4	0.85	0.18	49,58,60,64	0
26	CDL	C	305	58/100	0.85	0.22	44,65,131,156	0
21	EDO	J	102	4/4	0.85	0.24	52,52,100,116	0
19	PSC	A	607	27/52	0.86	0.22	36,66,100,129	0
21	EDO	C	320	4/4	0.86	0.26	32,56,75,112	0
21	EDO	Q	202	4/4	0.86	0.15	43,50,52,56	0
21	EDO	F	103	4/4	0.86	0.19	50,61,64,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	DMU	K	103	11/33	0.86	0.22	50,70,100,120	0
21	EDO	N	619	4/4	0.86	0.24	51,52,54,67	0
21	EDO	T	104	4/4	0.87	0.17	39,49,54,71	0
21	EDO	P	312	4/4	0.87	0.16	67,72,73,77	0
21	EDO	P	316	4/4	0.87	0.17	39,56,66,82	0
18	PGV	A	606	22/51	0.87	0.19	31,45,70,94	0
21	EDO	C	314	4/4	0.87	0.14	32,39,42,44	0
21	EDO	A	609	4/4	0.87	0.25	34,38,47,146	0
22	TGL	N	612	44/63	0.87	0.23	41,59,127,197	0
21	EDO	T	103	4/4	0.87	0.21	43,65,78,97	0
21	EDO	F	106	4/4	0.88	0.21	35,38,76,104	0
25	DMU	P	309	11/33	0.88	0.24	42,58,101,104	0
19	PSC	O	303	30/52	0.88	0.20	37,59,103,106	0
21	EDO	P	311	4/4	0.89	0.16	62,62,65,73	0
21	EDO	D	205	4/4	0.89	0.17	44,45,46,101	0
21	EDO	W	102	4/4	0.89	0.22	47,57,68,111	0
21	EDO	J	103	4/4	0.89	0.17	51,52,72,74	0
25	DMU	C	310	21/33	0.89	0.16	29,58,111,142	0
21	EDO	A	614	4/4	0.89	0.13	55,66,70,75	0
21	EDO	C	319	4/4	0.89	0.20	43,53,61,115	0
25	DMU	W	101	11/33	0.89	0.20	51,59,82,111	0
21	EDO	A	610	4/4	0.89	0.17	39,48,53,70	0
21	EDO	S	106	4/4	0.89	0.23	39,47,67,81	0
25	DMU	K	101	9/33	0.90	0.16	41,52,77,94	0
21	EDO	E	203	4/4	0.90	0.18	42,45,54,117	0
25	DMU	D	201	11/33	0.90	0.17	44,69,79,88	0
21	EDO	C	312	4/4	0.90	0.15	48,71,72,75	0
21	EDO	D	204	4/4	0.91	0.21	37,47,79,85	0
21	EDO	P	315	4/4	0.91	0.15	53,58,63,73	0
25	DMU	J	101	11/33	0.91	0.17	49,58,81,102	0
29	PO4	H	101	5/5	0.91	0.10	56,61,94,161	0
29	PO4	U	101	5/5	0.91	0.12	47,54,128,200	0
21	EDO	O	306	4/4	0.92	0.18	48,63,79,92	0
21	EDO	Y	102	4/4	0.92	0.16	48,57,57,83	0
21	EDO	Y	103	4/4	0.92	0.14	46,59,90,134	0
21	EDO	B	307	4/4	0.92	0.13	34,45,46,48	0
21	EDO	C	316	4/4	0.92	0.12	53,56,61,69	0
21	EDO	N	620	4/4	0.92	0.21	33,34,66,104	0
21	EDO	N	616	4/4	0.93	0.14	33,41,44,71	0
21	EDO	C	313	4/4	0.93	0.15	30,32,33,94	0
21	EDO	B	306	4/4	0.93	0.12	29,35,41,55	0
25	DMU	Z	101	33/33	0.93	0.10	38,46,79,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	N	621	4/4	0.93	0.12	46,52,52,62	0
21	EDO	O	305	4/4	0.93	0.17	42,46,51,95	0
25	DMU	M	101	33/33	0.93	0.10	31,40,53,69	0
21	EDO	C	318	4/4	0.94	0.15	40,60,63,111	0
21	EDO	D	206	4/4	0.94	0.12	36,38,58,71	0
21	EDO	A	612	4/4	0.94	0.11	28,31,32,38	0
21	EDO	A	618	4/4	0.94	0.15	33,34,39,87	0
21	EDO	F	105	4/4	0.94	0.14	39,44,64,96	0
21	EDO	C	317	4/4	0.94	0.12	55,56,72,75	0
24	CHD	C	304	29/29	0.94	0.08	26,29,35,41	0
21	EDO	A	616	4/4	0.95	0.15	30,42,68,94	0
21	EDO	A	617	4/4	0.95	0.13	37,39,46,63	0
21	EDO	N	613	4/4	0.95	0.09	28,29,29,32	0
21	EDO	N	614	4/4	0.95	0.09	37,38,39,44	0
21	EDO	N	615	4/4	0.95	0.12	37,40,41,67	0
21	EDO	P	313	4/4	0.95	0.14	34,37,39,39	0
21	EDO	P	314	4/4	0.95	0.12	30,35,40,62	0
20	PER	N	610[A]	2/2	0.95	0.16	28,28,28,28	2
21	EDO	C	315	4/4	0.95	0.14	28,35,50,72	0
18	PGV	N	608	51/51	0.95	0.12	23,34,69,80	0
20	PER	A	608[A]	2/2	0.95	0.12	23,23,23,23	2
21	EDO	O	304	4/4	0.95	0.08	30,31,32,32	0
21	EDO	S	102	4/4	0.96	0.08	23,25,25,25	0
24	CHD	B	303	29/29	0.96	0.07	21,26,31,46	0
18	PGV	C	301	51/51	0.96	0.10	22,32,67,80	0
24	CHD	G	101	29/29	0.96	0.07	21,26,35,42	0
21	EDO	B	305	4/4	0.96	0.11	32,34,45,103	0
27	PEK	C	307	53/53	0.96	0.12	26,42,102,136	0
24	CHD	P	301	29/29	0.96	0.07	24,29,35,40	0
21	EDO	T	102	4/4	0.96	0.12	31,32,37,40	0
27	PEK	P	306	53/53	0.96	0.12	28,41,84,122	0
21	EDO	E	202	4/4	0.96	0.08	31,38,43,45	0
21	EDO	N	617	4/4	0.96	0.08	22,29,30,32	0
21	EDO	N	618	4/4	0.96	0.11	31,41,43,47	0
21	EDO	A	613	4/4	0.97	0.12	28,39,46,48	0
21	EDO	B	304	4/4	0.97	0.07	24,25,27,29	0
18	PGV	P	307	51/51	0.97	0.11	23,32,97,138	0
17	NA	P	302	1/1	0.97	0.05	30,30,30,30	0
21	EDO	G	103	4/4	0.97	0.07	30,31,35,35	0
18	PGV	C	308	48/51	0.97	0.10	22,29,71,88	0
21	EDO	E	201	4/4	0.97	0.08	37,38,38,39	0
17	NA	C	302	1/1	0.97	0.06	31,31,31,31	0

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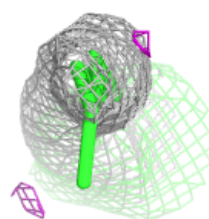
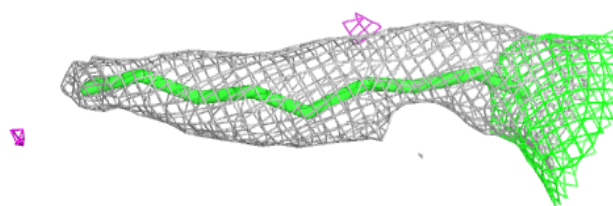
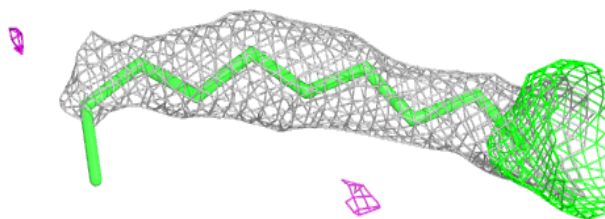
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	EDO	S	105	4/4	0.97	0.08	31,31,31,33	0
14	HEA	A	602	60/60	0.98	0.06	18,22,28,38	0
21	EDO	F	104	4/4	0.98	0.10	30,30,31,32	0
16	MG	A	604	1/1	0.98	0.07	19,19,19,19	0
21	EDO	S	103	4/4	0.98	0.07	32,33,38,41	0
21	EDO	F	102	4/4	0.98	0.06	24,25,26,27	0
14	HEA	A	601[A]	60/60	0.99	0.05	17,21,33,63	17
14	HEA	N	602[A]	60/60	0.99	0.06	20,25,38,46	17
14	HEA	N	602[B]	52/60	0.99	0.06	16,24,33,47	9
14	HEA	N	602[C]	52/60	0.99	0.06	20,24,40,52	9
14	HEA	N	603	60/60	0.99	0.06	19,23,29,38	0
21	EDO	A	611	4/4	0.99	0.07	22,24,27,28	0
14	HEA	A	601[B]	52/60	0.99	0.05	10,20,27,55	9
16	MG	N	605	1/1	0.99	0.07	21,21,21,21	0
17	NA	A	605	1/1	0.99	0.03	24,24,24,24	0
28	ZN	S	101	1/1	0.99	0.03	26,26,26,26	0
14	HEA	A	601[C]	52/60	0.99	0.05	17,21,31,57	9
17	NA	N	606	1/1	0.99	0.04	28,28,28,28	0
23	CUA	B	302	2/2	1.00	0.02	22,22,22,22	0
28	ZN	F	101	1/1	1.00	0.04	25,25,25,25	0
23	CUA	O	301	2/2	1.00	0.02	26,26,26,26	0
15	CU	N	604	1/1	1.00	0.02	24,24,24,24	0
15	CU	A	603	1/1	1.00	0.02	22,22,22,22	0

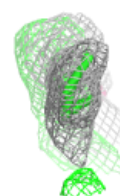
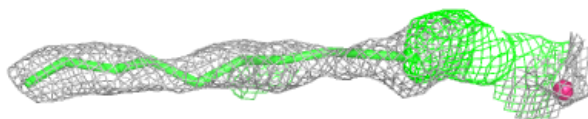
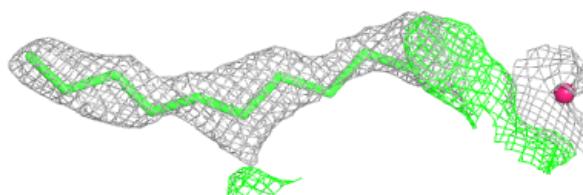
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DMU X 102:

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

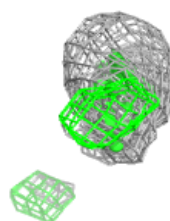
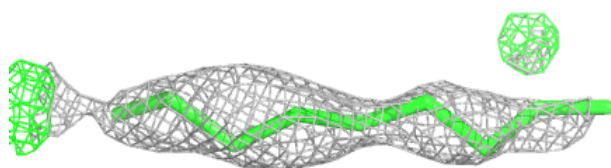
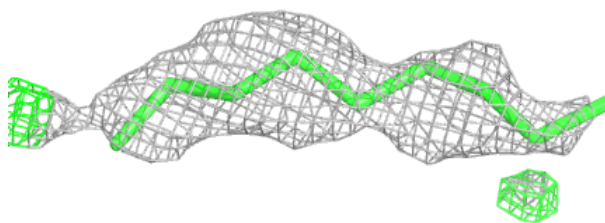
**Electron density around DMU D 203:**

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

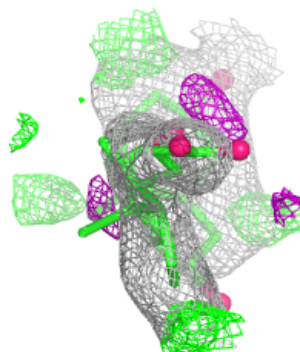
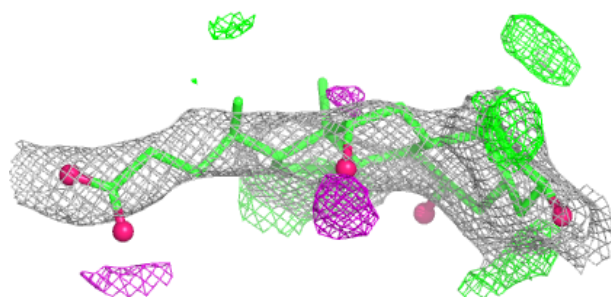
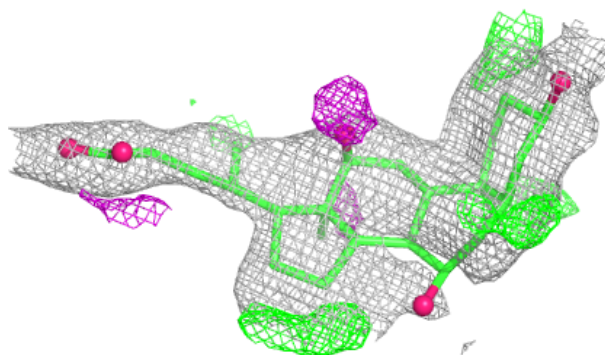


Electron density around DMU K 105:

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

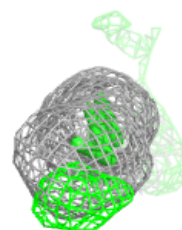
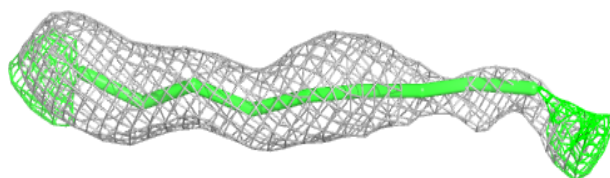
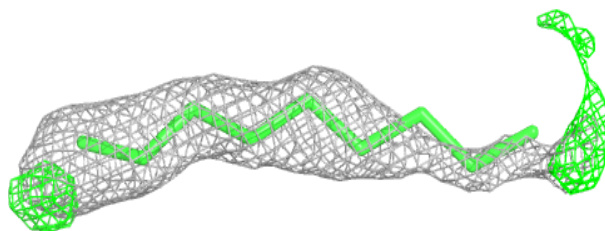
**Electron density around CHD Y 101:**

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

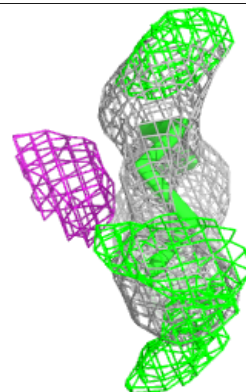
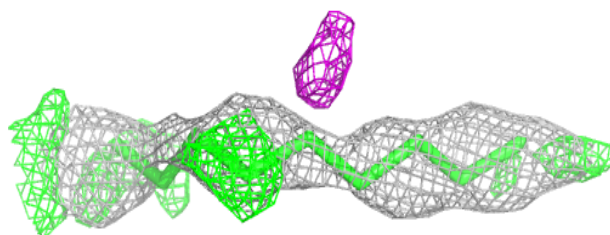
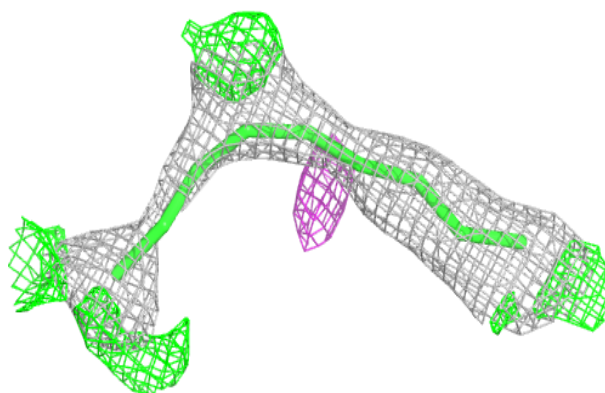


Electron density around DMU X 103:

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

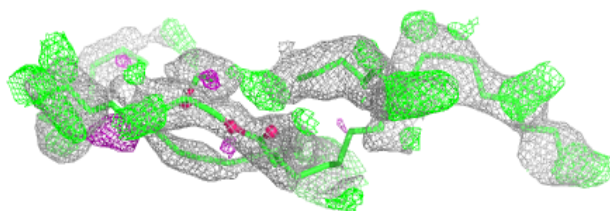
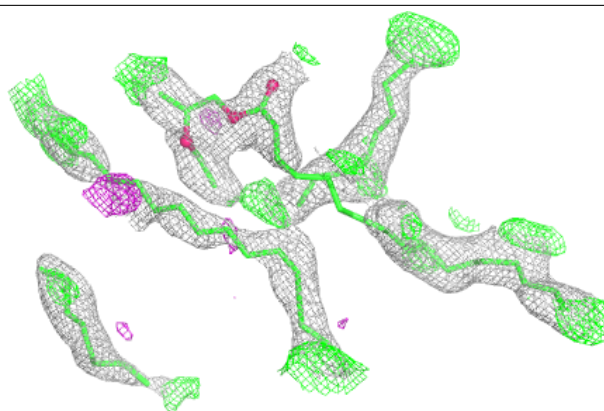
**Electron density around DMU K 104:**

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

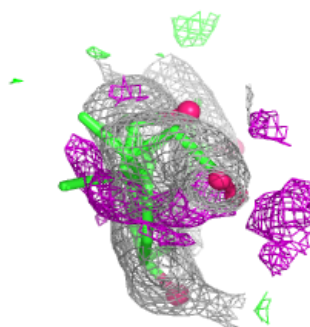
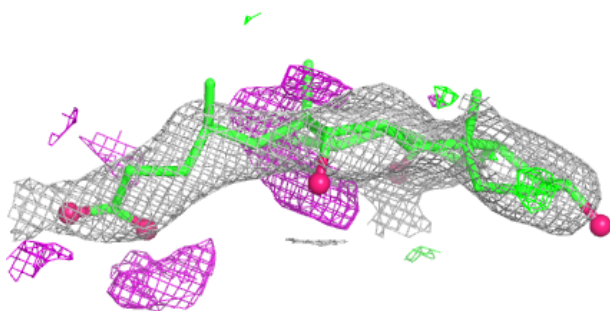
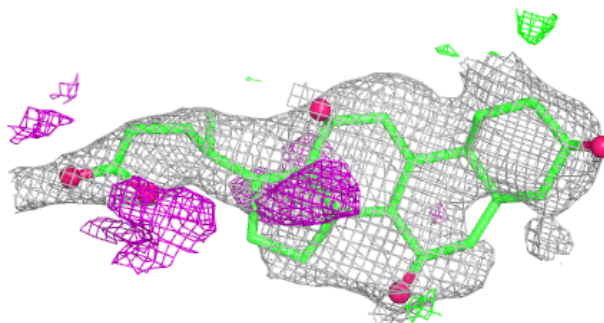


Electron density around CDL T 101:

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

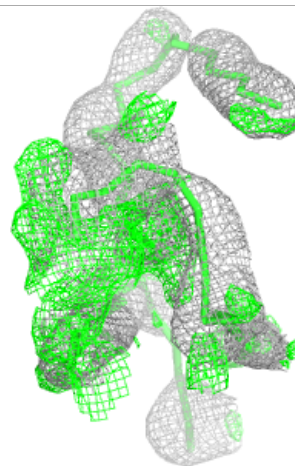
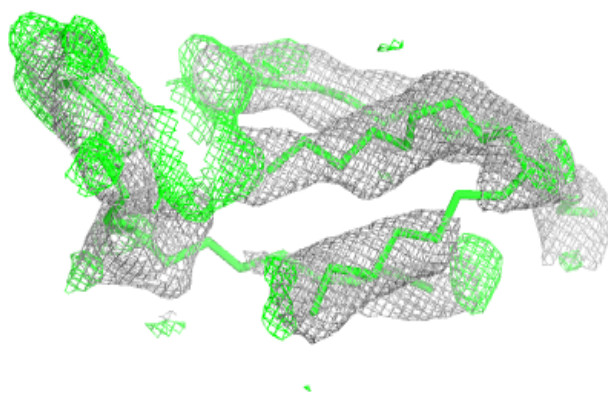
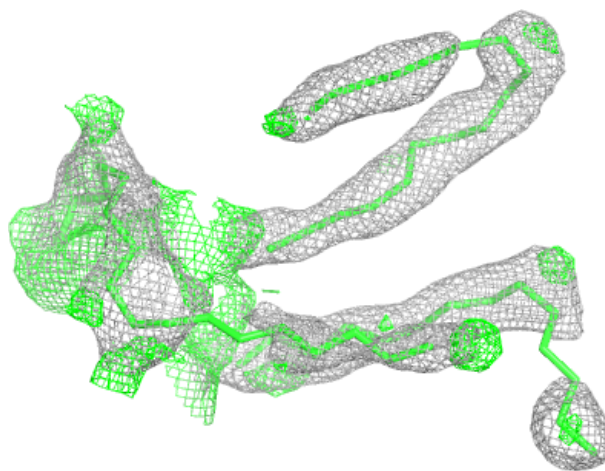
**Electron density around CHD L 102:**

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



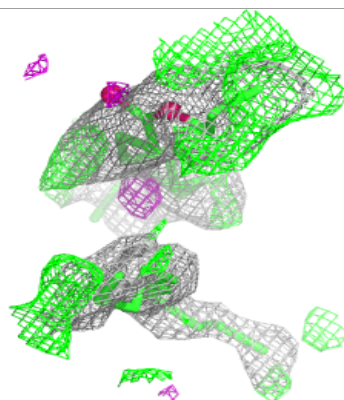
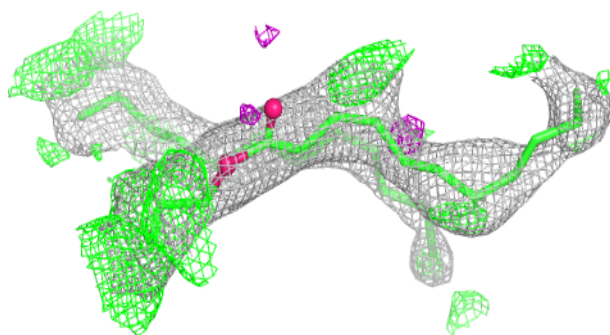
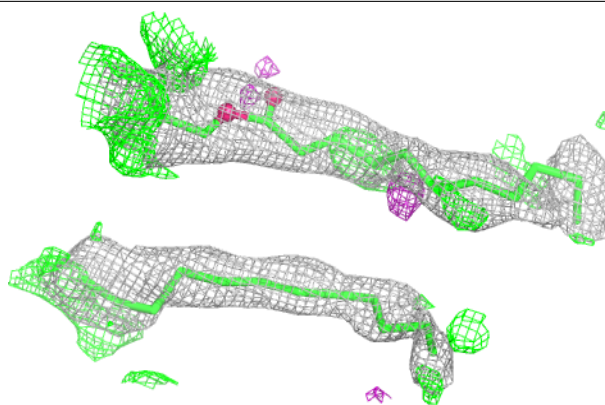
Electron density around TGL N 611:

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



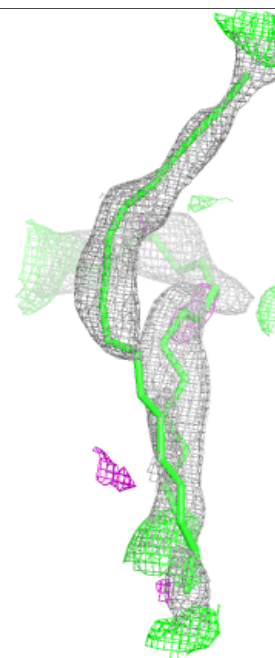
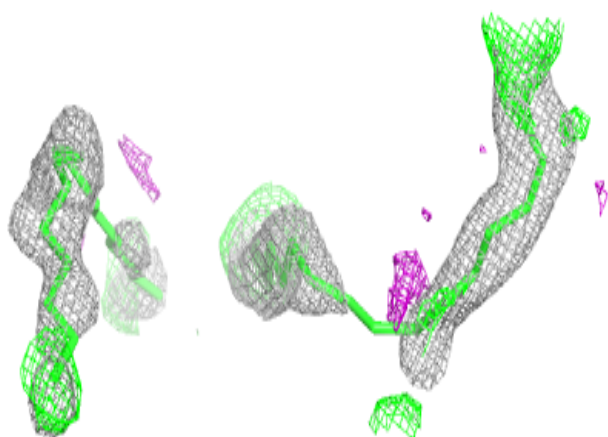
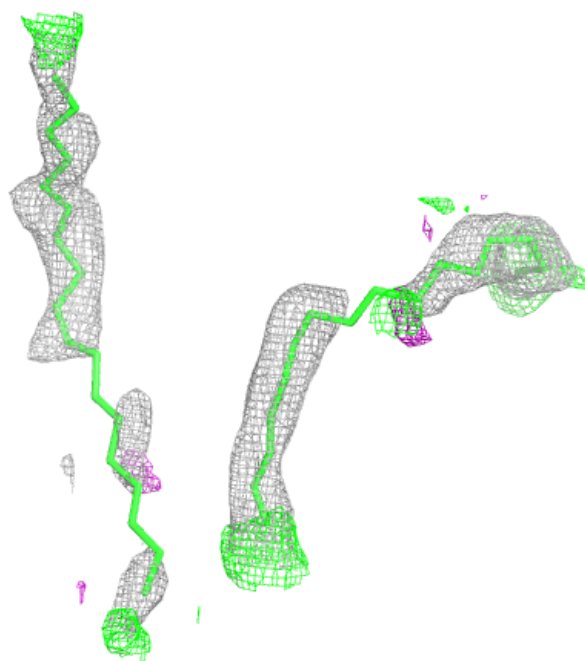
Electron density around PGV C 311:

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



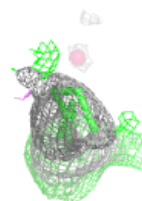
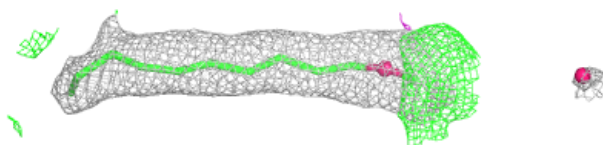
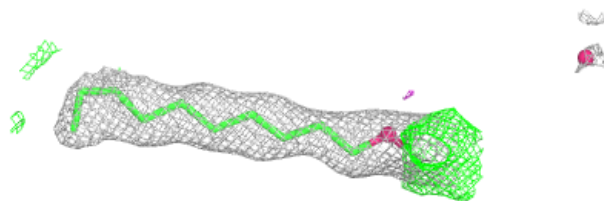
Electron density around PEK P 308:

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



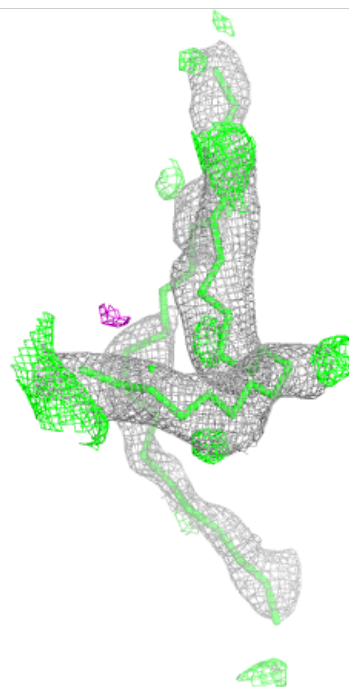
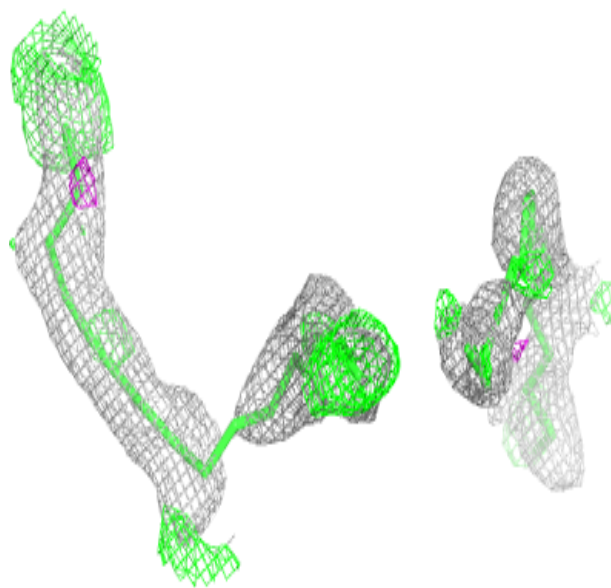
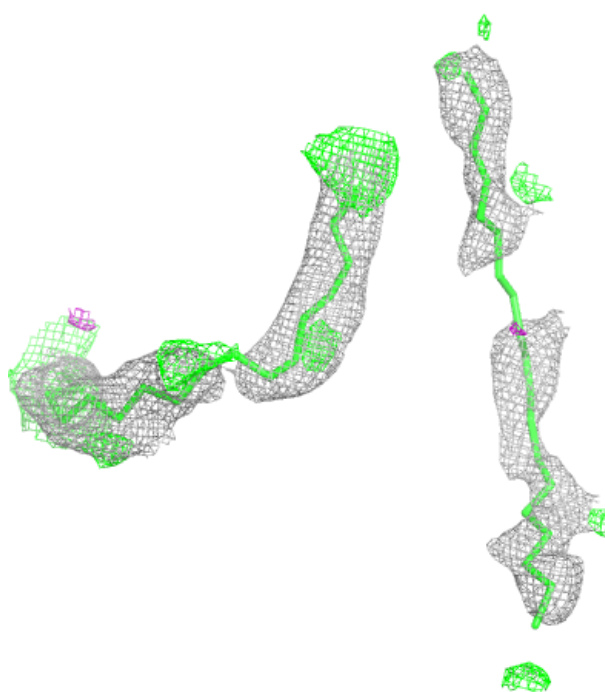
Electron density around DMU P 303:

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



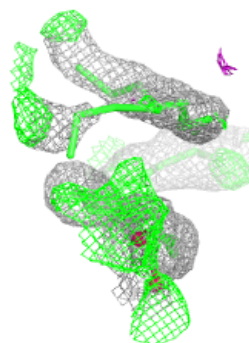
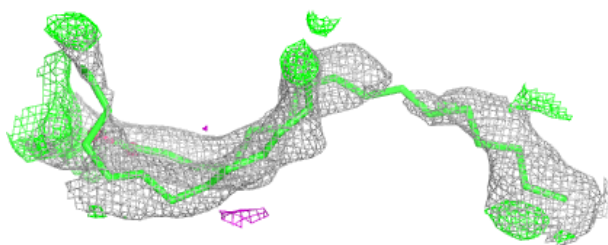
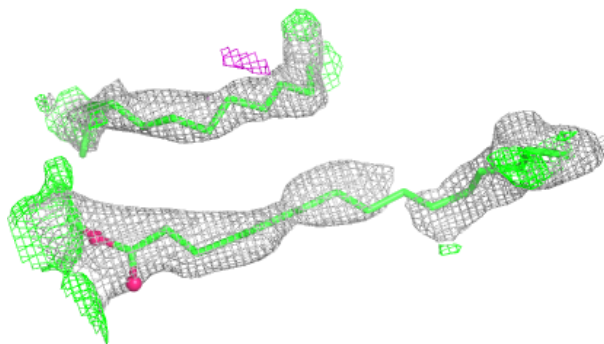
Electron density around PEK C 309:

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

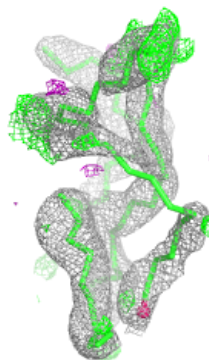
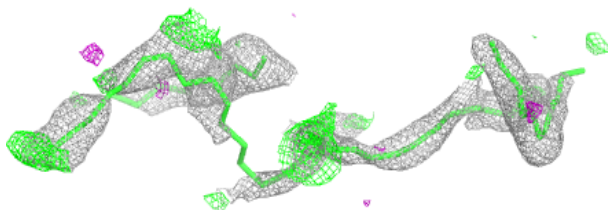
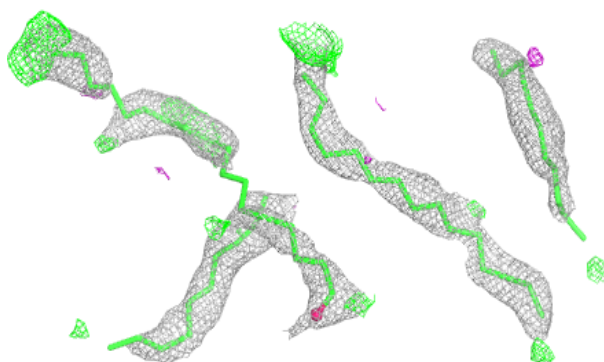


Electron density around PGV G 102:

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

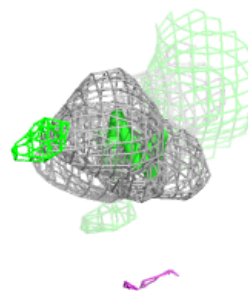
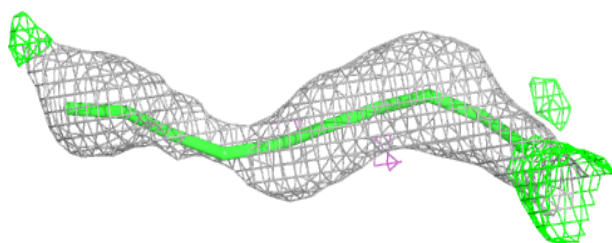
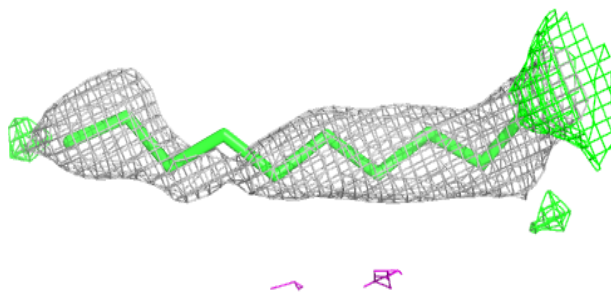
**Electron density around CDL N 601:**

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

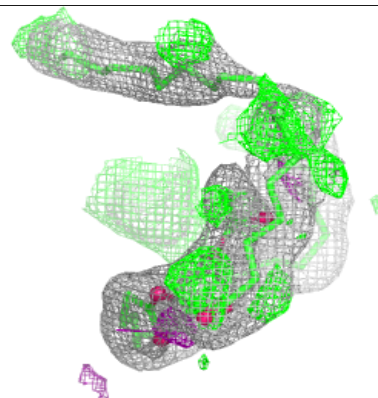
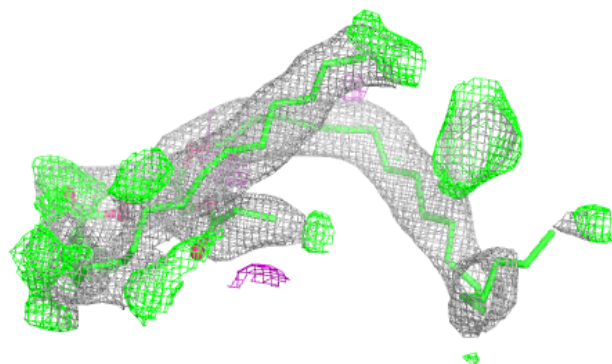
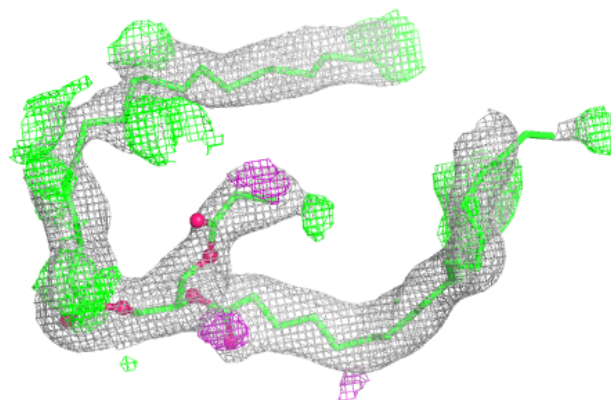


Electron density around DMU Q 201:

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

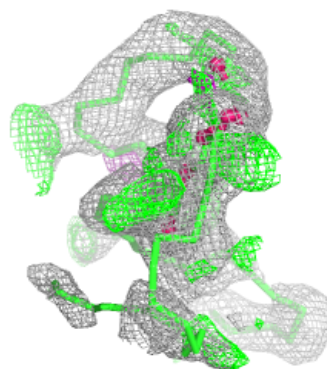
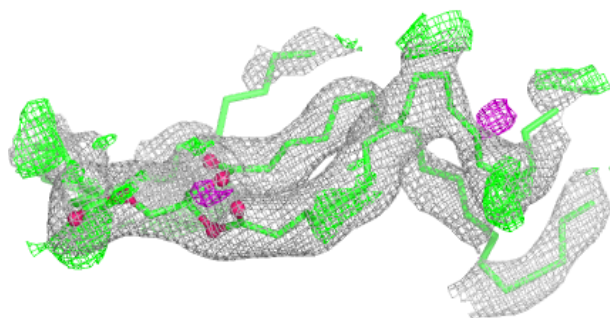
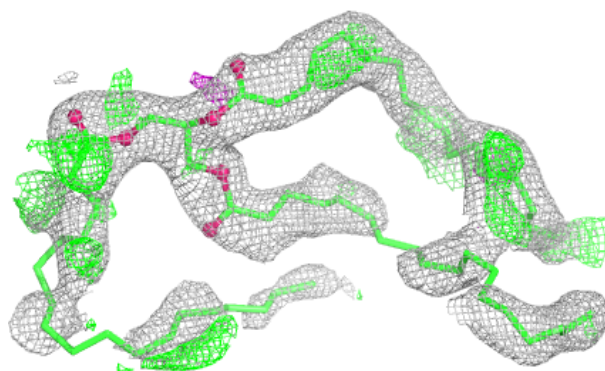
**Electron density around TGL B 301:**

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

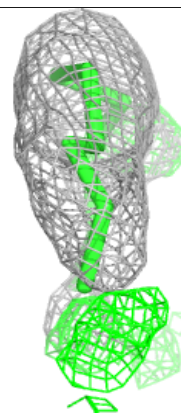
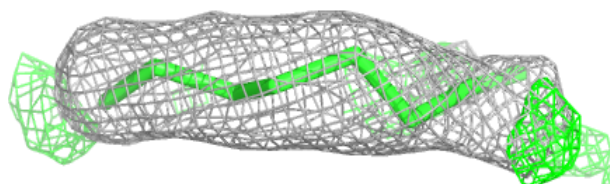
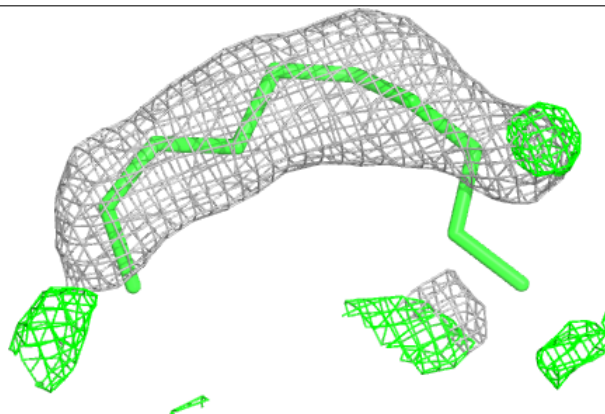


Electron density around TGL N 609:

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

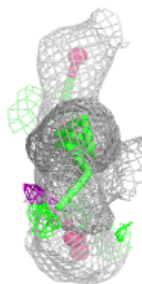
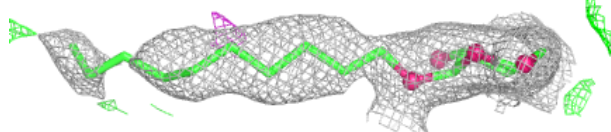
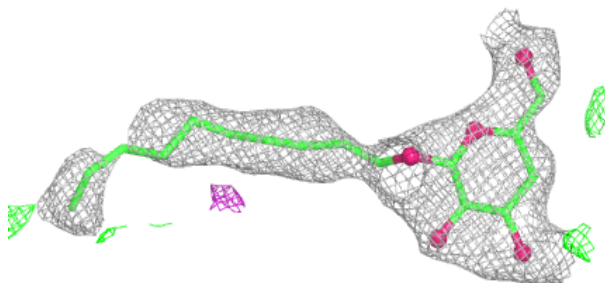
**Electron density around DMU K 106:**

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

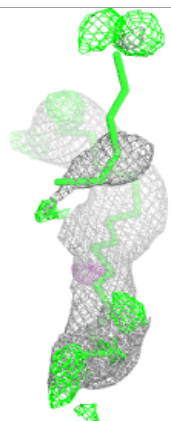
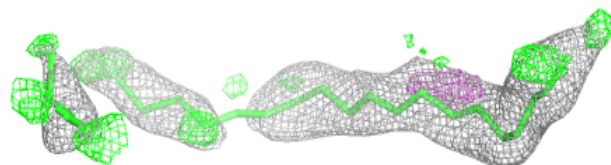
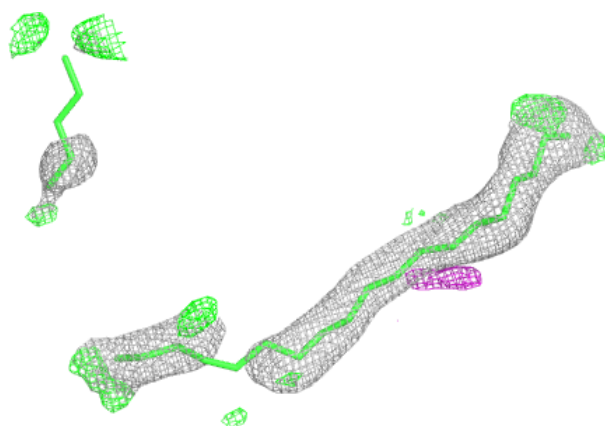


Electron density around DMU L 101:

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

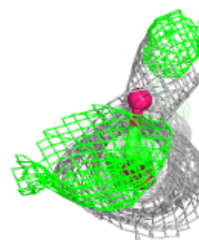
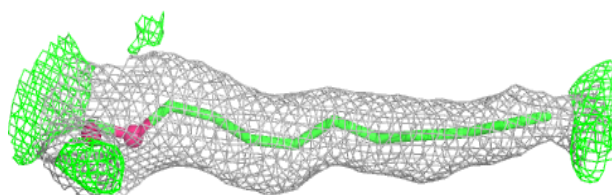
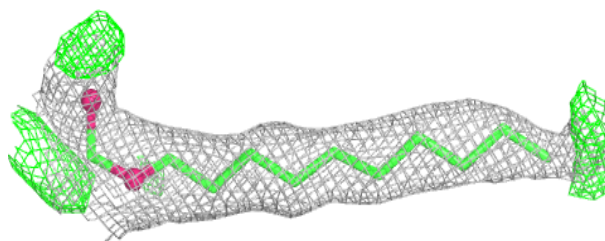
**Electron density around PEK C 306:**

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

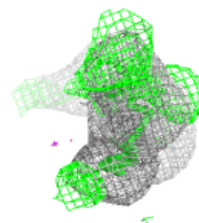
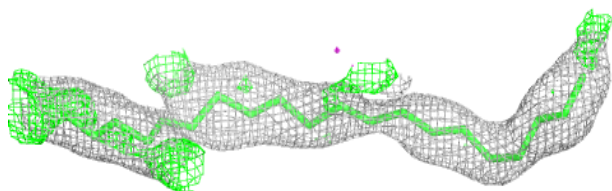
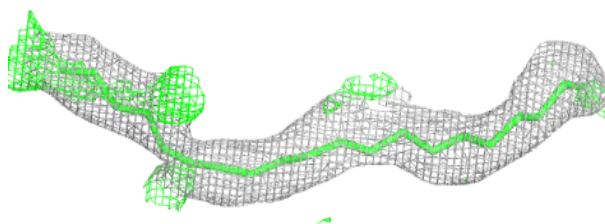


Electron density around DMU C 303:

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

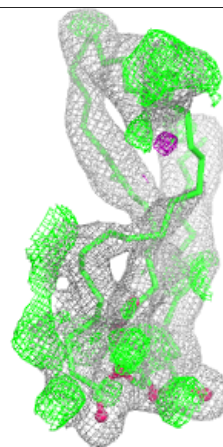
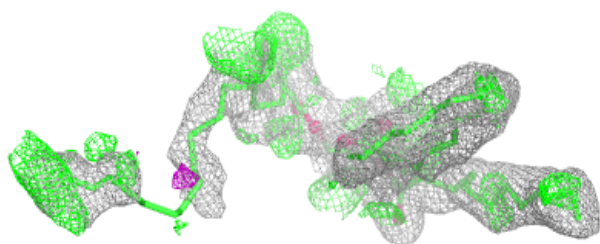
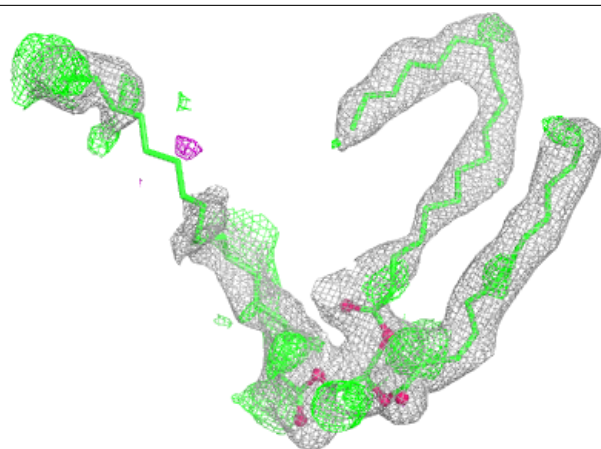
**Electron density around PEK P 305:**

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

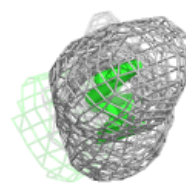
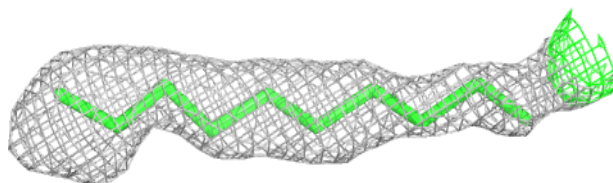
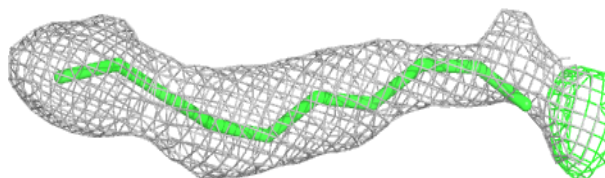


Electron density around TGL D 202:

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

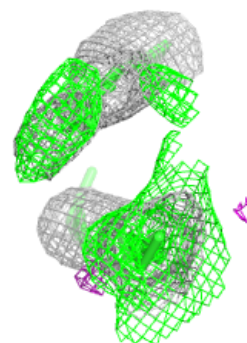
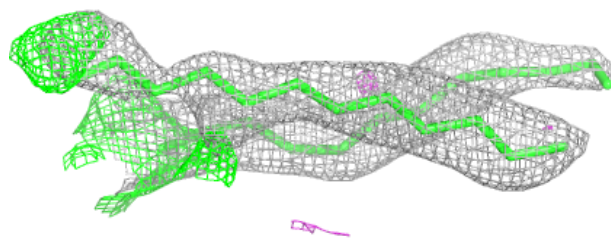
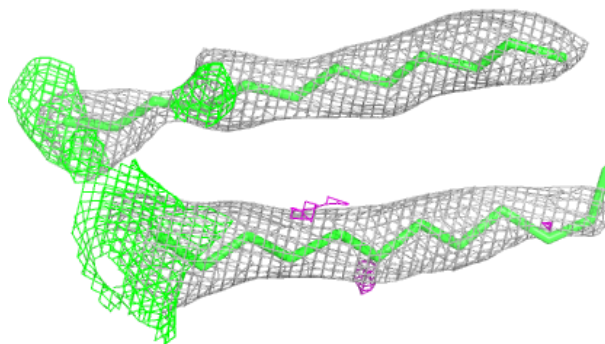
**Electron density around DMU K 102:**

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



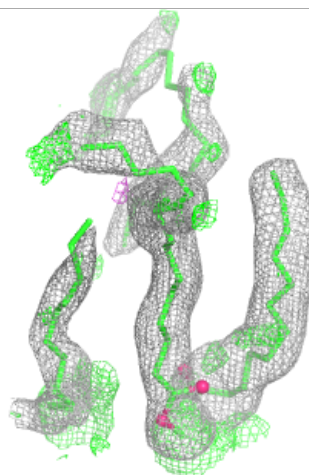
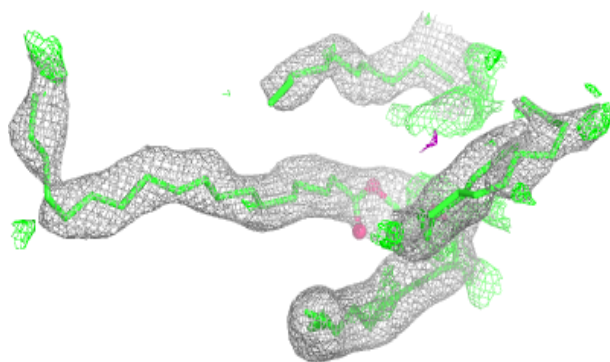
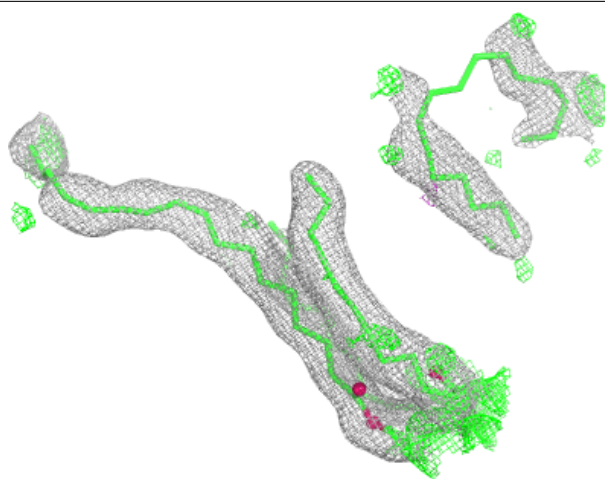
Electron density around PGV N 607:

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



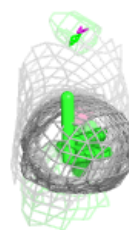
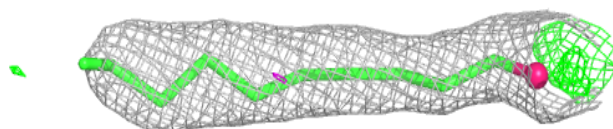
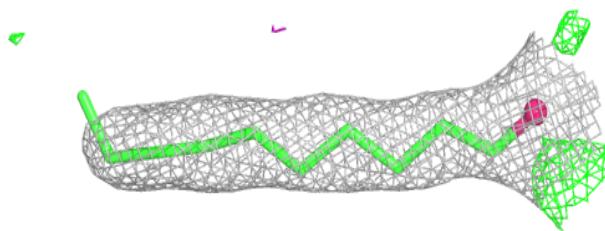
Electron density around CDL P 304:

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



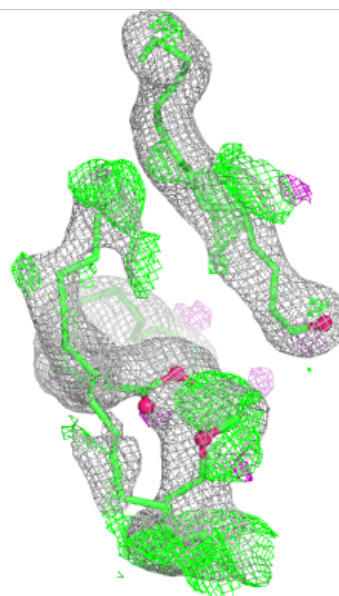
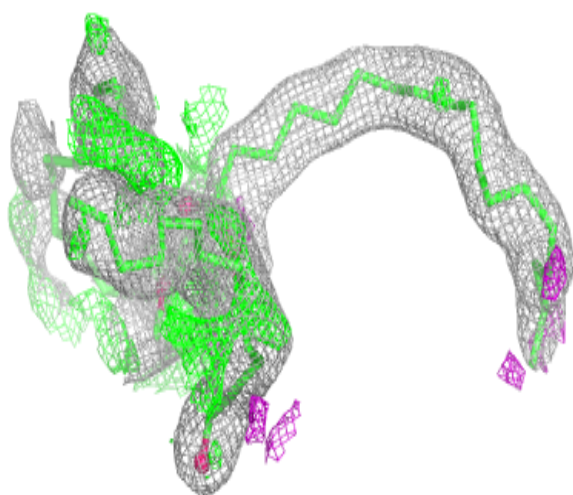
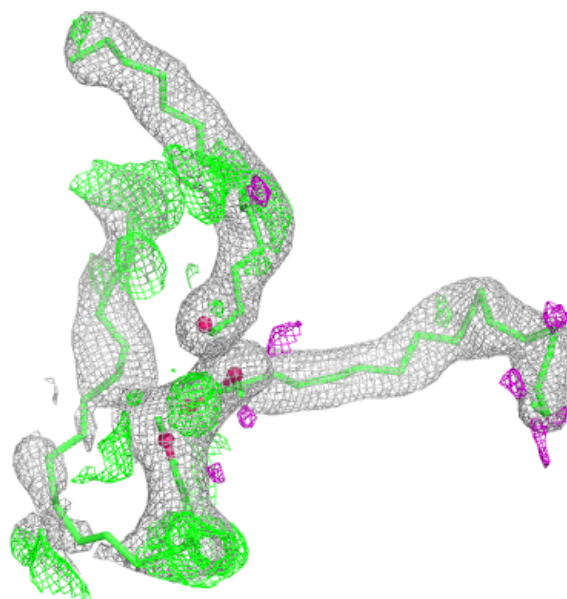
Electron density around DMU O 302:

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



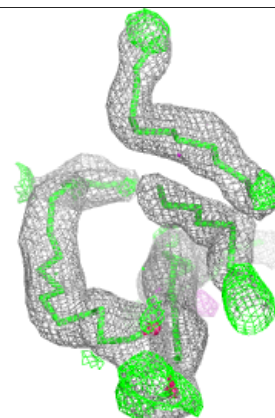
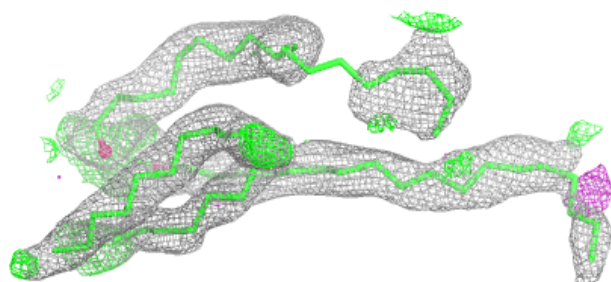
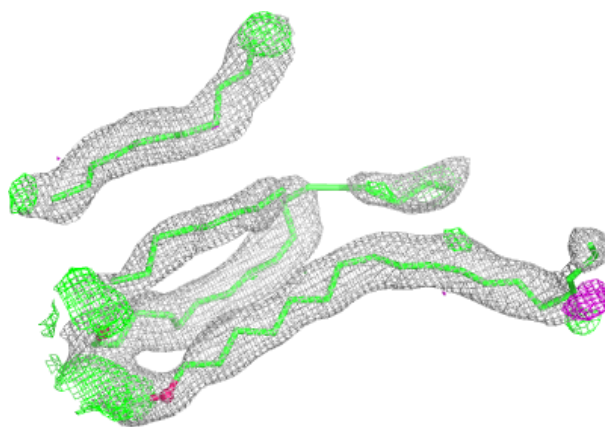
Electron density around TGL L 103:

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

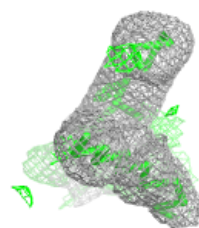
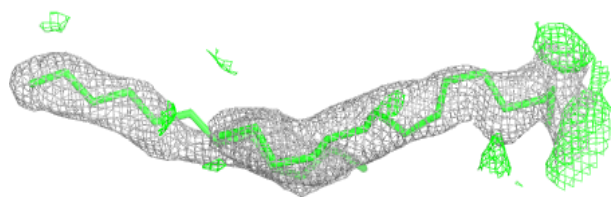
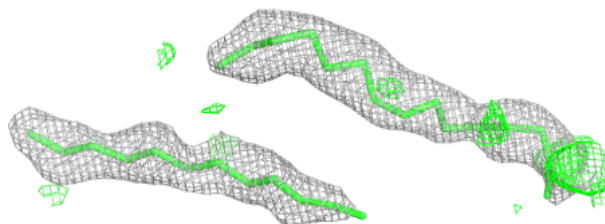


Electron density around CDL C 305:

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

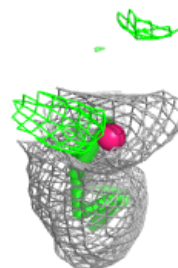
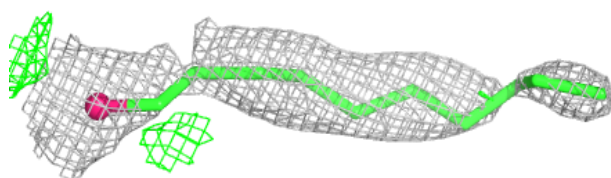
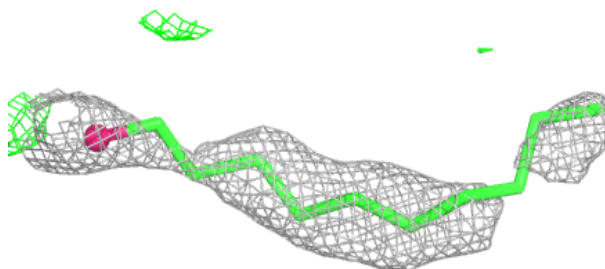
**Electron density around PSC A 607:**

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

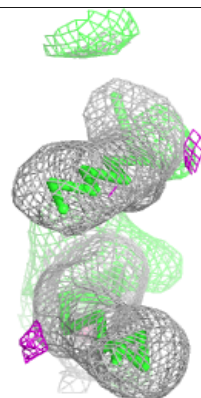
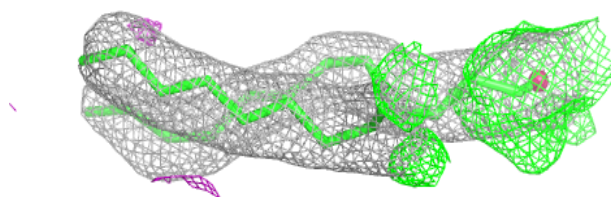
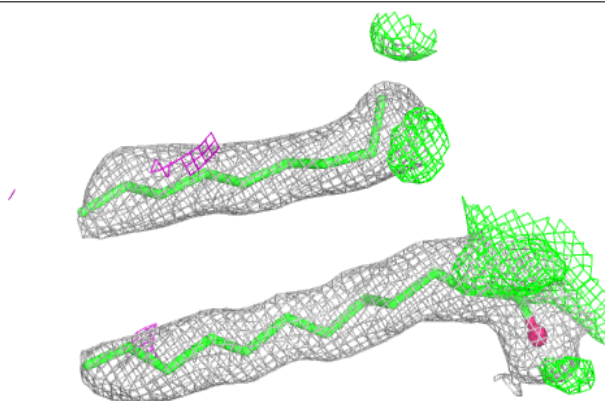


Electron density around DMU K 103:

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

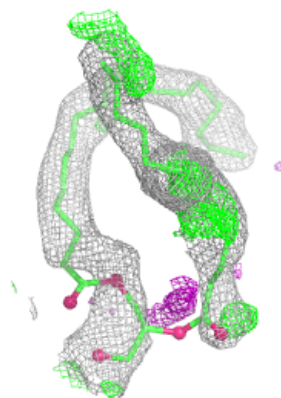
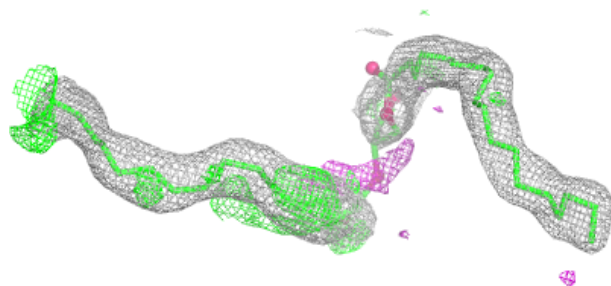
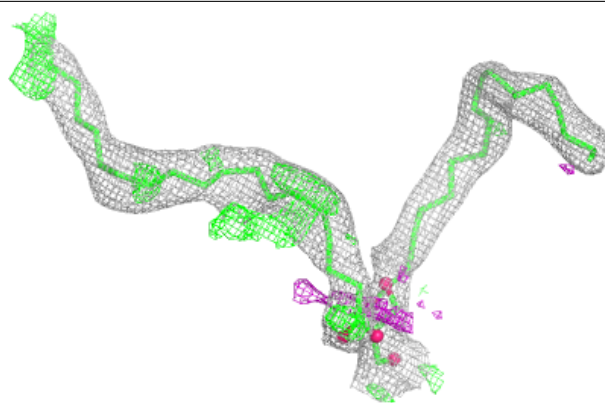
**Electron density around PGV A 606:**

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

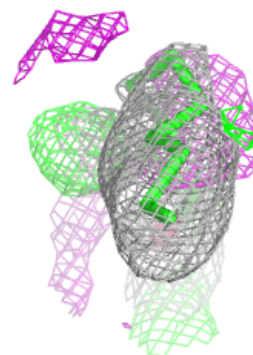
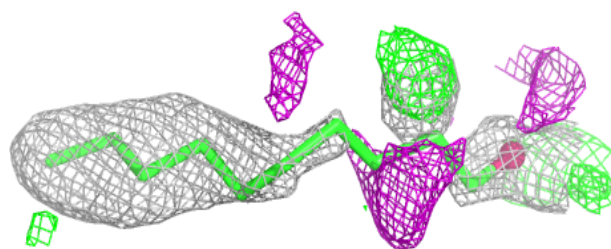
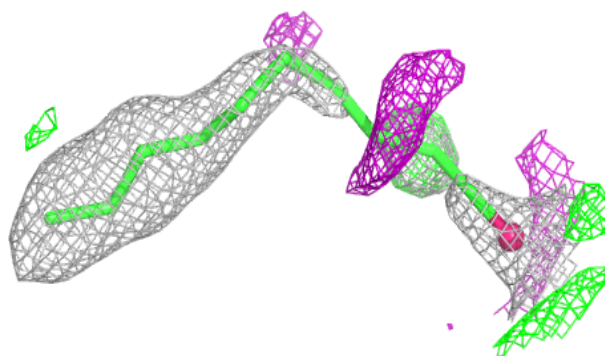


Electron density around TGL N 612:

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

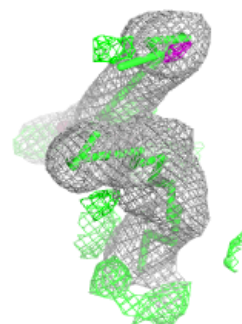
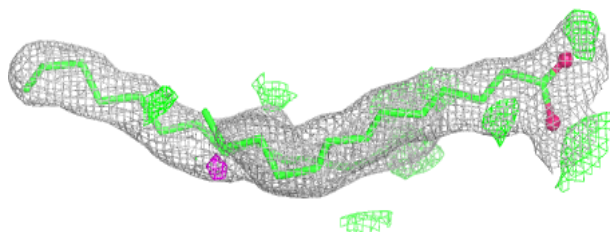
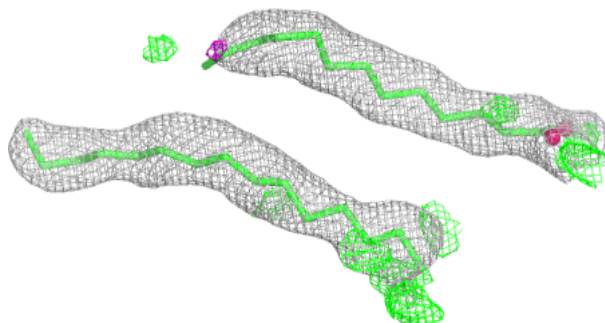
**Electron density around DMU P 309:**

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

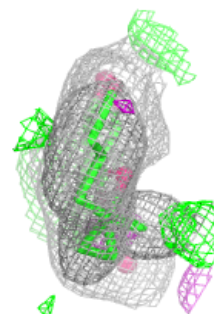
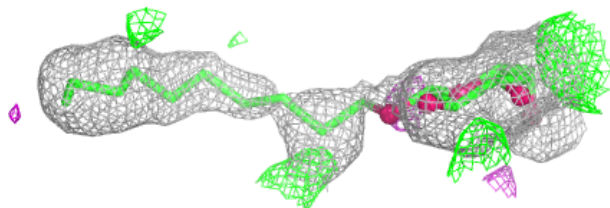
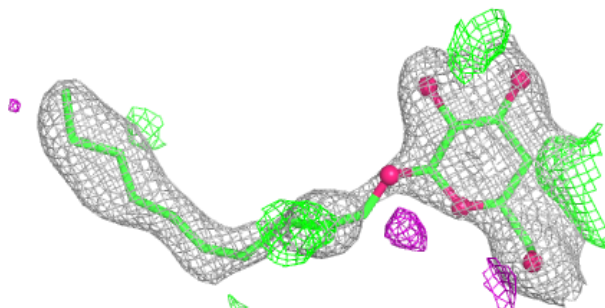


Electron density around PSC O 303:

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

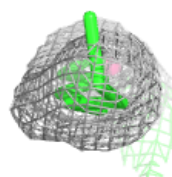
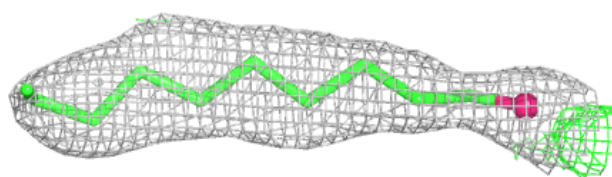
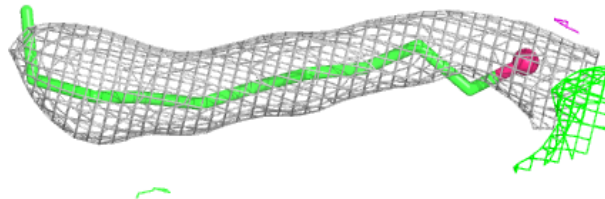
**Electron density around DMU C 310:**

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

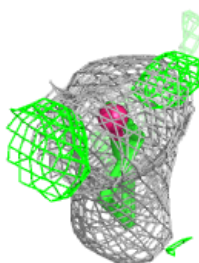
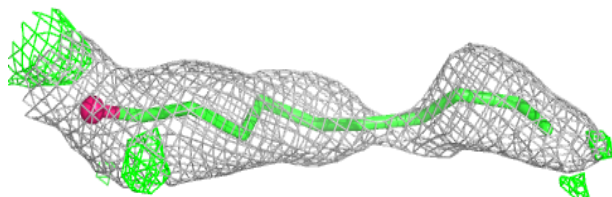
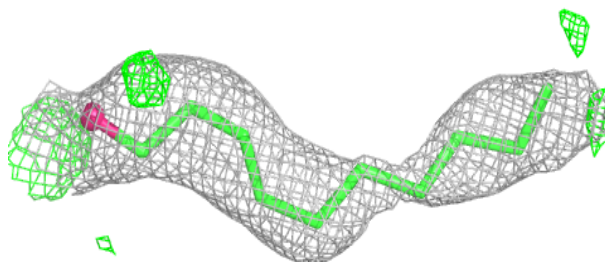


Electron density around DMU W 101:

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

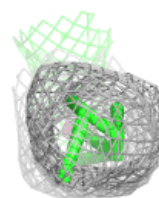
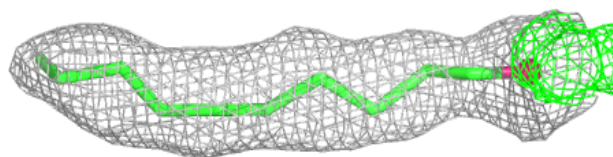
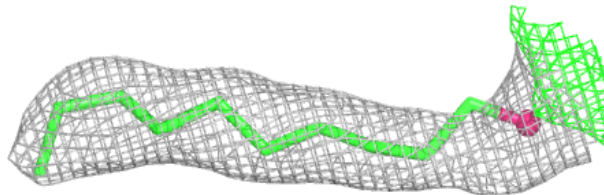
**Electron density around DMU D 201:**

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

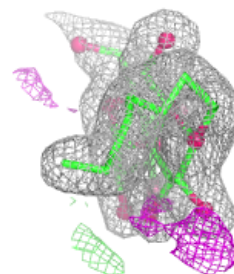
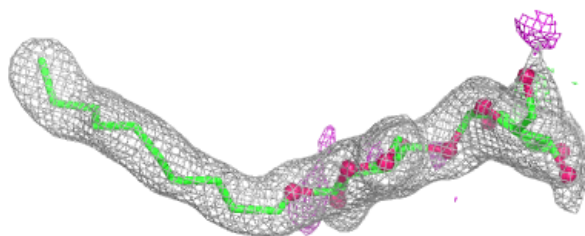
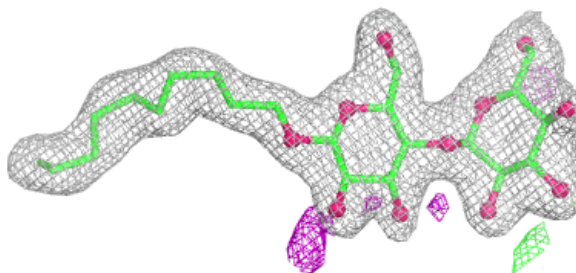


Electron density around DMU J 101:

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

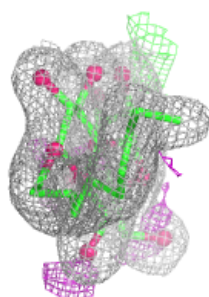
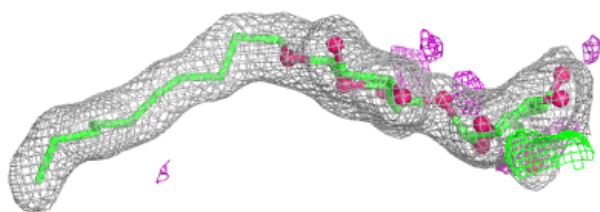
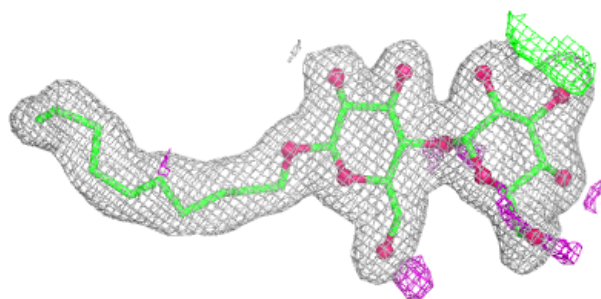
**Electron density around DMU Z 101:**

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

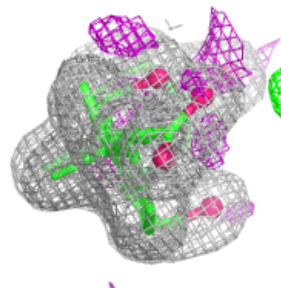
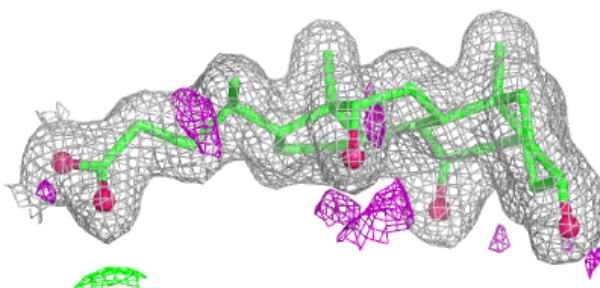
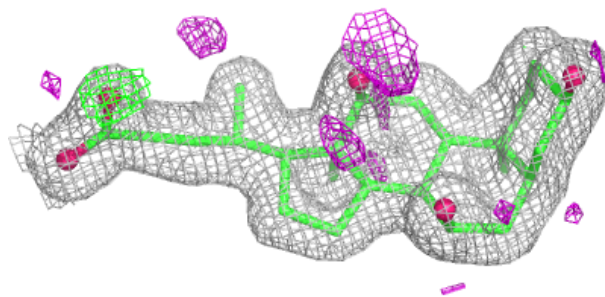


Electron density around DMU M 101:

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

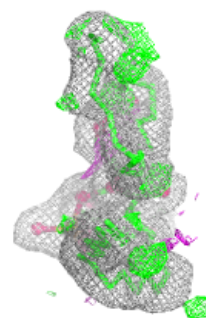
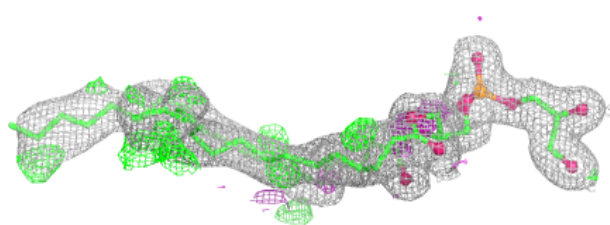
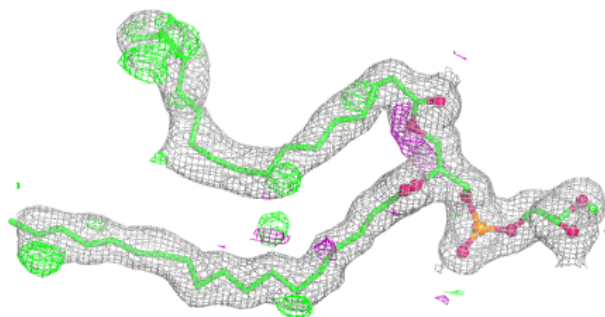
**Electron density around CHD C 304:**

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

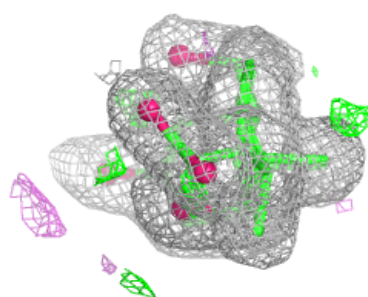
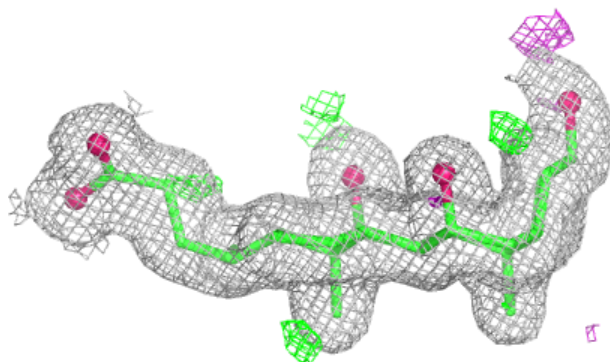
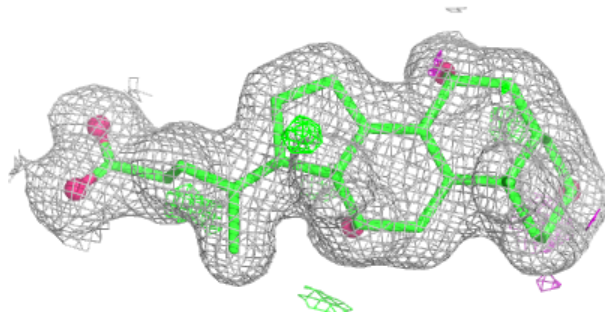


Electron density around PGV N 608:

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

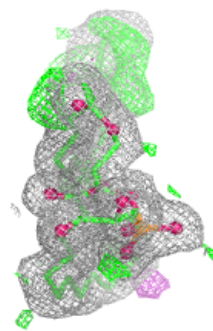
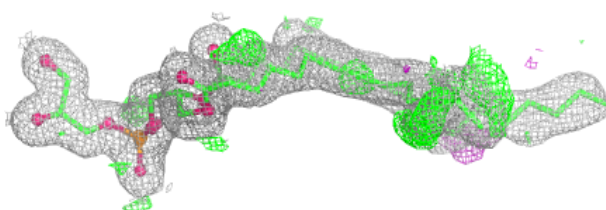
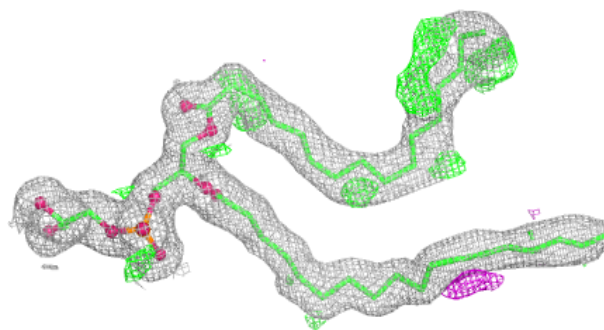
**Electron density around CHD B 303:**

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

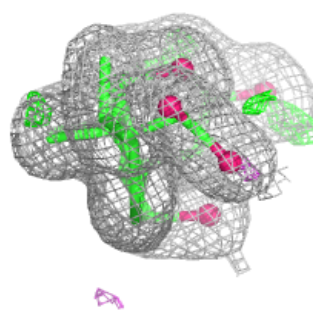
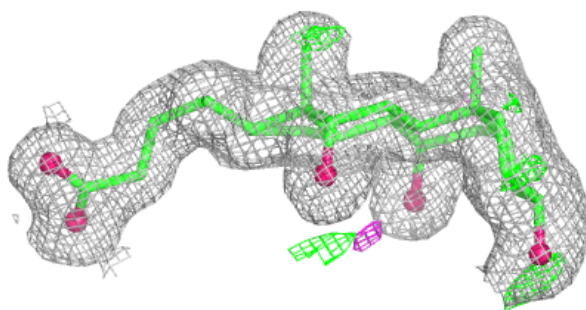
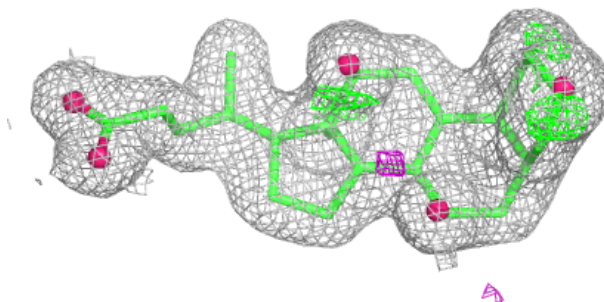


Electron density around PGV C 301:

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

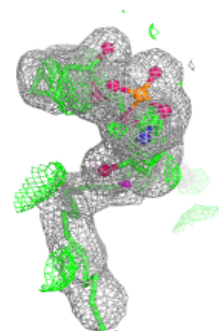
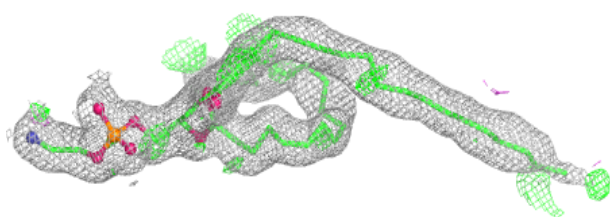
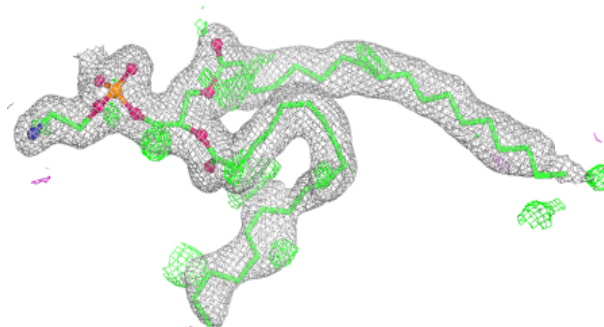
**Electron density around CHD G 101:**

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

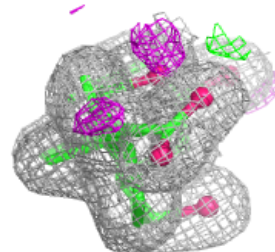
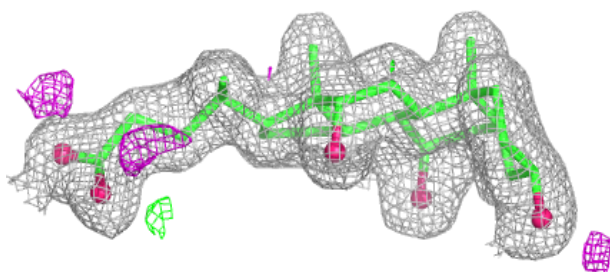
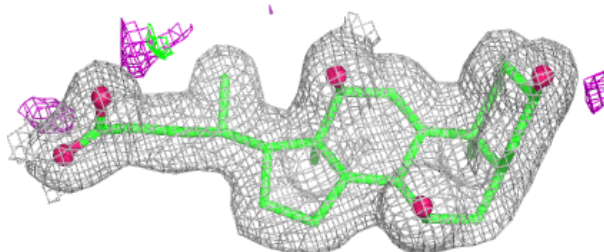


Electron density around PEK C 307:

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

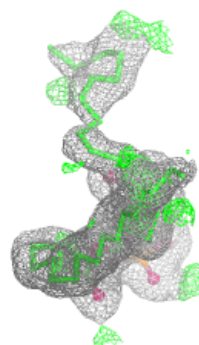
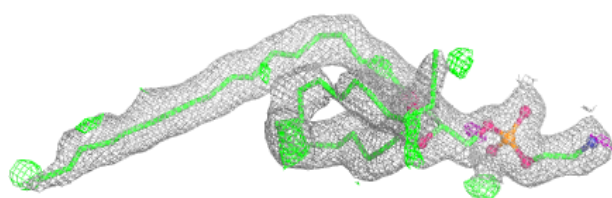
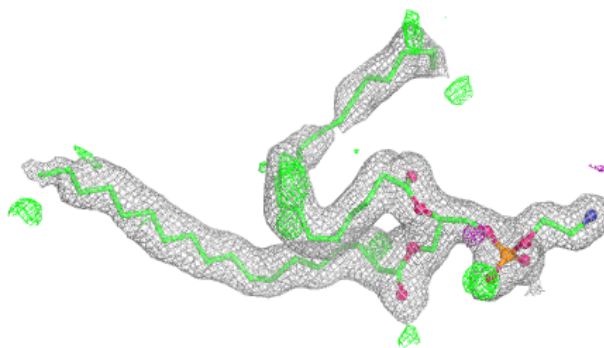
**Electron density around CHD P 301:**

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

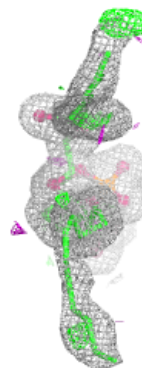
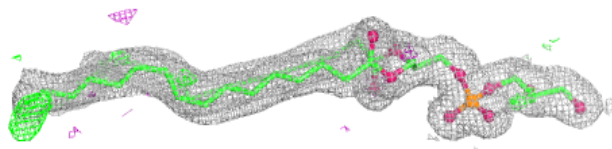
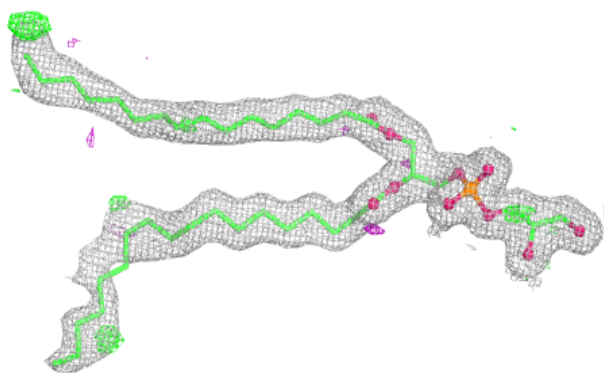


Electron density around PEK P 306:

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

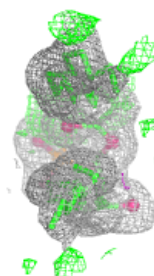
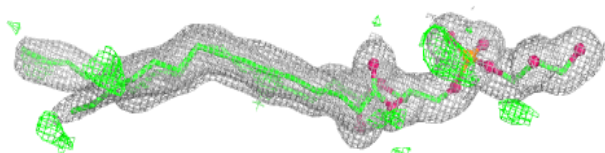
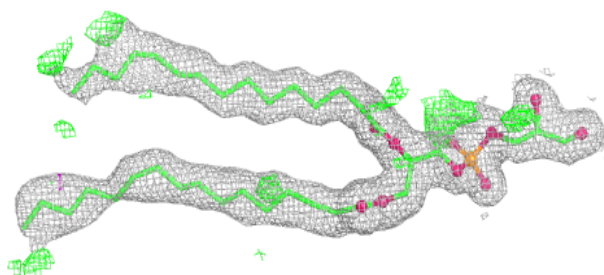
**Electron density around PGV P 307:**

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

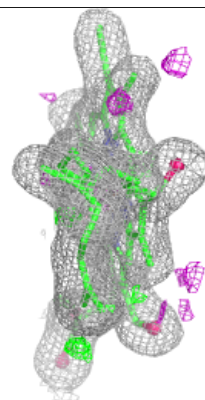
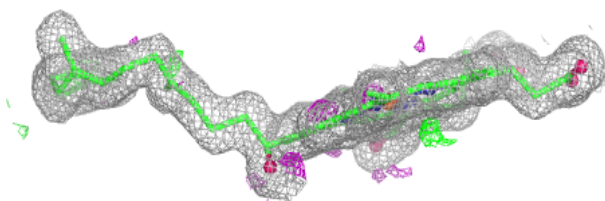
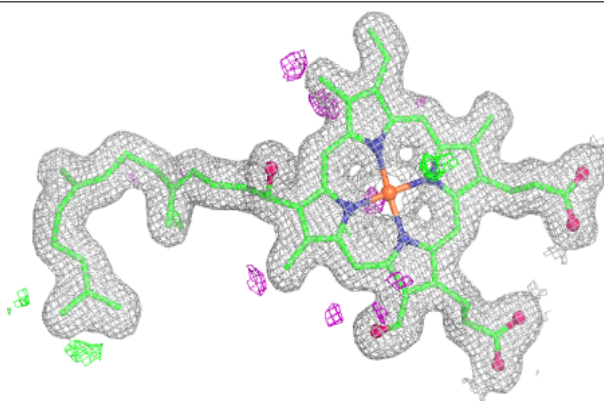


Electron density around PGV C 308:

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

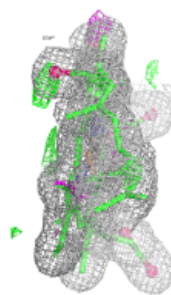
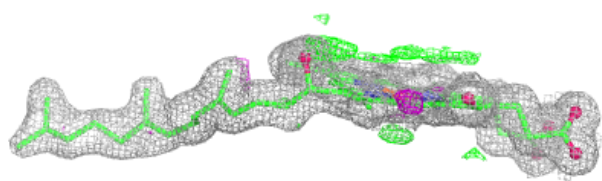
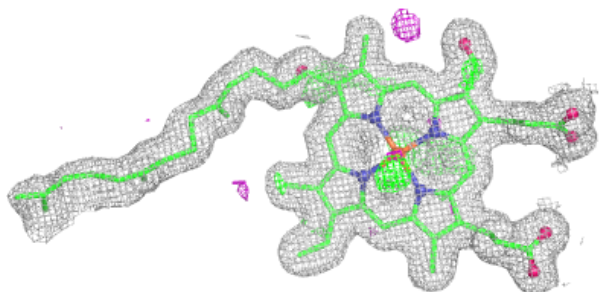
**Electron density around HEA A 602:**

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

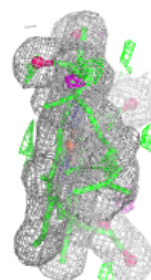
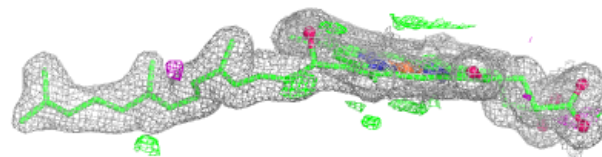
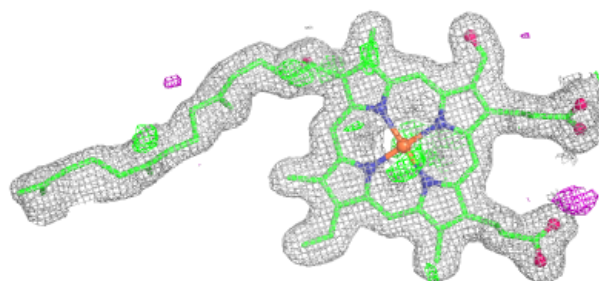


Electron density around HEA A 601 (A):

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

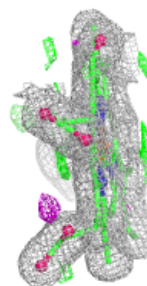
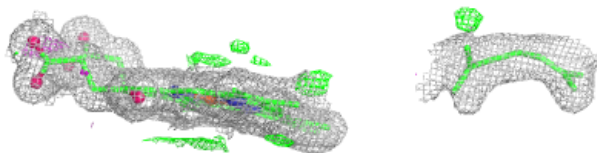
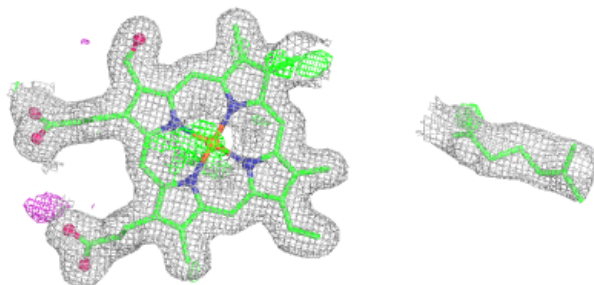
**Electron density around HEA N 602 (A):**

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

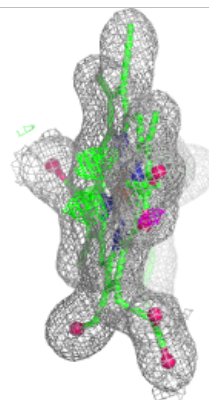
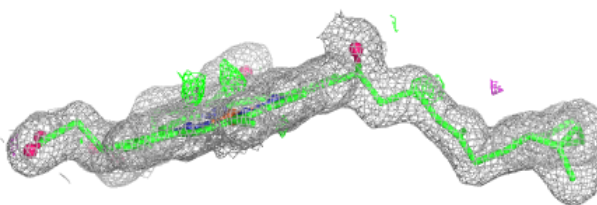
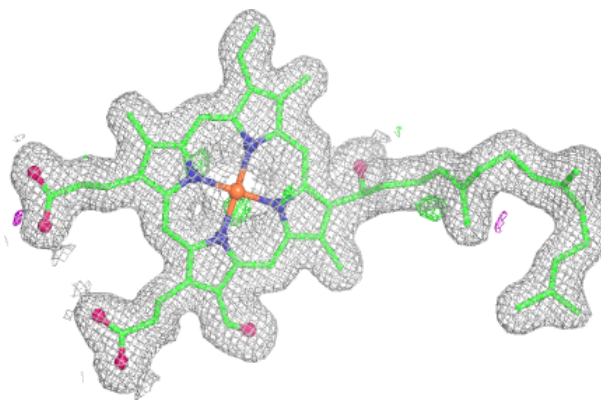


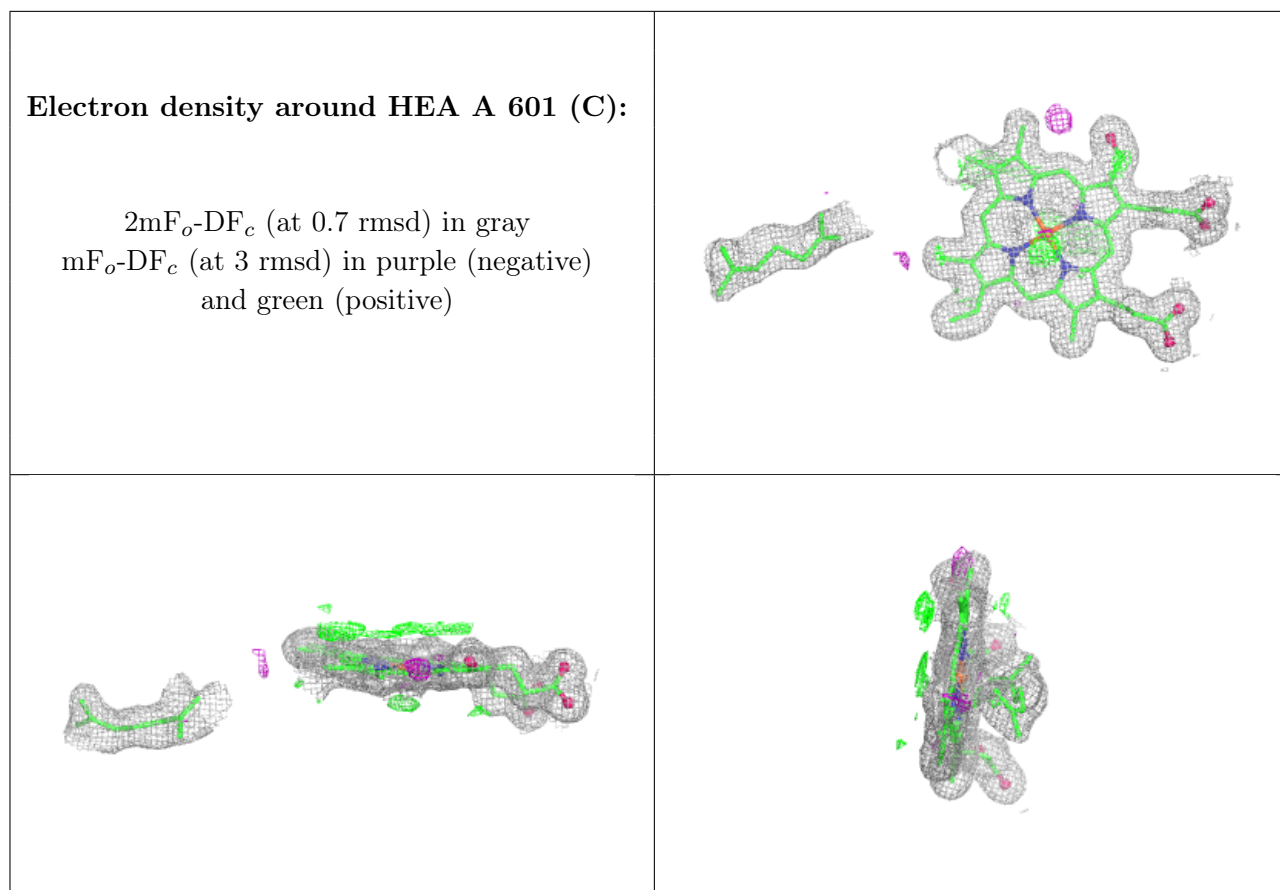
Electron density around HEA N 602 (C):

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

**Electron density around HEA N 603:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.