



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:28 AM UTC

PDB ID : 7D5W / pdb_00007d5w
Title : Bovine heart cytochrome c oxidase in a catalytic intermediate of O at 1.84 angstrom resolution
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2020-09-28
Resolution : 1.84 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

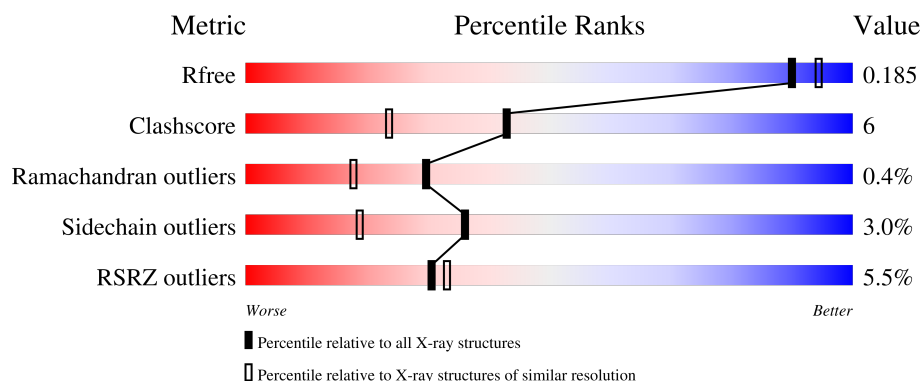
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	
1	N	514	
2	B	227	
2	O	227	
3	C	259	

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Mol	Chain	Length	Quality of chain
3	P	259	88% 12%
4	D	144	89% 10%
4	Q	144	89% 8%
5	E	105	98%
5	R	105	93% 7%
6	F	94	85% 13%
6	S	94	88% 12%
7	G	84	82% 14%
7	T	84	83% 13%
8	H	79	84% 11%
8	U	79	85% 11%
9	I	73	95% 5%
9	V	73	90% 10%
10	J	58	93% 7%
10	W	58	83% 17%
11	K	49	86% 14%
11	X	49	92% 8%
12	L	46	70% 30%
12	Y	46	85% 13%
13	M	43	91% 7%
13	Z	43	84% 16%

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 34545 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	34	0
			4193	2793	646	714	40			
1	N	514	Total	C	N	O	S	0	38	0
			4199	2799	644	714	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	8	0
			1851	1202	281	347	21			
2	O	227	Total	C	N	O	S	0	12	0
			1872	1217	288	346	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	11	0
			2144	1430	340	359	15			
3	P	259	Total	C	N	O	S	0	11	0
			2143	1431	341	357	14			

- 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
			1209	788	199	218	4			
4	Q	144	Total	C	N	O	S	0	1	0
			1197	779	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
			858	547	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
			731	451	129	145	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	5	0
			690	445	130	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
			665	418	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
			605	392	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
			462	297	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
			390	254	65	69	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

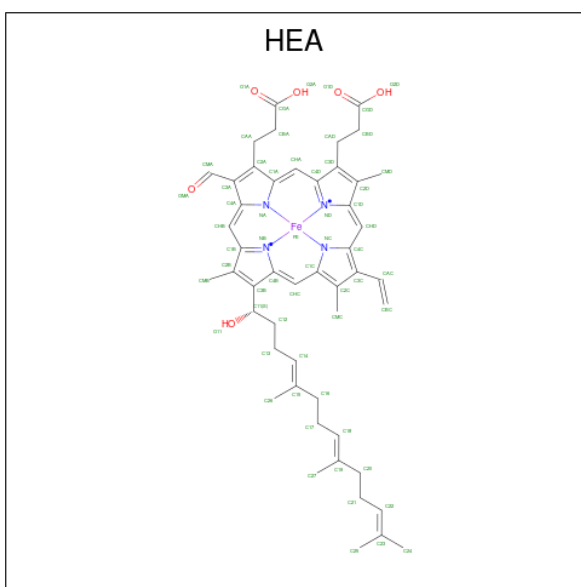
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	2	0
			386	259	64	60	3			
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 81	C 69	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 81	C 69	Fe 1	N 4	O 7	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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

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

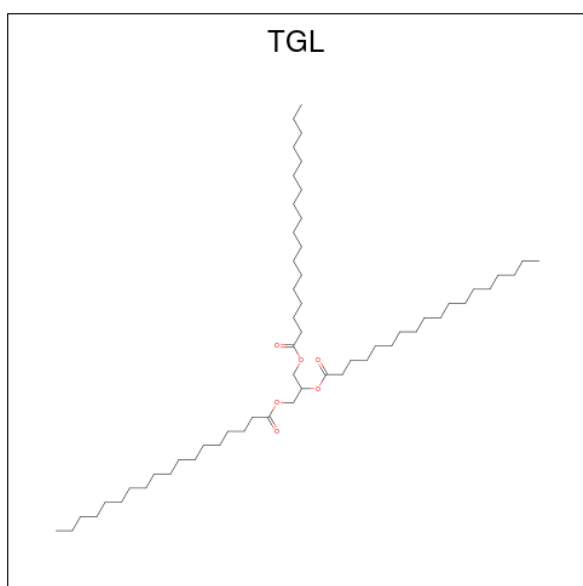
- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

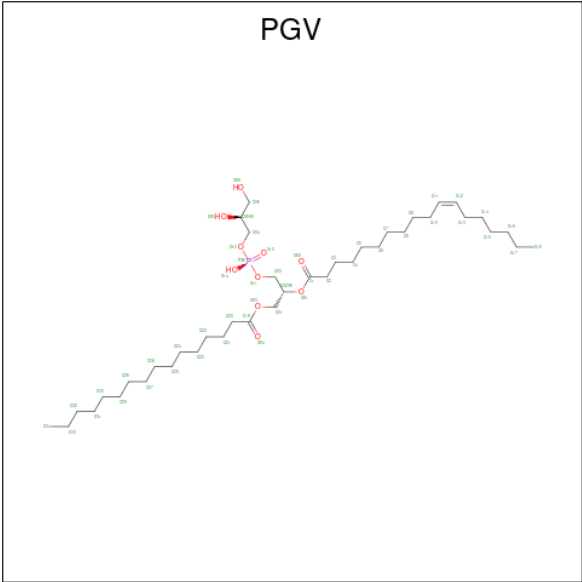
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



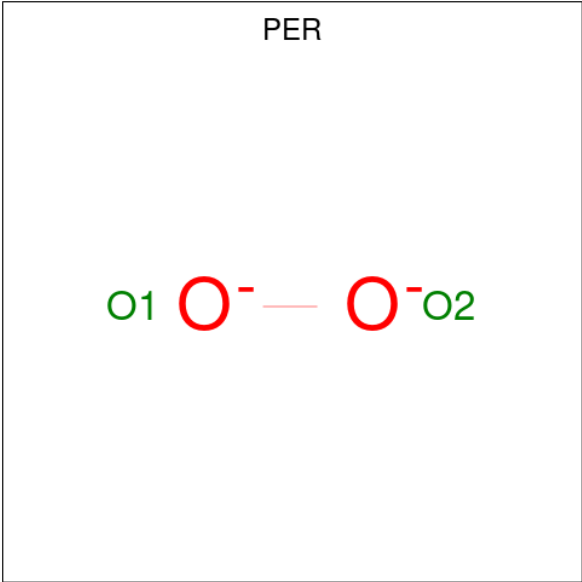
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	A	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			55	53	2		
18	N	1	Total	C	O	0	0
			55	53	2		

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



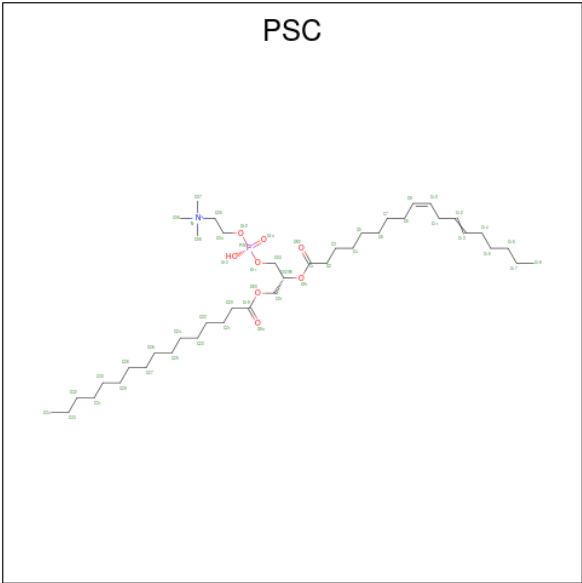
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	A	1	Total C O 34 32 2	0	0
19	A	1	Total C O P 51 40 10 1	0	0
19	C	1	Total C O P 48 37 10 1	0	0
19	C	1	Total C O 36 32 4	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	N	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O P 51 40 10 1	0	0
19	P	1	Total C O 31 29 2	0	0

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



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

- Molecule 21 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



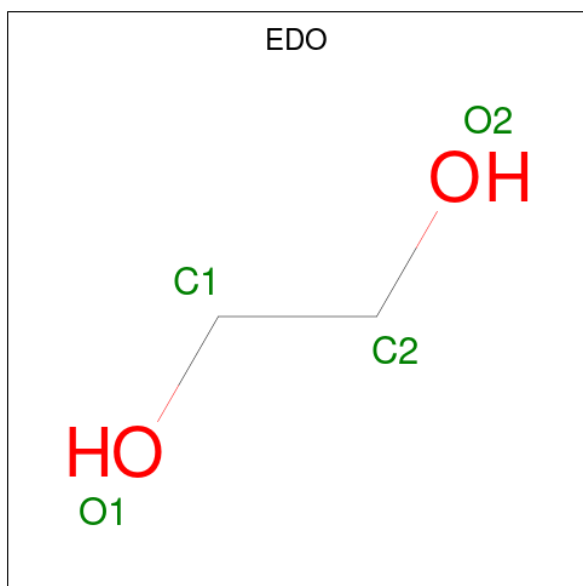
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total C 25 25	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	O	1	Total	C	O	0	0
			31	29	2		

- Molecule 22 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	E	1	Total 4	C 2	O 2	0	0
22	E	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	F	1	Total 4	C 2	O 2	0	0
22	G	1	Total 4	C 2	O 2	0	0
22	J	1	Total 4	C 2	O 2	0	0
22	J	1	Total 4	C 2	O 2	0	0
22	L	1	Total 4	C 2	O 2	0	0
22	L	1	Total 4	C 2	O 2	0	0
22	M	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0
22	N	1	Total 4	C 2	O 2	0	0

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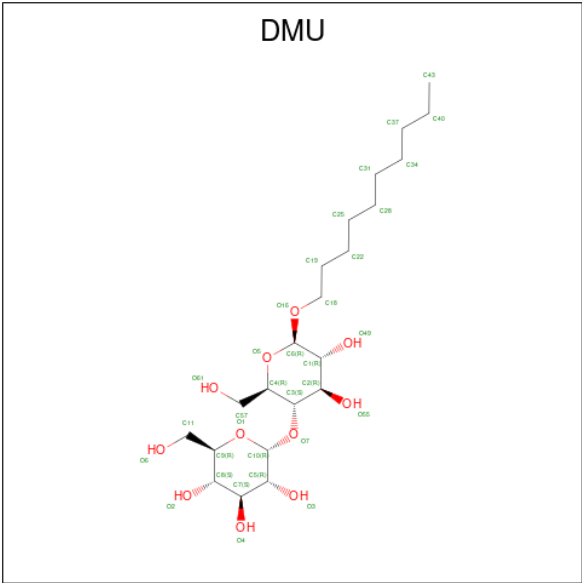
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	N	1	Total	C	O	0	0
			4	2	2		
22	O	1	Total	C	O	0	0
			4	2	2		
22	O	1	Total	C	O	0	0
			4	2	2		
22	O	1	Total	C	O	0	0
			4	2	2		
22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

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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



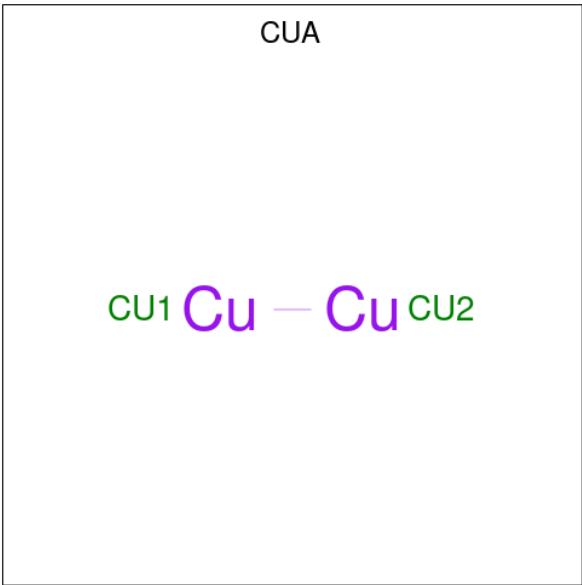
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			11	10	1		
23	C	1	Total	C	O	0	0
			33	22	11		
23	C	1	Total	C	O	0	0
			12	11	1		
23	D	1	Total	C	O	0	0
			33	22	11		

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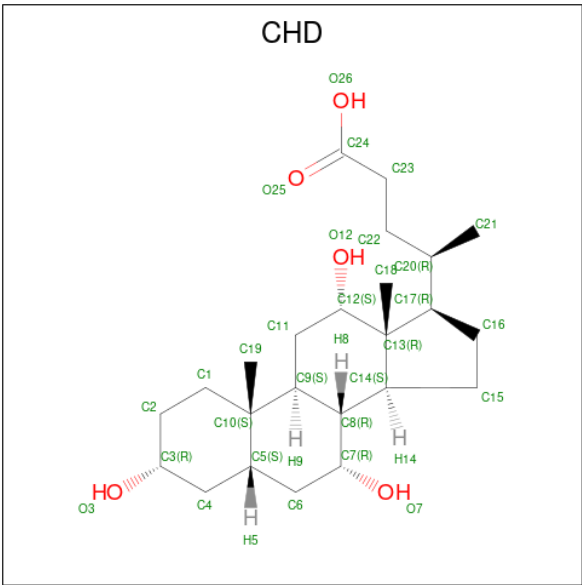
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	D	1	Total C O 11 10 1	0	0
23	J	1	Total C O 11 10 1	0	0
23	K	1	Total C 8 8	0	0
23	K	1	Total C O 11 10 1	0	0
23	K	1	Total C 10 10	0	0
23	K	1	Total C O 11 10 1	0	0
23	K	1	Total C 9 9	0	0
23	L	1	Total C O 21 16 5	0	0
23	M	1	Total C O 33 22 11	0	0
23	O	1	Total C O 13 11 2	0	0
23	P	1	Total C O 33 22 11	0	0
23	P	1	Total C O 21 16 5	0	0
23	P	1	Total C O 32 21 11	0	0
23	Q	1	Total C O 11 10 1	0	0
23	X	1	Total C 10 10	0	0
23	X	1	Total C 9 9	0	0
23	X	1	Total C 9 9	0	0
23	X	1	Total C O 22 16 6	0	0
23	Z	1	Total C O 33 22 11	0	0

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



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

- Molecule 25 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



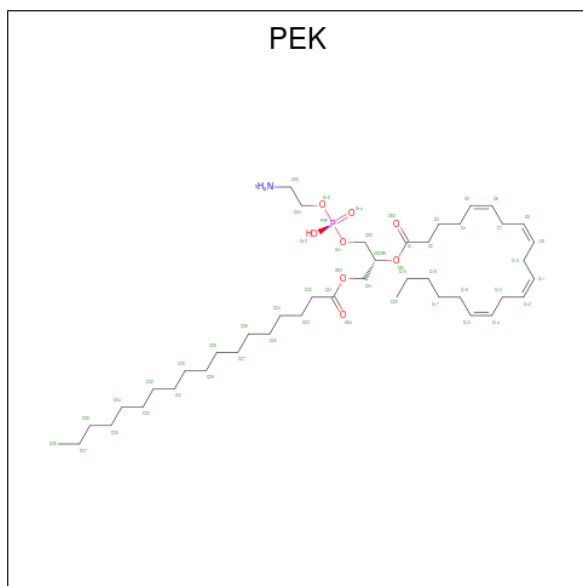
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	B	1	Total	C	O	0
			29	24	5	
25	C	1	Total	C	O	0
			29	24	5	

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

- Molecule 26 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).



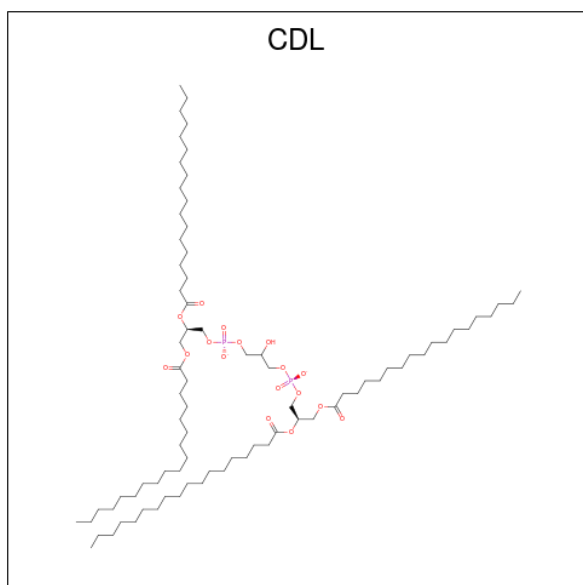
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	C	1	Total	C	N	O	P	0	0
			45	35	1	8	1		
26	C	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	C	1	Total	C				0	0
			36	36					
26	P	1	Total	C	N	O	P	0	0
			38	28	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	P	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	T	1	Total	C	O			0	0
			37	35	2				

- Molecule 27 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

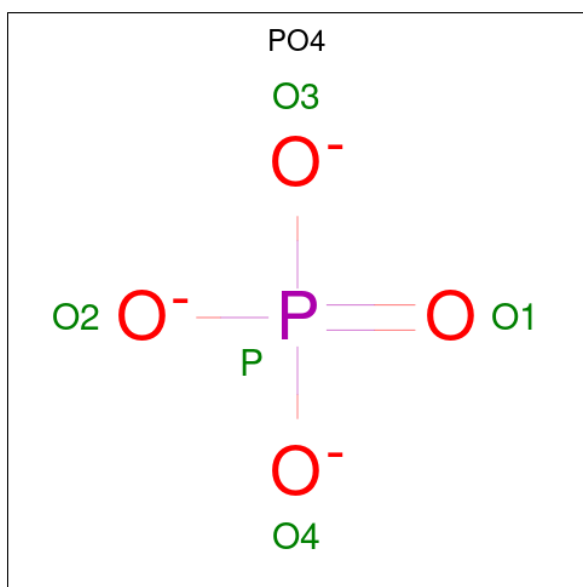


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			65	61	4		
27	N	1	Total	C	O	0	0
			62	60	2		
27	P	1	Total	C	O	0	0
			68	64	4		
27	T	1	Total	C	O	0	0
			61	59	2		

- 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	274	Total	O	0	14
			274	274		
30	B	229	Total	O	0	4
			229	229		
30	C	153	Total	O	0	0
			153	153		
30	D	206	Total	O	0	2
			207	207		
30	E	162	Total	O	0	0
			162	162		
30	F	161	Total	O	0	0
			161	161		
30	G	87	Total	O	0	0
			87	87		
30	H	92	Total	O	0	0
			92	92		
30	I	71	Total	O	0	0
			71	71		
30	J	61	Total	O	0	0
			61	61		

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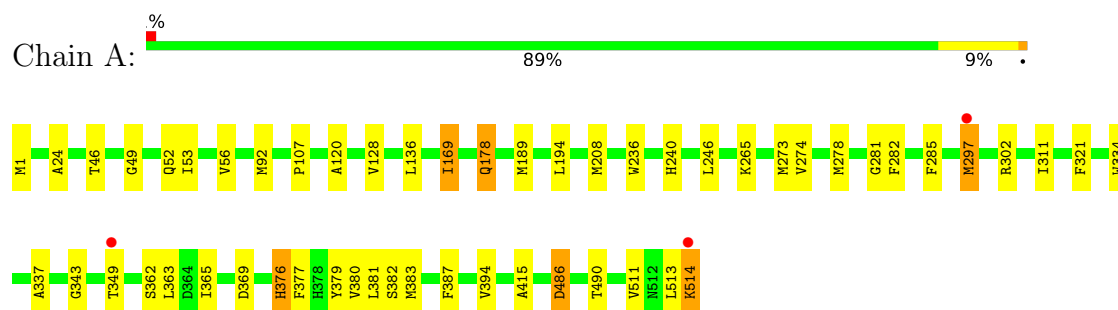
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	45	Total 45	O 45	0	0
30	L	40	Total 40	O 40	0	1
30	M	37	Total 37	O 37	0	0
30	N	282	Total 282	O 282	0	10
30	O	199	Total 199	O 199	0	2
30	P	161	Total 161	O 161	0	3
30	Q	119	Total 119	O 119	0	0
30	R	112	Total 113	O 113	0	1
30	S	141	Total 141	O 141	0	0
30	T	66	Total 66	O 66	0	0
30	U	96	Total 96	O 96	0	0
30	V	65	Total 66	O 66	0	1
30	W	41	Total 41	O 41	0	0
30	X	33	Total 33	O 33	0	0
30	Y	31	Total 31	O 31	0	1
30	Z	28	Total 28	O 28	0	0

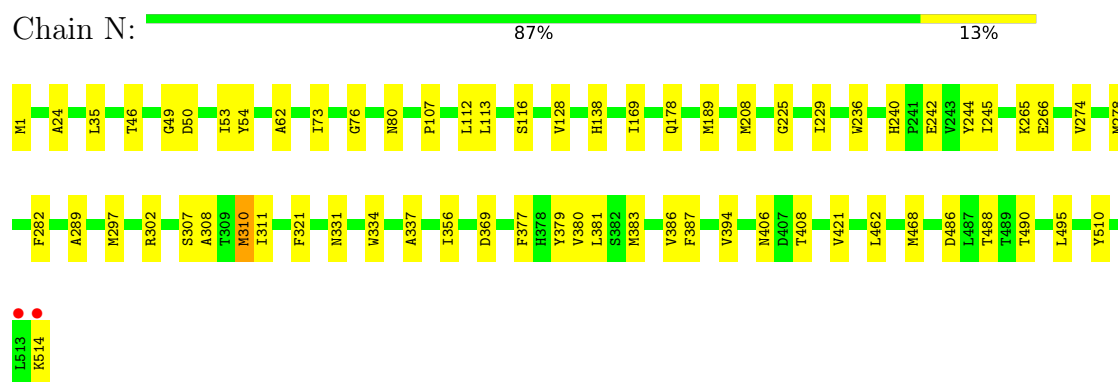
3 Residue-property plots [i](#)

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

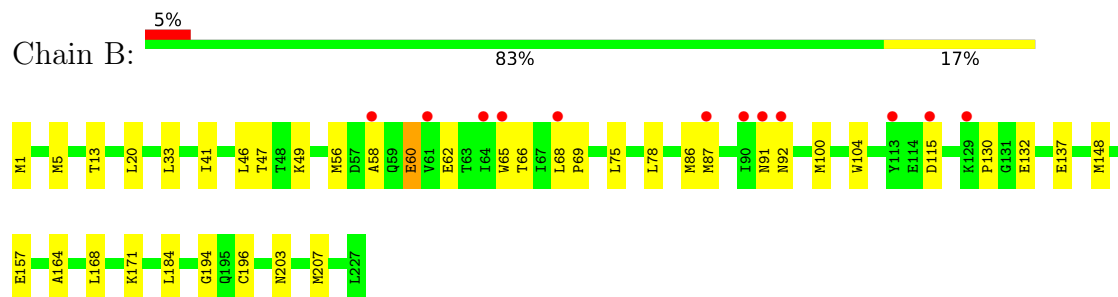
- Molecule 1: Cytochrome c oxidase subunit 1



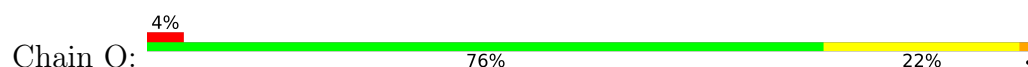
- Molecule 1: Cytochrome c oxidase subunit 1

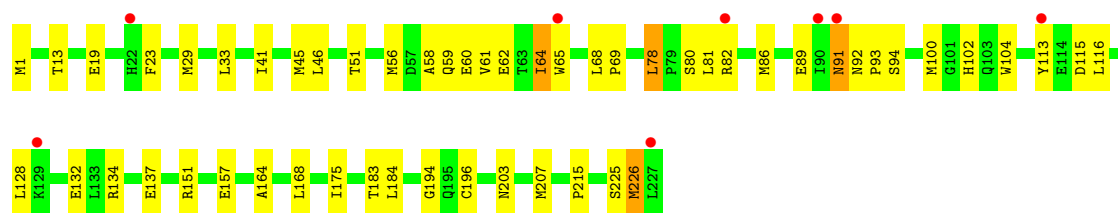


- Molecule 2: Cytochrome c oxidase subunit 2



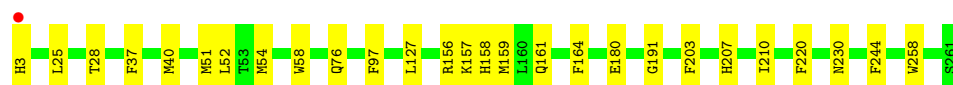
- Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 90% 10%



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 88% 12%



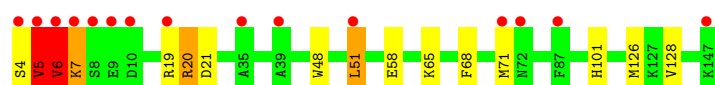
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 89% 10% 3%



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

Chain Q: 89% 8% 10%

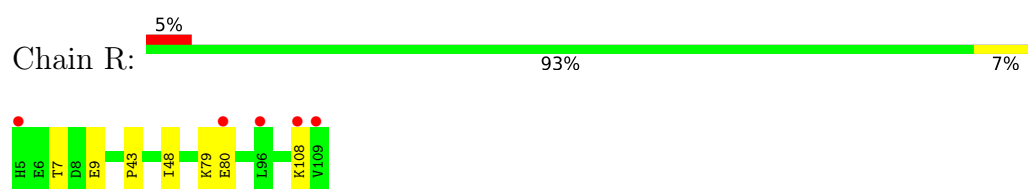


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

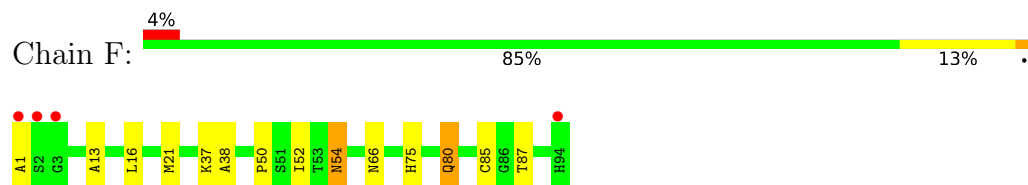
Chain E: 98% 3% 2%



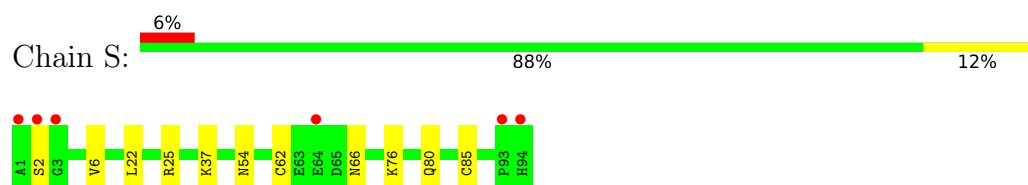
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



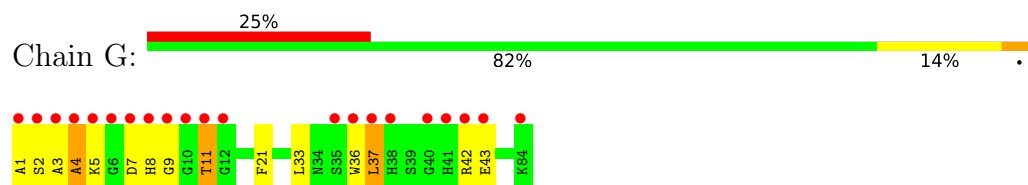
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



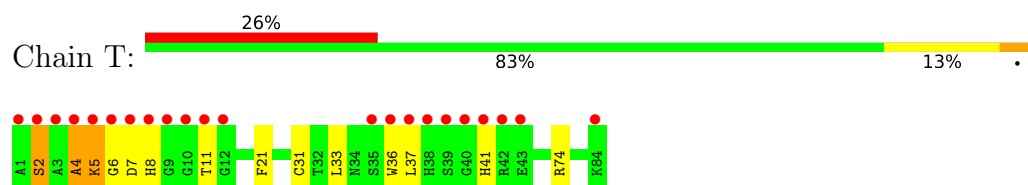
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



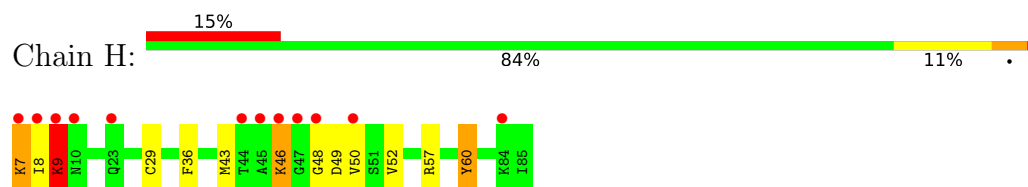
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



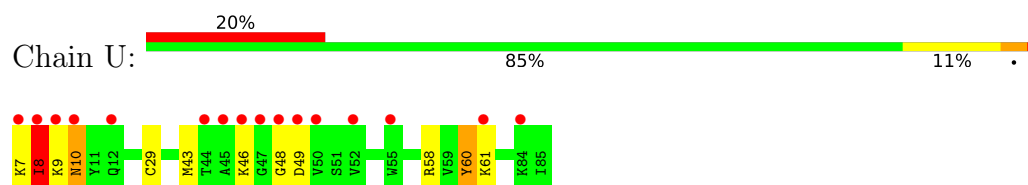
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



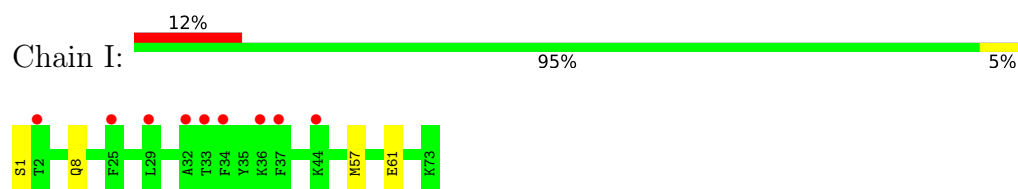
- Molecule 8: Cytochrome c oxidase subunit 6B1



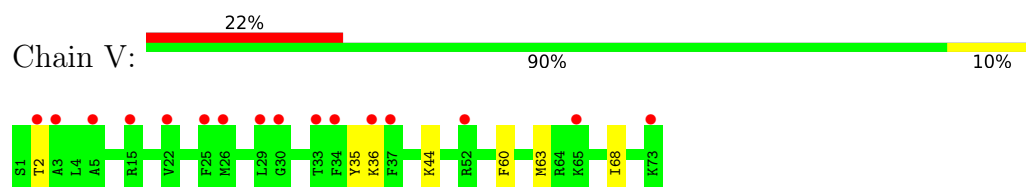
- Molecule 8: Cytochrome c oxidase subunit 6B1



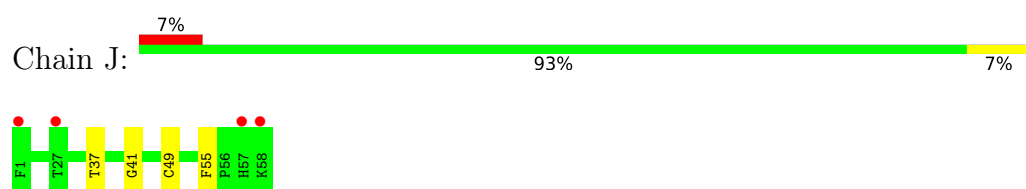
- Molecule 9: Cytochrome c oxidase subunit 6C



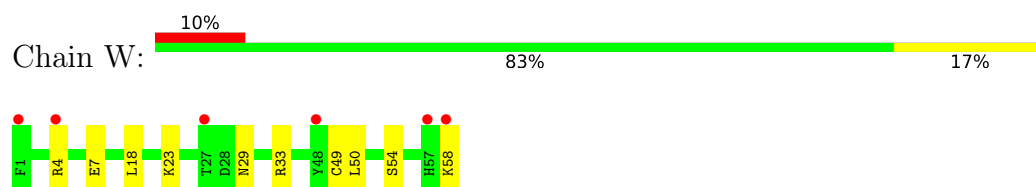
- Molecule 9: Cytochrome c oxidase subunit 6C



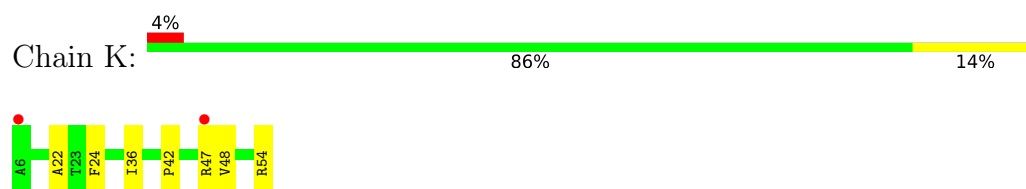
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



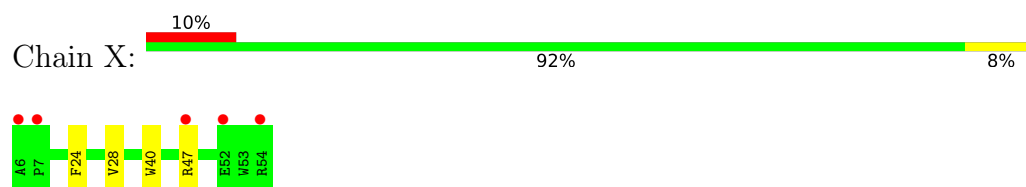
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



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

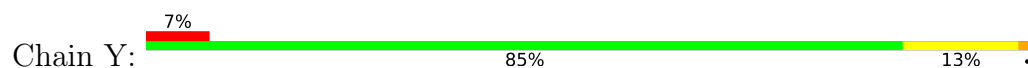


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

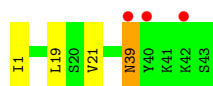




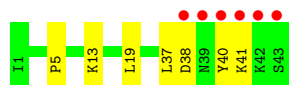
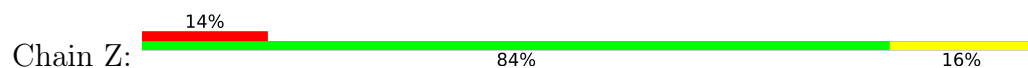
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.44Å 203.09Å 177.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 1.84 39.91 – 1.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-1.84) 99.8 (39.91-1.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.154 , 0.184 0.156 , 0.185	Depositor DCC
R_{free} test set	28294 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.805	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	34545	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PSC, PGV, PO4, NA, FME, DMU, CUA, HEA, PEK, TGL, PER, SAC, MG, CDL, CU, ZN, CHD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.76	0/4432	0.79	6/6043 (0.1%)
1	N	0.70	0/4457	0.75	3/6082 (0.0%)
2	B	0.65	0/1928	0.81	0/2623
2	O	0.56	0/1973	0.75	0/2686
3	C	0.65	0/2288	0.68	0/3125
3	P	0.62	0/2287	0.66	0/3124
4	D	0.60	0/1259	0.69	0/1698
4	Q	0.42	0/1236	0.58	0/1668
5	E	0.55	0/871	0.65	0/1182
5	R	0.46	0/882	0.58	0/1196
6	F	0.63	0/773	0.73	0/1048
6	S	0.65	0/732	0.74	0/993
7	G	0.58	0/743	0.74	0/1009
7	T	0.51	0/699	0.72	0/950
8	H	0.55	0/690	0.70	0/932
8	U	0.51	0/682	0.70	0/921
9	I	0.44	0/614	0.61	0/814
9	V	0.41	0/605	0.59	0/802
10	J	0.46	0/478	0.60	0/644
10	W	0.43	0/472	0.57	0/636
11	K	0.52	0/419	0.65	0/574
11	X	0.43	0/398	0.59	0/544
12	L	0.61	0/409	0.65	0/547
12	Y	0.51	0/393	0.65	0/526
13	M	0.63	0/346	0.63	0/470
13	Z	0.46	0/345	0.60	0/470
All	All	0.62	0/30411	0.71	9/41307 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-6.41	107.39	113.80
1	A	189	MET	CG-SD-CE	-5.91	87.90	100.90
1	A	240	HIS	CA-CB-CG	-5.80	108.00	113.80
1	N	310	MET	CG-SD-CE	-5.68	88.41	100.90
1	A	376	HIS	CA-C-N	-5.45	111.59	121.14
1	A	376	HIS	C-N-CA	-5.45	111.59	121.14
1	A	511	VAL	CA-C-N	-5.13	113.79	122.67
1	A	511	VAL	C-N-CA	-5.13	113.79	122.67
1	N	244	TYR	CA-CB-CG	-5.13	104.67	113.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4193	0	4162	55	0
1	N	4199	0	4190	61	0
2	B	1851	0	1858	25	0
2	O	1872	0	1876	31	0
3	C	2144	0	2062	27	0
3	P	2143	0	2069	28	0
4	D	1209	0	1202	17	0
4	Q	1197	0	1188	12	0
5	E	852	0	845	1	0
5	R	858	0	854	5	0
6	F	731	0	709	13	0
6	S	716	0	697	8	0
7	G	690	0	669	9	0
7	T	672	0	645	14	0
8	H	665	0	625	8	0
8	U	662	0	623	9	0
9	I	605	0	615	2	0
9	V	601	0	613	5	0
10	J	462	0	460	5	0
10	W	461	0	459	5	0
11	K	390	0	377	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	X	384	0	366	3	0
12	L	386	0	392	20	0
12	Y	380	0	380	5	0
13	M	336	0	352	6	0
13	Z	335	0	352	5	0
14	A	141	0	115	7	0
14	N	141	0	115	8	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	126	0	220	18	0
18	L	63	0	110	15	0
18	N	173	0	312	11	0
19	A	85	0	136	2	0
19	C	84	0	121	4	0
19	N	102	0	152	4	0
19	P	82	0	130	4	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	A	25	0	44	3	0
21	O	31	0	52	4	0
22	A	44	0	66	6	0
22	B	16	0	24	0	0
22	C	40	0	60	2	0
22	D	20	0	30	5	0
22	E	12	0	18	0	0
22	F	32	0	48	0	0
22	G	4	0	6	0	0
22	J	8	0	12	0	0
22	L	8	0	12	0	0
22	M	4	0	6	0	0
22	N	40	0	60	2	0
22	O	12	0	18	0	0
22	P	28	0	42	0	0
22	Q	4	0	6	0	0
22	S	24	0	36	1	0
22	T	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	8	0	12	0	0
22	Y	4	0	6	1	0
23	A	11	0	21	0	0
23	C	45	0	63	3	0
23	D	44	0	63	3	0
23	J	11	0	21	1	0
23	K	49	0	93	2	0
23	L	21	0	30	6	0
23	M	33	0	42	2	0
23	O	13	0	21	0	0
23	P	86	0	109	5	0
23	Q	11	0	21	2	0
23	X	50	0	84	2	0
23	Z	33	0	42	1	0
24	B	2	0	0	0	0
24	O	2	0	0	0	0
25	B	29	0	39	0	0
25	C	58	0	78	2	0
25	G	29	0	39	1	0
25	J	29	0	39	2	0
25	L	29	0	39	2	0
25	P	29	0	39	0	0
25	Y	29	0	39	0	0
26	C	133	0	192	7	0
26	P	90	0	116	2	0
26	T	37	0	59	6	0
27	C	65	0	113	8	0
27	N	62	0	109	5	0
27	P	68	0	119	7	0
27	T	61	0	110	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	274	0	0	7	0
30	B	229	0	0	1	0
30	C	153	0	0	5	0
30	D	207	0	0	1	0
30	E	162	0	0	0	0
30	F	161	0	0	2	0
30	G	87	0	0	1	0
30	H	92	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	71	0	0	1	0
30	J	61	0	0	0	0
30	K	45	0	0	0	0
30	L	40	0	0	2	0
30	M	37	0	0	0	0
30	N	282	0	0	7	0
30	O	199	0	0	1	0
30	P	161	0	0	0	0
30	Q	119	0	0	2	0
30	R	113	0	0	1	0
30	S	141	0	0	2	0
30	T	66	0	0	1	0
30	U	96	0	0	1	0
30	V	66	0	0	0	0
30	W	41	0	0	0	0
30	X	33	0	0	0	0
30	Y	31	0	0	0	0
30	Z	28	0	0	0	0
All	All	34545	0	32367	394	0

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

All (394) 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:A:609[A]:PER:O2	20:A:609[A]:PER:O1	1.55	1.24
20:N:611[A]:PER:O2	20:N:611[A]:PER:O1	1.55	1.21
12:L:20:ARG:HH22	18:L:101:TGL:HC52	1.31	0.95
1:N:113:LEU:HB2	18:N:608:TGL:H301	1.58	0.85
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.16	0.85
23:P:308:DMU:H9	10:W:49:CYS:HB3	1.57	0.85
18:A:607:TGL:HB21	4:D:78:TRP:HB3	1.57	0.84
1:A:178[B]:GLN:NE2	7:T:7:ASP:O	2.10	0.84
8:H:7:LYS:HD2	8:H:8:ILE:HG23	1.63	0.80
12:L:20:ARG:HH12	18:L:101:TGL:HC32	1.46	0.79
1:N:510:TYR:HA	22:N:621:EDO:H12	1.69	0.74
19:A:608:PGV:H311	13:M:19:LEU:HD23	1.71	0.73
27:C:308:CDL:H322	27:C:308:CDL:H471	1.70	0.72
13:M:39:ASN:HD22	13:M:39:ASN:H	1.38	0.72
27:T:102:CDL:H531	27:T:102:CDL:H251	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:304:PEK:H101	26:C:304:PEK:H42	1.72	0.69
1:A:194:LEU:HD11	7:T:4:ALA:HB1	1.75	0.69
12:L:14:SER:H	18:L:101:TGL:HC31	1.58	0.68
3:P:62:ILE:HD12	27:P:307:CDL:H522	1.77	0.67
5:R:80:GLU:N	5:R:80:GLU:OE1	2.28	0.67
27:P:307:CDL:H521	27:P:307:CDL:HB62	1.77	0.67
26:P:304:PEK:H101	26:P:304:PEK:H42	1.76	0.66
12:L:20:ARG:NH2	18:L:101:TGL:HC52	2.06	0.66
18:L:101:TGL:OC1	18:L:101:TGL:HC41	1.95	0.66
19:C:307:PGV:H21	19:C:307:PGV:H71	1.77	0.65
7:T:74:ARG:NH1	30:T:201:HOH:O	2.29	0.65
22:A:616:EDO:H22	30:A:912:HOH:O	1.97	0.65
2:B:100[B]:MET:HG2	2:B:157:GLU:HG3	1.78	0.65
18:A:607:TGL:HC71	2:B:49:LYS:HE3	1.80	0.64
12:L:25:MET:HG2	18:L:101:TGL:HA62	1.79	0.64
1:N:169:ILE:HG13	1:N:189[B]:MET:HE1	1.79	0.64
1:N:24:ALA:HB2	14:N:602[A]:HEA:H253	1.80	0.63
4:D:4:SER:HB2	22:D:204:EDO:O1	1.97	0.63
3:P:80[B]:ARG:NH2	3:P:236:GLU:OE1	2.31	0.63
3:P:34:TRP:HE1	23:P:316:DMU:H29	1.63	0.61
12:L:2:HIS:CG	12:L:3:TYR:H	2.18	0.61
13:M:39:ASN:H	13:M:39:ASN:ND2	1.99	0.61
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.83	0.61
3:P:33:MET:HE2	3:P:42:LEU:H	1.66	0.60
18:A:606:TGL:H322	18:A:606:TGL:H261	1.83	0.60
1:N:334:TRP:CD1	18:N:609:TGL:HC41	2.36	0.60
1:A:169:ILE:HG23	7:T:8:HIS:O	2.02	0.59
7:G:11:THR:HA	30:N:867:HOH:O	2.02	0.59
18:A:607:TGL:HA31	18:A:607:TGL:HB51	1.83	0.59
18:N:608:TGL:HC51	12:Y:20:ARG:NH2	2.17	0.59
27:T:102:CDL:H781	27:T:102:CDL:H561	1.83	0.59
7:G:37:LEU:HD23	27:N:601:CDL:H381	1.84	0.59
4:D:94:LEU:HB3	23:D:206:DMU:H18	1.85	0.59
7:G:1:ALA:HB2	19:P:306:PGV:H342	1.85	0.59
26:C:304:PEK:H14	30:C:535:HOH:O	2.03	0.59
9:I:8:GLN:HG2	30:I:140:HOH:O	2.02	0.59
1:N:514:LYS:OXT	6:S:37:LYS:NZ	2.34	0.59
3:C:203:PHE:CE1	26:C:304:PEK:H9	2.38	0.58
1:N:49[B]:GLY:HA3	13:Z:41:LYS:HE3	1.86	0.58
2:O:19:GLU:HG3	2:O:86[A]:MET:HE1	1.85	0.58
11:X:40:TRP:CD2	23:X:102:DMU:H14	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.86	0.58
6:F:54[A]:ASN:ND2	30:F:203:HOH:O	2.36	0.58
10:J:55:PHE:CE1	23:L:105:DMU:H29	2.39	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.85	0.57
1:N:35[B]:LEU:HD23	23:Z:101:DMU:H24	1.86	0.57
1:N:53[B]:ILE:HG12	30:N:895:HOH:O	2.04	0.57
1:N:308:ALA:O	1:N:311[A]:ILE:HG12	2.04	0.57
2:B:130:PRO:HB3	22:D:205:EDO:H21	1.85	0.57
3:C:127:LEU:HD22	27:N:601:CDL:HB61	1.87	0.57
1:N:297[C]:MET:HG2	1:N:302:ARG:HG3	1.85	0.57
12:L:24[B]:MET:HE1	18:L:101:TGL:HC81	1.87	0.56
1:A:194:LEU:CD1	7:T:4:ALA:HB1	2.35	0.56
3:P:168:THR:HG21	26:T:101:PEK:H12	1.87	0.56
30:C:411:HOH:O	6:F:52:ILE:HD11	2.05	0.56
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.88	0.56
4:Q:20:ARG:HG2	30:Q:386:HOH:O	2.05	0.56
1:N:274:VAL:HG12	1:N:278[A]:MET:HE2	1.87	0.56
1:A:321[A]:PHE:CD2	2:B:65:TRP:HB2	2.40	0.55
1:A:321[B]:PHE:CD1	21:A:610:PSC:H341	2.41	0.55
21:A:610:PSC:H242	2:B:56:MET:HB3	1.88	0.55
19:N:610:PGV:H311	13:Z:19:LEU:HD23	1.89	0.55
23:D:206:DMU:H29	11:K:36:ILE:HB	1.88	0.55
18:A:607:TGL:HC42	18:A:607:TGL:OG3	2.07	0.55
3:C:156:ARG:HE	25:C:309:CHD:C24	2.20	0.55
1:A:334:TRP:CD1	18:A:607:TGL:HC41	2.42	0.55
27:T:102:CDL:H561	27:T:102:CDL:H761	1.89	0.55
1:N:379:TYR:O	1:N:383[B]:MET:HB2	2.06	0.55
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.89	0.55
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.07	0.55
2:B:13:THR:HB	2:B:168:LEU:HD23	1.89	0.54
1:A:274:VAL:HG12	1:A:278[A]:MET:HE2	1.89	0.54
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.42	0.54
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.90	0.54
6:F:13:ALA:CB	6:F:21[B]:MET:HE1	2.37	0.54
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.88	0.54
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.90	0.54
19:N:612:PGV:H183	26:P:304:PEK:H342	1.90	0.54
1:N:331[B]:ASN:ND2	4:Q:21:ASP:HB3	2.22	0.53
1:A:278[B]:MET:HB3	7:T:5:LYS:HG2	1.90	0.53
3:C:210:ILE:HG12	19:C:306:PGV:H132	1.90	0.53
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24[B]:MET:SD	18:L:101:TGL:HC22	2.48	0.53
1:N:297[C]:MET:CG	1:N:302:ARG:HG3	2.38	0.53
7:T:41:HIS:HB3	7:T:74:ARG:NH2	2.24	0.53
1:N:514:LYS:HD2	30:S:278:HOH:O	2.07	0.53
26:T:101:PEK:H382	27:T:102:CDL:H273	1.91	0.53
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.90	0.53
1:N:113:LEU:HB2	18:N:608:TGL:C32	2.39	0.53
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.74	0.53
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.91	0.52
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.39	0.52
1:A:349:THR:OG1	1:A:349:THR:CA	2.57	0.52
1:N:488:THR:HB	1:N:495:LEU:HD13	1.91	0.52
4:D:120:THR:HG21	11:K:48[B]:VAL:CG1	2.40	0.52
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.91	0.52
10:J:41:GLY:HA3	23:J:104:DMU:H23	1.90	0.52
4:D:98:TRP:CE2	23:M:101:DMU:H11	2.44	0.52
3:C:52:LEU:HD21	27:C:308:CDL:H432	1.92	0.51
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.45	0.51
21:O:302:PSC:H111	21:O:302:PSC:H321	1.92	0.51
1:A:514[A]:LYS:HD2	30:A:731:HOH:O	2.11	0.51
30:A:787:HOH:O	12:L:7:PRO:HG3	2.09	0.51
1:A:379:TYR:O	1:A:383[B]:MET:HB2	2.11	0.51
27:N:601:CDL:H371	2:O:81:LEU:HD12	1.93	0.51
1:A:343:GLY:HA2	18:A:607:TGL:H212	1.93	0.50
1:A:53[A]:ILE:HD11	12:L:40:VAL:HG13	1.93	0.50
10:J:55:PHE:HE1	23:L:105:DMU:H29	1.75	0.50
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.94	0.50
4:D:86:MET:HE1	11:K:22:ALA:HB2	1.94	0.50
18:L:101:TGL:CC1	18:L:101:TGL:HC61	2.41	0.50
18:L:101:TGL:CC1	18:L:101:TGL:HG12	2.39	0.50
1:N:297[C]:MET:SD	1:N:302:ARG:HG3	2.51	0.50
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.91	0.50
1:A:46:THR:HG22	1:A:49[B]:GLY:H	1.77	0.50
26:C:305:PEK:H231	7:G:21:PHE:CD1	2.46	0.50
8:H:49:ASP:O	8:H:52:VAL:HG22	2.12	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.93	0.50
3:P:54:MET:HE1	19:P:305:PGV:H132	1.93	0.50
8:U:7:LYS:O	8:U:8:ILE:HB	2.11	0.50
3:P:33:MET:HE3	3:P:39:SER:OG	2.12	0.50
3:P:52:LEU:HD21	27:P:307:CDL:H412	1.94	0.50
2:O:78:LEU:O	2:O:82[B]:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180[B]:GLU:HG3	30:C:416:HOH:O	2.10	0.50
3:C:258:TRP:HZ3	27:N:601:CDL:H651	1.77	0.50
8:U:46:LYS:O	30:U:201:HOH:O	2.19	0.50
21:A:610:PSC:H342	2:B:41:ILE:HD13	1.93	0.49
3:C:37:PHE:CE2	23:C:310:DMU:H13	2.47	0.49
4:D:82:VAL:HG12	4:D:86:MET:HE2	1.94	0.49
7:T:31:CYS:SG	27:T:102:CDL:H532	2.52	0.49
23:L:105:DMU:H5	30:L:216:HOH:O	2.12	0.49
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.93	0.49
4:D:147:LYS:NZ	30:D:301:HOH:O	2.32	0.49
4:Q:65:LYS:HE3	30:Q:410:HOH:O	2.12	0.49
27:T:102:CDL:H781	27:T:102:CDL:C56	2.42	0.49
3:C:180[B]:GLU:HG2	30:C:422:HOH:O	2.11	0.49
8:H:43:MET:HE1	8:U:43:MET:HE1	1.94	0.49
11:X:40:TRP:CD1	23:X:102:DMU:H10	2.47	0.49
1:A:311:ILE:CD1	27:T:102:CDL:H441	2.42	0.49
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.48	0.49
1:N:113:LEU:CB	18:N:608:TGL:H301	2.36	0.49
1:A:513:LEU:O	1:A:514[A]:LYS:HB2	2.13	0.49
2:O:58:ALA:O	2:O:62:GLU:HG3	2.13	0.49
3:P:257:TYR:O	3:P:261:SER:HB3	2.12	0.49
1:N:468:MET:HG3	30:N:969:HOH:O	2.11	0.49
12:Y:3:TYR:CE2	22:Y:101:EDO:H21	2.48	0.49
3:P:33:MET:CE	3:P:42:LEU:H	2.25	0.49
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.48	0.49
2:O:13:THR:HB	2:O:168:LEU:HD23	1.95	0.49
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.94	0.49
3:C:258:TRP:CE3	22:C:315:EDO:H21	2.48	0.49
2:O:56:MET:HB3	21:O:302:PSC:H232	1.94	0.49
4:Q:101:HIS:ND1	23:Q:201:DMU:H6	2.28	0.49
1:N:383[C]:MET:O	1:N:387:PHE:N	2.46	0.48
4:Q:101:HIS:CG	23:Q:201:DMU:H6	2.48	0.48
1:A:273:MET:HE2	30:A:756:HOH:O	2.13	0.48
7:G:7:ASP:O	1:N:178[B]:GLN:NE2	2.46	0.48
25:L:102:CHD:H232	13:M:21:VAL:HG21	1.95	0.48
1:A:381[B]:LEU:HB2	14:A:602:HEA:CAC	2.43	0.48
1:N:46:THR:HG22	1:N:49[B]:GLY:H	1.78	0.48
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.48
8:U:43:MET:HE3	8:U:48:GLY:HA3	1.95	0.48
3:P:40:MET:SD	23:P:316:DMU:H6	2.54	0.48
3:P:210:ILE:HD13	19:P:305:PGV:H301	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:MET:HE2	30:B:417:HOH:O	2.14	0.48
12:L:24[A]:MET:SD	18:L:101:TGL:H152	2.54	0.48
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.48	0.48
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.48
4:D:120:THR:HG21	11:K:48[B]:VAL:HG11	1.95	0.48
1:A:321[B]:PHE:HB3	2:B:65:TRP:CE3	2.49	0.47
27:P:307:CDL:H161	27:P:307:CDL:H132	1.65	0.47
4:D:4:SER:HB2	22:D:204:EDO:C1	2.45	0.47
8:H:46:LYS:HE3	8:U:7:LYS:HB2	1.96	0.47
10:W:29:ASN:O	10:W:33:ARG:HG3	2.13	0.47
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	1.96	0.47
11:X:24:PHE:O	11:X:28:VAL:HG12	2.15	0.47
18:A:606:TGL:HA72	18:A:606:TGL:H142	1.96	0.47
3:C:54[B]:MET:HE1	19:C:306:PGV:H141	1.96	0.47
1:N:406:ASN:HD21	19:N:610:PGV:H21	1.79	0.47
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.38	0.47
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.96	0.47
1:N:486[B]:ASP:OD2	4:Q:19:ARG:NE	2.47	0.47
18:A:606:TGL:H142	18:A:606:TGL:H112	1.43	0.47
11:K:42:PRO:O	11:K:47:ARG:NH2	2.49	0.46
1:N:381[B]:LEU:HB2	14:N:603:HEA:CAC	2.46	0.46
2:O:61:VAL:O	2:O:64[A]:ILE:HG23	2.16	0.46
18:L:101:TGL:H261	18:L:101:TGL:H232	1.71	0.46
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.46
3:C:51[A]:MET:SD	27:C:308:CDL:H622	2.56	0.46
6:F:50:PRO:HG2	30:F:265:HOH:O	2.16	0.46
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.50	0.46
2:O:100:MET:HE3	2:O:157:GLU:HG3	1.97	0.46
3:C:220:PHE:HB2	27:C:308:CDL:H712	1.96	0.46
18:A:606:TGL:H101	18:A:606:TGL:C28	2.46	0.46
1:A:376:HIS:CE1	1:A:380[B]:VAL:HG11	2.50	0.46
1:A:383[C]:MET:O	1:A:387:PHE:N	2.48	0.46
26:C:304:PEK:H221	26:C:304:PEK:H251	1.54	0.46
27:C:308:CDL:H822	27:C:308:CDL:H851	1.66	0.46
2:O:89:GLU:O	2:O:91:ASN:ND2	2.49	0.46
18:N:607:TGL:HB91	18:N:607:TGL:H122	1.72	0.46
30:N:825:HOH:O	3:P:77:LYS:HE3	2.15	0.46
5:R:7:THR:HB	5:R:9:GLU:OE2	2.16	0.46
18:A:607:TGL:HB42	4:D:78:TRP:HA	1.98	0.46
18:N:608:TGL:H222	18:N:608:TGL:HA91	1.54	0.46
27:P:307:CDL:H821	27:P:307:CDL:H851	1.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:PHE:CE2	7:T:4:ALA:HB2	2.51	0.45
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.99	0.45
18:N:607:TGL:H222	18:N:607:TGL:H271	1.99	0.45
4:Q:68:PHE:HA	4:Q:71:MET:HE3	1.97	0.45
14:A:601[B]:HEA:H122	30:A:860:HOH:O	2.17	0.45
8:U:9:LYS:O	8:U:10:ASN:HB2	2.16	0.45
1:A:53[B]:ILE:HG12	30:L:235:HOH:O	2.17	0.45
5:E:90:ARG:NH2	5:E:103:GLU:OE2	2.49	0.45
1:N:408:THR:HB	19:N:610:PGV:H51	1.97	0.45
1:N:35[A]:LEU:HD11	1:N:462:LEU:HB2	1.98	0.45
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.99	0.45
3:P:224[B]:LYS:HE3	27:P:307:CDL:H131	1.98	0.45
14:A:602:HEA:H243	2:B:69:PRO:HB3	1.99	0.45
1:N:50[B]:ASP:CG	1:N:53[B]:ILE:HG13	2.42	0.45
1:N:297[C]:MET:SD	1:N:302:ARG:CG	3.05	0.45
1:N:383[A]:MET:HG2	1:N:421:VAL:HG21	1.99	0.45
6:S:22:LEU:HD12	30:S:306:HOH:O	2.15	0.45
2:O:65[B]:TRP:CD1	21:O:302:PSC:H12	2.52	0.45
1:A:285:PHE:CD2	7:T:4:ALA:HB2	2.52	0.45
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	1.98	0.45
3:P:116:TRP:HA	3:P:117:PRO:C	2.42	0.45
27:C:308:CDL:H662	27:C:308:CDL:H631	1.72	0.44
7:G:9:GLY:HA2	30:N:892:HOH:O	2.17	0.44
7:T:21:PHE:CG	26:T:101:PEK:H222	2.51	0.44
3:C:207:HIS:CE1	19:C:306:PGV:H343	2.52	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.17	0.44
6:S:76:LYS:HE3	6:S:76:LYS:HB3	1.69	0.44
3:C:164:PHE:CD1	25:C:309:CHD:H192	2.52	0.44
3:P:168:THR:HG22	26:T:101:PEK:H14	2.00	0.44
7:T:41:HIS:HB3	7:T:74:ARG:CZ	2.47	0.44
1:A:236:TRP:CH2	14:A:602:HEA:HBD1	2.51	0.44
1:A:334:TRP:CZ3	18:A:607:TGL:HA51	2.52	0.44
22:A:620:EDO:H22	6:F:66:ASN:ND2	2.31	0.44
8:U:60:TYR:CD1	8:U:60:TYR:C	2.95	0.44
1:A:311:ILE:HD11	27:T:102:CDL:H421	2.00	0.44
22:C:318:EDO:H11	6:F:16:LEU:HD13	1.99	0.44
12:L:24[B]:MET:CG	18:L:101:TGL:HA22	2.47	0.44
1:N:73:ILE:HD11	14:N:602[C]:HEA:H22	1.98	0.44
14:N:602[C]:HEA:H212	14:N:602[C]:HEA:H271	1.87	0.44
1:N:307:SER:O	1:N:311[A]:ILE:HG23	2.17	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.52	0.44
1:A:334:TRP:CE3	18:A:607:TGL:HA51	2.53	0.44
13:Z:37:LEU:HD23	13:Z:37:LEU:HA	1.86	0.44
1:A:281:GLY:C	7:T:4:ALA:HB3	2.43	0.44
1:A:136[B]:LEU:HD11	30:A:962:HOH:O	2.17	0.43
26:C:304:PEK:H42	26:C:304:PEK:H72	1.59	0.43
3:P:47:LEU:O	3:P:51[B]:MET:HG2	2.18	0.43
3:P:54:MET:HE1	19:P:305:PGV:C13	2.48	0.43
12:L:41:ARG:NH1	23:L:105:DMU:H2	2.33	0.43
3:P:168:THR:CG2	26:T:101:PEK:H12	2.46	0.43
2:B:164:ALA:O	2:B:194:GLY:HA3	2.17	0.43
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.00	0.43
1:N:377:PHE:O	1:N:381[B]:LEU:HB3	2.18	0.43
1:N:379:TYR:CZ	1:N:383[A]:MET:HE1	2.52	0.43
4:Q:5:VAL:H	13:Z:5:PRO:HD3	1.83	0.43
3:C:158:HIS:CE1	6:F:1:ALA:HB3	2.53	0.43
23:K:101:DMU:H21	23:K:102:DMU:H17	2.00	0.43
12:L:2:HIS:CG	12:L:3:TYR:N	2.85	0.43
1:N:76:GLY:O	1:N:80:ASN:HB2	2.18	0.43
1:A:334:TRP:HZ3	18:A:607:TGL:HA71	1.83	0.43
1:A:486[A]:ASP:OD1	22:A:612:EDO:O2	2.30	0.43
12:L:41:ARG:HH12	23:L:105:DMU:H2	1.83	0.43
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.54	0.43
3:P:59:ARG:HA	27:P:307:CDL:H522	1.99	0.43
5:R:79:LYS:HD2	5:R:79:LYS:HA	1.89	0.43
6:S:54:ASN:HB2	6:S:76:LYS:HE2	2.00	0.43
10:W:54:SER:O	12:Y:46:LYS:HD3	2.18	0.43
1:A:52[B]:GLN:O	1:A:56:VAL:HG23	2.19	0.43
3:C:37:PHE:CD2	23:C:310:DMU:H13	2.53	0.43
1:N:116:SER:HB3	30:N:834:HOH:O	2.18	0.43
1:A:362[B]:SER:HB2	2:B:20:LEU:HD21	2.01	0.43
22:A:612:EDO:H22	13:M:1:ILE:N	2.34	0.43
12:Y:45:LEU:HD21	13:Z:40:TYR:CD1	2.54	0.43
18:A:607:TGL:HG32	30:A:924:HOH:O	2.18	0.43
1:N:54[A]:TYR:HB2	30:N:788[A]:HOH:O	2.19	0.42
7:G:5:LYS:HB3	1:N:278[B]:MET:CE	2.49	0.42
8:U:43:MET:HE3	8:U:49:ASP:N	2.34	0.42
1:N:321:PHE:CD1	21:O:302:PSC:H341	2.54	0.42
14:N:603:HEA:H243	2:O:69:PRO:HB3	2.01	0.42
1:A:321[A]:PHE:HB3	2:B:65:TRP:CE3	2.54	0.42
18:A:607:TGL:HC92	2:B:47:THR:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:98:TRP:CD2	23:M:101:DMU:H11	2.54	0.42
23:L:105:DMU:H13	23:L:105:DMU:H18	1.62	0.42
2:B:196:CYS:CB	2:B:207:MET:HG3	2.50	0.42
1:N:266:GLU:OE1	22:S:106:EDO:H11	2.19	0.42
2:O:183:THR:HG22	30:O:567:HOH:O	2.19	0.42
10:W:4:ARG:O	10:W:7:GLU:HG2	2.20	0.42
14:A:601[C]:HEA:H212	14:A:601[C]:HEA:H271	1.69	0.42
3:P:47:LEU:O	3:P:51[A]:MET:HG3	2.19	0.42
2:B:58:ALA:O	2:B:62:GLU:HG3	2.20	0.42
3:C:58:TRP:HB2	27:C:308:CDL:H552	2.02	0.42
11:K:47:ARG:HG2	11:K:48[A]:VAL:HG23	2.02	0.42
2:O:168:LEU:HD13	2:O:184:LEU:HG	2.01	0.42
5:R:108:LYS:HB3	30:R:298:HOH:O	2.20	0.42
2:B:5:MET:HE2	2:B:5:MET:HB3	1.86	0.42
2:B:100[B]:MET:CG	2:B:157:GLU:HG3	2.49	0.42
3:C:244:PHE:HA	26:C:303:PEK:H101	2.01	0.42
4:D:115:TRP:HE3	22:D:205:EDO:H11	1.85	0.42
19:A:611:PGV:H182	3:C:28:THR:HG22	2.02	0.42
12:L:24[B]:MET:SD	18:L:101:TGL:CC2	3.07	0.42
18:N:607:TGL:H311	18:N:607:TGL:H141	1.77	0.42
3:C:158:HIS:HE1	6:F:1:ALA:HB3	1.85	0.41
3:C:191:GLY:HA3	30:G:212:HOH:O	2.19	0.41
12:L:24[B]:MET:HG2	18:L:101:TGL:HA22	2.02	0.41
1:A:311:ILE:CD1	27:T:102:CDL:H421	2.51	0.41
10:J:37:THR:HG23	25:J:101:CHD:H191	2.02	0.41
8:H:60:TYR:CD1	8:H:60:TYR:C	2.98	0.41
25:J:101:CHD:H21	25:J:101:CHD:H9	1.79	0.41
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.17	0.41
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.50	0.41
2:B:148[B]:MET:HE3	2:B:148[B]:MET:HB2	1.83	0.41
3:C:3:HIS:N	30:C:410:HOH:O	2.53	0.41
6:F:75:HIS:H	6:F:80[B]:GLN:HE22	1.68	0.41
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.55	0.41
1:A:379:TYR:CZ	1:A:383[A]:MET:HE1	2.55	0.41
4:D:19[B]:ARG:NH1	4:D:22:TYR:HB2	2.36	0.41
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.03	0.41
1:N:236:TRP:CH2	14:N:603:HEA:HBD1	2.56	0.41
1:N:310:MET:HE3	1:N:356:ILE:HG23	2.02	0.41
27:N:601:CDL:H801	27:N:601:CDL:H832	1.77	0.41
1:A:415:ALA:HB1	18:A:607:TGL:H131	2.02	0.41
2:O:102:HIS:O	2:O:104:TRP:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.41
9:V:63:MET:HB3	9:V:68:ILE:HG12	2.02	0.41
1:A:92:MET:HE2	22:A:616:EDO:H11	2.02	0.41
1:A:246:LEU:HD13	1:A:381[B]:LEU:HD11	2.02	0.41
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.52	0.41
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.02	0.41
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.02	0.41
25:L:102:CHD:H183	25:L:102:CHD:H212	2.02	0.41
3:P:165:ILE:HG12	26:T:101:PEK:H11	2.03	0.41
9:V:36:LYS:HE3	9:V:36:LYS:HB3	1.86	0.41
10:W:18:LEU:HB2	10:W:23:LYS:HG3	2.02	0.41
3:C:157:LYS:HE2	3:C:161[B]:GLN:NE2	2.35	0.41
25:G:101:CHD:H212	25:G:101:CHD:H12	2.02	0.41
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.02	0.41
23:P:308:DMU:H41	23:P:308:DMU:H36	1.74	0.41
23:P:308:DMU:H29	23:P:308:DMU:H32	2.03	0.41
1:A:120:ALA:HB2	22:A:618:EDO:H12	2.03	0.41
9:I:57:MET:O	9:I:61[B]:GLU:HG2	2.20	0.41
18:A:607:TGL:H132	18:A:607:TGL:H101	1.89	0.40
3:C:54[B]:MET:HE3	27:C:308:CDL:H601	2.03	0.40
18:N:608:TGL:HC31	12:Y:13:PHE:HA	2.04	0.40
3:P:207:HIS:HD2	3:P:241:TYR:OH	2.04	0.40
23:C:310:DMU:C22	10:J:49:CYS:HB3	2.51	0.40
4:D:5:VAL:H	22:D:204:EDO:C1	2.35	0.40
12:L:24[B]:MET:HE3	12:L:24[B]:MET:HB2	1.50	0.40
1:A:302[B]:ARG:HH22	1:A:365[B]:ILE:HD11	1.86	0.40
12:L:23:ALA:O	12:L:27[A]:LEU:HG	2.21	0.40
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.02	0.40
1:N:331[B]:ASN:ND2	2:O:51:THR:HG21	2.36	0.40
18:N:608:TGL:HC22	18:N:608:TGL:HC52	1.78	0.40
4:D:101:HIS:HB2	23:D:206:DMU:H30	2.03	0.40
11:K:24:PHE:HB2	23:K:103:DMU:H9	2.02	0.40
1:N:331[B]:ASN:HD21	4:Q:21:ASP:HB3	1.86	0.40
13:M:39:ASN:ND2	13:M:39:ASN:N	2.68	0.40
1:N:386[B]:VAL:HG21	14:N:602[B]:HEA:H162	2.04	0.40
22:N:620:EDO:H22	6:S:66:ASN:ND2	2.37	0.40
6:S:25:ARG:HE	6:S:25:ARG:HB2	1.68	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	548/514 (107%)	529 (96%)	19 (4%)	0	100	100
1	N	553/514 (108%)	534 (97%)	19 (3%)	0	100	100
2	B	233/227 (103%)	227 (97%)	5 (2%)	1 (0%)	30	18
2	O	237/227 (104%)	230 (97%)	5 (2%)	2 (1%)	16	5
3	C	268/259 (104%)	263 (98%)	5 (2%)	0	100	100
3	P	268/259 (104%)	263 (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%)	3 (2%)	2 (1%)	9	2
5	E	103/105 (98%)	102 (99%)	1 (1%)	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%)	90 (98%)	1 (1%)	1 (1%)	11	3
7	G	87/84 (104%)	77 (88%)	8 (9%)	2 (2%)	5	0
7	T	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	1	0
8	H	78/79 (99%)	73 (94%)	3 (4%)	2 (3%)	4	0
8	U	77/79 (98%)	72 (94%)	3 (4%)	2 (3%)	4	0
9	I	72/73 (99%)	71 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	57/58 (98%)	57 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
11	K	50/49 (102%)	49 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	46/46 (100%)	44 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
13	M	41/43 (95%)	40 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/43 (95%)	39 (95%)	2 (5%)	0	100	100
All	All	3640/3550 (102%)	3522 (97%)	102 (3%)	16 (0%)	30	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	2	SER
8	U	8	ILE
6	S	2	SER
8	H	9	LYS
8	H	48	GLY
2	O	92[A]	ASN
2	O	92[B]	ASN
7	G	3	ALA
7	T	4	ALA
8	U	10	ASN
7	T	5	LYS
4	Q	5	VAL
4	Q	6	VAL
7	T	6	GLY
2	B	92	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/426 (108%)	443 (97%)	15 (3%)	33	15
1	N	463/426 (109%)	460 (99%)	3 (1%)	78	72
2	B	218/210 (104%)	206 (94%)	12 (6%)	19	4
2	O	221/210 (105%)	210 (95%)	11 (5%)	22	6
3	C	235/224 (105%)	231 (98%)	4 (2%)	53	37
3	P	235/224 (105%)	231 (98%)	4 (2%)	53	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	131/128 (102%)	129 (98%)	2 (2%)	57	42
4	Q	129/128 (101%)	122 (95%)	7 (5%)	20	4
5	E	92/92 (100%)	91 (99%)	1 (1%)	65	54
5	R	93/92 (101%)	93 (100%)	0	100	100
6	F	83/78 (106%)	78 (94%)	5 (6%)	17	4
6	S	78/78 (100%)	77 (99%)	1 (1%)	61	47
7	G	73/68 (107%)	64 (88%)	9 (12%)	4	0
7	T	68/68 (100%)	63 (93%)	5 (7%)	13	2
8	H	72/71 (101%)	66 (92%)	6 (8%)	10	2
8	U	71/71 (100%)	67 (94%)	4 (6%)	19	4
9	I	58/57 (102%)	58 (100%)	0	100	100
9	V	57/57 (100%)	55 (96%)	2 (4%)	32	14
10	J	50/49 (102%)	50 (100%)	0	100	100
10	W	49/49 (100%)	47 (96%)	2 (4%)	27	10
11	K	42/39 (108%)	41 (98%)	1 (2%)	43	25
11	X	39/39 (100%)	38 (97%)	1 (3%)	40	23
12	L	41/39 (105%)	40 (98%)	1 (2%)	43	25
12	Y	39/39 (100%)	36 (92%)	3 (8%)	12	2
13	M	37/37 (100%)	36 (97%)	1 (3%)	39	22
13	Z	37/37 (100%)	35 (95%)	2 (5%)	20	4
All	All	3169/3036 (104%)	3067 (97%)	102 (3%)	36	17

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	A	169	ILE
1	A	178[A]	GLN
1	A	178[B]	GLN
1	A	297[A]	MET
1	A	297[B]	MET
1	A	363	LEU
1	A	369	ASP
1	A	382[A]	SER
1	A	382[B]	SER

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Mol	Chain	Res	Type
1	A	382[C]	SER
1	A	486[A]	ASP
1	A	486[B]	ASP
1	A	514[A]	LYS
1	A	514[B]	LYS
2	B	33	LEU
2	B	60[A]	GLU
2	B	60[B]	GLU
2	B	66	THR
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	86	MET
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	171	LYS
3	C	40	MET
3	C	76	GLN
3	C	159	MET
3	C	230	ASN
4	D	4	SER
4	D	31	LYS
5	E	90	ARG
6	F	37	LYS
6	F	54[A]	ASN
6	F	54[B]	ASN
6	F	80[A]	GLN
6	F	80[B]	GLN
7	G	2	SER
7	G	8	HIS
7	G	11	THR
7	G	33[A]	LEU
7	G	33[B]	LEU
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	43	GLU
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	46	LYS

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Mol	Chain	Res	Type
8	H	50	VAL
8	H	60	TYR
11	K	54	ARG
12	L	47	LYS
13	M	39	ASN
1	N	128	VAL
1	N	138	HIS
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	225	SER
2	O	226	MET
3	P	3	HIS
3	P	76	GLN
3	P	159	MET
3	P	230	ASN
4	Q	4	SER
4	Q	5	VAL
4	Q	6	VAL
4	Q	7	LYS
4	Q	20	ARG
4	Q	51	LEU
4	Q	58	GLU
6	S	80	GLN
7	T	2	SER
7	T	11	THR
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
8	U	8	ILE
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	2	THR
9	V	44	LYS

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	422	ASN
2	B	140	ASN
2	B	181	GLN
2	B	195	GLN
3	C	56	GLN
4	D	76	ASN
4	D	119	GLN
6	F	94	HIS
13	M	39	ASN
1	N	80	ASN
1	N	98	ASN
2	O	10	GLN
2	O	91	ASN
3	P	158	HIS
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
7	T	34	ASN
8	U	25	GLN
8	U	28	ASN
8	U	31	GLN
8	U	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	O	1	2	8,9,10	0.72	0	8,9,11	1.36	2 (25%)
9	SAC	I	1	9	7,8,9	0.67	0	7,9,11	1.09	1 (14%)
1	FME	A	1	1	8,9,10	0.45	0	8,9,11	1.35	2 (25%)
2	FME	B	1	2	8,9,10	0.78	0	8,9,11	1.96	1 (12%)
1	FME	N	1	1	8,9,10	0.47	0	8,9,11	1.20	1 (12%)
9	SAC	V	1	9	7,8,9	0.64	0	7,9,11	0.93	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
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	B	1	2	-	0/7/9/11	-
1	FME	N	1	1	-	2/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CG-CB-CA	-4.20	100.04	112.87
2	O	1	FME	CG-CB-CA	-2.85	104.15	112.87
1	A	1	FME	C-CA-N	2.36	114.06	109.50
9	I	1	SAC	O-C-CA	-2.20	119.11	124.77
1	A	1	FME	O1-CN-N	-2.18	119.69	125.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	O-C-CA	-2.07	119.45	124.77
1	N	1	FME	O1-CN-N	-2.00	120.15	125.32

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	O-C-CA-CB
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	C-CA-CB-OG
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 161 ligands modelled in this entry, 10 are monoatomic - leaving 151 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
25	CHD	P	301	-	32,32,32	0.78	0	51,51,51	1.36	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	A	621	-	3,3,3	0.58	0	2,2,2	0.54	0
22	EDO	A	620	-	3,3,3	0.66	0	2,2,2	0.19	0
22	EDO	A	622	-	3,3,3	0.53	0	2,2,2	0.64	0
22	EDO	N	619	-	3,3,3	0.52	0	2,2,2	0.18	0
21	PSC	A	610	-	23,23,51	0.85	1 (4%)	21,21,59	0.80	0
18	TGL	N	607	-	62,62,62	1.04	3 (4%)	65,65,65	1.21	5 (7%)
22	EDO	N	618	-	3,3,3	0.50	0	2,2,2	0.36	0
22	EDO	F	109	-	3,3,3	0.57	0	2,2,2	0.77	0
22	EDO	B	303	-	3,3,3	0.67	0	2,2,2	0.34	0
23	DMU	C	321	-	11,11,34	0.41	0	10,10,45	0.33	0
23	DMU	Q	201	-	10,10,34	0.37	0	9,9,45	0.36	0
23	DMU	X	101	-	9,9,34	0.32	0	8,8,45	0.52	0
23	DMU	A	623	-	10,10,34	0.31	0	9,9,45	0.48	0
19	PGV	C	307	-	35,35,50	1.31	2 (5%)	37,37,56	1.97	8 (21%)
22	EDO	P	313	-	3,3,3	0.40	0	2,2,2	0.98	0
22	EDO	D	203	-	3,3,3	0.46	0	2,2,2	0.27	0
23	DMU	X	102	-	8,8,34	0.30	0	7,7,45	0.49	0
22	EDO	Q	202	-	3,3,3	0.51	0	2,2,2	0.43	0
23	DMU	P	308	-	34,34,34	0.51	0	45,45,45	1.21	7 (15%)
22	EDO	N	617	-	3,3,3	0.43	0	2,2,2	0.19	0
22	EDO	A	619	-	3,3,3	0.45	0	2,2,2	0.22	0
22	EDO	A	612	-	3,3,3	0.69	0	2,2,2	0.33	0
22	EDO	A	613	-	3,3,3	0.77	0	2,2,2	0.70	0
20	PER	N	611[A]	15,14	1,1,1	0.89	0	-	-	-
22	EDO	O	304	-	3,3,3	0.61	0	2,2,2	0.09	0
22	EDO	A	614	-	3,3,3	0.42	0	2,2,2	0.32	0
14	HEA	A	601[A]	-	67,67,67	1.70	20 (29%)	81,103,103	1.81	17 (20%)
22	EDO	O	303	-	3,3,3	0.71	0	2,2,2	0.52	0
23	DMU	D	206	-	34,34,34	0.70	1 (2%)	45,45,45	1.40	8 (17%)
22	EDO	F	103	-	3,3,3	0.45	0	2,2,2	0.55	0
22	EDO	E	202	-	3,3,3	0.42	0	2,2,2	0.17	0
19	PGV	C	306	-	47,47,50	0.85	3 (6%)	50,53,56	0.91	3 (6%)
22	EDO	B	304	-	3,3,3	0.38	0	2,2,2	0.56	0
22	EDO	F	102	-	3,3,3	0.53	0	2,2,2	0.47	0
19	PGV	P	306	-	29,29,50	1.01	1 (3%)	28,28,56	0.91	2 (7%)
23	DMU	K	104	-	10,10,34	0.24	0	9,9,45	0.52	0
19	PGV	P	305	-	50,50,50	0.77	3 (6%)	53,56,56	1.01	1 (1%)
18	TGL	L	101	-	62,62,62	1.12	3 (4%)	65,65,65	1.40	8 (12%)
22	EDO	N	622	-	3,3,3	0.73	0	2,2,2	0.20	0
23	DMU	O	306	-	11,11,34	0.22	0	9,9,45	0.64	0
22	EDO	C	320	-	3,3,3	0.68	0	2,2,2	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	A	616	-	3,3,3	0.41	0	2,2,2	0.48	0
27	CDL	N	601	-	58,58,99	1.43	9 (15%)	55,55,111	1.00	4 (7%)
22	EDO	F	107	-	3,3,3	0.47	0	2,2,2	0.42	0
29	PO4	H	101	-	4,4,4	0.79	0	6,6,6	0.78	0
22	EDO	B	305	-	3,3,3	0.68	0	2,2,2	0.15	0
18	TGL	A	607	-	62,62,62	1.08	3 (4%)	65,65,65	1.12	6 (9%)
27	CDL	P	307	-	65,65,99	1.48	9 (13%)	64,64,111	1.26	6 (9%)
22	EDO	F	105	-	3,3,3	0.58	0	2,2,2	0.20	0
29	PO4	U	101	-	4,4,4	1.11	0	6,6,6	0.59	0
26	PEK	C	304	-	51,51,52	0.81	2 (3%)	54,56,57	1.17	5 (9%)
22	EDO	M	102	-	3,3,3	0.42	0	2,2,2	0.38	0
23	DMU	C	310	-	34,34,34	0.55	1 (2%)	45,45,45	1.21	7 (15%)
22	EDO	N	621	-	3,3,3	0.31	0	2,2,2	0.53	0
19	PGV	A	611	-	50,50,50	0.91	3 (6%)	53,56,56	1.22	5 (9%)
20	PER	A	609[A]	15,14	1,1,1	0.91	0	-	-	-
25	CHD	Y	102	-	32,32,32	0.68	0	51,51,51	2.21	15 (29%)
23	DMU	P	316	-	21,21,34	0.62	1 (4%)	24,25,45	0.83	1 (4%)
14	HEA	N	602[A]	-	67,67,67	1.70	17 (25%)	81,103,103	1.87	18 (22%)
22	EDO	N	615	-	3,3,3	0.50	0	2,2,2	0.38	0
22	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.62	0
22	EDO	L	103	-	3,3,3	0.22	0	2,2,2	1.02	0
22	EDO	L	104	-	3,3,3	0.57	0	2,2,2	0.52	0
22	EDO	D	205	-	3,3,3	0.35	0	2,2,2	0.43	0
22	EDO	S	104	-	3,3,3	0.45	0	2,2,2	0.79	0
19	PGV	N	610	-	50,50,50	0.97	2 (4%)	53,56,56	1.08	3 (5%)
22	EDO	S	105	-	3,3,3	0.58	0	2,2,2	0.74	0
18	TGL	N	608	-	52,52,62	0.75	1 (1%)	50,50,65	0.90	2 (4%)
23	DMU	K	101	-	7,7,34	0.24	0	6,6,45	0.39	0
22	EDO	S	106	-	3,3,3	0.36	0	2,2,2	0.92	0
22	EDO	Y	101	-	3,3,3	0.43	0	2,2,2	0.22	0
24	CUA	O	301	2	0,1,1	-	-	-	-	-
22	EDO	N	613	-	3,3,3	0.61	0	2,2,2	0.66	0
23	DMU	K	102	-	10,10,34	0.34	0	9,9,45	0.62	0
19	PGV	A	608	-	30,31,50	0.41	0	28,29,56	0.55	0
22	EDO	W	101	-	3,3,3	0.35	0	2,2,2	0.48	0
22	EDO	D	204	-	3,3,3	0.47	0	2,2,2	0.45	0
22	EDO	F	106	-	3,3,3	0.57	0	2,2,2	0.57	0
22	EDO	A	615	-	3,3,3	0.67	0	2,2,2	0.99	0
25	CHD	C	309	-	32,32,32	0.78	1 (3%)	51,51,51	1.25	6 (11%)
19	PGV	N	612	-	50,50,50	0.90	3 (6%)	53,56,56	1.14	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	EDO	C	313	-	3,3,3	0.76	0	2,2,2	0.31	0
21	PSC	O	302	-	27,27,51	0.78	1 (3%)	25,25,59	0.73	1 (4%)
23	DMU	X	103	-	8,8,34	0.31	0	7,7,45	0.62	0
22	EDO	C	311	-	3,3,3	0.50	0	2,2,2	0.21	0
22	EDO	S	103	-	3,3,3	0.56	0	2,2,2	0.18	0
27	CDL	T	102	-	57,57,99	1.39	8 (14%)	54,54,111	0.88	1 (1%)
23	DMU	K	103	-	9,9,34	0.35	0	8,8,45	0.34	0
22	EDO	F	108	-	3,3,3	0.44	0	2,2,2	0.41	0
22	EDO	B	306	-	3,3,3	0.55	0	2,2,2	0.36	0
22	EDO	W	102	-	3,3,3	0.46	0	2,2,2	0.49	0
22	EDO	C	317	-	3,3,3	0.51	0	2,2,2	0.19	0
22	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.35	0
26	PEK	C	305	-	34,34,52	0.33	0	32,32,57	0.59	0
26	PEK	P	304	-	51,51,52	0.77	3 (5%)	54,56,57	1.08	4 (7%)
22	EDO	S	102	-	3,3,3	0.73	0	2,2,2	0.74	0
26	PEK	C	303	-	44,44,52	1.22	2 (4%)	47,49,57	1.42	7 (14%)
22	EDO	J	103	-	3,3,3	0.33	0	2,2,2	0.77	0
22	EDO	T	103	-	3,3,3	0.69	0	2,2,2	0.41	0
22	EDO	T	104	-	3,3,3	0.46	0	2,2,2	0.32	0
22	EDO	P	312	-	3,3,3	0.41	0	2,2,2	0.97	0
22	EDO	C	314	-	3,3,3	0.31	0	2,2,2	0.68	0
24	CUA	B	301	2	0,1,1	-	-	-	-	-
22	EDO	N	614	-	3,3,3	0.63	0	2,2,2	0.23	0
22	EDO	N	620	-	3,3,3	0.57	0	2,2,2	0.17	0
14	HEA	N	603	20,1,30	67,67,67	1.70	20 (29%)	81,103,103	1.58	21 (25%)
22	EDO	T	105	-	3,3,3	0.59	0	2,2,2	0.36	0
22	EDO	C	315	-	3,3,3	0.53	0	2,2,2	0.17	0
14	HEA	A	602	20,1,30	67,67,67	1.62	19 (28%)	81,103,103	1.73	21 (25%)
23	DMU	K	105	-	8,8,34	0.30	0	7,7,45	0.57	0
22	EDO	E	203	-	3,3,3	0.43	0	2,2,2	0.44	0
25	CHD	L	102	-	32,32,32	0.68	0	51,51,51	2.42	22 (43%)
25	CHD	G	101	-	32,32,32	0.77	1 (3%)	51,51,51	1.14	3 (5%)
22	EDO	O	305	-	3,3,3	0.51	0	2,2,2	0.12	0
22	EDO	C	312	-	3,3,3	0.61	0	2,2,2	0.38	0
26	PEK	P	303	-	37,37,52	1.15	2 (5%)	40,42,57	1.23	4 (10%)
22	EDO	G	102	-	3,3,3	0.78	0	2,2,2	0.53	0
23	DMU	X	104	-	22,22,34	0.58	1 (4%)	27,27,45	0.77	0
23	DMU	Z	101	-	34,34,34	0.46	0	45,45,45	0.83	2 (4%)
23	DMU	P	317	-	33,33,34	0.73	1 (3%)	44,44,45	1.68	8 (18%)
25	CHD	B	302	-	32,32,32	0.88	0	51,51,51	1.40	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHD	J	101	-	32,32,32	0.72	0	51,51,51	2.72	19 (37%)
25	CHD	C	301	-	32,32,32	0.74	0	51,51,51	1.55	10 (19%)
22	EDO	D	201	-	3,3,3	0.54	0	2,2,2	0.34	0
22	EDO	C	319	-	3,3,3	0.57	0	2,2,2	0.35	0
22	EDO	P	310	-	3,3,3	0.51	0	2,2,2	0.22	0
22	EDO	J	102	-	3,3,3	0.49	0	2,2,2	0.22	0
22	EDO	P	314	-	3,3,3	0.54	0	2,2,2	0.19	0
26	PEK	T	101	-	35,35,52	0.88	1 (2%)	34,34,57	1.11	3 (8%)
23	DMU	J	104	-	10,10,34	0.34	0	9,9,45	0.41	0
22	EDO	P	315	-	3,3,3	0.49	0	2,2,2	0.17	0
22	EDO	N	616	-	3,3,3	0.38	0	2,2,2	0.71	0
22	EDO	P	311	-	3,3,3	0.68	0	2,2,2	0.17	0
23	DMU	D	207	-	10,10,34	0.33	0	9,9,45	0.57	0
22	EDO	C	318	-	3,3,3	0.52	0	2,2,2	0.38	0
23	DMU	M	101	-	34,34,34	0.45	0	45,45,45	1.03	1 (2%)
23	DMU	L	105	-	21,21,34	0.92	1 (4%)	24,25,45	2.06	6 (25%)
18	TGL	A	606	-	62,62,62	1.05	3 (4%)	65,65,65	1.30	8 (12%)
22	EDO	C	316	-	3,3,3	0.36	0	2,2,2	0.39	0
22	EDO	E	201	-	3,3,3	0.52	0	2,2,2	0.30	0
22	EDO	F	104	-	3,3,3	0.55	0	2,2,2	0.37	0
22	EDO	P	309	-	3,3,3	0.50	0	2,2,2	0.26	0
18	TGL	N	609	-	52,52,62	0.71	1 (1%)	50,50,65	0.71	2 (4%)
22	EDO	A	618	-	3,3,3	0.72	0	2,2,2	0.25	0
22	EDO	S	107	-	3,3,3	0.49	0	2,2,2	0.61	0
27	CDL	C	308	-	62,62,99	1.44	8 (12%)	61,61,111	1.43	11 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHD	P	301	-	-	1/9/74/74	0/4/4/4
22	EDO	A	621	-	-	0/1/1/1	-
22	EDO	A	620	-	-	1/1/1/1	-
22	EDO	A	622	-	-	0/1/1/1	-
22	EDO	N	619	-	-	1/1/1/1	-
21	PSC	A	610	-	-	11/19/19/55	-
18	TGL	N	607	-	-	32/65/65/65	-
22	EDO	N	618	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	F	109	-	-	0/1/1/1	-
22	EDO	B	303	-	-	0/1/1/1	-
23	DMU	C	321	-	-	0/9/9/59	-
23	DMU	Q	201	-	-	4/8/8/59	-
23	DMU	X	101	-	-	2/7/7/59	-
23	DMU	A	623	-	-	0/8/8/59	-
19	PGV	C	307	-	-	16/36/36/55	-
22	EDO	P	313	-	-	1/1/1/1	-
22	EDO	D	203	-	-	0/1/1/1	-
23	DMU	X	102	-	-	2/6/6/59	-
22	EDO	Q	202	-	-	0/1/1/1	-
23	DMU	P	308	-	-	8/19/59/59	0/2/2/2
22	EDO	N	617	-	-	0/1/1/1	-
22	EDO	A	619	-	-	1/1/1/1	-
22	EDO	A	612	-	-	1/1/1/1	-
22	EDO	A	613	-	-	0/1/1/1	-
22	EDO	O	304	-	-	0/1/1/1	-
22	EDO	A	614	-	-	1/1/1/1	-
14	HEA	A	601[A]	-	-	5/36/76/76	-
22	EDO	O	303	-	-	0/1/1/1	-
23	DMU	D	206	-	-	8/19/59/59	0/2/2/2
22	EDO	F	103	-	-	0/1/1/1	-
22	EDO	E	202	-	-	1/1/1/1	-
19	PGV	C	306	-	-	13/52/52/55	-
22	EDO	B	304	-	-	0/1/1/1	-
22	EDO	F	102	-	-	0/1/1/1	-
19	PGV	P	306	-	-	4/25/25/55	-
23	DMU	K	104	-	-	3/8/8/59	-
19	PGV	P	305	-	-	6/55/55/55	-
18	TGL	L	101	-	-	39/65/65/65	-
22	EDO	N	622	-	-	0/1/1/1	-
23	DMU	O	306	-	-	1/8/8/59	-
22	EDO	C	320	-	-	1/1/1/1	-
22	EDO	A	616	-	-	0/1/1/1	-
27	CDL	N	601	-	-	16/51/51/110	-
22	EDO	F	107	-	-	0/1/1/1	-
22	EDO	B	305	-	-	0/1/1/1	-
18	TGL	A	607	-	-	28/65/65/65	-
27	CDL	P	307	-	-	27/61/61/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	F	105	-	-	0/1/1/1	-
26	PEK	C	304	-	-	16/55/55/56	-
22	EDO	M	102	-	-	1/1/1/1	-
23	DMU	C	310	-	-	3/19/59/59	0/2/2/2
22	EDO	N	621	-	-	0/1/1/1	-
19	PGV	A	611	-	-	4/55/55/55	-
25	CHD	Y	102	-	-	3/9/74/74	0/4/4/4
23	DMU	P	316	-	-	4/13/29/59	0/1/1/2
14	HEA	N	602[A]	-	-	5/36/76/76	-
22	EDO	N	615	-	-	0/1/1/1	-
22	EDO	A	617	-	-	1/1/1/1	-
22	EDO	L	103	-	-	1/1/1/1	-
22	EDO	L	104	-	-	1/1/1/1	-
22	EDO	D	205	-	-	1/1/1/1	-
22	EDO	S	104	-	-	0/1/1/1	-
19	PGV	N	610	-	-	14/55/55/55	-
22	EDO	S	105	-	-	0/1/1/1	-
18	TGL	N	608	-	-	22/47/47/65	-
23	DMU	K	101	-	-	1/5/5/59	-
22	EDO	S	106	-	-	1/1/1/1	-
22	EDO	Y	101	-	-	0/1/1/1	-
22	EDO	N	613	-	-	0/1/1/1	-
23	DMU	K	102	-	-	4/8/8/59	-
19	PGV	A	608	-	-	9/27/27/55	-
22	EDO	W	101	-	-	1/1/1/1	-
22	EDO	D	204	-	-	1/1/1/1	-
22	EDO	F	106	-	-	0/1/1/1	-
22	EDO	A	615	-	-	0/1/1/1	-
25	CHD	C	309	-	-	5/9/74/74	0/4/4/4
19	PGV	N	612	-	-	6/55/55/55	-
22	EDO	C	313	-	-	0/1/1/1	-
21	PSC	O	302	-	-	5/23/23/55	-
23	DMU	X	103	-	-	0/6/6/59	-
22	EDO	C	311	-	-	0/1/1/1	-
22	EDO	S	103	-	-	0/1/1/1	-
27	CDL	T	102	-	-	18/50/50/110	-
23	DMU	K	103	-	-	2/7/7/59	-
22	EDO	F	108	-	-	1/1/1/1	-
22	EDO	B	306	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	W	102	-	-	1/1/1/1	-
22	EDO	C	317	-	-	0/1/1/1	-
22	EDO	D	202	-	-	1/1/1/1	-
26	PEK	C	305	-	-	13/30/30/56	-
26	PEK	P	304	-	-	10/55/55/56	-
22	EDO	S	102	-	-	0/1/1/1	-
26	PEK	C	303	-	-	17/48/48/56	-
22	EDO	J	103	-	-	1/1/1/1	-
22	EDO	T	103	-	-	0/1/1/1	-
22	EDO	T	104	-	-	1/1/1/1	-
22	EDO	P	312	-	-	1/1/1/1	-
22	EDO	C	314	-	-	0/1/1/1	-
22	EDO	N	614	-	-	0/1/1/1	-
22	EDO	N	620	-	-	0/1/1/1	-
14	HEA	N	603	20,1,30	-	9/36/76/76	-
22	EDO	T	105	-	-	1/1/1/1	-
22	EDO	C	315	-	-	0/1/1/1	-
14	HEA	A	602	20,1,30	-	7/36/76/76	-
23	DMU	K	105	-	-	0/6/6/59	-
22	EDO	E	203	-	-	0/1/1/1	-
25	CHD	L	102	-	-	5/9/74/74	0/4/4/4
25	CHD	G	101	-	-	2/9/74/74	0/4/4/4
22	EDO	O	305	-	-	0/1/1/1	-
22	EDO	C	312	-	-	0/1/1/1	-
26	PEK	P	303	-	-	13/41/41/56	-
22	EDO	G	102	-	-	0/1/1/1	-
23	DMU	X	104	-	-	2/13/33/59	0/1/1/2
23	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
23	DMU	P	317	-	-	3/18/58/59	0/2/2/2
25	CHD	B	302	-	-	2/9/74/74	0/4/4/4
25	CHD	J	101	-	-	7/9/74/74	0/4/4/4
25	CHD	C	301	-	-	1/9/74/74	0/4/4/4
22	EDO	D	201	-	-	0/1/1/1	-
22	EDO	C	319	-	-	0/1/1/1	-
22	EDO	P	310	-	-	0/1/1/1	-
22	EDO	J	102	-	-	1/1/1/1	-
22	EDO	P	314	-	-	0/1/1/1	-
26	PEK	T	101	-	-	14/32/32/56	-
23	DMU	J	104	-	-	2/8/8/59	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EDO	P	315	-	-	0/1/1/1	-
22	EDO	N	616	-	-	0/1/1/1	-
22	EDO	P	311	-	-	0/1/1/1	-
23	DMU	D	207	-	-	4/8/8/59	-
22	EDO	C	318	-	-	0/1/1/1	-
23	DMU	M	101	-	-	4/19/59/59	0/2/2/2
23	DMU	L	105	-	-	8/13/29/59	0/1/1/2
18	TGL	A	606	-	-	36/65/65/65	-
22	EDO	C	316	-	-	0/1/1/1	-
22	EDO	E	201	-	-	0/1/1/1	-
22	EDO	F	104	-	-	0/1/1/1	-
22	EDO	P	309	-	-	1/1/1/1	-
18	TGL	N	609	-	-	20/47/47/65	-
22	EDO	A	618	-	-	1/1/1/1	-
22	EDO	S	107	-	-	0/1/1/1	-
27	CDL	C	308	-	-	17/58/58/110	-

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	307	PGV	O03-C19	5.48	1.49	1.33
26	C	303	PEK	O03-C21	5.29	1.48	1.33
18	L	101	TGL	OG2-CB1	5.01	1.48	1.34
27	N	601	CDL	OB8-CB7	4.93	1.47	1.33
19	P	306	PGV	O03-C19	4.86	1.46	1.30
27	P	307	CDL	OB6-CB5	4.84	1.47	1.33
18	A	607	TGL	OG1-CA1	4.78	1.47	1.33
27	P	307	CDL	OB8-CB7	4.72	1.47	1.33
18	L	101	TGL	OG1-CA1	4.71	1.47	1.33
18	L	101	TGL	OG3-CC1	4.70	1.47	1.33
26	P	303	PEK	O03-C21	4.66	1.46	1.33
18	A	606	TGL	OG1-CA1	4.66	1.46	1.33
26	C	303	PEK	O01-C1	4.64	1.47	1.34
27	T	102	CDL	OB8-CB7	4.63	1.46	1.33
18	N	607	TGL	OG2-CB1	4.60	1.47	1.34
18	N	608	TGL	OG3-CC1	4.57	1.47	1.33
18	N	609	TGL	OG3-CC1	4.50	1.47	1.33
26	T	101	PEK	O03-C21	4.47	1.46	1.33
18	N	607	TGL	OG1-CA1	4.44	1.46	1.33
19	C	307	PGV	O01-C1	4.42	1.46	1.34
19	N	610	PGV	O03-C19	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	606	TGL	OG2-CB1	4.39	1.46	1.34
27	C	308	CDL	OB8-CB7	4.37	1.46	1.33
27	C	308	CDL	OB6-CB5	4.37	1.46	1.33
26	P	303	PEK	O01-C1	4.34	1.46	1.34
18	A	607	TGL	OG3-CC1	4.33	1.46	1.33
18	A	606	TGL	OG3-CC1	4.33	1.46	1.33
18	N	607	TGL	OG3-CC1	4.25	1.45	1.33
18	A	607	TGL	OG2-CB1	4.18	1.46	1.34
19	N	610	PGV	O01-C1	4.17	1.46	1.34
27	C	308	CDL	C59-C58	-4.05	1.31	1.51
14	N	602[A]	HEA	CHB-C4A	4.02	1.46	1.38
27	C	308	CDL	C82-C81	-3.98	1.32	1.51
21	A	610	PSC	C13-C12	3.83	1.53	1.31
27	C	308	CDL	C79-C78	-3.83	1.32	1.51
27	P	307	CDL	C82-C81	-3.81	1.32	1.51
21	O	302	PSC	C13-C12	3.81	1.53	1.31
27	C	308	CDL	C62-C61	-3.79	1.32	1.51
27	P	307	CDL	C79-C78	-3.72	1.33	1.51
27	T	102	CDL	C62-C61	-3.71	1.33	1.51
27	T	102	CDL	C82-C81	-3.69	1.33	1.51
27	T	102	CDL	C59-C58	-3.67	1.33	1.51
27	P	307	CDL	C59-C58	-3.66	1.33	1.51
27	N	601	CDL	C42-C41	-3.64	1.33	1.51
27	N	601	CDL	C62-C61	-3.62	1.33	1.51
27	P	307	CDL	C39-C38	-3.61	1.33	1.51
27	P	307	CDL	C42-C41	-3.61	1.33	1.51
19	A	611	PGV	O01-C1	3.61	1.44	1.34
26	C	304	PEK	O03-C21	3.61	1.43	1.33
27	C	308	CDL	C39-C38	-3.56	1.34	1.51
27	P	307	CDL	C22-C21	-3.55	1.34	1.51
27	C	308	CDL	C42-C41	-3.54	1.34	1.51
27	T	102	CDL	C79-C78	-3.52	1.34	1.51
19	N	612	PGV	O01-C1	3.51	1.44	1.34
27	N	601	CDL	C19-C18	-3.46	1.34	1.51
27	P	307	CDL	C19-C18	-3.45	1.34	1.51
27	T	102	CDL	C19-C18	-3.43	1.34	1.51
27	N	601	CDL	C82-C81	-3.43	1.34	1.51
27	N	601	CDL	C39-C38	-3.38	1.35	1.51
27	T	102	CDL	C22-C21	-3.37	1.35	1.51
27	N	601	CDL	C79-C78	-3.36	1.35	1.51
14	N	603	HEA	CHB-C4A	3.32	1.44	1.38
23	L	105	DMU	O16-C6	3.30	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	CHB-C4A	3.30	1.44	1.38
14	A	601[A]	HEA	C1A-C2A	-3.27	1.39	1.45
14	N	603	HEA	CHA-C1A	3.25	1.44	1.38
26	P	304	PEK	O03-C21	3.22	1.42	1.33
14	N	602[A]	HEA	CHA-C1A	3.22	1.44	1.38
14	N	603	HEA	C4D-C3D	-3.21	1.39	1.45
14	A	602	HEA	C4D-C3D	-3.13	1.39	1.45
14	A	601[A]	HEA	CHA-C4D	3.11	1.46	1.39
14	N	603	HEA	C4C-NC	-3.10	1.33	1.39
14	N	602[A]	HEA	C3A-C4A	-3.02	1.40	1.46
14	A	601[A]	HEA	CHC-C4B	2.94	1.44	1.38
27	N	601	CDL	C58-C59	-2.94	1.33	1.51
19	C	306	PGV	O01-C1	2.94	1.42	1.34
14	N	603	HEA	C4B-NB	-2.90	1.35	1.40
26	C	304	PEK	O01-C1	2.90	1.42	1.34
14	N	602[A]	HEA	C4C-NC	-2.87	1.34	1.39
14	N	603	HEA	FE-NA	2.87	2.04	1.95
14	A	602	HEA	C4C-NC	-2.85	1.34	1.39
27	T	102	CDL	C41-C42	-2.84	1.34	1.51
14	A	601[A]	HEA	CHD-C1D	2.84	1.44	1.38
19	A	611	PGV	O03-C19	2.80	1.41	1.33
19	N	612	PGV	O03-C19	2.80	1.41	1.33
14	A	602	HEA	CHD-C1D	2.76	1.44	1.38
14	A	601[A]	HEA	C4D-C3D	-2.75	1.40	1.45
27	N	601	CDL	C22-C21	-2.73	1.34	1.51
14	N	602[A]	HEA	CHC-C4B	2.71	1.43	1.38
14	N	602[A]	HEA	C1A-C2A	-2.70	1.40	1.45
14	A	601[A]	HEA	CHA-C1A	2.67	1.43	1.38
14	A	601[A]	HEA	CAD-C3D	2.66	1.58	1.51
14	N	602[A]	HEA	FE-ND	2.66	2.03	1.94
14	A	602	HEA	CHC-C4B	2.64	1.43	1.38
14	N	602[A]	HEA	CHD-C1D	2.64	1.43	1.38
23	D	206	DMU	O16-C6	2.63	1.44	1.40
14	A	601[A]	HEA	C4C-NC	-2.63	1.34	1.39
14	N	603	HEA	CHD-C1D	2.63	1.43	1.38
14	N	602[A]	HEA	C4B-NB	-2.62	1.35	1.40
14	N	603	HEA	C3A-C4A	-2.61	1.41	1.46
14	A	602	HEA	CHC-C1C	2.61	1.45	1.39
14	N	603	HEA	CHC-C4B	2.59	1.43	1.38
23	P	317	DMU	O16-C6	2.57	1.44	1.40
14	A	602	HEA	C4A-NA	-2.55	1.34	1.39
14	A	602	HEA	O11-C11	2.55	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	CHA-C4D	2.54	1.45	1.39
14	A	601[A]	HEA	FE-NA	2.54	2.03	1.95
19	P	305	PGV	O01-C1	2.52	1.41	1.34
19	P	305	PGV	O03-C19	2.51	1.40	1.33
14	A	602	HEA	CMC-C2C	2.51	1.55	1.50
14	N	603	HEA	CHA-C4D	2.50	1.44	1.39
14	A	601[A]	HEA	CHB-C4A	2.48	1.43	1.38
14	A	602	HEA	FE-NC	2.48	2.03	1.95
14	N	603	HEA	O11-C11	2.47	1.48	1.42
14	A	601[A]	HEA	C3A-C4A	-2.46	1.41	1.46
14	N	603	HEA	C4B-C3B	-2.46	1.40	1.44
14	A	601[A]	HEA	CMC-C2C	2.46	1.55	1.50
14	N	602[A]	HEA	FE-NC	2.45	2.03	1.95
14	N	602[A]	HEA	C1D-ND	-2.45	1.36	1.40
14	A	602	HEA	FE-ND	2.43	2.02	1.94
19	A	611	PGV	O01-C02	-2.42	1.40	1.46
19	C	306	PGV	O03-C19	2.42	1.40	1.33
14	N	603	HEA	FE-NC	2.41	2.03	1.95
14	A	601[A]	HEA	C4A-NA	-2.41	1.35	1.39
19	N	612	PGV	O01-C02	-2.41	1.40	1.46
14	A	602	HEA	C1A-C2A	-2.40	1.41	1.45
14	A	602	HEA	CHA-C1A	2.40	1.43	1.38
26	P	304	PEK	O01-C1	2.40	1.41	1.34
14	A	601[A]	HEA	C4B-NB	-2.37	1.36	1.40
14	A	601[A]	HEA	FE-ND	2.36	2.02	1.94
14	N	603	HEA	CBA-CGA	2.35	1.56	1.50
23	C	310	DMU	O16-C6	2.33	1.44	1.40
14	N	603	HEA	CHC-C1C	2.33	1.44	1.39
14	N	603	HEA	C1D-ND	-2.31	1.36	1.40
14	N	602[A]	HEA	FE-NA	2.30	2.02	1.95
14	N	603	HEA	CHB-C1B	2.29	1.44	1.39
14	N	602[A]	HEA	CHA-C4D	2.24	1.44	1.39
14	N	602[A]	HEA	O2D-CGD	-2.24	1.23	1.30
14	A	601[A]	HEA	CBD-CGD	2.23	1.55	1.50
14	A	602	HEA	CBA-CGA	2.23	1.55	1.50
14	N	602[A]	HEA	CBD-CGD	2.22	1.55	1.50
14	A	601[A]	HEA	C4B-C3B	-2.21	1.40	1.44
14	N	602[A]	HEA	C4A-NA	-2.20	1.35	1.39
23	X	104	DMU	O16-C6	2.19	1.43	1.40
14	A	602	HEA	FE-NA	2.17	2.02	1.95
14	N	603	HEA	FE-NB	2.14	2.01	1.94
14	A	602	HEA	C3A-C4A	-2.13	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602	HEA	C4B-C3B	-2.13	1.41	1.44
14	A	601[A]	HEA	FE-NB	2.13	2.01	1.94
14	N	603	HEA	C1A-NA	-2.13	1.35	1.39
25	G	101	CHD	O7-C7	2.12	1.47	1.43
14	A	602	HEA	C11-C3B	2.11	1.54	1.51
23	P	316	DMU	O16-C6	2.11	1.43	1.40
14	N	602[A]	HEA	O11-C11	2.10	1.47	1.42
14	N	603	HEA	C4A-NA	-2.07	1.35	1.39
19	C	306	PGV	O01-C02	-2.05	1.41	1.46
25	C	309	CHD	C10-C9	-2.05	1.52	1.56
14	A	601[A]	HEA	CMA-C3A	2.04	1.49	1.45
19	P	305	PGV	O01-C02	-2.03	1.41	1.46
26	P	304	PEK	C05-C04	2.02	1.58	1.49
14	A	601[A]	HEA	CBA-CGA	2.02	1.55	1.50

All (315) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	J	101	CHD	C14-C8-C9	-7.35	99.48	109.75
25	J	101	CHD	C14-C8-C7	7.35	121.60	111.85
25	J	101	CHD	C10-C9-C8	7.25	119.92	111.84
14	N	602[A]	HEA	C13-C12-C11	-6.64	103.78	114.39
18	A	606	TGL	OG2-CB1-CB2	6.39	125.30	111.48
19	C	307	PGV	O03-C19-C20	6.32	131.09	111.83
18	N	607	TGL	OG2-CB1-CB2	5.94	124.33	111.48
25	Y	102	CHD	C1-C10-C5	5.83	116.12	107.75
19	C	307	PGV	O01-C1-C2	5.67	123.75	111.48
25	L	102	CHD	C4-C5-C10	5.64	118.66	112.66
25	L	102	CHD	C21-C20-C17	5.52	121.17	112.88
25	J	101	CHD	C14-C13-C12	5.36	112.31	107.42
23	L	105	DMU	C18-O16-C6	5.26	122.67	113.68
25	C	301	CHD	C18-C13-C12	5.26	114.32	109.06
14	A	601[A]	HEA	C13-C12-C11	-5.24	106.02	114.39
25	Y	102	CHD	C9-C11-C12	-5.23	107.44	114.29
25	J	101	CHD	C9-C11-C12	-4.96	107.81	114.29
25	Y	102	CHD	C6-C5-C4	-4.73	105.82	111.23
23	L	105	DMU	O5-C6-O16	4.71	121.18	110.04
27	P	307	CDL	OB8-CB7-C71	4.71	126.19	111.83
23	P	317	DMU	C10-O1-C9	4.63	122.77	113.72
25	Y	102	CHD	C21-C20-C17	4.59	119.78	112.88
26	C	303	PEK	O03-C21-C22	4.59	125.82	111.83
25	Y	102	CHD	C14-C8-C7	4.54	117.87	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	C3D-C4D-ND	4.53	114.73	110.35
25	J	101	CHD	C22-C20-C17	4.50	119.65	110.33
19	C	307	PGV	C01-O03-C19	4.39	133.16	117.12
25	L	102	CHD	C5-C4-C3	4.37	119.30	112.71
26	C	303	PEK	O01-C1-C2	4.36	120.92	111.48
18	L	101	TGL	OG2-CB1-CB2	4.35	120.89	111.48
25	L	102	CHD	C13-C17-C20	4.33	124.72	119.48
14	A	601[A]	HEA	C3D-C4D-ND	4.25	114.45	110.35
19	N	610	PGV	C02-O01-C1	-4.24	107.65	117.80
25	L	102	CHD	C17-C13-C12	-4.23	113.86	117.67
25	L	102	CHD	C10-C9-C8	4.22	116.55	111.84
25	J	101	CHD	C9-C10-C5	4.22	114.37	108.51
26	P	303	PEK	O03-C21-C22	4.16	123.79	111.15
25	J	101	CHD	C13-C17-C20	4.16	124.53	119.48
14	A	601[A]	HEA	C2B-C1B-NB	4.09	114.63	109.90
25	L	102	CHD	C11-C9-C10	-4.07	109.57	113.70
25	B	302	CHD	C6-C5-C4	-4.01	106.65	111.23
25	Y	102	CHD	C19-C10-C1	-3.98	101.98	108.31
14	N	602[A]	HEA	C26-C15-C16	3.88	121.96	115.23
14	A	601[A]	HEA	C2D-C1D-ND	3.87	114.28	109.84
18	L	101	TGL	OG1-CA1-CA2	3.84	123.53	111.83
27	C	308	CDL	OB8-CB7-C71	3.80	123.41	111.83
27	C	308	CDL	C52-C51-CB5	-3.78	99.83	113.69
25	L	102	CHD	C6-C5-C4	-3.72	106.98	111.23
18	A	607	TGL	OG3-CC1-CC2	3.69	123.09	111.83
23	L	105	DMU	O5-C4-C57	3.68	112.73	106.83
26	T	101	PEK	O03-C21-C22	3.68	126.02	112.14
23	L	105	DMU	C3-C4-C57	-3.66	105.72	112.50
18	A	607	TGL	OG1-CA1-CA2	3.62	122.87	111.83
19	A	611	PGV	O03-C19-O04	-3.60	114.63	123.63
19	C	307	PGV	O03-C19-O04	-3.59	114.65	123.63
14	N	602[A]	HEA	C2D-C1D-ND	3.58	113.95	109.84
25	J	101	CHD	C1-C10-C9	-3.56	105.81	111.34
23	P	317	DMU	C10-C5-C7	3.56	117.49	110.01
14	N	602[A]	HEA	C2B-C1B-NB	3.55	114.01	109.90
14	N	602[A]	HEA	C3C-C2C-C1C	-3.55	102.99	107.17
18	L	101	TGL	CC3-CC2-CC1	3.54	126.66	113.69
25	Y	102	CHD	C14-C13-C12	3.53	110.64	107.42
25	J	101	CHD	C18-C13-C14	-3.52	105.69	111.20
25	L	102	CHD	C14-C13-C12	3.51	110.62	107.42
27	C	308	CDL	OB6-CB5-C51	3.50	122.50	111.83
14	A	602	HEA	C2B-C1B-NB	3.50	113.94	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M	101	DMU	C18-O16-C6	-3.46	107.77	113.68
18	A	606	TGL	CB3-CB2-CB1	-3.44	101.09	113.69
14	A	602	HEA	C3B-C4B-NB	3.43	113.78	109.84
23	P	317	DMU	C6-C1-C2	3.42	117.20	110.01
19	A	611	PGV	O03-C19-C20	3.40	122.20	111.83
23	P	317	DMU	O16-C6-C1	3.40	113.44	108.27
14	A	602	HEA	CAD-CBD-CGD	-3.39	104.67	113.67
25	C	301	CHD	C22-C20-C17	-3.39	103.31	110.33
23	P	317	DMU	O1-C9-C8	3.38	115.79	109.70
25	C	301	CHD	C1-C2-C3	-3.37	106.02	110.48
23	D	206	DMU	C6-O5-C4	3.36	120.28	113.72
25	Y	102	CHD	C4-C3-C2	-3.35	106.53	110.62
14	A	601[A]	HEA	O1A-CGA-CBA	-3.34	112.50	123.09
26	P	303	PEK	O01-C1-C2	3.32	118.67	111.48
27	P	307	CDL	OB8-CB7-OB9	-3.32	115.32	123.63
25	G	101	CHD	C6-C5-C4	-3.32	107.43	111.23
23	P	317	DMU	O1-C10-C5	3.30	117.16	110.37
19	P	305	PGV	O01-C1-O02	-3.30	115.98	123.70
25	J	101	CHD	C15-C14-C8	3.30	122.89	118.36
14	N	602[A]	HEA	C3C-C4C-NC	3.29	112.57	109.80
14	A	601[A]	HEA	O2A-CGA-CBA	3.27	124.33	114.00
18	A	607	TGL	OG3-CC1-OC1	-3.25	115.51	123.63
14	A	601[A]	HEA	CAA-CBA-CGA	-3.24	105.07	113.67
14	A	601[A]	HEA	CHA-C4D-C3D	-3.24	120.06	124.77
14	A	601[A]	HEA	C1B-C2B-C3B	-3.22	103.06	106.80
14	N	602[A]	HEA	C1D-ND-C4D	-3.21	101.41	105.21
18	L	101	TGL	CG3-CG2-CG1	-3.18	104.36	111.78
25	B	302	CHD	C13-C17-C20	-3.16	115.66	119.48
19	N	612	PGV	O03-C19-O04	-3.16	115.73	123.63
23	P	308	DMU	C18-O16-C6	-3.14	108.32	113.68
25	L	102	CHD	C1-C10-C5	3.13	112.24	107.75
26	C	304	PEK	O03-C21-C22	3.13	121.37	111.83
27	C	308	CDL	C61-C60-C59	-3.11	98.64	114.37
14	A	602	HEA	C1D-C2D-C3D	-3.07	103.75	106.98
14	A	601[A]	HEA	C1D-ND-C4D	-3.06	101.58	105.21
14	N	602[A]	HEA	C2C-C1C-NC	3.04	115.02	110.14
18	L	101	TGL	OG3-CC1-OC1	-3.00	116.14	123.63
25	Y	102	CHD	C10-C9-C8	2.98	115.17	111.84
25	L	102	CHD	C1-C10-C9	-2.96	106.74	111.34
14	A	602	HEA	C13-C12-C11	-2.95	109.68	114.39
14	N	602[A]	HEA	O2A-CGA-CBA	2.95	123.32	114.00
25	L	102	CHD	C9-C10-C5	2.95	112.61	108.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	L	102	CHD	C14-C8-C7	2.94	115.76	111.85
27	N	601	CDL	CB6-OB8-CB7	2.94	126.08	116.90
14	N	603	HEA	C3C-C4C-NC	2.93	112.27	109.80
26	T	101	PEK	C01-O03-C21	2.93	125.45	116.07
14	A	602	HEA	C20-C19-C18	-2.93	114.59	121.17
23	D	206	DMU	C10-O1-C9	2.93	119.44	113.72
25	J	101	CHD	C5-C6-C7	-2.92	110.92	114.40
14	N	602[A]	HEA	C3A-C2A-C1A	-2.92	104.29	107.05
23	P	317	DMU	O7-C10-C5	2.91	115.25	108.09
19	N	610	PGV	O01-C1-C2	2.89	117.74	111.48
27	T	102	CDL	OB8-CB7-C71	2.89	120.65	111.83
27	P	307	CDL	OB6-CB5-C51	2.89	120.64	111.83
19	N	610	PGV	O03-C19-C20	2.86	120.55	111.83
14	A	601[A]	HEA	C3C-C4C-NC	2.84	112.19	109.80
25	B	302	CHD	C16-C17-C13	2.84	106.29	103.54
23	C	310	DMU	C8-C7-C5	2.84	115.81	110.83
14	A	602	HEA	C4B-NB-C1B	-2.83	101.86	105.21
18	A	606	TGL	OG3-CC1-CC2	2.82	120.42	111.83
23	P	308	DMU	O7-C3-C2	2.81	114.38	107.23
25	C	309	CHD	C11-C9-C10	-2.79	110.87	113.70
19	C	307	PGV	O01-C1-O02	-2.79	117.19	123.70
25	B	302	CHD	C19-C10-C5	-2.79	105.78	110.44
14	A	602	HEA	CHB-C4A-NA	2.76	127.46	124.45
25	C	309	CHD	C19-C10-C9	-2.74	107.50	111.18
25	C	301	CHD	C18-C13-C17	-2.74	106.91	111.20
14	A	602	HEA	C3C-C2C-C1C	-2.73	103.95	107.17
27	C	308	CDL	OB8-CB7-OB9	-2.73	116.79	123.63
14	N	603	HEA	CHB-C1B-C2B	-2.73	120.72	125.03
14	N	602[A]	HEA	CAD-C3D-C2D	2.73	132.98	127.87
25	L	102	CHD	C18-C13-C14	-2.73	106.93	111.20
18	A	606	TGL	OG1-CA1-CA2	2.73	120.15	111.83
23	D	206	DMU	O1-C9-C8	2.73	114.61	109.70
18	N	608	TGL	OG3-CC1-OC1	-2.72	115.08	123.20
14	N	602[A]	HEA	C16-C15-C14	-2.72	115.06	121.17
19	N	612	PGV	O03-C19-C20	2.70	120.08	111.83
23	L	105	DMU	O5-C6-C1	-2.70	104.81	110.37
14	A	602	HEA	C2D-C1D-ND	2.70	112.94	109.84
18	L	101	TGL	OG1-CG1-CG2	2.69	116.17	108.40
14	N	602[A]	HEA	CAA-CBA-CGA	-2.69	106.52	113.67
26	C	303	PEK	C01-O03-C21	2.69	126.97	117.12
25	J	101	CHD	C13-C14-C8	-2.69	111.31	114.72
23	D	206	DMU	C11-C9-C8	-2.68	106.44	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	301	CHD	C22-C20-C17	-2.68	104.78	110.33
14	A	602	HEA	C27-C19-C20	2.67	119.87	115.23
19	P	306	PGV	O03-C19-C20	2.67	122.45	114.00
14	N	603	HEA	O2A-CGA-CBA	2.67	122.44	114.00
18	N	607	TGL	OG1-CA1-CA2	2.66	119.96	111.83
14	N	602[A]	HEA	C1B-C2B-C3B	-2.65	103.73	106.80
14	N	603	HEA	C13-C12-C11	-2.65	110.16	114.39
25	P	301	CHD	C11-C9-C10	-2.65	111.02	113.70
25	L	102	CHD	C11-C12-C13	2.63	113.94	111.26
26	C	303	PEK	O03-C21-O04	-2.63	117.06	123.63
25	P	301	CHD	C22-C23-C24	-2.62	105.50	112.49
19	P	306	PGV	O03-C19-O04	-2.62	116.60	123.33
25	Y	102	CHD	C13-C17-C20	2.62	122.65	119.48
26	T	101	PEK	O03-C21-O04	-2.61	115.40	123.20
25	J	101	CHD	C6-C5-C4	-2.60	108.26	111.23
14	N	603	HEA	C3B-C4B-NB	2.58	112.81	109.84
14	A	601[A]	HEA	CHB-C1B-NB	-2.56	121.67	124.42
26	P	304	PEK	O03-C21-C22	2.55	119.60	111.83
25	P	301	CHD	C6-C5-C10	-2.54	109.96	112.66
14	A	602	HEA	C13-C14-C15	-2.54	121.82	127.62
18	N	609	TGL	OG3-CC1-CC2	2.53	121.71	112.14
25	Y	102	CHD	C15-C14-C8	2.53	121.83	118.36
14	N	603	HEA	C4C-CHD-C1D	-2.53	120.31	126.25
18	N	608	TGL	OG3-CC1-CC2	2.52	121.67	112.14
26	P	304	PEK	C8-C7-C6	-2.52	99.63	112.02
26	C	303	PEK	O01-C1-O02	-2.51	117.84	123.70
14	N	603	HEA	C2C-C1C-NC	2.51	114.16	110.14
19	C	307	PGV	C21-C20-C19	-2.50	104.52	113.69
25	L	102	CHD	O25-C24-C23	-2.50	115.15	123.09
25	Y	102	CHD	C2-C1-C10	2.50	116.96	112.74
18	N	607	TGL	OG3-CC1-CC2	2.50	119.46	111.83
26	P	303	PEK	C01-O03-C21	2.50	126.24	117.12
23	D	206	DMU	C10-C5-C7	2.47	115.22	110.01
25	B	302	CHD	C11-C9-C10	-2.47	111.19	113.70
26	P	303	PEK	O03-C21-O04	-2.47	117.44	123.63
26	C	303	PEK	O03-C01-C02	2.46	115.48	108.40
19	C	307	PGV	O04-C19-C20	-2.46	114.17	123.78
14	N	603	HEA	C2B-C1B-NB	2.45	112.74	109.90
23	C	310	DMU	C10-C5-C7	2.44	115.15	110.01
18	A	607	TGL	OG2-CB1-CB2	2.44	116.77	111.48
23	C	310	DMU	O7-C10-C5	2.44	114.09	108.09
19	C	306	PGV	O03-C19-O04	-2.44	117.53	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602	HEA	C2C-C1C-NC	2.42	114.03	110.14
19	A	611	PGV	C32-C31-C30	-2.42	102.15	114.37
14	A	601[A]	HEA	C13-C14-C15	-2.41	122.10	127.62
14	N	603	HEA	C1D-C2D-C3D	-2.40	104.45	106.98
27	C	308	CDL	C80-C79-C78	2.40	126.51	114.37
27	C	308	CDL	C77-C76-C75	-2.40	102.25	114.37
27	P	307	CDL	C83-C82-C81	2.39	126.45	114.37
25	P	301	CHD	O12-C12-C13	-2.39	106.98	111.02
19	N	612	PGV	O01-C02-C01	-2.39	99.77	108.34
14	A	601[A]	HEA	C1D-C2D-C3D	-2.38	104.47	106.98
23	C	310	DMU	C10-O1-C9	-2.38	109.07	113.72
23	D	206	DMU	C7-C8-C9	2.38	114.55	110.23
25	Y	102	CHD	C16-C17-C13	-2.38	101.23	103.54
25	L	102	CHD	C15-C14-C8	2.37	121.61	118.36
23	P	308	DMU	C1-C2-C3	-2.37	104.31	109.68
25	C	301	CHD	C4-C5-C10	-2.37	110.14	112.66
23	C	310	DMU	C7-C8-C9	2.36	114.51	110.23
19	N	612	PGV	C01-O03-C19	-2.36	108.50	117.12
25	J	101	CHD	C11-C9-C8	-2.35	107.42	110.89
14	A	601[A]	HEA	C4B-NB-C1B	-2.35	102.43	105.21
14	N	603	HEA	O11-C11-C3B	-2.34	106.97	111.26
14	A	602	HEA	C4C-CHD-C1D	-2.34	120.75	126.25
25	L	102	CHD	C14-C8-C9	-2.33	106.49	109.75
14	N	603	HEA	C13-C14-C15	-2.33	122.29	127.62
25	G	101	CHD	C18-C13-C12	-2.33	106.72	109.06
27	C	308	CDL	C81-C80-C79	-2.33	102.60	114.37
14	N	603	HEA	C27-C19-C20	2.32	119.25	115.23
25	P	301	CHD	C18-C13-C12	2.31	111.37	109.06
23	Z	101	DMU	O1-C9-C8	2.31	113.86	109.70
23	P	317	DMU	C1-C2-C3	2.30	114.90	109.68
14	A	602	HEA	C26-C15-C16	2.30	119.22	115.23
23	D	206	DMU	O16-C6-C1	2.30	111.76	108.27
25	J	101	CHD	O7-C7-C8	2.29	114.78	109.52
27	C	308	CDL	CB4-OB6-CB5	-2.29	109.75	116.90
14	A	601[A]	HEA	C26-C15-C16	2.29	119.20	115.23
18	A	607	TGL	CG3-CG2-CG1	-2.29	106.45	111.78
25	C	301	CHD	C19-C10-C1	-2.28	104.68	108.31
26	C	304	PEK	O03-C21-O04	-2.28	117.94	123.63
26	P	304	PEK	C3-C2-C1	-2.27	105.39	113.69
27	N	601	CDL	C40-C39-C38	2.26	125.80	114.37
14	A	601[A]	HEA	C1A-CHA-C4D	-2.26	121.22	126.02
25	C	301	CHD	C11-C9-C10	-2.26	111.41	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	101	TGL	OG3-CC1-CC2	2.25	118.71	111.83
25	L	102	CHD	C18-C13-C12	2.25	111.31	109.06
27	C	308	CDL	C62-C61-C60	2.25	125.74	114.37
25	C	309	CHD	C14-C8-C9	-2.25	106.61	109.75
25	P	301	CHD	C18-C13-C17	-2.25	107.69	111.20
14	N	603	HEA	C3C-C2C-C1C	-2.24	104.53	107.17
26	C	303	PEK	C02-O01-C1	-2.24	112.44	117.80
23	P	308	DMU	C10-C5-C7	2.24	114.72	110.01
14	N	603	HEA	C2D-C1D-ND	2.24	112.41	109.84
26	C	304	PEK	C3-C2-C1	-2.24	105.50	113.69
25	C	301	CHD	C5-C4-C3	-2.23	109.34	112.71
18	N	607	TGL	OG2-CB1-OB1	-2.23	118.49	123.70
27	P	307	CDL	OB8-CB6-CB4	2.23	115.12	108.61
19	A	611	PGV	O01-C1-C2	2.22	116.29	111.48
14	N	603	HEA	CHC-C1C-C2C	-2.22	120.97	127.43
19	N	612	PGV	C9-C10-C11	-2.22	100.17	112.60
19	N	612	PGV	O01-C1-C2	2.20	116.25	111.48
25	G	101	CHD	C13-C14-C8	-2.19	111.95	114.72
25	L	102	CHD	C22-C20-C17	-2.17	105.82	110.33
25	J	101	CHD	C16-C17-C20	2.15	115.43	112.18
26	P	304	PEK	O03-C21-O04	-2.14	118.27	123.63
19	C	307	PGV	C03-C02-C01	-2.14	106.67	112.69
18	N	609	TGL	CG3-OG3-CC1	2.13	122.88	116.07
19	C	306	PGV	O03-C19-C20	2.12	118.31	111.83
14	N	603	HEA	CHA-C4D-C3D	-2.12	121.68	124.77
14	N	602[A]	HEA	CHA-C1A-C2A	-2.12	121.52	124.86
23	P	316	DMU	C3-C2-C1	2.12	113.72	110.67
25	C	309	CHD	C1-C10-C5	2.12	110.79	107.75
23	Z	101	DMU	C10-O7-C3	-2.12	112.96	117.98
25	Y	102	CHD	C21-C20-C22	-2.11	107.07	110.34
14	N	602[A]	HEA	O1A-CGA-CBA	-2.11	116.40	123.09
25	B	302	CHD	O26-C24-C23	2.11	120.66	114.00
14	A	602	HEA	CHC-C1C-C2C	-2.10	121.32	127.43
14	A	602	HEA	C4A-CHB-C1B	-2.10	121.55	126.02
14	A	602	HEA	CMB-C2B-C1B	2.10	128.31	125.03
25	L	102	CHD	C22-C23-C24	-2.10	106.89	112.49
23	C	310	DMU	C18-O16-C6	2.09	117.25	113.68
25	P	301	CHD	C16-C17-C20	-2.09	109.02	112.18
23	C	310	DMU	C10-O7-C3	-2.09	113.03	117.98
23	P	308	DMU	O1-C10-C5	2.08	114.65	110.37
25	L	102	CHD	C13-C14-C8	-2.08	112.08	114.72
14	N	603	HEA	C21-C22-C23	-2.08	120.70	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	302	PSC	C14-C13-C12	-2.08	109.25	124.83
25	P	301	CHD	C21-C20-C22	-2.08	107.12	110.34
25	C	301	CHD	C1-C10-C5	2.07	110.72	107.75
26	C	304	PEK	O01-C1-O02	-2.07	118.87	123.70
19	A	611	PGV	C34-C33-C32	-2.06	99.43	113.36
23	P	308	DMU	C7-C8-C9	2.06	113.97	110.23
27	N	601	CDL	C19-C18-C17	2.06	124.80	114.37
25	B	302	CHD	C13-C14-C8	-2.06	112.11	114.72
18	A	606	TGL	OB1-CB1-CB2	-2.06	115.72	123.78
14	N	603	HEA	O1A-CGA-CBA	-2.05	116.58	123.09
25	P	301	CHD	C5-C4-C3	-2.05	109.61	112.71
27	P	307	CDL	OB6-CB4-CB6	-2.05	102.61	108.61
14	N	603	HEA	CMB-C2B-C1B	2.05	128.23	125.03
27	N	601	CDL	C44-C43-C42	-2.05	104.03	114.37
23	D	206	DMU	O61-C57-C4	2.04	118.29	111.33
14	N	603	HEA	C3A-C2A-C1A	-2.04	105.11	107.05
26	C	304	PEK	O01-C1-C2	2.04	115.89	111.48
23	L	105	DMU	O61-C57-C4	2.04	117.01	111.77
14	N	602[A]	HEA	CMC-C2C-C1C	2.04	128.52	125.42
18	A	607	TGL	OG1-CA1-OA1	-2.03	118.54	123.63
19	C	306	PGV	O03-C01-C02	-2.03	102.53	108.40
14	N	603	HEA	CMC-C2C-C1C	2.03	128.51	125.42
23	P	308	DMU	C6-O5-C4	2.03	117.69	113.72
25	Y	102	CHD	O7-C7-C8	2.03	114.17	109.52
14	A	602	HEA	C3A-C2A-C1A	-2.03	105.13	107.05
25	P	301	CHD	C1-C10-C5	2.02	110.65	107.75
18	A	606	TGL	OG2-CB1-OB1	-2.02	118.97	123.70
25	J	101	CHD	O25-C24-C23	-2.02	116.67	123.09
25	C	309	CHD	C17-C13-C14	2.02	102.14	100.11
18	N	607	TGL	OG3-CC1-OC1	-2.02	118.57	123.63
25	C	309	CHD	C6-C5-C4	-2.02	108.92	111.23
18	A	606	TGL	CG3-CG2-CG1	-2.02	107.08	111.78
27	C	308	CDL	C84-C83-C82	-2.02	104.17	114.37
14	A	602	HEA	CAA-CBA-CGA	-2.02	108.32	113.67
25	C	301	CHD	O12-C12-C13	-2.02	107.62	111.02
18	A	606	TGL	CG2-OG2-CB1	-2.01	112.97	117.80
25	J	101	CHD	C23-C22-C20	-2.01	110.70	114.46
14	A	602	HEA	CBD-CAD-C3D	2.01	118.09	112.53
18	L	101	TGL	OG1-CA1-OA1	-2.00	118.61	123.63

There are no chirality outliers.

All (577) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C2A-C3A-CMA-OMA
14	N	602[A]	HEA	C2A-C3A-CMA-OMA
18	A	607	TGL	OB1-CB1-OG2-CG2
18	L	101	TGL	CB2-CB1-OG2-CG2
18	L	101	TGL	OB1-CB1-OG2-CG2
18	N	609	TGL	CC2-CC1-OG3-CG3
19	C	307	PGV	O04-C19-O03-C01
19	C	307	PGV	C20-C19-O03-C01
19	N	610	PGV	C04-O12-P-O11
19	N	610	PGV	C04-O12-P-O13
19	N	610	PGV	O04-C19-O03-C01
19	N	610	PGV	C20-C19-O03-C01
23	L	105	DMU	C3-C4-C57-O61
23	L	105	DMU	O5-C4-C57-O61
23	L	105	DMU	O5-C6-O16-C18
25	J	101	CHD	C13-C17-C20-C22
25	J	101	CHD	C16-C17-C20-C21
25	J	101	CHD	C16-C17-C20-C22
26	C	305	PEK	C13-C14-C15-C16
26	P	303	PEK	O04-C21-O03-C01
26	P	303	PEK	C22-C21-O03-C01
26	P	303	PEK	C5-C6-C7-C8
26	T	101	PEK	C6-C7-C8-C9
26	T	101	PEK	C11-C12-C13-C14
26	C	303	PEK	O04-C21-O03-C01
26	T	101	PEK	O04-C21-O03-C01
26	T	101	PEK	C22-C21-O03-C01
26	C	303	PEK	C22-C21-O03-C01
25	L	102	CHD	C13-C17-C20-C21
25	L	102	CHD	C16-C17-C20-C22
18	N	609	TGL	OC1-CC1-OG3-CG3
23	D	206	DMU	C3-C4-C57-O61
18	A	607	TGL	CB2-CB1-OG2-CG2
25	L	102	CHD	C16-C17-C20-C21
25	L	102	CHD	C13-C17-C20-C22
25	L	102	CHD	C20-C22-C23-C24
21	A	610	PSC	C11-C10-C9-C8
26	P	304	PEK	C7-C8-C9-C10
19	N	610	PGV	C2-C1-O01-C02
26	P	303	PEK	C2-C1-O01-C02
25	J	101	CHD	C21-C20-C22-C23
19	N	610	PGV	O02-C1-O01-C02
26	P	303	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
23	D	206	DMU	O5-C4-C57-O61
27	C	308	CDL	OB6-CB4-CB6-OB8
18	A	606	TGL	C22-C23-C24-C25
23	P	308	DMU	O6-C11-C9-O1
18	L	101	TGL	CC1-CC2-CC3-CC4
25	J	101	CHD	C17-C20-C22-C23
19	A	608	PGV	C10-C11-C12-C13
26	C	303	PEK	C4-C5-C6-C7
26	C	303	PEK	C7-C8-C9-C10
26	C	305	PEK	C4-C5-C6-C7
27	C	308	CDL	C37-C38-C39-C40
26	C	303	PEK	O02-C1-O01-C02
18	N	608	TGL	C16-C15-CC9-CC8
25	J	101	CHD	C13-C17-C20-C21
25	C	309	CHD	C17-C20-C22-C23
18	A	606	TGL	C11-C12-C13-C14
27	P	307	CDL	C20-C21-C22-C23
26	C	303	PEK	C2-C1-O01-C02
25	C	309	CHD	C21-C20-C22-C23
19	P	305	PGV	C10-C11-C12-C13
26	C	305	PEK	C10-C11-C12-C13
26	P	304	PEK	C4-C5-C6-C7
26	P	304	PEK	C10-C11-C12-C13
27	P	307	CDL	OB6-CB4-CB6-OB8
22	W	101	EDO	O1-C1-C2-O2
23	C	310	DMU	O16-C18-C19-C22
19	N	610	PGV	O12-C04-C05-O05
23	L	105	DMU	O16-C18-C19-C22
19	P	306	PGV	C10-C11-C12-C13
26	C	304	PEK	C7-C8-C9-C10
26	P	303	PEK	C4-C5-C6-C7
26	T	101	PEK	C13-C14-C15-C16
27	N	601	CDL	C80-C81-C82-C83
27	P	307	CDL	C82-C83-C84-C85
19	C	307	PGV	O02-C1-O01-C02
27	C	308	CDL	C51-CB5-OB6-CB4
18	L	101	TGL	C23-C24-C25-C26
26	C	304	PEK	C22-C23-C24-C25
18	L	101	TGL	CA9-C20-C21-C22
19	C	307	PGV	C2-C1-O01-C02
23	P	308	DMU	C4-C3-O7-C10
19	C	306	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	X	104	DMU	O16-C18-C19-C22
23	Z	101	DMU	O16-C18-C19-C22
23	D	206	DMU	C22-C25-C28-C31
23	P	308	DMU	C19-C22-C25-C28
23	P	308	DMU	O6-C11-C9-C8
23	P	308	DMU	C2-C3-O7-C10
19	C	307	PGV	C24-C25-C26-C27
23	K	102	DMU	C31-C34-C37-C40
23	K	103	DMU	C22-C25-C28-C31
23	M	101	DMU	C19-C22-C25-C28
27	T	102	CDL	C79-C80-C81-C82
23	P	316	DMU	O16-C18-C19-C22
23	C	310	DMU	C18-C19-C22-C25
18	A	606	TGL	C12-C13-C14-C29
26	C	303	PEK	C22-C23-C24-C25
21	O	302	PSC	C11-C10-C9-C8
18	L	101	TGL	C21-C22-C23-C24
18	L	101	TGL	C19-C33-C34-C35
18	A	607	TGL	CC5-CC6-CC7-CC8
18	A	607	TGL	C19-C33-C34-C35
18	L	101	TGL	CA5-CA6-CA7-CA8
19	C	306	PGV	C7-C8-C9-C10
19	C	307	PGV	C4-C5-C6-C7
26	C	304	PEK	C23-C24-C25-C26
18	N	607	TGL	OB1-CB1-OG2-CG2
18	N	607	TGL	C24-C25-C26-C27
27	P	307	CDL	C37-C38-C39-C40
18	N	607	TGL	CB9-C10-C11-C12
23	K	103	DMU	C25-C28-C31-C34
27	N	601	CDL	C37-C38-C39-C40
27	C	308	CDL	OB7-CB5-OB6-CB4
27	T	102	CDL	C60-C61-C62-C63
18	N	608	TGL	C19-C33-C34-C35
18	A	606	TGL	CA5-CA6-CA7-CA8
18	A	607	TGL	CC7-CC8-CC9-C15
18	N	607	TGL	CB3-CB4-CB5-CB6
27	C	308	CDL	C77-C78-C79-C80
23	Z	101	DMU	O6-C11-C9-C8
23	K	104	DMU	C25-C28-C31-C34
19	N	610	PGV	O12-C04-C05-C06
27	P	307	CDL	CB5-C51-C52-C53
18	A	607	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
18	N	609	TGL	CA6-CA7-CA8-CA9
18	N	609	TGL	CC9-C15-C16-C17
19	P	305	PGV	C30-C31-C32-C33
23	P	316	DMU	C31-C34-C37-C40
23	Z	101	DMU	C28-C31-C34-C37
27	N	601	CDL	C32-C33-C34-C35
22	A	612	EDO	O1-C1-C2-O2
22	J	103	EDO	O1-C1-C2-O2
22	L	103	EDO	O1-C1-C2-O2
18	L	101	TGL	C13-C14-C29-C30
27	T	102	CDL	C40-C41-C42-C43
23	L	105	DMU	C25-C28-C31-C34
18	A	606	TGL	CB2-CB1-OG2-CG2
18	N	607	TGL	CB2-CB1-OG2-CG2
27	P	307	CDL	CB6-CB4-OB6-CB5
27	T	102	CDL	C82-C83-C84-C85
27	P	307	CDL	C77-C78-C79-C80
18	A	606	TGL	CC7-CC8-CC9-C15
18	A	606	TGL	C17-C18-C19-C33
18	L	101	TGL	CB6-CB7-CB8-CB9
19	C	306	PGV	C20-C21-C22-C23
19	P	305	PGV	C7-C8-C9-C10
18	N	608	TGL	C21-C22-C23-C24
18	A	607	TGL	CB9-C10-C11-C12
18	A	607	TGL	CA9-C20-C21-C22
18	L	101	TGL	C11-C10-CB9-CB8
19	C	306	PGV	C19-C20-C21-C22
27	P	307	CDL	C51-CB5-OB6-CB4
27	P	307	CDL	C41-C42-C43-C44
21	A	610	PSC	C28-C29-C30-C31
27	P	307	CDL	C57-C58-C59-C60
18	N	609	TGL	C22-C23-C24-C25
27	N	601	CDL	C40-C41-C42-C43
18	N	608	TGL	CC3-CC4-CC5-CC6
21	A	610	PSC	C7-C8-C9-C10
18	N	607	TGL	CC5-CC6-CC7-CC8
23	L	105	DMU	C34-C37-C40-C43
18	N	609	TGL	CA9-C20-C21-C22
18	A	606	TGL	C21-C20-CA9-CA8
19	C	306	PGV	C27-C28-C29-C30
27	N	601	CDL	C17-C18-C19-C20
23	D	206	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
18	N	608	TGL	CB9-C10-C11-C12
26	T	101	PEK	C10-C11-C12-C13
18	N	608	TGL	C22-C23-C24-C25
18	N	607	TGL	C19-C33-C34-C35
23	Q	201	DMU	C18-C19-C22-C25
23	D	207	DMU	O16-C18-C19-C22
27	N	601	CDL	C33-C34-C35-C36
27	N	601	CDL	C77-C78-C79-C80
18	A	606	TGL	CB1-CB2-CB3-CB4
18	N	607	TGL	C20-C21-C22-C23
18	N	609	TGL	CC4-CC5-CC6-CC7
27	P	307	CDL	OB7-CB5-OB6-CB4
18	N	607	TGL	CB1-CB2-CB3-CB4
18	A	607	TGL	CC9-C15-C16-C17
18	N	608	TGL	CB4-CB5-CB6-CB7
27	T	102	CDL	C20-C21-C22-C23
18	L	101	TGL	C18-C19-C33-C34
18	N	608	TGL	C21-C20-CA9-CA8
25	C	309	CHD	C20-C22-C23-C24
18	A	607	TGL	C20-C21-C22-C23
18	N	607	TGL	C10-C11-C12-C13
18	N	607	TGL	C14-C29-C30-C31
19	N	610	PGV	C10-C11-C12-C13
21	O	302	PSC	C29-C30-C31-C32
18	N	607	TGL	C23-C24-C25-C26
19	P	306	PGV	C28-C29-C30-C31
23	Z	101	DMU	C25-C28-C31-C34
19	A	608	PGV	C11-C10-C9-C8
18	A	607	TGL	C16-C17-C18-C19
18	A	606	TGL	OB1-CB1-OG2-CG2
18	A	606	TGL	CC5-CC6-CC7-CC8
27	C	308	CDL	C55-C56-C57-C58
18	N	607	TGL	CA4-CA5-CA6-CA7
18	N	607	TGL	C17-C18-C19-C33
18	A	606	TGL	CC1-CC2-CC3-CC4
18	N	609	TGL	C23-C24-C25-C26
18	L	101	TGL	CC3-CC4-CC5-CC6
18	A	606	TGL	CA2-CA1-OG1-CG1
19	C	307	PGV	C10-C11-C12-C13
18	L	101	TGL	OG1-CG1-CG2-CG3
27	C	308	CDL	C59-C60-C61-C62
27	P	307	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
19	A	608	PGV	C4-C5-C6-C7
23	Z	101	DMU	C22-C25-C28-C31
22	D	204	EDO	O1-C1-C2-O2
22	L	104	EDO	O1-C1-C2-O2
22	N	619	EDO	O1-C1-C2-O2
18	N	609	TGL	CC5-CC6-CC7-CC8
27	N	601	CDL	C42-C43-C44-C45
19	N	612	PGV	C25-C26-C27-C28
18	N	609	TGL	CA4-CA5-CA6-CA7
18	L	101	TGL	C15-C16-C17-C18
19	C	306	PGV	C28-C29-C30-C31
18	A	606	TGL	CB9-C10-C11-C12
18	N	607	TGL	CB7-CB8-CB9-C10
18	A	606	TGL	C21-C22-C23-C24
27	N	601	CDL	C43-C44-C45-C46
14	A	602	HEA	C2A-C3A-CMA-OMA
14	N	603	HEA	C2A-C3A-CMA-OMA
23	Q	201	DMU	C19-C22-C25-C28
18	A	606	TGL	CC2-CC1-OG3-CG3
18	A	607	TGL	CC2-CC1-OG3-CG3
21	A	610	PSC	C29-C30-C31-C32
18	A	606	TGL	C16-C17-C18-C19
18	L	101	TGL	CC5-CC6-CC7-CC8
23	O	306	DMU	C25-C28-C31-C34
18	A	606	TGL	C18-C19-C33-C34
18	A	606	TGL	CB4-CB5-CB6-CB7
18	N	609	TGL	CC6-CC7-CC8-CC9
23	M	101	DMU	C22-C25-C28-C31
18	L	101	TGL	OG1-CA1-CA2-CA3
18	N	609	TGL	C11-C10-CB9-CB8
23	P	316	DMU	C28-C31-C34-C37
27	P	307	CDL	C81-C82-C83-C84
19	C	307	PGV	C23-C24-C25-C26
27	N	601	CDL	C20-C21-C22-C23
18	L	101	TGL	CA2-CA1-OG1-CG1
18	N	608	TGL	C29-C30-C31-C32
23	Z	101	DMU	C34-C37-C40-C43
18	N	608	TGL	CA3-CA4-CA5-CA6
27	P	307	CDL	C40-C41-C42-C43
19	P	305	PGV	C31-C32-C33-C34
18	N	608	TGL	C12-C13-C14-C29
19	A	611	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	C	304	PEK	C10-C11-C12-C13
26	P	304	PEK	C13-C14-C15-C16
18	A	607	TGL	CC3-CC4-CC5-CC6
27	P	307	CDL	C73-C74-C75-C76
18	N	607	TGL	CB4-CB5-CB6-CB7
23	L	105	DMU	C19-C18-O16-C6
23	K	104	DMU	C28-C31-C34-C37
19	A	608	PGV	C21-C22-C23-C24
27	P	307	CDL	C53-C54-C55-C56
23	M	101	DMU	C28-C31-C34-C37
25	Y	102	CHD	C13-C17-C20-C21
18	A	606	TGL	OA1-CA1-OG1-CG1
23	P	308	DMU	O5-C6-O16-C18
27	T	102	CDL	C71-CB7-OB8-CB6
23	D	207	DMU	C25-C28-C31-C34
26	C	305	PEK	C25-C26-C27-C28
23	L	105	DMU	C22-C25-C28-C31
18	A	606	TGL	CA1-CA2-CA3-CA4
19	C	307	PGV	C3-C4-C5-C6
27	C	308	CDL	C58-C59-C60-C61
27	N	601	CDL	C81-C82-C83-C84
23	P	308	DMU	O16-C18-C19-C22
22	A	614	EDO	O1-C1-C2-O2
22	J	102	EDO	O1-C1-C2-O2
22	P	313	EDO	O1-C1-C2-O2
18	A	606	TGL	CA2-CA3-CA4-CA5
27	T	102	CDL	C80-C81-C82-C83
18	L	101	TGL	CB4-CB5-CB6-CB7
26	T	101	PEK	C29-C30-C31-C32
18	L	101	TGL	C21-C20-CA9-CA8
18	N	607	TGL	C16-C15-CC9-CC8
19	C	307	PGV	C13-C14-C15-C16
18	A	607	TGL	C16-C15-CC9-CC8
21	A	610	PSC	C9-C10-C11-C12
21	A	610	PSC	C10-C11-C12-C13
21	O	302	PSC	C9-C10-C11-C12
21	O	302	PSC	C10-C11-C12-C13
26	C	303	PEK	C5-C6-C7-C8
26	C	303	PEK	C6-C7-C8-C9
26	C	303	PEK	C11-C10-C9-C8
26	C	303	PEK	C9-C10-C11-C12
26	C	303	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	C	303	PEK	C12-C13-C14-C15
26	C	304	PEK	C6-C7-C8-C9
26	C	304	PEK	C9-C10-C11-C12
26	C	304	PEK	C12-C13-C14-C15
26	C	305	PEK	C5-C6-C7-C8
26	C	305	PEK	C6-C7-C8-C9
26	C	305	PEK	C11-C10-C9-C8
26	C	305	PEK	C9-C10-C11-C12
26	C	305	PEK	C11-C12-C13-C14
26	C	305	PEK	C12-C13-C14-C15
26	P	303	PEK	C6-C7-C8-C9
26	P	303	PEK	C11-C10-C9-C8
26	P	303	PEK	C11-C12-C13-C14
26	P	303	PEK	C12-C13-C14-C15
26	P	304	PEK	C9-C10-C11-C12
26	P	304	PEK	C12-C13-C14-C15
26	T	101	PEK	C11-C10-C9-C8
26	T	101	PEK	C9-C10-C11-C12
26	T	101	PEK	C12-C13-C14-C15
18	N	608	TGL	CA2-CA3-CA4-CA5
18	N	607	TGL	CA7-CA8-CA9-C20
18	N	607	TGL	CC6-CC7-CC8-CC9
27	C	308	CDL	C36-C37-C38-C39
27	T	102	CDL	C78-C79-C80-C81
18	N	609	TGL	CA5-CA6-CA7-CA8
26	C	304	PEK	O03-C21-C22-C23
18	A	606	TGL	C13-C14-C29-C30
23	Q	201	DMU	C28-C31-C34-C37
18	L	101	TGL	OA1-CA1-OG1-CG1
18	L	101	TGL	CC4-CC5-CC6-CC7
19	P	305	PGV	C24-C25-C26-C27
27	T	102	CDL	OB9-CB7-OB8-CB6
27	T	102	CDL	C43-C44-C45-C46
27	C	308	CDL	C64-C65-C66-C67
19	C	307	PGV	C6-C7-C8-C9
18	L	101	TGL	C10-C11-C12-C13
18	L	101	TGL	CB3-CB4-CB5-CB6
18	A	607	TGL	OC1-CC1-OG3-CG3
18	A	607	TGL	CA6-CA7-CA8-CA9
26	P	304	PEK	C22-C23-C24-C25
18	N	607	TGL	C21-C20-CA9-CA8
18	A	607	TGL	C18-C19-C33-C34

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Mol	Chain	Res	Type	Atoms
18	N	608	TGL	C33-C34-C35-C36
19	A	608	PGV	C2-C3-C4-C5
21	A	610	PSC	C26-C27-C28-C29
23	D	206	DMU	C34-C37-C40-C43
18	A	607	TGL	OG1-CG1-CG2-OG2
18	L	101	TGL	OG2-CG2-CG3-OG3
18	N	607	TGL	CA2-CA3-CA4-CA5
18	N	608	TGL	C11-C12-C13-C14
27	N	601	CDL	C62-C63-C64-C65
18	N	608	TGL	CA9-C20-C21-C22
18	A	606	TGL	OC1-CC1-OG3-CG3
18	N	608	TGL	C10-C11-C12-C13
18	N	609	TGL	CA7-CA8-CA9-C20
18	A	606	TGL	C20-C21-C22-C23
18	L	101	TGL	C24-C25-C26-C27
26	T	101	PEK	C5-C6-C7-C8
19	A	608	PGV	C1-C2-C3-C4
21	A	610	PSC	C27-C28-C29-C30
23	M	101	DMU	C25-C28-C31-C34
19	C	306	PGV	C02-C03-O11-P
19	P	305	PGV	C02-C03-O11-P
19	P	306	PGV	C7-C8-C9-C10
23	P	317	DMU	C18-C19-C22-C25
26	T	101	PEK	C28-C29-C30-C31
14	A	601[A]	HEA	C4A-C3A-CMA-OMA
14	N	602[A]	HEA	C4A-C3A-CMA-OMA
14	N	603	HEA	C4A-C3A-CMA-OMA
26	C	304	PEK	C16-C17-C18-C19
18	L	101	TGL	OG1-CG1-CG2-OG2
18	N	607	TGL	OG2-CG2-CG3-OG3
18	A	607	TGL	CB1-CB2-CB3-CB4
18	L	101	TGL	CG1-CG2-CG3-OG3
18	N	607	TGL	CG1-CG2-CG3-OG3
19	N	612	PGV	C27-C28-C29-C30
23	X	102	DMU	C34-C37-C40-C43
19	A	611	PGV	C11-C12-C13-C14
22	F	108	EDO	O1-C1-C2-O2
27	C	308	CDL	C76-C77-C78-C79
18	L	101	TGL	CA6-CA7-CA8-CA9
27	P	307	CDL	C13-C14-C15-C16
18	N	607	TGL	C13-C14-C29-C30
14	A	601[A]	HEA	O11-C11-C3B-C2B

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Mol	Chain	Res	Type	Atoms
19	N	610	PGV	C04-O12-P-O14
26	C	303	PEK	C03-O11-P-O12
26	P	304	PEK	O12-C04-C05-N
27	T	102	CDL	CB3-CB4-CB6-OB8
18	A	607	TGL	CB3-CB4-CB5-CB6
18	L	101	TGL	CC2-CC3-CC4-CC5
27	P	307	CDL	C42-C43-C44-C45
26	C	304	PEK	C26-C27-C28-C29
27	N	601	CDL	C36-C37-C38-C39
19	N	610	PGV	C01-C02-O01-C1
19	C	306	PGV	C22-C23-C24-C25
19	C	307	PGV	C11-C12-C13-C14
26	C	305	PEK	C3-C4-C5-C6
18	L	101	TGL	C11-C12-C13-C14
23	K	101	DMU	C34-C37-C40-C43
23	K	102	DMU	C28-C31-C34-C37
23	P	317	DMU	C1-C6-O16-C18
25	Y	102	CHD	C16-C17-C20-C22
23	D	207	DMU	C28-C31-C34-C37
18	L	101	TGL	C17-C18-C19-C33
27	P	307	CDL	C72-C73-C74-C75
18	N	607	TGL	C16-C17-C18-C19
19	A	608	PGV	C11-C12-C13-C14
19	C	306	PGV	C11-C12-C13-C14
21	A	610	PSC	C12-C13-C14-C15
22	A	618	EDO	O1-C1-C2-O2
22	A	619	EDO	O1-C1-C2-O2
22	A	620	EDO	O1-C1-C2-O2
23	X	101	DMU	C28-C31-C34-C37
25	Y	102	CHD	C16-C17-C20-C21
23	J	104	DMU	C28-C31-C34-C37
27	P	307	CDL	C17-C18-C19-C20
23	P	308	DMU	C25-C28-C31-C34
19	C	306	PGV	C26-C27-C28-C29
19	N	612	PGV	C11-C12-C13-C14
18	A	606	TGL	C19-C33-C34-C35
27	P	307	CDL	C12-C13-C14-C15
23	K	102	DMU	C22-C25-C28-C31
14	A	602	HEA	CAD-CBD-CGD-O2D
23	D	207	DMU	C18-C19-C22-C25
18	L	101	TGL	C22-C23-C24-C25
18	N	609	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
18	L	101	TGL	CA1-CA2-CA3-CA4
14	A	602	HEA	C2D-C3D-CAD-CBD
27	C	308	CDL	C38-C39-C40-C41
18	N	608	TGL	CB6-CB7-CB8-CB9
19	N	612	PGV	C26-C27-C28-C29
26	C	304	PEK	C4-C5-C6-C7
27	C	308	CDL	C41-C42-C43-C44
25	G	101	CHD	C22-C23-C24-O26
19	C	307	PGV	C22-C23-C24-C25
14	N	603	HEA	CAD-CBD-CGD-O2D
25	P	301	CHD	C22-C23-C24-O25
23	Q	201	DMU	C31-C34-C37-C40
26	T	101	PEK	C32-C33-C34-C35
18	L	101	TGL	OA1-CA1-CA2-CA3
23	X	102	DMU	C22-C25-C28-C31
14	N	603	HEA	CAD-CBD-CGD-O1D
18	N	607	TGL	CA6-CA7-CA8-CA9
14	A	602	HEA	CAD-CBD-CGD-O1D
23	Z	101	DMU	O6-C11-C9-O1
22	A	617	EDO	O1-C1-C2-O2
22	E	202	EDO	O1-C1-C2-O2
27	P	307	CDL	C78-C79-C80-C81
25	B	302	CHD	C22-C23-C24-O25
25	G	101	CHD	C22-C23-C24-O25
23	D	206	DMU	C28-C31-C34-C37
14	A	602	HEA	CAA-CBA-CGA-O1A
18	N	607	TGL	CA3-CA4-CA5-CA6
18	N	607	TGL	C15-C16-C17-C18
18	A	606	TGL	CA7-CA8-CA9-C20
14	N	603	HEA	C26-C15-C16-C17
23	X	104	DMU	O5-C4-C57-O61
25	B	302	CHD	C22-C23-C24-O26
27	N	601	CDL	C72-C73-C74-C75
19	C	306	PGV	C9-C10-C11-C12
19	C	307	PGV	C9-C10-C11-C12
26	C	305	PEK	C14-C15-C16-C17
26	C	304	PEK	C11-C12-C13-C14
26	P	303	PEK	C9-C10-C11-C12
26	P	304	PEK	C11-C12-C13-C14
14	N	603	HEA	CAA-CBA-CGA-O1A
27	N	601	CDL	C31-C32-C33-C34
21	A	610	PSC	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	C	306	PGV	C24-C25-C26-C27
18	L	101	TGL	CC6-CC7-CC8-CC9
27	T	102	CDL	C59-C60-C61-C62
27	C	308	CDL	CB6-CB4-OB6-CB5
18	N	608	TGL	C18-C19-C33-C34
18	A	607	TGL	OG1-CG1-CG2-CG3
18	N	609	TGL	CC3-CC4-CC5-CC6
23	P	316	DMU	C34-C37-C40-C43
22	C	320	EDO	O1-C1-C2-O2
22	M	102	EDO	O1-C1-C2-O2
22	P	312	EDO	O1-C1-C2-O2
22	T	105	EDO	O1-C1-C2-O2
14	N	603	HEA	CAA-CBA-CGA-O2A
19	A	611	PGV	O03-C19-C20-C21
25	C	309	CHD	C22-C23-C24-O26
18	A	607	TGL	C24-C25-C26-C27
18	N	608	TGL	CC2-CC3-CC4-CC5
19	A	608	PGV	C22-C23-C24-C25
25	J	101	CHD	C22-C23-C24-O26
18	A	606	TGL	OG2-CG2-CG3-OG3
19	N	610	PGV	C9-C10-C11-C12
26	C	304	PEK	C14-C15-C16-C17
23	C	310	DMU	C28-C31-C34-C37
27	P	307	CDL	C43-C44-C45-C46
23	K	104	DMU	C18-C19-C22-C25
14	A	602	HEA	CAA-CBA-CGA-O2A
19	N	610	PGV	C11-C12-C13-C14
21	O	302	PSC	C12-C13-C14-C15
26	P	303	PEK	C3-C4-C5-C6
26	P	303	PEK	C14-C15-C16-C17
26	P	304	PEK	C14-C15-C16-C17
27	P	307	CDL	C52-C53-C54-C55
19	C	306	PGV	C1-C2-C3-C4
18	N	607	TGL	CC2-CC1-OG3-CG3
19	A	611	PGV	C26-C27-C28-C29
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
25	C	301	CHD	C22-C23-C24-O25
27	N	601	CDL	OB9-CB7-OB8-CB6
18	A	607	TGL	CB5-CB6-CB7-CB8
25	C	309	CHD	C22-C23-C24-O25
27	T	102	CDL	C55-C56-C57-C58
26	T	101	PEK	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	N	608	TGL	CB3-CB4-CB5-CB6
27	C	308	CDL	C40-C41-C42-C43
26	C	304	PEK	C34-C35-C36-C37
21	A	610	PSC	C23-C24-C25-C26
22	S	106	EDO	O1-C1-C2-O2
22	W	102	EDO	O1-C1-C2-O2
18	A	606	TGL	OG3-CC1-CC2-CC3
27	P	307	CDL	C58-C59-C60-C61
27	T	102	CDL	C17-C18-C19-C20
26	C	303	PEK	O03-C21-C22-C23
19	C	307	PGV	O01-C1-C2-C3
19	A	608	PGV	C9-C10-C11-C12
18	L	101	TGL	CB7-CB8-CB9-C10
19	P	306	PGV	C29-C30-C31-C32
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
19	N	612	PGV	O03-C19-C20-C21
18	N	607	TGL	C22-C23-C24-C25
26	C	305	PEK	C33-C34-C35-C36
14	N	603	HEA	C2D-C3D-CAD-CBD
18	A	606	TGL	OG1-CA1-CA2-CA3
27	C	308	CDL	C56-C57-C58-C59
14	N	603	HEA	C4D-C3D-CAD-CBD
18	A	607	TGL	C15-C16-C17-C18
26	C	303	PEK	C23-C24-C25-C26
18	A	606	TGL	CG1-CG2-CG3-OG3
18	N	608	TGL	CC5-CC6-CC7-CC8
27	T	102	CDL	C24-C25-C26-C27
23	P	317	DMU	O5-C6-O16-C18
18	N	609	TGL	C11-C12-C13-C14
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
18	N	608	TGL	C24-C25-C26-C27
18	N	609	TGL	C16-C15-CC9-CC8
23	K	102	DMU	O16-C18-C19-C22
22	D	205	EDO	O1-C1-C2-O2
22	N	618	EDO	O1-C1-C2-O2
22	T	104	EDO	O1-C1-C2-O2
18	A	606	TGL	C24-C25-C26-C27
27	P	307	CDL	C52-C51-CB5-OB6
27	C	308	CDL	C34-C35-C36-C37
26	C	304	PEK	O04-C21-C22-C23
23	D	206	DMU	C2-C3-O7-C10
14	N	602[A]	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
27	T	102	CDL	C72-C71-CB7-OB8
18	L	101	TGL	CA4-CA5-CA6-CA7
23	J	104	DMU	C18-C19-C22-C25
18	A	606	TGL	OC1-CC1-CC2-CC3
18	N	609	TGL	C10-C11-C12-C13
23	D	206	DMU	C4-C3-O7-C10
18	N	609	TGL	C13-C14-C29-C30
26	C	303	PEK	O04-C21-C22-C23
14	A	602	HEA	C4A-C3A-CMA-OMA
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
18	A	607	TGL	CA7-CA8-CA9-C20
27	P	307	CDL	C52-C51-CB5-OB7
18	A	606	TGL	C29-C30-C31-C32
18	A	606	TGL	OG1-CG1-CG2-OG2
19	N	610	PGV	O03-C19-C20-C21
18	A	607	TGL	C10-C11-C12-C13
27	T	102	CDL	C57-C58-C59-C60
19	C	307	PGV	O02-C1-C2-C3
18	N	607	TGL	OG3-CC1-CC2-CC3
26	C	304	PEK	C30-C31-C32-C33
18	A	607	TGL	C21-C22-C23-C24
18	N	607	TGL	CC7-CC8-CC9-C15
18	A	606	TGL	OA1-CA1-CA2-CA3
18	L	101	TGL	C14-C29-C30-C31
22	D	202	EDO	O1-C1-C2-O2
22	P	309	EDO	O1-C1-C2-O2
18	A	607	TGL	OG3-CC1-CC2-CC3
19	N	612	PGV	O04-C19-C20-C21
27	T	102	CDL	C72-C71-CB7-OB9
23	X	101	DMU	C19-C22-C25-C28

There are no ring outliers.

60 monomers are involved in 170 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	620	EDO	1	0
21	A	610	PSC	3	0
18	N	607	TGL	3	0
23	Q	201	DMU	2	0
19	C	307	PGV	1	0
23	X	102	DMU	2	0
23	P	308	DMU	3	0

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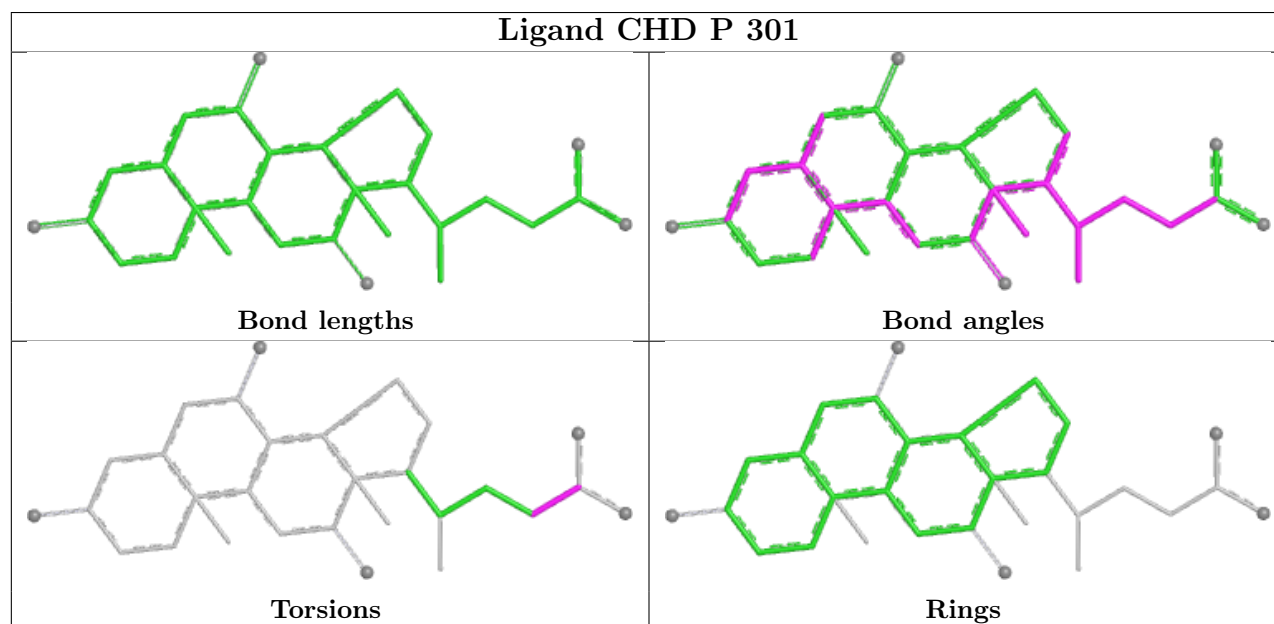
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22	A	612	EDO	2	0
20	N	611[A]	PER	1	0
14	A	601[A]	HEA	2	0
23	D	206	DMU	3	0
19	C	306	PGV	3	0
19	P	306	PGV	1	0
19	P	305	PGV	3	0
18	L	101	TGL	15	0
22	A	616	EDO	2	0
27	N	601	CDL	5	0
18	A	607	TGL	14	0
27	P	307	CDL	7	0
26	C	304	PEK	5	0
23	C	310	DMU	3	0
22	N	621	EDO	1	0
19	A	611	PGV	1	0
20	A	609[A]	PER	1	0
23	P	316	DMU	2	0
14	N	602[A]	HEA	2	0
22	D	205	EDO	2	0
19	N	610	PGV	3	0
18	N	608	TGL	7	0
23	K	101	DMU	1	0
22	S	106	EDO	1	0
22	Y	101	EDO	1	0
23	K	102	DMU	1	0
19	A	608	PGV	1	0
22	D	204	EDO	3	0
25	C	309	CHD	2	0
19	N	612	PGV	1	0
21	O	302	PSC	4	0
27	T	102	CDL	9	0
23	K	103	DMU	1	0
26	C	305	PEK	1	0
26	P	304	PEK	2	0
26	C	303	PEK	1	0
22	N	620	EDO	1	0
14	N	603	HEA	3	0
22	C	315	EDO	1	0
14	A	602	HEA	3	0
25	L	102	CHD	2	0
25	G	101	CHD	1	0

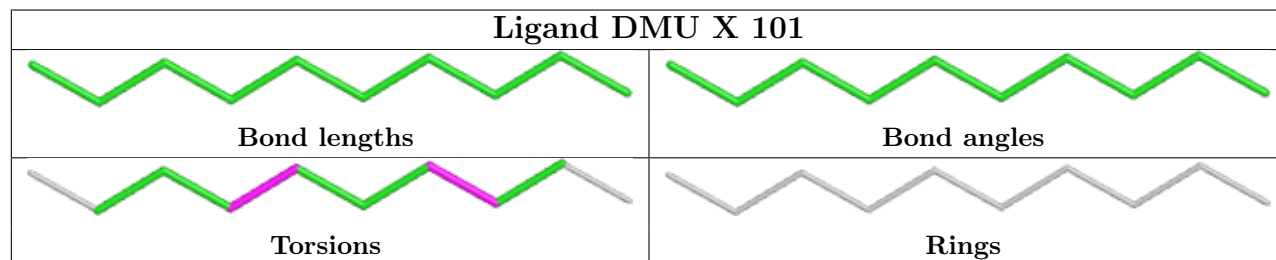
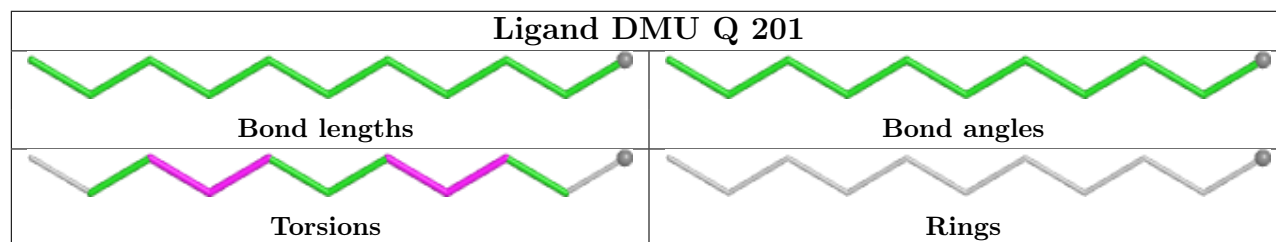
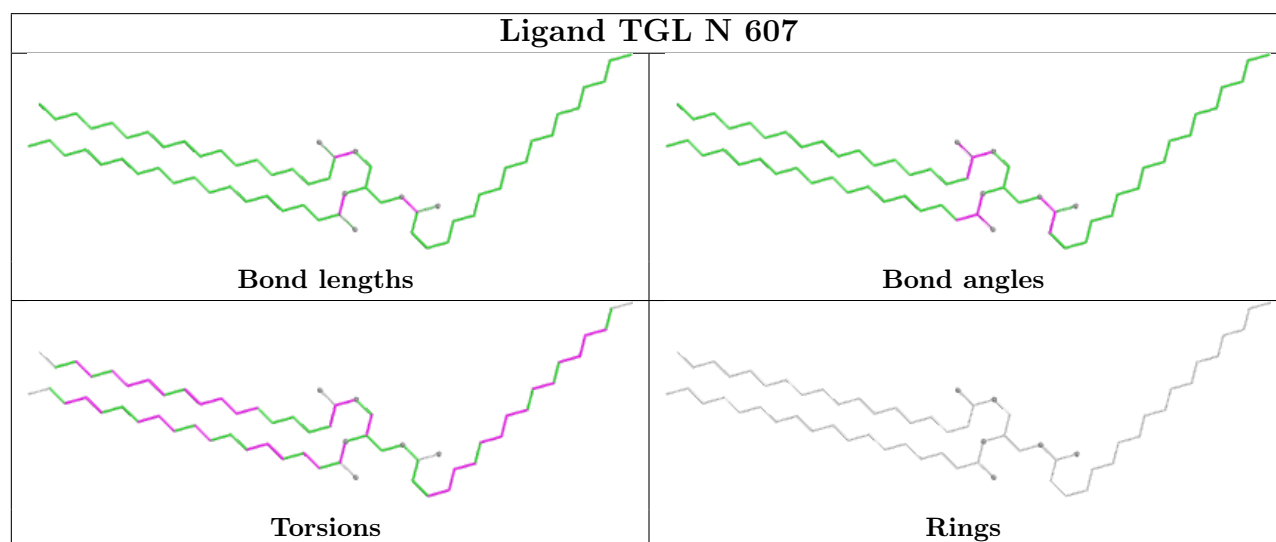
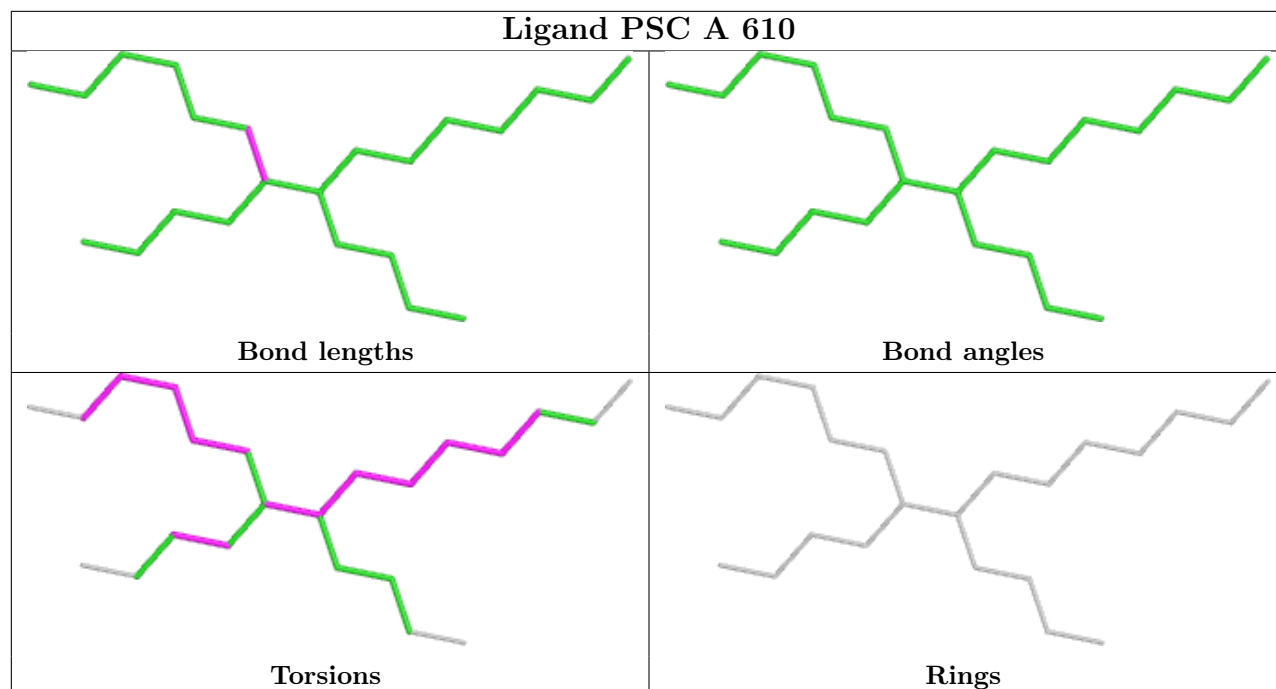
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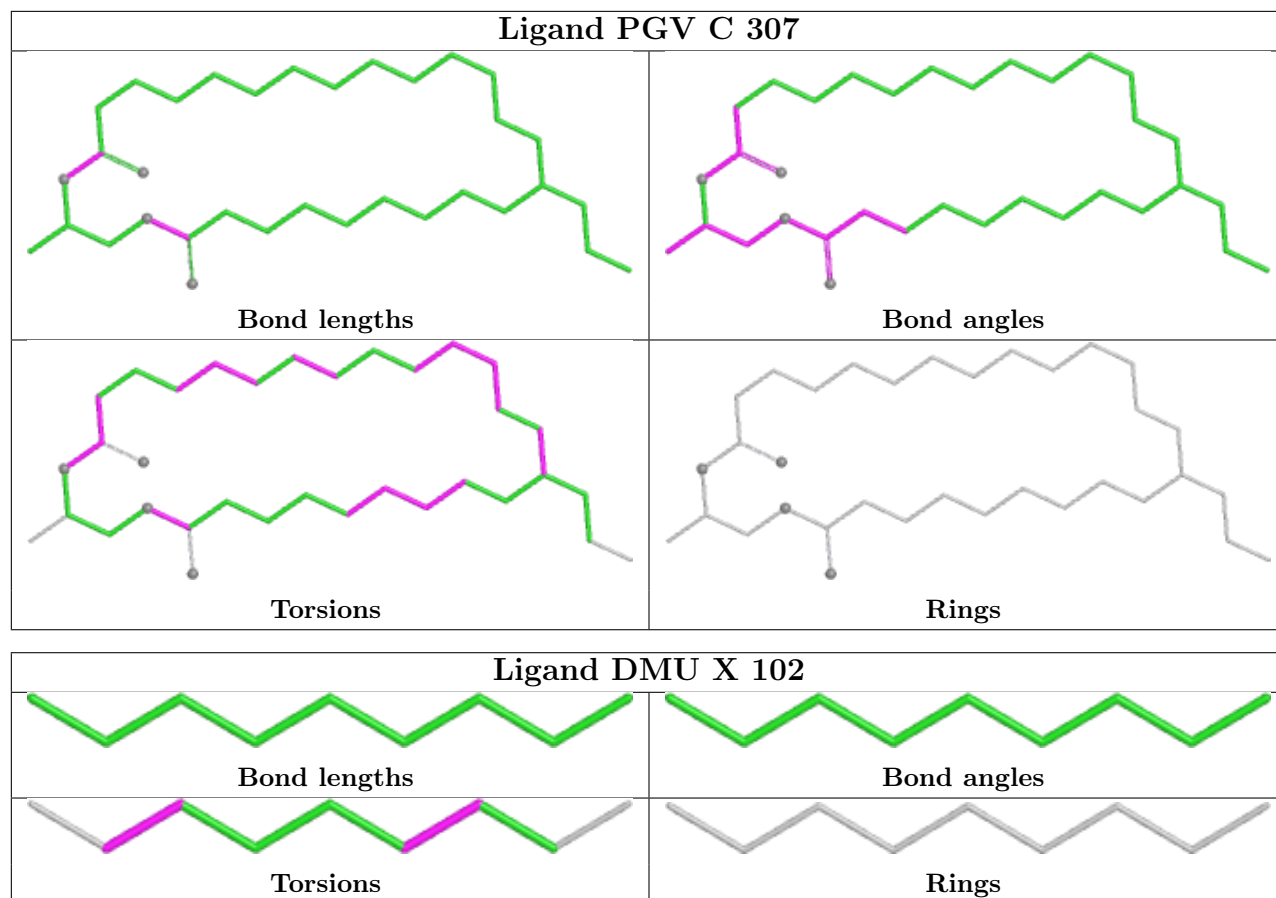
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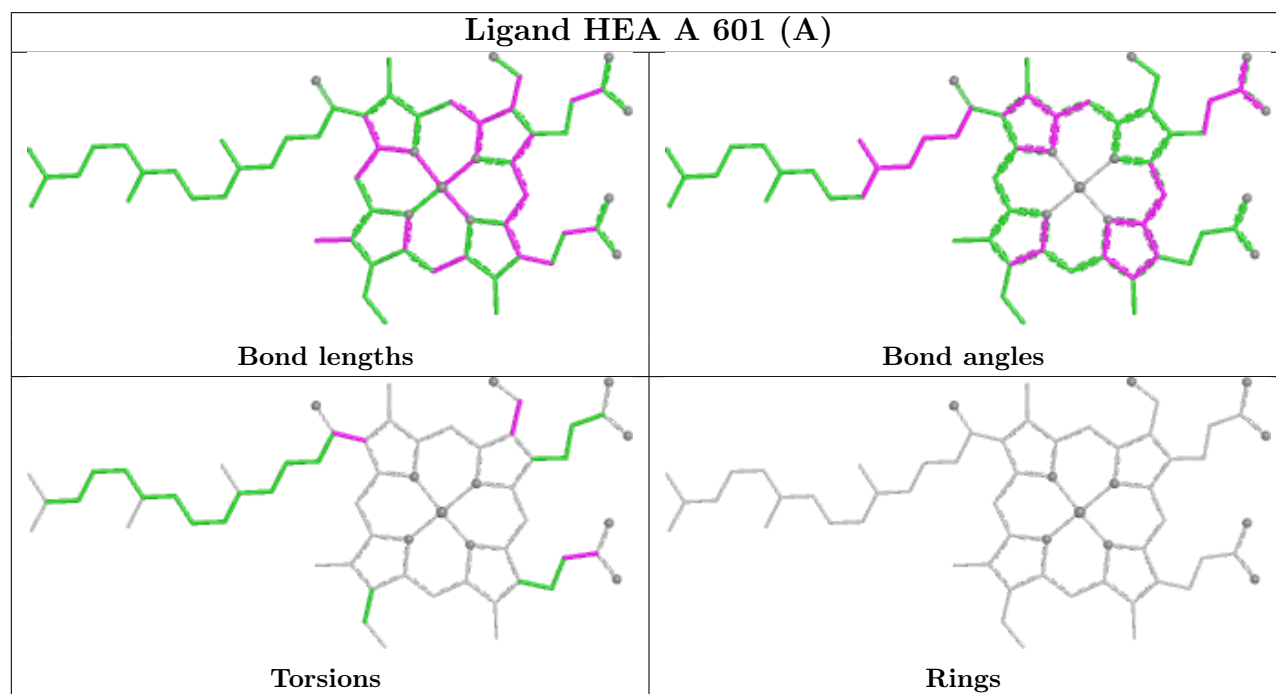
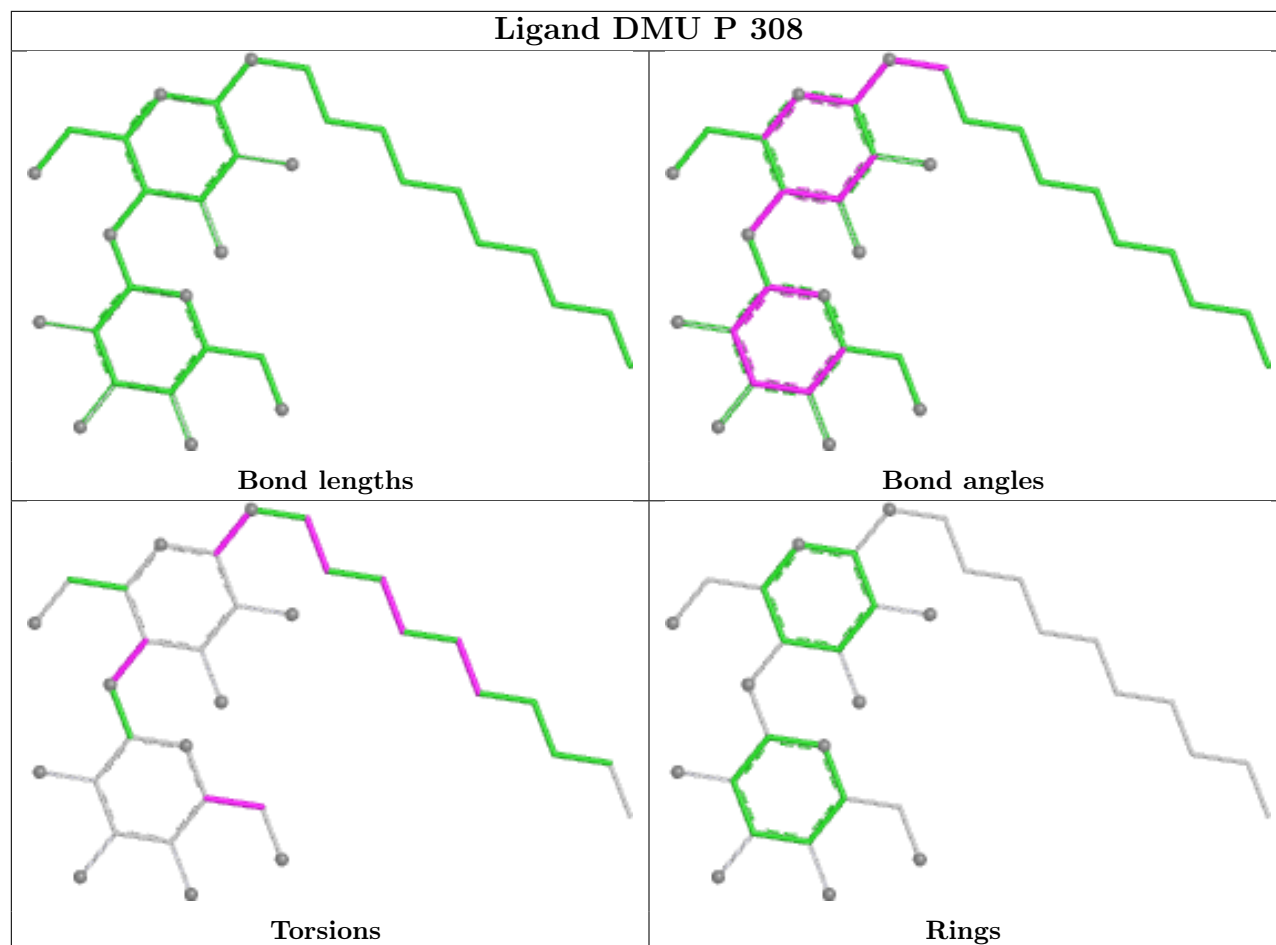
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	Z	101	DMU	1	0
25	J	101	CHD	2	0
26	T	101	PEK	6	0
23	J	104	DMU	1	0
22	C	318	EDO	1	0
23	M	101	DMU	2	0
23	L	105	DMU	6	0
18	A	606	TGL	4	0
18	N	609	TGL	1	0
22	A	618	EDO	1	0
27	C	308	CDL	8	0

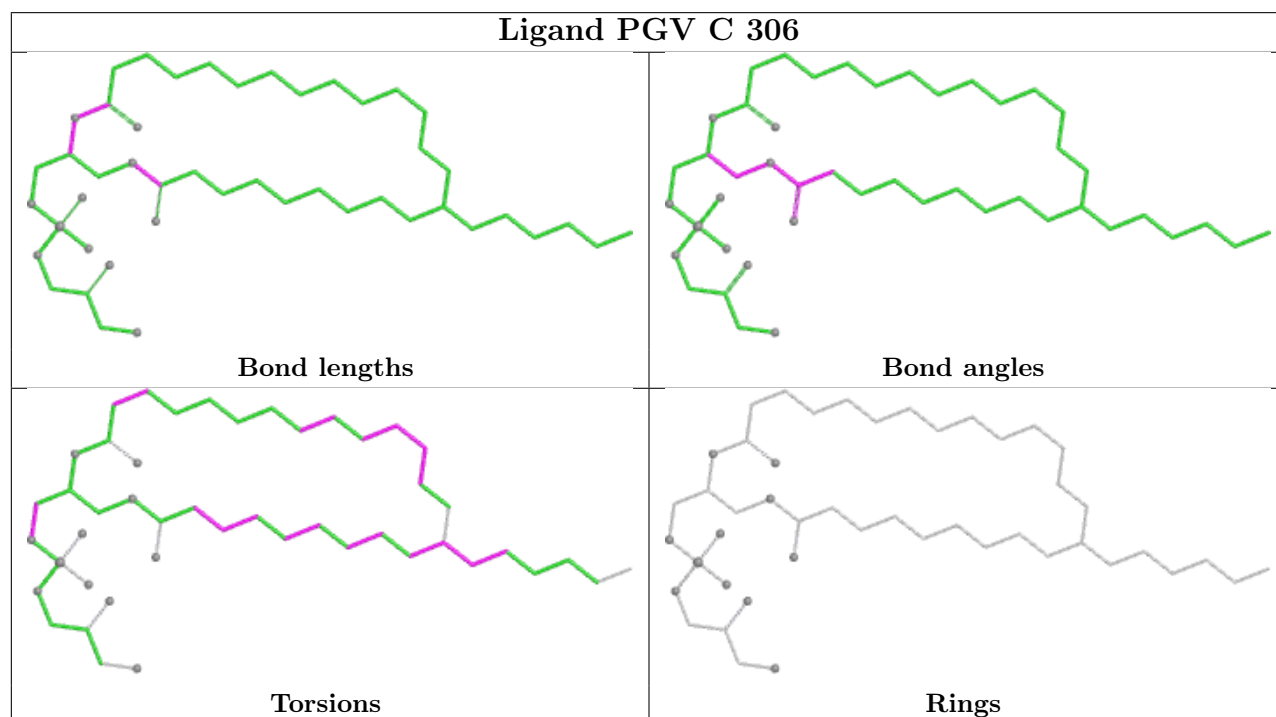
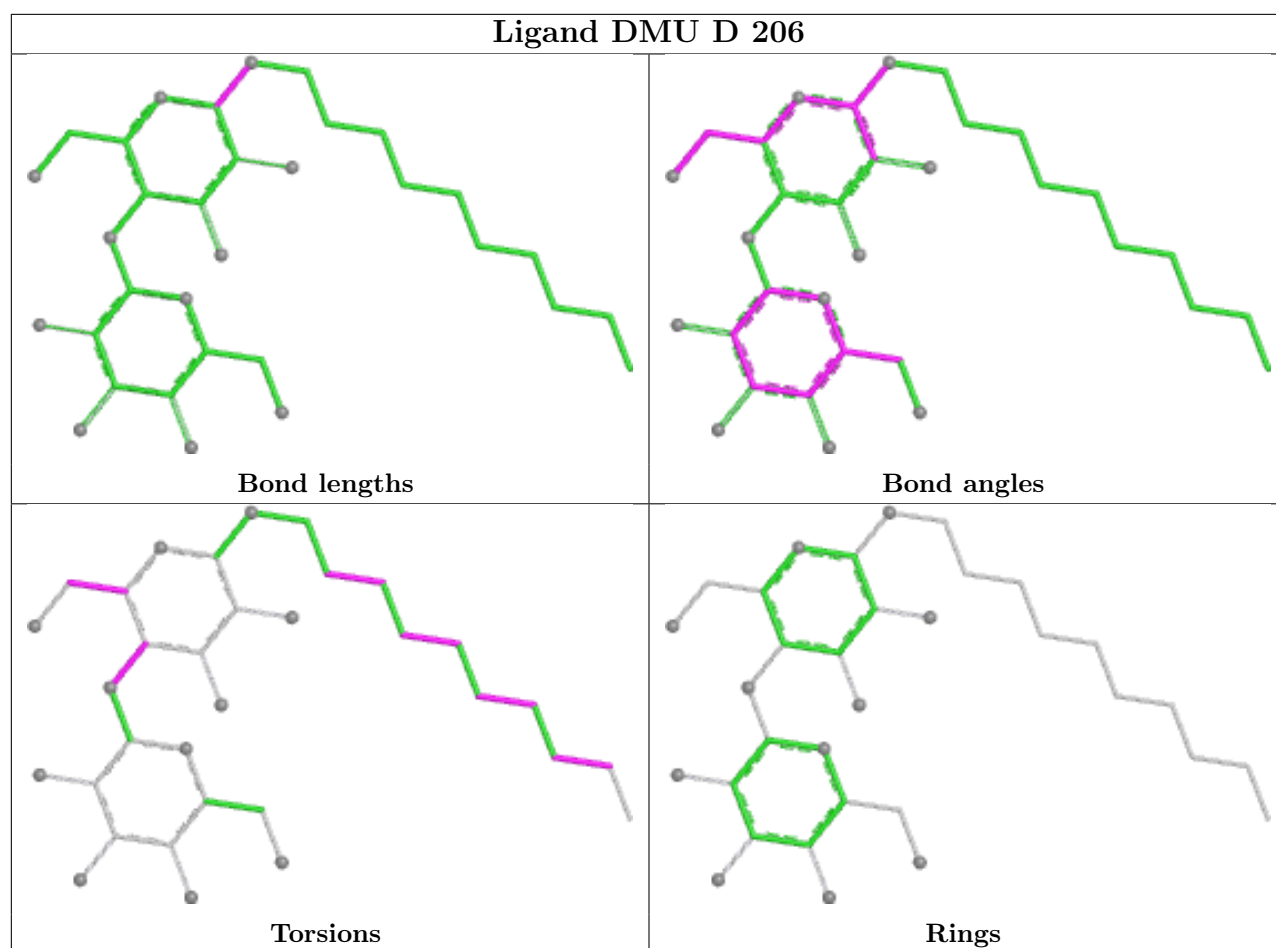
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

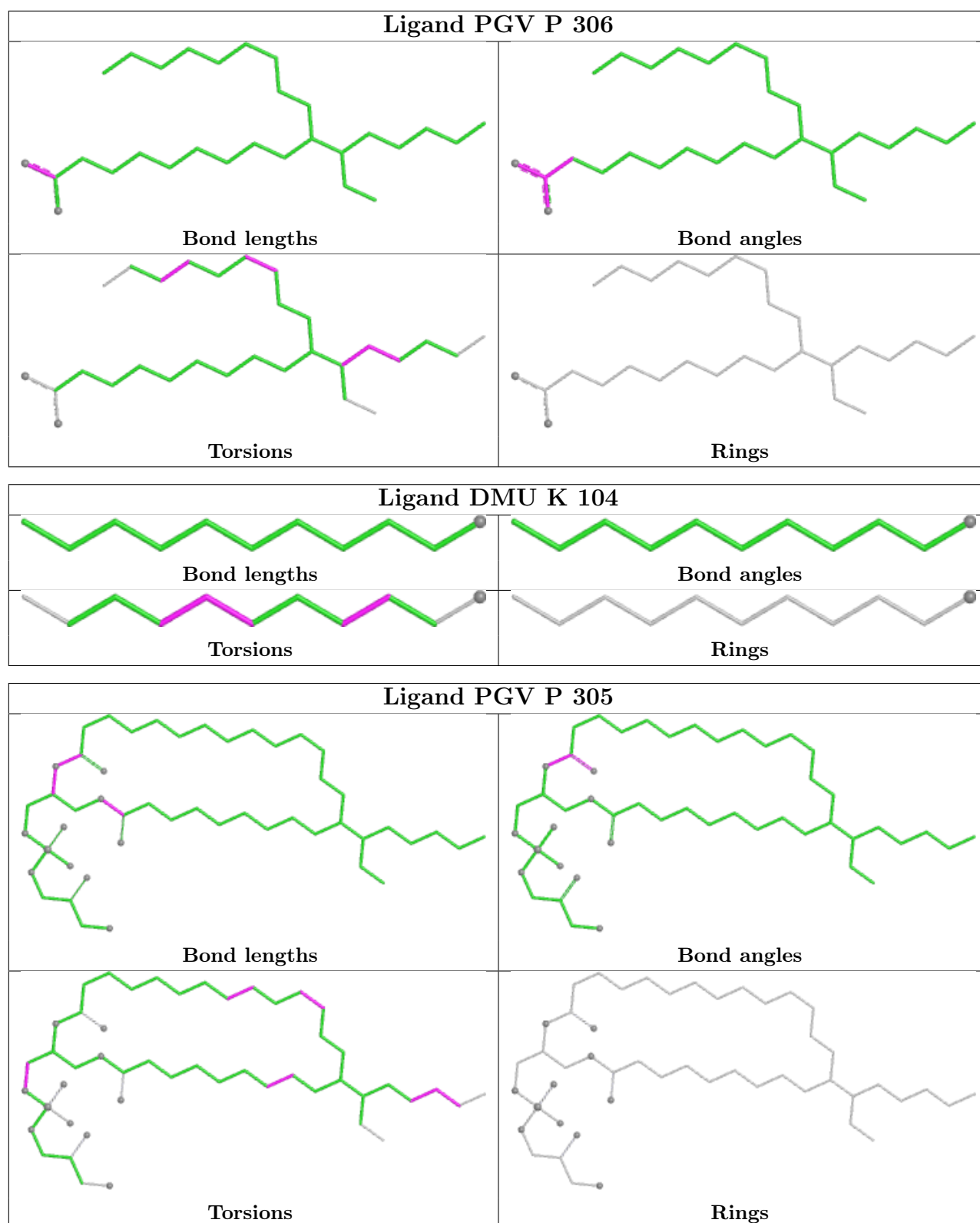


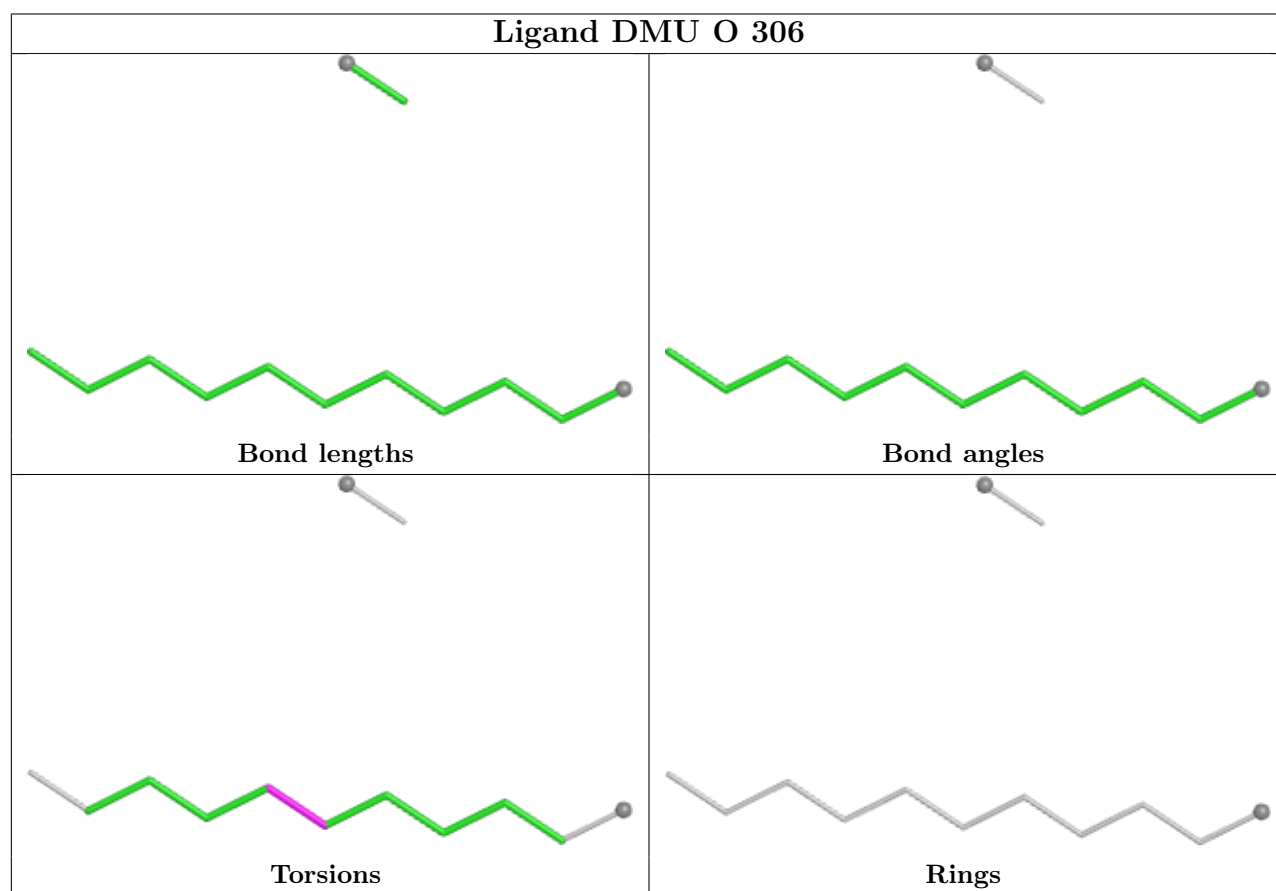
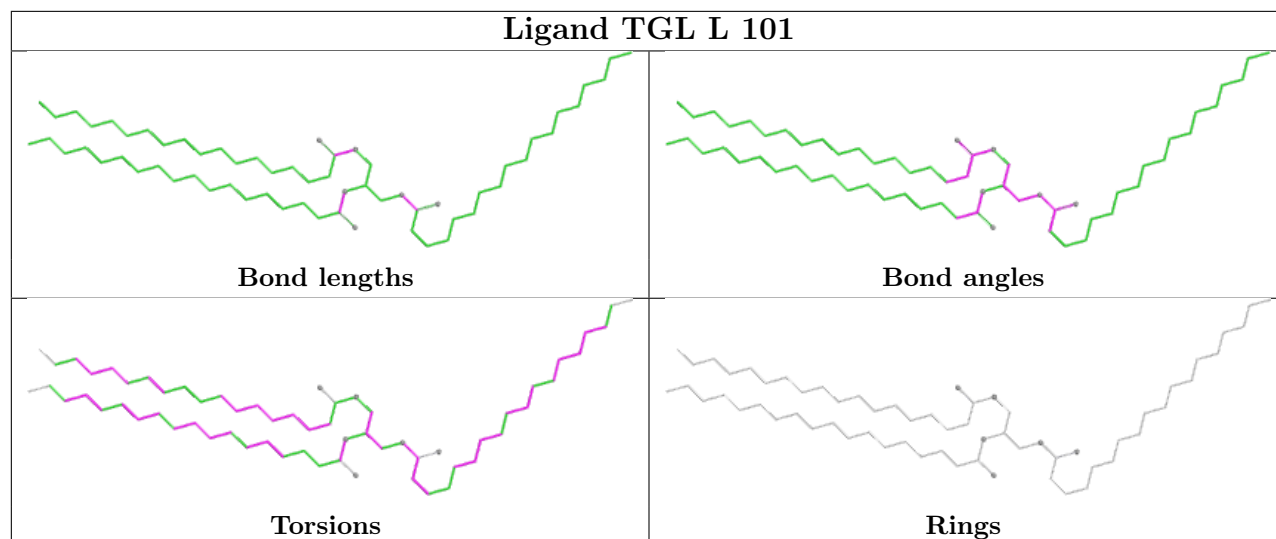


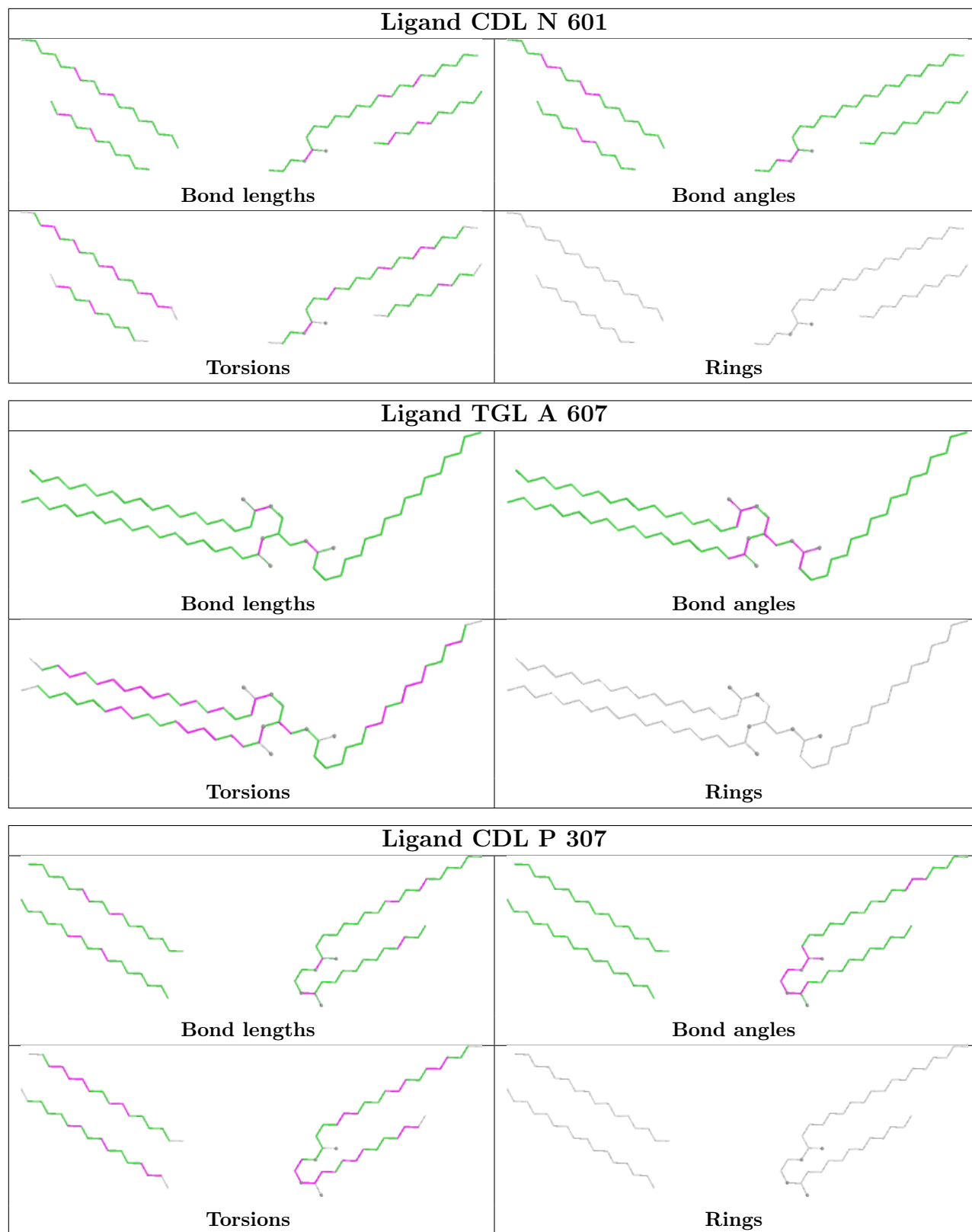


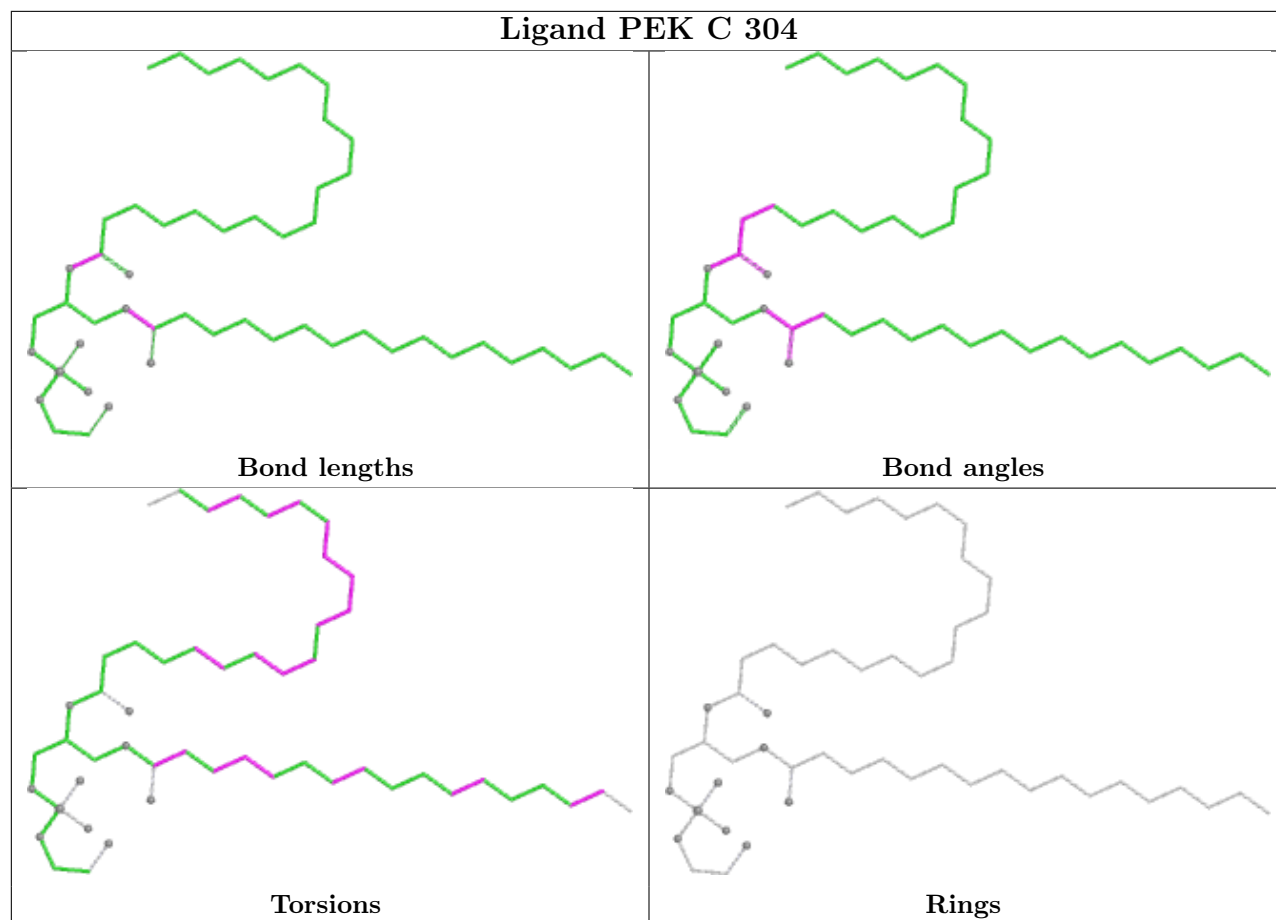


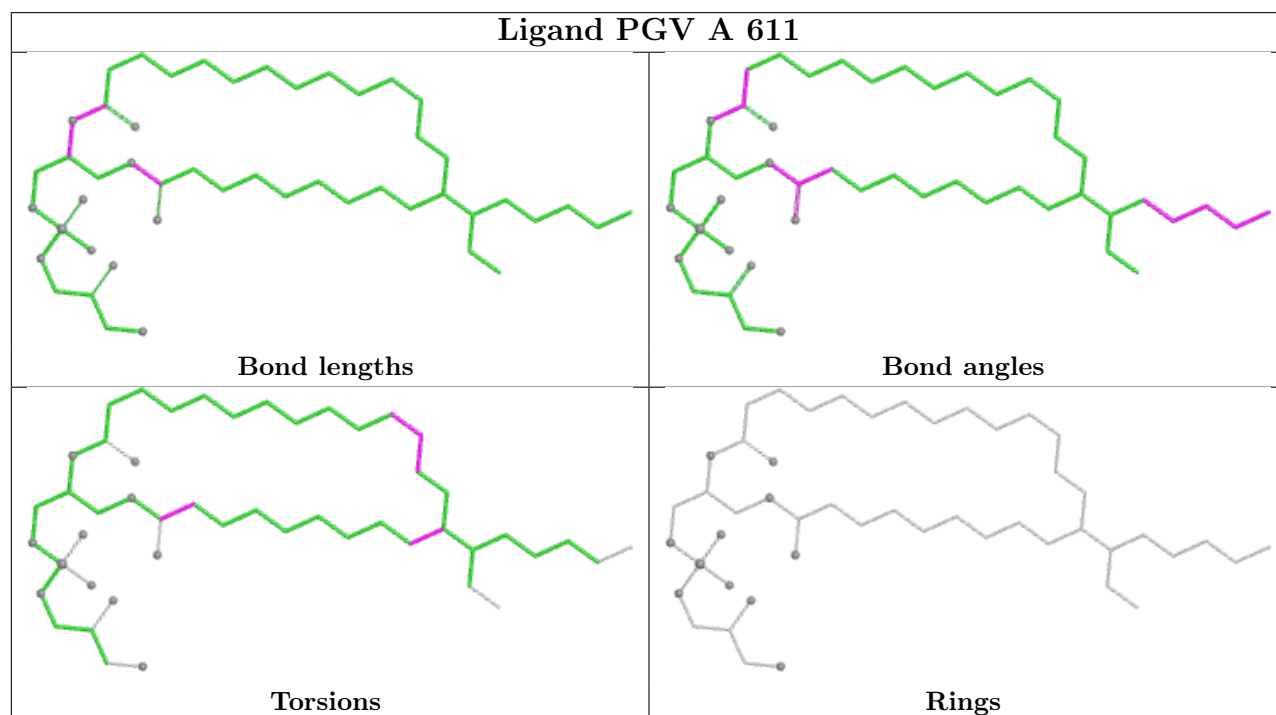
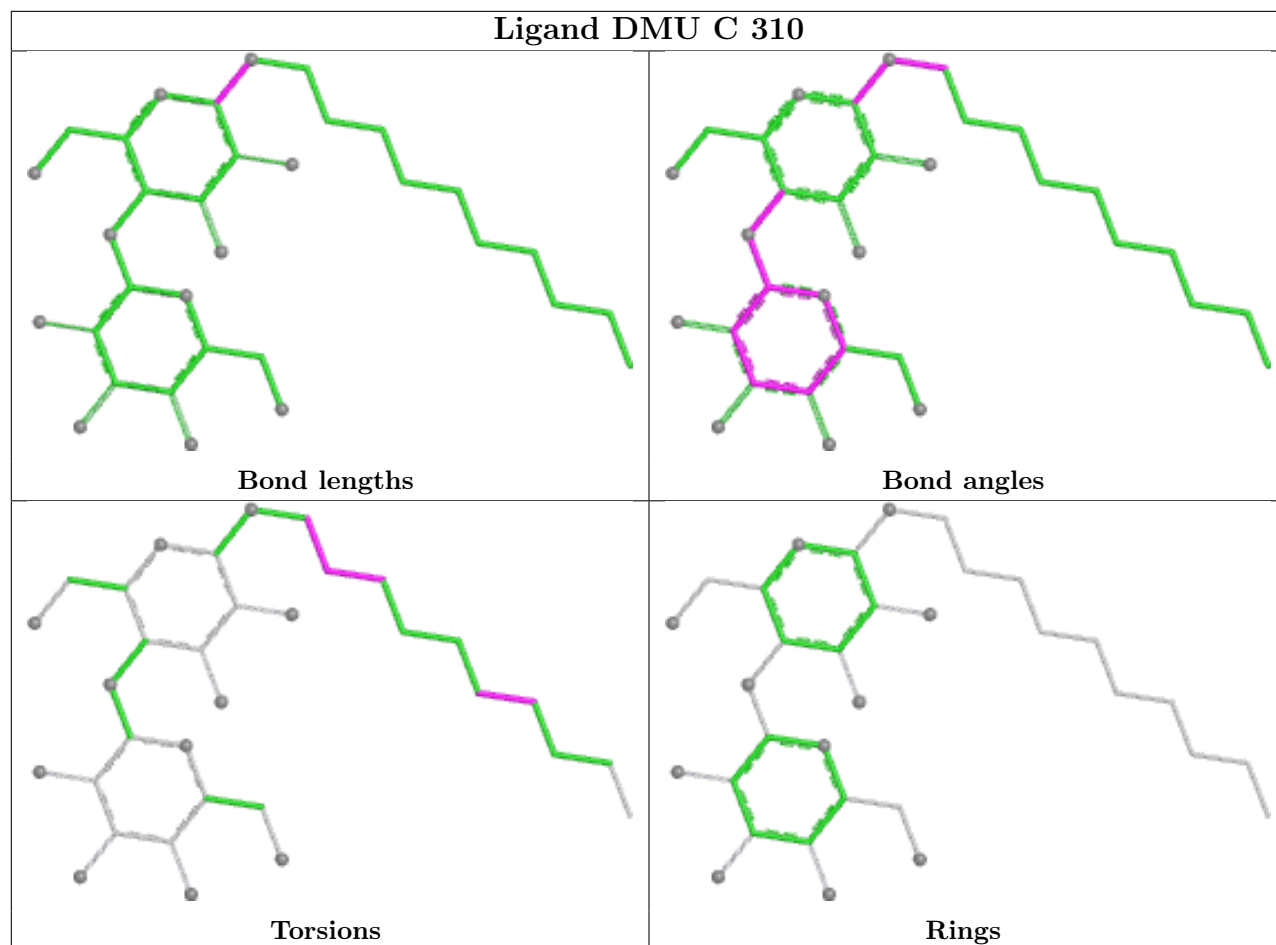


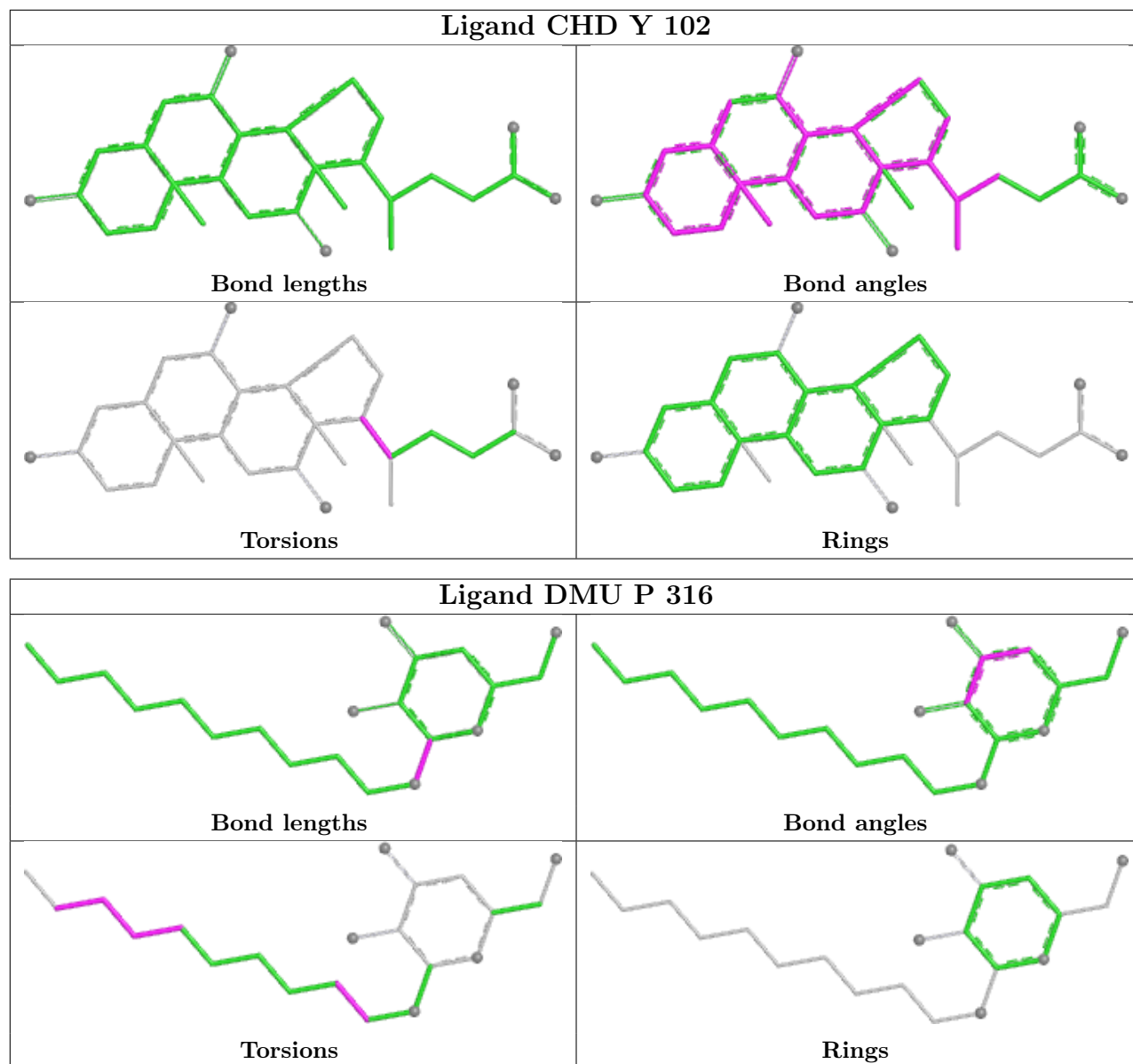


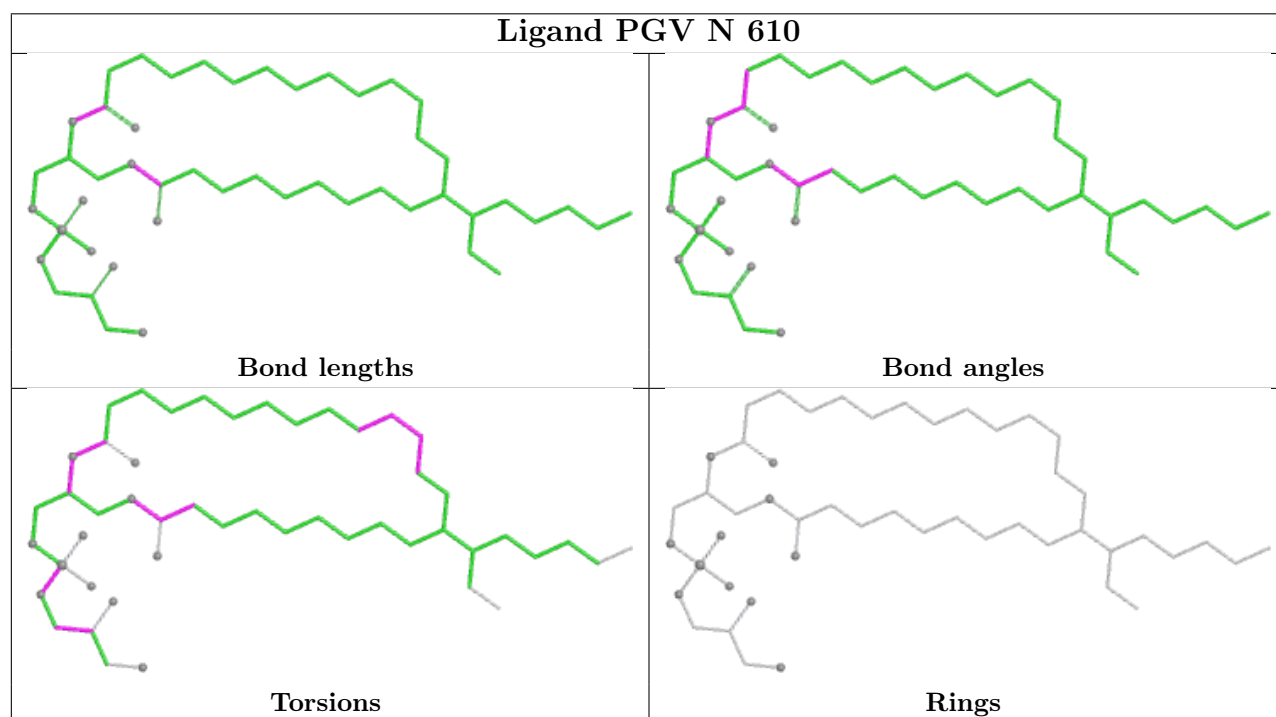
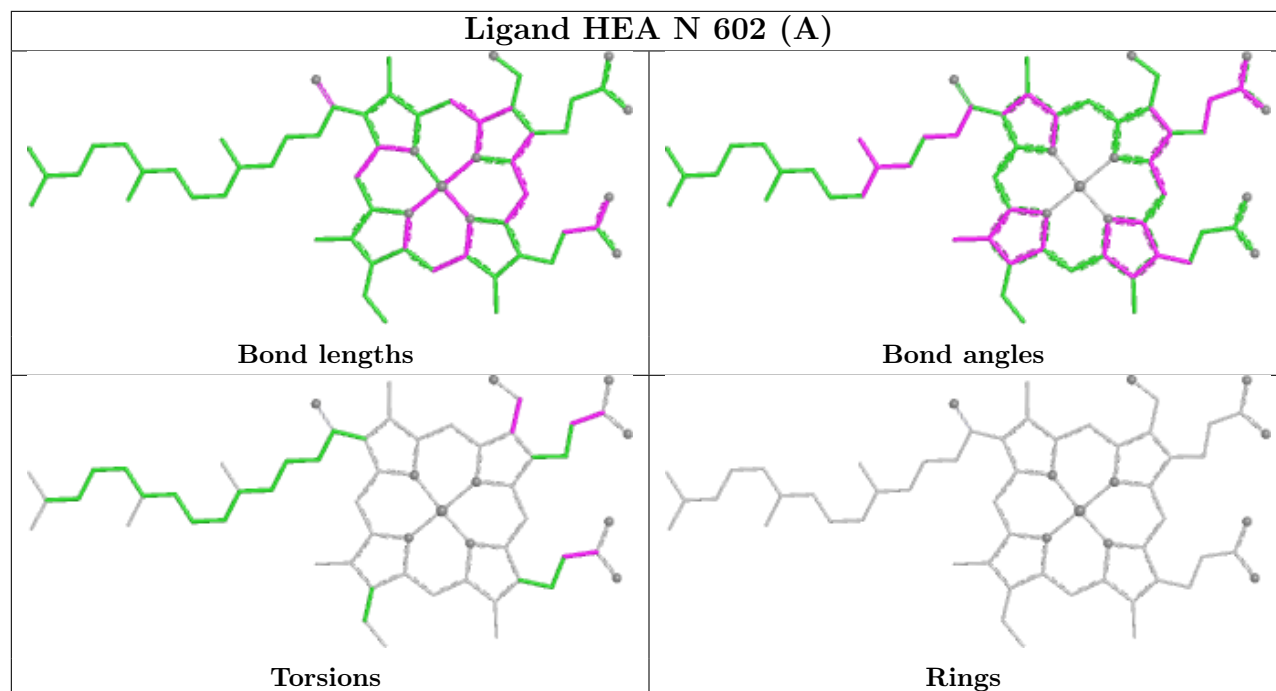


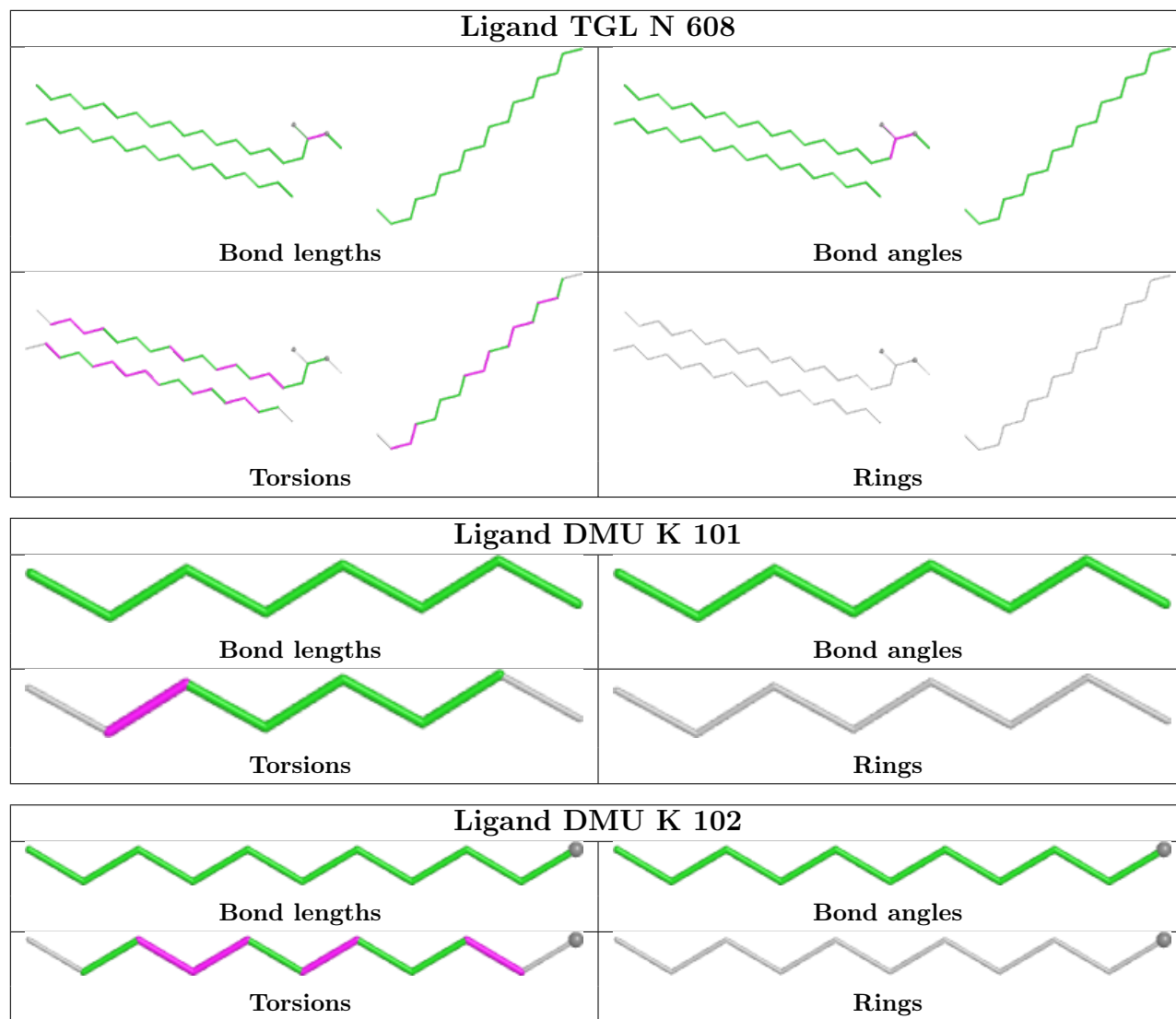


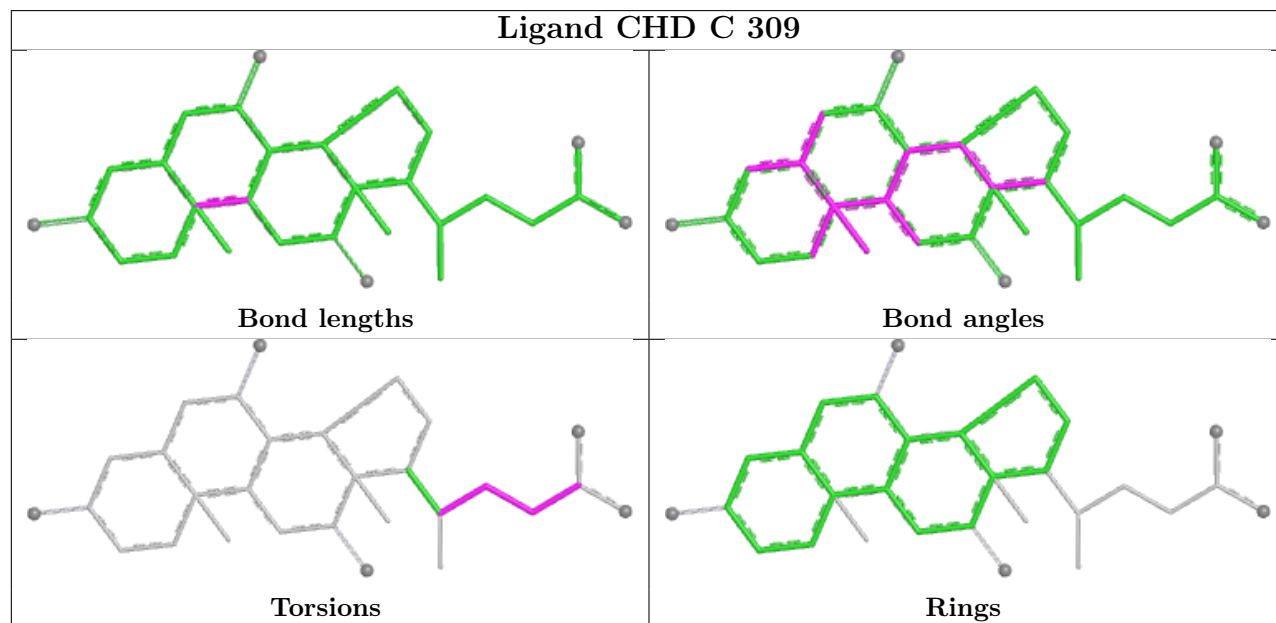
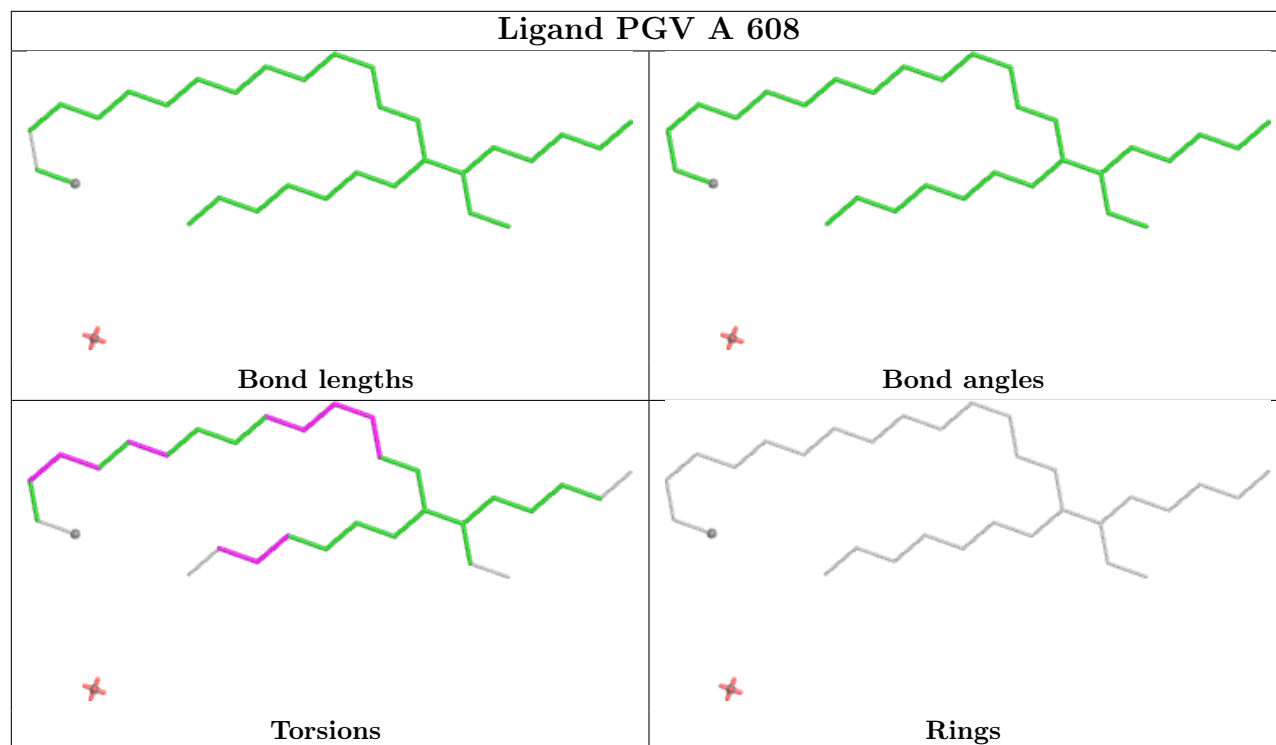


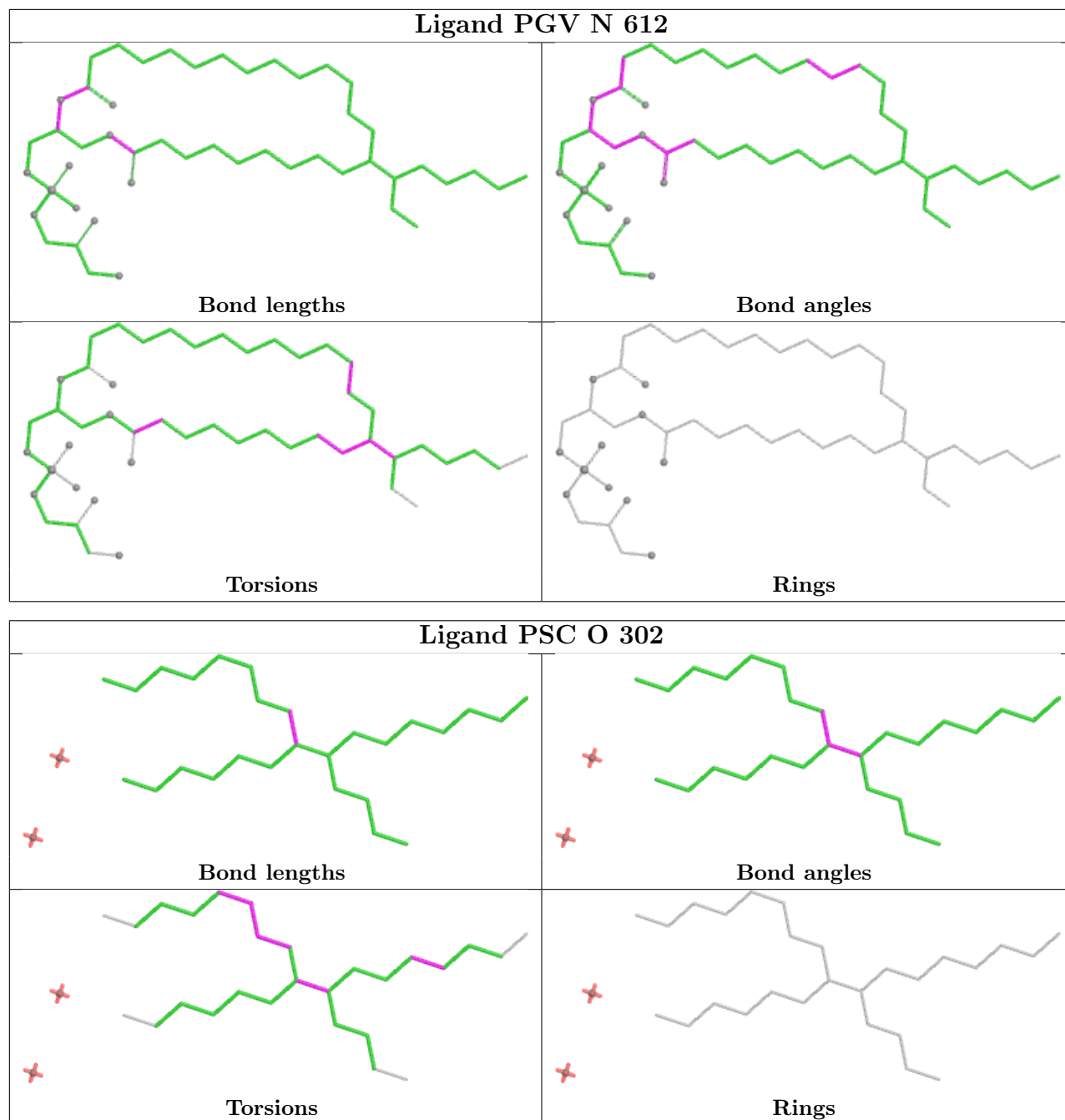


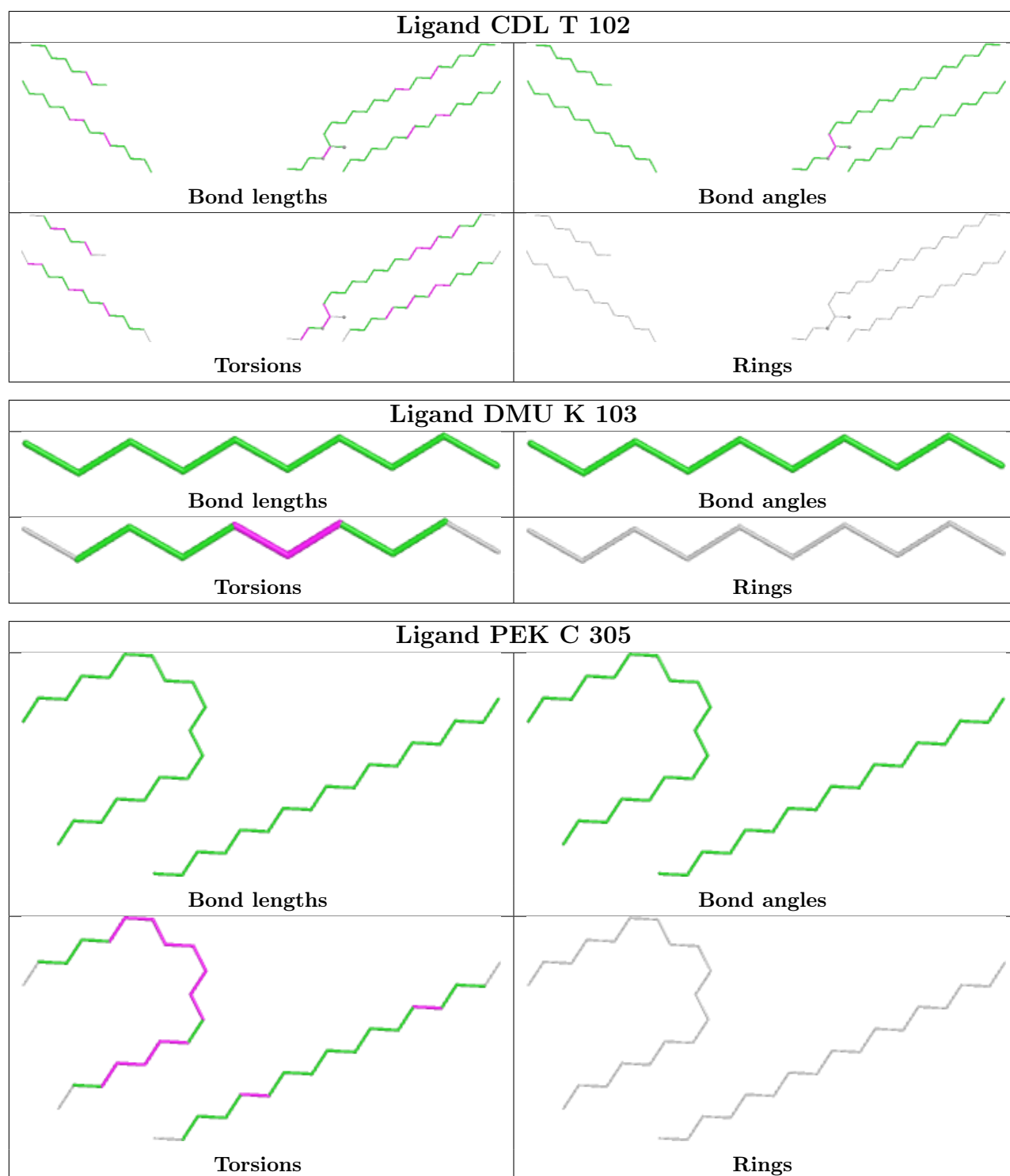


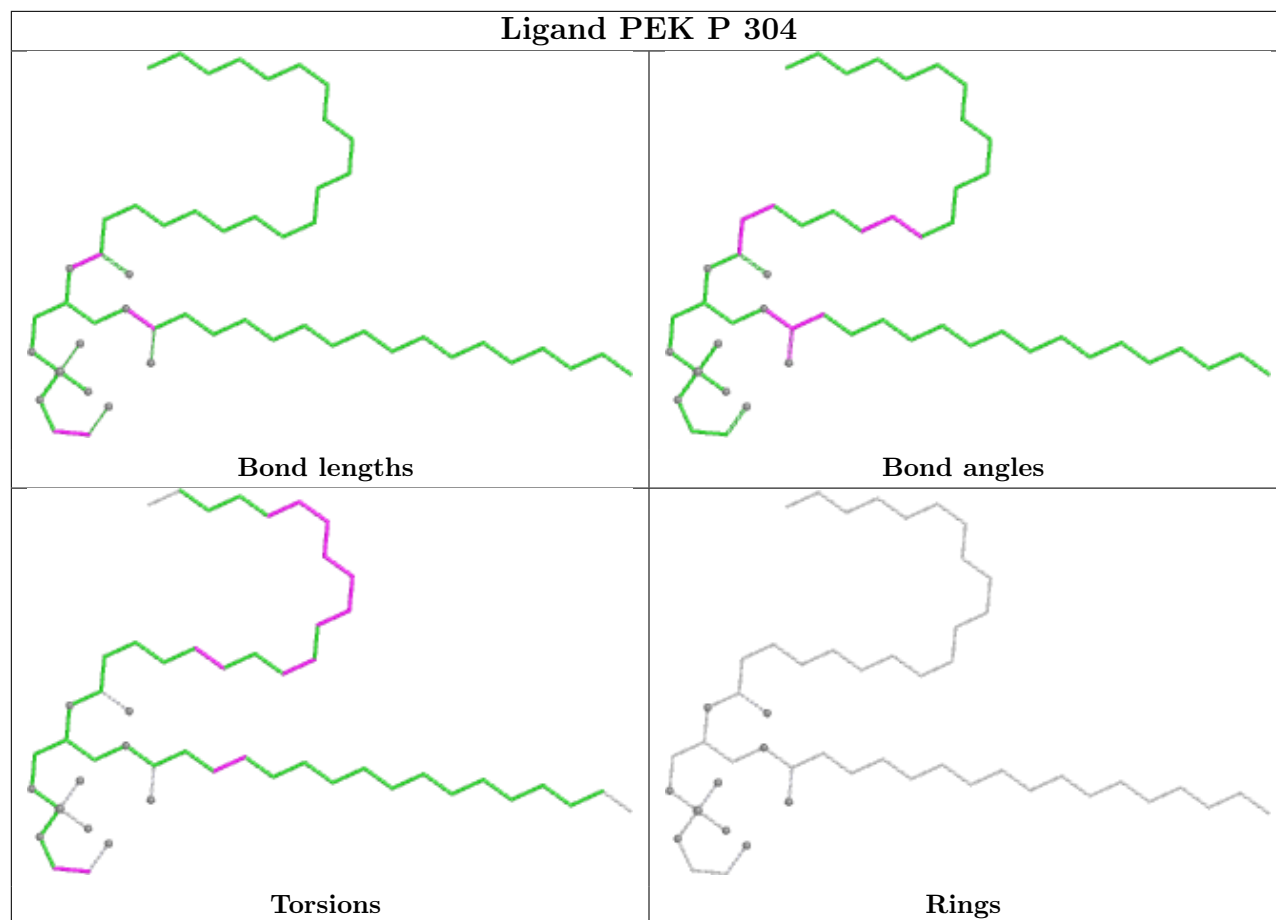


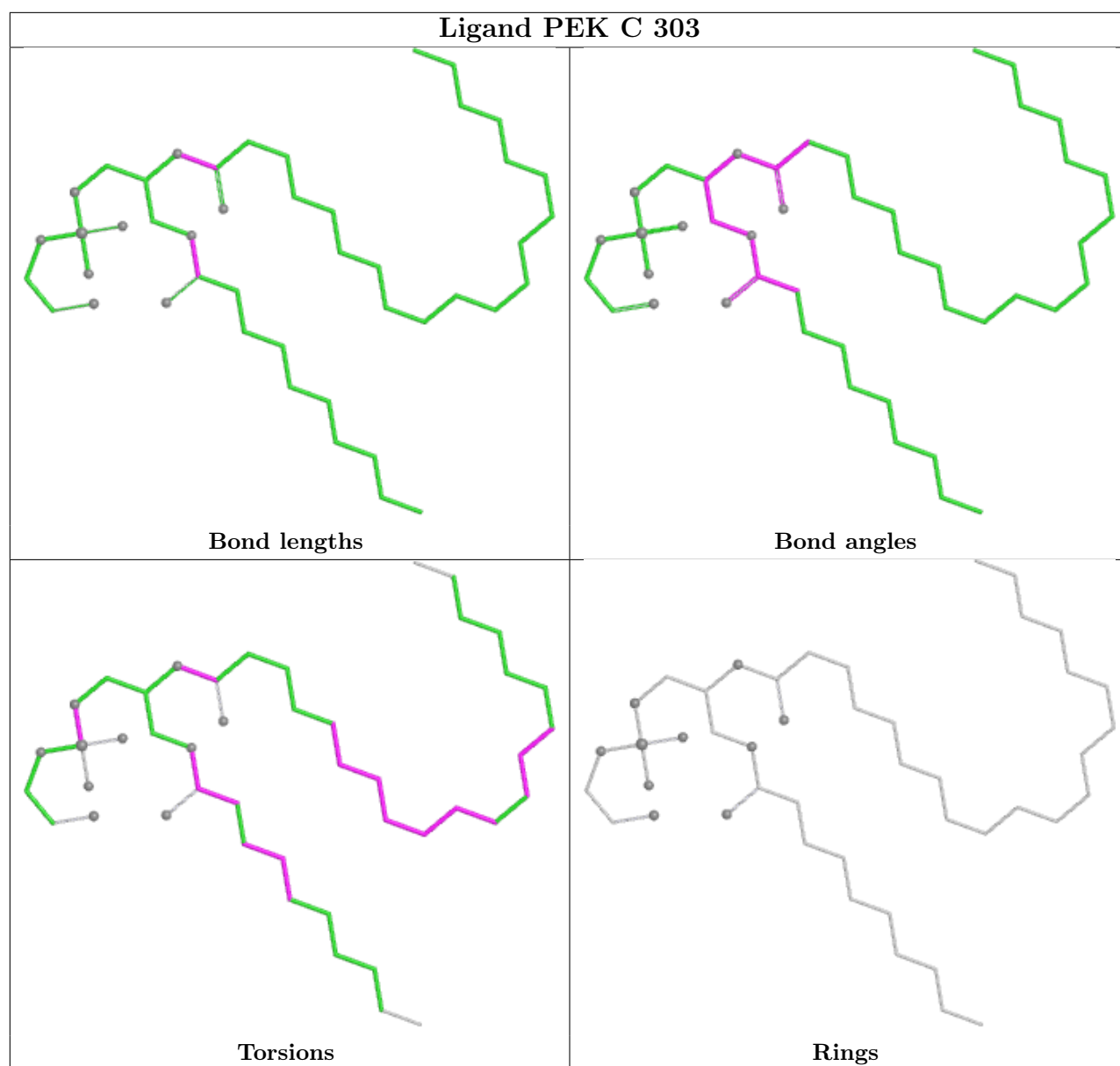


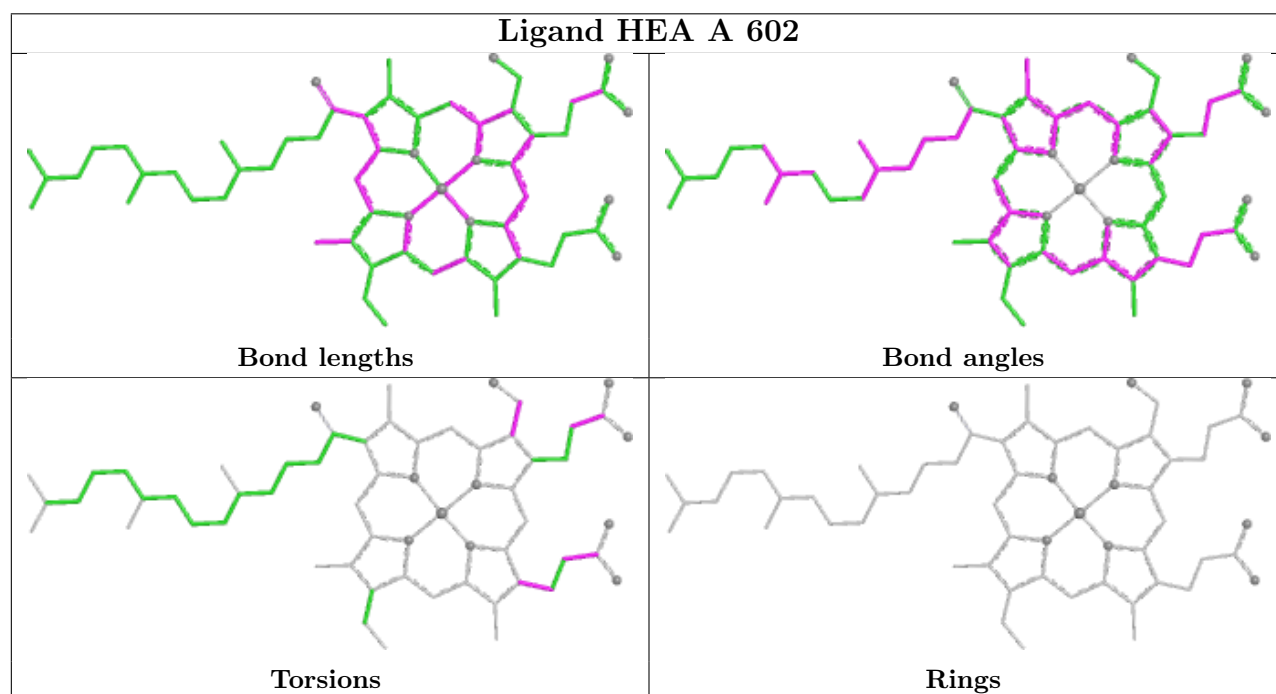
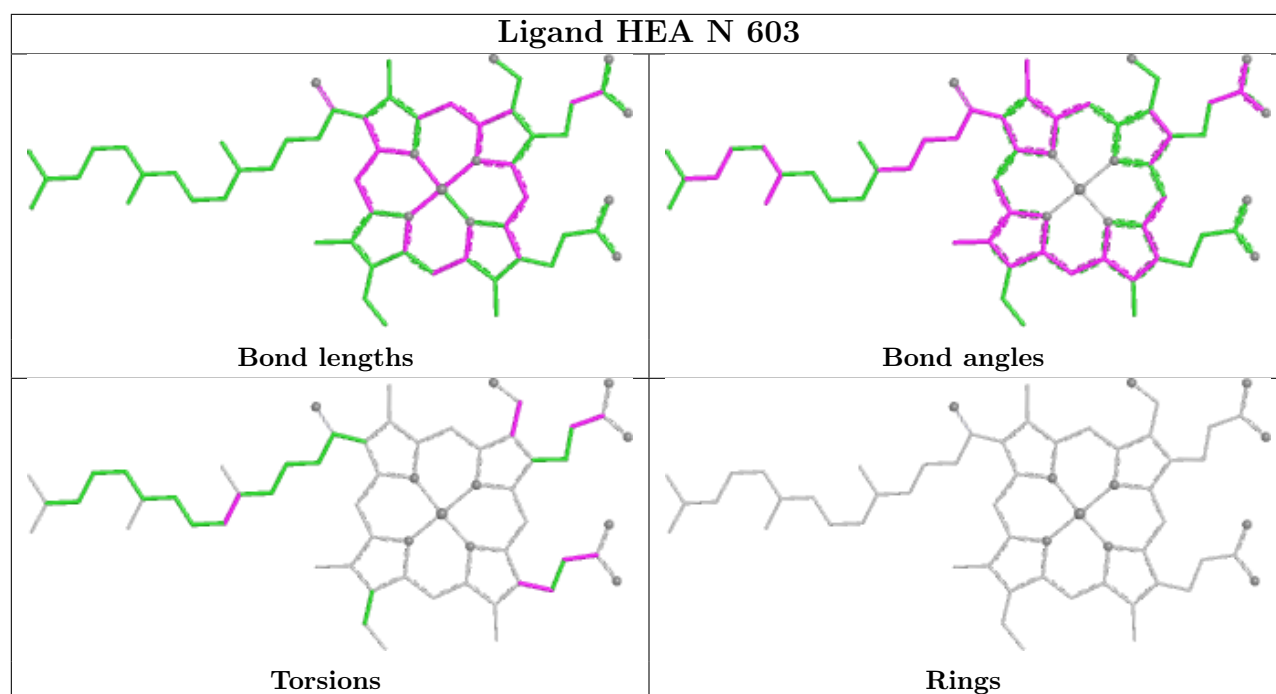




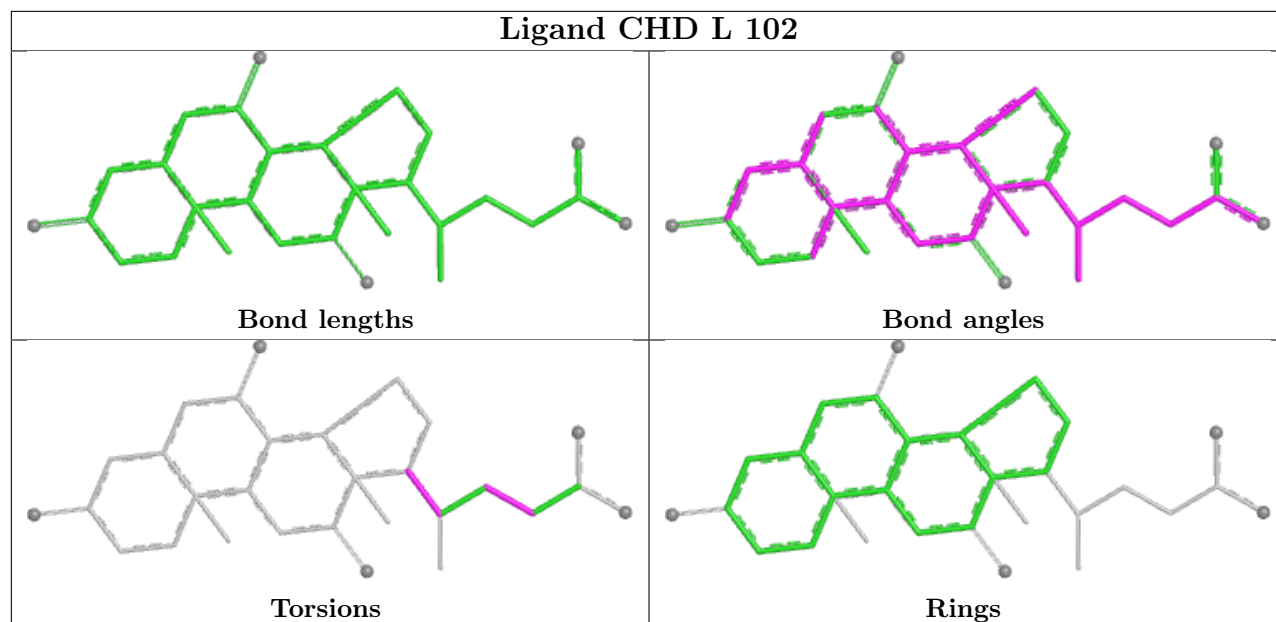




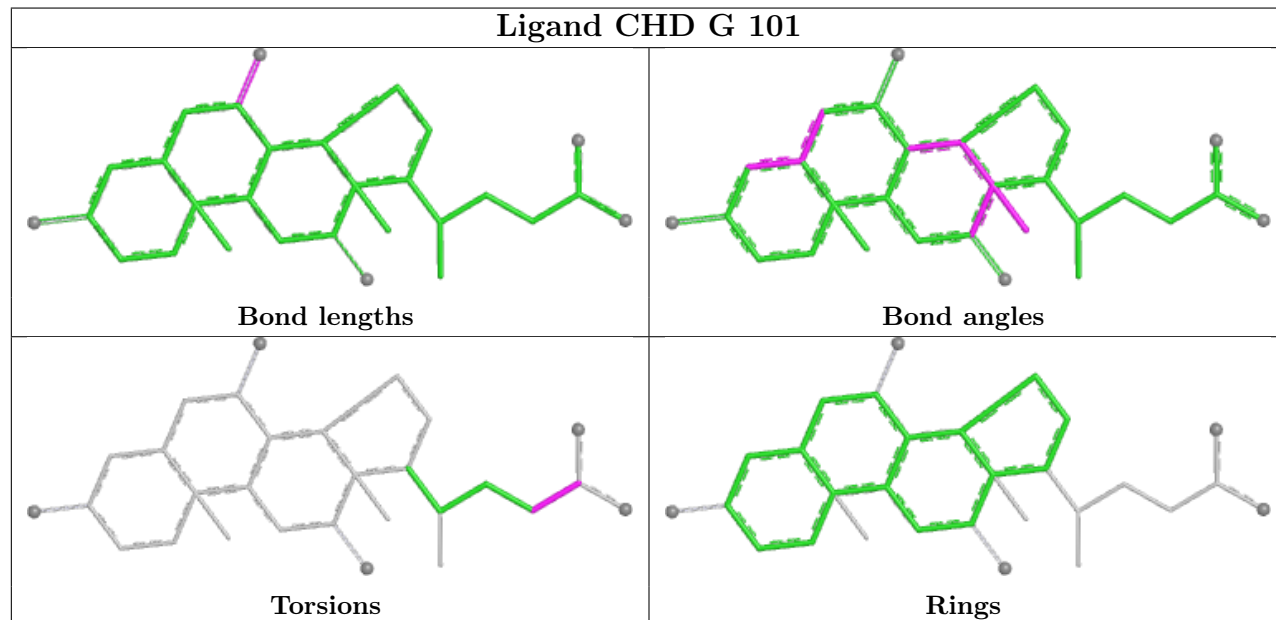


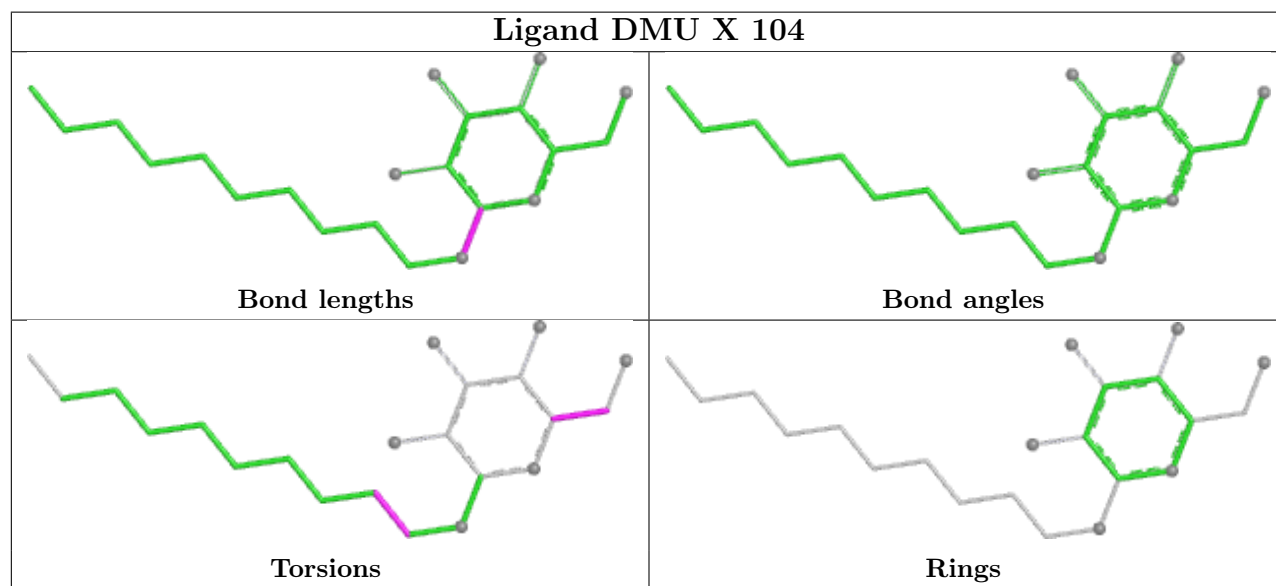
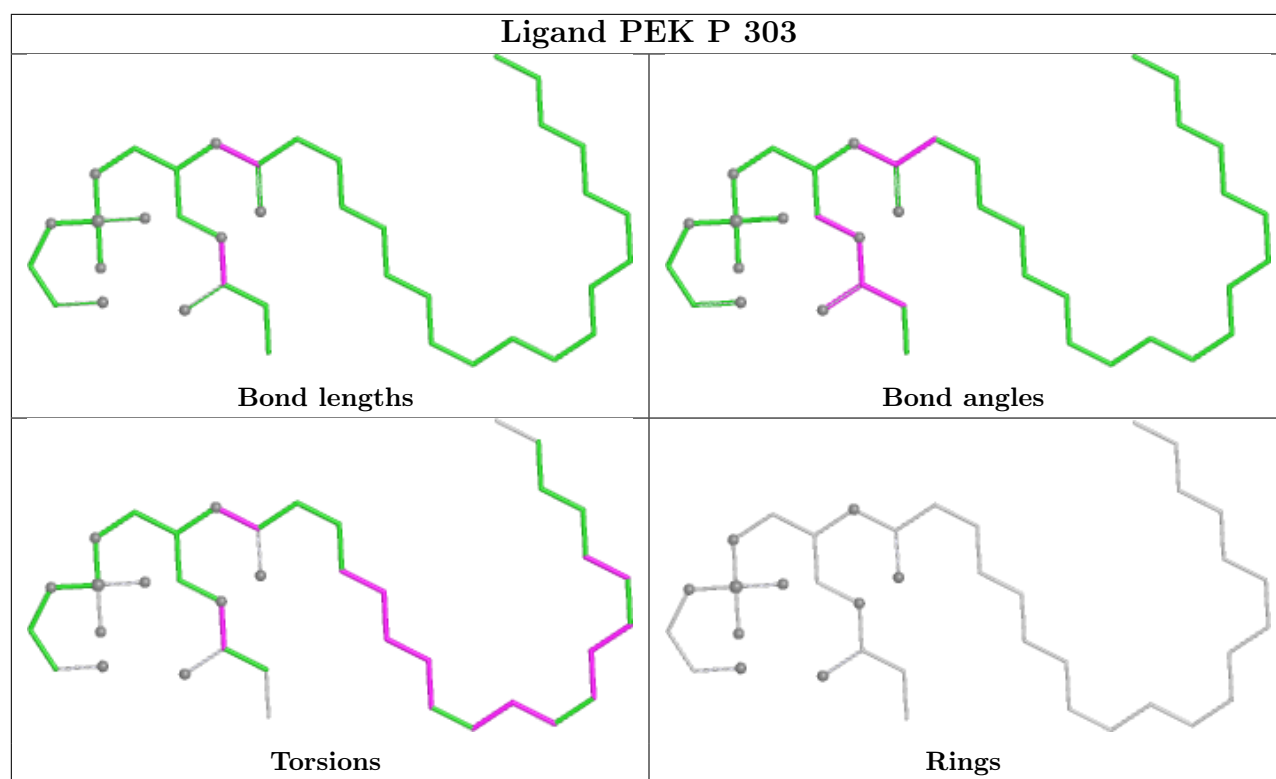


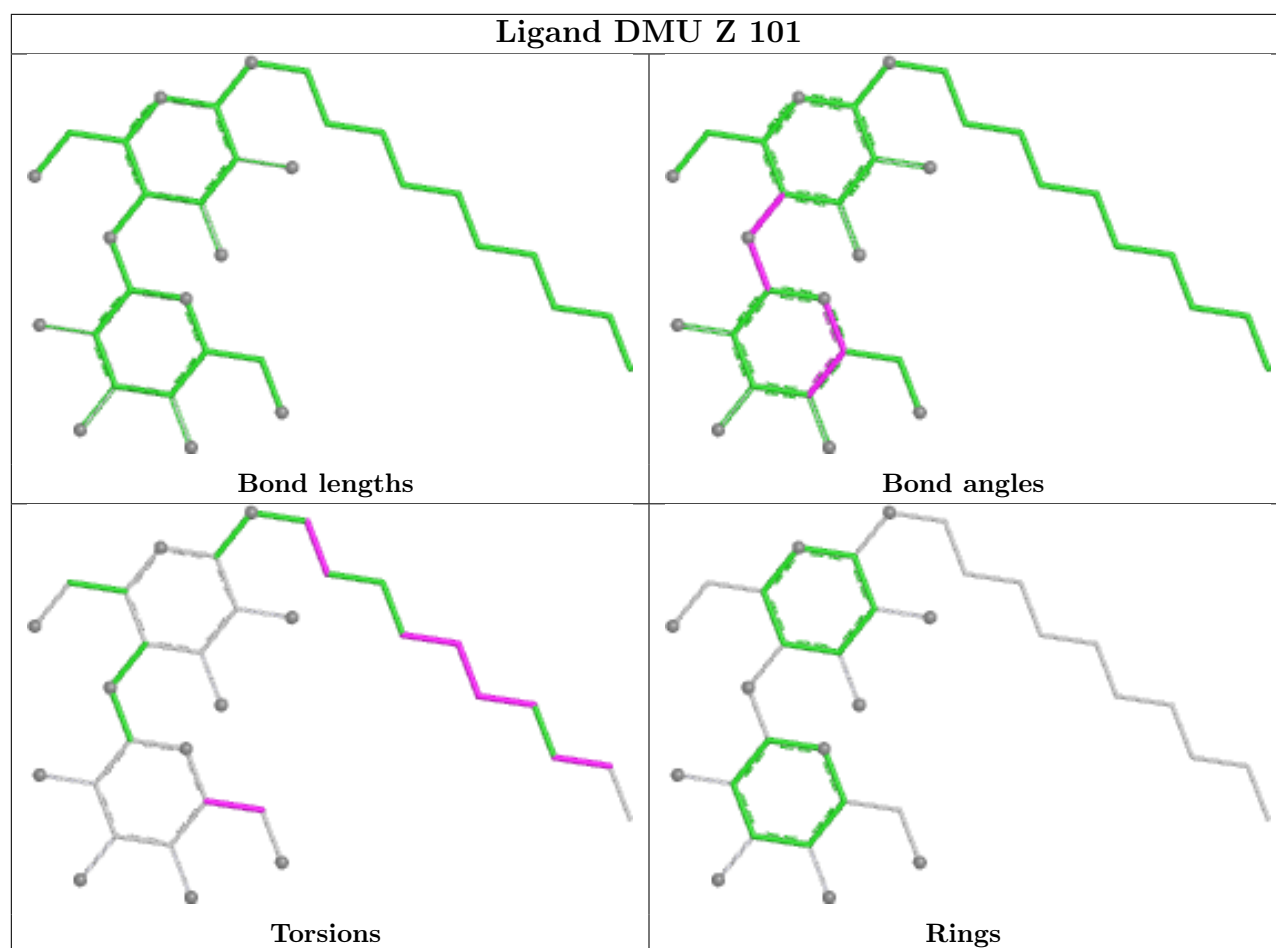
Ligand CHD L 102

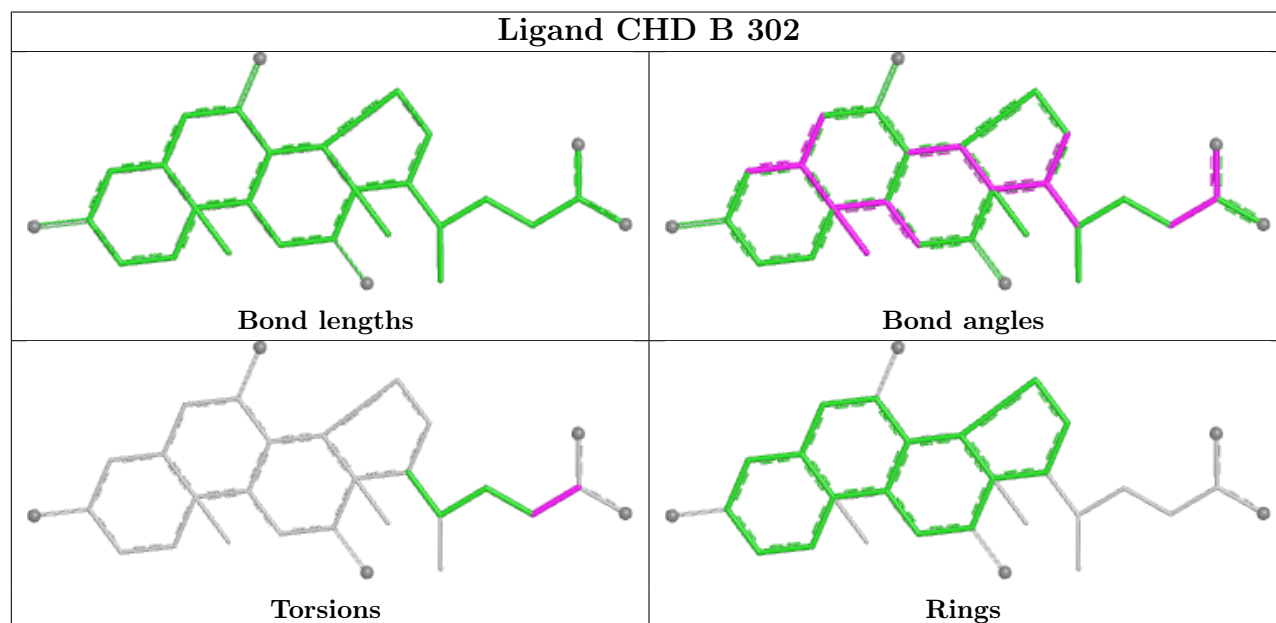
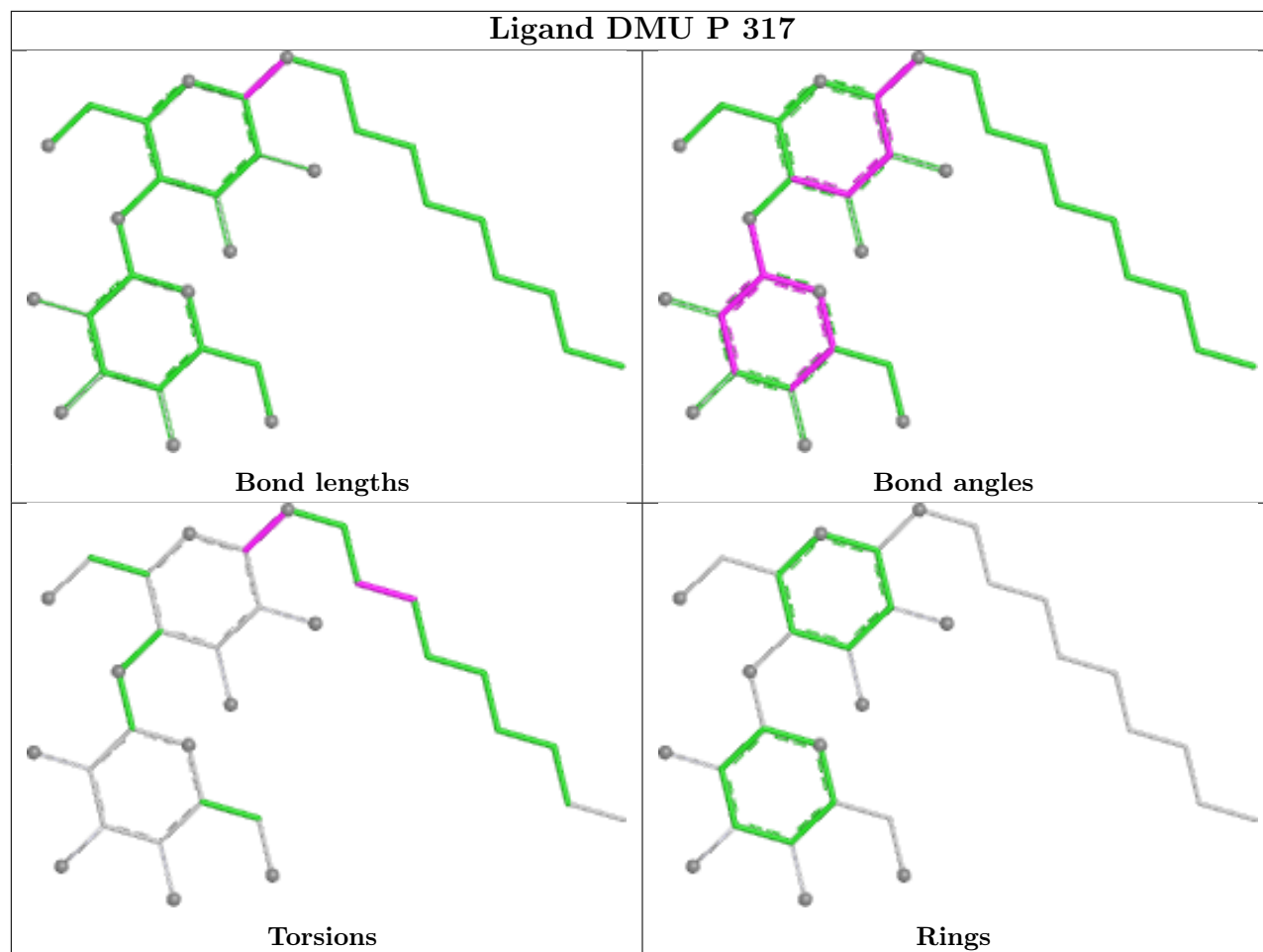


Ligand CHD G 101

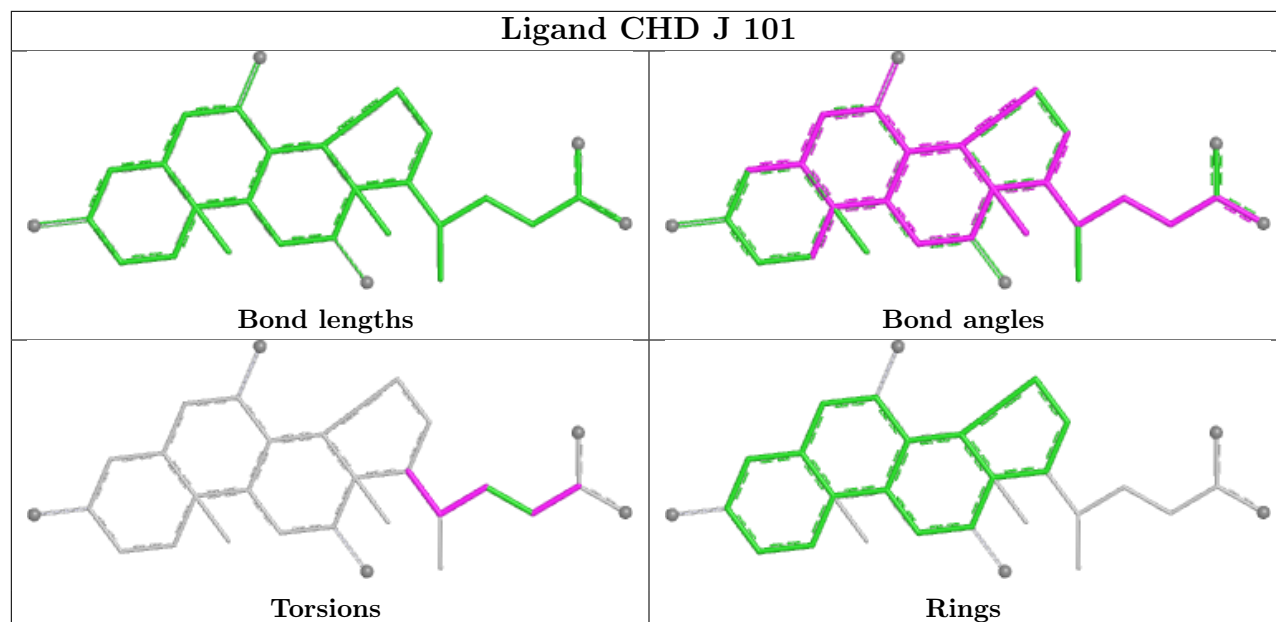




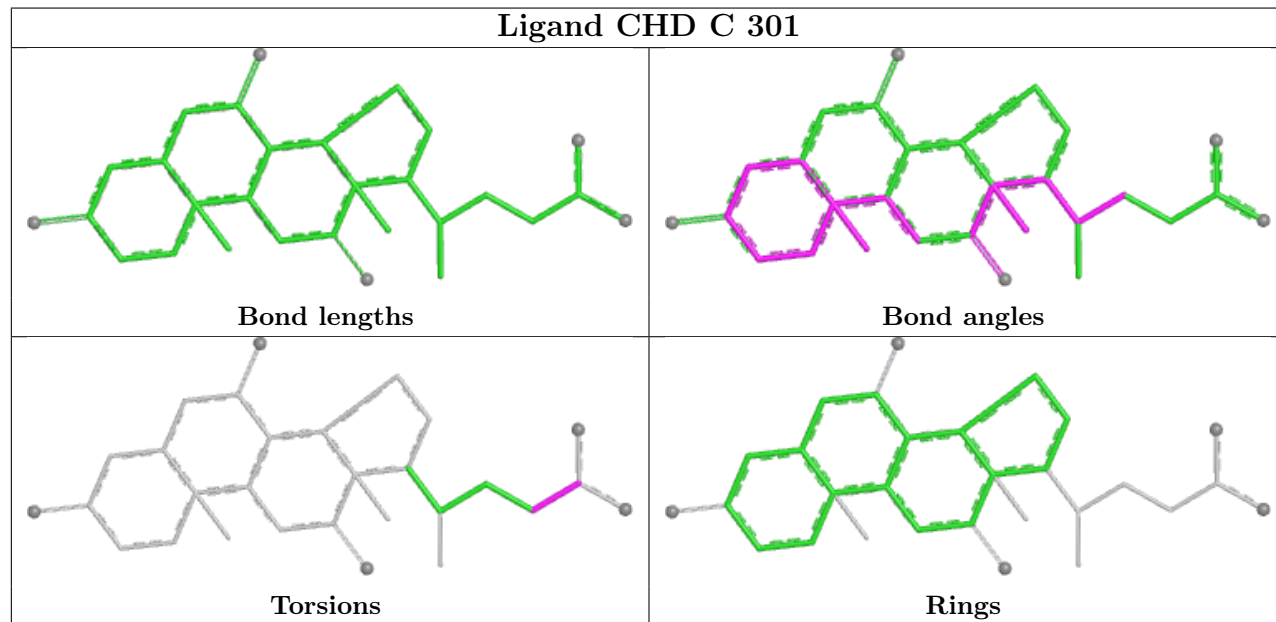


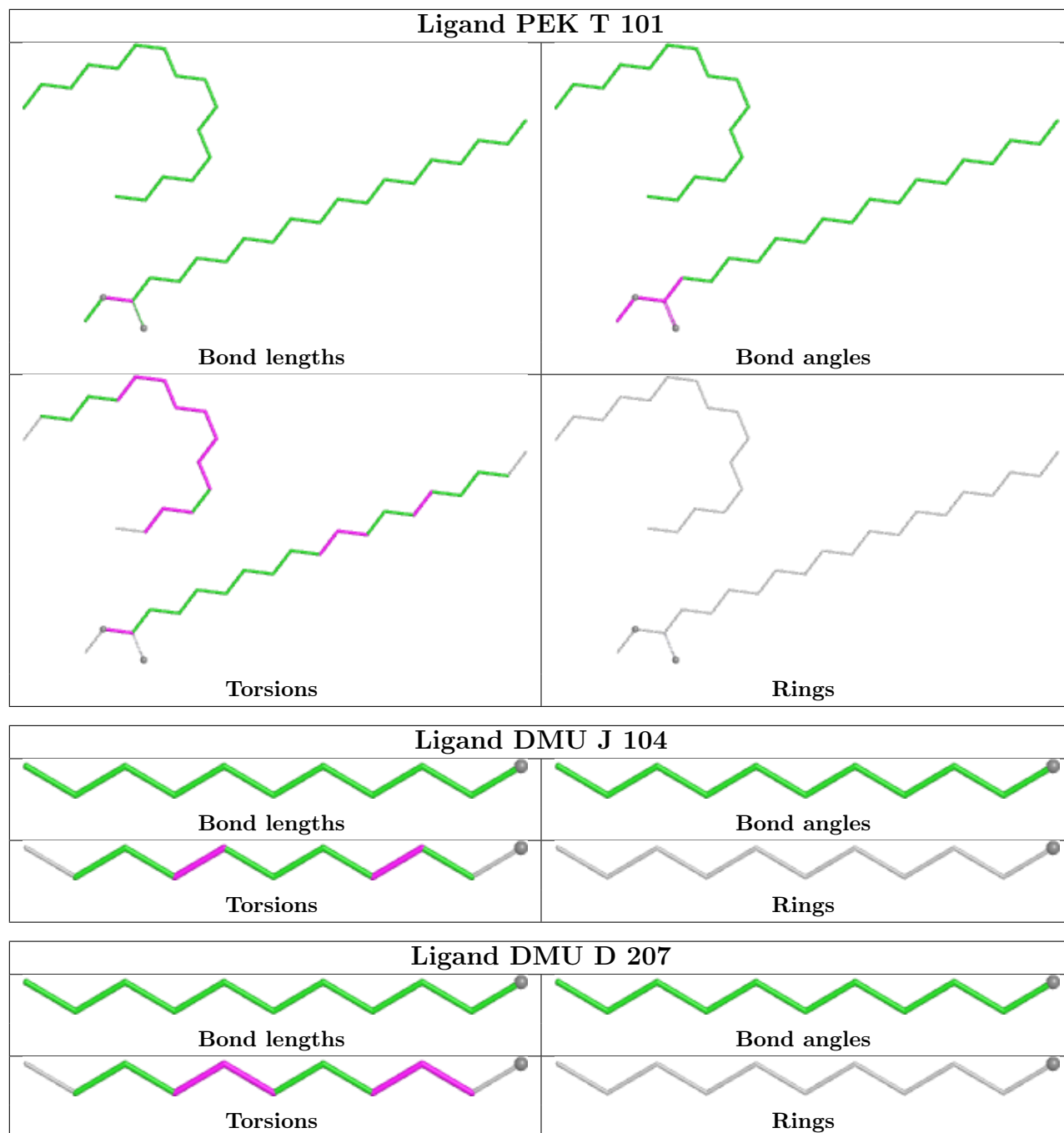


Ligand CHD J 101

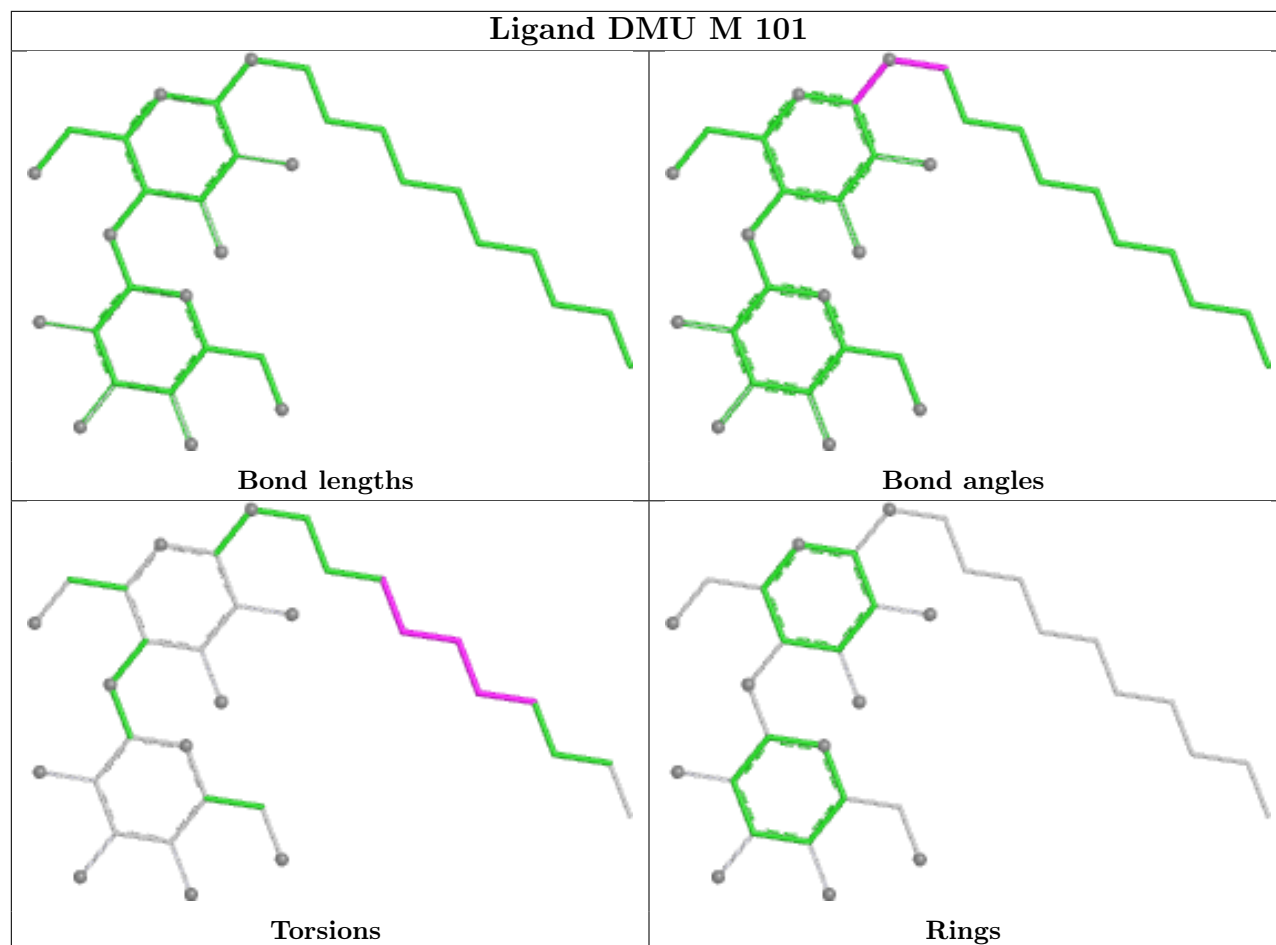


Ligand CHD C 301

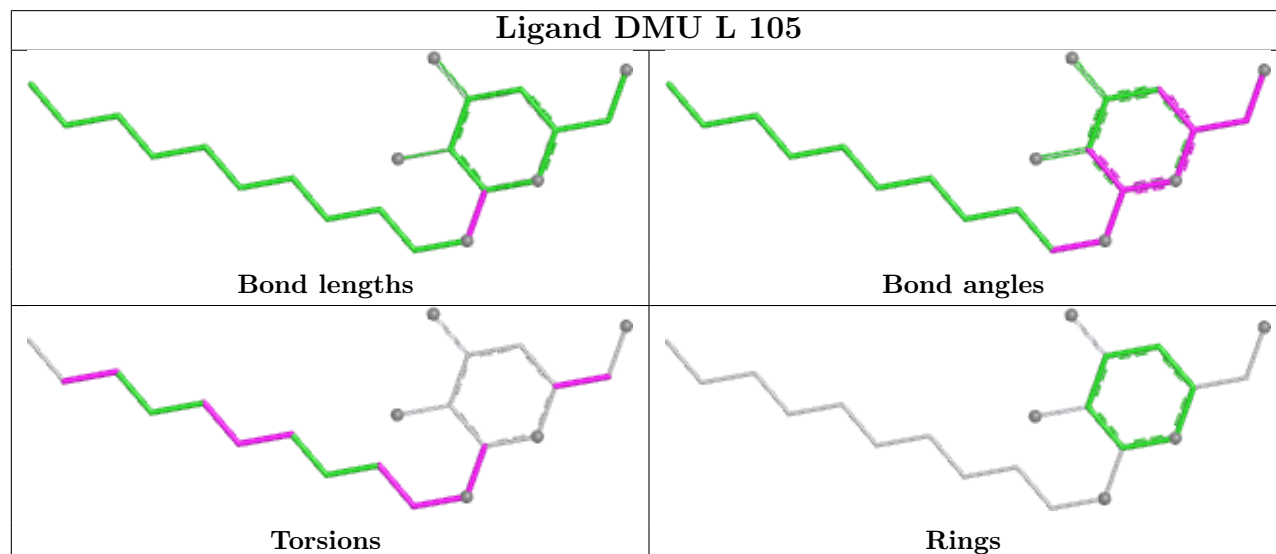


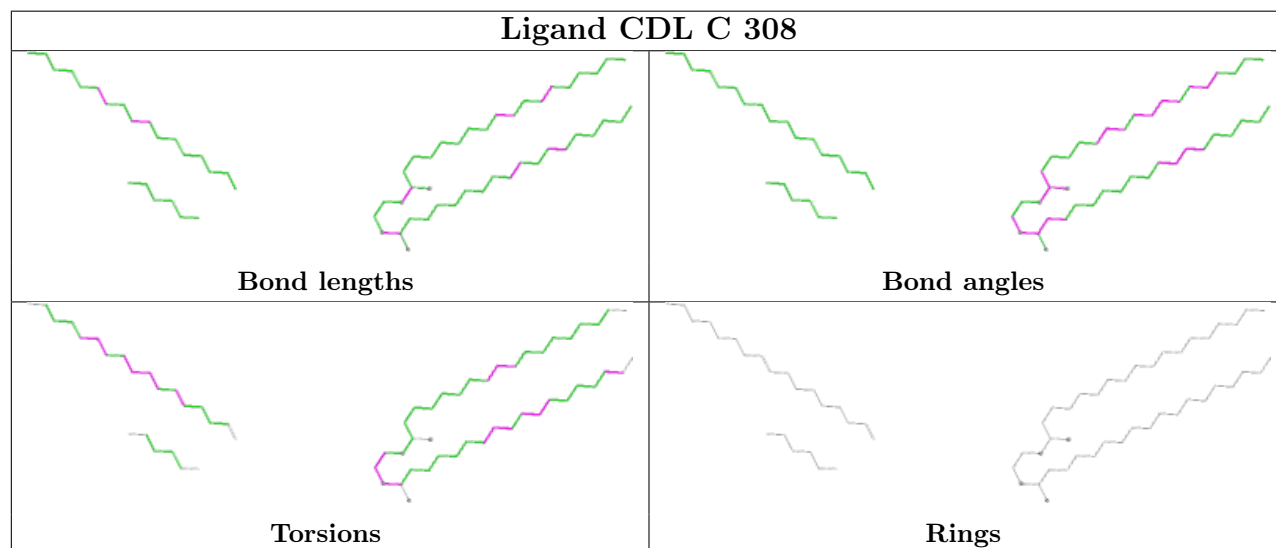
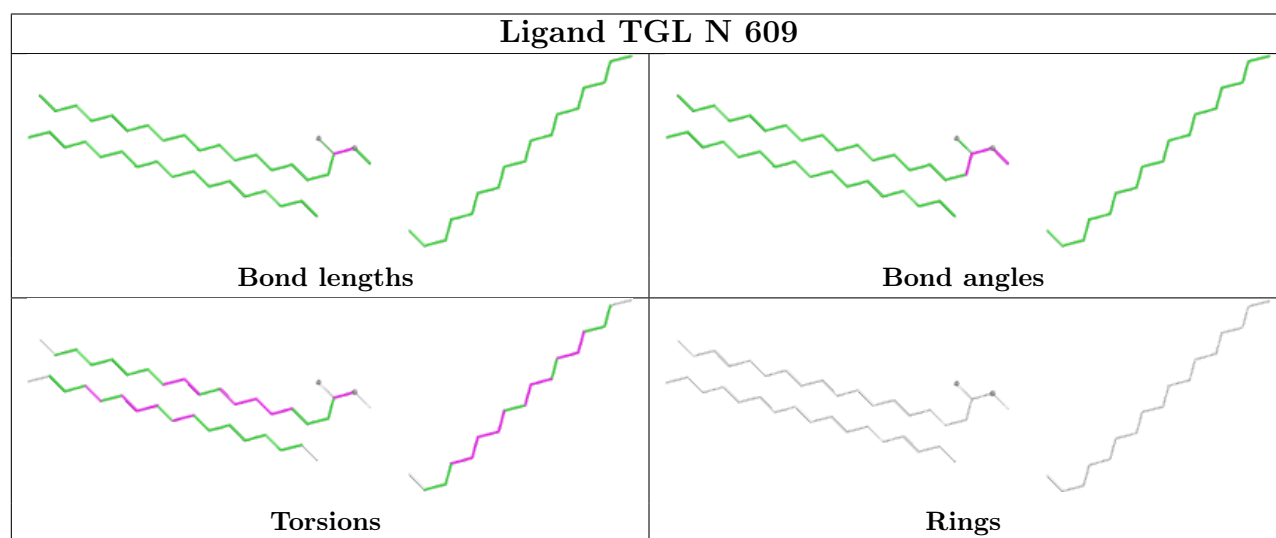
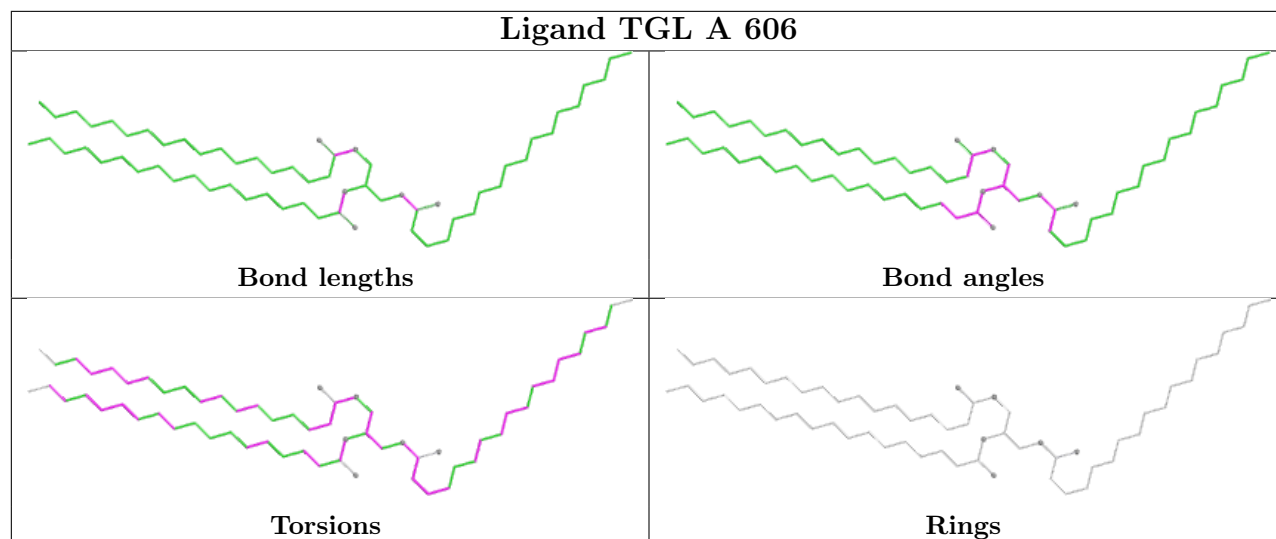


Ligand DMU M 101



Ligand DMU L 105





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%)	-0.50	3 (0%)	85 90	9, 24, 31, 65	34 (6%)
1	N	513/514 (99%)	-0.46	2 (0%)	88 93	10, 26, 35, 80	38 (7%)
2	B	226/227 (99%)	0.08	12 (5%)	32 34	22, 32, 61, 110	8 (3%)
2	O	226/227 (99%)	0.16	8 (3%)	47 51	23, 35, 68, 115	12 (5%)
3	C	259/259 (100%)	-0.28	1 (0%)	88 93	17, 27, 40, 93	11 (4%)
3	P	259/259 (100%)	-0.27	3 (1%)	76 82	17, 28, 43, 90	11 (4%)
4	D	144/144 (100%)	0.01	5 (3%)	47 51	22, 33, 56, 93	3 (2%)
4	Q	144/144 (100%)	0.91	15 (10%)	11 12	30, 48, 96, 243	1 (0%)
5	E	105/105 (100%)	0.02	3 (2%)	53 58	27, 33, 69, 156	0
5	R	105/105 (100%)	0.28	5 (4%)	35 37	29, 41, 77, 169	1 (0%)
6	F	94/94 (100%)	0.15	4 (4%)	40 42	23, 32, 65, 130	5 (5%)
6	S	94/94 (100%)	0.22	6 (6%)	25 26	22, 31, 66, 125	0
7	G	84/84 (100%)	1.31	21 (25%)	2 2	22, 35, 140, 183	5 (5%)
7	T	84/84 (100%)	1.18	22 (26%)	1 1	25, 39, 127, 194	0
8	H	79/79 (100%)	0.66	12 (15%)	5 6	26, 38, 112, 179	1 (1%)
8	U	79/79 (100%)	0.71	16 (20%)	3 2	31, 42, 117, 215	0
9	I	72/73 (98%)	0.88	9 (12%)	8 8	27, 48, 86, 102	1 (1%)
9	V	72/73 (98%)	1.16	16 (22%)	2 2	29, 55, 95, 161	0
10	J	58/58 (100%)	0.39	4 (6%)	23 24	27, 37, 88, 175	1 (1%)
10	W	58/58 (100%)	0.43	6 (10%)	12 12	28, 39, 86, 171	0
11	K	49/49 (100%)	0.29	2 (4%)	41 44	27, 38, 59, 72	3 (6%)
11	X	49/49 (100%)	0.80	5 (10%)	12 13	36, 47, 86, 100	0
12	L	46/46 (100%)	0.05	3 (6%)	25 26	25, 29, 56, 105	2 (4%)
12	Y	46/46 (100%)	0.24	3 (6%)	25 26	28, 36, 74, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/43 (100%)	0.06	3 (6%) 22 23	25, 30, 86, 141	0
13	Z	43/43 (100%)	0.55	6 (13%) 6 6	33, 38, 122, 190	0
All	All	3544/3550 (99%)	0.06	195 (5%) 30 33	9, 31, 76, 243	137 (3%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	1	ALA	12.5
7	T	3	ALA	12.3
7	G	3	ALA	10.9
4	Q	5	VAL	9.8
7	G	36	TRP	9.6
7	G	6	GLY	9.5
4	Q	6	VAL	9.2
6	S	1	ALA	8.8
7	G	11	THR	7.9
7	G	7	ASP	7.5
7	G	8	HIS	7.3
7	G	9	GLY	7.1
7	T	2	SER	6.8
7	G	4	ALA	6.7
7	T	5	LYS	6.6
6	F	2	SER	6.6
7	T	11	THR	6.5
7	T	36	TRP	6.5
8	H	8	ILE	6.2
9	V	2	THR	6.1
7	G	5	LYS	6.1
6	S	94	HIS	5.9
3	P	3	HIS	5.8
4	Q	7	LYS	5.8
7	T	10	GLY	5.8
7	T	1	ALA	5.8
7	T	6	GLY	5.8
8	U	46	LYS	5.4
7	T	8	HIS	5.3
7	G	2	SER	5.3
8	U	45	ALA	5.2
4	Q	8	SER	5.1
6	S	2	SER	5.1
9	I	2	THR	5.0

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Mol	Chain	Res	Type	RSRZ
6	S	3	GLY	5.0
2	O	113	TYR	4.9
12	Y	2	HIS	4.7
7	T	7	ASP	4.7
7	T	38	HIS	4.7
10	J	1	PHE	4.7
7	G	10	GLY	4.7
6	S	93	PRO	4.6
12	L	2	HIS	4.6
9	I	37	PHE	4.5
6	F	3	GLY	4.3
4	D	4	SER	4.2
9	I	29	LEU	4.2
2	B	65	TRP	4.1
9	V	37	PHE	4.1
10	W	1	PHE	4.1
7	T	40	GLY	4.1
1	A	514[A]	LYS	4.0
4	Q	4	SER	4.0
7	T	4	ALA	4.0
8	U	8	ILE	3.9
8	U	48	GLY	3.9
2	B	61	VAL	3.9
8	H	9	LYS	3.8
8	H	45	ALA	3.7
3	C	3	HIS	3.6
13	Z	40	TYR	3.6
8	H	46	LYS	3.5
2	O	227	LEU	3.5
8	U	47	GLY	3.5
8	H	44	THR	3.5
11	X	7	PRO	3.5
7	G	1	ALA	3.4
8	U	50	VAL	3.4
4	Q	10	ASP	3.4
7	G	42	ARG	3.4
9	V	3	ALA	3.4
13	M	40	TYR	3.3
1	N	513	LEU	3.3
11	X	6	ALA	3.3
8	U	84	LYS	3.3
7	T	9	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
8	H	48	GLY	3.3
5	E	5	HIS	3.3
4	Q	51	LEU	3.3
2	B	90	ILE	3.2
9	V	15	ARG	3.2
4	Q	147	LYS	3.2
5	R	109	VAL	3.2
9	I	44	LYS	3.2
13	Z	43	SER	3.2
4	Q	9	GLU	3.2
4	Q	35	ALA	3.1
4	Q	72	ASN	3.1
13	Z	42	LYS	3.1
13	Z	39	ASN	3.1
11	K	47	ARG	3.1
9	I	32	ALA	3.1
10	W	48	TYR	3.0
8	H	47	GLY	3.0
7	G	37	LEU	3.0
7	G	38	HIS	3.0
2	O	82[B]	ARG	2.9
13	Z	41	LYS	2.9
3	P	37	PHE	2.9
9	V	34	PHE	2.9
11	K	6	ALA	2.9
7	T	41	HIS	2.9
11	X	54	ARG	2.9
13	Z	38	ASP	2.9
10	W	27	THR	2.8
10	W	58	LYS	2.8
10	J	58	LYS	2.8
7	T	39	SER	2.8
2	B	91	ASN	2.8
7	G	41	HIS	2.8
7	T	12	GLY	2.8
9	I	25	PHE	2.7
5	R	5	HIS	2.7
2	B	129	LYS	2.7
10	J	27	THR	2.7
7	T	42	ARG	2.6
4	D	7	LYS	2.6
8	U	10	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
7	T	84	LYS	2.6
8	H	7	LYS	2.6
4	Q	87	PHE	2.6
6	S	64	GLU	2.6
8	H	23	GLN	2.6
7	G	40	GLY	2.6
5	E	109	VAL	2.5
8	H	50	VAL	2.5
2	B	87	MET	2.5
1	A	297[A]	MET	2.5
7	G	43	GLU	2.5
7	G	84	LYS	2.5
12	Y	47	LYS	2.5
4	Q	19	ARG	2.5
9	V	5	ALA	2.5
4	D	143	ASN	2.4
5	E	39	TYR	2.4
9	V	29	LEU	2.4
8	U	12	GLN	2.4
4	Q	39	ALA	2.4
8	U	49	ASP	2.4
8	U	52	VAL	2.4
10	W	57	HIS	2.4
8	U	7	LYS	2.4
8	U	61	LYS	2.4
10	J	57	HIS	2.4
7	G	35	SER	2.4
7	T	35	SER	2.4
8	U	55	TRP	2.4
7	T	37	LEU	2.3
12	L	45	LEU	2.3
8	U	44	THR	2.3
9	V	36	LYS	2.3
9	V	22	VAL	2.3
2	B	115[A]	ASP	2.3
2	O	65[A]	TRP	2.3
9	V	25	PHE	2.3
3	P	122	HIS	2.3
6	F	94	HIS	2.3
9	I	36	LYS	2.3
9	V	65	LYS	2.3
5	R	80	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	22[A]	HIS	2.3
13	M	39	ASN	2.3
12	L	47	LYS	2.3
10	W	4	ARG	2.3
11	X	52	GLU	2.3
1	N	514	LYS	2.3
2	B	68	LEU	2.3
8	H	84	LYS	2.3
7	G	12	GLY	2.2
9	I	33	THR	2.2
2	B	64	ILE	2.2
2	B	92	ASN	2.2
9	V	73	LYS	2.2
1	A	349	THR	2.2
5	R	96	LEU	2.2
2	B	113	TYR	2.2
2	O	90	ILE	2.2
8	H	10[A]	ASN	2.2
13	M	42	LYS	2.2
2	B	58	ALA	2.2
7	T	43	GLU	2.1
9	V	26	MET	2.1
11	X	47	ARG	2.1
2	O	129	LYS	2.1
8	U	9	LYS	2.1
4	Q	71	MET	2.1
12	Y	24	MET	2.1
2	O	91	ASN	2.1
9	V	52	ARG	2.1
5	R	108	LYS	2.0
9	I	34	PHE	2.0
9	V	33	THR	2.0
9	V	30	GLY	2.0
4	D	5	VAL	2.0
4	D	31	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SAC	V	1	9/10	0.45	0.22	201,217,238,247	0
9	SAC	I	1	9/10	0.64	0.24	129,147,176,183	0
1	FME	N	1	10/11	0.93	0.14	36,45,97,109	0
2	FME	B	1	10/11	0.95	0.12	28,31,40,126	0
1	FME	A	1	10/11	0.95	0.09	37,51,85,99	0
2	FME	O	1	10/11	0.96	0.10	31,36,44,111	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	CDL	N	601	62/100	0.68	0.32	44,76,103,117	0
25	CHD	J	101	29/29	0.70	0.21	50,120,146,151	0
22	EDO	L	104	4/4	0.70	0.29	50,51,79,128	0
23	DMU	X	102	9/33	0.71	0.29	65,70,82,86	0
23	DMU	X	104	22/33	0.71	0.20	58,94,150,157	0
23	DMU	A	623	11/33	0.72	0.23	62,76,106,114	0
25	CHD	Y	102	29/29	0.72	0.24	56,91,135,152	0
23	DMU	K	103	10/33	0.72	0.31	62,75,106,112	0
22	EDO	L	103	4/4	0.76	0.25	42,49,64,119	0
23	DMU	X	103	9/33	0.76	0.23	56,62,103,104	0
23	DMU	L	105	21/33	0.76	0.22	54,80,107,120	0
25	CHD	C	309	29/29	0.77	0.18	47,86,113,140	0
25	CHD	L	102	29/29	0.77	0.21	51,95,117,134	0
22	EDO	A	614	4/4	0.78	0.28	51,61,65,80	0
26	PEK	C	303	45/53	0.78	0.20	44,95,175,209	0
23	DMU	P	317	32/33	0.78	0.17	52,107,133,136	0
27	CDL	T	102	61/100	0.78	0.25	42,77,110,117	0
26	PEK	P	303	38/53	0.79	0.21	49,79,163,172	0
18	TGL	N	609	55/63	0.79	0.27	46,72,112,119	0
22	EDO	P	315	4/4	0.79	0.20	66,95,100,113	0
23	DMU	D	206	33/33	0.80	0.17	46,95,141,151	0
22	EDO	A	612	4/4	0.80	0.21	51,51,71,101	0
19	PGV	C	307	36/51	0.80	0.26	41,74,140,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	PEK	C	305	36/53	0.81	0.25	42,76,101,118	0
21	PSC	O	302	31/52	0.81	0.25	36,62,106,153	0
22	EDO	F	105	4/4	0.81	0.22	56,58,67,70	0
19	PGV	A	608	34/51	0.81	0.26	32,57,110,126	0
23	DMU	P	316	21/33	0.82	0.19	51,81,126,136	0
22	EDO	A	618	4/4	0.82	0.20	52,59,65,85	0
22	EDO	C	320	4/4	0.82	0.26	33,68,70,73	0
18	TGL	N	607	63/63	0.82	0.24	40,79,108,125	0
18	TGL	A	606	63/63	0.82	0.22	39,72,108,119	0
19	PGV	P	306	31/51	0.82	0.23	32,72,96,109	0
23	DMU	O	306	13/33	0.82	0.23	45,66,128,139	0
22	EDO	A	617	4/4	0.83	0.19	57,70,72,73	0
23	DMU	Q	201	11/33	0.83	0.24	49,70,93,95	0
23	DMU	D	207	11/33	0.83	0.22	58,81,115,120	0
19	PGV	N	610	51/51	0.83	0.22	40,83,151,204	0
22	EDO	O	305	4/4	0.83	0.21	49,61,62,105	0
26	PEK	T	101	37/53	0.83	0.24	43,75,105,131	0
18	TGL	A	607	63/63	0.83	0.23	32,68,117,128	0
20	PER	N	611[A]	2/2	0.83	0.16	20,20,20,31	2
22	EDO	C	315	4/4	0.84	0.20	65,78,87,99	0
23	DMU	P	308	33/33	0.84	0.17	37,102,137,160	0
27	CDL	P	307	68/100	0.84	0.23	39,76,127,157	0
21	PSC	A	610	25/52	0.84	0.25	44,70,88,111	0
22	EDO	D	204	4/4	0.85	0.24	41,43,50,59	0
22	EDO	J	103	4/4	0.85	0.18	59,62,62,75	0
22	EDO	T	104	4/4	0.85	0.27	56,73,98,107	0
18	TGL	N	608	55/63	0.86	0.22	38,64,110,123	0
18	TGL	L	101	63/63	0.86	0.22	25,60,114,165	0
22	EDO	C	319	4/4	0.86	0.20	43,47,61,111	0
23	DMU	K	102	11/33	0.87	0.20	55,70,95,105	0
22	EDO	Y	101	4/4	0.87	0.16	48,51,53,64	0
22	EDO	D	205	4/4	0.87	0.14	53,58,59,61	0
27	CDL	C	308	65/100	0.87	0.21	37,69,123,156	0
23	DMU	X	101	10/33	0.87	0.19	41,60,84,103	0
22	EDO	C	313	4/4	0.87	0.15	30,39,40,49	0
22	EDO	J	102	4/4	0.87	0.20	48,48,91,98	0
23	DMU	C	310	33/33	0.88	0.15	35,81,151,167	0
22	EDO	M	102	4/4	0.88	0.21	68,86,88,93	0
22	EDO	N	620	4/4	0.88	0.22	52,52,53,80	0
22	EDO	W	101	4/4	0.88	0.18	54,56,71,77	0
22	EDO	F	107	4/4	0.88	0.17	45,50,81,119	0
23	DMU	K	104	11/33	0.88	0.19	50,68,100,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	EDO	P	309	4/4	0.88	0.16	60,63,63,69	0
22	EDO	F	109	4/4	0.89	0.15	35,36,71,71	0
22	EDO	T	105	4/4	0.89	0.14	37,48,58,62	0
23	DMU	C	321	12/33	0.89	0.17	51,66,84,89	0
22	EDO	P	314	4/4	0.89	0.15	37,53,55,74	0
22	EDO	F	102	4/4	0.89	0.21	33,36,53,121	0
29	PO4	U	101	5/5	0.89	0.10	51,53,120,124	0
22	EDO	C	317	4/4	0.90	0.15	60,67,70,80	0
22	EDO	A	620	4/4	0.90	0.21	44,52,61,82	0
22	EDO	E	203	4/4	0.90	0.15	49,49,49,75	0
22	EDO	S	104	4/4	0.90	0.14	44,46,48,54	0
22	EDO	S	106	4/4	0.90	0.21	37,52,72,76	0
22	EDO	C	311	4/4	0.90	0.15	44,65,68,73	0
22	EDO	O	304	4/4	0.90	0.14	46,46,48,52	0
22	EDO	F	103	4/4	0.90	0.15	44,51,53,59	0
23	DMU	Z	101	33/33	0.91	0.11	37,47,68,72	0
22	EDO	B	306	4/4	0.91	0.13	38,47,48,48	0
23	DMU	K	105	9/33	0.91	0.16	38,52,70,105	0
22	EDO	P	310	4/4	0.91	0.14	71,72,75,80	0
23	DMU	J	104	11/33	0.91	0.16	49,60,84,99	0
22	EDO	D	202	4/4	0.91	0.15	43,43,57,86	0
22	EDO	W	102	4/4	0.91	0.15	46,63,67,113	0
22	EDO	Q	202	4/4	0.92	0.13	41,46,48,52	0
22	EDO	A	621	4/4	0.92	0.21	37,40,40,52	0
22	EDO	B	305	4/4	0.92	0.14	28,36,44,63	0
23	DMU	M	101	33/33	0.92	0.10	35,41,54,65	0
22	EDO	N	619	4/4	0.92	0.21	40,78,80,94	0
22	EDO	P	312	4/4	0.92	0.14	28,39,39,57	0
22	EDO	P	313	4/4	0.92	0.16	49,54,61,76	0
22	EDO	C	316	4/4	0.92	0.12	49,55,70,77	0
29	PO4	H	101	5/5	0.92	0.10	62,62,77,101	0
22	EDO	D	201	4/4	0.92	0.16	39,49,70,82	0
22	EDO	C	318	4/4	0.93	0.14	40,60,68,94	0
22	EDO	F	108	4/4	0.93	0.17	37,42,79,101	0
22	EDO	A	622	4/4	0.94	0.15	32,37,42,42	0
23	DMU	K	101	8/33	0.94	0.17	48,63,77,85	0
22	EDO	N	615	4/4	0.94	0.11	38,41,42,58	0
22	EDO	N	616	4/4	0.94	0.16	33,40,44,86	0
22	EDO	D	203	4/4	0.94	0.12	37,40,57,68	0
22	EDO	A	616	4/4	0.94	0.31	31,40,42,78	0
22	EDO	N	621	4/4	0.94	0.17	39,41,43,116	0
22	EDO	N	622	4/4	0.94	0.17	30,34,50,92	0

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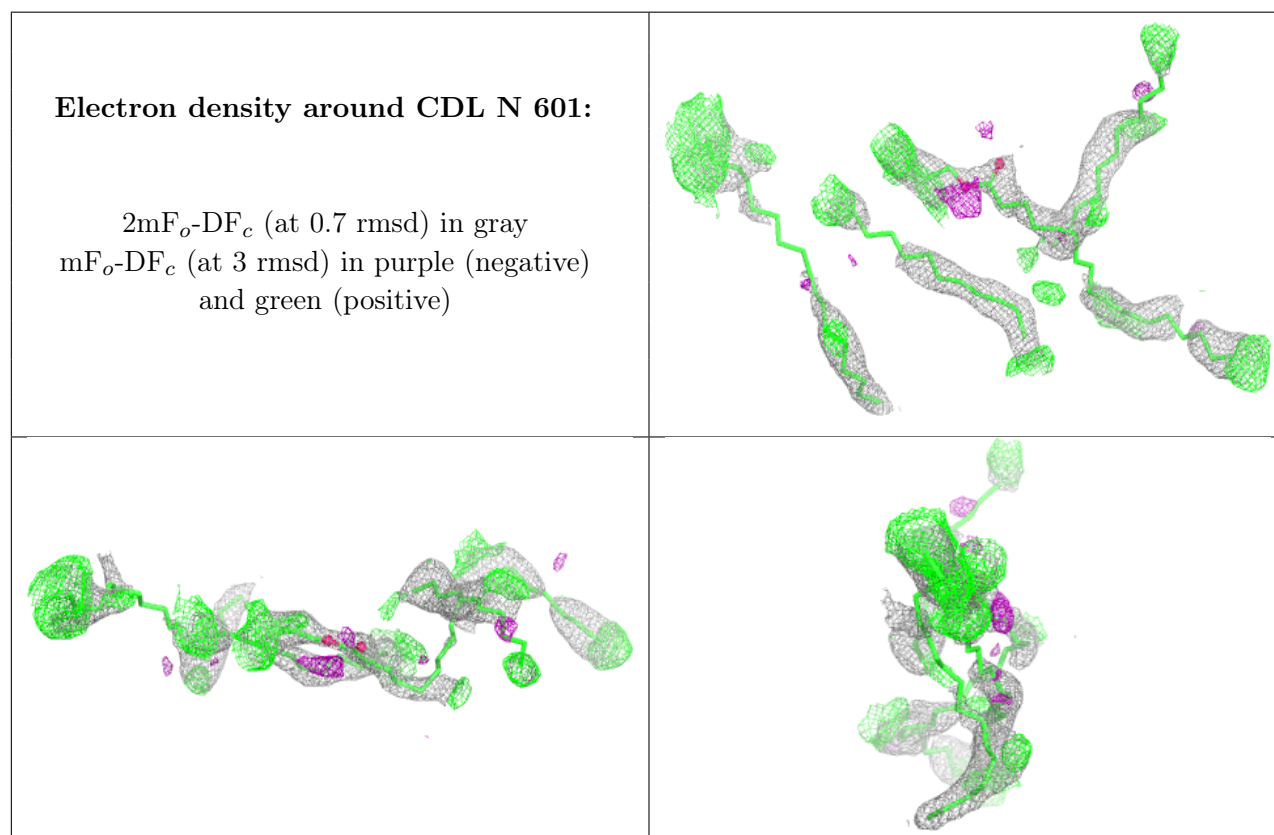
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	EDO	C	314	4/4	0.95	0.12	31,35,53,60	0
22	EDO	P	311	4/4	0.95	0.11	33,37,37,44	0
22	EDO	S	107	4/4	0.95	0.12	28,45,48,62	0
22	EDO	T	103	4/4	0.95	0.08	30,30,38,40	0
22	EDO	A	619	4/4	0.95	0.15	28,42,71,95	0
25	CHD	C	301	29/29	0.95	0.07	26,29,39,44	0
22	EDO	E	202	4/4	0.95	0.08	37,37,41,43	0
20	PER	A	609[A]	2/2	0.95	0.10	20,20,20,24	2
19	PGV	N	612	51/51	0.95	0.13	24,31,73,93	0
22	EDO	A	615	4/4	0.95	0.09	26,26,28,33	0
22	EDO	E	201	4/4	0.96	0.09	38,39,40,40	0
26	PEK	P	304	52/53	0.96	0.13	28,43,96,117	0
17	NA	C	302	1/1	0.96	0.07	36,36,36,36	0
19	PGV	A	611	51/51	0.96	0.11	19,30,73,90	0
25	CHD	P	301	29/29	0.96	0.07	26,30,35,44	0
22	EDO	C	312	4/4	0.96	0.12	32,33,33,82	0
22	EDO	N	613	4/4	0.96	0.08	24,27,28,32	0
26	PEK	C	304	52/53	0.96	0.12	25,42,97,111	0
17	NA	P	302	1/1	0.96	0.07	38,38,38,38	0
22	EDO	N	618	4/4	0.97	0.10	29,42,46,46	0
19	PGV	P	305	51/51	0.97	0.11	22,31,87,120	0
22	EDO	F	106	4/4	0.97	0.08	30,31,32,32	0
22	EDO	B	303	4/4	0.97	0.07	21,25,26,32	0
22	EDO	B	304	4/4	0.97	0.09	33,43,55,80	0
22	EDO	S	102	4/4	0.97	0.07	20,22,22,24	0
22	EDO	S	103	4/4	0.97	0.07	32,33,43,43	0
22	EDO	O	303	4/4	0.97	0.09	25,29,30,31	0
22	EDO	S	105	4/4	0.97	0.10	29,31,32,32	0
19	PGV	C	306	48/51	0.97	0.10	21,28,66,92	0
22	EDO	N	614	4/4	0.97	0.08	38,39,40,40	0
22	EDO	G	102	4/4	0.97	0.06	25,32,32,34	0
25	CHD	B	302	29/29	0.97	0.07	21,27,36,50	0
16	MG	A	604	1/1	0.97	0.10	18,18,18,18	0
22	EDO	N	617	4/4	0.97	0.07	20,26,28,31	0
25	CHD	G	101	29/29	0.97	0.06	20,26,34,40	0
22	EDO	A	613	4/4	0.98	0.10	21,24,30,30	0
14	HEA	N	603	60/60	0.98	0.06	18,23,28,37	0
22	EDO	F	104	4/4	0.98	0.05	22,24,25,27	0
14	HEA	N	602[B]	54/60	0.99	0.06	15,24,33,40	12
14	HEA	N	602[C]	51/60	0.99	0.06	16,24,28,33	9
14	HEA	A	601[A]	60/60	0.99	0.05	17,21,40,61	18
14	HEA	A	601[B]	54/60	0.99	0.05	9,20,29,45	12

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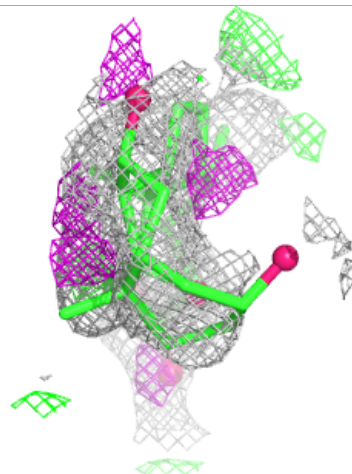
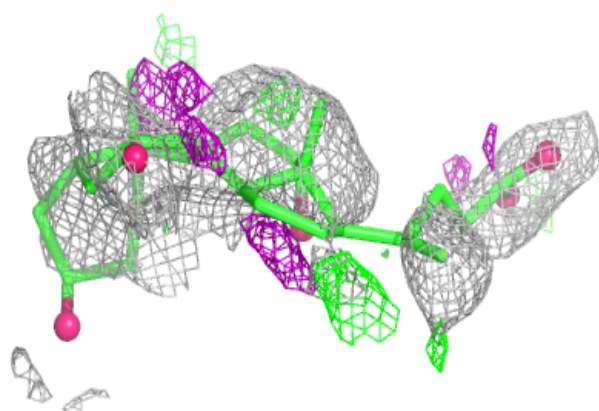
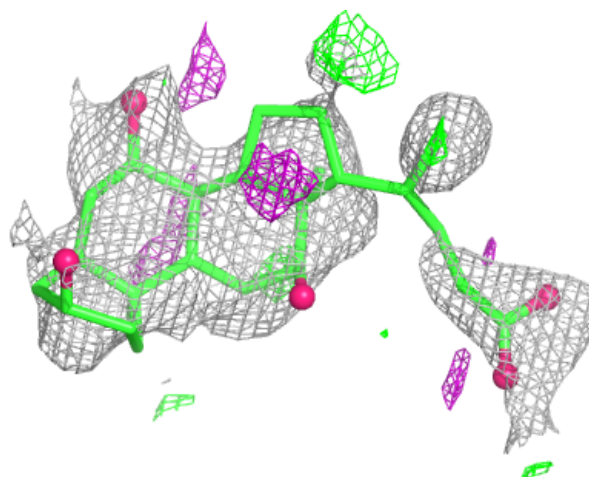
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	MG	N	605	1/1	0.99	0.06	21,21,21,21	0
17	NA	A	605	1/1	0.99	0.05	24,24,24,24	0
14	HEA	A	601[C]	51/60	0.99	0.05	9,20,24,40	9
17	NA	N	606	1/1	0.99	0.05	30,30,30,30	0
14	HEA	A	602	60/60	0.99	0.06	16,21,30,37	0
14	HEA	N	602[A]	60/60	0.99	0.06	18,24,38,44	18
15	CU	N	604	1/1	1.00	0.02	24,24,24,24	0
15	CU	A	603	1/1	1.00	0.01	23,23,23,23	0
28	ZN	F	101	1/1	1.00	0.03	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.03	25,25,25,25	0
24	CUA	B	301	2/2	1.00	0.01	22,22,22,23	0
24	CUA	O	301	2/2	1.00	0.02	26,26,26,26	0

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



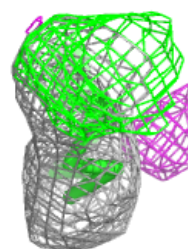
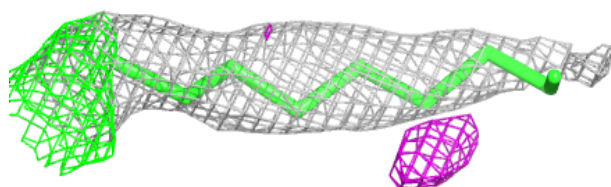
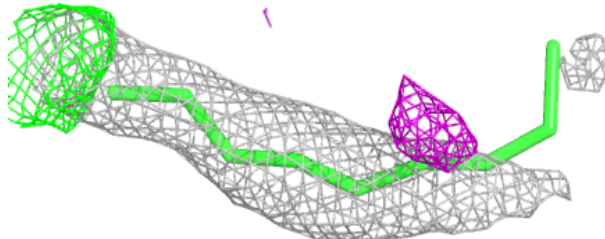
Electron density around CHD J 101:

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

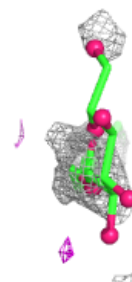
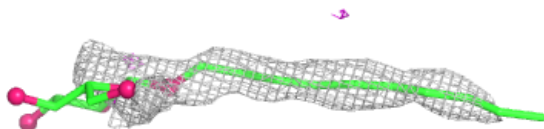
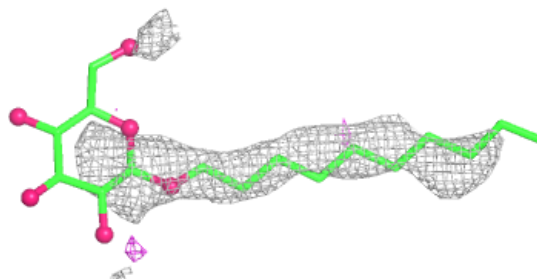


Electron density around DMU X 102:

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

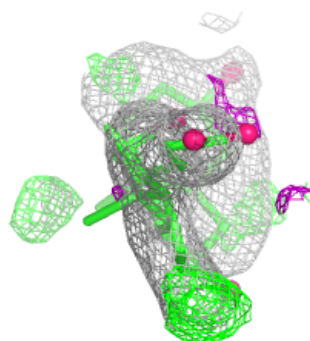
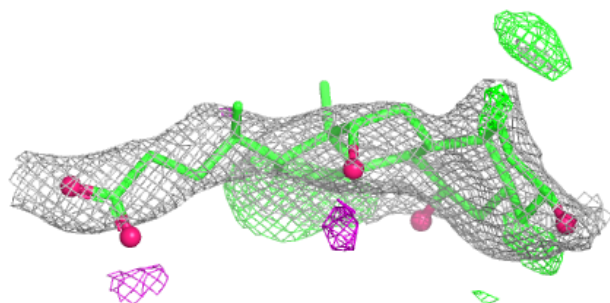
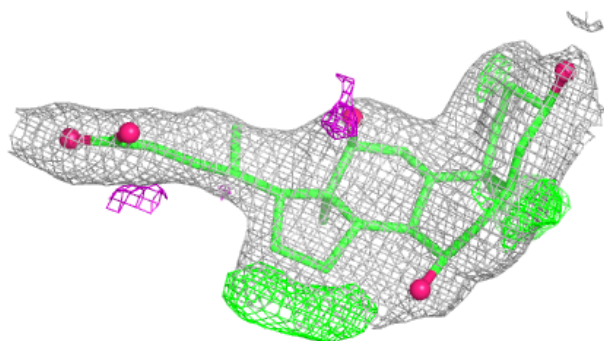
**Electron density around DMU X 104:**

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

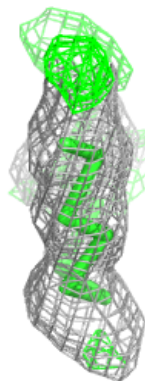
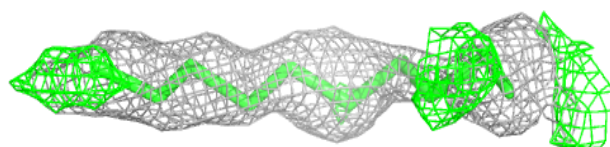
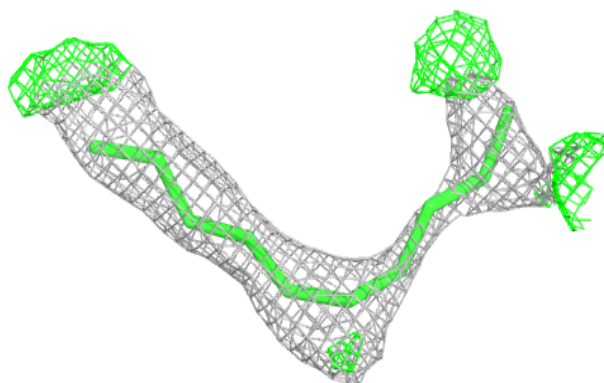


Electron density around CHD Y 102:

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

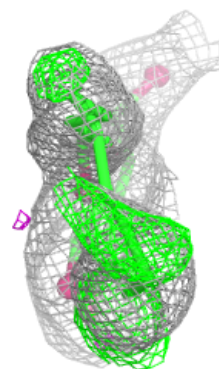
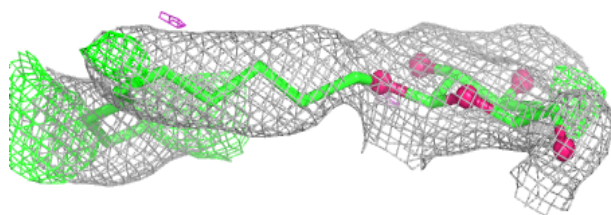
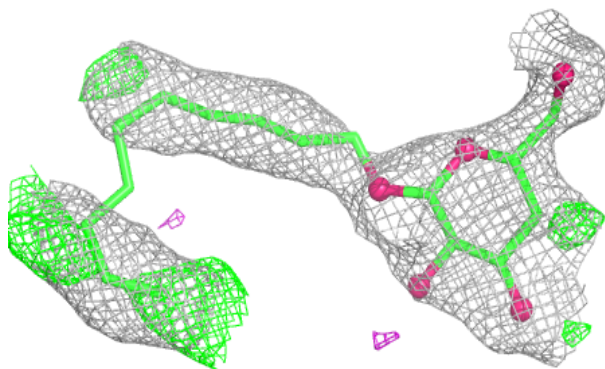
**Electron density around DMU K 103:**

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

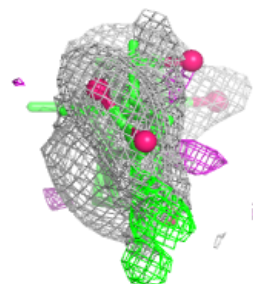
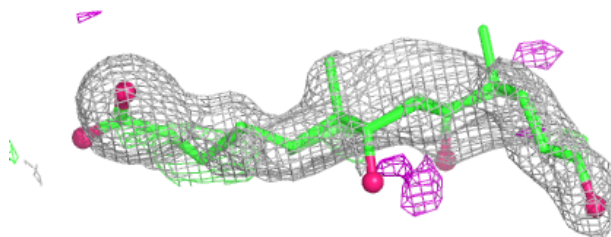
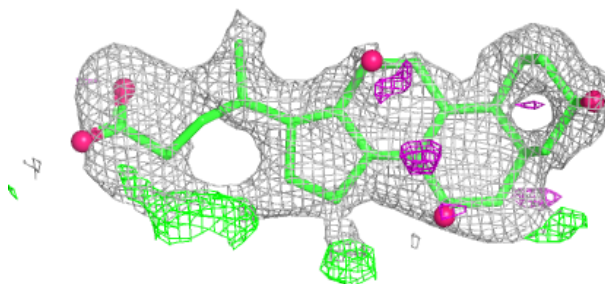


Electron density around DMU L 105:

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

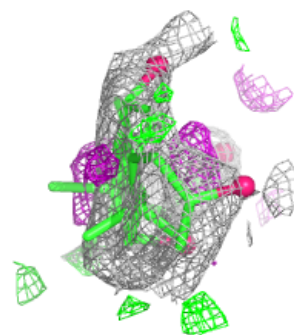
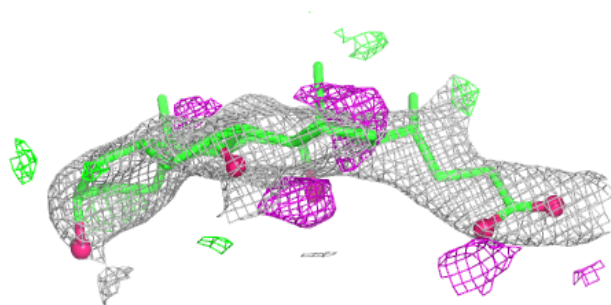
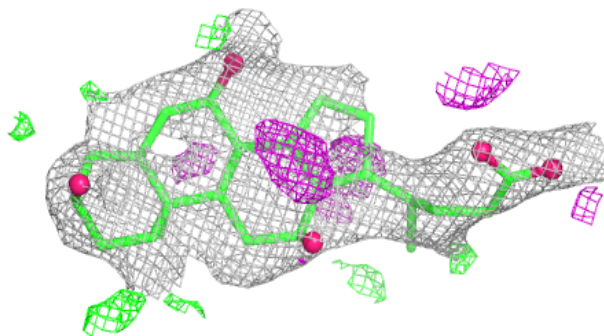
**Electron density around CHD C 309:**

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



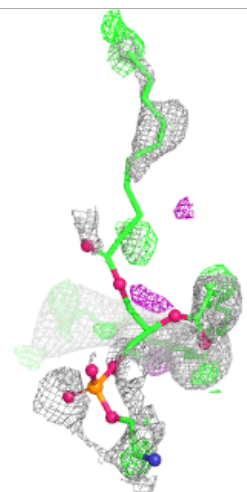
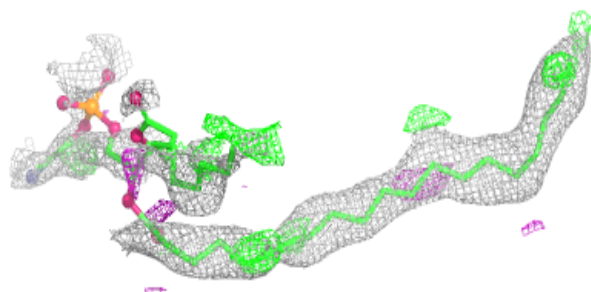
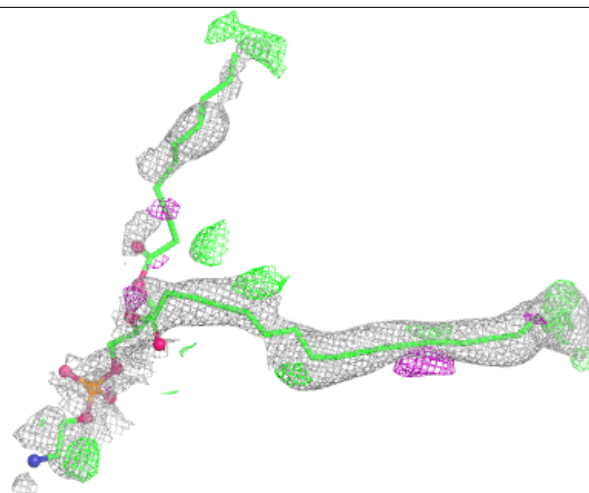
Electron density around CHD L 102:

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



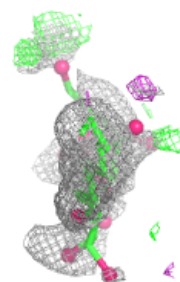
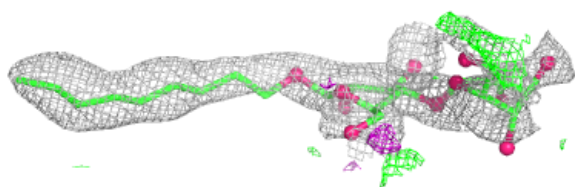
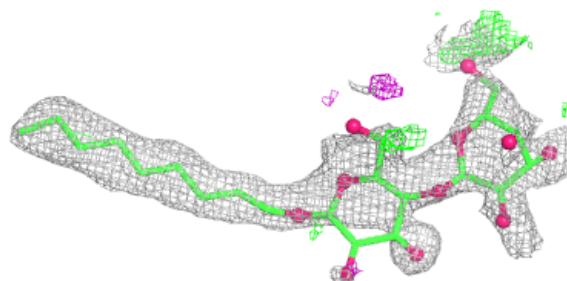
Electron density around PEK C 303:

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

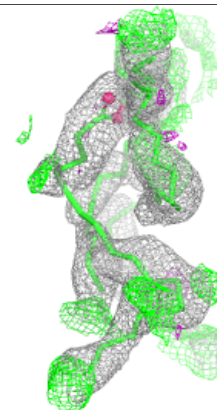
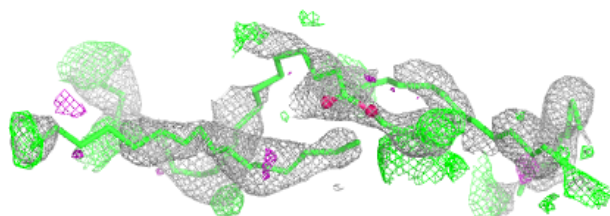
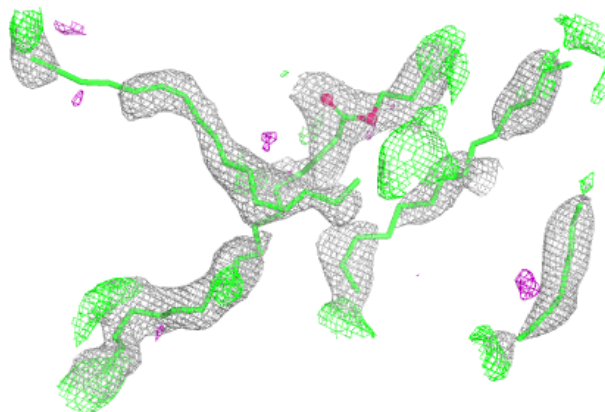


Electron density around DMU P 317:

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

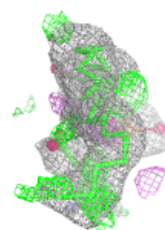
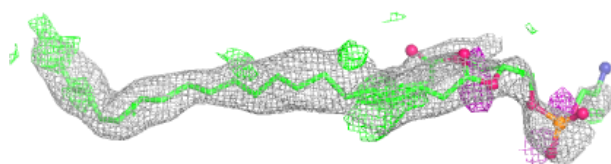
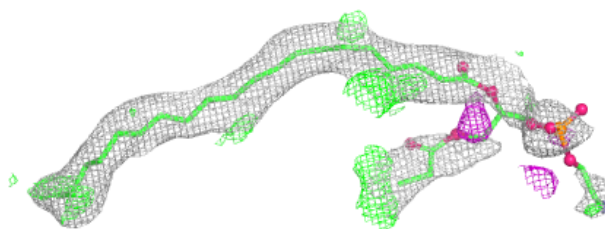
**Electron density around CDL T 102:**

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

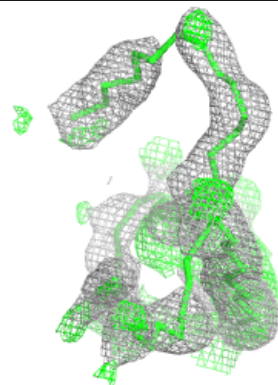
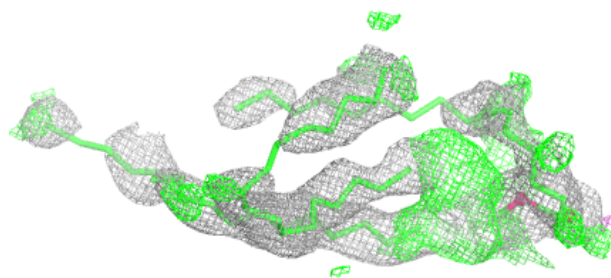
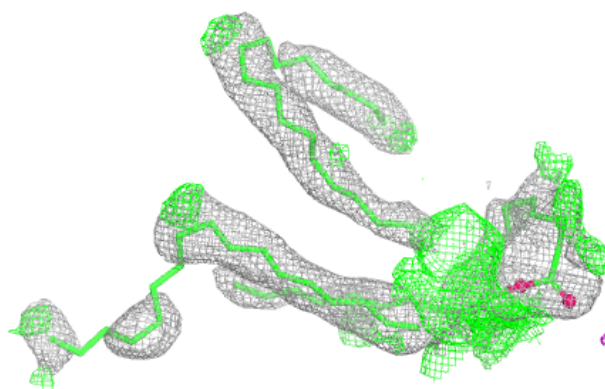


Electron density around PEK P 303:

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

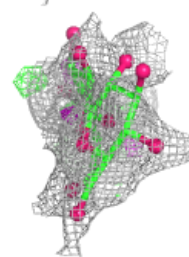
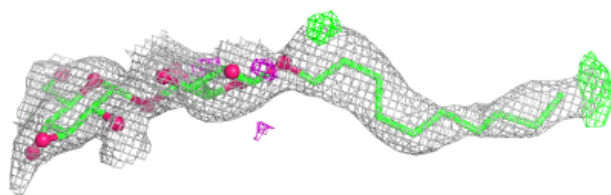
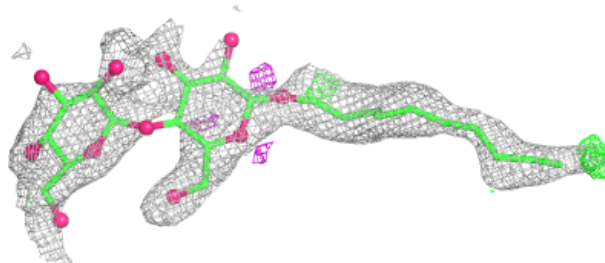
**Electron density around TGL N 609:**

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

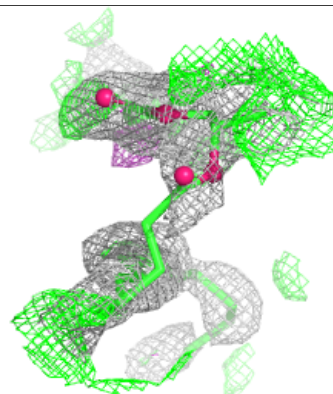
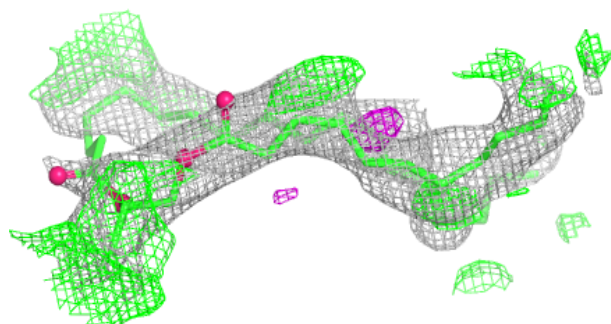
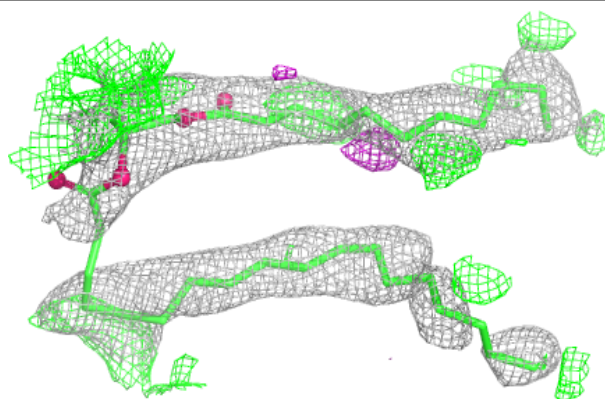


Electron density around DMU D 206:

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

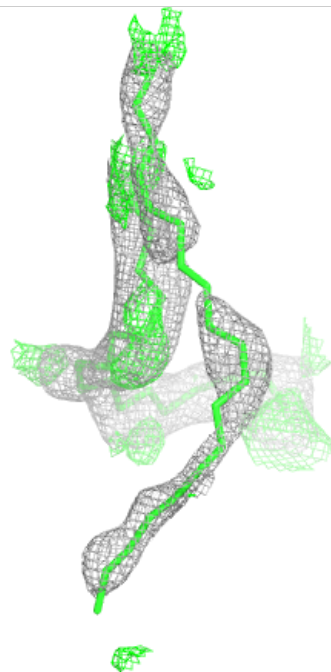
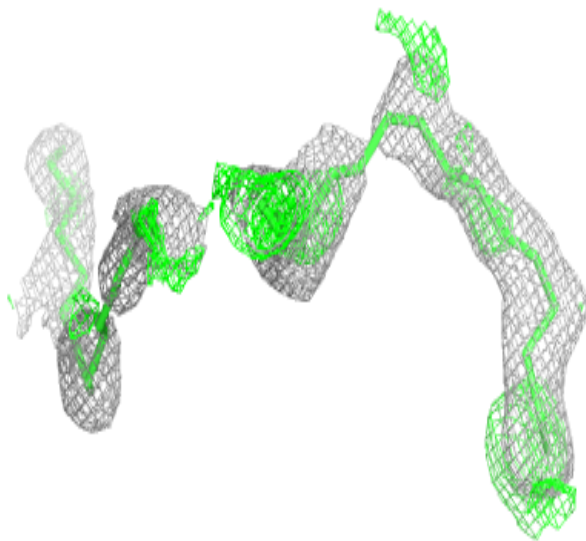
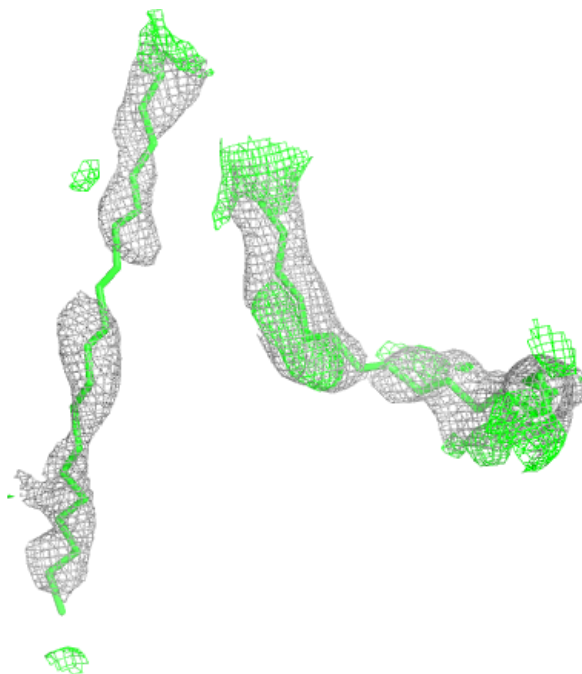
**Electron density around PGV C 307:**

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



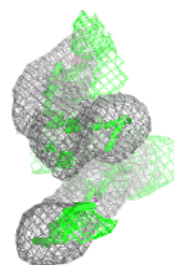
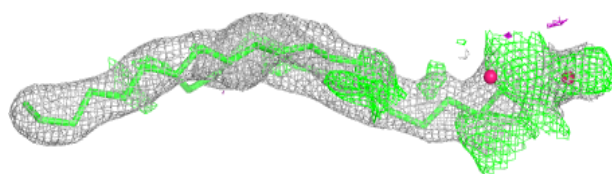
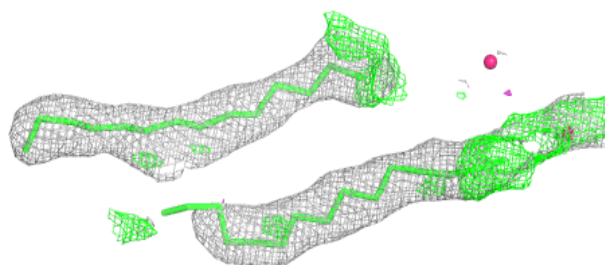
Electron density around PEK C 305:

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

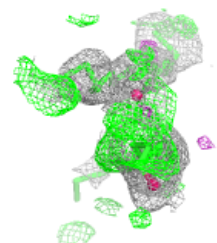
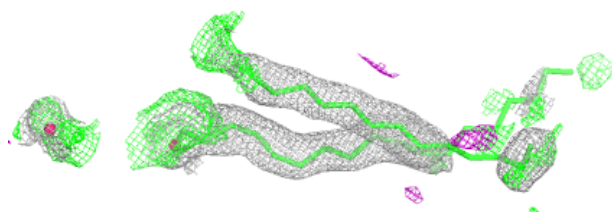
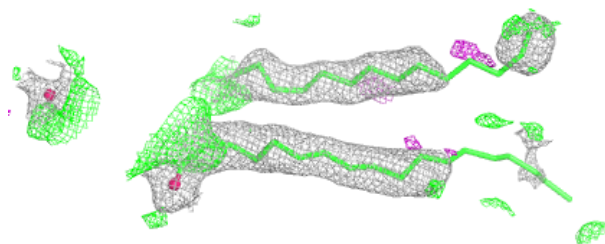


Electron density around PSC O 302:

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

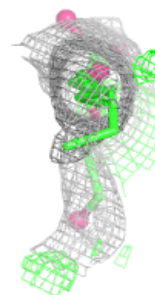
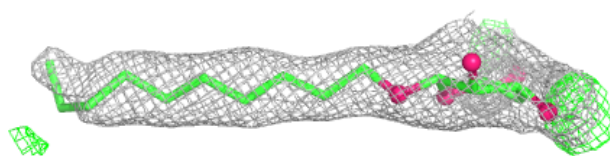
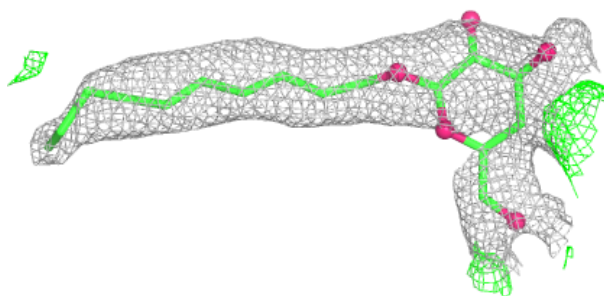
**Electron density around PGV A 608:**

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

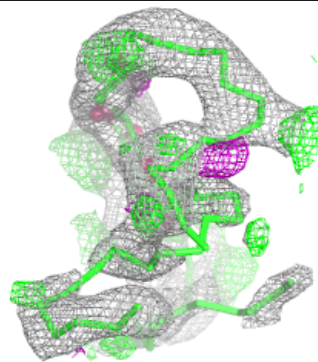
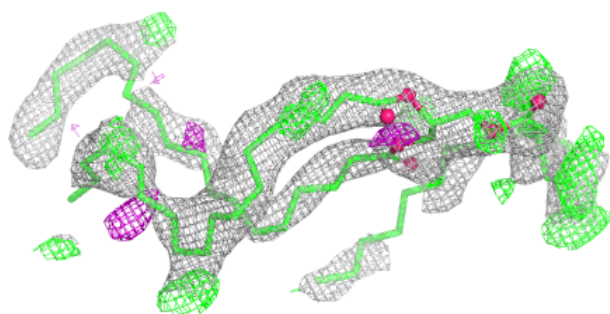
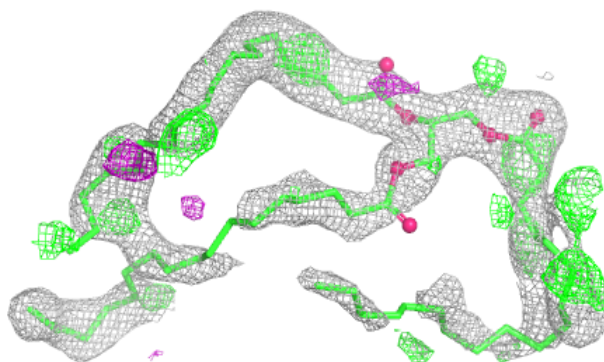


Electron density around DMU P 316:

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

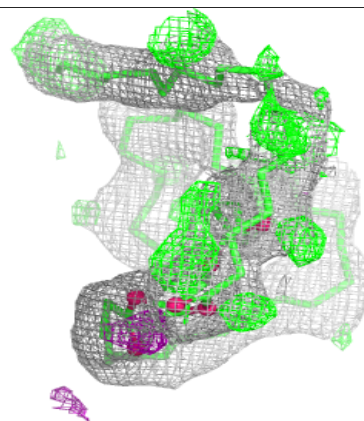
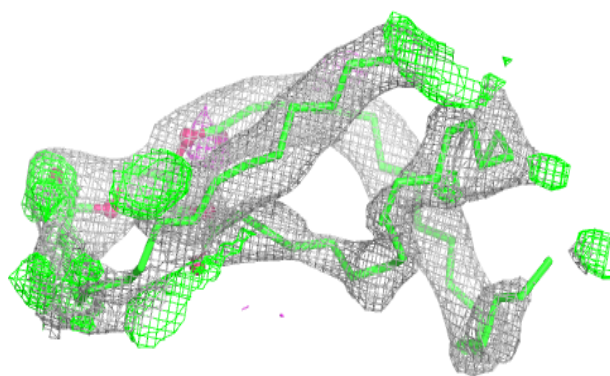
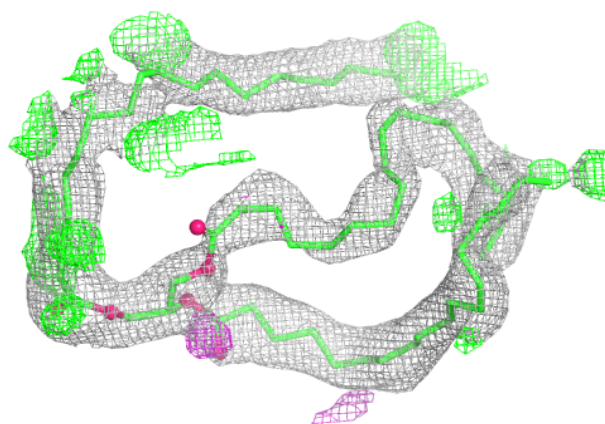
**Electron density around TGL N 607:**

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

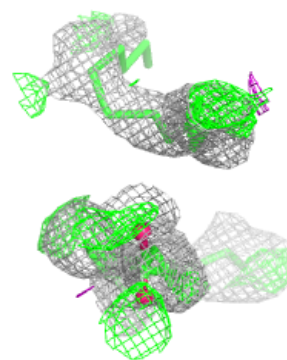
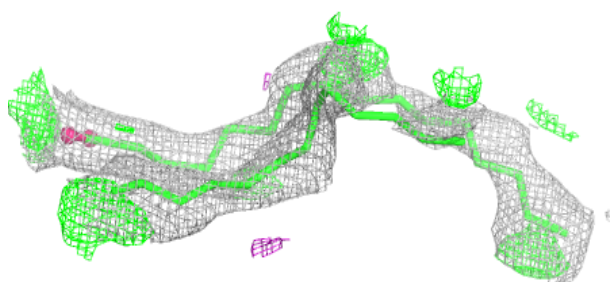
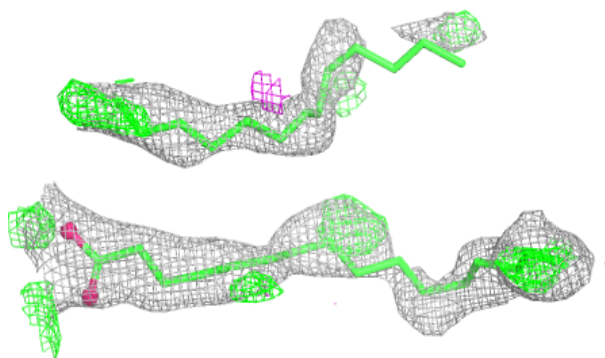


Electron density around TGL A 606:

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

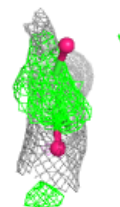
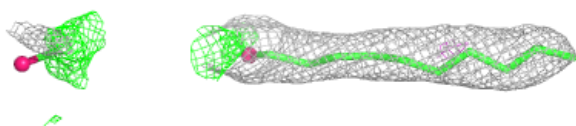
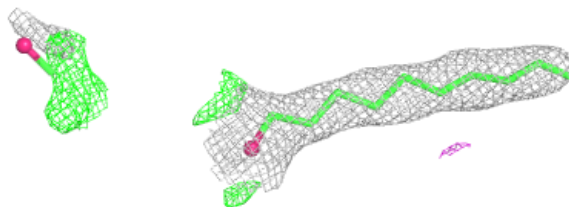
**Electron density around PGV P 306:**

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

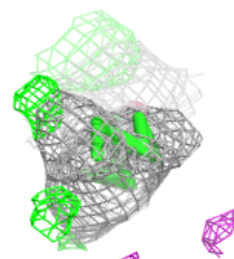
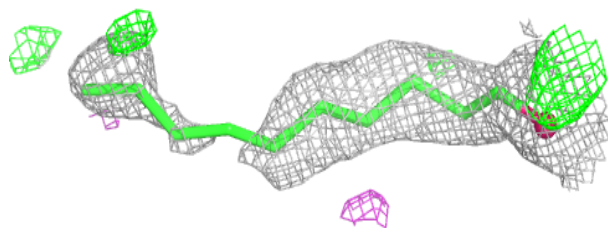
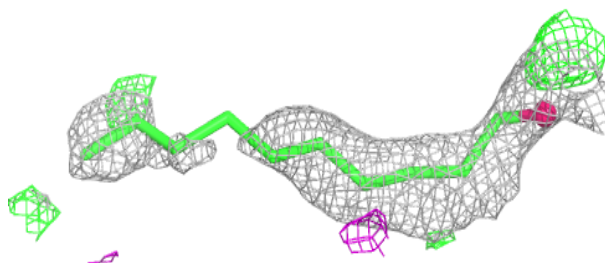


Electron density around DMU O 306:

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

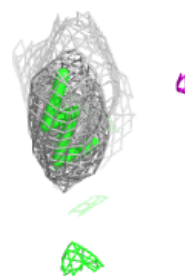
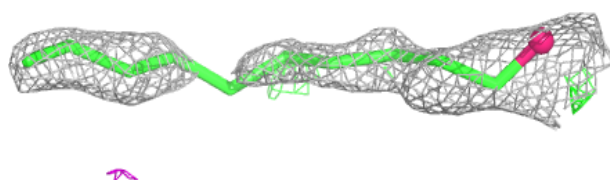
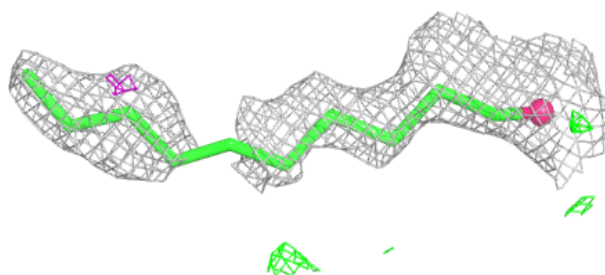
**Electron density around DMU Q 201:**

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

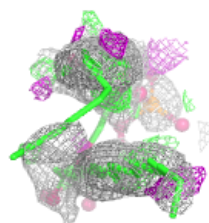
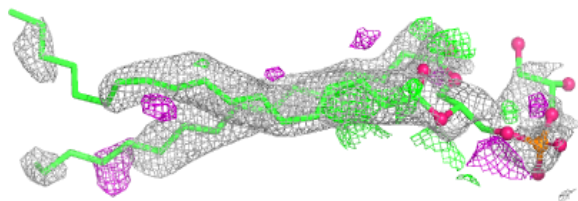
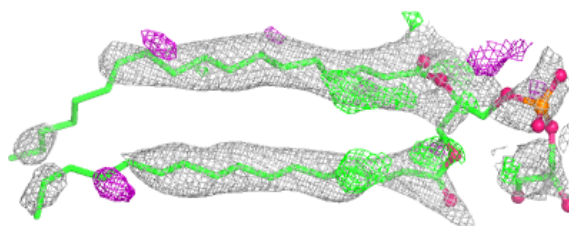


Electron density around DMU D 207:

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

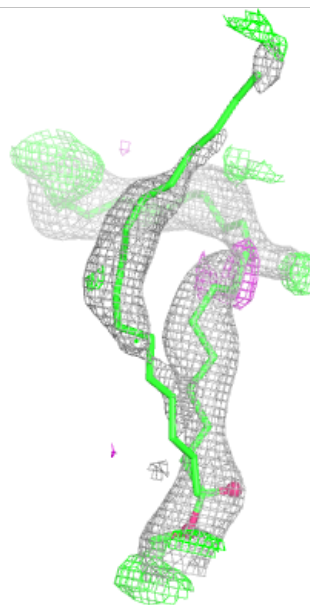
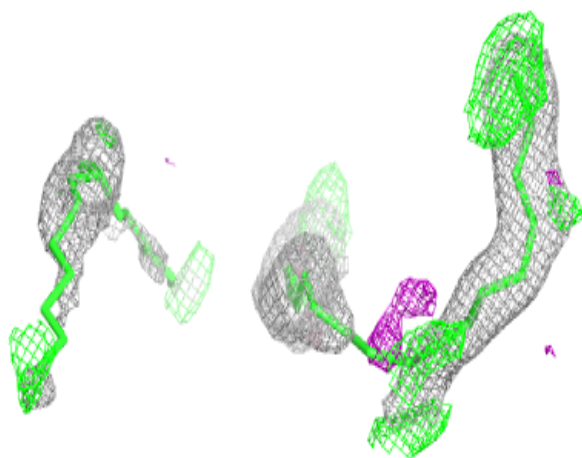
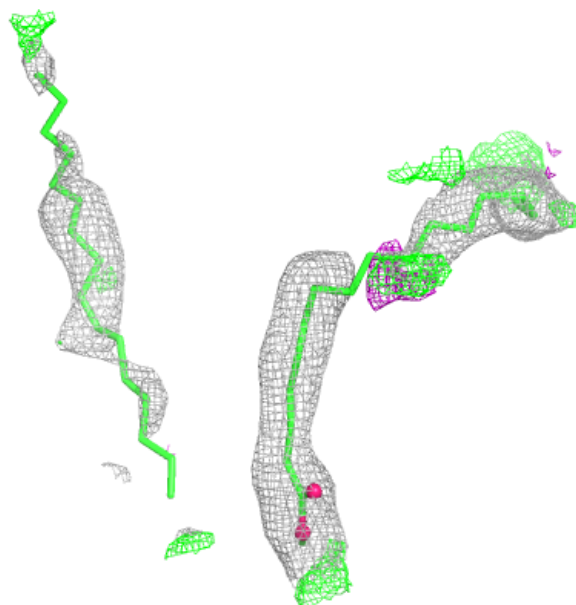
**Electron density around PGV N 610:**

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



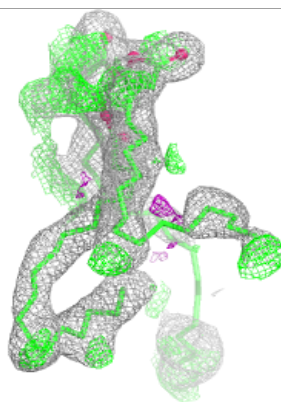
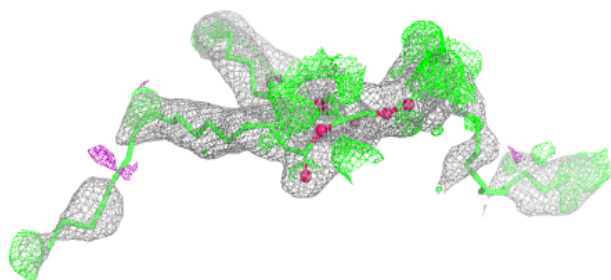
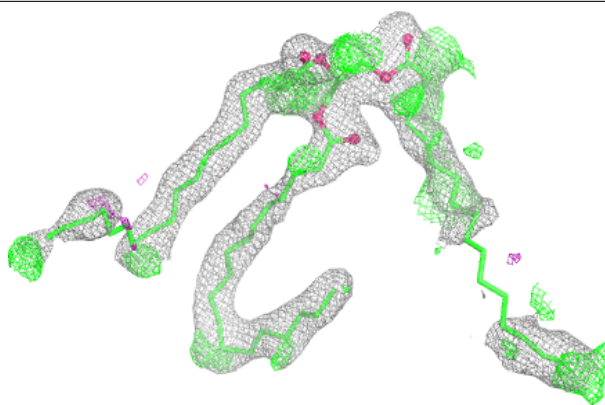
Electron density around PEK T 101:

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

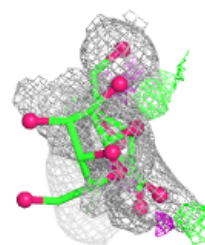
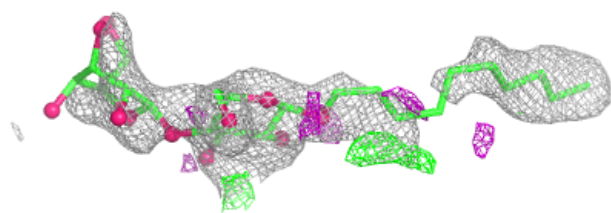
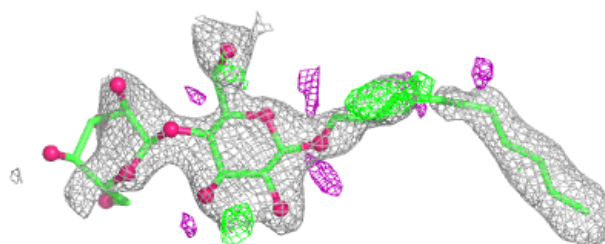


Electron density around TGL A 607:

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

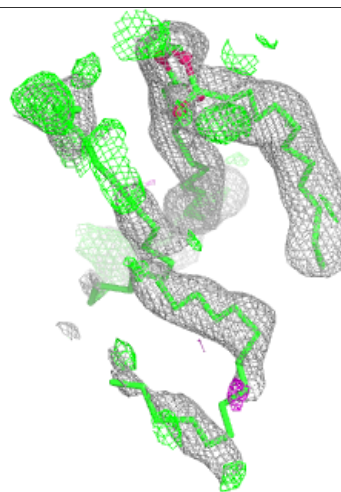
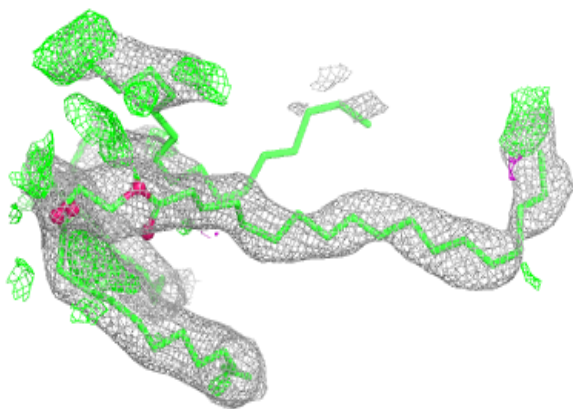
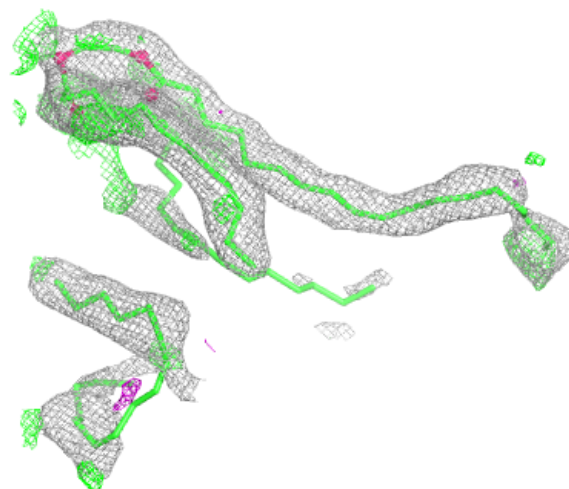
**Electron density around DMU P 308:**

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



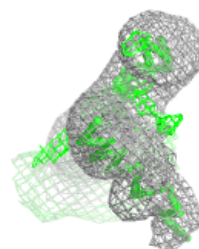
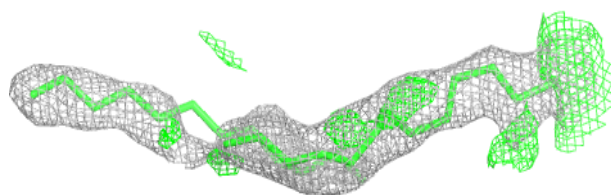
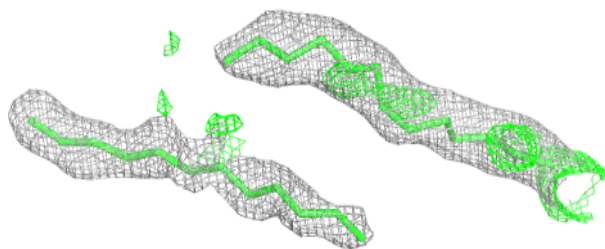
Electron density around CDL P 307:

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



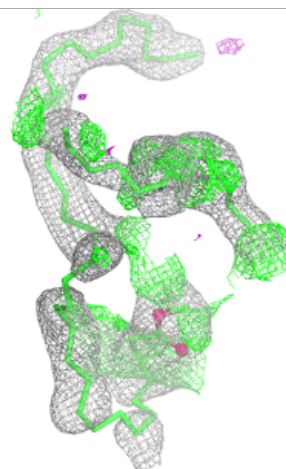
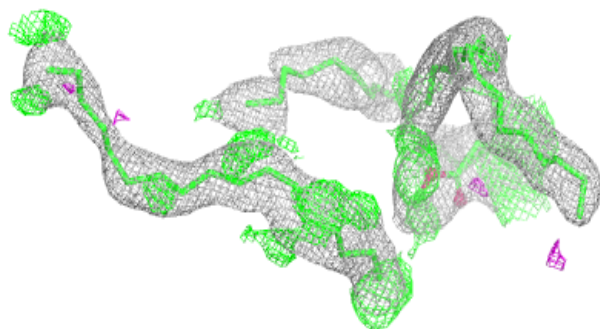
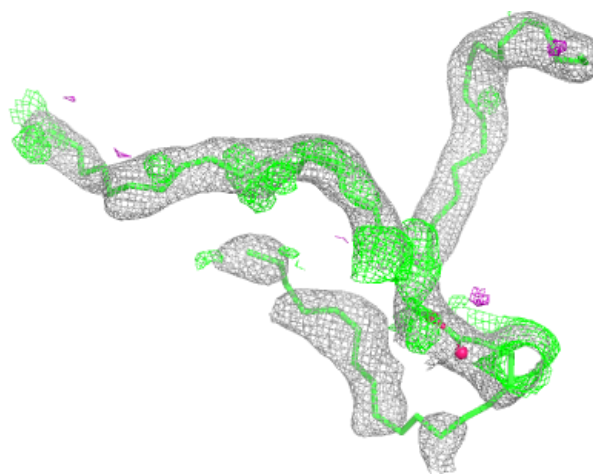
Electron density around PSC A 610:

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



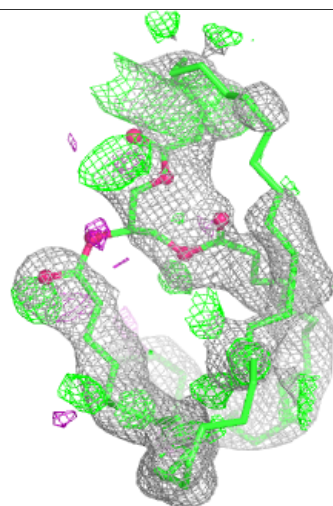
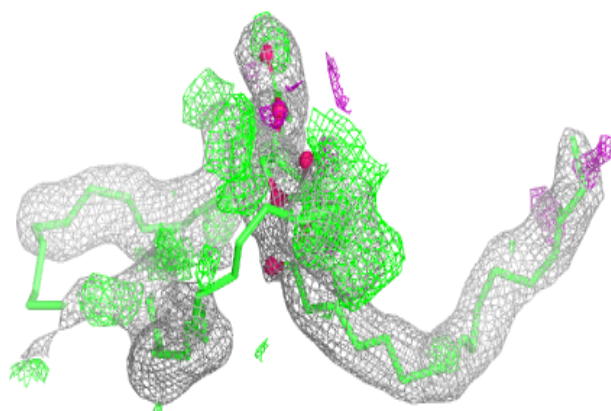
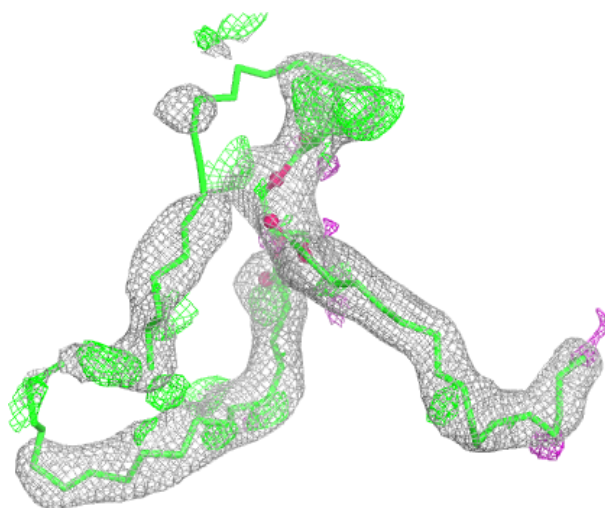
Electron density around TGL N 608:

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



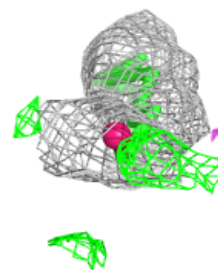
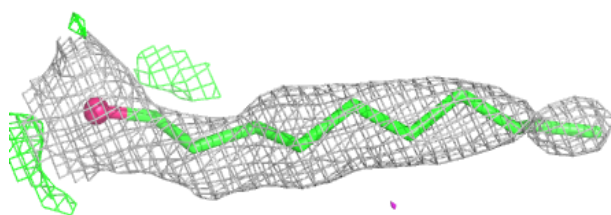
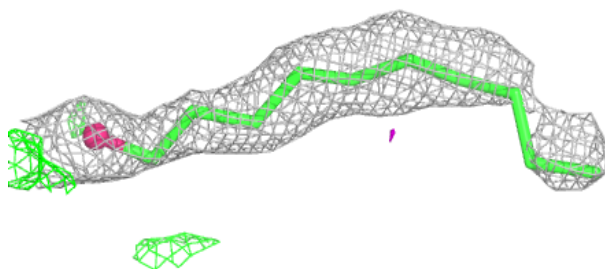
Electron density around TGL L 101:

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



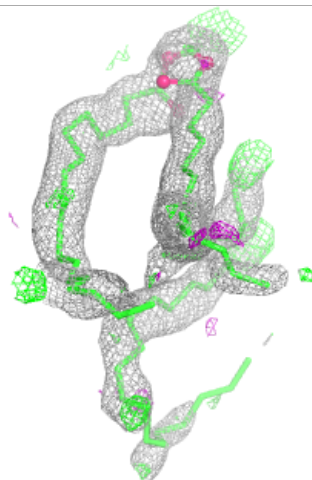
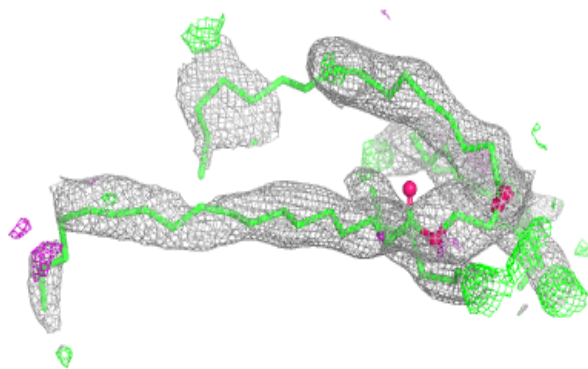
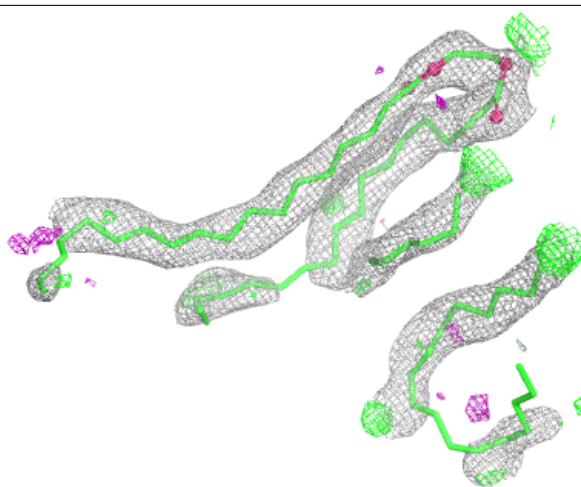
Electron density around DMU K 102:

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



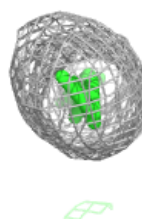
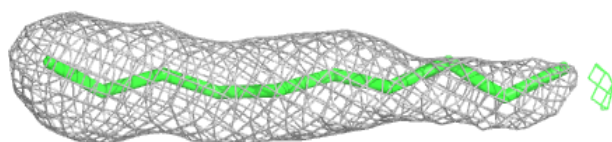
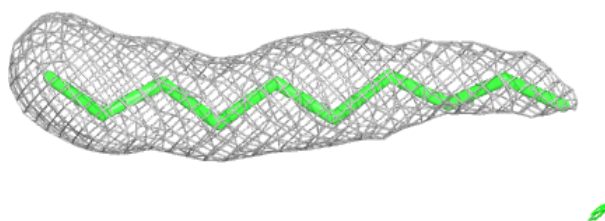
Electron density around CDL C 308:

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

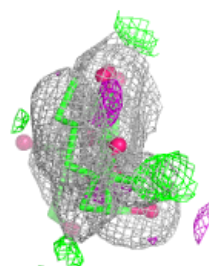
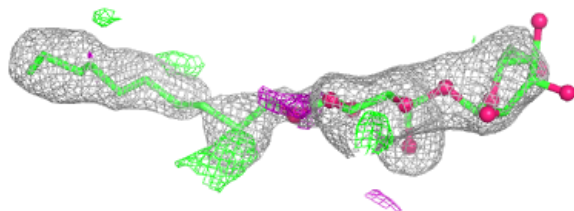
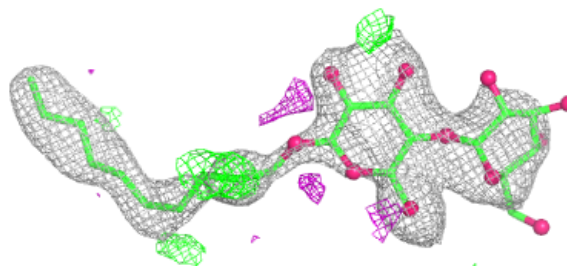


Electron density around DMU X 101:

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

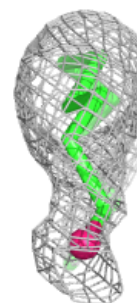
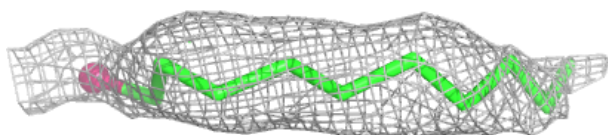
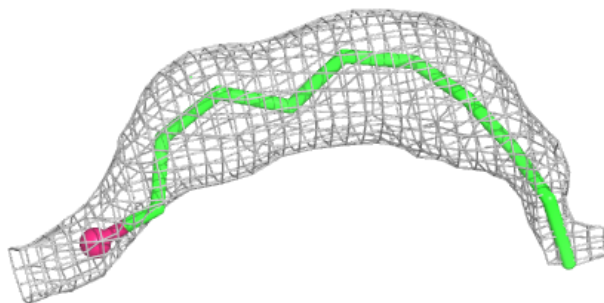
**Electron density around DMU C 310:**

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

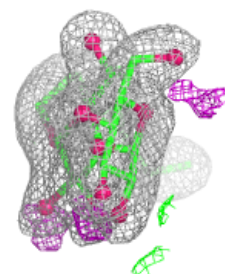
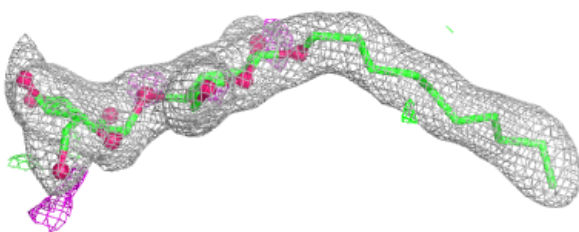
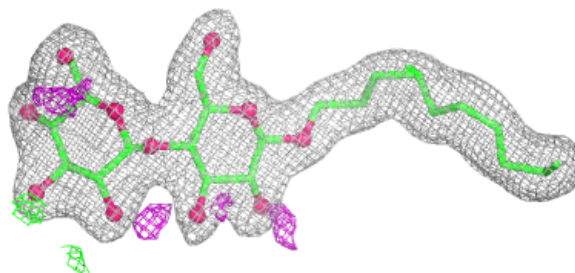


Electron density around DMU K 104:

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

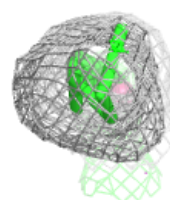
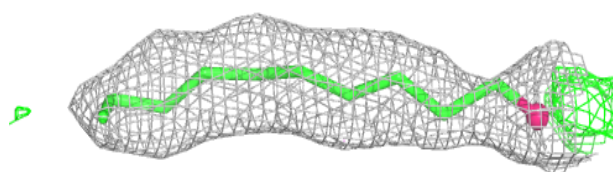
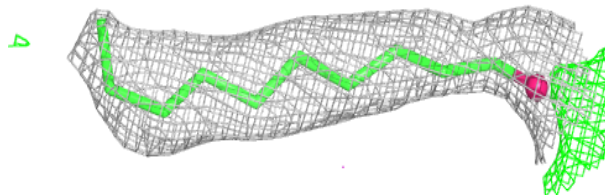
**Electron density around DMU Z 101:**

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

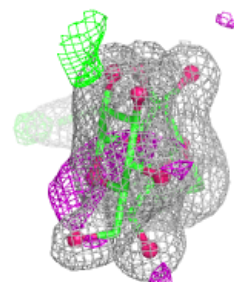
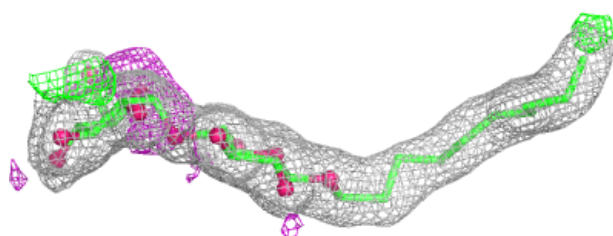
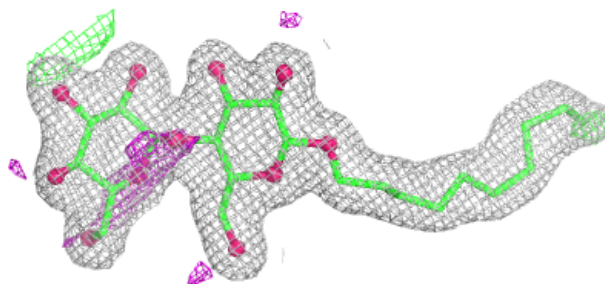


Electron density around DMU J 104:

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

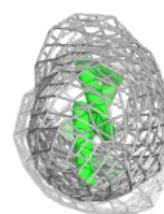
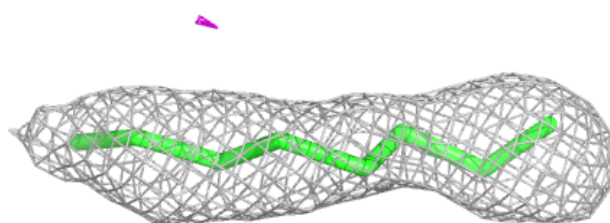
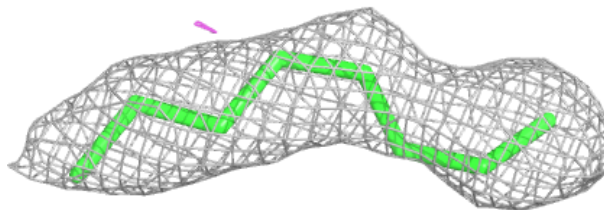
**Electron density around DMU M 101:**

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

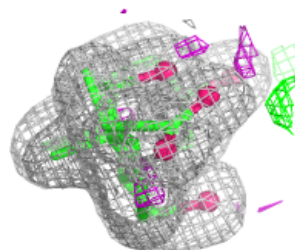
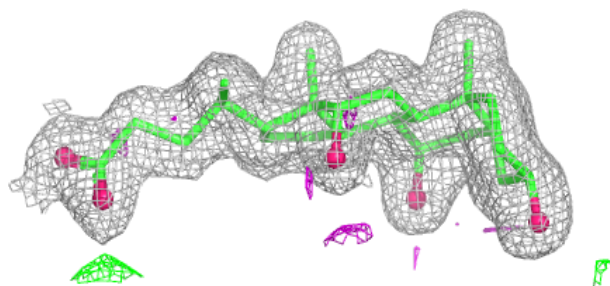
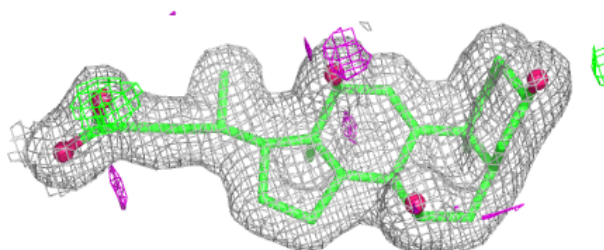


Electron density around DMU K 101:

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

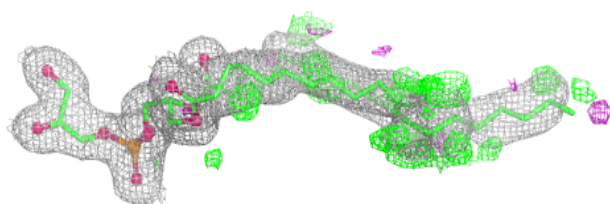
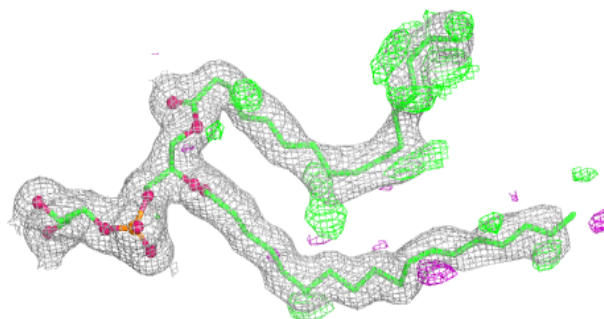
**Electron density around CHD C 301:**

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

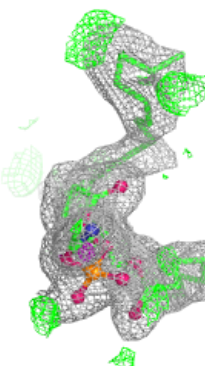
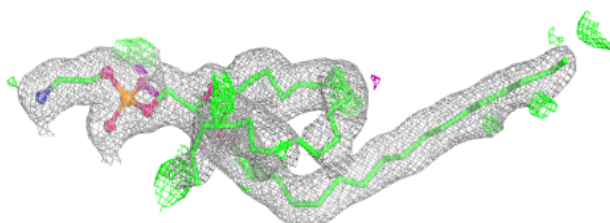
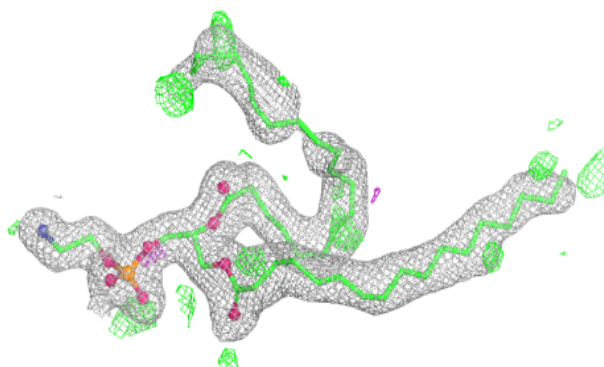


Electron density around PGV N 612:

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

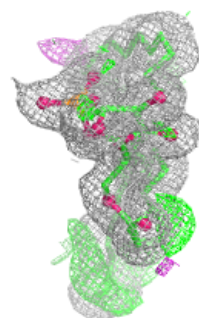
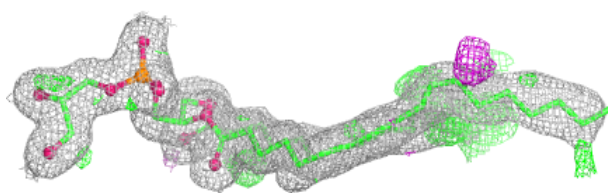
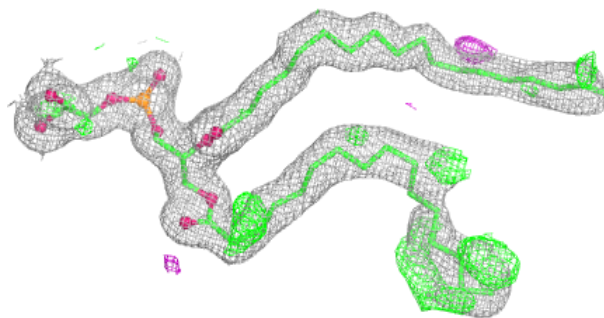
**Electron density around PEK P 304:**

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

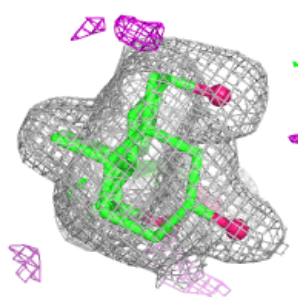
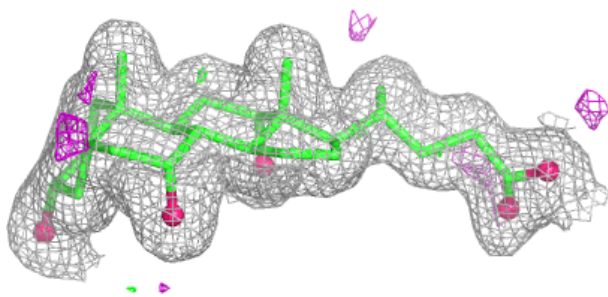
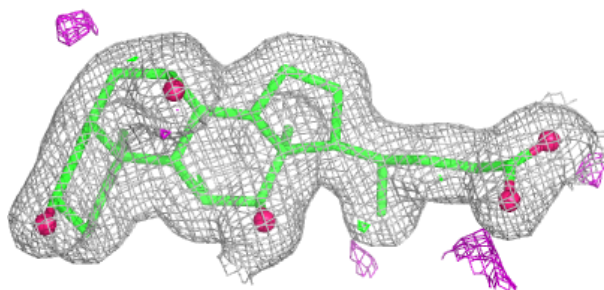


Electron density around PGV A 611:

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

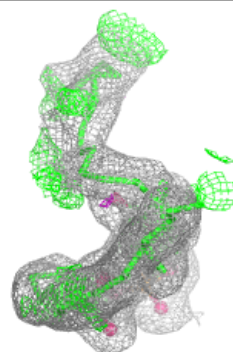
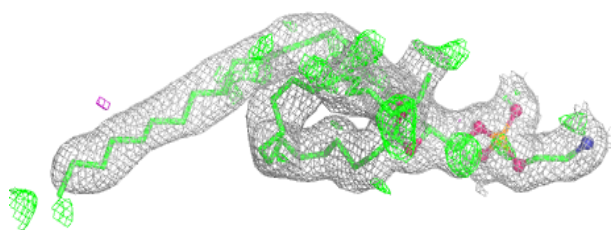
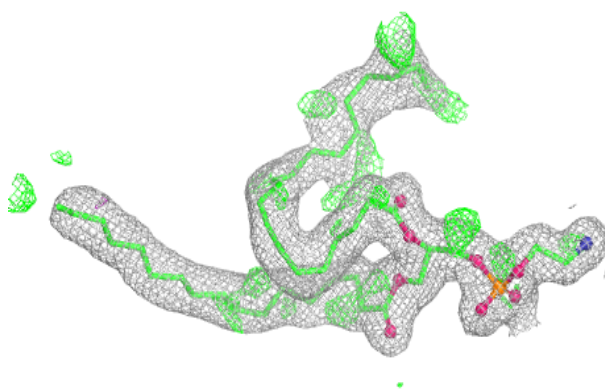
**Electron density around CHD P 301:**

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

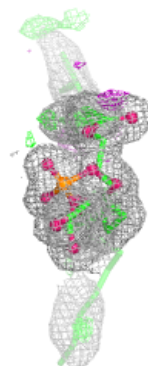
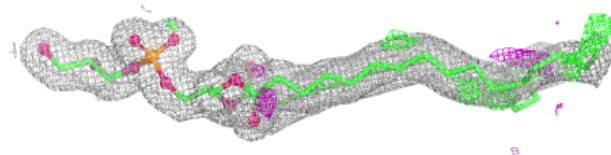
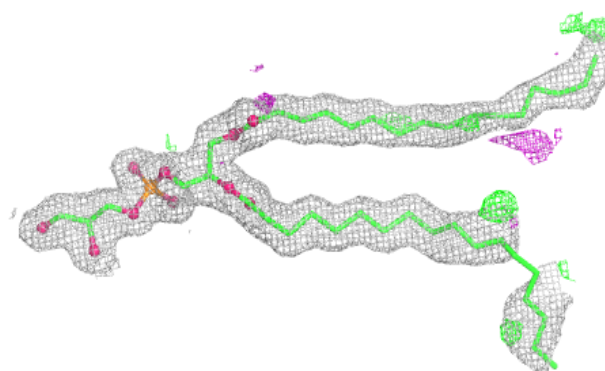


Electron density around PEK C 304:

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

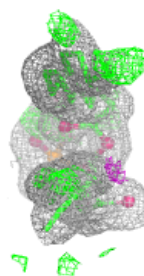
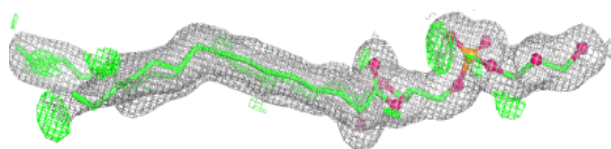
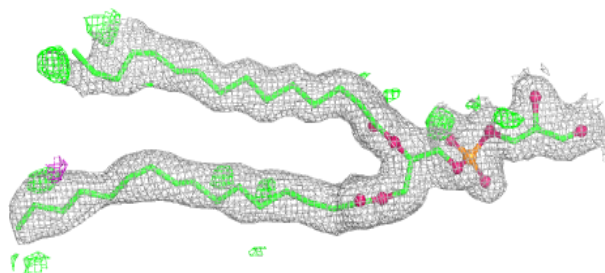
**Electron density around PGV P 305:**

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

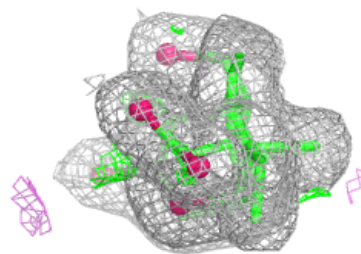
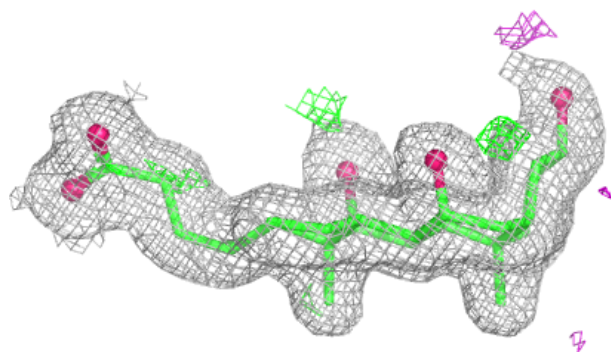
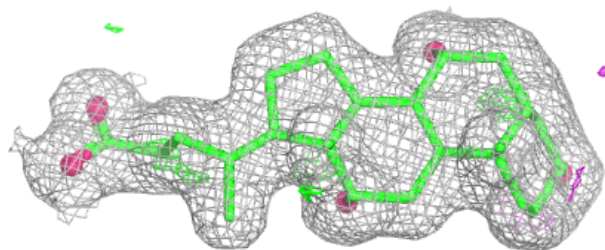


Electron density around PGV C 306:

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

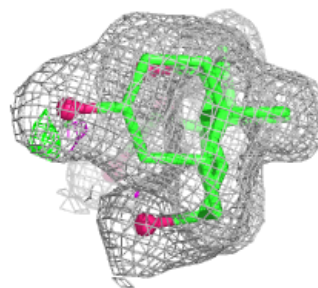
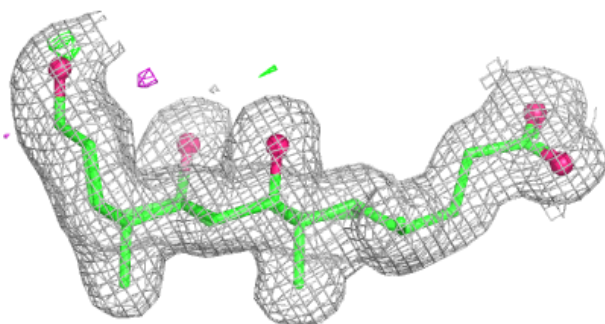
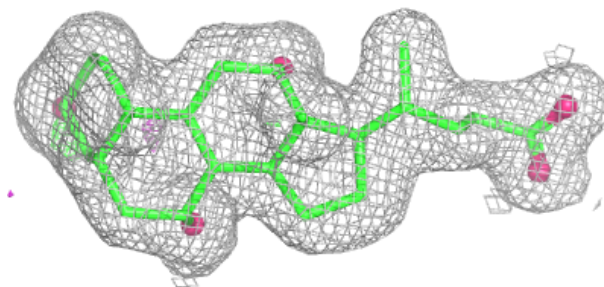
**Electron density around CHD B 302:**

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

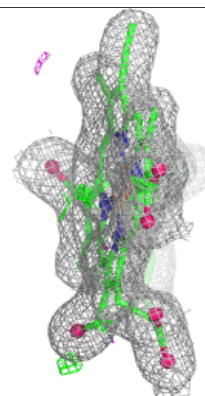
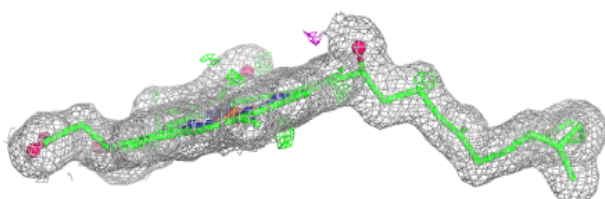
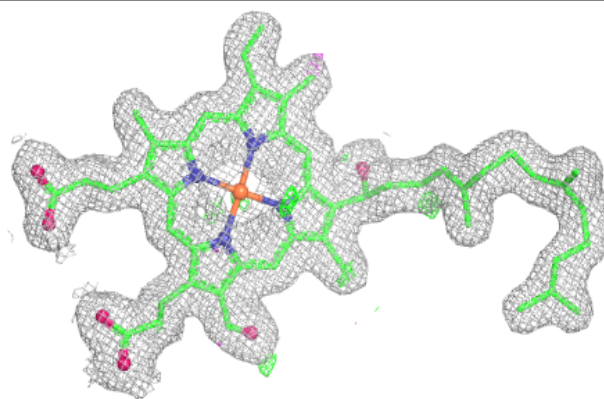


Electron density around CHD G 101:

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

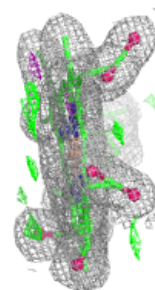
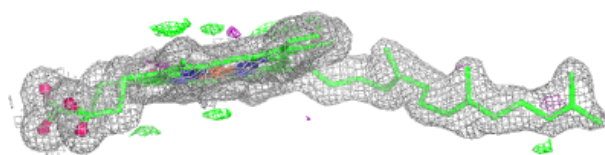
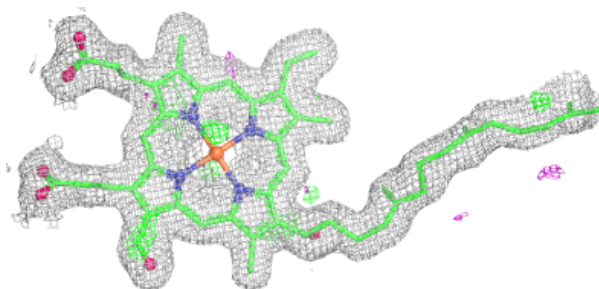
**Electron density around HEA N 603:**

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

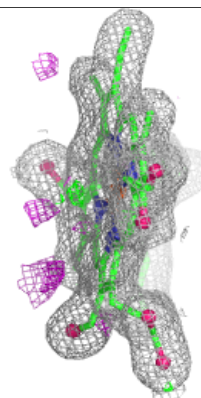
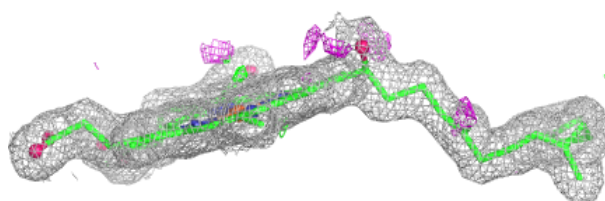
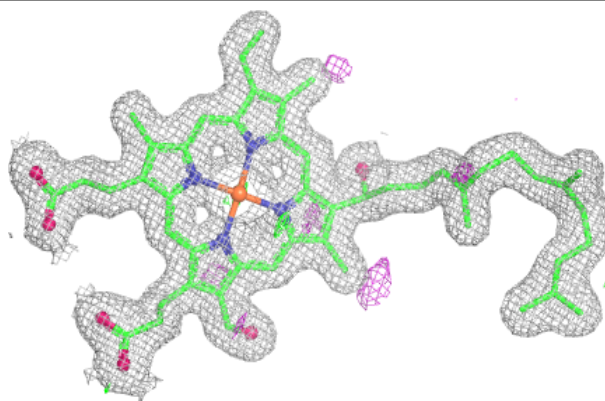


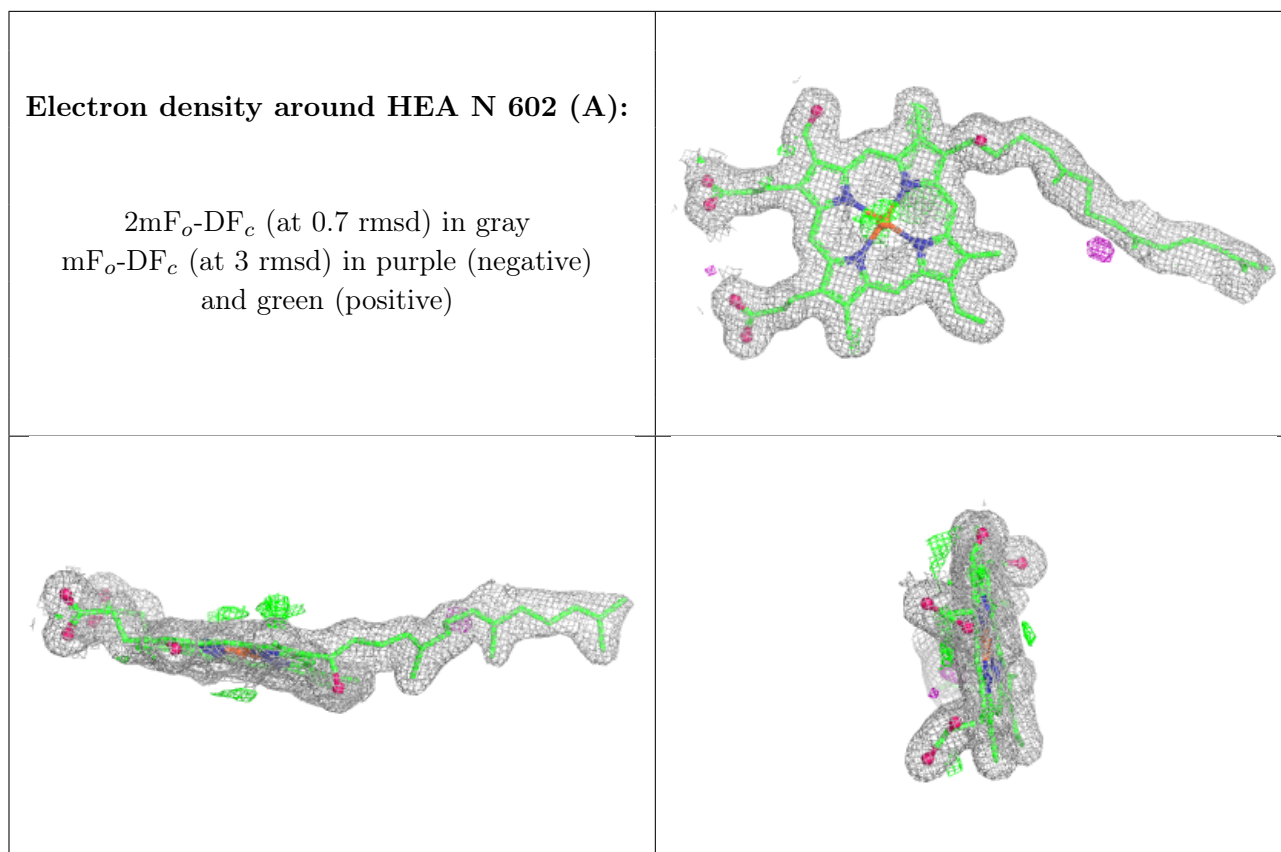
Electron density around HEA A 601 (A):

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

**Electron density around HEA A 602:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.