



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:14 PM UTC

PDB ID : 7TIH / pdb_00007tih
Title : Structure of oxidized bovine cytochrome c oxidase with reduced metal centers induced by synchrotron X-ray exposure
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.; Russi, S.; Cohen, A.
Deposited on : 2022-01-13
Resolution : 2.35 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

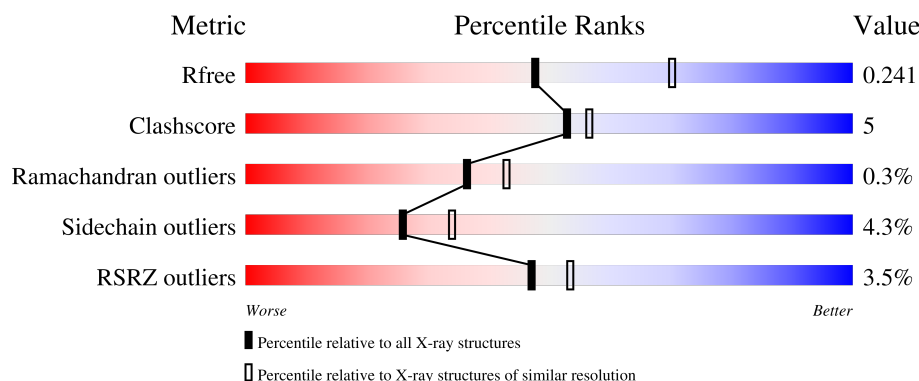
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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.



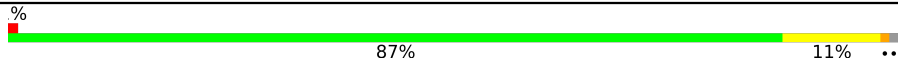
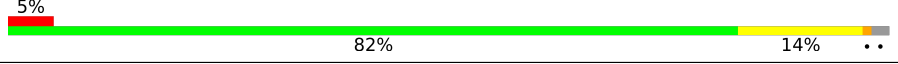
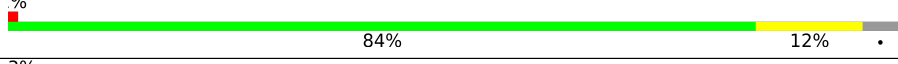
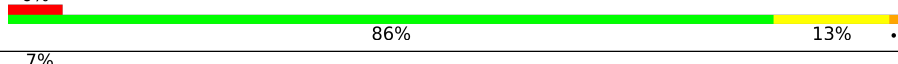
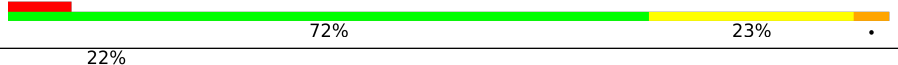
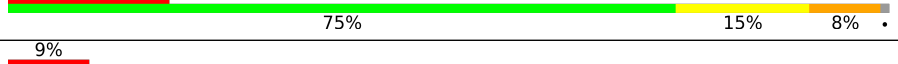
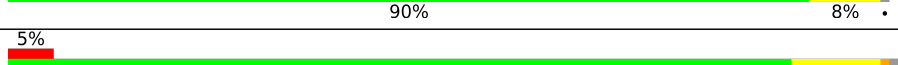
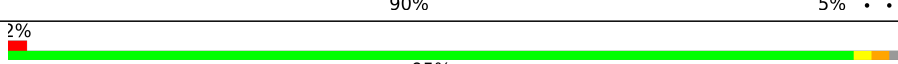
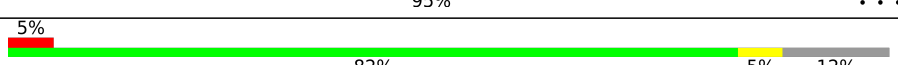
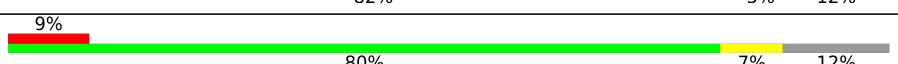
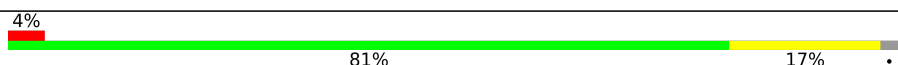
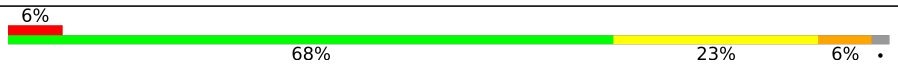
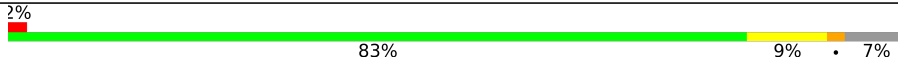
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	514	 88% 12%
1	N	514	 84% 16%
2	B	227	 3% 80% 19%
2	O	227	 3% 82% 17%
3	C	261	 90% 9%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	PSC	R	201	X	-	-	-

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32721 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			
9	V	72	Total	C	N	O	S	0	0	0
			592	385	106	97	4			

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

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

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

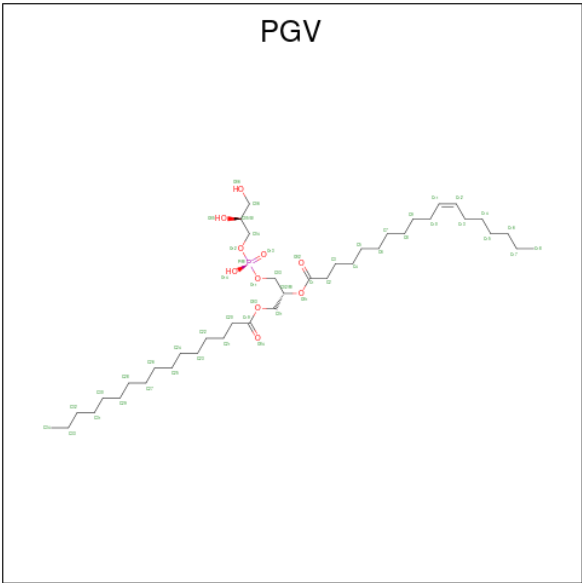
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

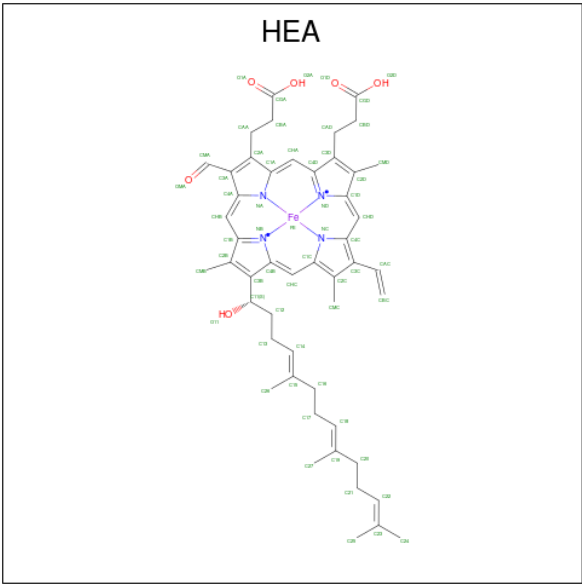
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

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



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

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	G	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	I	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	J	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	K	1	Total 4	C 2	O 2	0	0
19	L	1	Total 4	C 2	O 2	0	0
19	M	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0
19	N	1	Total 4	C 2	O 2	0	0

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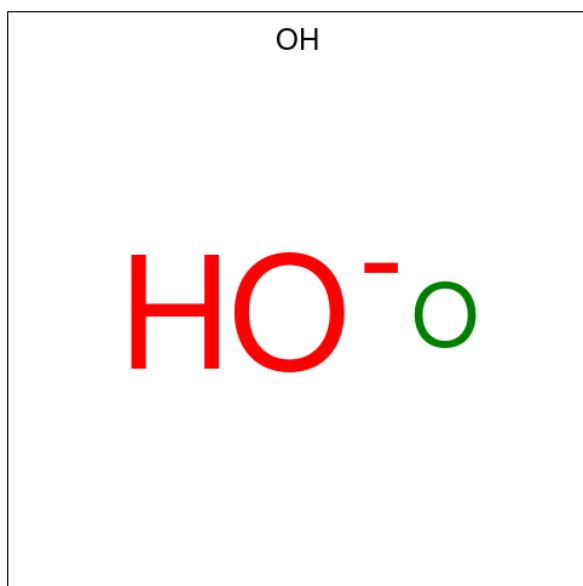
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	N	1	Total C O 4 2 2	0	0
19	O	1	Total C O 4 2 2	0	0
19	O	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4 2 2	0	0
19	P	1	Total C O 4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

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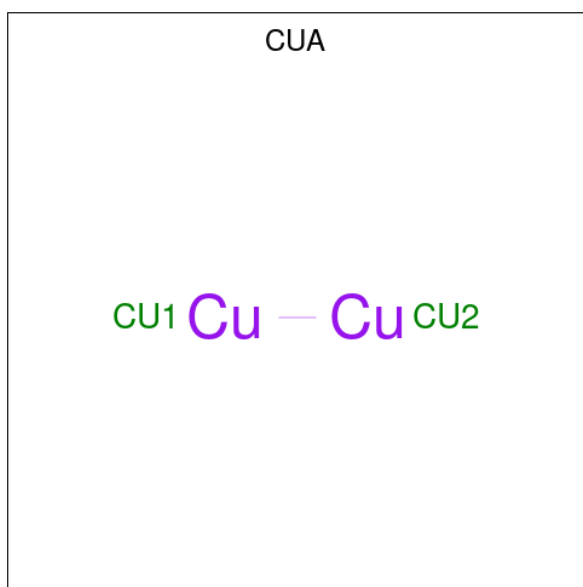
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	S	1	Total C O 4 2 2	0	0
19	T	1	Total C O 4 2 2	0	0
19	V	1	Total C O 4 2 2	0	0
19	V	1	Total C O 4 2 2	0	0
19	W	1	Total C O 4 2 2	0	0
19	W	1	Total C O 4 2 2	0	0
19	Z	1	Total C O 4 2 2	0	0

- Molecule 20 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



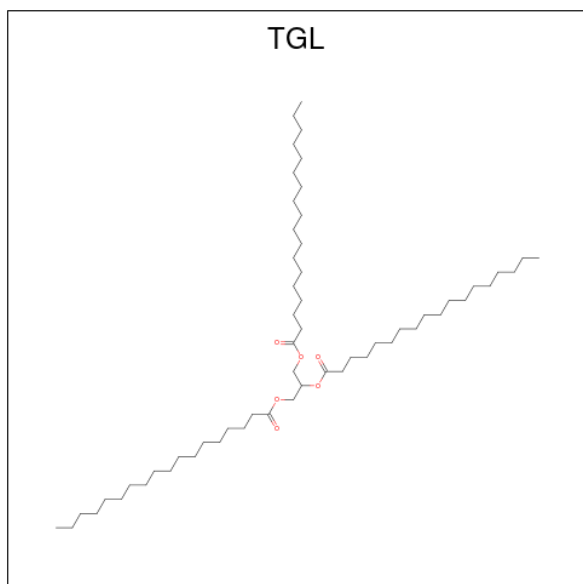
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total O 1 1	0	0
20	N	1	Total O 1 1	0	0

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

- Molecule 22 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$) (labeled as "Ligand of Interest" by depositor).



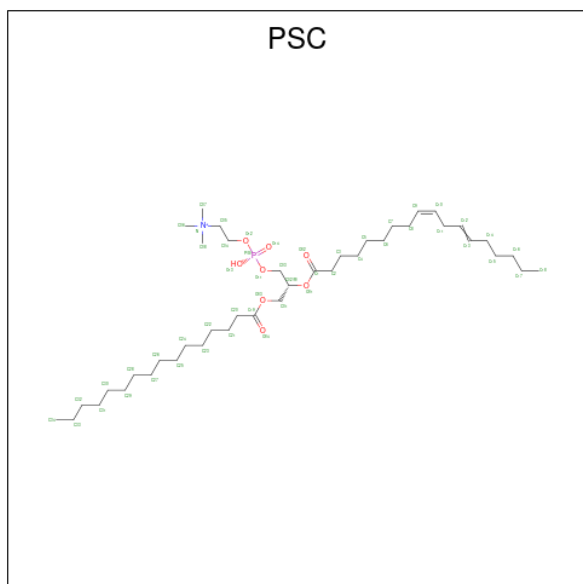
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		

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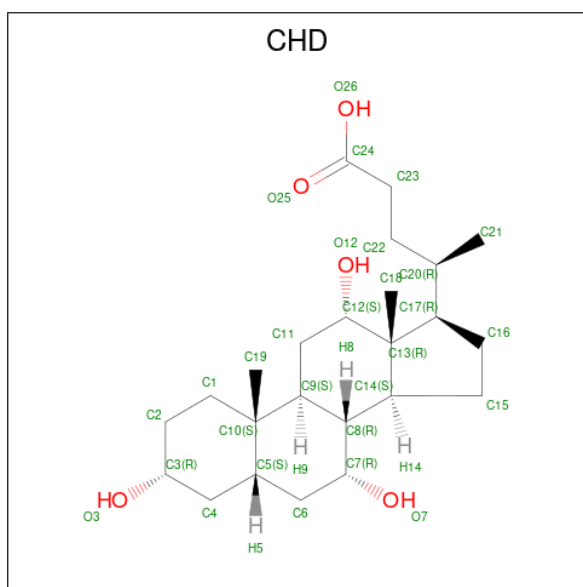
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	D	1	Total	C	O	0	0
			63	57	6		
22	L	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	Q	1	Total	C	O	0	0
			63	57	6		
22	Y	1	Total	C	O	0	0
			63	57	6		

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



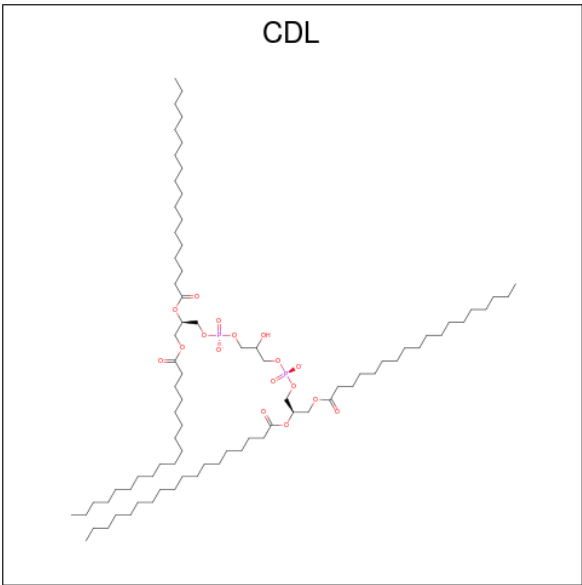
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



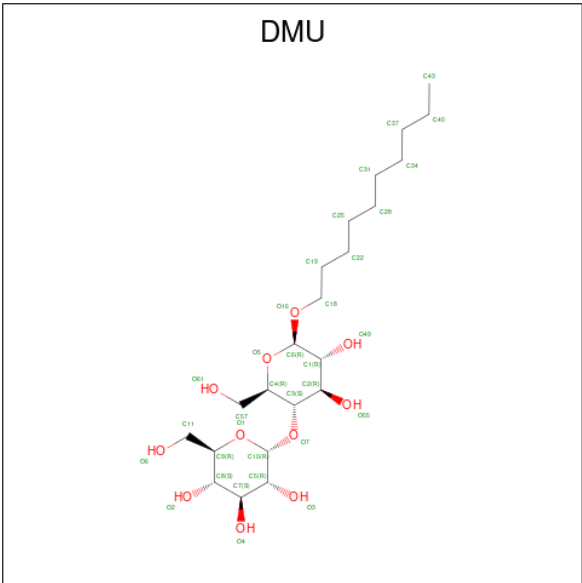
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	G	1	Total C O 29 24 5	0	0
24	J	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	W	1	Total C O 29 24 5	0	0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

- Molecule 25 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



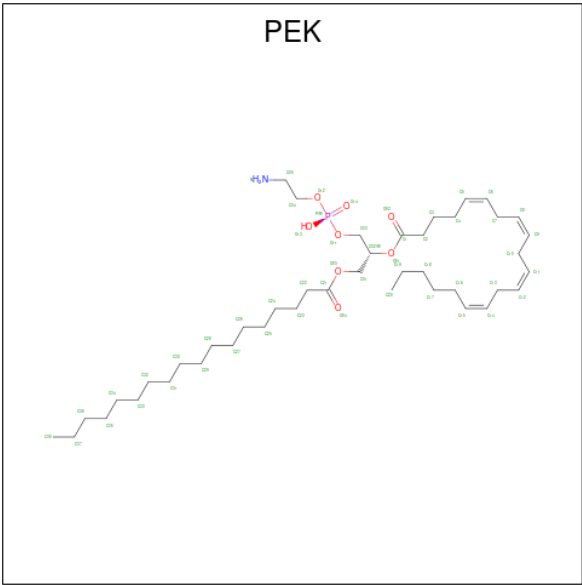
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	C	1	Total	C	O	P	0	0
			100	81	17	2		
25	P	1	Total	C	O	P	0	0
			100	81	17	2		
25	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 26 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	C	1	Total	C	O	0	0
			33	22	11		
26	D	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	Q	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



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

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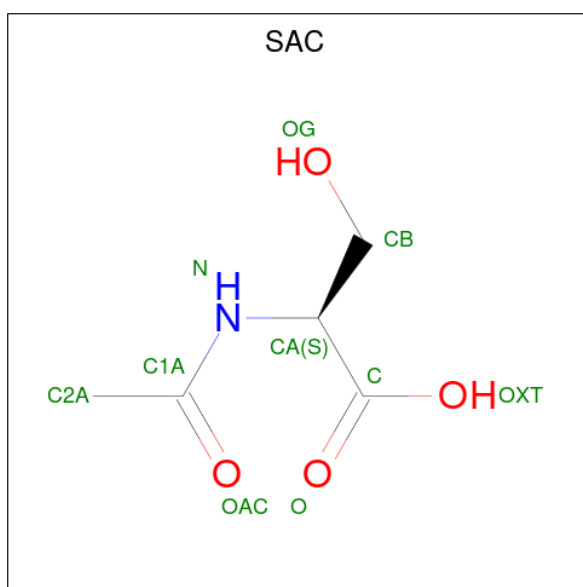
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- 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 N-ACETYL-SERINE (CCD ID: SAC) (formula: C₅H₉NO₄).



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

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	188	Total	O	0	0
			188	188		
30	B	107	Total	O	0	0
			107	107		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	C	107	Total 107	O 107	0	0
30	D	89	Total 89	O 89	0	0
30	E	71	Total 71	O 71	0	0
30	F	68	Total 68	O 68	0	0
30	G	32	Total 32	O 32	0	0
30	H	41	Total 41	O 41	0	0
30	I	31	Total 31	O 31	0	0
30	J	23	Total 23	O 23	0	0
30	K	19	Total 19	O 19	0	0
30	L	25	Total 25	O 25	0	0
30	M	18	Total 18	O 18	0	0
30	N	167	Total 167	O 167	0	0
30	O	90	Total 90	O 90	0	0
30	P	105	Total 105	O 105	0	0
30	Q	69	Total 69	O 69	0	0
30	R	52	Total 52	O 52	0	0
30	S	81	Total 81	O 81	0	0
30	T	43	Total 43	O 43	0	0
30	U	34	Total 34	O 34	0	0
30	V	17	Total 17	O 17	0	0
30	W	26	Total 26	O 26	0	0

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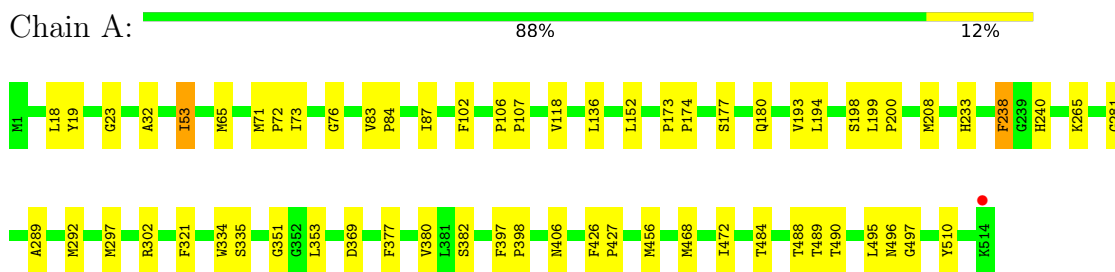
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	X	14	Total 14	O 14	0	0
30	Y	4	Total 4	O 4	0	0
30	Z	8	Total 8	O 8	0	0

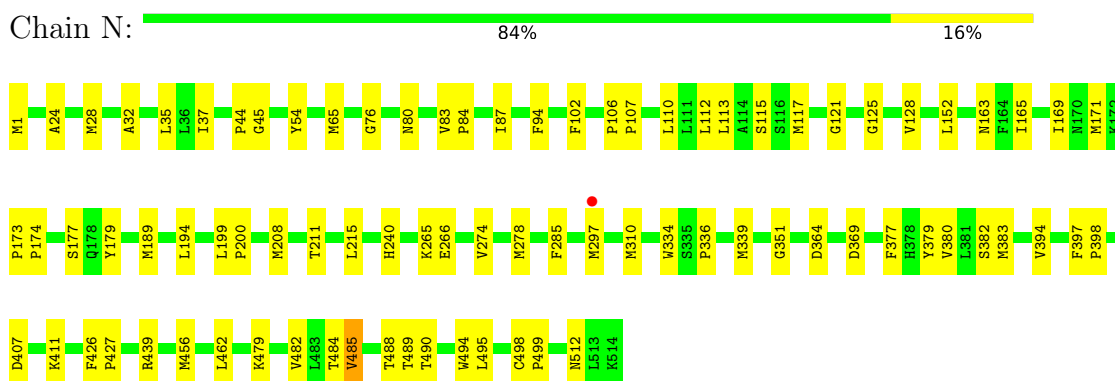
3 Residue-property plots

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

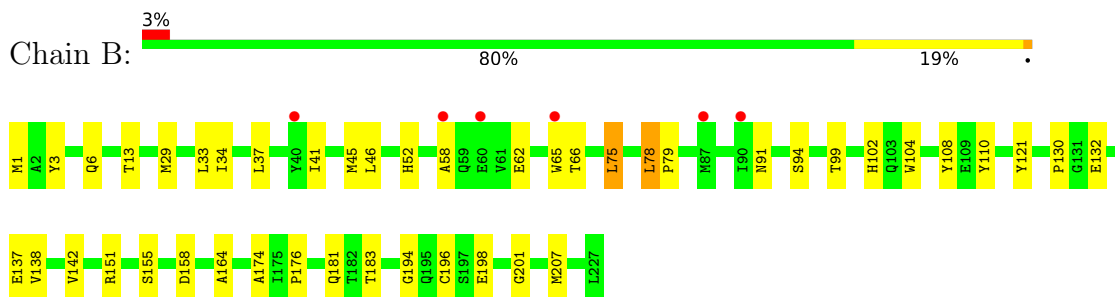
• Molecule 1: Cytochrome c oxidase subunit 1



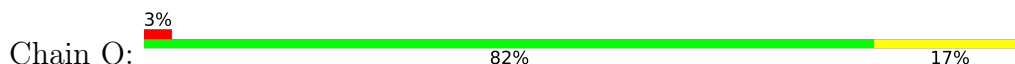
• Molecule 1: Cytochrome c oxidase subunit 1

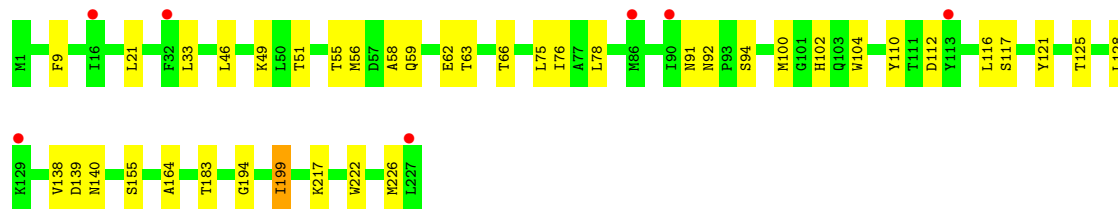


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 90% 9% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 11% ..



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

Chain D: 87% 10% ..



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

Chain Q: 82% 14% ..

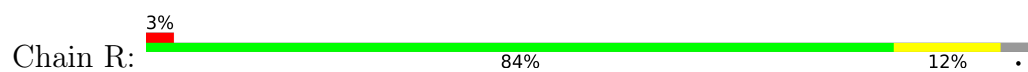


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

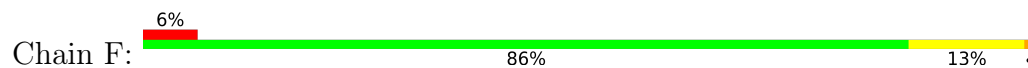
Chain E: 84% 12% .



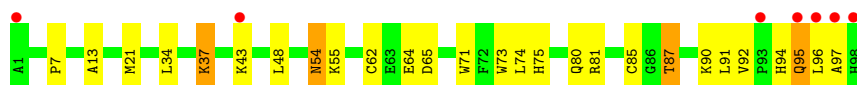
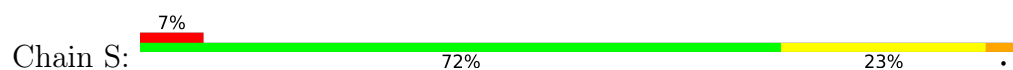
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



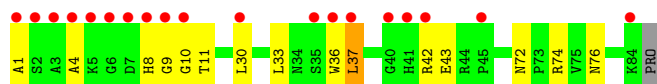
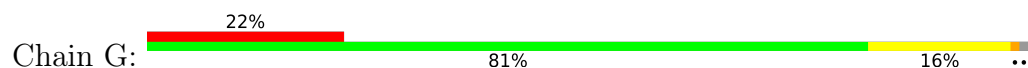
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



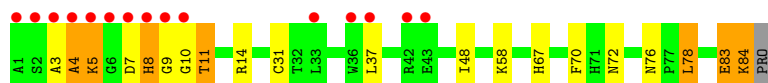
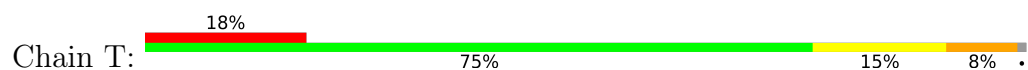
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



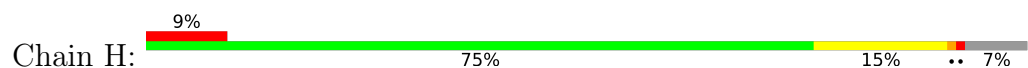
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



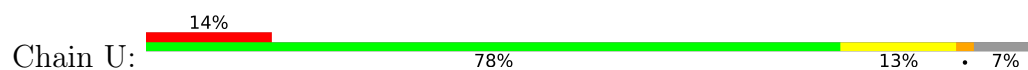
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



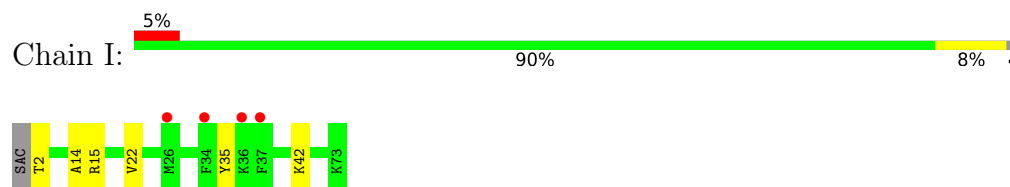
- Molecule 8: Cytochrome c oxidase subunit 6B1



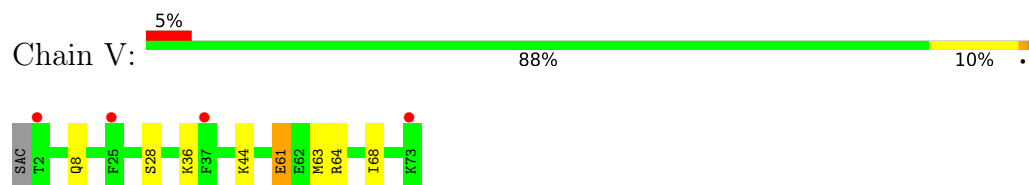
- Molecule 8: Cytochrome c oxidase subunit 6B1



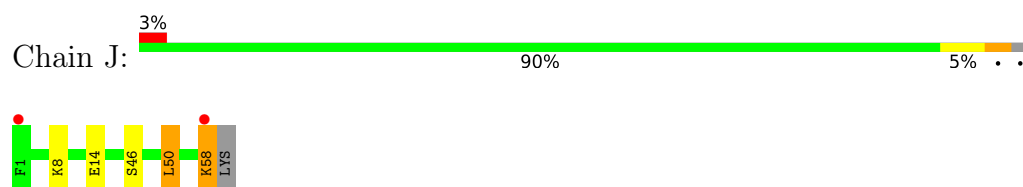
- Molecule 9: Cytochrome c oxidase subunit 6C



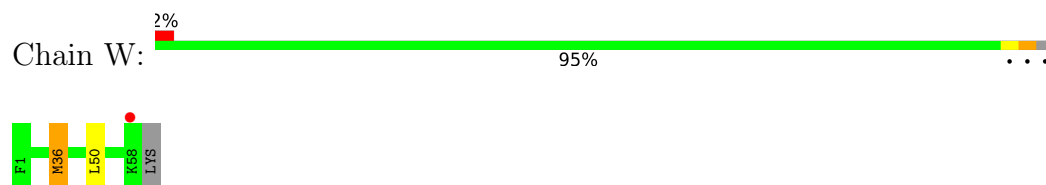
- Molecule 9: Cytochrome c oxidase subunit 6C



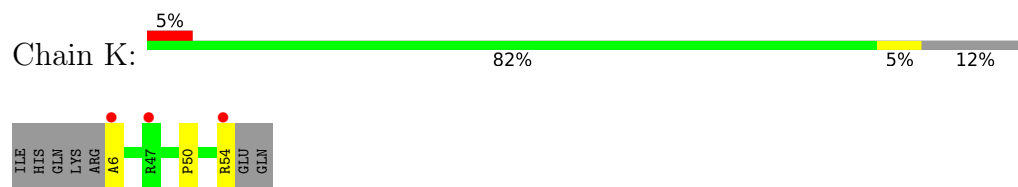
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



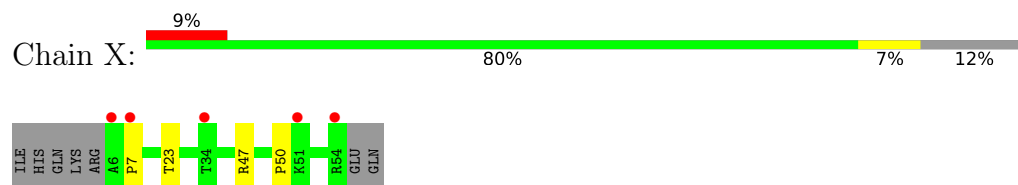
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



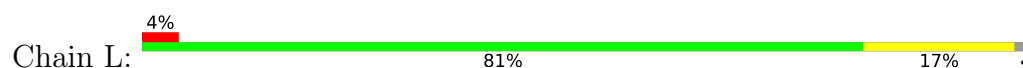
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

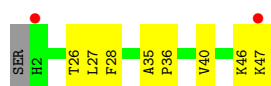


- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial

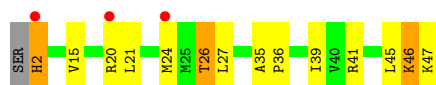


- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

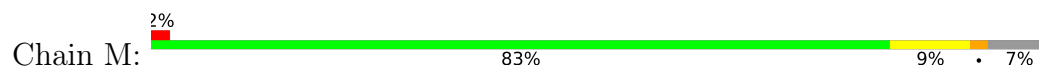




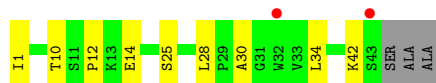
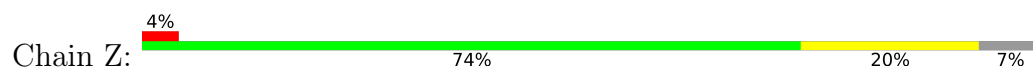
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	178.04Å 182.70Å 205.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.34 – 2.35 39.34 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.34-2.35) 99.9 (39.34-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.193 , 0.235 0.203 , 0.241	Depositor DCC
R_{free} test set	13603 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32721	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.98	1/4156 (0.0%)	1.40	8/5678 (0.1%)
1	N	1.00	0/4156	1.41	6/5678 (0.1%)
2	B	1.01	1/1860 (0.1%)	1.39	6/2534 (0.2%)
2	O	1.01	0/1860	1.39	2/2534 (0.1%)
3	C	0.94	0/2197	1.42	2/3005 (0.1%)
3	P	0.97	0/2197	1.41	4/3005 (0.1%)
4	D	1.01	0/1229	1.36	0/1658
4	Q	1.02	0/1229	1.44	0/1658
5	E	0.99	0/871	1.45	1/1182 (0.1%)
5	R	1.00	0/871	1.50	0/1182
6	F	1.03	0/765	1.39	0/1038
6	S	1.04	0/765	1.34	0/1038
7	G	0.99	0/690	1.37	0/937
7	T	1.01	1/690 (0.1%)	1.37	2/937 (0.2%)
8	H	0.98	0/682	1.44	0/921
8	U	0.98	0/682	1.51	0/921
9	I	0.97	0/605	1.58	0/802
9	V	0.98	0/605	1.58	2/802 (0.2%)
10	J	0.98	0/471	1.52	1/636 (0.2%)
10	W	1.00	0/471	1.49	0/636
11	K	1.06	0/398	1.44	0/546
11	X	1.06	0/398	1.50	0/546
12	L	0.95	0/393	1.36	0/526
12	Y	0.96	0/393	1.42	1/526 (0.2%)
13	M	0.97	0/345	1.53	0/470
13	Z	0.96	0/345	1.47	0/470
All	All	0.99	3/29324 (0.0%)	1.42	35/39866 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	T	0	1
8	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	5.64	1.30	1.23
7	T	48	ILE	N-CA	5.44	1.50	1.45
1	A	174	PRO	C-O	-5.20	1.17	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CA-CB-CG	-8.21	105.59	113.80
1	A	377	PHE	CA-CB-CG	7.47	121.27	113.80
1	N	240	HIS	CA-CB-CG	-6.70	107.10	113.80
1	N	377	PHE	CA-CB-CG	6.49	120.29	113.80
12	Y	39	ILE	N-CA-C	-5.99	105.02	110.82
1	A	102	PHE	CA-CB-CG	-5.80	108.00	113.80
2	O	51	THR	CA-C-N	5.79	129.44	121.33
2	O	51	THR	C-N-CA	5.79	129.44	121.33
3	P	145	THR	CA-CB-OG1	-5.76	100.96	109.60
2	B	183	THR	CA-CB-OG1	-5.73	101.01	109.60
7	T	37	LEU	CA-C-N	5.64	128.86	120.17
7	T	37	LEU	C-N-CA	5.64	128.86	120.17
3	P	35	PHE	CA-CB-CG	5.63	119.43	113.80
2	B	13	THR	CB-CA-C	5.58	119.08	109.15
2	B	201	GLY	CA-C-N	5.52	127.95	120.38
2	B	201	GLY	C-N-CA	5.52	127.95	120.38
1	N	125	GLY	CA-C-O	-5.48	117.85	122.29
2	B	99	THR	CA-CB-OG1	-5.38	101.52	109.60
3	P	159	MET	N-CA-C	-5.37	105.33	111.07
3	P	204	HIS	CA-CB-CG	-5.36	108.44	113.80
1	A	240	HIS	N-CA-CB	5.32	116.70	110.42
2	B	13	THR	N-CA-C	-5.23	107.55	114.04
1	A	456	MET	CA-C-N	5.21	125.76	119.98
1	A	456	MET	C-N-CA	5.21	125.76	119.98
9	V	28	SER	CA-C-N	5.20	127.56	120.54
9	V	28	SER	C-N-CA	5.20	127.56	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	25	ASP	CA-CB-CG	5.07	117.67	112.60
1	N	240	HIS	N-CA-CB	5.07	116.40	110.42
1	N	102	PHE	CA-CB-CG	-5.06	108.74	113.80
3	C	128	GLU	CA-C-N	5.05	123.42	120.24
3	C	128	GLU	C-N-CA	5.05	123.42	120.24
1	N	45	GLY	O-C-N	5.05	127.24	122.90
10	J	14	GLU	CA-C-O	-5.04	115.47	120.96
1	A	238	PHE	CA-C-N	5.01	125.54	119.98
1	A	238	PHE	C-N-CA	5.01	125.54	119.98

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	H	9	LYS	Peptide
7	T	83	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	43	0
1	N	4027	0	4001	50	0
2	B	1824	0	1833	21	0
2	O	1824	0	1833	22	0
3	C	2110	0	2027	14	0
3	P	2110	0	2027	22	0
4	D	1195	0	1183	12	0
4	Q	1195	0	1183	15	0
5	E	852	0	845	7	0
5	R	852	0	845	4	0
6	F	748	0	728	6	0
6	S	748	0	728	16	0
7	G	675	0	643	10	0
7	T	675	0	644	22	0
8	H	662	0	623	11	0
8	U	662	0	623	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	592	0	604	2	0
9	V	592	0	604	2	0
10	J	460	0	459	3	0
10	W	460	0	459	1	0
11	K	384	0	366	2	0
11	X	384	0	366	1	0
12	L	380	0	380	5	0
12	Y	380	0	380	10	0
13	M	335	0	352	3	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	102	0	152	1	0
17	C	102	0	152	3	0
17	N	51	0	76	4	0
17	P	153	0	228	4	0
18	A	120	0	108	3	0
18	N	120	0	108	9	0
19	A	40	0	60	3	0
19	B	32	0	48	1	0
19	C	16	0	24	1	0
19	D	24	0	36	0	0
19	E	20	0	30	0	0
19	F	12	0	18	0	0
19	G	20	0	30	0	0
19	I	8	0	12	0	0
19	J	16	0	24	0	0
19	K	8	0	12	0	0
19	L	4	0	6	0	0
19	M	4	0	6	0	0
19	N	40	0	60	4	0
19	O	8	0	12	0	0
19	P	20	0	30	0	0
19	Q	16	0	24	2	0
19	R	8	0	12	0	0
19	S	16	0	24	1	0
19	T	4	0	6	0	0
19	V	8	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	W	8	0	12	0	0
19	Z	4	0	6	0	0
20	A	1	0	0	1	0
20	N	1	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	0	0
22	D	63	0	110	3	0
22	L	63	0	110	2	0
22	N	63	0	110	0	0
22	Q	63	0	110	1	0
22	Y	63	0	110	2	0
23	B	52	0	80	3	0
23	R	52	0	80	2	0
24	C	58	0	78	1	0
24	G	29	0	39	0	0
24	J	29	0	39	1	0
24	P	58	0	78	1	0
24	T	58	0	78	12	0
24	W	29	0	39	1	0
24	Y	29	0	39	4	0
25	C	200	0	312	4	0
25	P	100	0	156	2	0
25	T	100	0	156	6	0
26	C	66	0	84	2	0
26	D	33	0	42	3	0
26	G	33	0	42	0	0
26	P	33	0	42	0	0
26	Q	33	0	42	2	0
27	C	53	0	77	1	0
27	G	106	0	154	5	0
27	P	106	0	154	4	0
27	T	53	0	77	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	0	0
29	V	9	0	8	2	0
30	A	188	0	0	6	0
30	B	107	0	0	0	0
30	C	107	0	0	1	0
30	D	89	0	0	2	0
30	E	71	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	F	68	0	0	0	0
30	G	32	0	0	0	0
30	H	41	0	0	1	0
30	I	31	0	0	1	0
30	J	23	0	0	1	0
30	K	19	0	0	1	0
30	L	25	0	0	1	0
30	M	18	0	0	0	0
30	N	167	0	0	6	0
30	O	90	0	0	1	0
30	P	105	0	0	5	0
30	Q	69	0	0	1	0
30	R	52	0	0	0	0
30	S	81	0	0	1	0
30	T	43	0	0	3	0
30	U	34	0	0	1	0
30	V	17	0	0	0	0
30	W	26	0	0	0	0
30	X	14	0	0	0	0
30	Y	4	0	0	1	0
30	Z	8	0	0	1	0
All	All	32721	0	31981	318	0

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

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:43:MET:HE2	8:U:52:VAL:HG21	1.51	0.92
12:Y:24:MET:SD	22:Y:101:TGL:HC42	2.14	0.87
27:P:305:PEK:H381	25:T:103:CDL:H271	1.56	0.85
7:G:76:ASN:HD21	27:G:102:PEK:HN2	1.21	0.85
20:A:618:OH:O	30:A:701:HOH:O	1.99	0.81
20:N:618:OH:O	30:N:701:HOH:O	1.98	0.81
24:T:105:CHD:H183	24:T:105:CHD:H231	1.64	0.79
25:C:304:CDL:H1	25:C:304:CDL:OA5	1.82	0.78
3:C:246:ASP:HB2	30:C:476:HOH:O	1.85	0.77
7:T:72:ASN:H	7:T:76:ASN:HD22	1.30	0.76
7:G:72:ASN:H	7:G:76:ASN:HD22	1.31	0.75
8:H:43:MET:HE1	8:U:43:MET:HE1	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:GLY:HA2	19:A:608:EDO:H21	1.72	0.71
1:A:297:MET:HG3	1:A:302:ARG:HG3	1.73	0.70
27:P:305:PEK:H381	25:T:103:CDL:C27	2.20	0.70
3:P:149:HIS:CE1	24:T:105:CHD:H182	2.28	0.69
1:A:468:MET:HE1	18:A:607:HEA:H212	1.74	0.69
7:T:8:HIS:O	24:T:105:CHD:H42	1.93	0.69
7:T:76:ASN:HD21	27:T:102:PEK:HN2	1.39	0.68
7:G:8:HIS:HB3	1:N:179:TYR:OH	1.94	0.67
2:O:58:ALA:O	2:O:62:GLU:HG3	1.95	0.66
7:T:31:CYS:SG	25:T:103:CDL:C54	2.84	0.66
27:G:102:PEK:C12	27:G:102:PEK:H161	2.27	0.64
17:N:617:PGV:C5	17:N:617:PGV:C1	2.77	0.63
1:A:472:ILE:HG21	22:L:101:TGL:H202	1.80	0.63
1:A:281:GLY:C	7:T:4:ALA:HB3	2.24	0.63
17:C:303:PGV:H11	17:C:303:PGV:H42	1.79	0.63
7:T:31:CYS:SG	25:T:103:CDL:H542	2.39	0.63
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.82	0.62
3:C:103:HIS:ND1	24:C:301:CHD:O26	2.29	0.62
1:N:336:PRO:HB2	1:N:394:VAL:HG11	1.81	0.62
12:L:28:PHE:CD1	22:L:101:TGL:HA32	2.35	0.62
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.81	0.62
3:P:246:ASP:HB2	30:P:477:HOH:O	2.00	0.61
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.82	0.61
3:P:116:TRP:HA	3:P:117:PRO:C	2.24	0.61
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.83	0.61
1:A:497:GLY:HA2	19:A:608:EDO:C2	2.31	0.61
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.35	0.61
3:P:149:HIS:NE2	24:T:105:CHD:C18	2.64	0.60
3:C:149:HIS:NE2	26:C:311:DMU:H2	2.17	0.60
6:F:87:THR:HG22	6:F:89:TYR:CE1	2.36	0.60
2:O:121:TYR:O	2:O:138:VAL:HA	2.01	0.60
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.60
29:V:101:SAC:C	29:V:101:SAC:H2A1	2.32	0.60
3:P:54:MET:HE1	17:P:306:PGV:H131	1.83	0.59
12:Y:24:MET:SD	22:Y:101:TGL:CC4	2.89	0.59
6:S:13:ALA:CB	6:S:21:MET:HE1	2.32	0.59
7:T:9:GLY:N	30:T:201:HOH:O	2.36	0.58
8:U:27:ARG:NH1	30:U:101:HOH:O	2.36	0.58
25:P:308:CDL:OA2	30:P:401:HOH:O	2.17	0.57
2:B:58:ALA:O	2:B:62:GLU:HG3	2.05	0.57
1:A:193:VAL:HG21	7:T:5:LYS:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASN:O	30:A:702:HOH:O	2.17	0.56
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.40	0.56
2:O:56:MET:HA	23:R:201:PSC:H202	1.88	0.56
2:O:116:LEU:HD12	2:O:117:SER:N	2.20	0.56
19:N:611:EDO:O2	30:N:702:HOH:O	2.10	0.55
6:F:55:LYS:HA	6:F:74:LEU:O	2.07	0.55
12:L:46:LYS:HA	30:L:213:HOH:O	2.07	0.55
18:N:606:HEA:HMC1	18:N:606:HEA:HBC1	1.89	0.55
3:P:3:HIS:HB2	30:P:479:HOH:O	2.07	0.55
6:S:92:VAL:O	6:S:92:VAL:HG23	2.07	0.55
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.88	0.55
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.41	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.88	0.54
8:H:43:MET:CE	8:U:43:MET:HE1	2.35	0.54
25:T:103:CDL:H531	25:T:103:CDL:H211	1.90	0.54
1:A:194:LEU:CD2	7:T:4:ALA:HB1	2.37	0.54
10:J:58:LYS:HA	30:J:216:HOH:O	2.07	0.54
24:T:105:CHD:C18	24:T:105:CHD:H222	2.37	0.54
3:C:58:TRP:HB3	17:C:302:PGV:H31	1.88	0.54
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.91	0.53
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.08	0.53
19:N:614:EDO:H12	30:N:732:HOH:O	2.09	0.53
1:N:87:ILE:O	1:N:173:PRO:HD3	2.09	0.52
1:N:117:MET:HE1	24:Y:102:CHD:H222	1.91	0.52
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.90	0.52
19:N:612:EDO:H11	30:N:771:HOH:O	2.09	0.52
1:A:87:ILE:O	1:A:173:PRO:HD3	2.08	0.52
2:B:78:LEU:CB	2:B:79:PRO:CD	2.87	0.52
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.91	0.52
5:E:84:TYR:OH	30:E:301:HOH:O	2.19	0.52
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.36	0.52
17:N:617:PGV:H282	13:Z:12:PRO:HG3	1.91	0.52
24:T:105:CHD:H183	24:T:105:CHD:C23	2.37	0.52
25:C:310:CDL:H452	7:G:37:LEU:HD23	1.92	0.52
7:T:70:PHE:O	27:T:102:PEK:N	2.43	0.51
27:G:103:PEK:H231	2:O:59:GLN:HE22	1.75	0.51
6:S:75:HIS:H	6:S:80:GLN:HE22	1.57	0.51
13:Z:30:ALA:N	30:Z:1701:HOH:O	2.40	0.51
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.45	0.51
8:H:43:MET:HE1	8:U:43:MET:CE	2.37	0.51
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:35:PHE:O	7:T:58:LYS:NZ	2.43	0.51
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.51
7:T:5:LYS:NZ	30:T:204:HOH:O	2.44	0.51
2:B:121:TYR:O	2:B:138:VAL:HA	2.10	0.51
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.76	0.51
1:N:364:ASP:OD1	18:N:605:HEA:O2A	2.29	0.51
3:C:116:TRP:HA	3:C:117:PRO:C	2.34	0.51
1:N:211:THR:HG22	1:N:215:LEU:HD12	1.93	0.51
12:Y:2:HIS:N	30:Y:201:HOH:O	2.44	0.51
1:N:479:LYS:HD3	30:N:759:HOH:O	2.12	0.50
24:T:105:CHD:H222	24:T:105:CHD:H181	1.93	0.50
1:N:397:PHE:N	1:N:398:PRO:CD	2.74	0.50
1:A:484:THR:HG22	30:A:813:HOH:O	2.11	0.50
3:P:124:LEU:HD13	3:P:180:GLU:OE1	2.12	0.50
6:S:54:ASN:HD22	6:S:54:ASN:C	2.19	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.11	0.50
1:N:407:ASP:O	1:N:411:LYS:HG3	2.11	0.50
3:P:95:THR:HG21	17:P:307:PGV:H302	1.92	0.50
1:A:65:MET:HB3	18:A:607:HEA:CAC	2.42	0.49
1:N:112:LEU:HD23	1:N:112:LEU:C	2.37	0.49
17:N:617:PGV:H241	17:N:617:PGV:H202	1.93	0.49
23:R:201:PSC:H341	23:R:201:PSC:H142	1.94	0.49
1:N:174:PRO:HD2	19:N:612:EDO:H11	1.92	0.49
27:P:301:PEK:O02	27:P:301:PEK:H031	2.12	0.49
29:V:101:SAC:C	29:V:101:SAC:C2A	2.89	0.49
1:N:28:MET:HE2	1:N:28:MET:N	2.27	0.49
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.28	0.49
4:D:123:MET:HE2	4:D:134:PHE:CZ	2.48	0.49
4:Q:123:MET:HE2	4:Q:134:PHE:CE2	2.47	0.49
13:M:28:LEU:HB2	13:M:29:PRO:HD3	1.95	0.49
24:Y:102:CHD:H192	24:Y:102:CHD:H3	1.95	0.48
1:N:489:THR:HA	6:S:71:TRP:O	2.13	0.48
8:H:9:LYS:HG3	30:H:113:HOH:O	2.12	0.48
1:N:310:MET:HE1	2:O:76:ILE:HB	1.95	0.48
24:T:105:CHD:C18	24:T:105:CHD:C22	2.91	0.48
4:D:98:TRP:CE2	26:D:208:DMU:H8	2.49	0.48
4:D:123:MET:HE2	4:D:134:PHE:CE2	2.48	0.48
1:N:24:ALA:HB2	18:N:606:HEA:H253	1.94	0.48
3:P:3:HIS:CB	30:P:479:HOH:O	2.62	0.48
3:P:103:HIS:HA	17:P:307:PGV:O04	2.12	0.48
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:HA	22:D:201:TGL:HB52	1.94	0.48
2:B:155:SER:O	2:B:174:ALA:HB1	2.14	0.48
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.96	0.48
3:P:149:HIS:NE2	24:T:105:CHD:H182	2.27	0.48
8:H:60:TYR:CD1	8:H:60:TYR:C	2.92	0.47
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.96	0.47
1:A:489:THR:HA	6:F:71:TRP:O	2.13	0.47
1:N:199:LEU:N	1:N:200:PRO:CD	2.77	0.47
19:A:608:EDO:H12	30:A:735:HOH:O	2.14	0.47
12:Y:41:ARG:HH22	24:Y:102:CHD:H191	1.80	0.47
7:T:31:CYS:SG	25:T:103:CDL:H541	2.54	0.47
11:K:6:ALA:N	30:K:204:HOH:O	2.48	0.47
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.49	0.47
5:R:82:TYR:HB3	5:R:83:PRO:HD3	1.96	0.47
1:A:83:VAL:HB	1:A:84:PRO:HD3	1.97	0.47
1:A:194:LEU:HD21	7:T:4:ALA:HB1	1.95	0.47
1:N:339:MET:HE1	1:N:411:LYS:HD3	1.96	0.47
7:G:4:ALA:HB1	1:N:194:LEU:HD23	1.96	0.47
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.15	0.47
7:T:67:HIS:NE2	7:T:84:LYS:HB3	2.30	0.47
25:P:308:CDL:CA2	30:P:401:HOH:O	2.63	0.47
1:A:353:LEU:HD11	2:B:34:ILE:HG22	1.97	0.47
3:C:129:VAL:N	3:C:130:PRO:CD	2.78	0.47
26:C:312:DMU:H26	26:C:312:DMU:H18	1.73	0.47
18:N:605:HEA:CMC	18:N:605:HEA:HBC1	2.45	0.46
12:Y:45:LEU:O	12:Y:46:LYS:C	2.57	0.46
2:B:29:MET:HG3	9:I:35:TYR:CD1	2.50	0.46
4:Q:7:LYS:HA	4:Q:10:ASP:HB2	1.98	0.46
1:A:19:TYR:CD1	1:A:76:GLY:HA3	2.50	0.46
12:L:35:ALA:HB3	12:L:36:PRO:HD3	1.97	0.46
1:A:406:ASN:HD21	17:A:604:PGV:H31	1.81	0.46
7:G:76:ASN:ND2	27:G:102:PEK:HN2	2.01	0.46
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.97	0.46
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.51	0.46
2:O:102:HIS:O	2:O:104:TRP:HA	2.15	0.46
7:G:4:ALA:CB	1:N:285:PHE:CE2	2.99	0.46
1:N:379:TYR:O	1:N:383:MET:HB2	2.15	0.46
18:N:606:HEA:H122	18:N:606:HEA:HHC	1.98	0.46
3:P:149:HIS:CE1	24:T:105:CHD:C18	2.98	0.46
24:P:309:CHD:H212	24:P:309:CHD:H183	1.98	0.46
6:S:94:HIS:O	30:S:201:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.45	0.46
3:P:228:THR:HA	6:S:7:PRO:O	2.15	0.46
4:Q:123:MET:HE2	4:Q:134:PHE:CZ	2.51	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.15	0.45
2:O:116:LEU:HD12	2:O:117:SER:H	1.80	0.45
2:O:125:THR:HA	2:O:128:LEU:HD12	1.98	0.45
1:A:302:ARG:NH2	8:H:23:GLN:HE21	2.13	0.45
27:T:102:PEK:H32	27:T:102:PEK:H101	1.98	0.45
1:A:233:HIS:CE1	1:A:292:MET:HE1	2.52	0.45
2:B:158:ASP:HB2	19:B:305:EDO:H22	1.97	0.45
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.52	0.45
17:C:303:PGV:H22	17:C:303:PGV:H141	1.97	0.45
26:D:208:DMU:C11	30:D:301:HOH:O	2.65	0.45
27:T:102:PEK:H32	27:T:102:PEK:H71	1.99	0.45
10:W:36:MET:HE3	10:W:36:MET:HA	1.99	0.45
1:A:488:THR:HB	1:A:495:LEU:HD13	1.98	0.45
3:C:55:TYR:HA	25:C:304:CDL:H551	1.98	0.45
12:Y:45:LEU:HD12	24:Y:102:CHD:H7	1.99	0.45
23:B:303:PSC:O03	23:B:303:PSC:H232	2.17	0.44
6:S:64:GLU:O	6:S:65:ASP:HB2	2.18	0.44
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.44
4:D:127:LYS:HD2	30:I:226:HOH:O	2.17	0.44
7:T:9:GLY:CA	30:T:201:HOH:O	2.64	0.44
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.32	0.44
1:N:115:SER:O	1:N:121:GLY:HA2	2.17	0.44
4:Q:46:ALA:O	4:Q:47:SER:C	2.60	0.44
24:T:101:CHD:O7	24:T:101:CHD:H41	2.17	0.44
5:E:12:ASP:OD2	5:E:44:GLU:HG3	2.16	0.44
1:A:335:SER:HB2	30:A:839:HOH:O	2.18	0.44
2:B:158:ASP:O	2:B:176:PRO:HG3	2.18	0.44
3:C:173:PHE:CD1	3:C:173:PHE:C	2.94	0.44
1:N:83:VAL:HB	1:N:84:PRO:HD3	1.99	0.44
2:B:75:LEU:HD12	2:B:75:LEU:HA	1.88	0.44
5:R:67:ILE:O	5:R:71:VAL:HG23	2.17	0.44
2:B:78:LEU:CB	2:B:79:PRO:HD3	2.48	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.00	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.17	0.43
7:T:67:HIS:NE2	7:T:84:LYS:HG2	2.32	0.43
10:J:50:LEU:C	10:J:50:LEU:HD22	2.43	0.43
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.00	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:63:SER:O	5:E:67:ILE:HG13	2.19	0.43
1:N:37:ILE:HG21	18:N:606:HEA:CMA	2.49	0.43
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	2.01	0.43
3:P:22:LEU:O	3:P:25:LEU:HB3	2.19	0.43
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.00	0.43
2:B:52:HIS:CE1	23:B:303:PSC:H02	2.54	0.43
6:F:64:GLU:O	6:F:65:ASP:HB2	2.19	0.43
26:Q:206:DMU:H6	13:Z:28:LEU:HD23	2.00	0.43
24:T:105:CHD:H183	24:T:105:CHD:C22	2.48	0.43
7:G:1:ALA:HB2	27:P:301:PEK:C37	2.49	0.43
8:H:52:VAL:HG12	8:U:46:LYS:HB3	1.99	0.43
2:B:108:TYR:CE2	2:B:142:VAL:HG21	2.54	0.43
24:J:101:CHD:H17	24:J:101:CHD:H232	1.88	0.42
1:N:76:GLY:O	1:N:80:ASN:HB2	2.19	0.42
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.18	0.42
4:Q:81:VAL:HG11	22:Q:201:TGL:HB82	2.01	0.42
1:N:110:LEU:HD12	1:N:113:LEU:HD23	2.02	0.42
30:N:745:HOH:O	6:S:37:LYS:HG3	2.19	0.42
8:H:17:ASP:C	8:H:17:ASP:OD1	2.62	0.42
1:A:397:PHE:N	1:A:398:PRO:CD	2.83	0.42
4:D:138:TRP:CH2	11:K:50:PRO:HG2	2.55	0.42
1:N:65:MET:HB3	18:N:606:HEA:CAC	2.49	0.42
2:O:139:ASP:OD1	2:O:140:ASN:N	2.52	0.42
1:N:94:PHE:HB2	1:N:163:ASN:ND2	2.34	0.42
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.01	0.42
2:O:199:ILE:HG23	2:O:199:ILE:O	2.18	0.42
3:P:129:VAL:N	3:P:130:PRO:CD	2.83	0.42
8:H:37:HIS:CD2	8:H:76:ARG:CZ	3.02	0.42
1:N:171:MET:HE3	3:P:8:TYR:CD1	2.55	0.42
3:P:192:VAL:HA	3:P:195:SER:HB2	2.02	0.42
1:A:351:GLY:HA3	1:A:380:VAL:HG13	2.00	0.42
1:A:426:PHE:N	1:A:427:PRO:CD	2.83	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.18	0.42
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.01	0.42
1:N:266:GLU:OE2	2:O:55:THR:OG1	2.26	0.42
4:Q:7:LYS:HD2	19:Q:204:EDO:O2	2.19	0.42
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.49	0.42
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.02	0.42
27:C:313:PEK:H302	7:T:3:ALA:HB3	2.02	0.42
10:J:8:LYS:HD3	10:J:8:LYS:HA	1.85	0.42
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
7:T:78:LEU:HD22	7:T:84:LYS:HB2	2.02	0.42
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.02	0.42
1:A:302:ARG:HD2	30:A:879:HOH:O	2.20	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.19	0.42
3:C:158:HIS:CB	19:C:306:EDO:H11	2.50	0.42
4:D:122:ARG:HG2	4:D:126:MET:HE3	2.02	0.42
7:G:10:GLY:CA	1:N:177:SER:HB2	2.50	0.42
8:H:39:CYS:O	8:H:43:MET:HG2	2.19	0.42
6:S:34:LEU:O	19:S:105:EDO:H21	2.19	0.42
1:A:23:GLY:HA3	1:A:73:ILE:HG13	2.02	0.41
7:G:1:ALA:HA	17:P:307:PGV:H312	2.02	0.41
2:O:222:TRP:NE1	2:O:226:MET:HE3	2.36	0.41
4:Q:98:TRP:CE2	26:Q:206:DMU:H11	2.55	0.41
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.56	0.41
13:M:34:LEU:HD12	13:M:34:LEU:HA	1.88	0.41
1:N:165:ILE:O	1:N:169:ILE:HG12	2.20	0.41
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.55	0.41
1:N:274:VAL:HG12	1:N:278:MET:HE2	2.02	0.41
1:N:498:CYS:HA	1:N:499:PRO:HA	1.88	0.41
2:O:112:ASP:OD1	8:U:13:THR:OG1	2.27	0.41
19:Q:205:EDO:H11	30:Q:365:HOH:O	2.20	0.41
6:S:81:ARG:HA	6:S:87:THR:O	2.20	0.41
12:Y:15:VAL:HG12	12:Y:21:LEU:HD22	2.01	0.41
18:A:607:HEA:HMC1	18:A:607:HEA:HBC1	2.03	0.41
3:C:62:ILE:HD12	25:C:304:CDL:H511	2.02	0.41
4:D:98:TRP:CE3	26:D:208:DMU:H13	2.56	0.41
18:N:606:HEA:H172	18:N:606:HEA:H261	1.79	0.41
2:B:3:TYR:CZ	2:B:6:GLN:HG3	2.55	0.41
1:N:456:MET:HG2	4:Q:96:LEU:HD13	2.02	0.41
1:N:485:VAL:HG21	1:N:494:TRP:CE3	2.55	0.41
4:D:77:GLU:HB3	22:D:201:TGL:HB32	2.02	0.41
1:A:18:LEU:HD23	1:A:18:LEU:HA	1.93	0.41
1:A:199:LEU:N	1:A:200:PRO:CD	2.84	0.41
30:D:345:HOH:O	13:M:4:LYS:HE2	2.20	0.41
5:E:90:ARG:HD3	5:E:90:ARG:HA	1.98	0.41
6:F:85:CYS:SG	6:F:87:THR:HB	2.61	0.41
23:B:303:PSC:H32	9:I:14:ALA:CB	2.50	0.41
1:N:426:PHE:N	1:N:427:PRO:CD	2.83	0.41
17:N:617:PGV:H241	17:N:617:PGV:H012	2.03	0.41
1:N:54:TYR:OH	18:N:606:HEA:O2A	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:100:MET:SD	2:O:155:SER:HB3	2.60	0.40
1:A:198:SER:HB2	1:A:238:PHE:HA	2.03	0.40
1:A:297:MET:O	1:A:302:ARG:NH2	2.54	0.40
1:A:510:TYR:CD1	1:A:510:TYR:C	3.00	0.40
27:G:102:PEK:C12	27:G:102:PEK:C16	2.96	0.40
24:W:302:CHD:H161	24:W:302:CHD:O25	2.20	0.40
5:R:52:LEU:O	5:R:55:CYS:HB2	2.21	0.40
7:T:11:TPO:HG23	7:T:14:ARG:HB2	2.02	0.40
1:A:281:GLY:C	7:T:4:ALA:CB	2.92	0.40
3:C:16:TRP:N	3:C:17:PRO:CD	2.84	0.40
4:D:78:TRP:N	22:D:201:TGL:HB32	2.35	0.40
3:P:31:LEU:HD23	3:P:31:LEU:HA	1.91	0.40
8:U:49:ASP:O	8:U:52:VAL:HG22	2.21	0.40
1:A:321:PHE:HB3	2:B:65:TRP:CE2	2.56	0.40
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.87	0.40
5:E:82:TYR:N	5:E:83:PRO:CD	2.84	0.40
1:N:35:LEU:HD13	1:N:462:LEU:HD22	2.03	0.40
2:O:226:MET:HE1	30:O:450:HOH:O	2.21	0.40
6:S:92:VAL:O	6:S:92:VAL:CG2	2.68	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	512/514 (100%)	498 (97%)	14 (3%)	0	100	100
1	N	512/514 (100%)	494 (96%)	18 (4%)	0	100	100
2	B	225/227 (99%)	215 (96%)	10 (4%)	0	100	100
2	O	225/227 (99%)	214 (95%)	11 (5%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	131 (92%)	11 (8%)	0	100	100
5	E	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
6	S	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	5	4
7	G	81/85 (95%)	69 (85%)	10 (12%)	2 (2%)	4	3
7	T	81/85 (95%)	66 (82%)	13 (16%)	2 (2%)	4	3
8	H	77/85 (91%)	68 (88%)	7 (9%)	2 (3%)	4	2
8	U	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	9	8
9	I	70/73 (96%)	70 (100%)	0	0	100	100
9	V	70/73 (96%)	66 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	44 (94%)	2 (4%)	1 (2%)	5	4
12	L	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
12	Y	44/47 (94%)	41 (93%)	2 (4%)	1 (2%)	5	3
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3502/3614 (97%)	3351 (96%)	140 (4%)	11 (0%)	36	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	8	ILE
8	H	45	ALA
7	G	43	GLU
12	Y	46	LYS
6	S	95	GLN
6	S	97	ALA
7	T	8	HIS
11	X	7	PRO
7	T	4	ALA

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Mol	Chain	Res	Type
7	G	9	GLY
8	U	8	ILE

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	426/426 (100%)	419 (98%)	7 (2%)	55	70
1	N	426/426 (100%)	417 (98%)	9 (2%)	47	61
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	34
2	O	210/210 (100%)	198 (94%)	12 (6%)	18	23
3	C	224/226 (99%)	219 (98%)	5 (2%)	45	59
3	P	224/226 (99%)	217 (97%)	7 (3%)	35	47
4	D	128/129 (99%)	123 (96%)	5 (4%)	28	39
4	Q	128/129 (99%)	122 (95%)	6 (5%)	23	30
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	44
5	R	92/95 (97%)	87 (95%)	5 (5%)	20	24
6	F	81/81 (100%)	76 (94%)	5 (6%)	16	19
6	S	81/81 (100%)	73 (90%)	8 (10%)	7	7
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	9
7	T	67/68 (98%)	62 (92%)	5 (8%)	12	13
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	15
8	U	71/75 (95%)	64 (90%)	7 (10%)	7	7
9	I	57/57 (100%)	53 (93%)	4 (7%)	14	15
9	V	57/57 (100%)	53 (93%)	4 (7%)	14	15
10	J	49/50 (98%)	46 (94%)	3 (6%)	17	20
10	W	49/50 (98%)	47 (96%)	2 (4%)	27	36
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	54
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	39/40 (98%)	36 (92%)	3 (8%)	12	13
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	4
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	24
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	24
All	All	3040/3082 (99%)	2908 (96%)	132 (4%)	26	34

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ILE
1	A	118	VAL
1	A	136	LEU
1	A	152	LEU
1	A	180	GLN
1	A	369	ASP
1	A	382	SER
2	B	33	LEU
2	B	37	LEU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	110	TYR
2	B	130	PRO
3	C	42	LEU
3	C	127	LEU
3	C	159	MET
3	C	223	LEU
3	C	230	ASN
4	D	4	SER
4	D	36	SER
4	D	45	LYS
4	D	51	LEU
4	D	121	LYS
5	E	7	THR
5	E	70	VAL
5	E	108	LYS
6	F	26	LYS
6	F	48	LEU
6	F	87	THR

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Mol	Chain	Res	Type
6	F	96	LEU
6	F	98	HIS
7	G	30	LEU
7	G	33	LEU
7	G	36	TRP
7	G	37	LEU
7	G	42	ARG
7	G	74	ARG
8	H	7	LYS
8	H	9	LYS
8	H	29	CYS
8	H	60	TYR
8	H	84	LYS
9	I	2	THR
9	I	15	ARG
9	I	22	VAL
9	I	42	LYS
10	J	46	SER
10	J	50	LEU
10	J	58	LYS
11	K	54	ARG
12	L	26	THR
12	L	27	LEU
12	L	47	LYS
13	M	13	LYS
13	M	34	LEU
1	N	128	VAL
1	N	152	LEU
1	N	189	MET
1	N	297	MET
1	N	369	ASP
1	N	382	SER
1	N	484	THR
1	N	485	VAL
1	N	512	ASN
2	O	33	LEU
2	O	63	THR
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	92	ASN

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Mol	Chain	Res	Type
2	O	94	SER
2	O	110	TYR
2	O	183	THR
2	O	199	ILE
2	O	217	LYS
3	P	3	HIS
3	P	33	MET
3	P	127	LEU
3	P	144	ILE
3	P	159	MET
3	P	223	LEU
3	P	230	ASN
4	Q	4	SER
4	Q	7	LYS
4	Q	15	SER
4	Q	19	ARG
4	Q	31	LYS
4	Q	58	GLU
5	R	5	HIS
5	R	7	THR
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
6	S	37	LYS
6	S	43	LYS
6	S	48	LEU
6	S	54	ASN
6	S	87	THR
6	S	90	LYS
6	S	91	LEU
6	S	95	GLN
7	T	5	LYS
7	T	7	ASP
7	T	78	LEU
7	T	83	GLU
7	T	84	LYS
8	U	7	LYS
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	43	MET
8	U	60	TYR

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Mol	Chain	Res	Type
8	U	61	LYS
9	V	8	GLN
9	V	36	LYS
9	V	44	LYS
9	V	61	GLU
10	W	36	MET
10	W	50	LEU
11	X	23	THR
11	X	47	ARG
12	Y	2	HIS
12	Y	20	ARG
12	Y	26	THR
12	Y	27	LEU
12	Y	47	LYS
13	Z	34	LEU
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	178	GLN
1	A	180	GLN
2	B	10	GLN
2	B	22	HIS
2	B	91	ASN
2	B	140	ASN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
4	D	29	HIS
4	D	119	GLN
5	E	94	ASN
7	G	8	HIS
7	G	76	ASN
8	H	10	ASN
8	H	31	GLN
10	J	29	ASN
1	N	178	GLN
1	N	232	GLN
1	N	512	ASN

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Mol	Chain	Res	Type
2	O	59	GLN
2	O	91	ASN
3	P	56	GLN
3	P	68	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	72	ASN
4	Q	101	HIS
4	Q	143	ASN
5	R	94	ASN
6	S	28	GLN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	76	ASN
8	U	31	GLN
8	U	32	ASN
10	W	57	HIS
11	X	35	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	TPO	G	11	7	8,10,11	0.96	1 (12%)	10,14,16	0.73	0
2	FME	O	1	2	8,9,10	0.53	0	8,9,11	0.73	0
1	FME	A	1	1	8,9,10	0.68	0	8,9,11	0.87	0
1	FME	N	1	1	8,9,10	0.47	0	8,9,11	0.96	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TPO	T	11	7	8,10,11	0.98	1 (12%)	10,14,16	0.81	0
2	FME	B	1	2	8,9,10	0.60	0	8,9,11	0.92	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	TPO	G	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
2	FME	B	1	2	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-OG1	2.18	1.63	1.59
7	T	11	TPO	P-OG1	2.07	1.63	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	2.16	113.66	109.50
1	N	1	FME	O-C-CA	-2.03	119.54	124.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
7	G	11	TPO	O-C-CA-CB
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	O-C-CA-CB
7	T	11	TPO	CA-CB-OG1-P
2	B	1	FME	CA-CB-CG-SD
1	A	1	FME	CA-CB-CG-SD
2	B	1	FME	C-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	CB-CG-SD-CE
1	N	1	FME	C-CA-CB-CG
2	B	1	FME	N-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	T	11	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 134 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	$\# Z > 2$
24	CHD	Y	102	-	32,32,32	0.70	0	51,51,51	1.20	7 (13%)
19	EDO	P	311	-	3,3,3	0.14	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	I	103	-	3,3,3	0.13	0	2,2,2	0.10	0
22	TGL	D	201	-	62,62,62	0.34	0	65,65,65	0.33	0
19	EDO	O	303	-	3,3,3	0.21	0	2,2,2	0.41	0
19	EDO	S	105	-	3,3,3	0.18	0	2,2,2	0.27	0
19	EDO	C	306	-	3,3,3	0.73	0	2,2,2	0.74	0
27	PEK	T	102	-	52,52,52	0.31	0	55,57,57	0.58	1 (1%)
19	EDO	N	616	-	3,3,3	0.04	0	2,2,2	0.27	0
19	EDO	D	202	-	3,3,3	0.26	0	2,2,2	0.42	0
19	EDO	N	613	-	3,3,3	0.15	0	2,2,2	0.20	0
24	CHD	T	105	-	32,32,32	0.69	0	51,51,51	1.26	4 (7%)
24	CHD	T	101	-	32,32,32	0.66	0	51,51,51	1.05	2 (3%)
19	EDO	G	107	-	3,3,3	0.05	0	2,2,2	0.08	0
19	EDO	A	611	-	3,3,3	0.32	0	2,2,2	0.38	0
25	CDL	C	310	-	99,99,99	0.38	0	105,111,111	0.44	0
18	HEA	A	607	1	67,67,67	2.35	26 (38%)	81,103,103	2.46	30 (37%)
19	EDO	N	611	-	3,3,3	0.16	0	2,2,2	0.12	0
19	EDO	R	203	-	3,3,3	0.12	0	2,2,2	0.11	0
22	TGL	Y	101	-	62,62,62	0.29	0	65,65,65	0.40	1 (1%)
19	EDO	B	310	-	3,3,3	0.19	0	2,2,2	0.25	0
24	CHD	J	101	-	32,32,32	0.66	1 (3%)	51,51,51	0.78	1 (1%)
26	DMU	P	303	-	34,34,34	1.70	8 (23%)	45,45,45	1.55	9 (20%)
19	EDO	R	202	-	3,3,3	0.14	0	2,2,2	0.21	0
19	EDO	B	307	-	3,3,3	0.07	0	2,2,2	0.13	0
19	EDO	P	312	-	3,3,3	0.11	0	2,2,2	0.25	0
24	CHD	C	301	-	32,32,32	0.54	0	51,51,51	0.71	1 (1%)
18	HEA	A	606	1	67,67,67	2.32	27 (40%)	81,103,103	2.44	29 (35%)
19	EDO	G	104	-	3,3,3	0.26	0	2,2,2	0.33	0
17	PGV	C	302	-	50,50,50	0.39	0	53,56,56	0.52	0
19	EDO	J	103	-	3,3,3	0.78	0	2,2,2	0.77	0
19	EDO	O	302	-	3,3,3	0.22	0	2,2,2	0.34	0
19	EDO	W	303	-	3,3,3	0.11	0	2,2,2	0.07	0
25	CDL	C	304	-	99,99,99	0.35	0	105,111,111	0.52	0
19	EDO	N	608	-	3,3,3	0.72	0	2,2,2	0.58	0
19	EDO	N	612	-	3,3,3	0.26	0	2,2,2	0.49	0
24	CHD	C	305	-	32,32,32	0.64	0	51,51,51	0.92	1 (1%)
19	EDO	E	202	-	3,3,3	0.14	0	2,2,2	0.11	0
24	CHD	W	302	-	32,32,32	0.65	0	51,51,51	0.86	0
19	EDO	Q	204	-	3,3,3	0.25	0	2,2,2	0.31	0
19	EDO	F	703	-	3,3,3	0.12	0	2,2,2	0.16	0
19	EDO	A	616	-	3,3,3	0.09	0	2,2,2	0.29	0
17	PGV	N	617	-	50,50,50	0.37	0	53,56,56	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	J	104	-	3,3,3	0.17	0	2,2,2	0.21	0
17	PGV	A	604	-	50,50,50	0.39	0	53,56,56	0.51	0
19	EDO	Z	1601	-	3,3,3	0.18	0	2,2,2	0.26	0
19	EDO	N	609	-	3,3,3	0.17	0	2,2,2	0.44	0
19	EDO	A	609	-	3,3,3	0.24	0	2,2,2	0.21	0
19	EDO	A	612	-	3,3,3	0.35	0	2,2,2	0.31	0
17	PGV	P	302	-	50,50,50	0.36	0	53,56,56	0.62	1 (1%)
17	PGV	C	303	-	50,50,50	0.43	0	53,56,56	0.56	1 (1%)
19	EDO	E	203	-	3,3,3	0.16	0	2,2,2	0.25	0
19	EDO	M	701	-	3,3,3	0.09	0	2,2,2	0.15	0
19	EDO	D	206	-	3,3,3	0.24	0	2,2,2	0.36	0
19	EDO	K	102	-	3,3,3	0.17	0	2,2,2	0.19	0
18	HEA	N	606	1	67,67,67	2.36	28 (41%)	81,103,103	2.68	31 (38%)
19	EDO	P	310	-	3,3,3	0.11	0	2,2,2	0.16	0
19	EDO	P	314	-	3,3,3	0.09	0	2,2,2	0.17	0
19	EDO	C	307	-	3,3,3	0.15	0	2,2,2	0.17	0
19	EDO	S	103	-	3,3,3	0.09	0	2,2,2	0.07	0
19	EDO	E	204	-	3,3,3	0.25	0	2,2,2	0.22	0
29	SAC	V	101	-	7,8,9	0.51	0	7,9,11	1.41	1 (14%)
19	EDO	Q	203	-	3,3,3	0.20	0	2,2,2	0.27	0
19	EDO	K	101	-	3,3,3	0.09	0	2,2,2	0.09	0
19	EDO	D	207	-	3,3,3	0.24	0	2,2,2	0.22	0
19	EDO	G	106	-	3,3,3	0.12	0	2,2,2	0.25	0
19	EDO	B	311	-	3,3,3	0.11	0	2,2,2	0.10	0
24	CHD	P	309	-	32,32,32	0.55	0	51,51,51	0.85	1 (1%)
19	EDO	S	104	-	3,3,3	0.07	0	2,2,2	0.02	0
19	EDO	B	306	-	3,3,3	0.11	0	2,2,2	0.06	0
22	TGL	N	604	-	62,62,62	0.32	0	65,65,65	0.53	1 (1%)
25	CDL	P	308	-	99,99,99	0.38	0	105,111,111	0.53	1 (0%)
18	HEA	N	605	1	67,67,67	2.19	29 (43%)	81,103,103	2.53	35 (43%)
22	TGL	B	302	-	62,62,62	0.38	0	65,65,65	0.42	1 (1%)
23	PSC	B	303	-	51,51,51	0.34	0	57,59,59	0.40	0
19	EDO	N	610	-	3,3,3	0.25	0	2,2,2	0.19	0
19	EDO	S	102	-	3,3,3	0.34	0	2,2,2	0.34	0
19	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.39	0
26	DMU	C	312	-	34,34,34	1.19	3 (8%)	45,45,45	1.32	6 (13%)
19	EDO	Q	202	-	3,3,3	0.10	0	2,2,2	0.17	0
19	EDO	J	102	-	3,3,3	0.11	0	2,2,2	0.08	0
23	PSC	R	201	-	51,51,51	0.35	0	57,59,59	0.49	0
19	EDO	G	105	-	3,3,3	0.20	0	2,2,2	0.22	0
21	CUA	B	301	2	0,1,1	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	D	203	-	3,3,3	0.08	0	2,2,2	0.03	0
19	EDO	N	607	-	3,3,3	0.13	0	2,2,2	0.19	0
19	EDO	P	313	-	3,3,3	0.13	0	2,2,2	0.05	0
19	EDO	Q	205	-	3,3,3	0.16	0	2,2,2	0.27	0
24	CHD	G	108	-	32,32,32	0.62	0	51,51,51	0.83	0
19	EDO	E	205	-	3,3,3	0.06	0	2,2,2	0.04	0
19	EDO	C	309	-	3,3,3	0.10	0	2,2,2	0.09	0
27	PEK	P	301	-	52,52,52	0.37	0	55,57,57	0.49	0
19	EDO	W	301	-	3,3,3	0.09	0	2,2,2	0.11	0
27	PEK	C	313	-	52,52,52	0.41	0	55,57,57	0.54	1 (1%)
21	CUA	O	301	2	0,1,1	-	-	-	-	-
19	EDO	N	615	-	3,3,3	0.14	0	2,2,2	0.16	0
17	PGV	A	605	-	50,50,50	0.40	0	53,56,56	0.56	0
26	DMU	C	311	-	34,34,34	2.11	8 (23%)	45,45,45	1.78	9 (20%)
19	EDO	V	102	-	3,3,3	0.13	0	2,2,2	0.16	0
19	EDO	I	102	-	3,3,3	0.08	0	2,2,2	0.10	0
19	EDO	N	614	-	3,3,3	0.60	0	2,2,2	0.72	0
25	CDL	T	103	-	99,99,99	0.41	0	105,111,111	0.49	1 (0%)
19	EDO	B	304	-	3,3,3	0.05	0	2,2,2	0.13	0
19	EDO	E	201	-	3,3,3	0.13	0	2,2,2	0.24	0
19	EDO	J	105	-	3,3,3	0.05	0	2,2,2	0.19	0
26	DMU	D	208	-	34,34,34	1.06	2 (5%)	45,45,45	2.71	8 (17%)
19	EDO	A	617	-	3,3,3	0.16	0	2,2,2	0.25	0
27	PEK	P	305	-	52,52,52	0.36	0	55,57,57	0.58	0
19	EDO	B	308	-	3,3,3	0.24	0	2,2,2	0.25	0
22	TGL	L	101	-	62,62,62	0.34	0	65,65,65	0.37	0
19	EDO	F	701	-	3,3,3	0.11	0	2,2,2	0.47	0
17	PGV	P	306	-	50,50,50	0.34	0	53,56,56	0.50	0
27	PEK	G	102	-	52,52,52	0.32	0	55,57,57	0.58	0
19	EDO	A	613	-	3,3,3	0.09	0	2,2,2	0.09	0
19	EDO	B	309	-	3,3,3	0.37	0	2,2,2	0.41	0
26	DMU	Q	206	-	34,34,34	1.02	1 (2%)	45,45,45	1.20	6 (13%)
19	EDO	F	704	-	3,3,3	0.24	0	2,2,2	0.27	0
19	EDO	D	204	-	3,3,3	0.13	0	2,2,2	0.17	0
22	TGL	Q	201	-	62,62,62	0.34	0	65,65,65	0.38	0
19	EDO	C	308	-	3,3,3	0.13	0	2,2,2	0.20	0
19	EDO	D	205	-	3,3,3	0.10	0	2,2,2	0.15	0
19	EDO	G	109	-	3,3,3	0.10	0	2,2,2	0.23	0
19	EDO	A	614	-	3,3,3	0.07	0	2,2,2	0.18	0
29	SAC	I	101	-	7,8,9	0.56	0	7,9,11	1.25	1 (14%)
26	DMU	G	101	-	34,34,34	2.41	8 (23%)	45,45,45	2.06	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	T	104	-	3,3,3	0.16	0	2,2,2	0.16	0
19	EDO	A	615	-	3,3,3	0.11	0	2,2,2	0.16	0
19	EDO	A	610	-	3,3,3	0.19	0	2,2,2	0.29	0
19	EDO	V	103	-	3,3,3	0.18	0	2,2,2	0.26	0
27	PEK	G	103	-	52,52,52	0.37	0	55,57,57	0.51	0
24	CHD	P	304	-	32,32,32	0.58	0	51,51,51	0.68	0
17	PGV	P	307	-	50,50,50	0.34	0	53,56,56	0.43	0
19	EDO	A	608	-	3,3,3	0.70	0	2,2,2	0.82	0
19	EDO	L	102	-	3,3,3	0.24	0	2,2,2	0.31	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
24	CHD	Y	102	-	-	4/9/74/74	1/4/4/4
19	EDO	P	311	-	-	1/1/1/1	-
19	EDO	I	103	-	-	1/1/1/1	-
22	TGL	D	201	-	-	41/65/65/65	-
19	EDO	O	303	-	-	1/1/1/1	-
19	EDO	S	105	-	-	1/1/1/1	-
19	EDO	C	306	-	-	0/1/1/1	-
27	PEK	T	102	-	-	16/56/56/56	-
19	EDO	N	616	-	-	0/1/1/1	-
19	EDO	D	202	-	-	1/1/1/1	-
19	EDO	N	613	-	-	1/1/1/1	-
24	CHD	T	105	-	-	7/9/74/74	0/4/4/4
24	CHD	T	101	-	-	3/9/74/74	0/4/4/4
19	EDO	G	107	-	-	1/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
25	CDL	C	310	-	-	56/110/110/110	-
18	HEA	A	607	1	-	6/36/76/76	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	R	203	-	-	1/1/1/1	-
22	TGL	Y	101	-	-	37/65/65/65	-
19	EDO	B	310	-	-	1/1/1/1	-
24	CHD	J	101	-	-	1/9/74/74	0/4/4/4
26	DMU	P	303	-	-	9/19/59/59	0/2/2/2
19	EDO	R	202	-	-	0/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	P	312	-	-	1/1/1/1	-
24	CHD	C	301	-	-	1/9/74/74	0/4/4/4
18	HEA	A	606	1	-	9/36/76/76	-
19	EDO	G	104	-	-	1/1/1/1	-
17	PGV	C	302	-	-	16/55/55/55	-
19	EDO	J	103	-	-	0/1/1/1	-
19	EDO	O	302	-	-	1/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-
25	CDL	C	304	-	-	53/110/110/110	-
19	EDO	N	608	-	-	0/1/1/1	-
19	EDO	N	612	-	-	0/1/1/1	-
24	CHD	C	305	-	-	2/9/74/74	0/4/4/4
19	EDO	E	202	-	-	1/1/1/1	-
24	CHD	W	302	-	-	2/9/74/74	0/4/4/4
19	EDO	Q	204	-	-	1/1/1/1	-
19	EDO	F	703	-	-	1/1/1/1	-
19	EDO	A	616	-	-	0/1/1/1	-
17	PGV	N	617	-	-	29/55/55/55	-
19	EDO	J	104	-	-	1/1/1/1	-
17	PGV	A	604	-	-	31/55/55/55	-
19	EDO	Z	1601	-	-	1/1/1/1	-
19	EDO	N	609	-	-	0/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
19	EDO	A	612	-	-	1/1/1/1	-
17	PGV	P	302	-	-	15/55/55/55	-
17	PGV	C	303	-	-	32/55/55/55	-
19	EDO	E	203	-	-	0/1/1/1	-
19	EDO	M	701	-	-	0/1/1/1	-
19	EDO	D	206	-	-	1/1/1/1	-
19	EDO	K	102	-	-	1/1/1/1	-
18	HEA	N	606	1	-	6/36/76/76	-
19	EDO	P	310	-	-	0/1/1/1	-
19	EDO	P	314	-	-	1/1/1/1	-
19	EDO	C	307	-	-	1/1/1/1	-
19	EDO	S	103	-	-	0/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
29	SAC	V	101	-	-	6/7/8/10	-
19	EDO	Q	203	-	-	0/1/1/1	-
19	EDO	K	101	-	-	1/1/1/1	-
19	EDO	D	207	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	G	106	-	-	0/1/1/1	-
19	EDO	B	311	-	-	1/1/1/1	-
24	CHD	P	309	-	-	3/9/74/74	0/4/4/4
19	EDO	S	104	-	-	1/1/1/1	-
19	EDO	B	306	-	-	0/1/1/1	-
22	TGL	N	604	-	-	31/65/65/65	-
25	CDL	P	308	-	-	54/110/110/110	-
18	HEA	N	605	1	-	7/36/76/76	-
22	TGL	B	302	-	-	34/65/65/65	-
23	PSC	B	303	-	-	29/55/55/55	-
19	EDO	N	610	-	-	1/1/1/1	-
19	EDO	S	102	-	-	0/1/1/1	-
19	EDO	B	305	-	-	1/1/1/1	-
26	DMU	C	312	-	-	9/19/59/59	0/2/2/2
19	EDO	Q	202	-	-	1/1/1/1	-
19	EDO	J	102	-	-	1/1/1/1	-
23	PSC	R	201	-	1/1/5/9	29/55/55/55	-
19	EDO	G	105	-	-	1/1/1/1	-
19	EDO	D	203	-	-	1/1/1/1	-
19	EDO	N	607	-	-	1/1/1/1	-
19	EDO	P	313	-	-	1/1/1/1	-
19	EDO	Q	205	-	-	1/1/1/1	-
24	CHD	G	108	-	-	2/9/74/74	0/4/4/4
19	EDO	E	205	-	-	0/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
27	PEK	P	301	-	-	25/56/56/56	-
19	EDO	W	301	-	-	1/1/1/1	-
27	PEK	C	313	-	-	24/56/56/56	-
19	EDO	N	615	-	-	1/1/1/1	-
17	PGV	A	605	-	-	15/55/55/55	-
26	DMU	C	311	-	-	9/19/59/59	0/2/2/2
19	EDO	V	102	-	-	1/1/1/1	-
19	EDO	I	102	-	-	0/1/1/1	-
19	EDO	N	614	-	-	1/1/1/1	-
25	CDL	T	103	-	-	55/110/110/110	-
19	EDO	B	304	-	-	0/1/1/1	-
19	EDO	E	201	-	-	0/1/1/1	-
19	EDO	J	105	-	-	1/1/1/1	-
26	DMU	D	208	-	-	10/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	A	617	-	-	0/1/1/1	-
27	PEK	P	305	-	-	27/56/56/56	-
19	EDO	B	308	-	-	1/1/1/1	-
22	TGL	L	101	-	-	30/65/65/65	-
19	EDO	F	701	-	-	0/1/1/1	-
17	PGV	P	306	-	-	11/55/55/55	-
27	PEK	G	102	-	-	23/56/56/56	-
19	EDO	A	613	-	-	1/1/1/1	-
19	EDO	B	309	-	-	0/1/1/1	-
26	DMU	Q	206	-	-	10/19/59/59	0/2/2/2
19	EDO	F	704	-	-	0/1/1/1	-
19	EDO	D	204	-	-	0/1/1/1	-
22	TGL	Q	201	-	-	38/65/65/65	-
19	EDO	C	308	-	-	1/1/1/1	-
19	EDO	D	205	-	-	1/1/1/1	-
19	EDO	G	109	-	-	1/1/1/1	-
19	EDO	A	614	-	-	1/1/1/1	-
29	SAC	I	101	-	-	4/7/8/10	-
26	DMU	G	101	-	-	6/19/59/59	0/2/2/2
19	EDO	T	104	-	-	0/1/1/1	-
19	EDO	A	615	-	-	0/1/1/1	-
19	EDO	A	610	-	-	0/1/1/1	-
19	EDO	V	103	-	-	1/1/1/1	-
27	PEK	G	103	-	-	27/56/56/56	-
24	CHD	P	304	-	-	1/9/74/74	0/4/4/4
17	PGV	P	307	-	-	27/55/55/55	-
19	EDO	A	608	-	-	0/1/1/1	-
19	EDO	L	102	-	-	0/1/1/1	-

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	311	DMU	O16-C6	8.03	1.53	1.40
26	G	101	DMU	O16-C6	8.02	1.53	1.40
18	N	606	HEA	C3B-C2B	5.27	1.46	1.34
18	N	605	HEA	C3D-C2D	4.91	1.47	1.36
26	G	101	DMU	O5-C6	4.91	1.54	1.41
18	A	607	HEA	FE-NA	4.89	2.11	1.95
26	G	101	DMU	O7-C10	4.89	1.55	1.41
18	N	606	HEA	CHB-C4A	4.85	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	605	HEA	C3B-C2B	4.81	1.45	1.34
18	N	606	HEA	C3D-C2D	4.70	1.46	1.36
18	N	606	HEA	FE-NC	4.68	2.10	1.95
18	A	606	HEA	FE-NC	4.63	2.10	1.95
18	A	606	HEA	C3D-C2D	4.59	1.46	1.36
18	A	607	HEA	CHA-C1A	4.53	1.47	1.38
18	A	607	HEA	C1D-ND	-4.44	1.32	1.40
18	A	607	HEA	C3B-C2B	4.43	1.44	1.34
18	A	606	HEA	C3B-C2B	4.38	1.44	1.34
18	N	606	HEA	FE-ND	4.35	2.08	1.94
18	A	606	HEA	C1B-NB	-4.35	1.30	1.38
18	N	606	HEA	FE-NB	4.30	2.08	1.94
18	A	607	HEA	C3D-C2D	4.30	1.46	1.36
18	A	607	HEA	FE-NB	4.26	2.08	1.94
18	A	607	HEA	C3A-C2A	4.25	1.46	1.37
26	C	311	DMU	O7-C10	4.24	1.53	1.41
18	A	607	HEA	CHB-C4A	4.23	1.46	1.38
26	G	101	DMU	O1-C10	4.21	1.52	1.41
18	A	606	HEA	CHA-C1A	4.21	1.46	1.38
18	A	607	HEA	FE-NC	4.18	2.09	1.95
18	N	606	HEA	C3A-C2A	4.12	1.46	1.37
18	A	606	HEA	FE-NA	4.11	2.08	1.95
18	A	607	HEA	CHD-C1D	4.10	1.46	1.38
18	A	606	HEA	CHB-C4A	4.02	1.46	1.38
18	A	606	HEA	FE-ND	4.00	2.07	1.94
18	N	605	HEA	FE-NC	3.99	2.08	1.95
26	P	303	DMU	O7-C10	3.97	1.53	1.41
18	N	606	HEA	CHC-C4B	3.96	1.46	1.38
18	A	606	HEA	C1D-ND	-3.92	1.33	1.40
18	N	605	HEA	CHB-C4A	3.85	1.45	1.38
18	N	606	HEA	C4D-ND	-3.85	1.31	1.38
26	C	312	DMU	O16-C6	3.83	1.46	1.40
18	A	606	HEA	CHD-C1D	3.79	1.46	1.38
26	C	311	DMU	O7-C3	3.74	1.53	1.43
18	A	606	HEA	C4B-NB	-3.72	1.33	1.40
18	A	606	HEA	CHC-C4B	3.71	1.45	1.38
18	A	607	HEA	CHC-C4B	3.70	1.45	1.38
18	N	606	HEA	CHA-C1A	3.69	1.45	1.38
18	N	605	HEA	CHD-C1D	3.68	1.45	1.38
26	G	101	DMU	O5-C4	3.65	1.53	1.44
18	A	607	HEA	FE-ND	3.64	2.06	1.94
26	P	303	DMU	C8-C9	3.61	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	606	HEA	CHD-C4C	3.61	1.47	1.39
18	A	607	HEA	C4B-NB	-3.59	1.34	1.40
26	P	303	DMU	O16-C6	3.57	1.46	1.40
18	A	606	HEA	FE-NB	3.57	2.05	1.94
18	N	606	HEA	CHC-C1C	3.56	1.47	1.39
18	A	607	HEA	C4B-C3B	3.55	1.51	1.44
26	P	303	DMU	O1-C10	3.53	1.50	1.41
18	A	606	HEA	C4A-NA	-3.51	1.33	1.39
18	A	606	HEA	C3A-C2A	3.50	1.45	1.37
18	N	605	HEA	C1B-NB	-3.49	1.32	1.38
26	Q	206	DMU	O16-C6	3.49	1.46	1.40
26	G	101	DMU	O7-C3	3.48	1.52	1.43
18	N	606	HEA	CHD-C1D	3.46	1.45	1.38
18	N	605	HEA	C3A-C2A	3.46	1.45	1.37
18	N	605	HEA	CHD-C4C	3.42	1.47	1.39
18	N	605	HEA	FE-NA	3.40	2.06	1.95
18	A	606	HEA	C1A-NA	-3.39	1.33	1.39
18	N	606	HEA	FE-NA	3.39	2.06	1.95
18	N	606	HEA	C4A-NA	-3.38	1.33	1.39
18	N	605	HEA	FE-NB	3.36	2.05	1.94
18	N	605	HEA	C1A-NA	-3.35	1.33	1.39
18	N	606	HEA	C1A-NA	-3.34	1.33	1.39
18	N	606	HEA	C1D-ND	-3.33	1.34	1.40
18	N	605	HEA	CHA-C1A	3.31	1.44	1.38
18	N	605	HEA	FE-ND	3.26	2.05	1.94
18	N	605	HEA	C4B-NB	-3.26	1.34	1.40
18	A	607	HEA	C4C-NC	-3.16	1.33	1.39
18	A	607	HEA	CHB-C1B	3.16	1.46	1.39
18	A	607	HEA	C1C-NC	-3.15	1.33	1.39
18	A	606	HEA	C4C-NC	-3.14	1.33	1.39
18	N	605	HEA	CHC-C4B	3.11	1.44	1.38
18	A	607	HEA	CHA-C4D	3.11	1.46	1.39
18	N	606	HEA	C4B-C3B	3.10	1.50	1.44
18	A	607	HEA	CHD-C4C	3.10	1.46	1.39
18	A	606	HEA	CHD-C4C	3.10	1.46	1.39
26	P	303	DMU	O1-C9	3.08	1.51	1.44
18	N	605	HEA	CHA-C4D	3.06	1.46	1.39
18	N	605	HEA	C4A-NA	-3.04	1.33	1.39
26	P	303	DMU	O7-C3	2.98	1.51	1.43
18	N	606	HEA	C1C-C2C	2.98	1.50	1.43
18	A	606	HEA	CHA-C4D	2.97	1.46	1.39
18	N	606	HEA	C1B-NB	-2.92	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	606	HEA	CHB-C1B	2.92	1.45	1.39
18	A	606	HEA	CHC-C1C	2.87	1.45	1.39
26	D	208	DMU	O5-C4	2.85	1.51	1.44
18	A	607	HEA	C11-C3B	-2.85	1.47	1.51
18	A	607	HEA	C4A-NA	-2.85	1.34	1.39
18	A	607	HEA	C4D-ND	-2.83	1.33	1.38
18	N	605	HEA	C4D-ND	-2.82	1.33	1.38
18	A	607	HEA	C1B-NB	-2.78	1.33	1.38
18	N	606	HEA	CHA-C4D	2.78	1.45	1.39
18	A	607	HEA	CHC-C1C	2.67	1.45	1.39
18	N	605	HEA	C1C-NC	-2.64	1.34	1.39
18	N	605	HEA	C1B-C2B	2.64	1.49	1.44
26	C	311	DMU	C3-C4	2.63	1.60	1.52
18	N	605	HEA	CHC-C1C	2.62	1.45	1.39
18	N	605	HEA	CHB-C1B	2.59	1.45	1.39
18	A	606	HEA	C1A-C2A	2.59	1.49	1.45
18	A	606	HEA	C1C-NC	-2.58	1.34	1.39
18	A	606	HEA	C11-C3B	-2.56	1.48	1.51
18	N	606	HEA	C4C-NC	-2.55	1.34	1.39
18	N	605	HEA	C11-C3B	-2.54	1.48	1.51
18	A	606	HEA	CHB-C1B	2.54	1.45	1.39
18	A	606	HEA	C4D-ND	-2.53	1.33	1.38
26	G	101	DMU	C6-C1	2.52	1.59	1.52
18	N	606	HEA	C1A-C2A	2.51	1.49	1.45
18	N	605	HEA	C1D-ND	-2.49	1.35	1.40
18	A	607	HEA	C1A-NA	-2.45	1.35	1.39
18	N	606	HEA	C11-C3B	-2.39	1.48	1.51
18	N	605	HEA	C4B-C3B	2.38	1.48	1.44
26	C	311	DMU	C2-C3	2.31	1.58	1.52
18	N	605	HEA	C1C-C2C	2.31	1.48	1.43
26	C	311	DMU	C10-C5	2.30	1.59	1.52
26	C	312	DMU	O1-C10	2.23	1.47	1.41
18	A	607	HEA	C1C-C2C	2.21	1.48	1.43
18	N	606	HEA	C3C-C4C	2.20	1.49	1.42
26	C	311	DMU	O5-C4	2.19	1.49	1.44
18	A	606	HEA	C4B-C3B	2.16	1.48	1.44
26	P	303	DMU	C2-C1	2.15	1.57	1.52
24	J	101	CHD	O26-C24	-2.14	1.23	1.30
18	N	605	HEA	C3C-C4C	2.13	1.48	1.42
26	C	312	DMU	O49-C1	2.10	1.48	1.43
26	C	311	DMU	O1-C10	2.08	1.47	1.41
26	P	303	DMU	C11-C9	2.06	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	606	HEA	C1C-NC	-2.04	1.35	1.39
26	G	101	DMU	O1-C9	2.04	1.49	1.44
26	D	208	DMU	O1-C10	2.03	1.47	1.41
18	N	606	HEA	C4B-NB	-2.02	1.36	1.40
18	A	606	HEA	C1B-C2B	2.02	1.48	1.44
18	N	605	HEA	C4C-NC	-2.02	1.35	1.39
18	N	605	HEA	C1A-C2A	2.02	1.48	1.45

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	208	DMU	C18-O16-C6	15.37	139.93	113.68
18	N	606	HEA	C3A-C2A-C1A	-8.47	99.03	107.05
18	N	605	HEA	C2A-C1A-NA	6.96	117.03	110.32
18	N	605	HEA	C3A-C2A-C1A	-6.92	100.50	107.05
18	N	606	HEA	C2A-C1A-NA	6.90	116.98	110.32
18	A	607	HEA	C3A-C2A-C1A	-6.36	101.03	107.05
18	N	605	HEA	C3B-C4B-NB	6.27	117.05	109.84
18	A	606	HEA	C3A-C2A-C1A	-6.09	101.28	107.05
18	N	606	HEA	C3D-C4D-ND	6.01	116.16	110.35
18	N	606	HEA	C1D-C2D-C3D	-5.99	100.68	106.98
18	A	606	HEA	C3C-C2C-C1C	-5.86	100.26	107.17
18	N	606	HEA	C2D-C1D-ND	5.75	116.45	109.84
18	N	606	HEA	C3C-C2C-C1C	-5.73	100.42	107.17
26	G	101	DMU	O5-C4-C57	5.72	120.62	106.44
18	A	606	HEA	C2B-C1B-NB	5.66	116.44	109.90
18	A	607	HEA	C2B-C1B-NB	5.62	116.40	109.90
18	A	607	HEA	C3C-C4C-NC	5.56	114.48	109.80
18	A	607	HEA	C2D-C1D-ND	5.56	116.23	109.84
18	N	605	HEA	C3C-C4C-NC	5.46	114.39	109.80
18	A	607	HEA	C2A-C1A-NA	5.35	115.48	110.32
18	N	605	HEA	C2B-C1B-NB	5.33	116.06	109.90
18	A	606	HEA	C2A-C1A-NA	5.32	115.45	110.32
26	D	208	DMU	O5-C6-O16	5.31	122.59	110.04
18	A	606	HEA	C3B-C4B-NB	5.25	115.87	109.84
18	A	607	HEA	C3D-C4D-ND	5.16	115.34	110.35
26	C	311	DMU	C18-O16-C6	5.14	122.46	113.68
18	N	605	HEA	C3D-C4D-ND	5.10	115.28	110.35
18	A	607	HEA	C3B-C4B-NB	5.04	115.63	109.84
18	N	606	HEA	C3C-C4C-NC	4.95	113.97	109.80
18	N	606	HEA	C3B-C4B-NB	4.84	115.40	109.84
18	A	607	HEA	C1D-C2D-C3D	-4.78	101.95	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	606	HEA	C3D-C4D-ND	4.77	114.96	110.35
18	N	606	HEA	C2B-C1B-NB	4.74	115.38	109.90
18	A	606	HEA	CMB-C2B-C1B	4.62	132.26	125.03
18	A	607	HEA	C3C-C2C-C1C	-4.62	101.73	107.17
18	N	606	HEA	C17-C18-C19	-4.48	117.37	127.62
18	N	605	HEA	C3C-C2C-C1C	-4.46	101.92	107.17
18	N	605	HEA	C2D-C1D-ND	4.44	114.95	109.84
26	G	101	DMU	C6-O5-C4	4.42	122.36	113.72
18	A	606	HEA	C3C-C4C-NC	4.42	113.52	109.80
18	A	606	HEA	C1D-C2D-C3D	-4.41	102.34	106.98
26	G	101	DMU	C2-C3-C4	-4.38	101.22	110.93
18	A	606	HEA	C2D-C1D-ND	4.22	114.69	109.84
18	A	606	HEA	C2C-C1C-NC	4.21	116.89	110.14
18	N	605	HEA	C1D-C2D-C3D	-4.09	102.68	106.98
18	N	606	HEA	C2C-C1C-NC	4.04	116.62	110.14
26	G	101	DMU	C18-O16-C6	4.01	120.53	113.68
26	P	303	DMU	C18-O16-C6	4.00	120.51	113.68
26	C	311	DMU	C10-O7-C3	3.96	127.36	117.98
18	N	605	HEA	C2C-C1C-NC	3.90	116.39	110.14
18	N	606	HEA	C4B-C3B-C2B	-3.90	100.89	107.44
26	C	311	DMU	C1-C2-C3	3.90	118.52	109.68
18	A	607	HEA	OMA-CMA-C3A	-3.86	116.91	125.62
26	P	303	DMU	O7-C10-O1	3.82	120.75	110.69
26	G	101	DMU	C10-O1-C9	3.81	121.16	113.72
18	N	605	HEA	C4B-C3B-C2B	-3.78	101.09	107.44
26	G	101	DMU	O7-C10-O1	3.78	120.63	110.69
18	A	607	HEA	CHB-C1B-C2B	-3.76	119.09	125.03
18	A	606	HEA	CAD-CBD-CGD	-3.70	103.84	113.67
26	C	312	DMU	O1-C9-C11	3.69	115.59	106.44
18	N	605	HEA	CAA-C2A-C1A	3.68	132.32	124.85
18	A	606	HEA	C1B-C2B-C3B	-3.65	102.56	106.80
18	N	606	HEA	OMA-CMA-C3A	-3.52	117.68	125.62
18	A	607	HEA	C4B-C3B-C2B	-3.50	101.56	107.44
18	A	607	HEA	CAA-CBA-CGA	-3.48	104.45	113.67
18	A	606	HEA	C4B-C3B-C2B	-3.41	101.70	107.44
26	P	303	DMU	C10-O1-C9	3.41	120.38	113.72
26	G	101	DMU	O7-C3-C4	3.38	118.36	109.48
18	N	606	HEA	C26-C15-C16	3.36	121.06	115.23
18	N	605	HEA	CHA-C4D-C3D	-3.33	119.92	124.77
26	C	311	DMU	O5-C6-O16	3.32	117.89	110.04
18	N	606	HEA	CAA-C2A-C1A	3.29	131.55	124.85
18	A	606	HEA	CHA-C4D-C3D	-3.28	120.00	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	604	TGL	OG2-CB1-CB2	3.27	118.55	111.48
18	N	606	HEA	C27-C19-C20	3.26	120.89	115.23
26	G	101	DMU	O7-C3-C2	3.23	115.43	107.23
18	N	605	HEA	C1B-C2B-C3B	-3.22	103.06	106.80
26	C	311	DMU	O5-C4-C3	3.22	116.38	109.72
18	A	607	HEA	C2C-C1C-NC	3.12	115.14	110.14
18	A	607	HEA	C4C-C3C-C2C	-3.08	103.48	107.30
18	A	607	HEA	CHA-C4D-C3D	-3.05	120.33	124.77
24	T	105	CHD	C14-C8-C7	3.05	115.89	111.85
18	N	606	HEA	CMC-C2C-C1C	3.04	130.04	125.42
18	N	605	HEA	CHB-C1B-C2B	-3.03	120.24	125.03
18	A	606	HEA	C4A-C3A-C2A	-3.03	104.19	106.81
18	N	605	HEA	C27-C19-C20	3.03	120.49	115.23
18	A	606	HEA	C13-C12-C11	-3.00	109.60	114.39
18	A	607	HEA	C13-C12-C11	-2.99	109.61	114.39
18	A	607	HEA	C1B-C2B-C3B	-2.96	103.37	106.80
26	P	303	DMU	C7-C8-C9	2.94	115.56	110.23
26	Q	206	DMU	C18-O16-C6	2.93	118.68	113.68
18	N	605	HEA	CHA-C1A-NA	-2.92	121.27	124.45
29	V	101	SAC	O-C-CA	-2.92	117.26	124.77
18	A	606	HEA	CAA-C2A-C1A	2.91	130.77	124.85
18	N	606	HEA	CHA-C4D-C3D	-2.90	120.55	124.77
18	N	605	HEA	OMA-CMA-C3A	-2.90	119.09	125.62
29	I	101	SAC	O-C-CA	-2.89	117.34	124.77
24	Y	102	CHD	C5-C6-C7	-2.87	110.98	114.40
25	P	308	CDL	OB6-CB5-C51	2.86	117.67	111.48
18	A	607	HEA	CMB-C2B-C1B	2.84	129.47	125.03
26	C	311	DMU	O7-C10-O1	2.84	118.17	110.69
18	A	607	HEA	C4D-C3D-C2D	-2.83	102.77	106.89
18	N	606	HEA	C16-C15-C14	-2.82	114.84	121.17
26	D	208	DMU	O1-C9-C11	2.80	113.39	106.44
18	A	606	HEA	CHB-C1B-C2B	-2.80	120.60	125.03
18	N	605	HEA	C4D-C3D-C2D	-2.76	102.88	106.89
18	N	605	HEA	C20-C19-C18	-2.74	115.02	121.17
18	N	606	HEA	CHD-C1D-C2D	-2.73	119.18	126.95
18	N	606	HEA	C13-C12-C11	-2.73	110.03	114.39
26	D	208	DMU	O16-C6-C1	-2.73	104.13	108.27
18	N	605	HEA	CAD-CBD-CGD	-2.72	106.45	113.67
18	N	606	HEA	C12-C13-C14	-2.71	105.05	112.16
18	N	605	HEA	C4C-C3C-C2C	-2.69	103.95	107.30
18	N	605	HEA	CMB-C2B-C1B	2.65	129.18	125.03
24	Y	102	CHD	C13-C14-C8	2.65	118.07	114.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	208	DMU	C22-C19-C18	-2.65	101.96	113.47
18	N	605	HEA	CHC-C1C-C2C	-2.64	119.77	127.43
18	A	606	HEA	CMB-C2B-C3B	-2.64	125.18	130.28
18	N	606	HEA	CHB-C1B-C2B	-2.63	120.88	125.03
18	A	607	HEA	C27-C19-C20	2.60	119.73	115.23
18	A	606	HEA	CHC-C4B-C3B	-2.59	119.27	125.80
18	N	605	HEA	CHC-C4B-C3B	-2.57	119.31	125.80
26	P	303	DMU	O1-C9-C11	2.57	112.82	106.44
18	A	606	HEA	OMA-CMA-C3A	-2.57	119.82	125.62
25	T	103	CDL	OB6-CB5-C51	2.57	117.03	111.48
18	A	607	HEA	CHD-C1D-C2D	-2.57	119.66	126.95
24	T	105	CHD	C5-C6-C7	-2.56	111.36	114.40
26	D	208	DMU	O5-C4-C57	2.56	112.77	106.44
26	G	101	DMU	O5-C6-O16	2.55	116.06	110.04
22	Y	101	TGL	OG2-CB1-CB2	2.52	116.94	111.48
18	N	606	HEA	CHA-C1A-NA	-2.52	121.71	124.45
24	T	105	CHD	C9-C11-C12	2.52	117.59	114.29
26	P	303	DMU	O7-C3-C2	2.51	113.60	107.23
18	A	606	HEA	CHC-C1C-C2C	-2.50	120.16	127.43
24	Y	102	CHD	C14-C8-C9	2.50	113.24	109.75
26	C	311	DMU	O5-C6-C1	-2.50	105.23	110.37
18	A	606	HEA	CMD-C2D-C1D	2.49	128.93	125.03
18	A	606	HEA	C4D-C3D-C2D	-2.49	103.27	106.89
26	C	312	DMU	C6-C1-C2	2.49	115.24	110.01
18	N	605	HEA	O11-C11-C3B	-2.46	106.75	111.26
18	N	606	HEA	CHC-C1C-C2C	-2.45	120.31	127.43
18	N	606	HEA	C21-C22-C23	-2.43	119.53	127.64
24	Y	102	CHD	C17-C13-C14	-2.41	97.69	100.11
26	P	303	DMU	C1-C2-C3	2.40	115.13	109.68
18	N	605	HEA	CHD-C1D-C2D	-2.39	120.17	126.95
26	C	312	DMU	O4-C7-C5	-2.38	104.77	110.38
18	N	606	HEA	C4D-C3D-C2D	-2.37	103.44	106.89
26	D	208	DMU	C6-O5-C4	-2.37	109.09	113.72
18	N	606	HEA	CMD-C2D-C3D	2.35	132.52	126.15
26	G	101	DMU	O5-C4-C3	-2.35	104.86	109.72
18	A	606	HEA	O11-C11-C3B	-2.35	106.95	111.26
18	A	606	HEA	CAA-CBA-CGA	-2.34	107.45	113.67
27	C	313	PEK	O01-C1-C2	2.34	116.55	111.48
18	N	605	HEA	C4A-C3A-C2A	-2.34	104.78	106.81
18	N	605	HEA	C13-C12-C11	-2.32	110.69	114.39
26	Q	206	DMU	O49-C1-C2	-2.31	104.92	110.38
26	P	303	DMU	O1-C10-C5	-2.31	105.62	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	312	DMU	C28-C25-C22	-2.30	102.72	114.37
24	P	309	CHD	C10-C9-C8	2.29	114.39	111.84
18	A	607	HEA	CHA-C1A-C2A	-2.28	121.26	124.86
26	C	312	DMU	C1-C2-C3	2.27	114.83	109.68
18	N	606	HEA	CHA-C1A-C2A	-2.27	121.29	124.86
26	C	311	DMU	C25-C22-C19	-2.26	102.93	114.37
18	A	606	HEA	CMC-C2C-C1C	2.25	128.84	125.42
18	N	605	HEA	CAD-C3D-C2D	2.24	132.07	127.87
24	Y	102	CHD	C13-C17-C20	2.24	122.19	119.48
18	A	607	HEA	O11-C11-C3B	-2.23	107.18	111.26
26	C	311	DMU	O16-C6-C1	2.23	111.65	108.27
18	A	607	HEA	C4A-C3A-C2A	-2.22	104.89	106.81
26	Q	206	DMU	C10-O1-C9	2.21	118.04	113.72
24	T	101	CHD	C18-C13-C14	2.21	114.67	111.20
26	Q	206	DMU	O16-C6-C1	2.20	111.62	108.27
18	A	607	HEA	CHC-C1C-C2C	-2.18	121.10	127.43
26	Q	206	DMU	O7-C10-C5	2.18	113.45	108.09
18	A	606	HEA	CHB-C4A-NA	-2.17	122.09	124.45
18	A	607	HEA	CHC-C4B-NB	-2.16	121.69	124.37
18	N	606	HEA	CAA-CBA-CGA	-2.15	107.97	113.67
18	N	606	HEA	C21-C20-C19	-2.14	106.09	113.19
27	T	102	PEK	O13-P-O14	2.14	122.39	112.44
24	Y	102	CHD	C17-C13-C12	2.13	119.58	117.67
26	C	312	DMU	C22-C19-C18	-2.12	104.25	113.47
26	Q	206	DMU	O5-C6-O16	-2.12	105.05	110.04
17	C	303	PGV	O01-C1-C2	2.11	116.04	111.48
24	T	101	CHD	C4-C3-C2	2.10	113.18	110.62
18	N	605	HEA	C4B-NB-C1B	-2.10	102.72	105.21
26	D	208	DMU	C25-C22-C19	-2.09	103.79	114.37
18	N	605	HEA	CMC-C2C-C1C	2.09	128.61	125.42
18	A	607	HEA	CMC-C2C-C3C	2.09	131.46	126.55
18	A	607	HEA	C16-C15-C14	-2.09	116.48	121.17
18	A	607	HEA	C17-C18-C19	-2.08	122.86	127.62
24	C	305	CHD	C4-C5-C10	2.08	114.87	112.66
24	J	101	CHD	C5-C4-C3	2.08	115.84	112.71
18	N	605	HEA	C12-C11-C3B	2.08	115.37	112.12
24	C	301	CHD	O25-C24-C23	-2.05	116.58	123.09
22	B	302	TGL	OG2-CB1-CB2	2.05	115.92	111.48
18	N	605	HEA	O2D-CGD-CBD	2.05	120.48	114.00
24	T	105	CHD	C10-C9-C8	2.05	114.12	111.84
24	Y	102	CHD	C16-C17-C13	-2.04	101.57	103.54
18	N	605	HEA	CHA-C1A-C2A	-2.01	121.70	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	303	DMU	O2-C8-C7	-2.01	105.65	110.38
17	P	302	PGV	O01-C1-C2	2.00	115.81	111.48

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	R	201	PSC	C02

All (973) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	A	604	PGV	C03-O11-P-O12
17	A	604	PGV	C03-O11-P-O13
17	A	604	PGV	C04-O12-P-O11
17	A	604	PGV	C04-O12-P-O14
17	A	604	PGV	O12-C04-C05-O05
17	C	303	PGV	C03-O11-P-O12
17	C	303	PGV	C03-O11-P-O14
17	C	303	PGV	O01-C02-C03-O11
17	C	303	PGV	O12-C04-C05-C06
17	C	303	PGV	C04-C05-C06-O06
17	N	617	PGV	C03-O11-P-O14
17	N	617	PGV	O02-C1-O01-C02
17	N	617	PGV	C2-C1-O01-C02
17	P	307	PGV	C03-O11-P-O12
17	P	307	PGV	C03-O11-P-O13
17	P	307	PGV	C04-C05-C06-O06
18	A	606	HEA	C2A-C3A-CMA-OMA
18	A	607	HEA	C2A-C3A-CMA-OMA
18	A	607	HEA	C19-C20-C21-C22
18	N	605	HEA	C2D-C3D-CAD-CBD
18	N	606	HEA	C2A-C3A-CMA-OMA
22	D	201	TGL	CB2-CB1-OG2-CG2
22	L	101	TGL	CB2-CB1-OG2-CG2
22	Q	201	TGL	OG2-CG2-CG3-OG3
22	Y	101	TGL	CB2-CB1-OG2-CG2
22	Y	101	TGL	OB1-CB1-OG2-CG2
23	B	303	PSC	C03-O11-P-O14
23	B	303	PSC	C04-O12-P-O11
23	B	303	PSC	C04-O12-P-O13
23	R	201	PSC	C03-O11-P-O12
23	R	201	PSC	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
23	R	201	PSC	C04-O12-P-O11
23	R	201	PSC	C04-O12-P-O14
23	R	201	PSC	O12-C04-C05-N
23	R	201	PSC	C2-C1-O01-C02
25	C	304	CDL	C1-CA2-OA2-PA1
25	C	304	CDL	CA3-OA5-PA1-OA2
25	C	304	CDL	CA3-OA5-PA1-OA3
25	C	304	CDL	OA7-CA5-OA6-CA4
25	C	304	CDL	C11-CA5-OA6-CA4
25	C	310	CDL	CA2-C1-CB2-OB2
25	C	310	CDL	CA2-OA2-PA1-OA3
25	C	310	CDL	CA2-OA2-PA1-OA5
25	C	310	CDL	C11-CA5-OA6-CA4
25	C	310	CDL	CB3-OB5-PB2-OB2
25	P	308	CDL	C1-CA2-OA2-PA1
25	P	308	CDL	CA2-OA2-PA1-OA3
25	P	308	CDL	CA3-OA5-PA1-OA2
25	P	308	CDL	CA3-OA5-PA1-OA3
25	P	308	CDL	CA3-OA5-PA1-OA4
25	P	308	CDL	CB2-OB2-PB2-OB3
25	P	308	CDL	CB2-OB2-PB2-OB5
25	T	103	CDL	O1-C1-CA2-OA2
25	T	103	CDL	CB2-OB2-PB2-OB3
25	T	103	CDL	CB2-OB2-PB2-OB4
25	T	103	CDL	CB2-OB2-PB2-OB5
26	C	311	DMU	C1-C6-O16-C18
26	C	311	DMU	O5-C6-O16-C18
26	D	208	DMU	C19-C18-O16-C6
27	C	313	PEK	C03-O11-P-O12
27	C	313	PEK	O12-C04-C05-N
27	G	102	PEK	C6-C7-C8-C9
27	G	102	PEK	C12-C13-C14-C15
27	G	103	PEK	C03-O11-P-O12
27	G	103	PEK	O02-C1-O01-C02
27	G	103	PEK	C11-C10-C9-C8
27	P	301	PEK	C04-O12-P-O13
27	P	301	PEK	O12-C04-C05-N
27	P	301	PEK	C11-C12-C13-C14
27	P	305	PEK	C04-O12-P-O14
27	P	305	PEK	O12-C04-C05-N
27	P	305	PEK	O02-C1-O01-C02
27	T	102	PEK	O12-C04-C05-N

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Mol	Chain	Res	Type	Atoms
27	T	102	PEK	C9-C10-C11-C12
29	I	101	SAC	C2A-C1A-N-CA
29	I	101	SAC	N-CA-CB-OG
29	I	101	SAC	C-CA-CB-OG
29	V	101	SAC	C2A-C1A-N-CA
29	V	101	SAC	C-CA-N-C1A
29	V	101	SAC	O-C-CA-CB
29	V	101	SAC	C-CA-CB-OG
17	N	617	PGV	O04-C19-O03-C01
22	Q	201	TGL	OC1-CC1-OG3-CG3
23	B	303	PSC	O04-C19-O03-C01
26	P	303	DMU	O1-C10-O7-C3
22	Q	201	TGL	CC2-CC1-OG3-CG3
23	B	303	PSC	C20-C19-O03-C01
26	C	311	DMU	O1-C10-O7-C3
25	T	103	CDL	OA9-CA7-OA8-CA6
27	G	103	PEK	O04-C21-O03-C01
17	A	604	PGV	O02-C1-O01-C02
22	D	201	TGL	OB1-CB1-OG2-CG2
22	L	101	TGL	OB1-CB1-OG2-CG2
23	R	201	PSC	O02-C1-O01-C02
25	C	310	CDL	OA7-CA5-OA6-CA4
29	V	101	SAC	OAC-C1A-N-CA
17	N	617	PGV	C20-C19-O03-C01
25	P	308	CDL	C31-CA7-OA8-CA6
25	T	103	CDL	C31-CA7-OA8-CA6
27	G	103	PEK	C22-C21-O03-C01
17	A	604	PGV	C2-C1-O01-C02
27	G	103	PEK	C2-C1-O01-C02
27	P	305	PEK	C2-C1-O01-C02
22	D	201	TGL	OC1-CC1-OG3-CG3
18	A	607	HEA	C26-C15-C16-C17
18	A	607	HEA	C14-C15-C16-C17
17	P	307	PGV	C20-C19-O03-C01
22	D	201	TGL	CC2-CC1-OG3-CG3
25	C	310	CDL	OA9-CA7-OA8-CA6
25	P	308	CDL	OA9-CA7-OA8-CA6
27	P	305	PEK	O04-C21-O03-C01
18	N	605	HEA	C4D-C3D-CAD-CBD
29	I	101	SAC	OAC-C1A-N-CA
25	P	308	CDL	O1-C1-CB2-OB2
17	A	604	PGV	C20-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
26	D	208	DMU	O6-C11-C9-O1
25	P	308	CDL	C51-CB5-OB6-CB4
26	C	311	DMU	O5-C4-C57-O61
26	G	101	DMU	O6-C11-C9-O1
25	C	310	CDL	C31-CA7-OA8-CA6
27	P	305	PEK	C22-C21-O03-C01
17	P	307	PGV	O04-C19-O03-C01
26	D	208	DMU	O6-C11-C9-C8
17	A	604	PGV	C05-C04-O12-P
26	C	312	DMU	O5-C6-O16-C18
26	Q	206	DMU	O5-C6-O16-C18
17	C	303	PGV	C20-C19-O03-C01
22	Y	101	TGL	CA2-CA1-OG1-CG1
23	B	303	PSC	C19-C20-C21-C22
24	Y	102	CHD	C17-C20-C22-C23
17	N	617	PGV	C1-C2-C3-C4
17	A	604	PGV	C23-C24-C25-C26
24	Y	102	CHD	C21-C20-C22-C23
17	A	604	PGV	O04-C19-O03-C01
22	Y	101	TGL	OA1-CA1-OG1-CG1
27	P	301	PEK	O04-C21-O03-C01
25	P	308	CDL	OB7-CB5-OB6-CB4
17	A	604	PGV	O12-C04-C05-C06
25	P	308	CDL	CA2-C1-CB2-OB2
25	C	310	CDL	C71-CB7-OB8-CB6
27	P	301	PEK	C22-C21-O03-C01
26	P	303	DMU	O6-C11-C9-C8
22	Y	101	TGL	C11-C12-C13-C14
24	T	105	CHD	C17-C20-C22-C23
22	N	604	TGL	C21-C22-C23-C24
18	N	606	HEA	C26-C15-C16-C17
18	N	606	HEA	C14-C15-C16-C17
26	C	312	DMU	C1-C6-O16-C18
26	Q	206	DMU	C1-C6-O16-C18
17	C	303	PGV	O12-C04-C05-O05
25	C	310	CDL	O1-C1-CB2-OB2
22	L	101	TGL	CA3-CA4-CA5-CA6
26	C	311	DMU	C3-C4-C57-O61
26	G	101	DMU	O5-C4-C57-O61
25	T	103	CDL	OB6-CB4-CB6-OB8
26	C	312	DMU	O5-C4-C57-O61
17	C	303	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
22	N	604	TGL	CC1-CC2-CC3-CC4
27	P	301	PEK	C25-C26-C27-C28
22	D	201	TGL	C14-C29-C30-C31
17	A	604	PGV	C1-C2-C3-C4
22	Y	101	TGL	CA1-CA2-CA3-CA4
27	C	313	PEK	C1-C2-C3-C4
24	W	302	CHD	C20-C22-C23-C24
24	T	105	CHD	C21-C20-C22-C23
17	C	303	PGV	C19-C20-C21-C22
25	C	310	CDL	CB5-C51-C52-C53
25	T	103	CDL	CB7-C71-C72-C73
27	T	102	PEK	C1-C2-C3-C4
25	C	310	CDL	OB9-CB7-OB8-CB6
26	D	208	DMU	O5-C6-O16-C18
17	C	303	PGV	C13-C14-C15-C16
17	N	617	PGV	C25-C26-C27-C28
22	Y	101	TGL	CC9-C15-C16-C17
17	P	307	PGV	O12-C04-C05-O05
25	C	304	CDL	O1-C1-CA2-OA2
27	G	103	PEK	C1-C2-C3-C4
17	C	302	PGV	C12-C13-C14-C15
27	P	301	PEK	C13-C14-C15-C16
22	D	201	TGL	CC1-CC2-CC3-CC4
25	P	308	CDL	CA7-C31-C32-C33
23	B	303	PSC	C21-C22-C23-C24
25	C	304	CDL	CB7-C71-C72-C73
27	G	102	PEK	C1-C2-C3-C4
17	A	604	PGV	C21-C22-C23-C24
22	Y	101	TGL	CC6-CC7-CC8-CC9
22	B	302	TGL	CC1-CC2-CC3-CC4
22	N	604	TGL	CB1-CB2-CB3-CB4
27	C	313	PEK	O02-C1-O01-C02
17	P	307	PGV	O12-C04-C05-C06
25	C	304	CDL	CB2-C1-CA2-OA2
25	T	103	CDL	CB2-C1-CA2-OA2
18	N	606	HEA	C27-C19-C20-C21
27	C	313	PEK	C2-C1-O01-C02
17	C	303	PGV	C10-C11-C12-C13
25	P	308	CDL	O1-C1-CA2-OA2
24	Y	102	CHD	C20-C22-C23-C24
25	C	310	CDL	CB7-C71-C72-C73
24	T	105	CHD	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
17	P	302	PGV	C5-C6-C7-C8
17	P	302	PGV	C30-C31-C32-C33
22	L	101	TGL	CB6-CB7-CB8-CB9
22	Q	201	TGL	C21-C20-CA9-CA8
25	C	304	CDL	C37-C38-C39-C40
25	C	310	CDL	C15-C16-C17-C18
26	Q	206	DMU	O16-C18-C19-C22
22	B	302	TGL	CA3-CA4-CA5-CA6
22	N	604	TGL	C11-C12-C13-C14
27	G	102	PEK	C27-C28-C29-C30
27	T	102	PEK	C33-C34-C35-C36
17	A	604	PGV	C4-C5-C6-C7
17	C	303	PGV	C28-C29-C30-C31
22	N	604	TGL	CB9-C10-C11-C12
22	Y	101	TGL	CC2-CC3-CC4-CC5
22	Y	101	TGL	C23-C24-C25-C26
25	C	310	CDL	C57-C58-C59-C60
22	D	201	TGL	CC5-CC6-CC7-CC8
22	L	101	TGL	C12-C13-C14-C29
22	Q	201	TGL	CA5-CA6-CA7-CA8
22	Q	201	TGL	C20-C21-C22-C23
22	Y	101	TGL	CB6-CB7-CB8-CB9
25	C	304	CDL	C62-C63-C64-C65
25	T	103	CDL	C81-C82-C83-C84
17	C	303	PGV	O05-C05-C06-O06
17	P	307	PGV	O05-C05-C06-O06
22	B	302	TGL	CA6-CA7-CA8-CA9
22	L	101	TGL	C16-C17-C18-C19
25	P	308	CDL	C36-C37-C38-C39
17	P	307	PGV	C3-C4-C5-C6
22	B	302	TGL	CC3-CC4-CC5-CC6
25	C	304	CDL	C19-C20-C21-C22
17	C	303	PGV	C6-C7-C8-C9
25	C	304	CDL	C17-C18-C19-C20
25	T	103	CDL	C15-C16-C17-C18
23	B	303	PSC	C2-C1-O01-C02
27	P	301	PEK	C2-C1-O01-C02
27	C	313	PEK	C30-C31-C32-C33
27	C	313	PEK	C29-C30-C31-C32
27	P	301	PEK	C28-C29-C30-C31
27	P	305	PEK	C28-C29-C30-C31
22	Q	201	TGL	CC1-CC2-CC3-CC4

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Mol	Chain	Res	Type	Atoms
23	R	201	PSC	C28-C29-C30-C31
25	C	304	CDL	C13-C14-C15-C16
25	P	308	CDL	C20-C21-C22-C23
25	T	103	CDL	C33-C34-C35-C36
27	G	102	PEK	C28-C29-C30-C31
25	P	308	CDL	C13-C14-C15-C16
26	G	101	DMU	C31-C34-C37-C40
29	V	101	SAC	N-CA-CB-OG
26	P	303	DMU	O6-C11-C9-O1
17	A	604	PGV	C02-C01-O03-C19
26	C	312	DMU	C25-C28-C31-C34
17	A	604	PGV	C20-C21-C22-C23
22	B	302	TGL	CA9-C20-C21-C22
25	P	308	CDL	CB2-C1-CA2-OA2
22	Y	101	TGL	CC2-CC1-OG3-CG3
26	C	312	DMU	C3-C4-C57-O61
17	C	303	PGV	C4-C5-C6-C7
22	D	201	TGL	C17-C18-C19-C33
23	B	303	PSC	C25-C26-C27-C28
25	C	304	CDL	C31-C32-C33-C34
26	D	208	DMU	C25-C28-C31-C34
23	R	201	PSC	C20-C21-C22-C23
25	C	310	CDL	C75-C76-C77-C78
25	P	308	CDL	C58-C59-C60-C61
27	P	305	PEK	C27-C28-C29-C30
17	P	302	PGV	C6-C7-C8-C9
22	D	201	TGL	CC7-CC8-CC9-C15
25	C	304	CDL	C59-C60-C61-C62
25	P	308	CDL	C81-C82-C83-C84
25	T	103	CDL	C17-C18-C19-C20
19	A	614	EDO	O1-C1-C2-O2
19	B	305	EDO	O1-C1-C2-O2
19	C	307	EDO	O1-C1-C2-O2
19	C	308	EDO	O1-C1-C2-O2
19	E	204	EDO	O1-C1-C2-O2
19	G	105	EDO	O1-C1-C2-O2
19	J	102	EDO	O1-C1-C2-O2
19	J	104	EDO	O1-C1-C2-O2
19	Q	202	EDO	O1-C1-C2-O2
19	Q	204	EDO	O1-C1-C2-O2
19	Q	205	EDO	O1-C1-C2-O2
19	R	203	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
22	D	201	TGL	CA6-CA7-CA8-CA9
25	P	308	CDL	C59-C60-C61-C62
25	P	308	CDL	C82-C83-C84-C85
27	C	313	PEK	C28-C29-C30-C31
27	C	313	PEK	C34-C35-C36-C37
17	C	302	PGV	C1-C2-C3-C4
22	B	302	TGL	C18-C19-C33-C34
25	C	310	CDL	C81-C82-C83-C84
26	Q	206	DMU	C28-C31-C34-C37
17	C	303	PGV	C2-C1-O01-C02
22	B	302	TGL	C21-C22-C23-C24
25	T	103	CDL	C78-C79-C80-C81
25	T	103	CDL	C35-C36-C37-C38
27	G	103	PEK	C16-C17-C18-C19
17	A	605	PGV	C19-C20-C21-C22
22	D	201	TGL	CB4-CB5-CB6-CB7
22	N	604	TGL	CA4-CA5-CA6-CA7
22	Q	201	TGL	CC5-CC6-CC7-CC8
25	C	310	CDL	C33-C34-C35-C36
27	P	301	PEK	O02-C1-O01-C02
22	B	302	TGL	CC4-CC5-CC6-CC7
25	T	103	CDL	C51-C52-C53-C54
26	D	208	DMU	C22-C25-C28-C31
26	D	208	DMU	C31-C34-C37-C40
18	N	606	HEA	C18-C19-C20-C21
24	T	105	CHD	C13-C17-C20-C21
22	N	604	TGL	CC5-CC6-CC7-CC8
25	C	304	CDL	C18-C19-C20-C21
22	B	302	TGL	CC2-CC1-OG3-CG3
17	A	605	PGV	C5-C6-C7-C8
22	Y	101	TGL	C16-C17-C18-C19
25	C	304	CDL	C81-C82-C83-C84
27	G	103	PEK	C31-C32-C33-C34
17	A	605	PGV	C7-C8-C9-C10
17	P	306	PGV	C6-C7-C8-C9
25	C	310	CDL	C40-C41-C42-C43
25	P	308	CDL	C17-C18-C19-C20
22	Y	101	TGL	OC1-CC1-OG3-CG3
22	L	101	TGL	CC2-CC3-CC4-CC5
22	Y	101	TGL	CA6-CA7-CA8-CA9
26	C	312	DMU	C22-C25-C28-C31
22	D	201	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	N	604	TGL	C16-C15-CC9-CC8
22	Y	101	TGL	CA3-CA4-CA5-CA6
17	P	307	PGV	C14-C15-C16-C17
22	D	201	TGL	CA9-C20-C21-C22
22	B	302	TGL	CB2-CB1-OG2-CG2
25	C	304	CDL	C51-CB5-OB6-CB4
25	C	310	CDL	C51-CB5-OB6-CB4
25	T	103	CDL	C51-CB5-OB6-CB4
25	P	308	CDL	C22-C23-C24-C25
23	B	303	PSC	O02-C1-O01-C02
17	A	604	PGV	C22-C23-C24-C25
22	D	201	TGL	CB2-CB3-CB4-CB5
22	N	604	TGL	C14-C29-C30-C31
22	N	604	TGL	CA7-CA8-CA9-C20
25	P	308	CDL	C56-C57-C58-C59
25	T	103	CDL	C61-C62-C63-C64
22	D	201	TGL	C16-C17-C18-C19
25	C	304	CDL	C83-C84-C85-C86
25	C	310	CDL	C16-C17-C18-C19
25	C	310	CDL	C32-C33-C34-C35
17	N	617	PGV	C3-C4-C5-C6
22	N	604	TGL	CB6-CB7-CB8-CB9
25	C	310	CDL	C79-C80-C81-C82
22	B	302	TGL	CB5-CB6-CB7-CB8
25	C	304	CDL	C54-C55-C56-C57
25	P	308	CDL	C52-C53-C54-C55
26	P	303	DMU	C28-C31-C34-C37
17	P	302	PGV	C7-C8-C9-C10
25	C	304	CDL	C55-C56-C57-C58
25	T	103	CDL	C38-C39-C40-C41
25	C	304	CDL	C56-C57-C58-C59
25	C	310	CDL	C72-C73-C74-C75
22	L	101	TGL	CC9-C15-C16-C17
17	A	605	PGV	C6-C7-C8-C9
22	N	604	TGL	CB2-CB1-OG2-CG2
17	N	617	PGV	C6-C7-C8-C9
17	P	302	PGV	C23-C24-C25-C26
22	L	101	TGL	C21-C20-CA9-CA8
27	T	102	PEK	C24-C25-C26-C27
17	N	617	PGV	C19-C20-C21-C22
23	B	303	PSC	C1-C2-C3-C4
22	B	302	TGL	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
27	G	102	PEK	C15-C16-C17-C18
22	B	302	TGL	CC7-CC8-CC9-C15
25	C	304	CDL	C76-C77-C78-C79
27	G	102	PEK	C30-C31-C32-C33
25	P	308	CDL	C31-C32-C33-C34
26	Q	206	DMU	C22-C25-C28-C31
27	P	301	PEK	C14-C15-C16-C17
17	P	307	PGV	C28-C29-C30-C31
25	C	304	CDL	C22-C23-C24-C25
25	P	308	CDL	C78-C79-C80-C81
25	T	103	CDL	C58-C59-C60-C61
24	T	105	CHD	C16-C17-C20-C21
22	B	302	TGL	OB1-CB1-OG2-CG2
25	T	103	CDL	OB7-CB5-OB6-CB4
25	C	304	CDL	CA2-C1-CB2-OB2
17	A	604	PGV	C3-C4-C5-C6
22	N	604	TGL	CA6-CA7-CA8-CA9
25	T	103	CDL	C31-C32-C33-C34
27	P	301	PEK	C34-C35-C36-C37
25	C	310	CDL	C80-C81-C82-C83
27	T	102	PEK	C32-C33-C34-C35
26	C	311	DMU	O6-C11-C9-O1
17	P	306	PGV	C20-C21-C22-C23
22	N	604	TGL	CA9-C20-C21-C22
25	C	304	CDL	C61-C62-C63-C64
27	G	102	PEK	C24-C25-C26-C27
17	C	303	PGV	C7-C8-C9-C10
23	B	303	PSC	C13-C14-C15-C16
27	G	103	PEK	C2-C3-C4-C5
27	P	305	PEK	C15-C16-C17-C18
27	T	102	PEK	C15-C16-C17-C18
17	P	302	PGV	C29-C30-C31-C32
22	Q	201	TGL	CC4-CC5-CC6-CC7
26	P	303	DMU	C19-C22-C25-C28
17	C	303	PGV	C01-C02-C03-O11
25	C	304	CDL	OA5-CA3-CA4-CA6
25	T	103	CDL	OA5-CA3-CA4-CA6
27	C	313	PEK	C01-C02-C03-O11
17	C	303	PGV	O02-C1-O01-C02
25	C	304	CDL	OB7-CB5-OB6-CB4
25	C	310	CDL	OB7-CB5-OB6-CB4
26	P	303	DMU	C31-C34-C37-C40

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Mol	Chain	Res	Type	Atoms
17	P	307	PGV	C7-C8-C9-C10
17	P	307	PGV	C27-C28-C29-C30
23	R	201	PSC	C23-C24-C25-C26
25	T	103	CDL	C34-C35-C36-C37
17	P	307	PGV	C25-C26-C27-C28
22	Q	201	TGL	C19-C33-C34-C35
25	T	103	CDL	C11-CA5-OA6-CA4
17	C	302	PGV	C5-C6-C7-C8
22	N	604	TGL	CC6-CC7-CC8-CC9
22	Q	201	TGL	CA2-CA1-OG1-CG1
22	Y	101	TGL	C16-C15-CC9-CC8
22	N	604	TGL	OB1-CB1-OG2-CG2
27	T	102	PEK	C7-C8-C9-C10
17	A	604	PGV	O03-C01-C02-C03
22	B	302	TGL	OG1-CG1-CG2-CG3
22	D	201	TGL	CG1-CG2-CG3-OG3
22	L	101	TGL	CG1-CG2-CG3-OG3
22	Q	201	TGL	CG1-CG2-CG3-OG3
25	P	308	CDL	CB3-CB4-CB6-OB8
25	T	103	CDL	CB3-CB4-CB6-OB8
22	B	302	TGL	C21-C20-CA9-CA8
17	P	307	PGV	C11-C10-C9-C8
27	P	301	PEK	C15-C16-C17-C18
17	C	302	PGV	C6-C7-C8-C9
22	Y	101	TGL	C10-C11-C12-C13
27	C	313	PEK	C22-C23-C24-C25
19	A	611	EDO	O1-C1-C2-O2
19	A	612	EDO	O1-C1-C2-O2
19	B	307	EDO	O1-C1-C2-O2
19	D	206	EDO	O1-C1-C2-O2
19	F	703	EDO	O1-C1-C2-O2
19	G	107	EDO	O1-C1-C2-O2
19	K	101	EDO	O1-C1-C2-O2
19	K	102	EDO	O1-C1-C2-O2
19	O	303	EDO	O1-C1-C2-O2
19	P	313	EDO	O1-C1-C2-O2
19	Z	1601	EDO	O1-C1-C2-O2
22	D	201	TGL	CC2-CC3-CC4-CC5
27	P	301	PEK	C22-C23-C24-C25
27	P	305	PEK	C23-C24-C25-C26
22	B	302	TGL	OC1-CC1-OG3-CG3
27	P	301	PEK	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
27	P	305	PEK	C32-C33-C34-C35
17	P	307	PGV	C2-C3-C4-C5
25	C	310	CDL	C59-C60-C61-C62
17	N	617	PGV	C02-C03-O11-P
22	N	604	TGL	CB5-CB6-CB7-CB8
26	G	101	DMU	O6-C11-C9-C8
22	Q	201	TGL	C16-C17-C18-C19
25	P	308	CDL	C42-C43-C44-C45
25	T	103	CDL	C77-C78-C79-C80
22	L	101	TGL	CB7-CB8-CB9-C10
22	Y	101	TGL	CB2-CB3-CB4-CB5
25	C	304	CDL	C77-C78-C79-C80
17	N	617	PGV	C2-C3-C4-C5
17	N	617	PGV	C7-C8-C9-C10
25	T	103	CDL	C72-C73-C74-C75
25	T	103	CDL	C76-C77-C78-C79
27	C	313	PEK	C33-C34-C35-C36
23	R	201	PSC	C2-C3-C4-C5
26	D	208	DMU	C18-C19-C22-C25
22	B	302	TGL	CB4-CB5-CB6-CB7
22	N	604	TGL	CA2-CA3-CA4-CA5
25	T	103	CDL	C43-C44-C45-C46
25	P	308	CDL	C71-CB7-OB8-CB6
26	G	101	DMU	C3-C4-C57-O61
17	C	303	PGV	C2-C3-C4-C5
17	N	617	PGV	C21-C22-C23-C24
17	P	307	PGV	C5-C6-C7-C8
22	D	201	TGL	CC9-C15-C16-C17
23	B	303	PSC	C4-C5-C6-C7
25	C	310	CDL	C35-C36-C37-C38
23	R	201	PSC	C26-C27-C28-C29
17	N	617	PGV	C28-C29-C30-C31
22	D	201	TGL	C10-C11-C12-C13
22	L	101	TGL	C11-C12-C13-C14
25	T	103	CDL	C55-C56-C57-C58
27	G	103	PEK	C26-C27-C28-C29
25	C	304	CDL	C24-C25-C26-C27
25	C	310	CDL	C20-C21-C22-C23
25	C	310	CDL	C78-C79-C80-C81
25	T	103	CDL	C59-C60-C61-C62
26	C	312	DMU	C28-C31-C34-C37
22	B	302	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	L	101	TGL	CC7-CC8-CC9-C15
17	C	303	PGV	C31-C32-C33-C34
22	Y	101	TGL	CC1-CC2-CC3-CC4
22	D	201	TGL	C16-C15-CC9-CC8
22	B	302	TGL	CB3-CB4-CB5-CB6
18	N	605	HEA	C3B-C11-C12-C13
25	C	310	CDL	C60-C61-C62-C63
27	P	305	PEK	C17-C18-C19-C20
22	Y	101	TGL	CC4-CC5-CC6-CC7
25	C	310	CDL	C37-C38-C39-C40
26	D	208	DMU	C19-C22-C25-C28
27	P	305	PEK	C31-C32-C33-C34
22	L	101	TGL	C29-C30-C31-C32
25	C	304	CDL	C41-C42-C43-C44
22	D	201	TGL	CC4-CC5-CC6-CC7
27	G	102	PEK	C17-C18-C19-C20
27	P	305	PEK	C13-C14-C15-C16
17	N	617	PGV	C4-C5-C6-C7
17	N	617	PGV	C15-C16-C17-C18
17	C	302	PGV	C25-C26-C27-C28
25	T	103	CDL	C82-C83-C84-C85
25	T	103	CDL	OA7-CA5-OA6-CA4
26	P	303	DMU	C19-C18-O16-C6
26	Q	206	DMU	C19-C18-O16-C6
27	P	301	PEK	C02-C03-O11-P
22	L	101	TGL	C21-C22-C23-C24
25	C	310	CDL	C22-C23-C24-C25
25	T	103	CDL	C71-CB7-OB8-CB6
17	P	307	PGV	C26-C27-C28-C29
22	Q	201	TGL	C12-C13-C14-C29
27	P	305	PEK	C16-C17-C18-C19
25	C	310	CDL	OA5-CA3-CA4-CA6
25	P	308	CDL	OA5-CA3-CA4-CA6
22	L	101	TGL	C19-C33-C34-C35
22	Q	201	TGL	C29-C30-C31-C32
22	B	302	TGL	C33-C34-C35-C36
17	A	604	PGV	C27-C28-C29-C30
22	L	101	TGL	CA6-CA7-CA8-CA9
22	N	604	TGL	CC3-CC4-CC5-CC6
26	Q	206	DMU	C25-C28-C31-C34
22	Q	201	TGL	OA1-CA1-OG1-CG1
25	P	308	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
22	B	302	TGL	CB9-C10-C11-C12
22	B	302	TGL	C20-C21-C22-C23
25	P	308	CDL	C15-C16-C17-C18
22	Q	201	TGL	C22-C23-C24-C25
26	Q	206	DMU	C34-C37-C40-C43
25	T	103	CDL	C12-C13-C14-C15
17	C	302	PGV	C15-C16-C17-C18
22	D	201	TGL	CB1-CB2-CB3-CB4
25	P	308	CDL	C44-C45-C46-C47
25	P	308	CDL	C54-C55-C56-C57
23	B	303	PSC	O03-C01-C02-C03
25	C	310	CDL	CB3-CB4-CB6-OB8
25	C	310	CDL	C41-C42-C43-C44
17	P	307	PGV	C30-C31-C32-C33
22	Y	101	TGL	CC5-CC6-CC7-CC8
25	C	310	CDL	C39-C40-C41-C42
25	T	103	CDL	C22-C23-C24-C25
19	J	105	EDO	O1-C1-C2-O2
19	N	614	EDO	O1-C1-C2-O2
19	S	105	EDO	O1-C1-C2-O2
23	B	303	PSC	C3-C4-C5-C6
26	P	303	DMU	C25-C28-C31-C34
22	N	604	TGL	C25-C26-C27-C28
23	B	303	PSC	C15-C16-C17-C18
27	C	313	PEK	C16-C17-C18-C19
22	B	302	TGL	C23-C24-C25-C26
27	C	313	PEK	C15-C16-C17-C18
17	C	302	PGV	C02-C03-O11-P
25	C	304	CDL	CA4-CA3-OA5-PA1
25	T	103	CDL	C1-CA2-OA2-PA1
17	A	604	PGV	C25-C26-C27-C28
27	T	102	PEK	C26-C27-C28-C29
23	R	201	PSC	C14-C15-C16-C17
22	L	101	TGL	C15-C16-C17-C18
27	G	102	PEK	C34-C35-C36-C37
25	C	310	CDL	OB6-CB4-CB6-OB8
25	P	308	CDL	OB6-CB4-CB6-OB8
23	B	303	PSC	C9-C10-C11-C12
23	B	303	PSC	C10-C11-C12-C13
23	R	201	PSC	C9-C10-C11-C12
23	R	201	PSC	C10-C11-C12-C13
27	C	313	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
27	C	313	PEK	C11-C12-C13-C14
27	C	313	PEK	C12-C13-C14-C15
27	G	103	PEK	C6-C7-C8-C9
27	G	103	PEK	C12-C13-C14-C15
27	P	301	PEK	C5-C6-C7-C8
27	P	301	PEK	C6-C7-C8-C9
27	P	301	PEK	C11-C10-C9-C8
27	P	305	PEK	C5-C6-C7-C8
27	P	305	PEK	C6-C7-C8-C9
27	P	305	PEK	C11-C10-C9-C8
27	P	305	PEK	C9-C10-C11-C12
17	N	617	PGV	C26-C27-C28-C29
22	L	101	TGL	C13-C14-C29-C30
22	Q	201	TGL	CC9-C15-C16-C17
25	P	308	CDL	C61-C62-C63-C64
22	B	302	TGL	CC6-CC7-CC8-CC9
22	L	101	TGL	CB2-CB3-CB4-CB5
22	Q	201	TGL	C18-C19-C33-C34
25	C	304	CDL	C71-C72-C73-C74
27	P	305	PEK	C14-C15-C16-C17
25	P	308	CDL	C37-C38-C39-C40
17	C	303	PGV	C5-C6-C7-C8
23	R	201	PSC	C13-C14-C15-C16
22	Q	201	TGL	C10-C11-C12-C13
23	B	303	PSC	C5-C6-C7-C8
26	C	312	DMU	O6-C11-C9-C8
22	Y	101	TGL	CB7-CB8-CB9-C10
22	Q	201	TGL	C33-C34-C35-C36
27	G	103	PEK	C32-C33-C34-C35
25	C	304	CDL	C44-C45-C46-C47
27	C	313	PEK	C17-C18-C19-C20
17	A	604	PGV	C6-C7-C8-C9
17	N	617	PGV	C29-C30-C31-C32
22	D	201	TGL	C19-C33-C34-C35
23	R	201	PSC	C01-C02-C03-O11
25	C	304	CDL	OB5-CB3-CB4-CB6
25	T	103	CDL	OB5-CB3-CB4-CB6
26	Q	206	DMU	C18-C19-C22-C25
17	P	306	PGV	C9-C10-C11-C12
25	T	103	CDL	OB9-CB7-OB8-CB6
22	Y	101	TGL	CA9-C20-C21-C22
25	P	308	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
25	C	304	CDL	C57-C58-C59-C60
24	T	101	CHD	C17-C20-C22-C23
25	P	308	CDL	C55-C56-C57-C58
23	B	303	PSC	C28-C29-C30-C31
25	P	308	CDL	OB9-CB7-OB8-CB6
27	T	102	PEK	C29-C30-C31-C32
22	N	604	TGL	CC9-C15-C16-C17
23	R	201	PSC	O01-C02-C03-O11
25	P	308	CDL	OA5-CA3-CA4-OA6
25	P	308	CDL	OB5-CB3-CB4-OB6
22	Y	101	TGL	C24-C25-C26-C27
22	N	604	TGL	CG1-CG2-CG3-OG3
22	B	302	TGL	CB1-CB2-CB3-CB4
27	P	305	PEK	C35-C36-C37-C38
22	B	302	TGL	C19-C33-C34-C35
26	G	101	DMU	C25-C28-C31-C34
27	P	301	PEK	C05-C04-O12-P
27	G	103	PEK	C10-C11-C12-C13
22	B	302	TGL	CA4-CA5-CA6-CA7
19	D	205	EDO	O1-C1-C2-O2
19	P	314	EDO	O1-C1-C2-O2
19	V	102	EDO	O1-C1-C2-O2
17	A	604	PGV	O03-C01-C02-O01
17	A	604	PGV	C12-C13-C14-C15
22	L	101	TGL	OG2-CG2-CG3-OG3
23	B	303	PSC	O03-C01-C02-O01
17	A	604	PGV	C2-C3-C4-C5
25	C	310	CDL	C74-C75-C76-C77
17	P	306	PGV	O04-C19-O03-C01
27	G	103	PEK	C35-C36-C37-C38
17	P	302	PGV	C13-C14-C15-C16
17	C	302	PGV	C3-C4-C5-C6
22	D	201	TGL	OA1-CA1-OG1-CG1
25	T	103	CDL	C54-C55-C56-C57
22	Y	101	TGL	CA4-CA5-CA6-CA7
23	B	303	PSC	C29-C30-C31-C32
22	D	201	TGL	CA2-CA3-CA4-CA5
17	C	302	PGV	C24-C25-C26-C27
27	G	102	PEK	C7-C8-C9-C10
27	T	102	PEK	C3-C4-C5-C6
17	N	617	PGV	C30-C31-C32-C33
23	R	201	PSC	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
26	C	312	DMU	C19-C18-O16-C6
25	T	103	CDL	C52-C53-C54-C55
26	P	303	DMU	O16-C18-C19-C22
22	L	101	TGL	C14-C29-C30-C31
27	P	301	PEK	C2-C3-C4-C5
25	C	304	CDL	C38-C39-C40-C41
22	Q	201	TGL	CB4-CB5-CB6-CB7
22	Y	101	TGL	C17-C18-C19-C33
25	P	308	CDL	OB5-CB3-CB4-CB6
25	C	304	CDL	C23-C24-C25-C26
22	Y	101	TGL	CA2-CA3-CA4-CA5
17	C	303	PGV	C20-C21-C22-C23
27	T	102	PEK	C31-C32-C33-C34
22	D	201	TGL	C20-C21-C22-C23
22	Y	101	TGL	C19-C33-C34-C35
17	P	302	PGV	C14-C15-C16-C17
22	D	201	TGL	C21-C20-CA9-CA8
22	L	101	TGL	CC6-CC7-CC8-CC9
25	C	304	CDL	OA5-CA3-CA4-OA6
25	C	304	CDL	OB5-CB3-CB4-OB6
25	T	103	CDL	OA5-CA3-CA4-OA6
25	T	103	CDL	OB5-CB3-CB4-OB6
27	C	313	PEK	O01-C02-C03-O11
27	P	305	PEK	O01-C02-C03-O11
17	C	303	PGV	C11-C10-C9-C8
24	P	309	CHD	C20-C22-C23-C24
17	A	605	PGV	C31-C32-C33-C34
18	A	606	HEA	C4A-C3A-CMA-OMA
18	A	607	HEA	C4A-C3A-CMA-OMA
18	N	606	HEA	C4A-C3A-CMA-OMA
17	P	306	PGV	C11-C12-C13-C14
26	C	311	DMU	C31-C34-C37-C40
22	D	201	TGL	OG2-CG2-CG3-OG3
22	N	604	TGL	OG2-CG2-CG3-OG3
25	C	304	CDL	OB6-CB4-CB6-OB8
23	R	201	PSC	O03-C01-C02-C03
25	C	304	CDL	CA3-CA4-CA6-OA8
25	C	304	CDL	CB3-CB4-CB6-OB8
22	L	101	TGL	C10-C11-C12-C13
25	P	308	CDL	C23-C24-C25-C26
22	N	604	TGL	C10-C11-C12-C13
17	A	605	PGV	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
25	C	310	CDL	C62-C63-C64-C65
17	P	306	PGV	C20-C19-O03-C01
22	Q	201	TGL	CB7-CB8-CB9-C10
17	C	302	PGV	C4-C5-C6-C7
19	B	310	EDO	O1-C1-C2-O2
22	D	201	TGL	C22-C23-C24-C25
25	C	304	CDL	C82-C83-C84-C85
17	A	604	PGV	C03-O11-P-O14
17	N	617	PGV	C03-O11-P-O12
17	N	617	PGV	C03-O11-P-O13
17	P	302	PGV	C04-O12-P-O13
17	P	307	PGV	C03-O11-P-O14
23	B	303	PSC	C03-O11-P-O12
25	C	304	CDL	CB2-OB2-PB2-OB3
25	C	304	CDL	CB2-OB2-PB2-OB4
25	C	304	CDL	CB2-OB2-PB2-OB5
25	C	310	CDL	CB2-OB2-PB2-OB3
25	C	310	CDL	CB3-OB5-PB2-OB3
25	P	308	CDL	CB2-OB2-PB2-OB4
25	T	103	CDL	CA2-OA2-PA1-OA3
25	T	103	CDL	CB3-OB5-PB2-OB3
27	C	313	PEK	C03-O11-P-O14
27	G	103	PEK	C03-O11-P-O14
17	P	302	PGV	C4-C5-C6-C7
25	C	304	CDL	C72-C73-C74-C75
17	A	604	PGV	C02-C03-O11-P
17	P	306	PGV	C02-C03-O11-P
17	C	303	PGV	C14-C15-C16-C17
17	P	307	PGV	C11-C12-C13-C14
22	N	604	TGL	C29-C30-C31-C32
25	P	308	CDL	C51-C52-C53-C54
17	A	605	PGV	C02-C01-O03-C19
25	C	310	CDL	CB6-CB4-OB6-CB5
27	T	102	PEK	C23-C24-C25-C26
18	A	606	HEA	C4D-C3D-CAD-CBD
27	P	305	PEK	C25-C26-C27-C28
25	C	310	CDL	OA5-CA3-CA4-OA6
22	Q	201	TGL	CB3-CB4-CB5-CB6
25	C	310	CDL	C63-C64-C65-C66
22	N	604	TGL	CA3-CA4-CA5-CA6
22	B	302	TGL	C13-C14-C29-C30
22	Q	201	TGL	CA3-CA4-CA5-CA6

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Mol	Chain	Res	Type	Atoms
17	N	617	PGV	C20-C21-C22-C23
22	Q	201	TGL	C11-C10-CB9-CB8
17	C	303	PGV	C22-C23-C24-C25
25	C	310	CDL	O1-C1-CA2-OA2
22	Y	101	TGL	C18-C19-C33-C34
25	T	103	CDL	C63-C64-C65-C66
26	D	208	DMU	O16-C18-C19-C22
17	P	307	PGV	C12-C13-C14-C15
22	D	201	TGL	CA1-CA2-CA3-CA4
25	C	310	CDL	C21-C22-C23-C24
19	B	311	EDO	O1-C1-C2-O2
26	C	311	DMU	C19-C18-O16-C6
25	C	310	CDL	C77-C78-C79-C80
17	P	306	PGV	C19-C20-C21-C22
27	P	305	PEK	C1-C2-C3-C4
25	P	308	CDL	C18-C19-C20-C21
25	T	103	CDL	C20-C21-C22-C23
22	D	201	TGL	CA2-CA1-OG1-CG1
25	T	103	CDL	CA4-CA3-OA5-PA1
22	Q	201	TGL	CA4-CA5-CA6-CA7
17	P	306	PGV	C25-C26-C27-C28
17	P	302	PGV	C9-C10-C11-C12
27	G	103	PEK	C14-C15-C16-C17
27	C	313	PEK	O04-C21-O03-C01
22	D	201	TGL	C21-C22-C23-C24
17	A	605	PGV	C27-C28-C29-C30
22	Y	101	TGL	C13-C14-C29-C30
25	C	304	CDL	C63-C64-C65-C66
17	A	605	PGV	O03-C19-C20-C21
22	Y	101	TGL	C11-C10-CB9-CB8
17	C	303	PGV	C25-C26-C27-C28
17	C	303	PGV	C12-C13-C14-C15
26	Q	206	DMU	C19-C22-C25-C28
17	P	307	PGV	C21-C22-C23-C24
22	D	201	TGL	CB5-CB6-CB7-CB8
23	R	201	PSC	O03-C19-C20-C21
24	G	108	CHD	C22-C23-C24-O25
24	T	101	CHD	C22-C23-C24-O25
23	R	201	PSC	C3-C4-C5-C6
17	P	307	PGV	C10-C11-C12-C13
22	Y	101	TGL	C33-C34-C35-C36
25	C	310	CDL	CA3-CA4-OA6-CA5

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	CA6-CA4-OA6-CA5
27	P	301	PEK	C03-C02-O01-C1
22	L	101	TGL	C11-C10-CB9-CB8
19	B	308	EDO	O1-C1-C2-O2
19	V	103	EDO	O1-C1-C2-O2
18	A	606	HEA	CAD-CBD-CGD-O1D
18	A	606	HEA	CAA-CBA-CGA-O1A
18	A	606	HEA	CAD-CBD-CGD-O2D
18	N	605	HEA	CAD-CBD-CGD-O1D
24	T	101	CHD	C22-C23-C24-O26
24	T	105	CHD	C22-C23-C24-O25
23	R	201	PSC	C7-C8-C9-C10
17	P	302	PGV	C15-C16-C17-C18
17	C	303	PGV	C05-C04-O12-P
27	G	103	PEK	C4-C5-C6-C7
18	N	605	HEA	O11-C11-C12-C13
24	C	305	CHD	C22-C23-C24-O25
25	C	304	CDL	C80-C81-C82-C83
22	Q	201	TGL	CC2-CC3-CC4-CC5
25	C	310	CDL	C19-C20-C21-C22
25	C	310	CDL	C61-C62-C63-C64
23	B	303	PSC	C27-C28-C29-C30
25	C	310	CDL	C11-C12-C13-C14
24	P	309	CHD	C22-C23-C24-O25
25	C	304	CDL	C15-C16-C17-C18
27	G	102	PEK	C11-C10-C9-C8
27	G	103	PEK	C5-C6-C7-C8
27	P	305	PEK	C11-C12-C13-C14
25	P	308	CDL	C43-C44-C45-C46
22	N	604	TGL	CC2-CC3-CC4-CC5
17	P	302	PGV	C27-C28-C29-C30
22	N	604	TGL	CC4-CC5-CC6-CC7
22	L	101	TGL	CA4-CA5-CA6-CA7
27	P	305	PEK	C30-C31-C32-C33
18	A	606	HEA	CAA-CBA-CGA-O2A
27	G	102	PEK	C2-C1-O01-C02
18	A	606	HEA	C2D-C3D-CAD-CBD
22	D	201	TGL	OG2-CB1-CB2-CB3
22	D	201	TGL	OG1-CG1-CG2-CG3
26	C	311	DMU	C22-C25-C28-C31
18	N	605	HEA	CAD-CBD-CGD-O2D
22	Y	101	TGL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	G	102	PEK	O02-C1-O01-C02
27	G	102	PEK	C32-C33-C34-C35
19	C	309	EDO	O1-C1-C2-O2
19	D	202	EDO	O1-C1-C2-O2
19	G	104	EDO	O1-C1-C2-O2
19	I	103	EDO	O1-C1-C2-O2
19	O	302	EDO	O1-C1-C2-O2
19	P	311	EDO	O1-C1-C2-O2
19	P	312	EDO	O1-C1-C2-O2
19	S	104	EDO	O1-C1-C2-O2
19	W	301	EDO	O1-C1-C2-O2
22	N	604	TGL	C21-C20-CA9-CA8
22	Q	201	TGL	C11-C12-C13-C14
17	C	302	PGV	C20-C21-C22-C23
27	P	301	PEK	C35-C36-C37-C38
22	Q	201	TGL	OB1-CB1-OG2-CG2
22	D	201	TGL	C29-C30-C31-C32
22	D	201	TGL	CA3-CA4-CA5-CA6
17	C	302	PGV	C13-C14-C15-C16
24	P	309	CHD	C22-C23-C24-O26
22	L	101	TGL	C20-C21-C22-C23
17	C	302	PGV	C11-C12-C13-C14
27	C	313	PEK	C3-C4-C5-C6
22	D	201	TGL	CC3-CC4-CC5-CC6
25	P	308	CDL	C57-C58-C59-C60
27	C	313	PEK	C22-C21-O03-C01
17	A	605	PGV	C12-C13-C14-C15
22	L	101	TGL	CA5-CA6-CA7-CA8
17	P	302	PGV	C11-C12-C13-C14
23	B	303	PSC	C7-C8-C9-C10
23	B	303	PSC	C12-C13-C14-C15
27	C	313	PEK	C14-C15-C16-C17
24	J	101	CHD	C20-C22-C23-C24
24	G	108	CHD	C22-C23-C24-O26
24	T	105	CHD	C22-C23-C24-O26
17	P	302	PGV	O03-C19-C20-C21
17	A	605	PGV	C15-C16-C17-C18
27	G	102	PEK	C3-C4-C5-C6
25	P	308	CDL	C62-C63-C64-C65
18	N	605	HEA	C2A-C3A-CMA-OMA
23	R	201	PSC	C30-C31-C32-C33
17	N	617	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	T	103	CDL	C37-C38-C39-C40
17	N	617	PGV	C9-C10-C11-C12
23	R	201	PSC	C12-C13-C14-C15
22	B	302	TGL	C24-C25-C26-C27
25	T	103	CDL	C18-C19-C20-C21
22	Y	101	TGL	C15-C16-C17-C18
27	G	102	PEK	C25-C26-C27-C28
27	G	103	PEK	C17-C18-C19-C20
22	Y	101	TGL	CB5-CB6-CB7-CB8
17	P	306	PGV	C7-C8-C9-C10
17	C	302	PGV	C31-C32-C33-C34
17	A	604	PGV	O03-C19-C20-C21
23	B	303	PSC	C31-C32-C33-C34
19	D	203	EDO	O1-C1-C2-O2
19	G	109	EDO	O1-C1-C2-O2
19	N	610	EDO	O1-C1-C2-O2
19	N	613	EDO	O1-C1-C2-O2
19	W	303	EDO	O1-C1-C2-O2
17	C	303	PGV	C27-C28-C29-C30
27	G	103	PEK	O03-C01-C02-O01
24	W	302	CHD	C22-C23-C24-O25
17	A	605	PGV	C9-C10-C11-C12
27	P	301	PEK	C3-C4-C5-C6
27	P	305	PEK	C01-C02-C03-O11
22	N	604	TGL	CB4-CB5-CB6-CB7
27	T	102	PEK	O01-C1-C2-C3
23	R	201	PSC	O04-C19-O03-C01
22	D	201	TGL	OG1-CA1-CA2-CA3
17	C	302	PGV	C9-C10-C11-C12
17	N	617	PGV	C11-C12-C13-C14
17	P	307	PGV	C9-C10-C11-C12
17	P	307	PGV	C24-C25-C26-C27
22	D	201	TGL	C11-C10-CB9-CB8
23	R	201	PSC	C21-C22-C23-C24
25	C	310	CDL	C64-C65-C66-C67
27	T	102	PEK	C14-C15-C16-C17
25	C	304	CDL	O1-C1-CB2-OB2
22	Q	201	TGL	CB2-CB1-OG2-CG2
22	Q	201	TGL	OG3-CC1-CC2-CC3
27	G	103	PEK	C27-C28-C29-C30
23	B	303	PSC	O03-C19-C20-C21
27	G	102	PEK	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	B	302	TGL	CB6-CB7-CB8-CB9
22	L	101	TGL	CC4-CC5-CC6-CC7
22	Q	201	TGL	CC7-CC8-CC9-C15
25	C	310	CDL	C55-C56-C57-C58
18	A	607	HEA	CAA-CBA-CGA-O2A
25	C	310	CDL	C13-C14-C15-C16
27	G	103	PEK	O03-C01-C02-C03
22	Q	201	TGL	OG2-CB1-CB2-CB3
22	N	604	TGL	C24-C25-C26-C27
27	G	103	PEK	C29-C30-C31-C32
22	B	302	TGL	CC9-C15-C16-C17
17	N	617	PGV	O03-C19-C20-C21
27	P	301	PEK	C26-C27-C28-C29
19	A	613	EDO	O1-C1-C2-O2
19	E	202	EDO	O1-C1-C2-O2
19	N	607	EDO	O1-C1-C2-O2
19	N	615	EDO	O1-C1-C2-O2
17	C	303	PGV	C23-C24-C25-C26
22	B	302	TGL	OG3-CC1-CC2-CC3
23	R	201	PSC	C20-C19-O03-C01
17	A	605	PGV	C24-C25-C26-C27
17	C	303	PGV	C26-C27-C28-C29
25	C	304	CDL	C34-C35-C36-C37
25	T	103	CDL	C83-C84-C85-C86
22	Q	201	TGL	CB2-CB3-CB4-CB5
27	G	103	PEK	C02-C03-O11-P
24	C	305	CHD	C22-C23-C24-O26
18	A	606	HEA	C26-C15-C16-C17
17	A	605	PGV	C26-C27-C28-C29
17	N	617	PGV	O01-C02-C03-O11
22	Q	201	TGL	C17-C18-C19-C33
17	C	302	PGV	O01-C1-C2-C3
24	P	304	CHD	C22-C23-C24-O26
27	G	102	PEK	O02-C1-C2-C3
22	D	201	TGL	OA1-CA1-CA2-CA3
22	Q	201	TGL	OC1-CC1-CC2-CC3
27	T	102	PEK	O02-C1-C2-C3
25	P	308	CDL	C64-C65-C66-C67
17	N	617	PGV	O04-C19-C20-C21
22	B	302	TGL	OC1-CC1-CC2-CC3
22	Q	201	TGL	OB1-CB1-CB2-CB3
27	G	102	PEK	O03-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
27	G	102	PEK	C4-C5-C6-C7
17	A	604	PGV	O04-C19-C20-C21
22	Y	101	TGL	C21-C22-C23-C24
24	C	301	CHD	C22-C23-C24-O26
17	P	307	PGV	C31-C32-C33-C34
17	A	605	PGV	C13-C14-C15-C16
23	B	303	PSC	O04-C19-C20-C21
25	T	103	CDL	C19-C20-C21-C22
27	G	103	PEK	C34-C35-C36-C37
24	Y	102	CHD	C22-C23-C24-O26
23	R	201	PSC	O01-C1-C2-C3
25	T	103	CDL	C52-C51-CB5-OB6
27	G	102	PEK	C23-C24-C25-C26
22	L	101	TGL	CA9-C20-C21-C22
17	A	604	PGV	C19-C20-C21-C22
17	P	306	PGV	C1-C2-C3-C4
25	C	310	CDL	C36-C37-C38-C39
27	G	102	PEK	C33-C34-C35-C36

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	Y	102	CHD	C10-C5-C6-C7-C8-C9

46 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	Y	102	CHD	4	0
22	D	201	TGL	3	0
19	S	105	EDO	1	0
19	C	306	EDO	1	0
27	T	102	PEK	4	0
24	T	105	CHD	11	0
24	T	101	CHD	1	0
25	C	310	CDL	1	0
18	A	607	HEA	3	0
19	N	611	EDO	1	0
22	Y	101	TGL	2	0
24	J	101	CHD	1	0
24	C	301	CHD	1	0
17	C	302	PGV	1	0
25	C	304	CDL	3	0

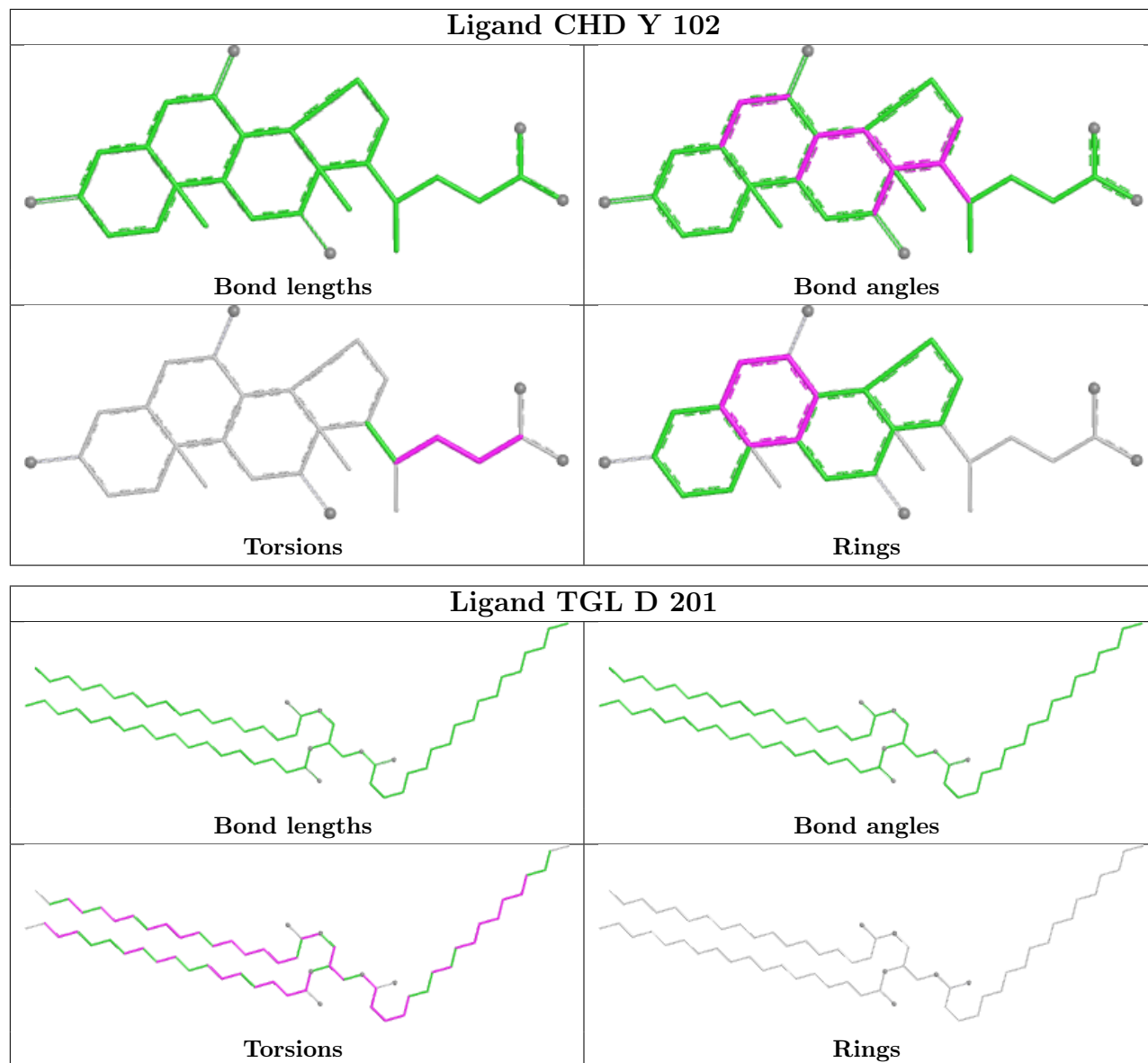
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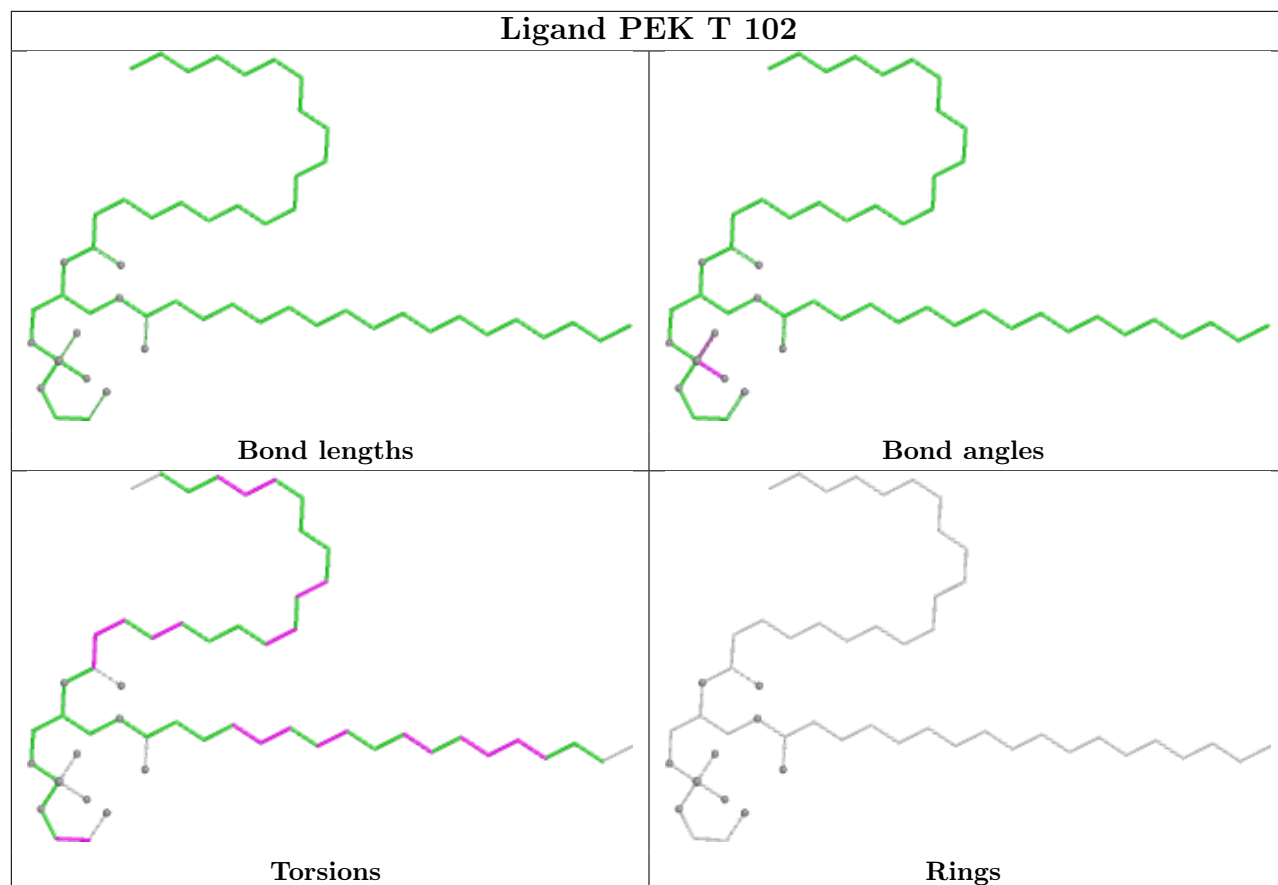
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	612	EDO	2	0
24	W	302	CHD	1	0
19	Q	204	EDO	1	0
17	N	617	PGV	4	0
17	A	604	PGV	1	0
17	C	303	PGV	2	0
18	N	606	HEA	7	0
29	V	101	SAC	2	0
24	P	309	CHD	1	0
25	P	308	CDL	2	0
18	N	605	HEA	2	0
23	B	303	PSC	3	0
19	B	305	EDO	1	0
26	C	312	DMU	1	0
23	R	201	PSC	2	0
19	Q	205	EDO	1	0
27	P	301	PEK	2	0
27	C	313	PEK	1	0
26	C	311	DMU	1	0
19	N	614	EDO	1	0
25	T	103	CDL	6	0
26	D	208	DMU	3	0
27	P	305	PEK	2	0
22	L	101	TGL	2	0
17	P	306	PGV	1	0
27	G	102	PEK	4	0
26	Q	206	DMU	2	0
22	Q	201	TGL	1	0
27	G	103	PEK	1	0
17	P	307	PGV	3	0
19	A	608	EDO	3	0

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

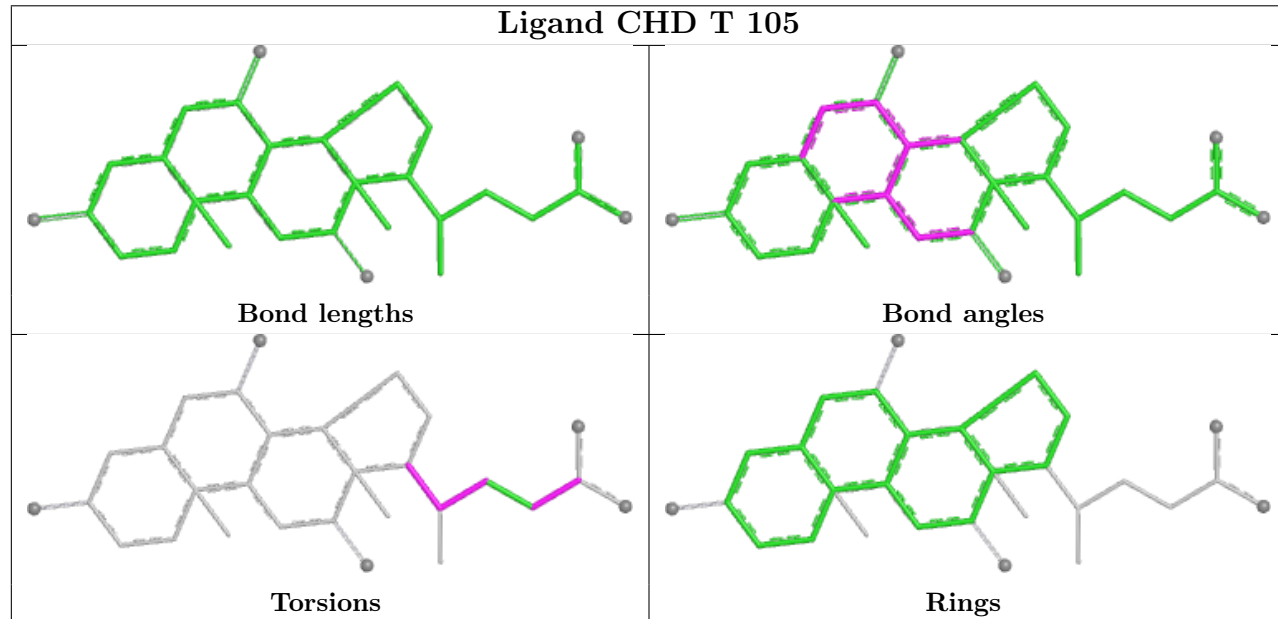
equivalents in the CSD to analyse the geometry.

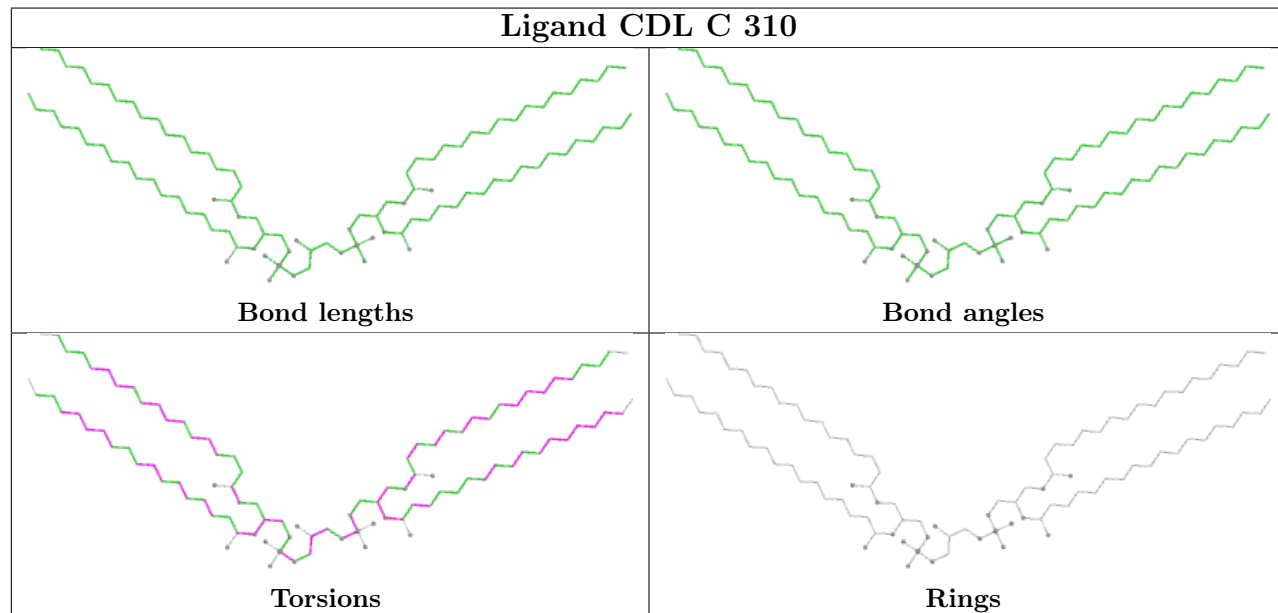
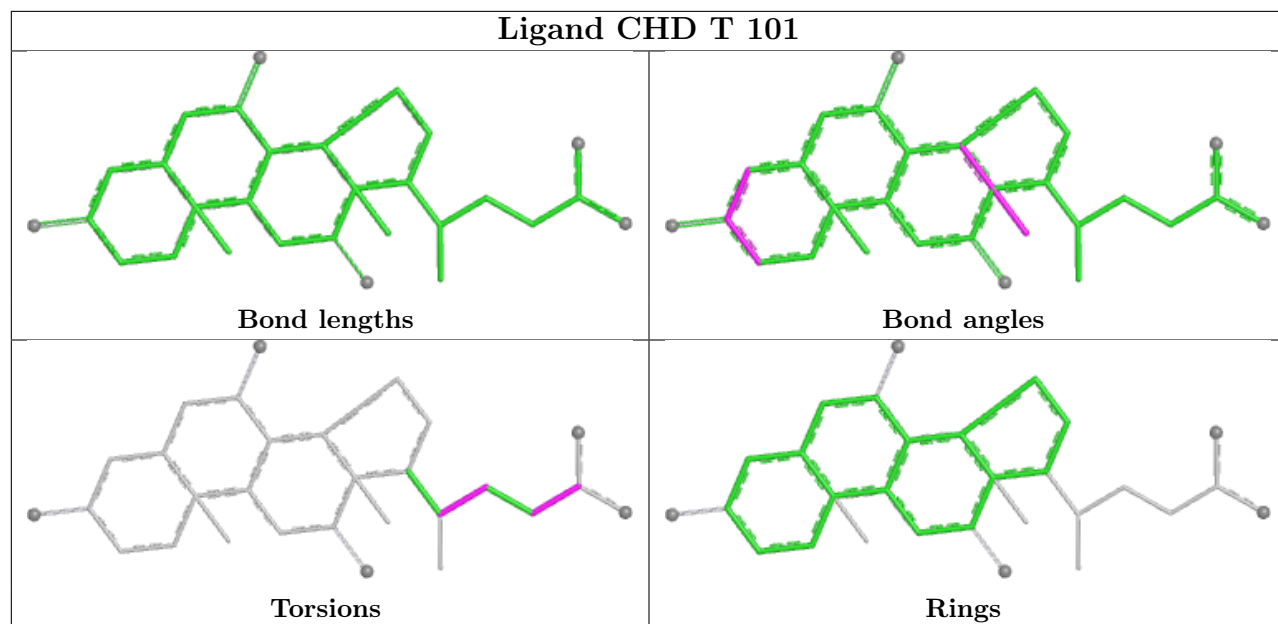


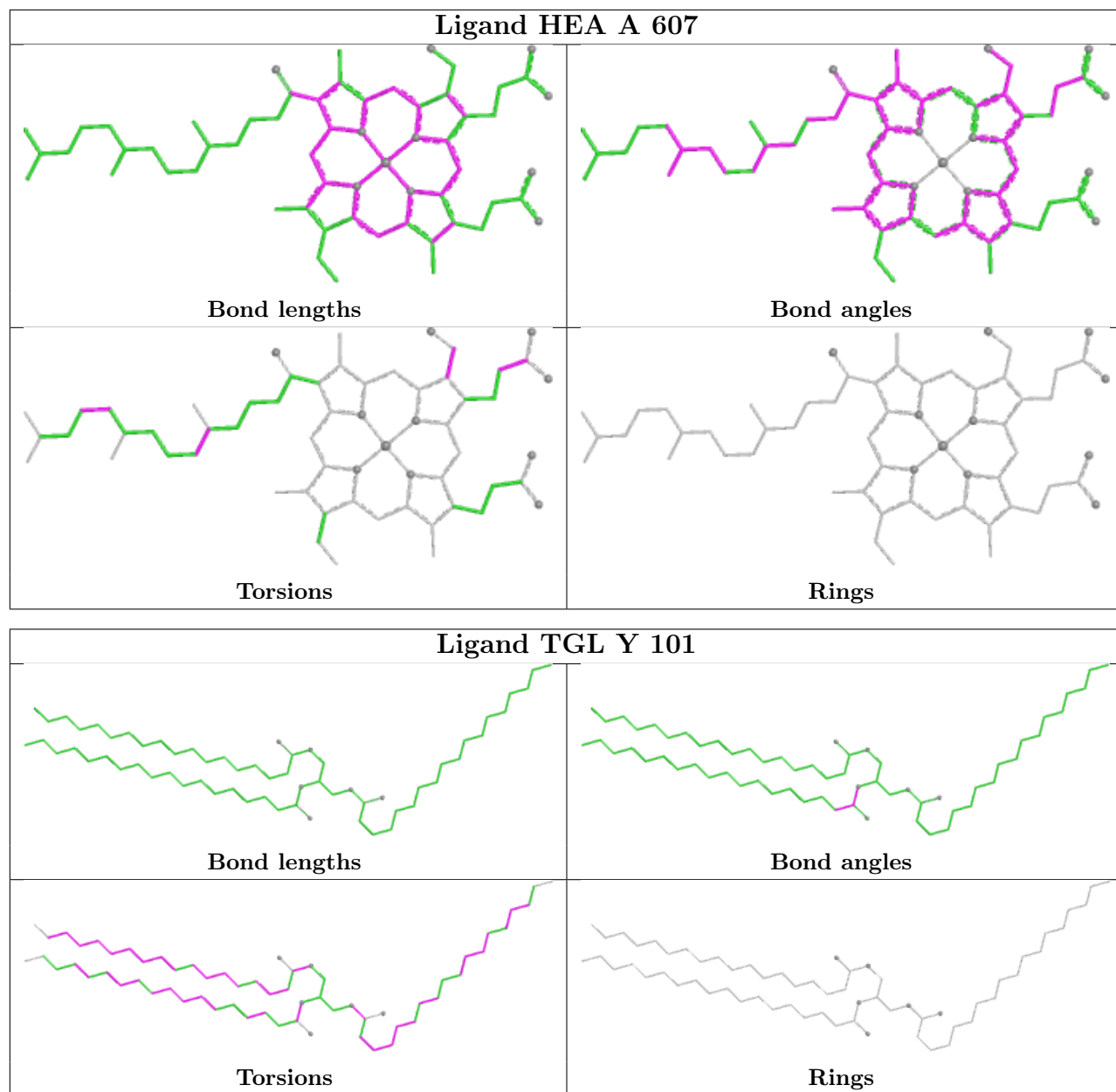
Ligand PEK T 102



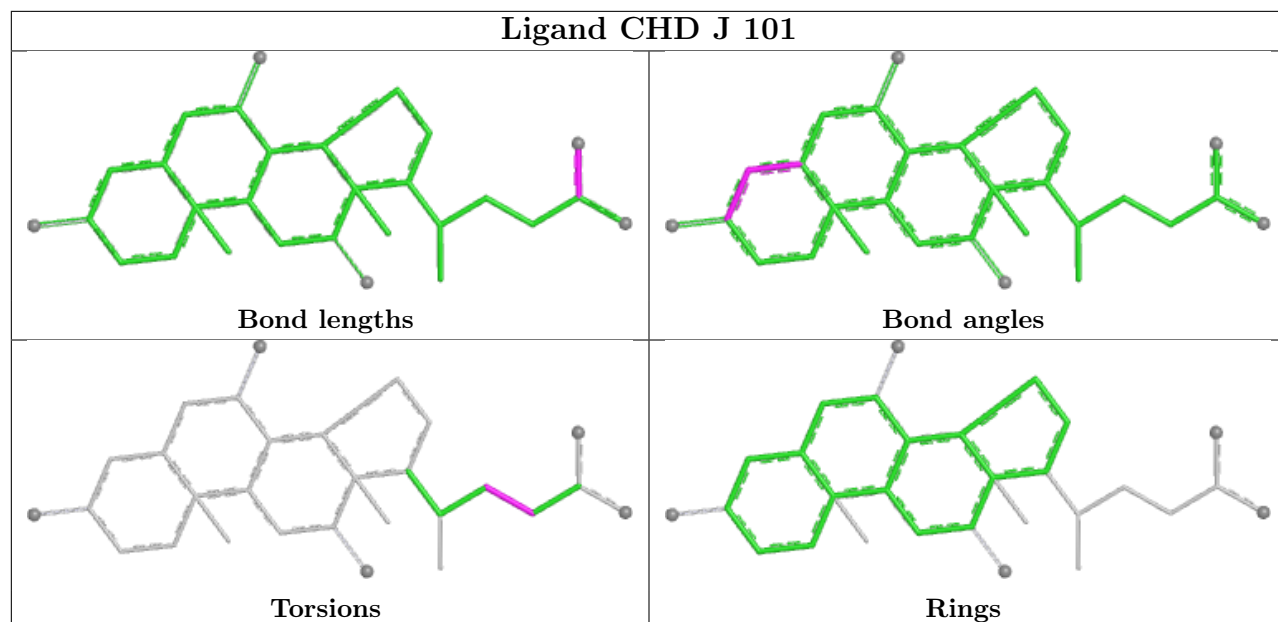
Ligand CHD T 105



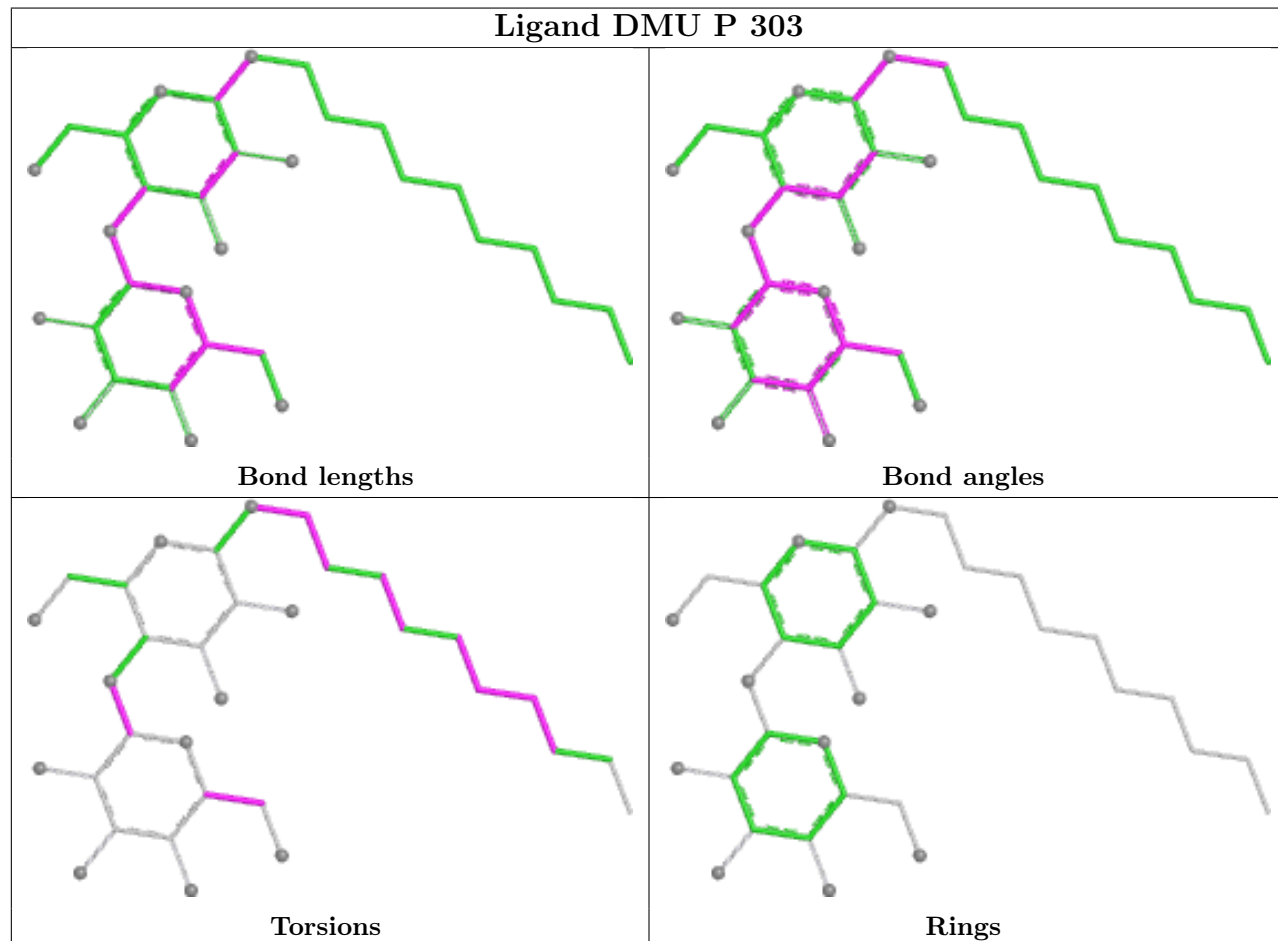


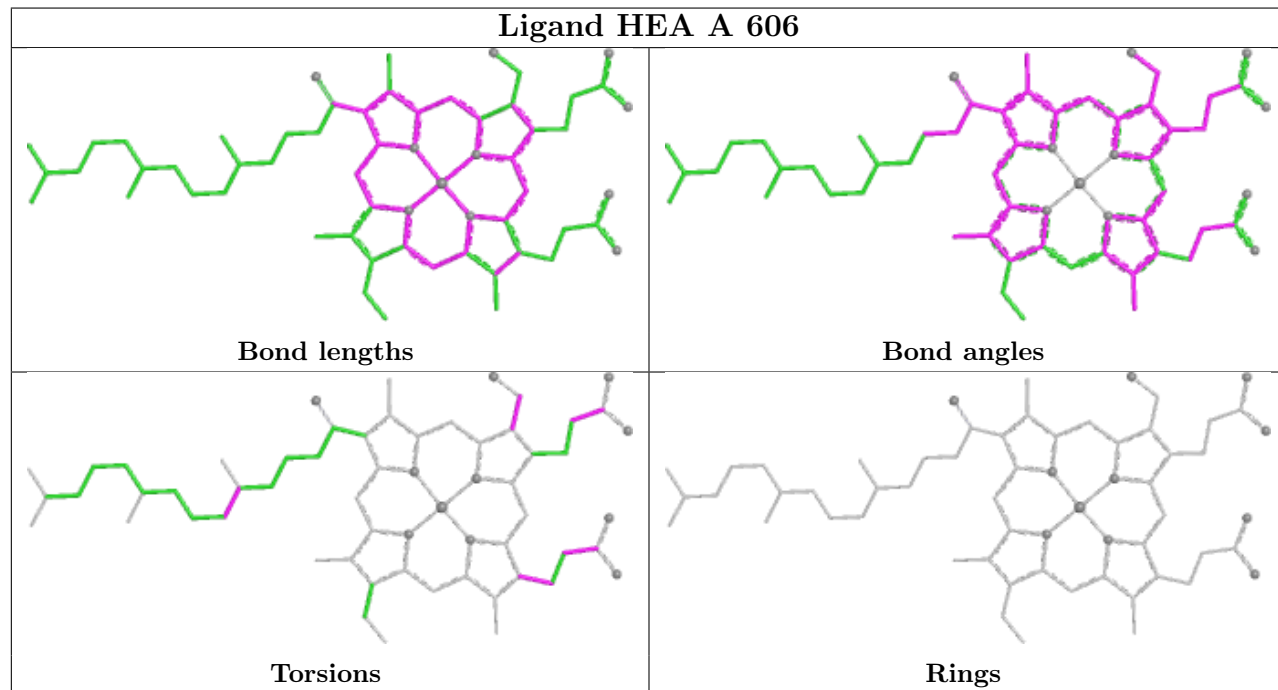
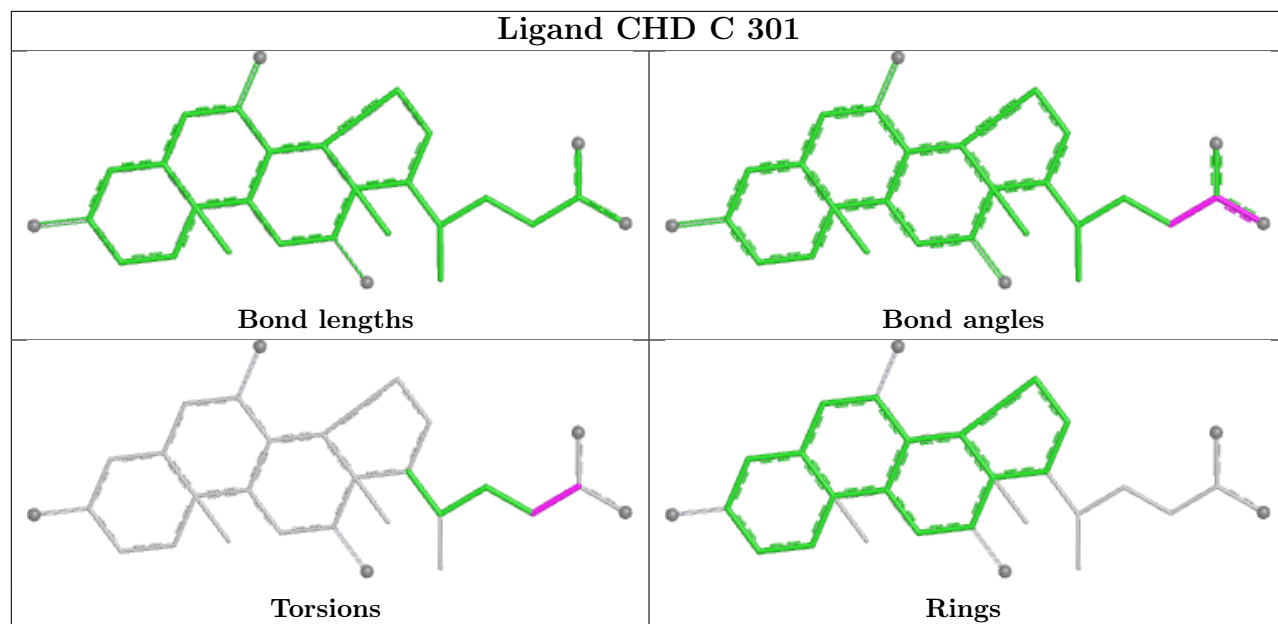


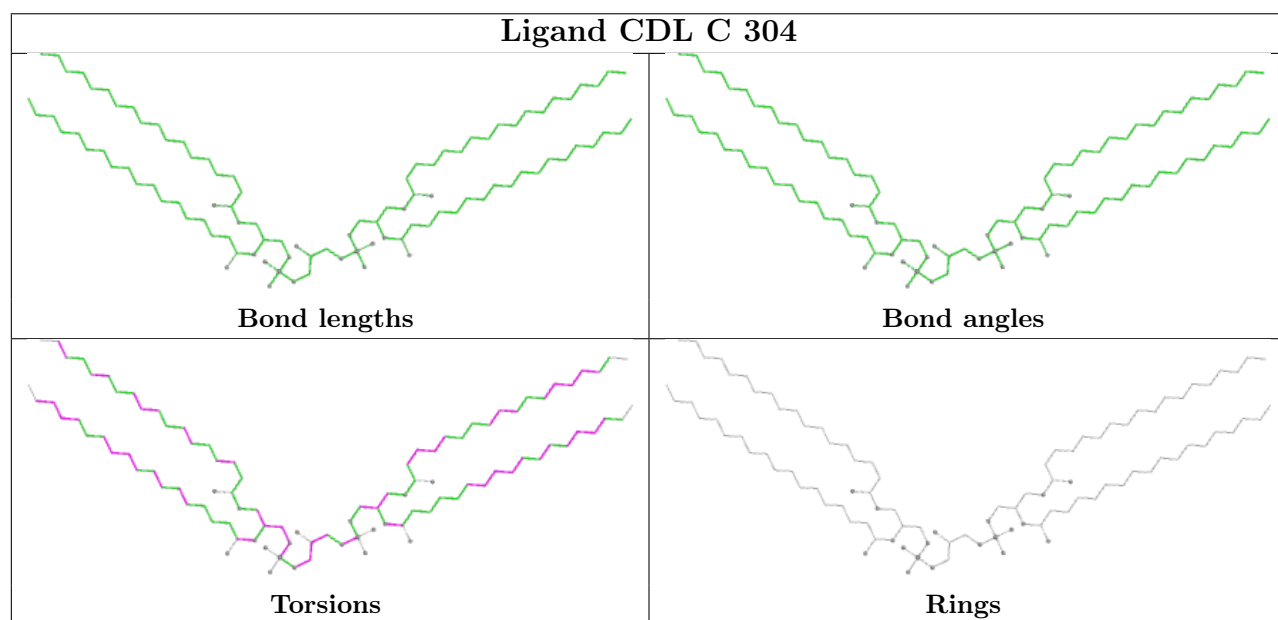
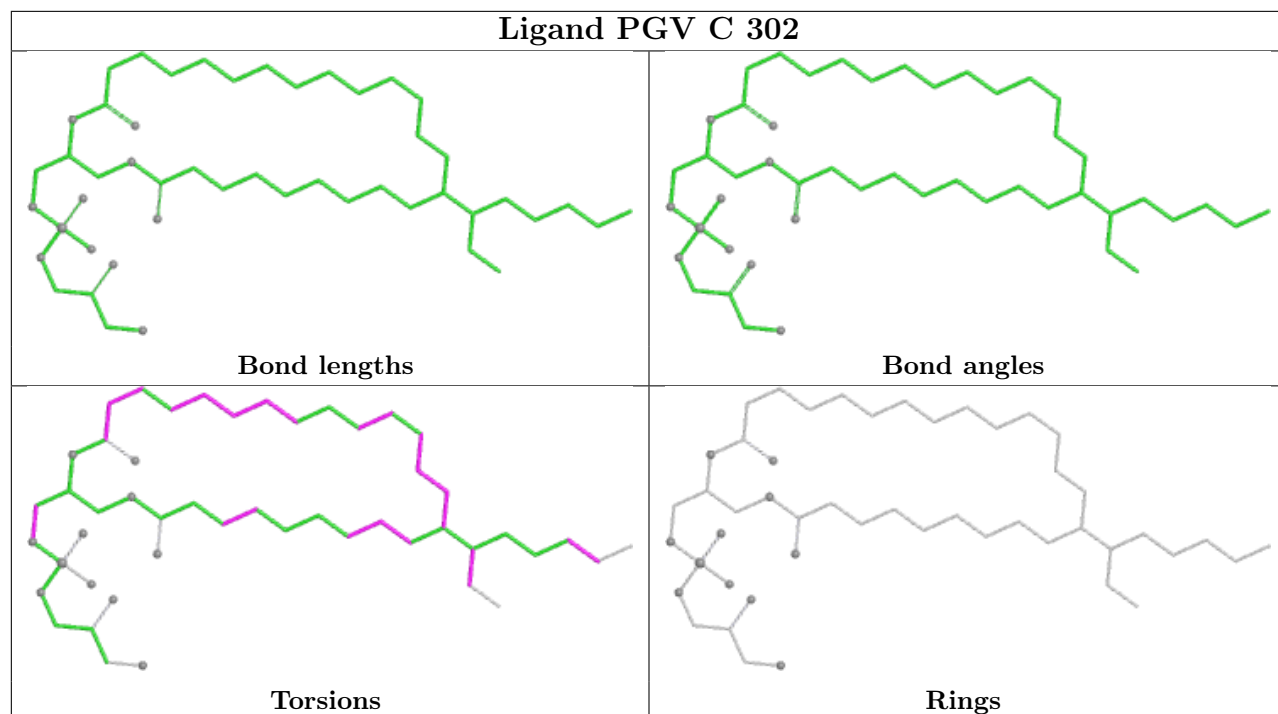
Ligand CHD J 101

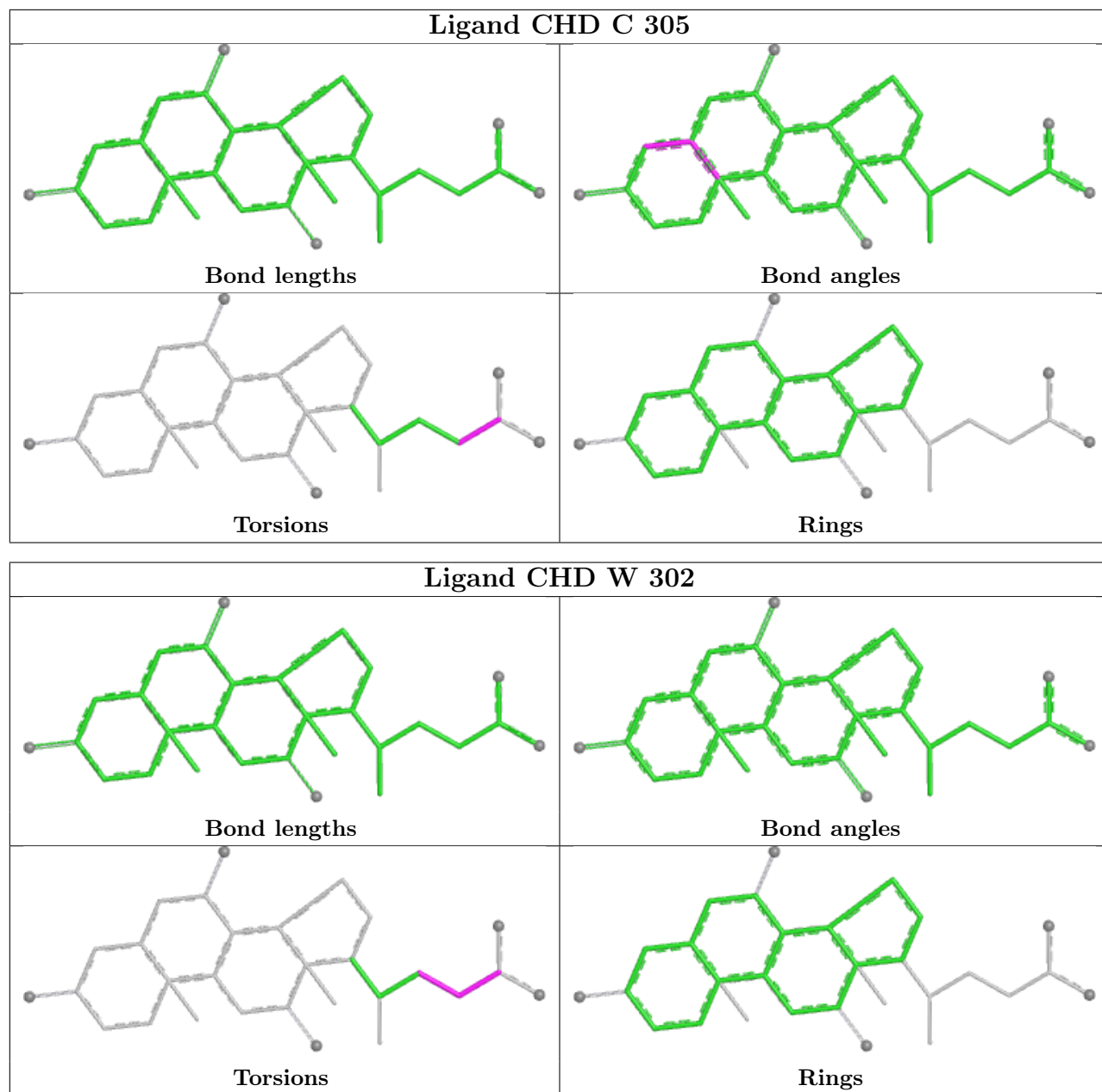


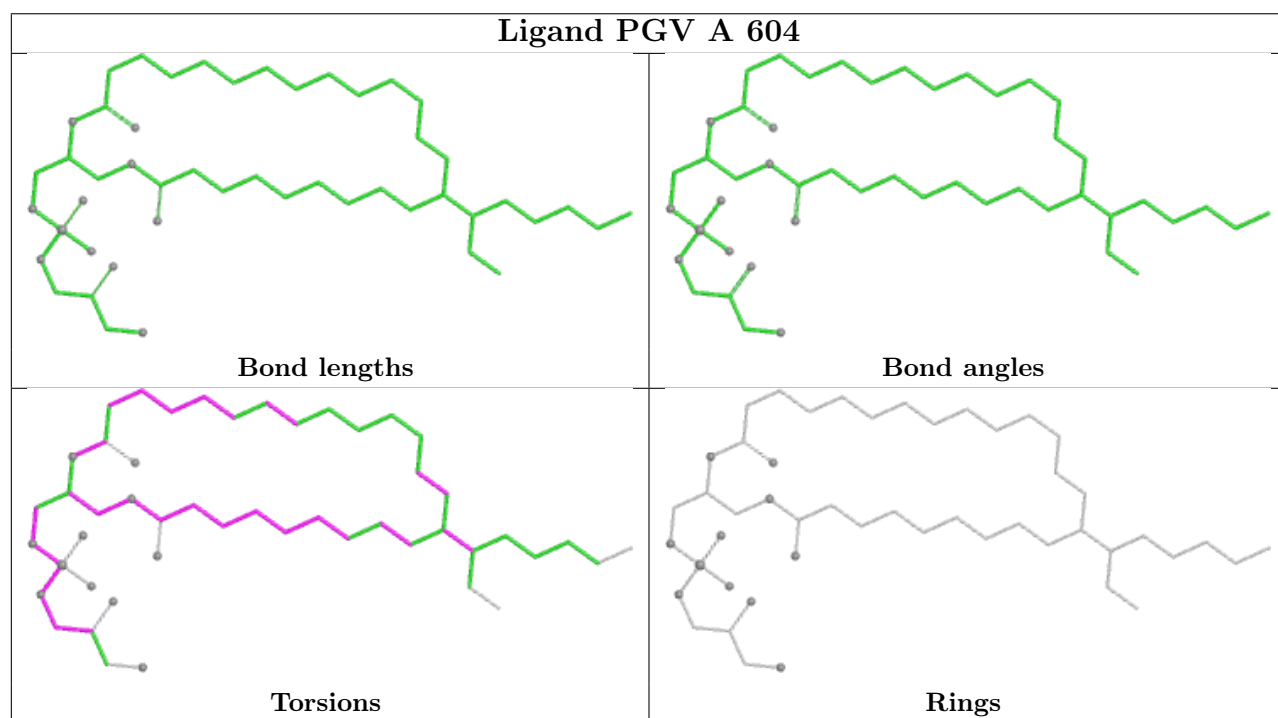
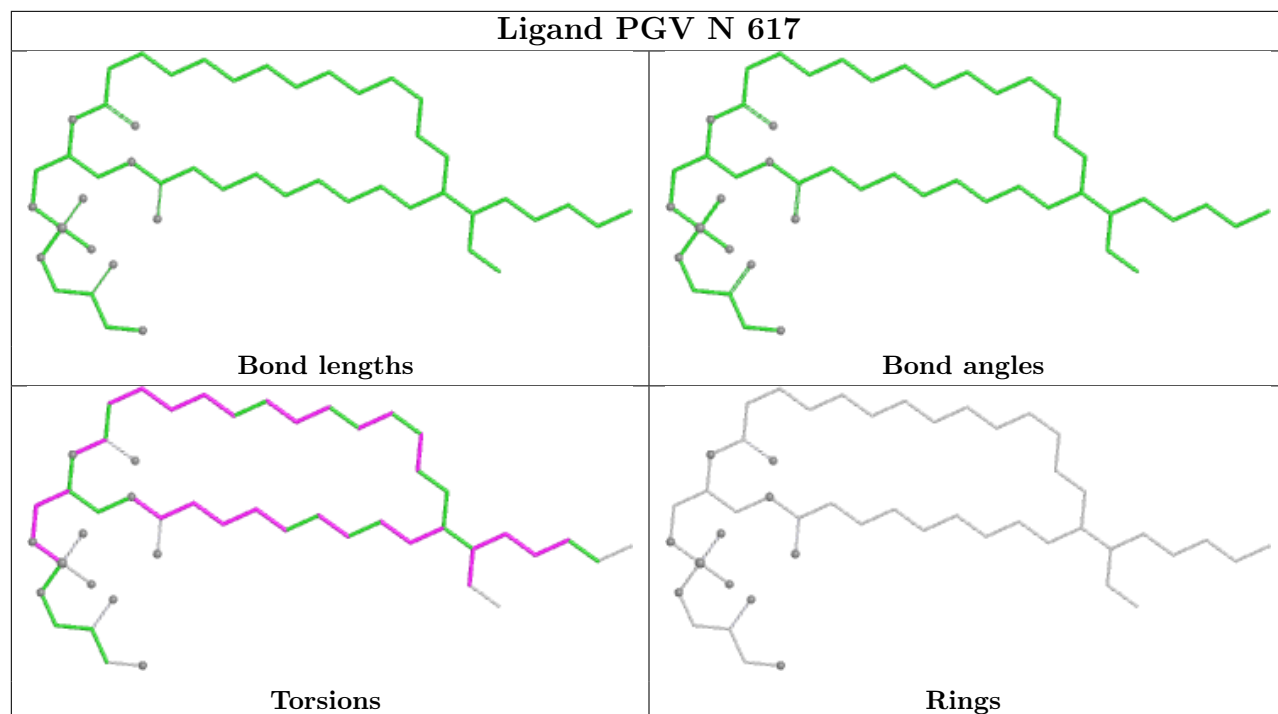
Ligand DMU P 303

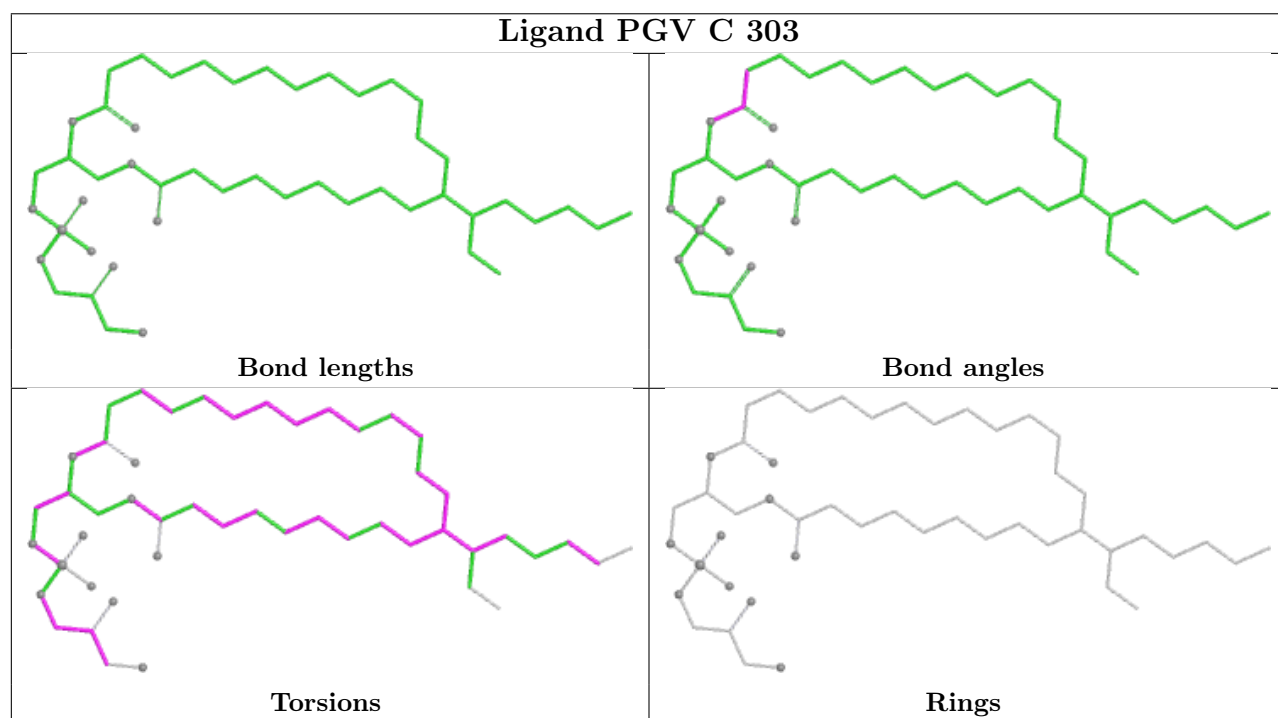
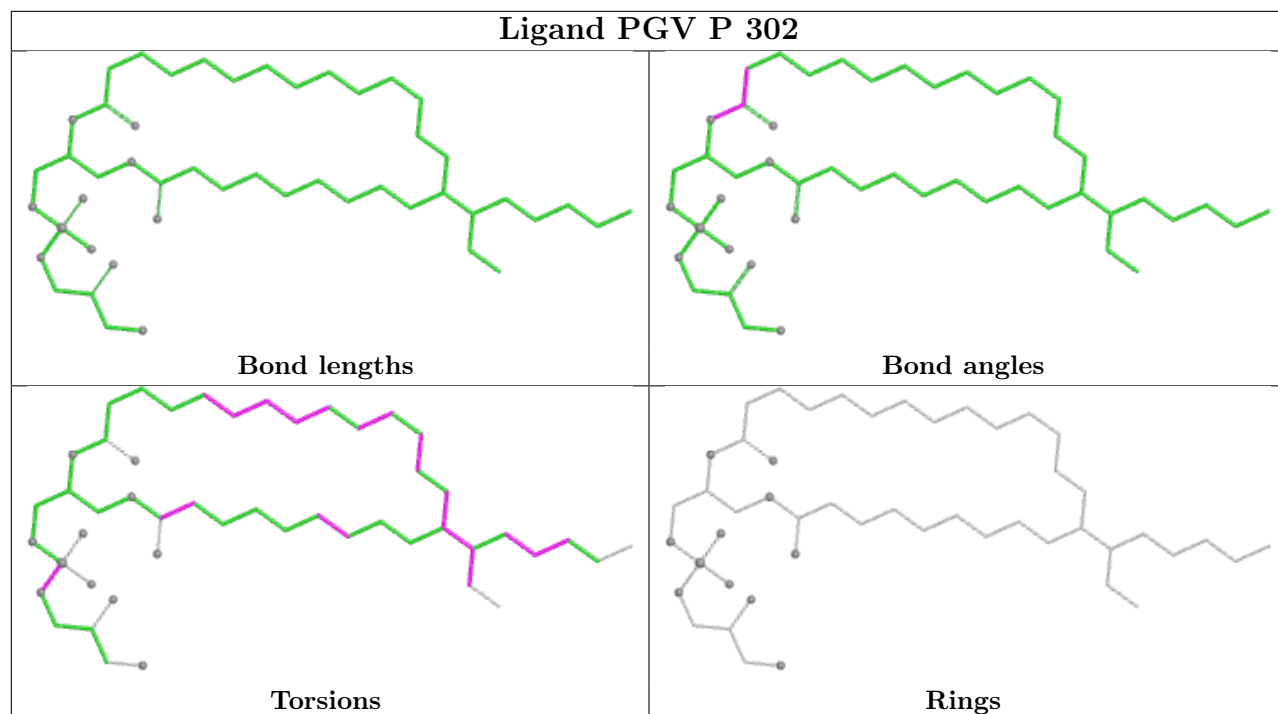


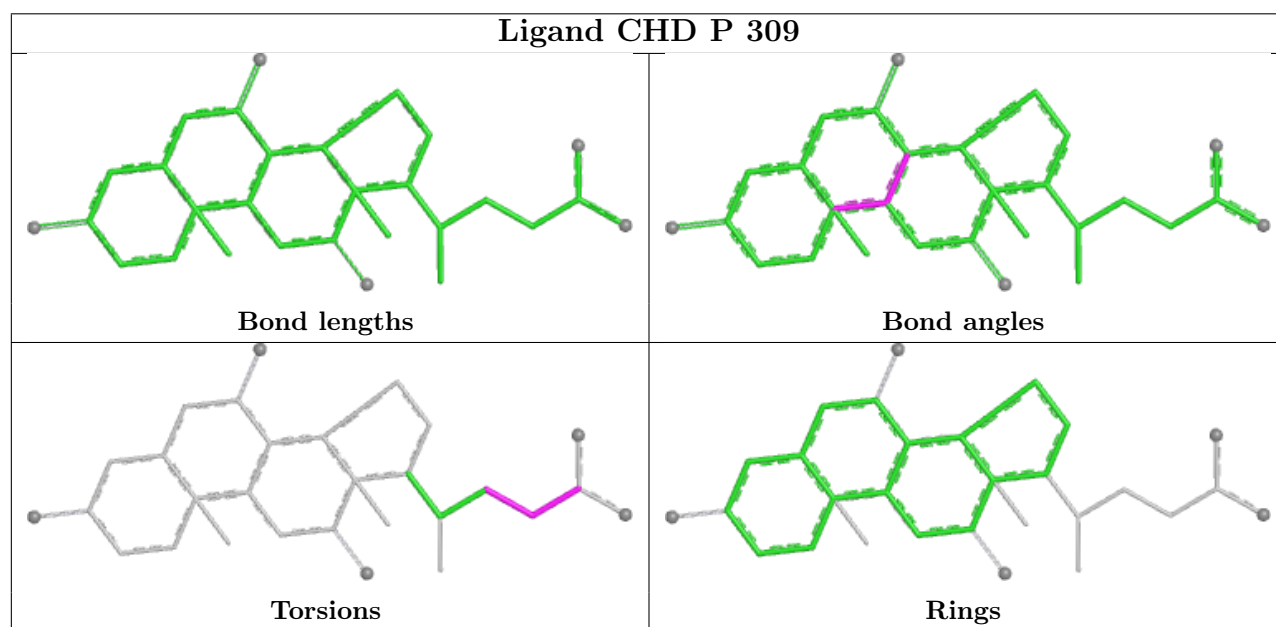
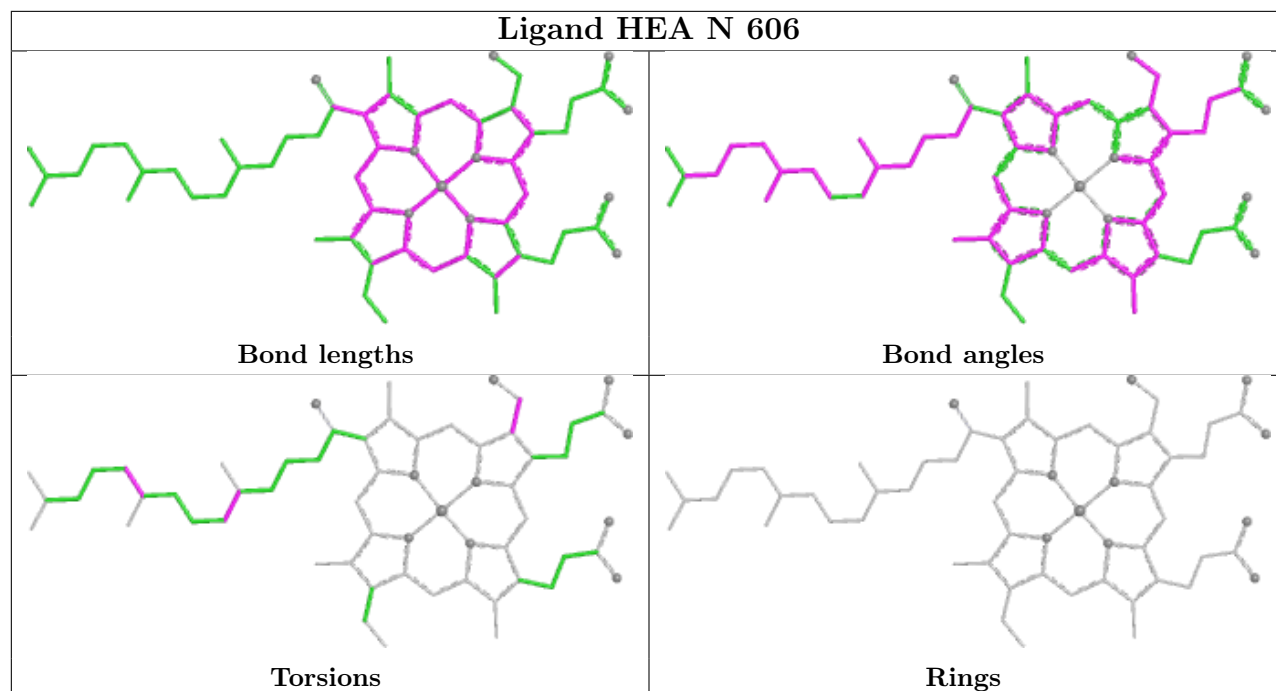


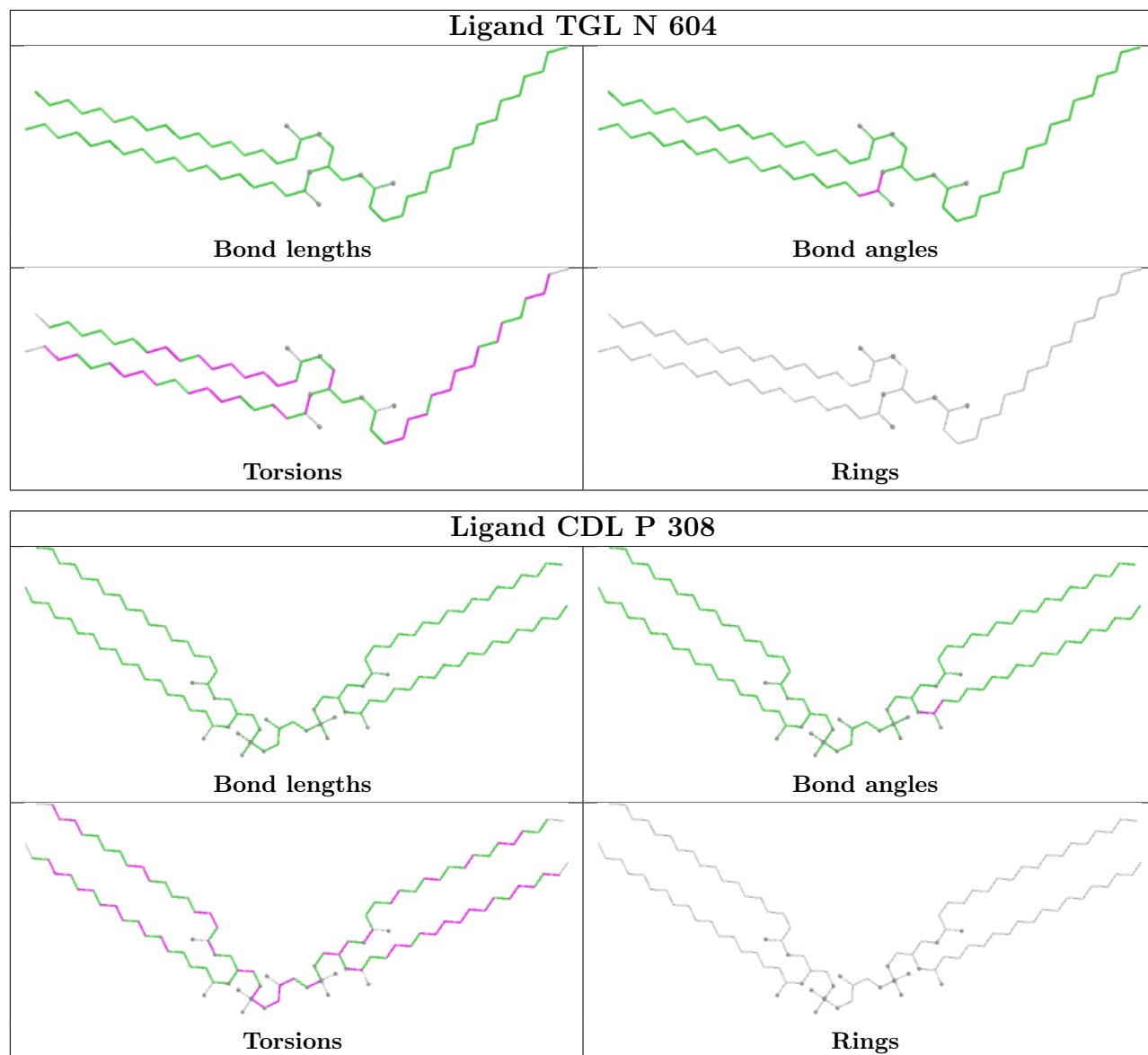


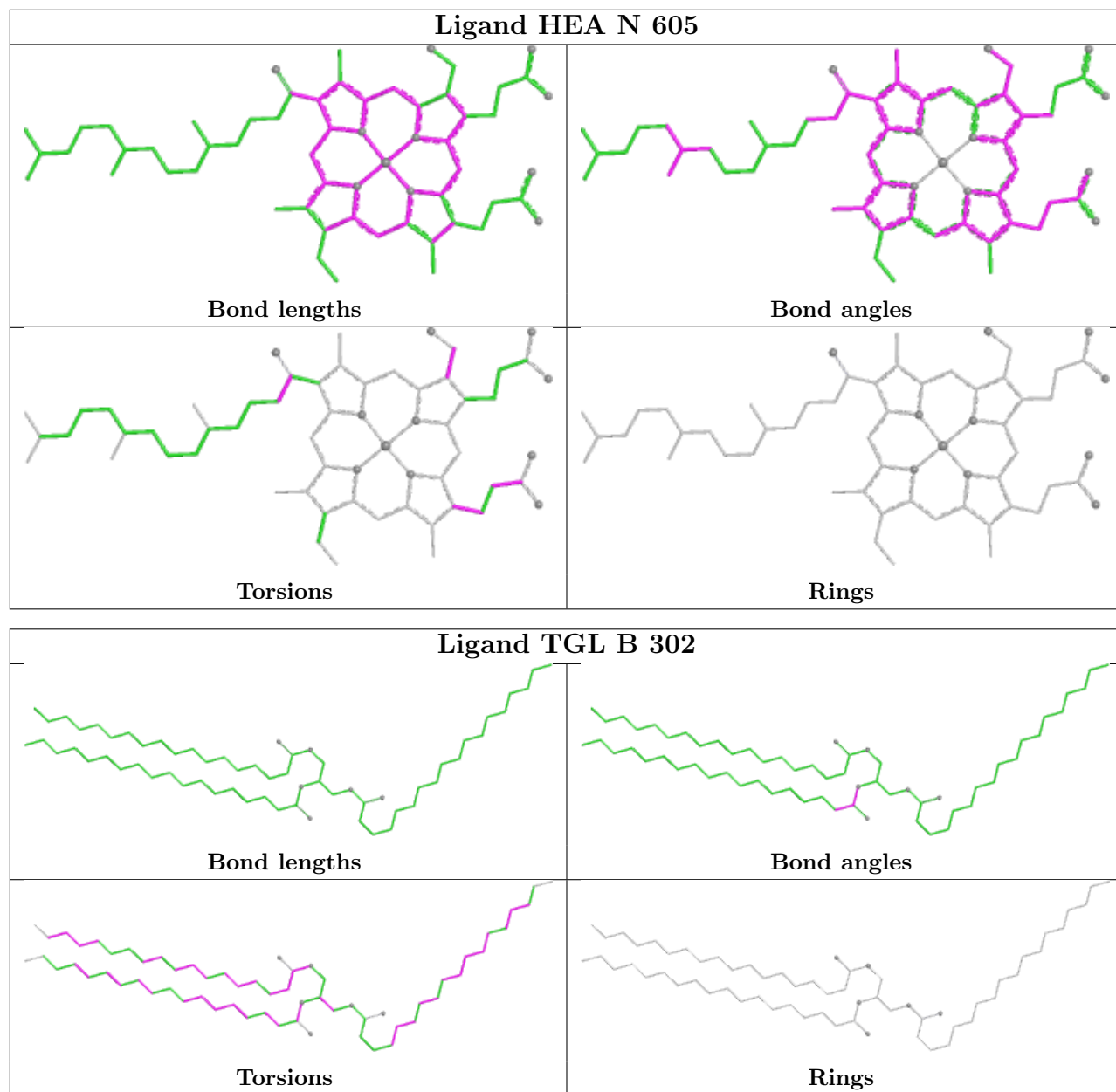




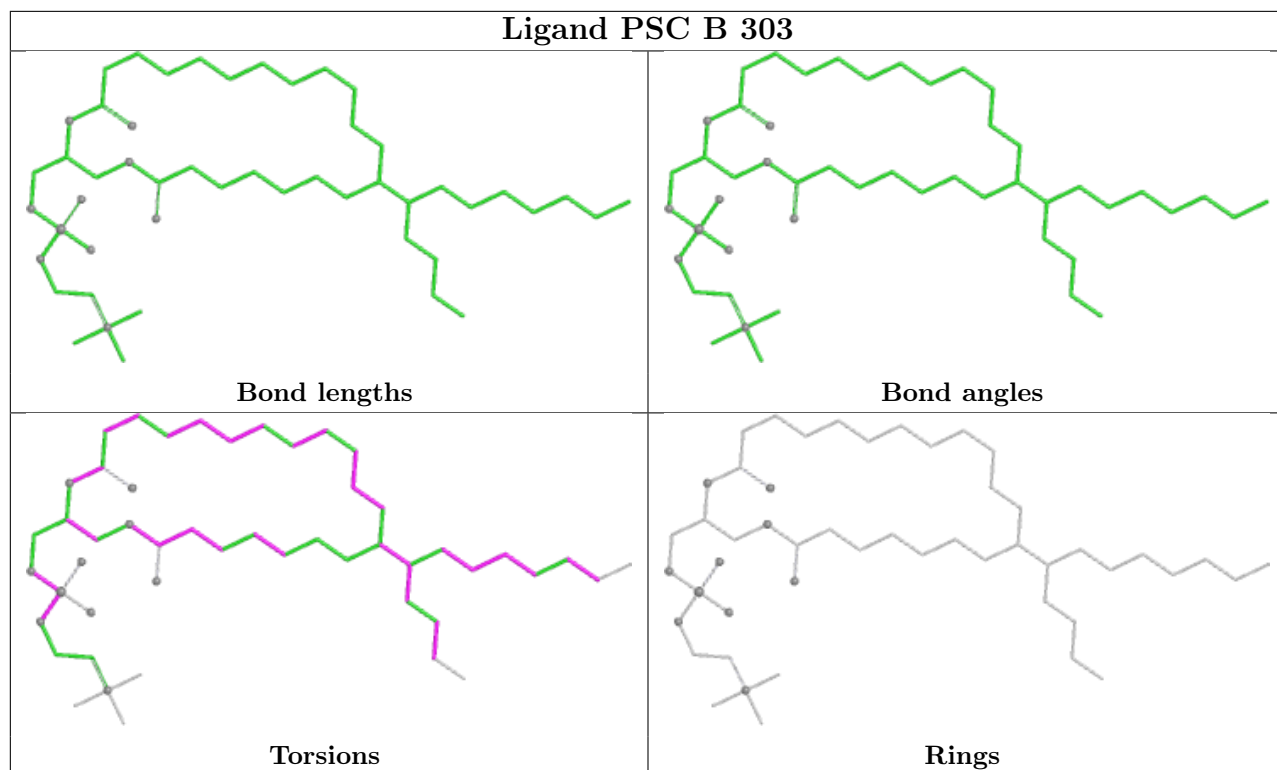




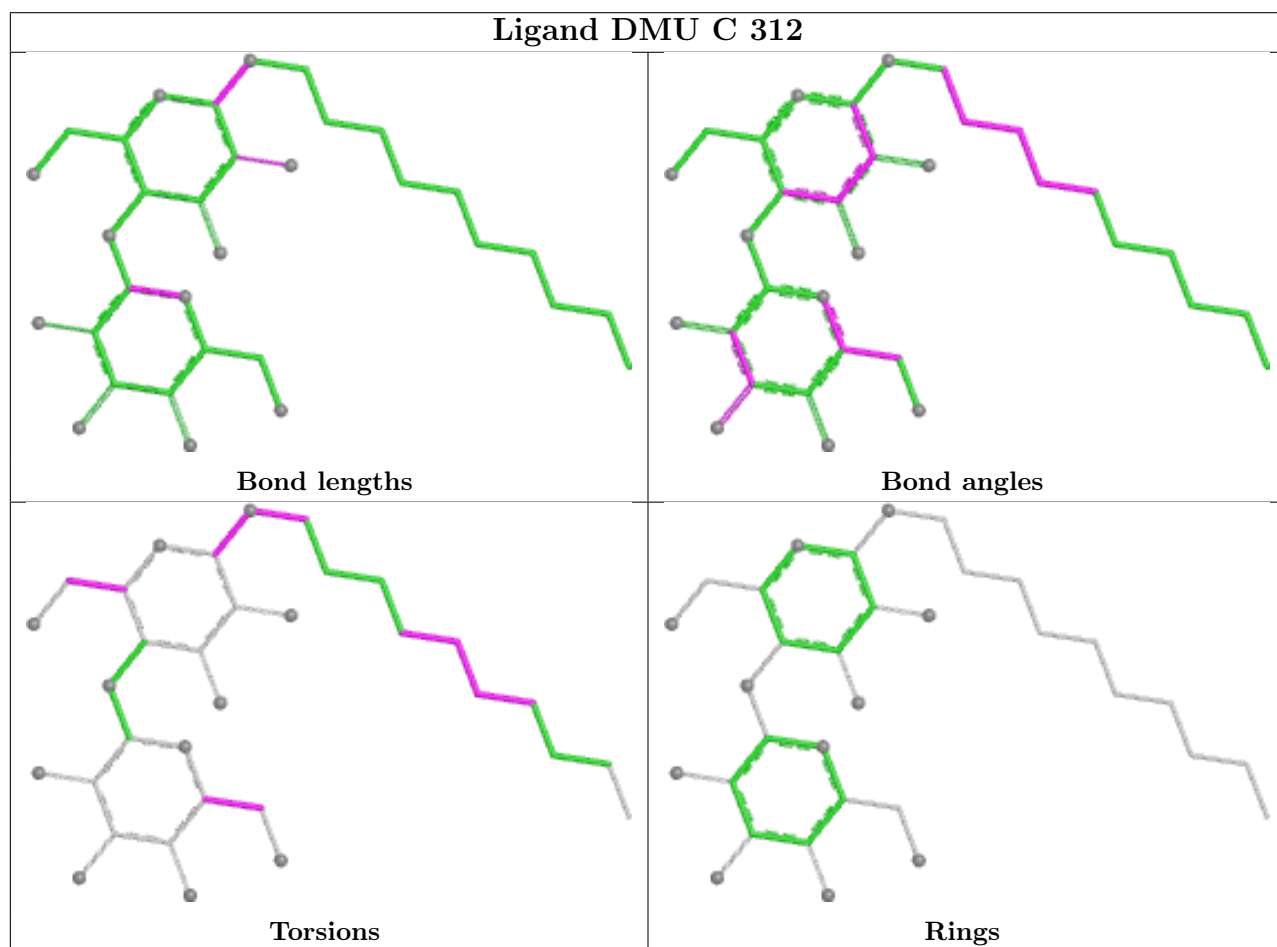




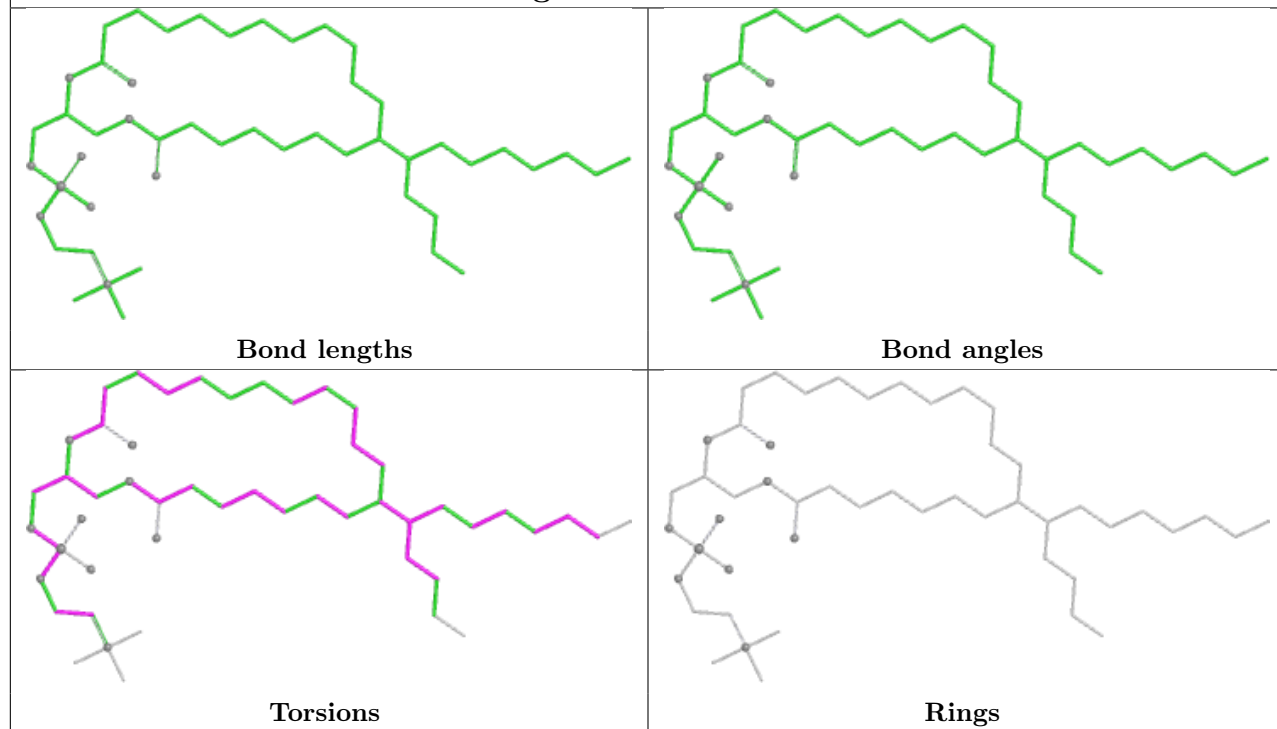
Ligand PSC B 303



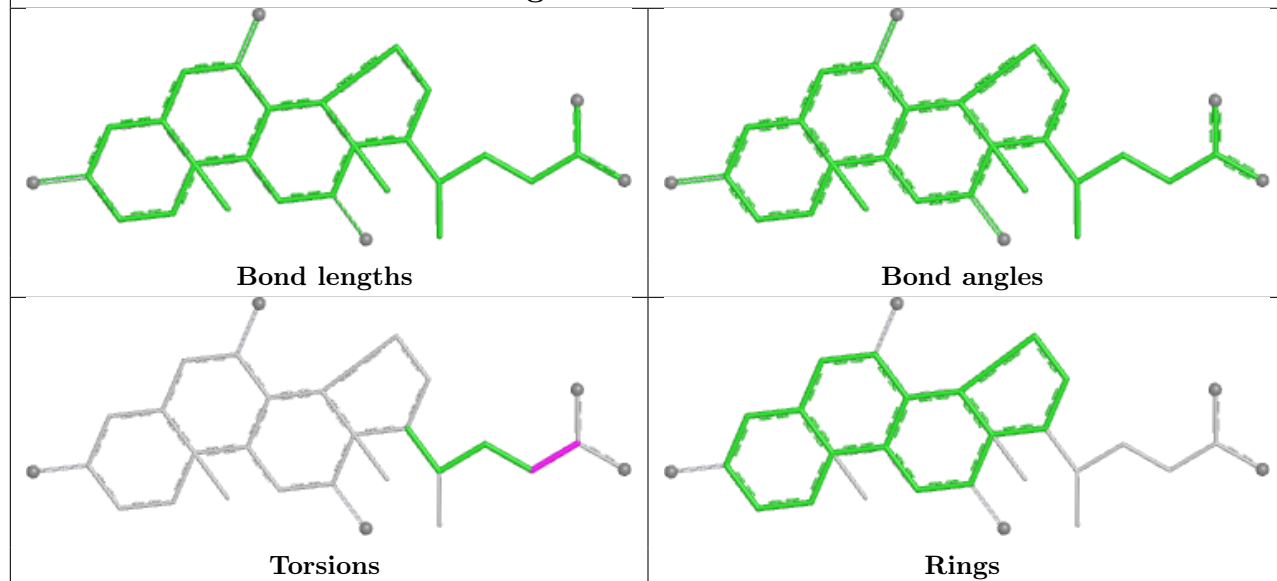
Ligand DMU C 312



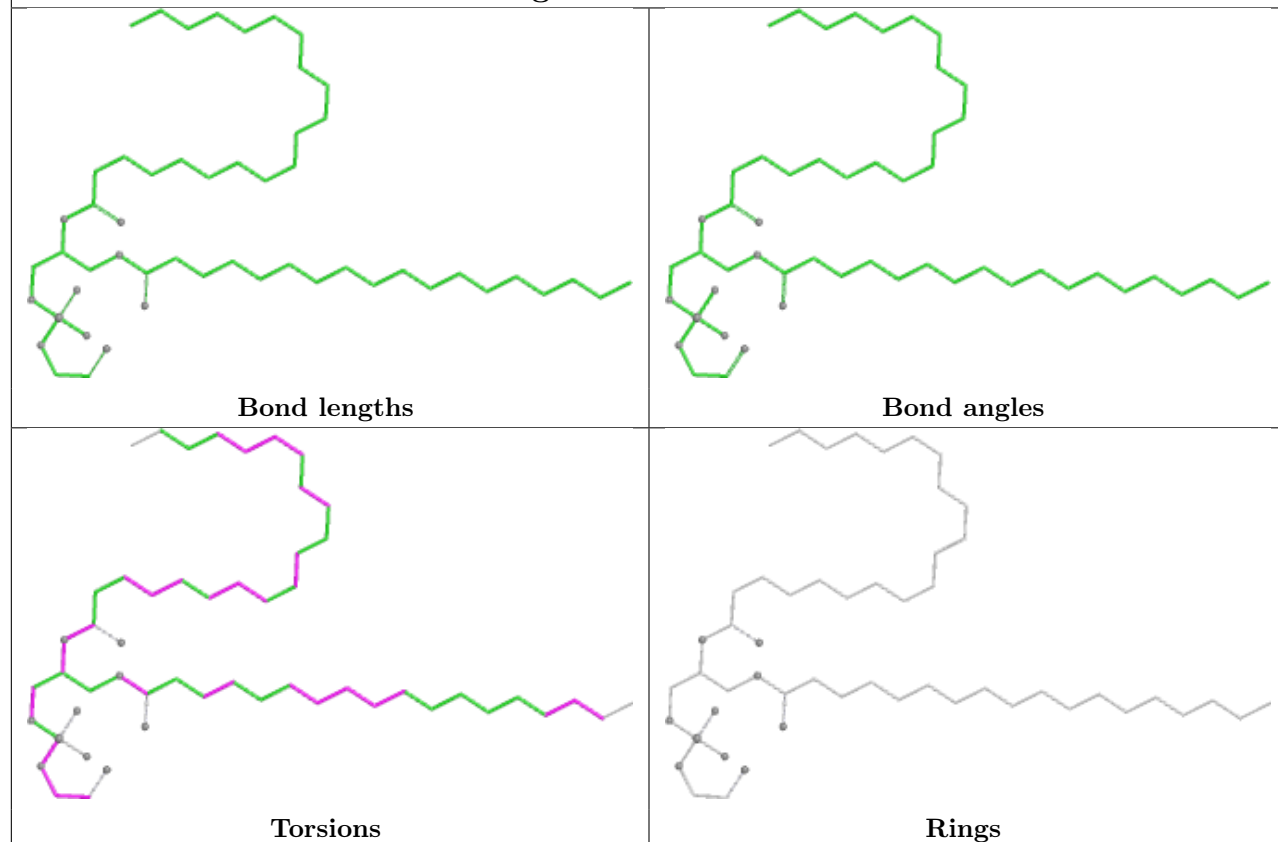
Ligand PSC R 201



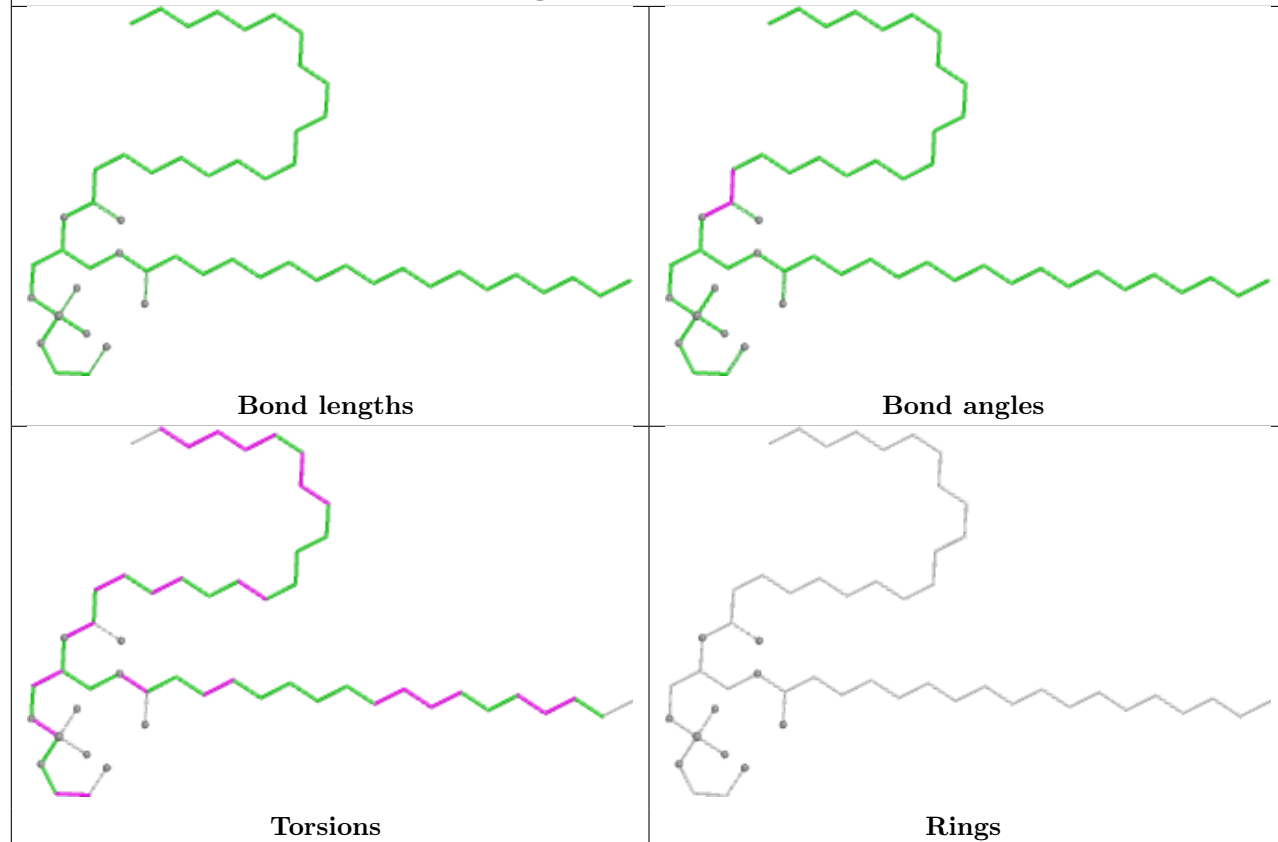
Ligand CHD G 108

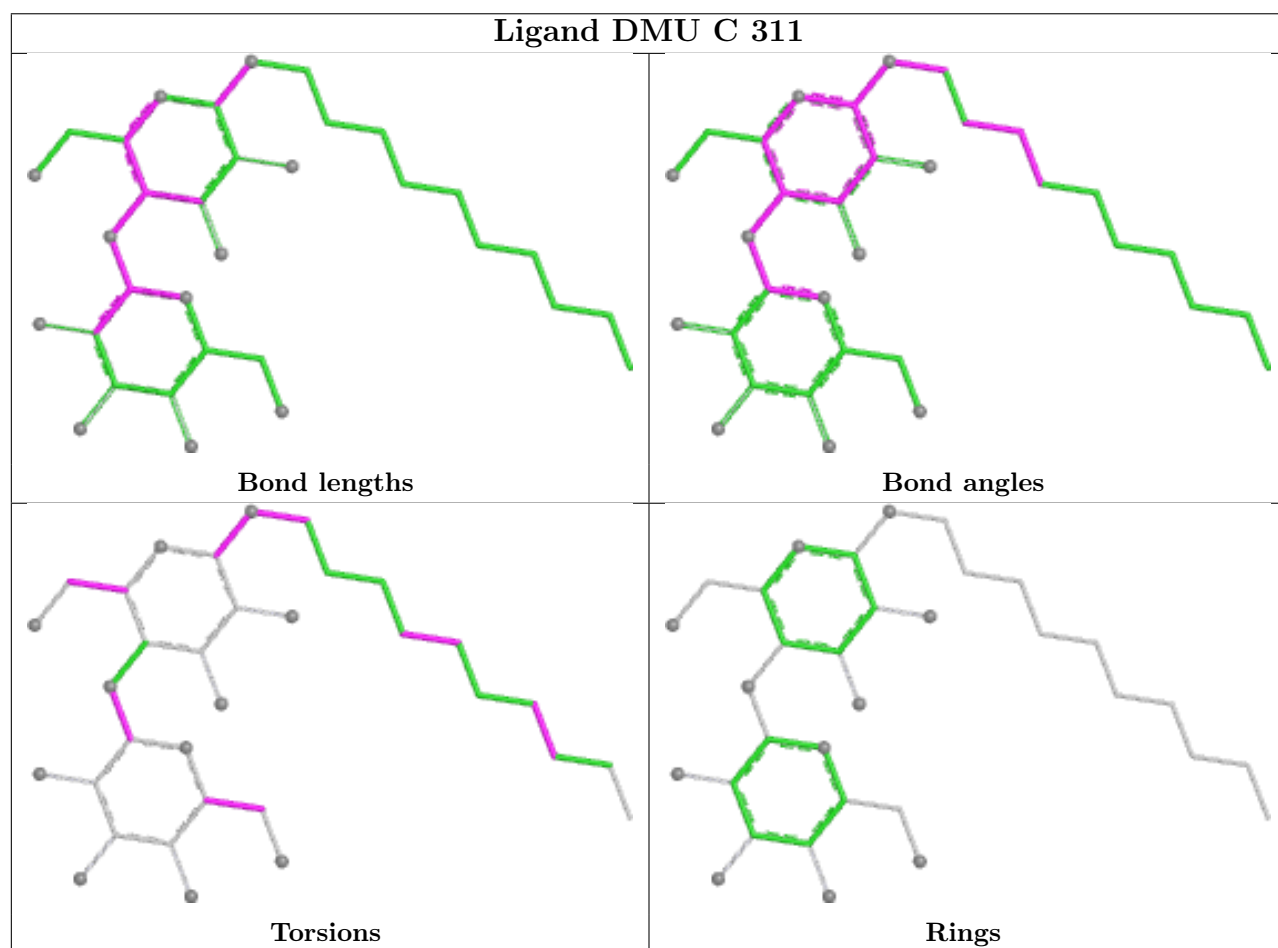
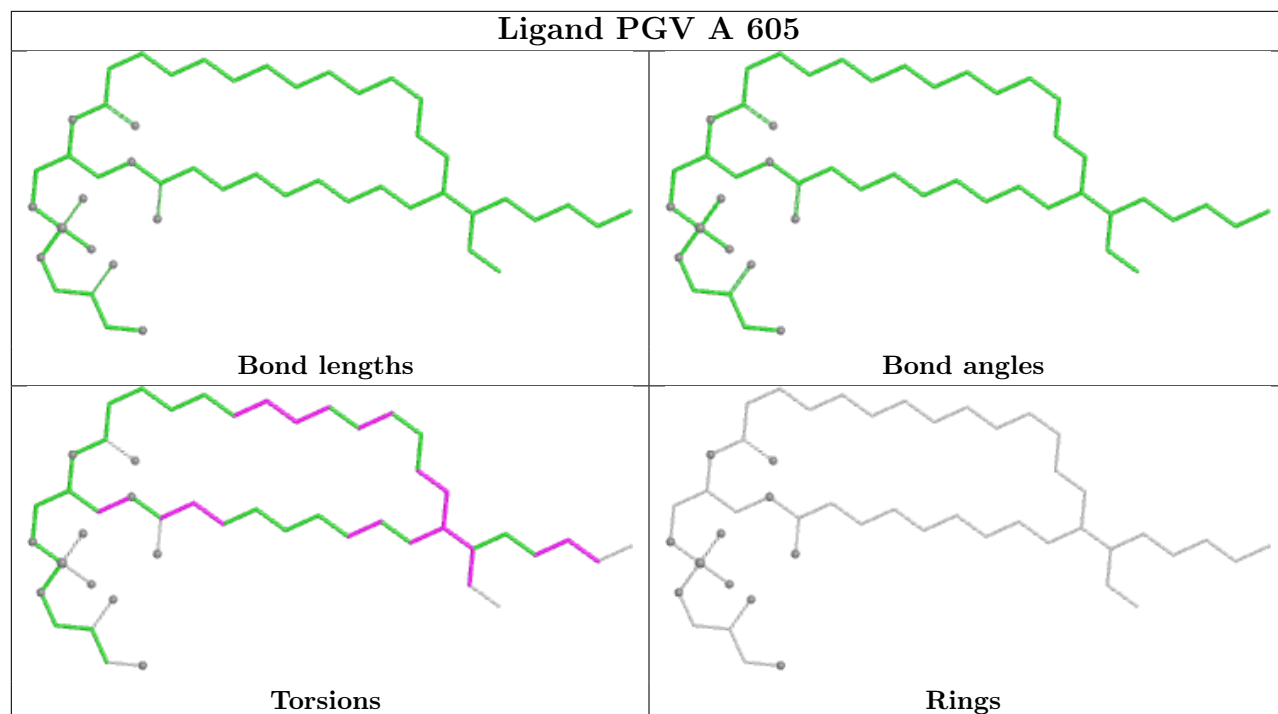


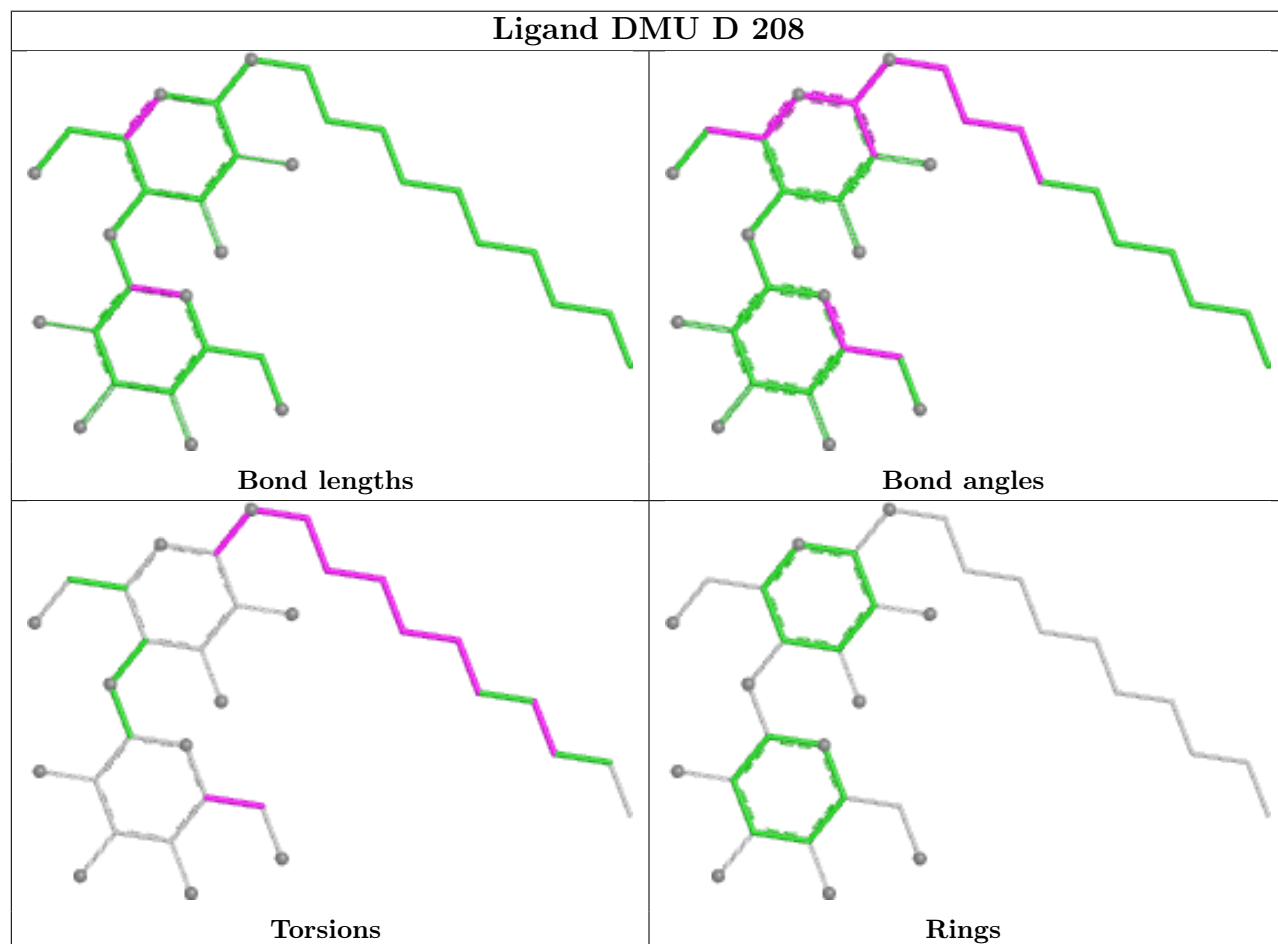
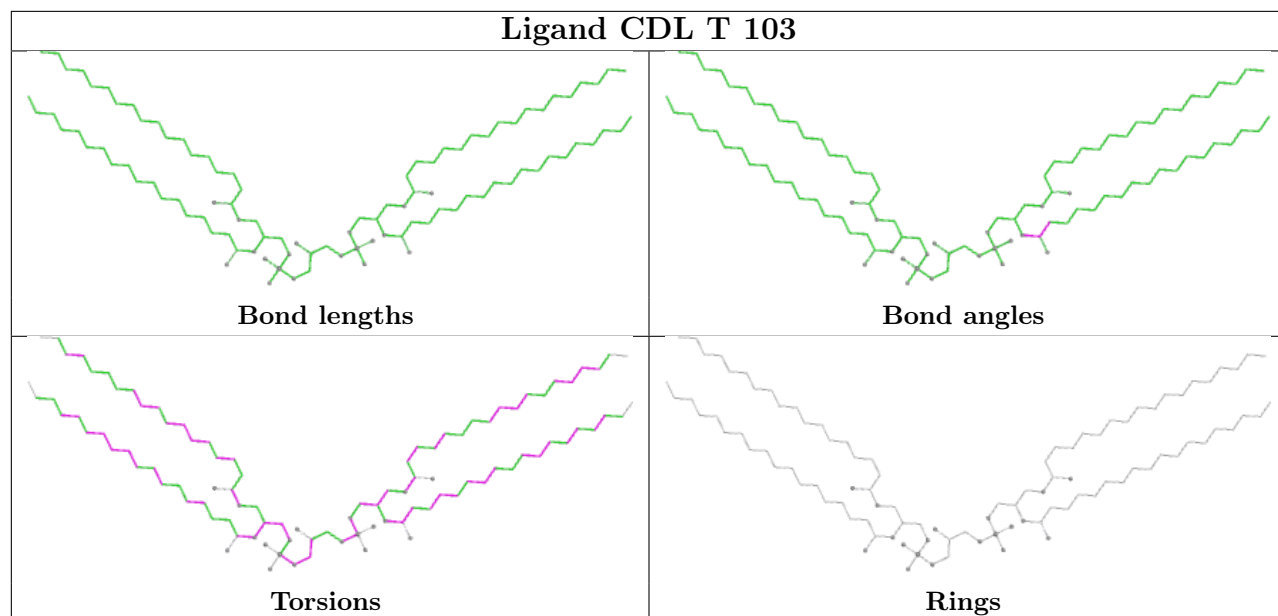
Ligand PEK P 301



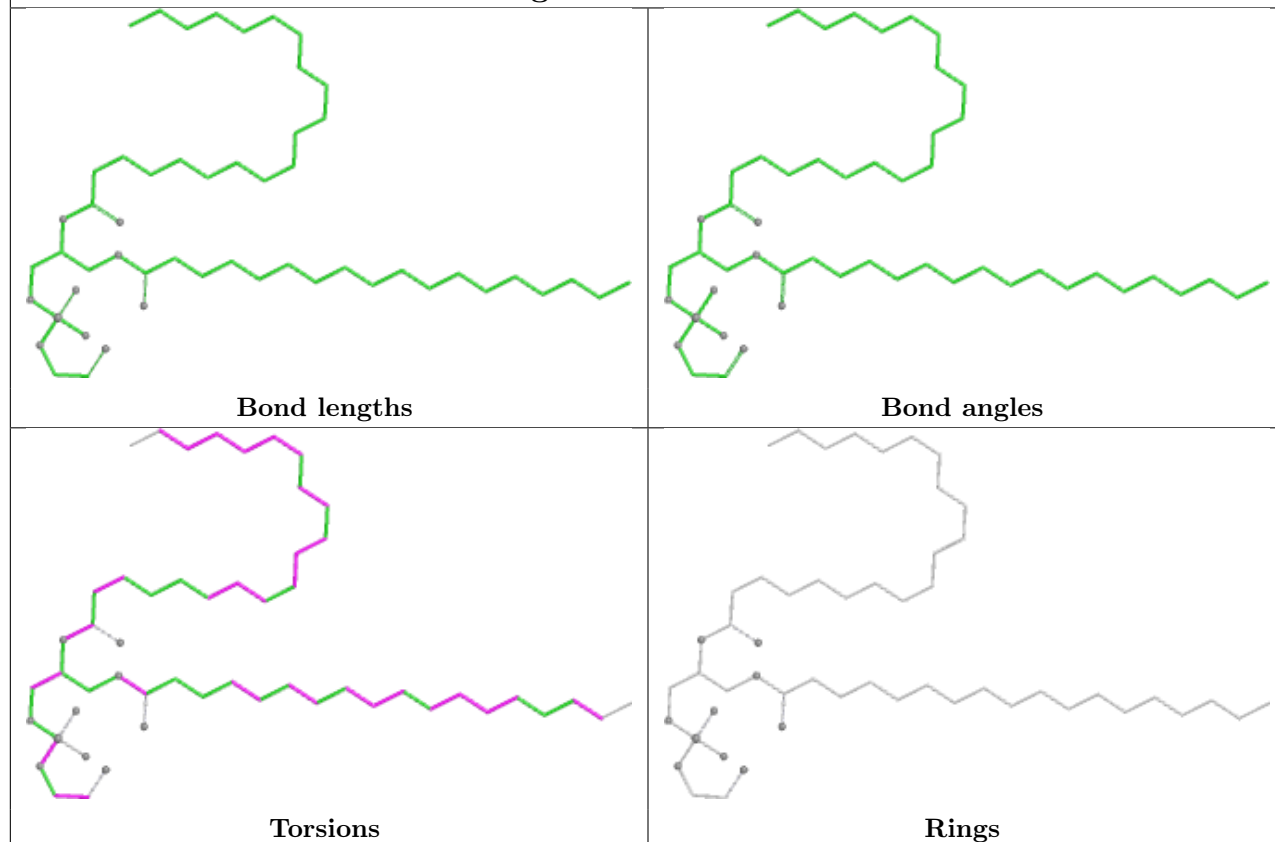
Ligand PEK C 313



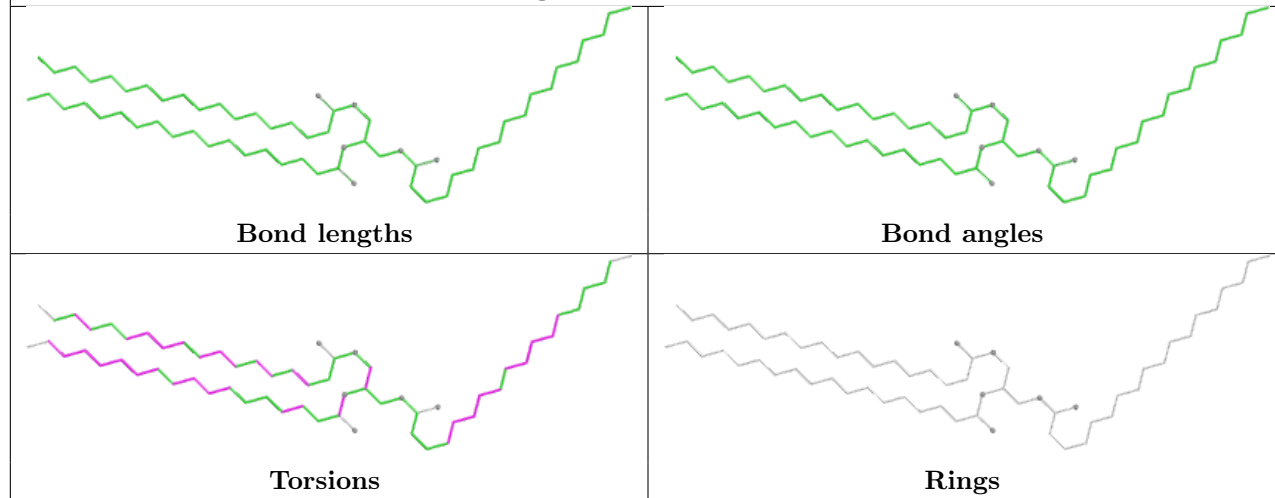


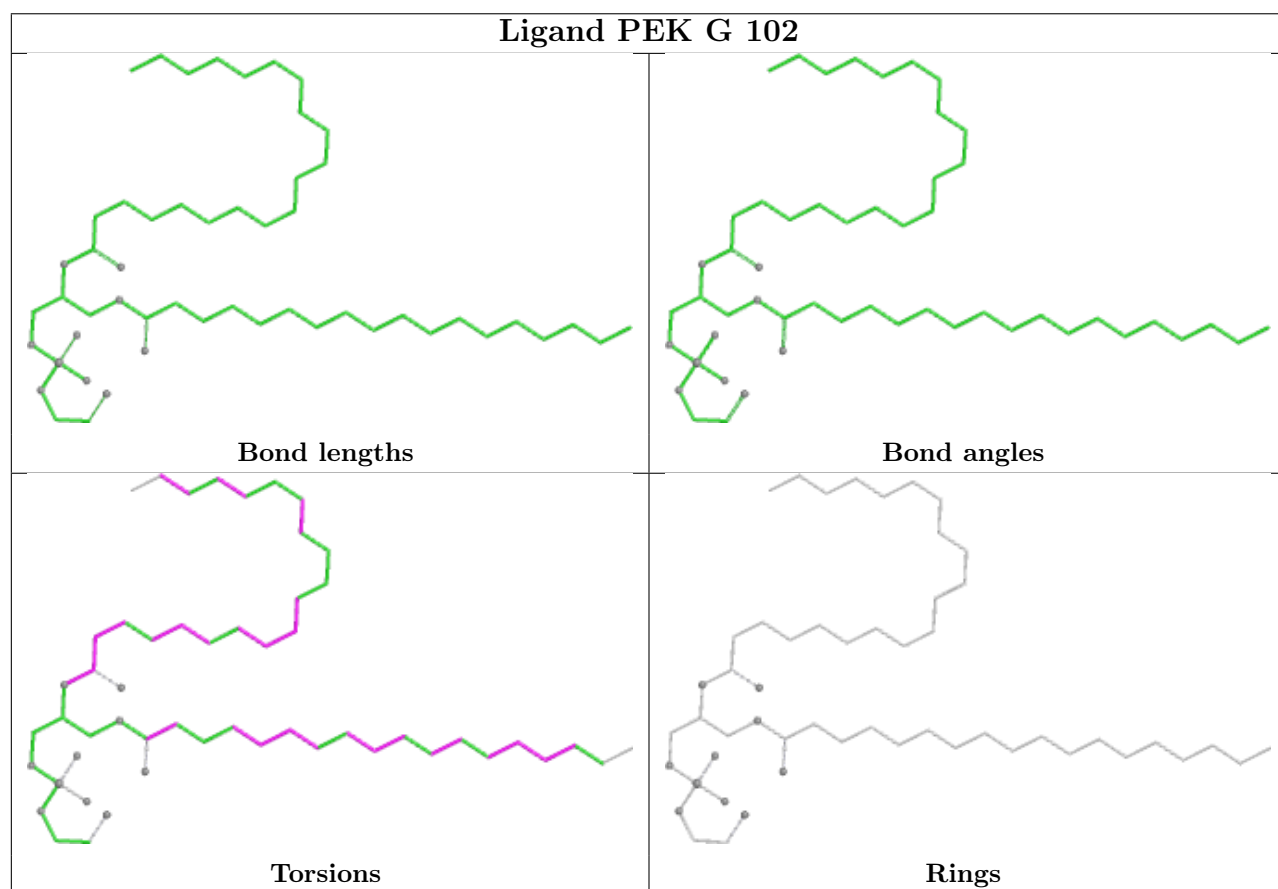
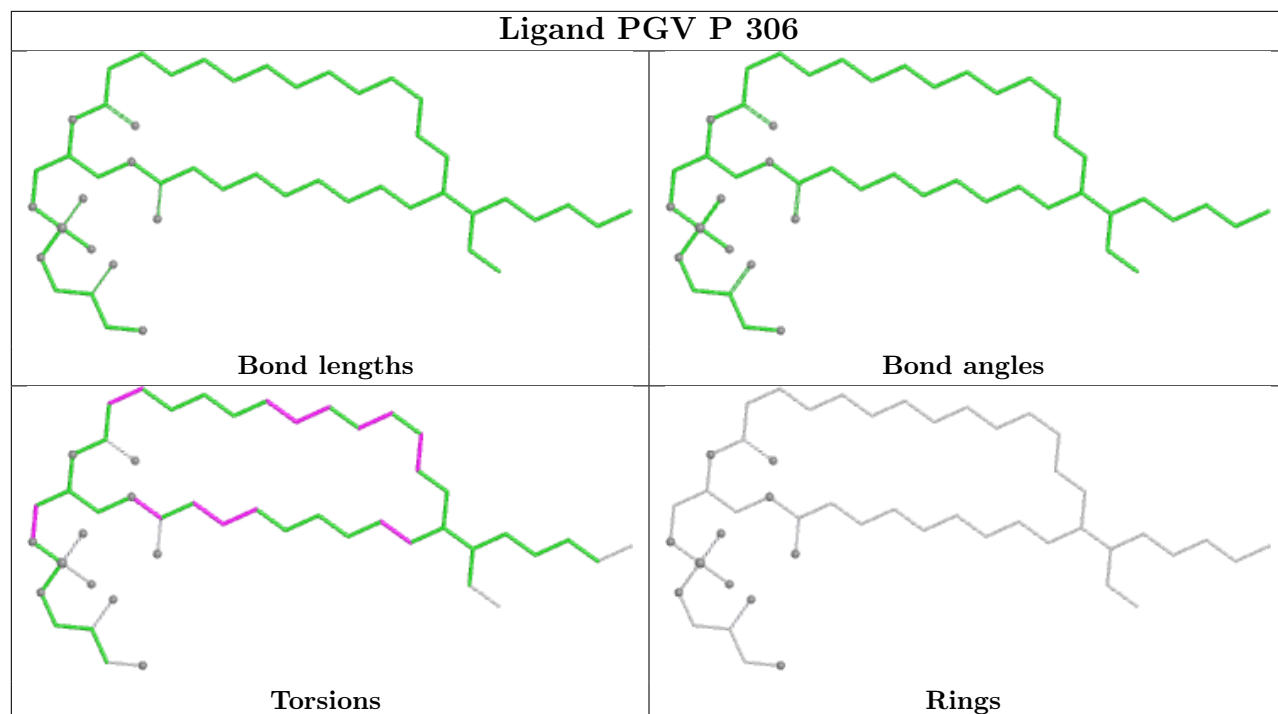


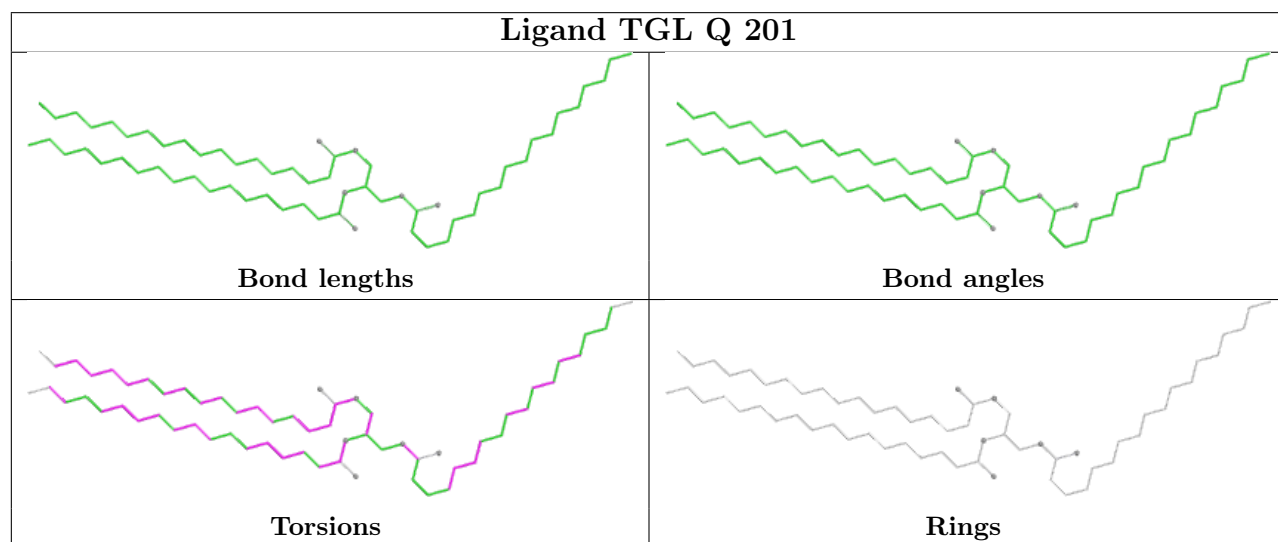
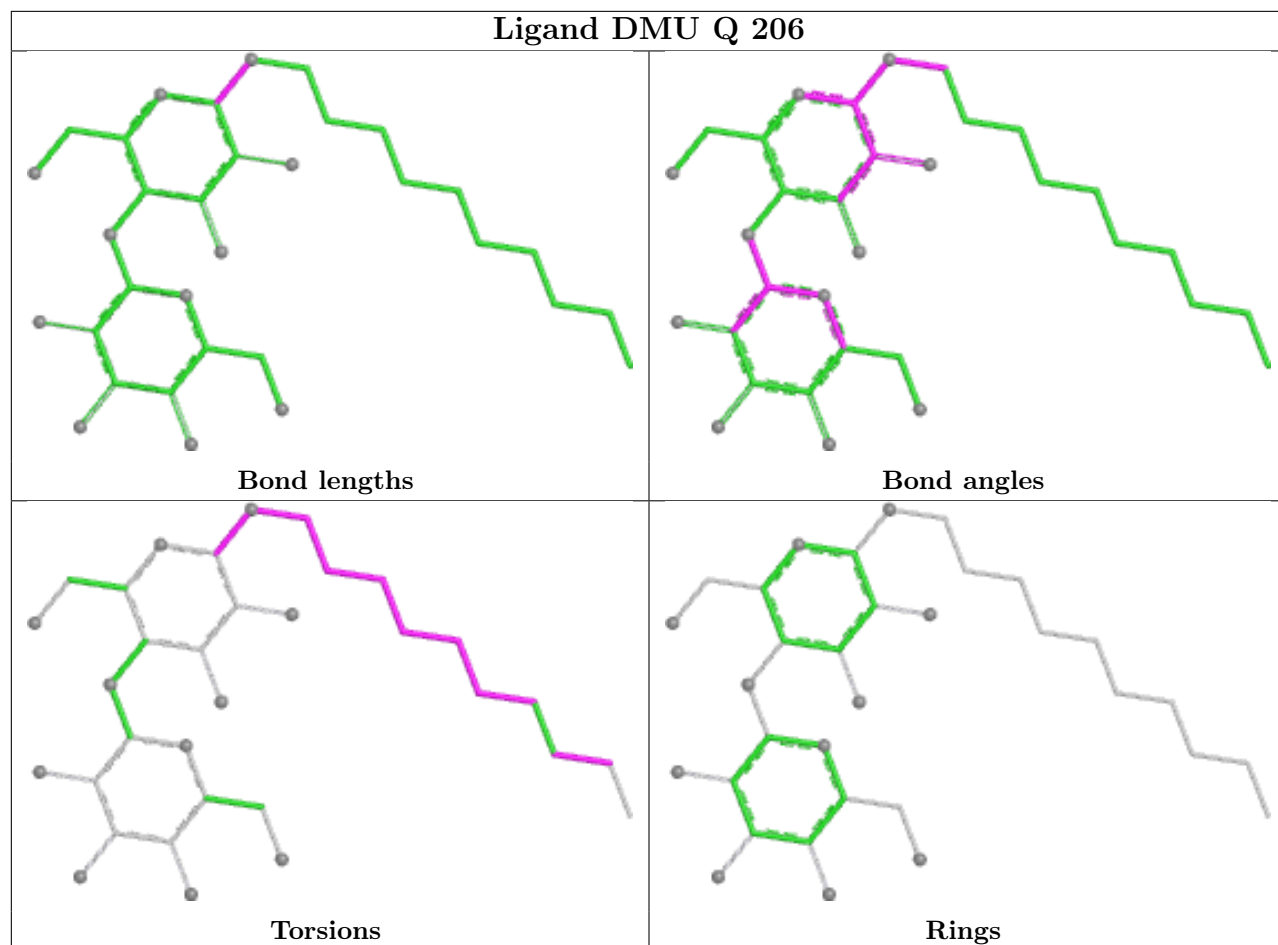
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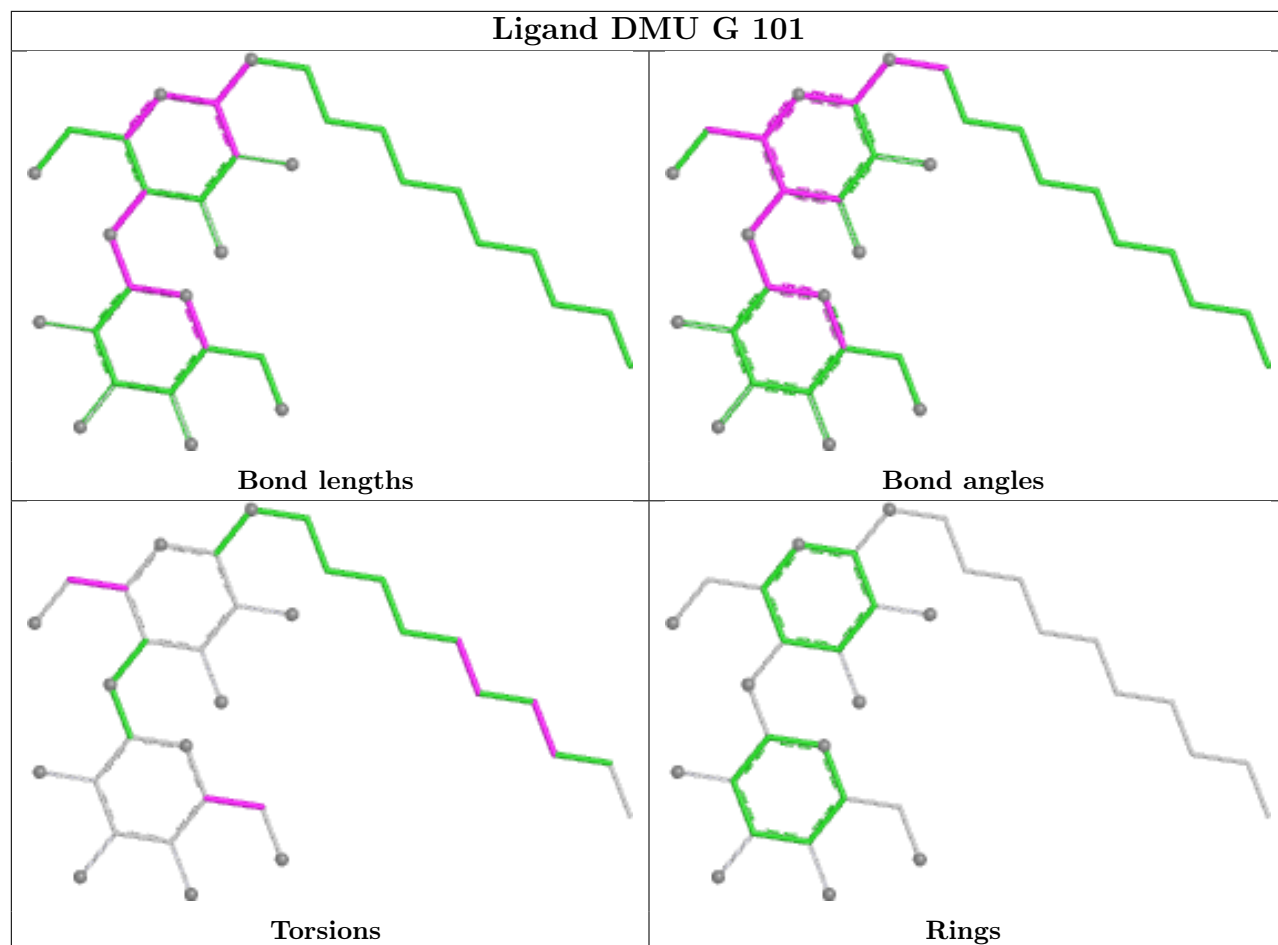


Ligand TGL L 101

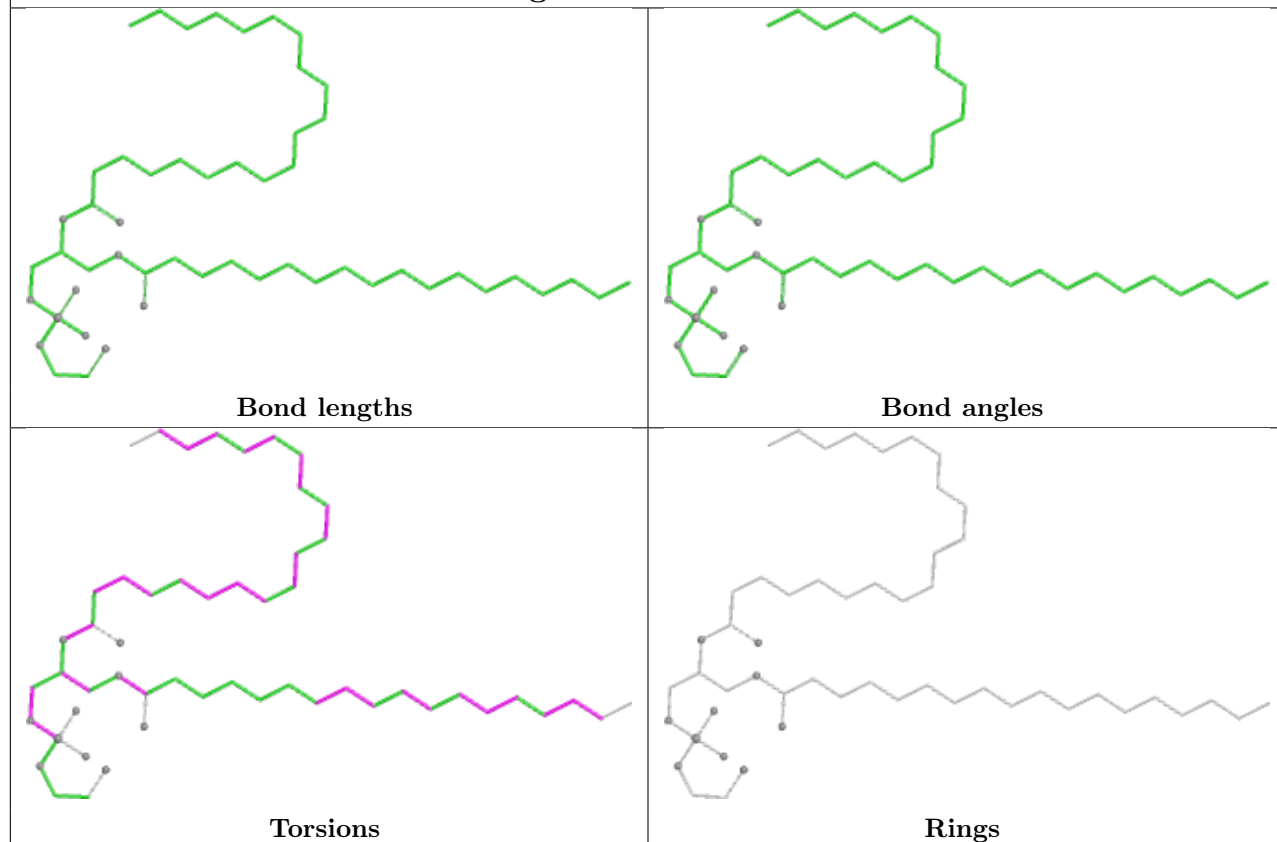




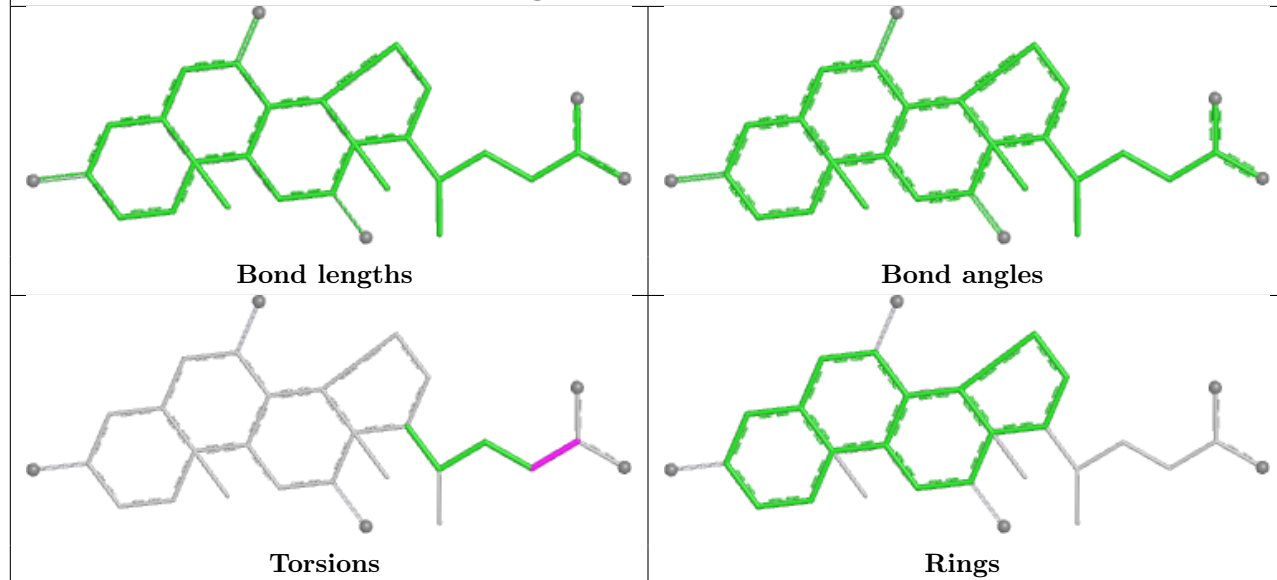


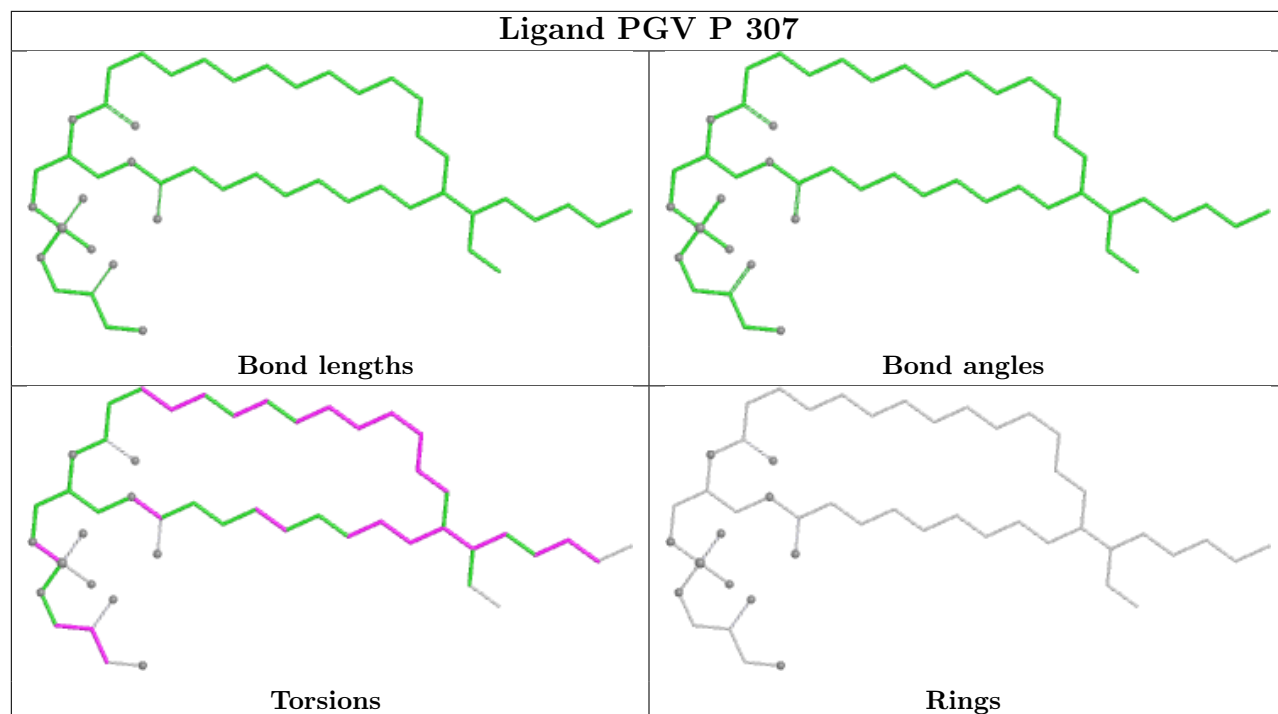


Ligand PEK G 103



Ligand CHD P 304





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.36	1 (0%) 91 92	26, 32, 41, 78	0
1	N	513/514 (99%)	-0.26	1 (0%) 91 92	28, 36, 47, 75	0
2	B	226/227 (99%)	-0.01	6 (2%) 56 63	27, 39, 73, 116	0
2	O	226/227 (99%)	0.12	7 (3%) 51 58	32, 45, 76, 100	0
3	C	259/261 (99%)	-0.31	1 (0%) 88 91	27, 36, 49, 93	0
3	P	259/261 (99%)	-0.26	2 (0%) 82 86	30, 37, 54, 93	0
4	D	144/147 (97%)	-0.14	2 (1%) 73 78	31, 41, 63, 89	0
4	Q	144/147 (97%)	0.66	8 (5%) 30 35	39, 56, 89, 170	0
5	E	105/109 (96%)	-0.17	1 (0%) 79 83	33, 42, 68, 114	0
5	R	105/109 (96%)	0.13	3 (2%) 53 60	38, 50, 73, 112	0
6	F	98/98 (100%)	0.16	6 (6%) 27 31	31, 41, 94, 178	0
6	S	98/98 (100%)	0.13	7 (7%) 22 25	32, 43, 99, 135	0
7	G	83/85 (97%)	0.96	19 (22%) 2 1	32, 44, 113, 120	0
7	T	83/85 (97%)	0.89	15 (18%) 3 3	33, 48, 112, 144	0
8	H	79/85 (92%)	0.53	8 (10%) 12 14	32, 45, 104, 110	0
8	U	79/85 (92%)	0.73	12 (15%) 5 6	37, 51, 110, 154	0
9	I	72/73 (98%)	0.36	4 (5%) 30 35	34, 51, 82, 107	0
9	V	72/73 (98%)	0.54	4 (5%) 30 35	40, 58, 82, 98	0
10	J	58/59 (98%)	0.05	2 (3%) 48 55	35, 46, 73, 110	0
10	W	58/59 (98%)	0.18	1 (1%) 69 74	38, 51, 86, 128	0
11	K	49/56 (87%)	0.20	3 (6%) 27 31	33, 45, 64, 70	0
11	X	49/56 (87%)	0.72	5 (10%) 12 13	45, 55, 81, 110	0
12	L	46/47 (97%)	-0.07	2 (4%) 40 45	30, 37, 56, 112	0
12	Y	46/47 (97%)	0.26	3 (6%) 25 28	36, 47, 78, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.00	1 (2%) 61 66	31, 38, 74, 96	0
13	Z	43/46 (93%)	0.26	2 (4%) 36 42	40, 48, 83, 126	0
All	All	3550/3614 (98%)	0.01	126 (3%) 47 53	26, 40, 77, 178	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	9.6
4	Q	6	VAL	9.5
6	F	1	ALA	9.2
6	S	1	ALA	8.4
7	G	3	ALA	8.4
7	G	2	SER	7.7
7	T	1	ALA	7.5
6	F	97	ALA	7.0
8	U	8	ILE	6.9
8	H	8	ILE	6.7
6	F	96	LEU	5.6
7	G	36	TRP	5.4
7	G	5	LYS	5.4
7	T	6	GLY	5.3
7	T	3	ALA	5.3
4	Q	4	SER	5.2
7	G	1	ALA	5.2
11	X	6	ALA	5.1
7	G	9	GLY	5.0
8	U	45	ALA	4.9
7	G	4	ALA	4.9
7	T	10	GLY	4.9
12	L	2	HIS	4.9
4	Q	7	LYS	4.7
7	T	5	LYS	4.7
7	T	8	HIS	4.7
7	T	36	TRP	4.6
7	T	9	GLY	4.6
4	Q	8	SER	4.6
8	U	7	LYS	4.6
9	I	37	PHE	4.5
3	C	3	HIS	4.4
7	G	10	GLY	4.4
4	D	4	SER	4.4

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Mol	Chain	Res	Type	RSRZ
8	U	9	LYS	4.3
9	V	2	THR	4.3
6	F	2	SER	4.2
9	V	37	PHE	4.2
2	B	90	ILE	4.2
10	J	1	PHE	4.1
7	G	6	GLY	4.0
2	B	60	GLU	4.0
8	H	44	THR	3.9
11	X	51	LYS	3.9
7	T	2	SER	3.8
8	H	7	LYS	3.7
11	X	7	PRO	3.7
2	O	90	ILE	3.7
8	U	46	LYS	3.6
3	P	3	HIS	3.6
6	F	98	HIS	3.5
7	T	4	ALA	3.4
7	G	7	ASP	3.4
10	W	58	LYS	3.4
1	N	297	MET	3.3
6	S	93	PRO	3.3
5	E	5	HIS	3.3
6	S	97	ALA	3.2
2	O	113	TYR	3.2
12	L	47	LYS	3.2
8	H	46	LYS	3.1
7	G	40	GLY	3.1
10	J	58	LYS	3.1
6	S	95	GLN	3.1
6	S	96	LEU	3.1
7	G	41	HIS	3.1
11	K	6	ALA	3.1
7	T	37	LEU	3.1
7	T	42	ARG	3.0
7	G	8	HIS	3.0
6	S	43	LYS	3.0
7	G	84	LYS	3.0
8	H	45	ALA	2.9
12	Y	2	HIS	2.9
9	I	36	LYS	2.8
7	T	33	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	Q	35	ALA	2.8
8	H	42	ALA	2.8
8	U	16	PHE	2.8
2	B	87	MET	2.7
5	R	109	VAL	2.7
6	S	98	HIS	2.7
6	F	95	GLN	2.7
8	U	47	GLY	2.7
2	O	86	MET	2.7
5	R	5	HIS	2.6
2	B	58	ALA	2.6
8	H	9	LYS	2.6
2	O	32	PHE	2.6
2	O	227	LEU	2.5
8	H	48	GLY	2.5
7	G	37	LEU	2.4
8	U	10	ASN	2.4
7	T	7	ASP	2.4
13	Z	43	SER	2.4
4	D	5	VAL	2.4
2	O	129	LYS	2.3
7	G	35	SER	2.3
9	V	25	PHE	2.3
11	K	54	ARG	2.3
4	Q	9	GLU	2.3
9	V	73	LYS	2.3
2	B	65	TRP	2.2
7	G	42	ARG	2.2
2	B	40	TYR	2.2
13	Z	32	TRP	2.2
12	Y	24	MET	2.2
7	T	43	GLU	2.2
13	M	42	LYS	2.2
5	R	108	LYS	2.2
8	U	44	THR	2.2
11	X	34	THR	2.2
2	O	16	ILE	2.1
7	G	30	LEU	2.1
9	I	34	PHE	2.1
9	I	26	MET	2.1
1	A	514	LYS	2.1
8	U	80	THR	2.1

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Mol	Chain	Res	Type	RSRZ
11	K	47	ARG	2.1
8	U	18	SER	2.1
3	P	230	ASN	2.0
11	X	54	ARG	2.0
4	Q	31	LYS	2.0
8	U	42	ALA	2.0
7	G	45	PRO	2.0
12	Y	20	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	TPO	G	11	11/12	0.55	0.22	65,112,161,163	0
7	TPO	T	11	11/12	0.63	0.18	86,110,136,136	0
1	FME	A	1	10/11	0.90	0.15	44,54,81,85	0
1	FME	N	1	10/11	0.91	0.14	49,54,81,82	0
2	FME	O	1	10/11	0.94	0.12	43,47,55,60	0
2	FME	B	1	10/11	0.97	0.08	38,39,50,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	SAC	V	101	9/10	0.39	0.21	113,120,131,132	0
29	SAC	I	101	9/10	0.50	0.28	98,111,125,128	0
24	CHD	Y	102	29/29	0.64	0.30	82,140,163,186	0
19	EDO	G	109	4/4	0.65	0.27	91,103,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	W	303	4/4	0.67	0.31	82,85,85,86	0
19	EDO	J	102	4/4	0.67	0.22	74,77,77,79	0
19	EDO	V	103	4/4	0.68	0.39	82,90,92,93	0
19	EDO	Z	1601	4/4	0.70	0.28	77,84,85,86	0
17	PGV	C	303	51/51	0.72	0.30	66,98,125,151	0
27	PEK	C	313	53/53	0.73	0.28	60,84,139,156	0
25	CDL	C	310	100/100	0.73	0.35	61,107,147,165	0
26	DMU	G	101	33/33	0.73	0.24	78,110,150,153	0
19	EDO	G	105	4/4	0.74	0.21	76,80,85,86	0
19	EDO	C	308	4/4	0.75	0.25	74,78,79,80	0
26	DMU	C	312	33/33	0.75	0.17	70,103,119,133	0
19	EDO	A	617	4/4	0.76	0.32	94,103,106,110	0
26	DMU	C	311	33/33	0.77	0.23	82,113,128,132	0
23	PSC	B	303	52/52	0.78	0.28	59,111,180,194	0
24	CHD	T	105	29/29	0.78	0.28	88,161,180,184	0
27	PEK	G	103	53/53	0.79	0.29	65,97,166,172	0
19	EDO	N	614	4/4	0.80	0.34	63,63,67,73	0
17	PGV	N	617	51/51	0.80	0.23	51,90,145,155	0
19	EDO	N	608	4/4	0.80	0.27	47,51,52,56	0
19	EDO	N	612	4/4	0.80	0.36	78,79,85,87	0
27	PEK	P	301	53/53	0.80	0.21	59,87,135,155	0
25	CDL	T	103	100/100	0.80	0.28	59,107,145,164	0
22	TGL	Q	201	63/63	0.80	0.29	66,92,121,137	0
23	PSC	R	201	52/52	0.81	0.29	56,99,184,199	0
17	PGV	A	604	51/51	0.81	0.24	48,83,126,130	0
27	PEK	P	305	53/53	0.81	0.28	63,98,164,174	0
26	DMU	P	303	33/33	0.81	0.14	54,103,121,129	0
19	EDO	J	103	4/4	0.81	0.22	52,57,63,64	0
19	EDO	B	309	4/4	0.82	0.23	65,72,78,81	0
22	TGL	D	201	63/63	0.82	0.26	48,82,100,115	0
22	TGL	N	604	63/63	0.82	0.28	58,91,131,137	0
19	EDO	E	204	4/4	0.82	0.23	64,64,64,70	0
19	EDO	F	703	4/4	0.82	0.24	53,69,73,77	0
19	EDO	I	102	4/4	0.83	0.23	60,65,66,68	0
17	PGV	P	307	51/51	0.83	0.25	69,104,132,144	0
22	TGL	B	302	63/63	0.84	0.27	49,85,110,116	0
19	EDO	C	306	4/4	0.84	0.19	44,45,48,49	0
19	EDO	E	205	4/4	0.85	0.16	60,69,70,70	0
19	EDO	A	612	4/4	0.85	0.21	54,63,65,65	0
19	EDO	O	303	4/4	0.85	0.20	69,73,77,81	0
22	TGL	Y	101	63/63	0.85	0.23	52,69,126,140	0
19	EDO	V	102	4/4	0.85	0.20	72,80,81,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	CDL	P	308	100/100	0.86	0.22	51,90,120,128	0
19	EDO	S	104	4/4	0.86	0.19	71,79,81,82	0
19	EDO	A	611	4/4	0.86	0.18	64,65,67,68	0
19	EDO	O	302	4/4	0.86	0.21	68,74,75,80	0
19	EDO	D	205	4/4	0.86	0.26	91,98,101,105	0
19	EDO	R	203	4/4	0.86	0.17	64,65,66,68	0
22	TGL	L	101	63/63	0.87	0.22	43,70,121,131	0
19	EDO	D	202	4/4	0.87	0.18	53,67,72,74	0
25	CDL	C	304	100/100	0.87	0.22	52,92,118,123	0
19	EDO	N	610	4/4	0.87	0.20	66,69,69,72	0
19	EDO	B	306	4/4	0.88	0.14	55,59,62,65	0
19	EDO	B	311	4/4	0.88	0.21	91,92,93,96	0
19	EDO	P	314	4/4	0.88	0.19	67,74,77,79	0
24	CHD	J	101	29/29	0.89	0.13	53,72,92,93	0
19	EDO	Q	204	4/4	0.89	0.19	68,76,83,84	0
19	EDO	G	107	4/4	0.89	0.20	60,62,62,62	0
26	DMU	Q	206	33/33	0.89	0.13	53,68,83,92	0
19	EDO	G	106	4/4	0.89	0.14	54,60,62,69	0
19	EDO	A	613	4/4	0.90	0.20	56,65,70,76	0
19	EDO	B	308	4/4	0.90	0.20	63,65,72,74	0
19	EDO	N	611	4/4	0.90	0.20	65,68,70,73	0
19	EDO	J	104	4/4	0.90	0.17	67,74,78,79	0
19	EDO	K	102	4/4	0.90	0.11	62,64,64,66	0
19	EDO	N	615	4/4	0.90	0.16	56,57,60,60	0
19	EDO	S	105	4/4	0.90	0.14	67,68,70,71	0
24	CHD	W	302	29/29	0.90	0.12	66,74,96,98	0
19	EDO	B	307	4/4	0.91	0.18	64,68,70,70	0
19	EDO	Q	205	4/4	0.91	0.18	61,69,79,83	0
19	EDO	D	203	4/4	0.91	0.15	53,57,61,62	0
19	EDO	B	305	4/4	0.91	0.14	55,62,66,67	0
19	EDO	D	206	4/4	0.91	0.13	55,56,57,61	0
19	EDO	A	615	4/4	0.91	0.14	61,66,67,68	0
19	EDO	C	307	4/4	0.92	0.12	66,66,70,76	0
19	EDO	J	105	4/4	0.92	0.11	58,62,62,66	0
19	EDO	N	613	4/4	0.92	0.16	51,64,70,75	0
19	EDO	K	101	4/4	0.92	0.12	58,60,61,61	0
19	EDO	D	207	4/4	0.92	0.19	64,65,68,73	0
19	EDO	T	104	4/4	0.92	0.17	58,60,63,64	0
19	EDO	L	102	4/4	0.92	0.15	63,64,64,65	0
24	CHD	P	309	29/29	0.92	0.10	55,63,68,74	0
19	EDO	A	610	4/4	0.92	0.13	41,42,45,49	0
19	EDO	P	313	4/4	0.92	0.13	51,52,54,59	0

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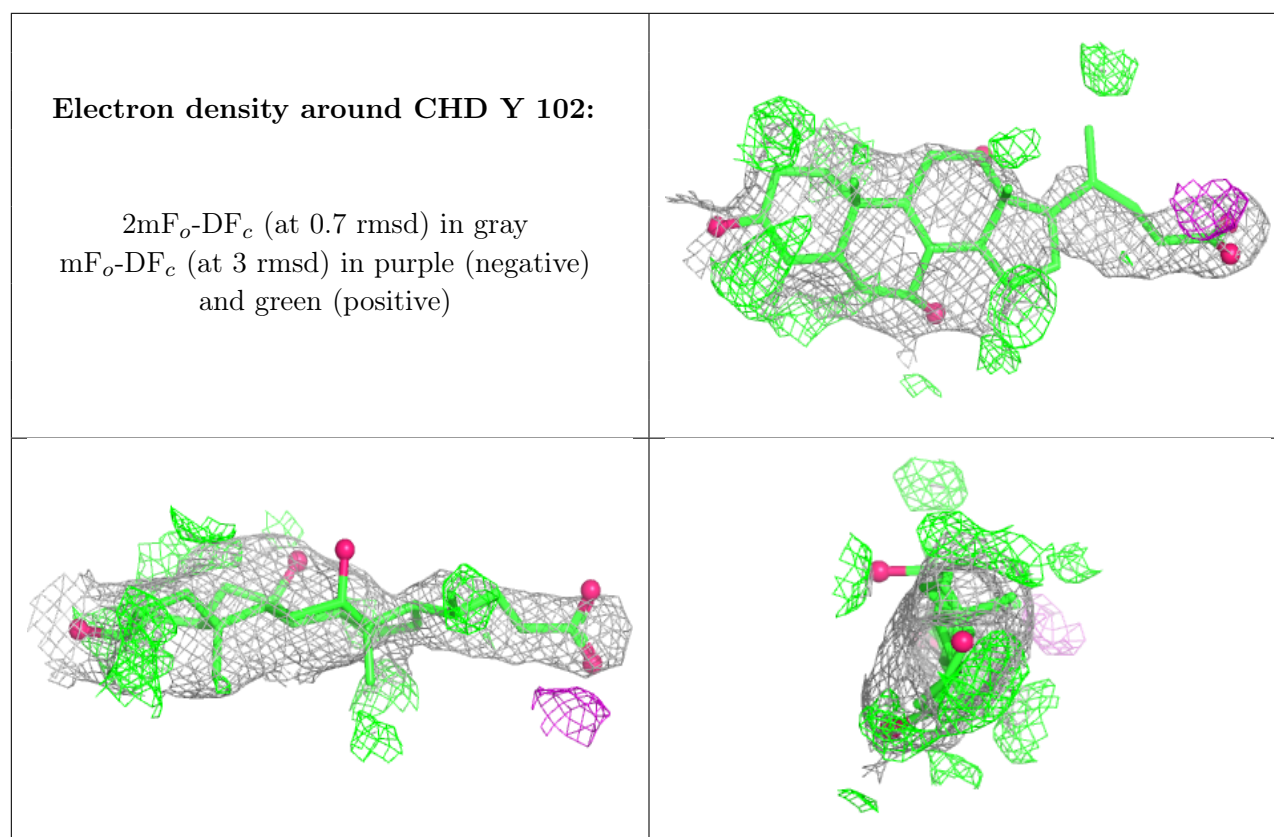
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	C	309	4/4	0.92	0.15	78,78,78,81	0
19	EDO	Q	202	4/4	0.92	0.16	61,64,68,76	0
19	EDO	Q	203	4/4	0.92	0.12	58,62,64,66	0
19	EDO	P	312	4/4	0.93	0.13	53,56,57,58	0
19	EDO	A	608	4/4	0.93	0.15	47,56,59,61	0
19	EDO	S	103	4/4	0.93	0.17	73,74,74,77	0
19	EDO	B	310	4/4	0.93	0.11	57,60,62,64	0
24	CHD	C	305	29/29	0.93	0.09	53,55,59,63	0
19	EDO	A	614	4/4	0.93	0.16	55,56,57,57	0
19	EDO	P	310	4/4	0.93	0.13	61,67,71,78	0
19	EDO	P	311	4/4	0.93	0.15	68,72,74,76	0
26	DMU	D	208	33/33	0.93	0.09	42,53,75,76	0
19	EDO	R	202	4/4	0.94	0.10	57,58,60,60	0
19	EDO	D	204	4/4	0.94	0.14	65,67,69,70	0
19	EDO	W	301	4/4	0.94	0.15	69,75,80,80	0
19	EDO	M	701	4/4	0.94	0.12	67,69,70,75	0
19	EDO	I	103	4/4	0.94	0.12	61,62,67,68	0
27	PEK	T	102	53/53	0.94	0.15	35,54,100,105	0
19	EDO	G	104	4/4	0.94	0.13	37,39,40,42	0
19	EDO	E	203	4/4	0.94	0.12	54,55,58,59	0
24	CHD	T	101	29/29	0.95	0.08	32,38,43,47	0
27	PEK	G	102	53/53	0.95	0.14	32,53,88,100	0
19	EDO	A	616	4/4	0.95	0.18	68,69,72,72	0
15	MG	N	602	1/1	0.95	0.05	35,35,35,35	0
24	CHD	C	301	29/29	0.95	0.08	35,37,40,44	0
19	EDO	N	616	4/4	0.95	0.16	70,70,73,74	0
19	EDO	F	701	4/4	0.95	0.10	43,44,45,46	0
19	EDO	S	102	4/4	0.95	0.11	37,38,39,39	0
19	EDO	A	609	4/4	0.96	0.08	30,33,33,35	0
19	EDO	B	304	4/4	0.96	0.10	32,35,36,39	0
17	PGV	P	302	51/51	0.96	0.11	28,51,74,75	0
17	PGV	A	605	51/51	0.96	0.11	28,44,72,73	0
19	EDO	E	201	4/4	0.96	0.07	47,48,49,49	0
19	EDO	N	607	4/4	0.96	0.06	35,35,36,36	0
19	EDO	E	202	4/4	0.96	0.09	49,53,54,54	0
19	EDO	N	609	4/4	0.96	0.14	51,52,53,53	0
17	PGV	C	302	51/51	0.96	0.12	30,44,100,102	0
17	PGV	P	306	51/51	0.97	0.10	30,45,87,88	0
24	CHD	P	304	29/29	0.97	0.06	31,35,38,40	0
19	EDO	F	704	4/4	0.97	0.08	37,39,41,42	0
15	MG	A	602	1/1	0.97	0.04	31,31,31,31	0
24	CHD	G	108	29/29	0.97	0.05	32,35,39,41	0

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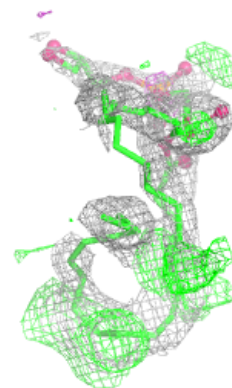
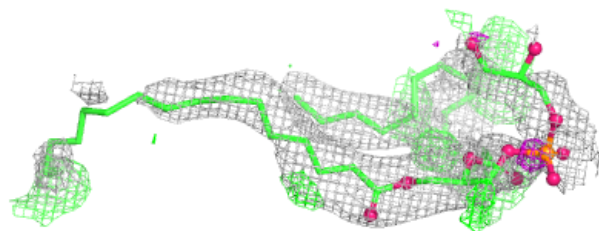
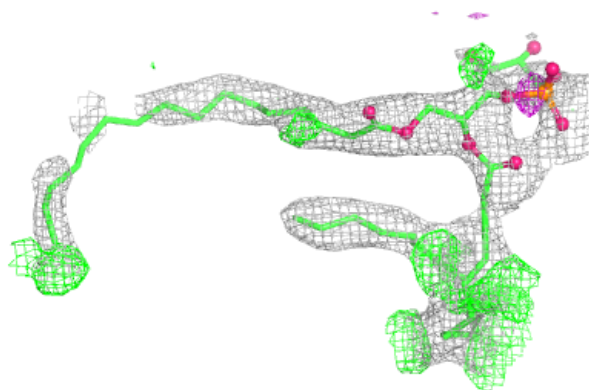
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	HEA	A	606	60/60	0.98	0.06	25,28,37,40	0
18	HEA	A	607	60/60	0.98	0.07	25,31,54,63	0
18	HEA	N	605	60/60	0.98	0.07	28,31,38,40	0
18	HEA	N	606	60/60	0.98	0.07	25,37,47,59	0
16	NA	N	603	1/1	0.99	0.04	32,32,32,32	0
20	OH	N	618	1/1	0.99	0.07	18,18,18,18	1
21	CUA	B	301	2/2	0.99	0.02	30,30,30,31	0
21	CUA	O	301	2/2	0.99	0.03	35,35,35,37	0
16	NA	A	603	1/1	0.99	0.08	30,30,30,30	0
14	CU	A	601	1/1	1.00	0.02	31,31,31,31	0
28	ZN	F	702	1/1	1.00	0.01	36,36,36,36	0
28	ZN	S	101	1/1	1.00	0.02	39,39,39,39	0
14	CU	N	601	1/1	1.00	0.02	33,33,33,33	0
20	OH	A	618	1/1	1.00	0.04	21,21,21,21	1

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.

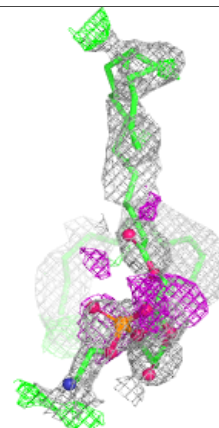
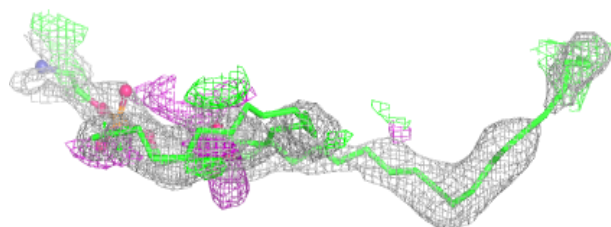
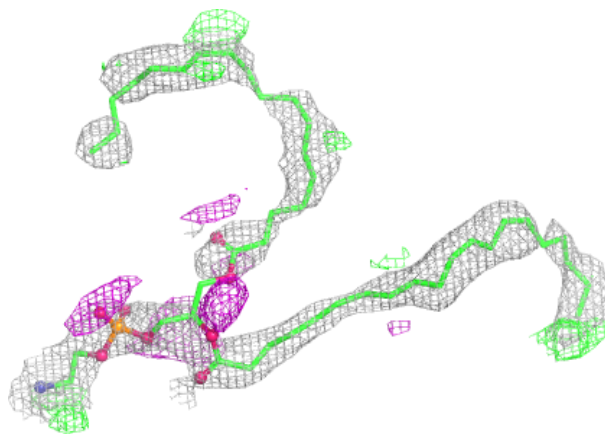


Electron density around PGV C 303:

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

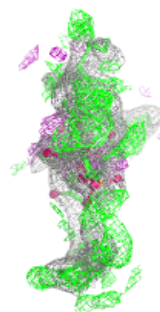
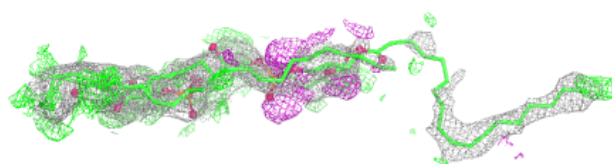
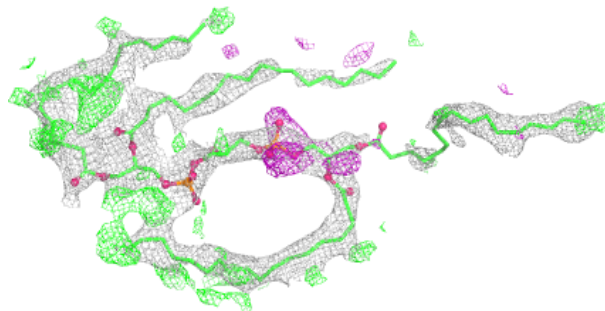
**Electron density around PEK C 313:**

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

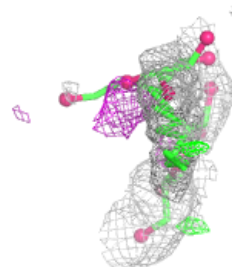
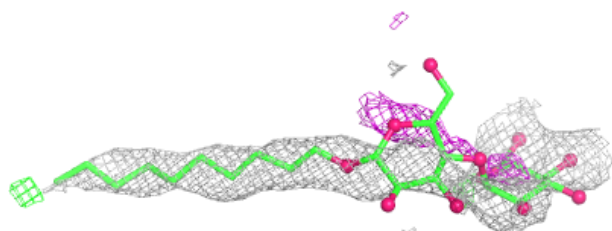
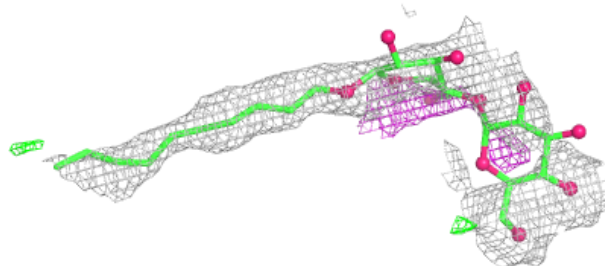


Electron density around CDL C 310:

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

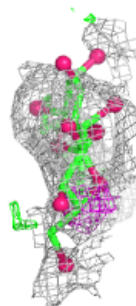
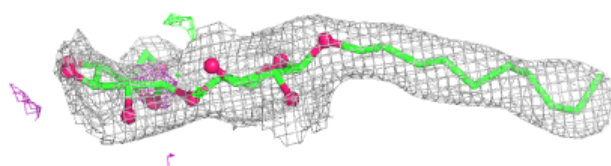
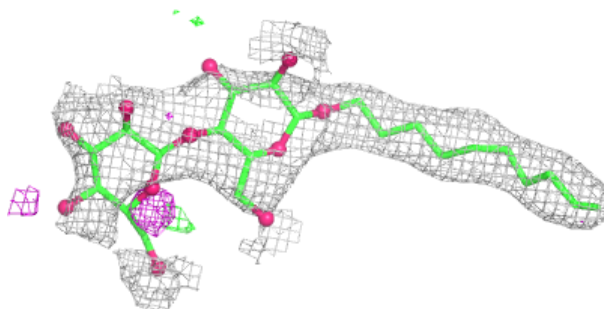
**Electron density around DMU G 101:**

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

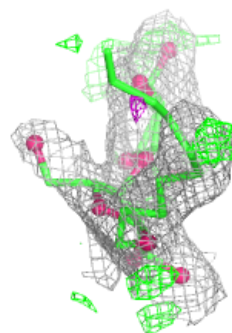
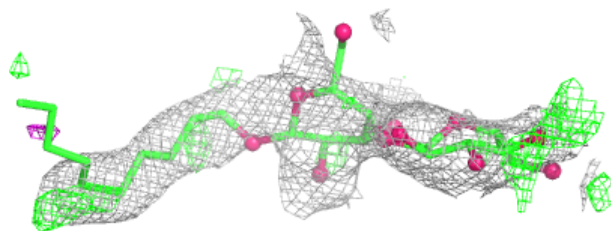
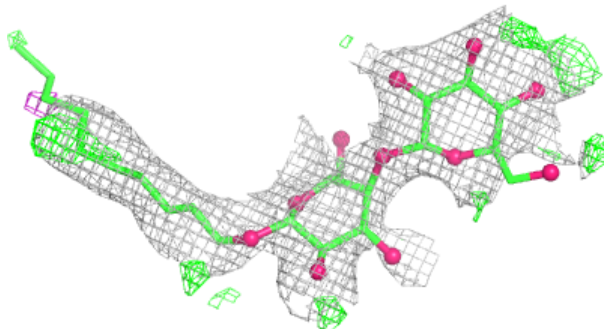


Electron density around DMU C 312:

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

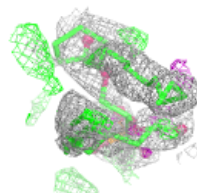
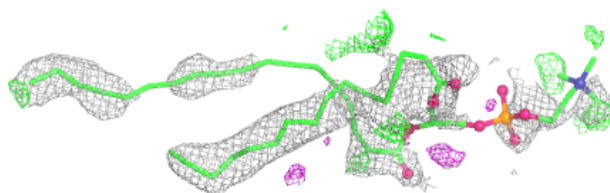
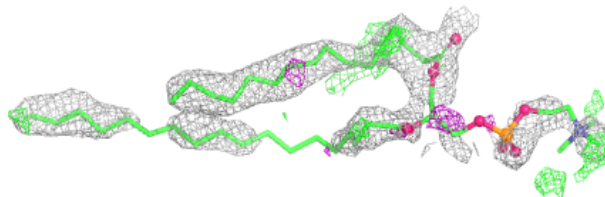
**Electron density around DMU C 311:**

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

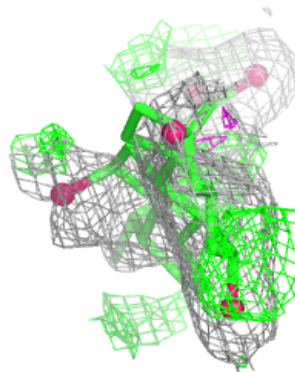
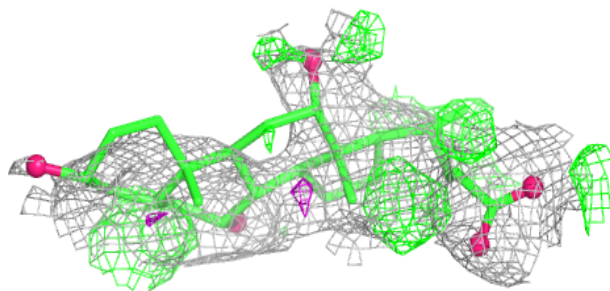
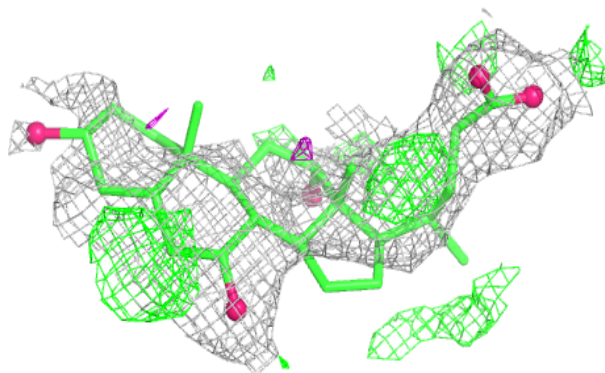


Electron density around PSC B 303:

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

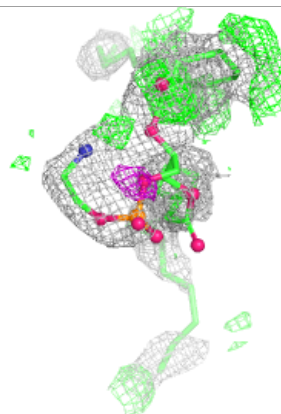
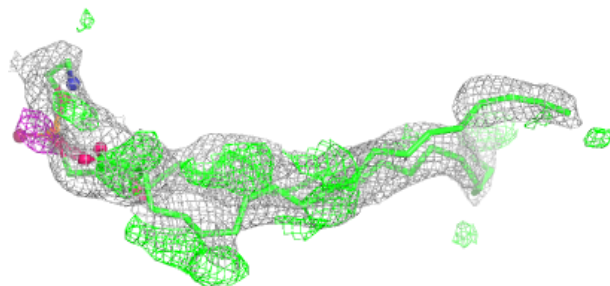
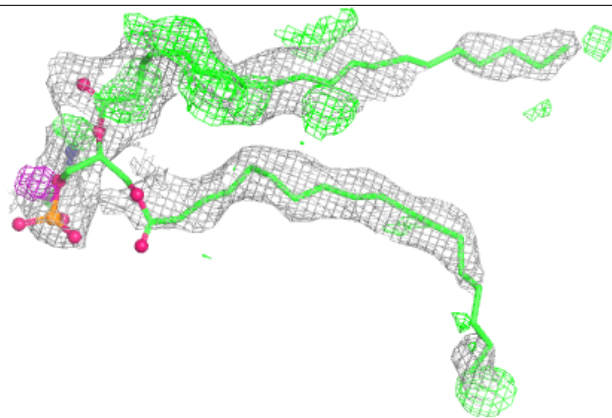
**Electron density around CHD T 105:**

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

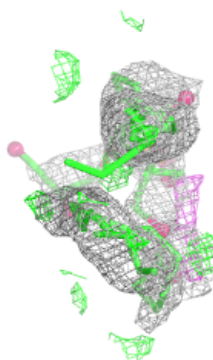
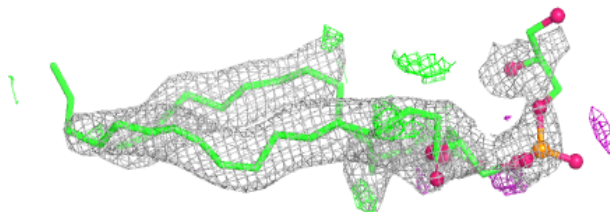
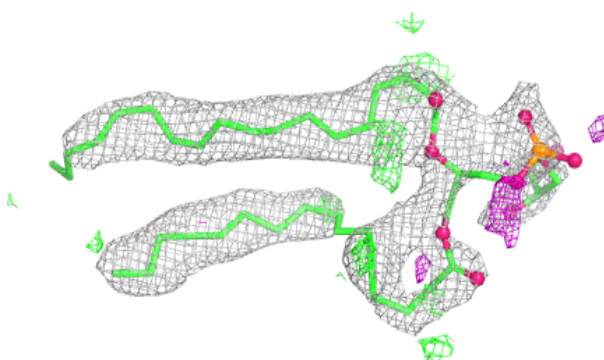


Electron density around PEK G 103:

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

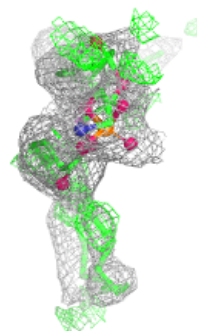
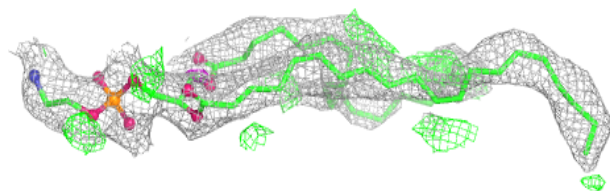
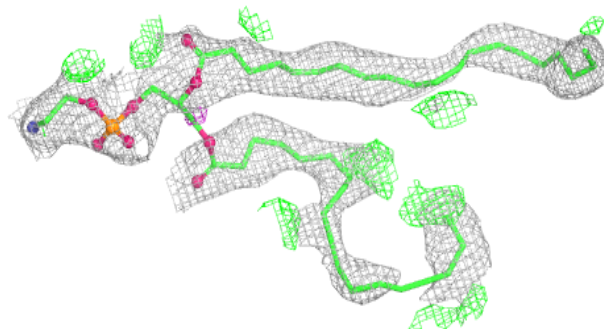
**Electron density around PGV N 617:**

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

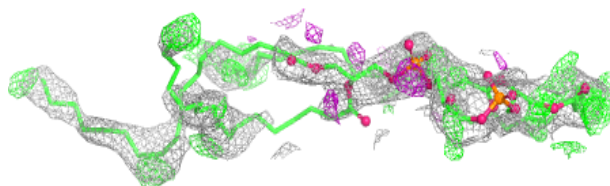
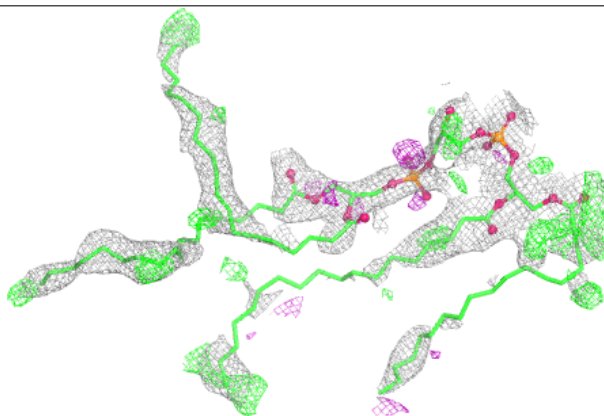


Electron density around PEK P 301:

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

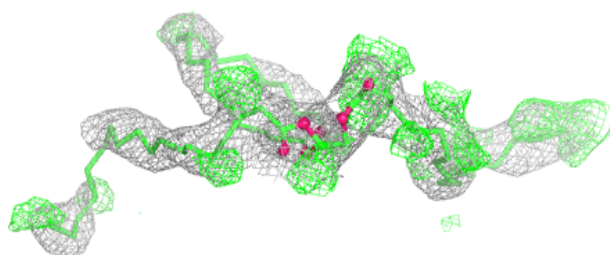
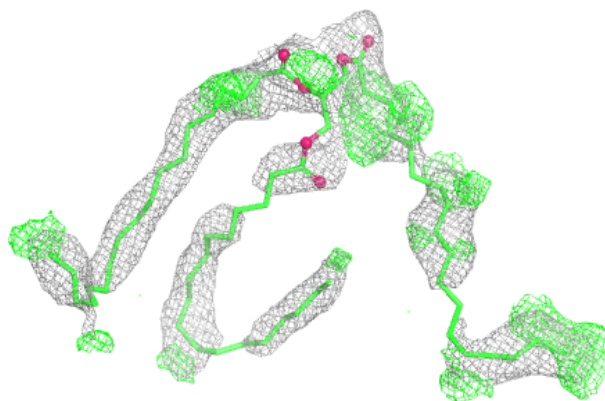
**Electron density around CDL T 103:**

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

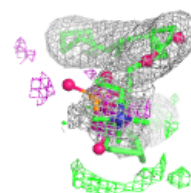
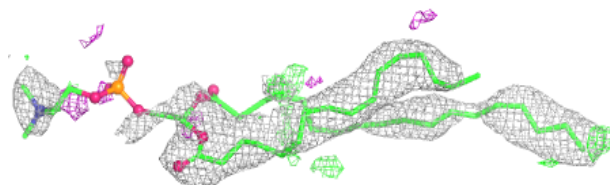
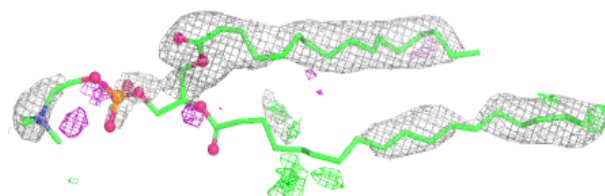


Electron density around TGL Q 201:

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

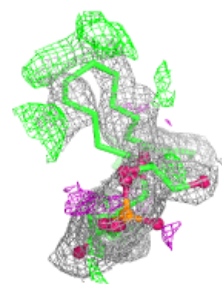
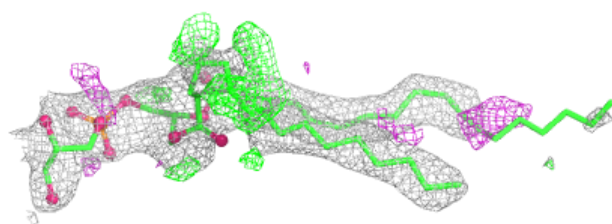
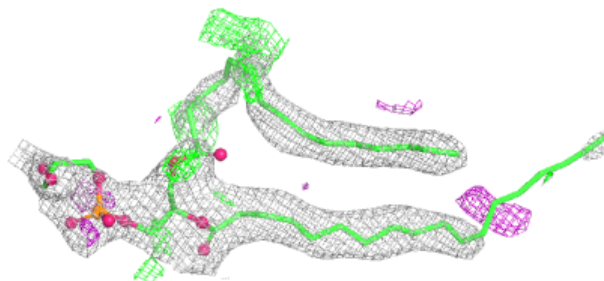
**Electron density around PSC R 201:**

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

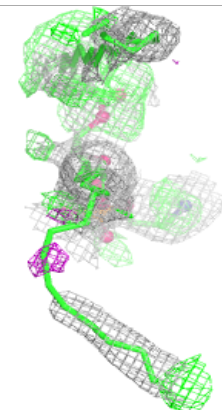
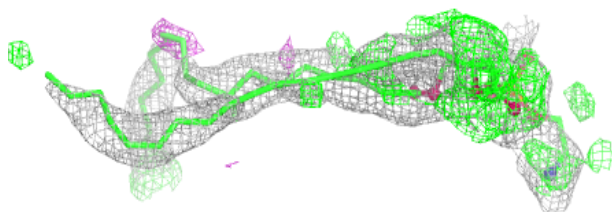
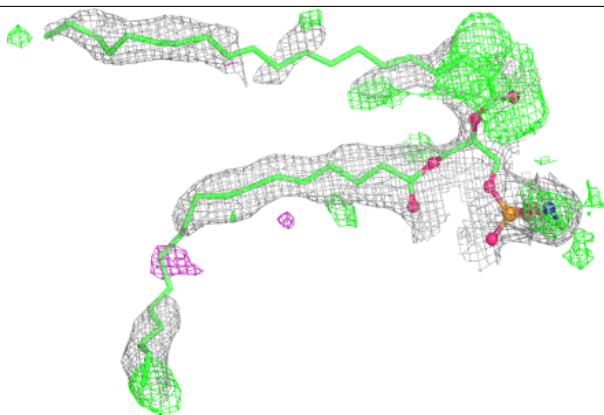


Electron density around PGV A 604:

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

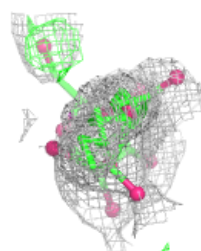
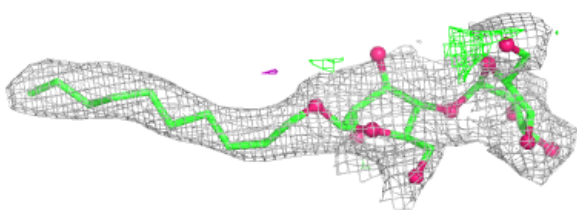
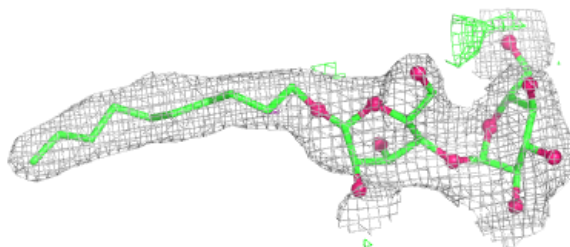
**Electron density around PEK P 305:**

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

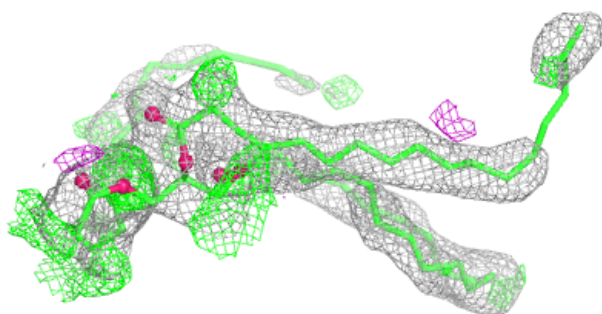
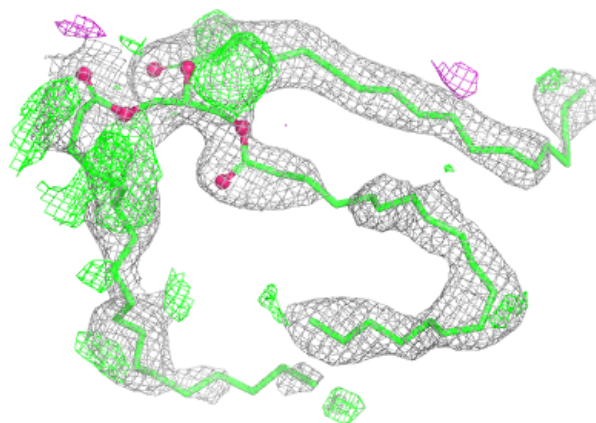


Electron density around DMU P 303:

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

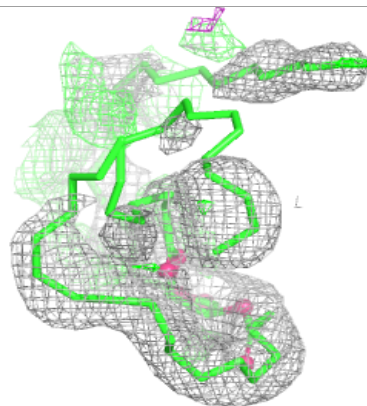
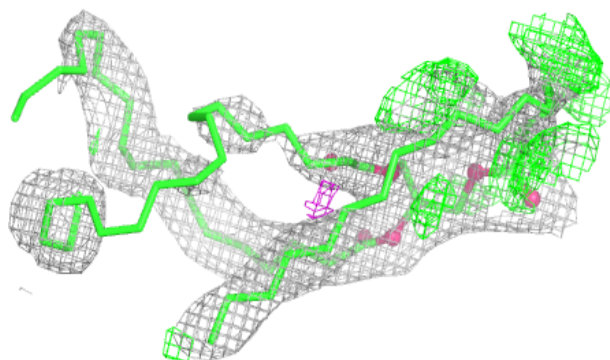
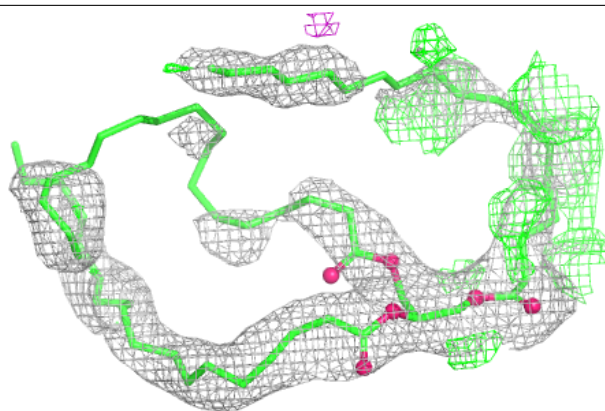
**Electron density around TGL D 201:**

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

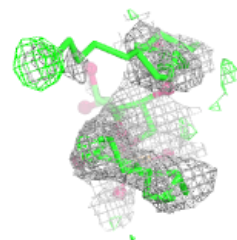
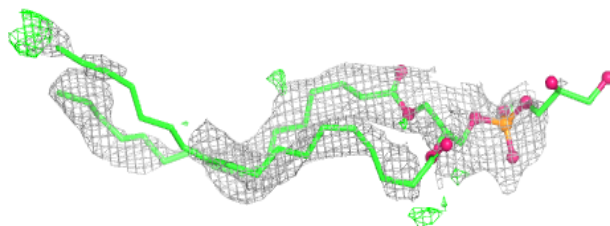
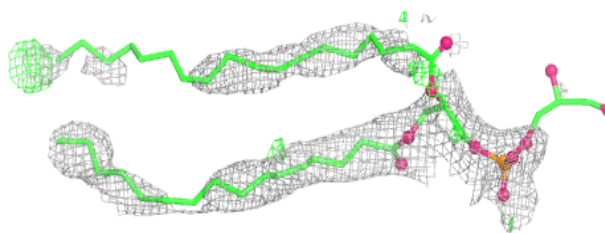


Electron density around TGL N 604:

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

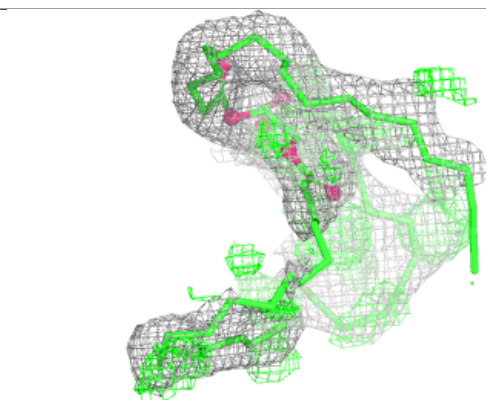
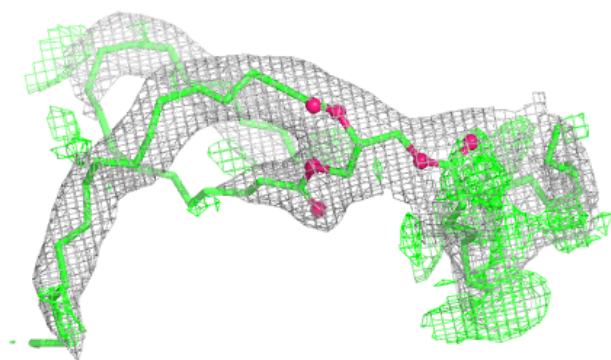
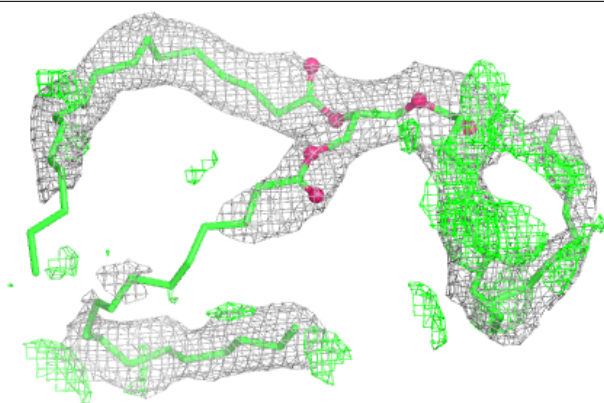
**Electron density around PGV P 307:**

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

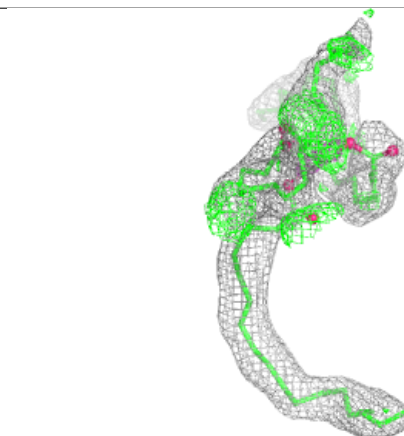
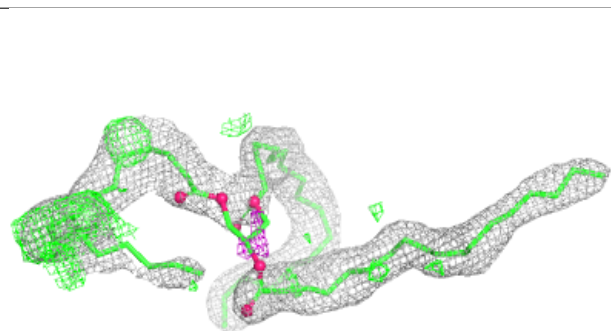
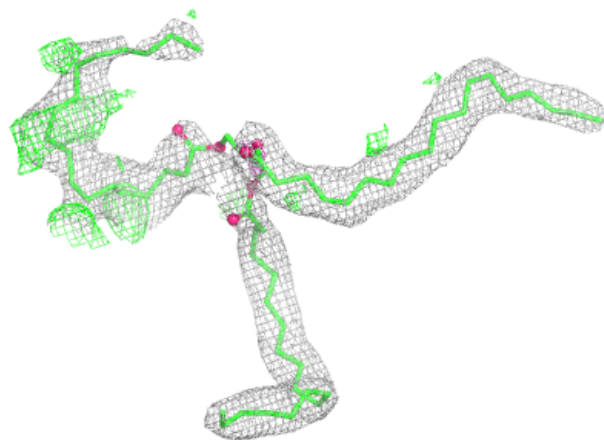


Electron density around TGL B 302:

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

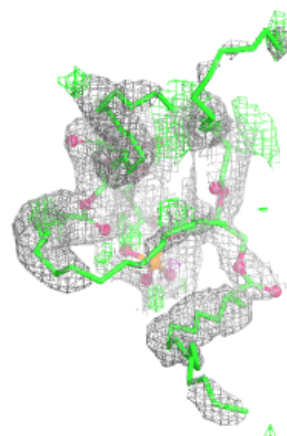
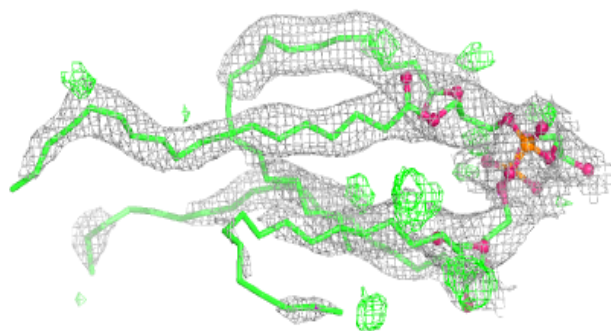
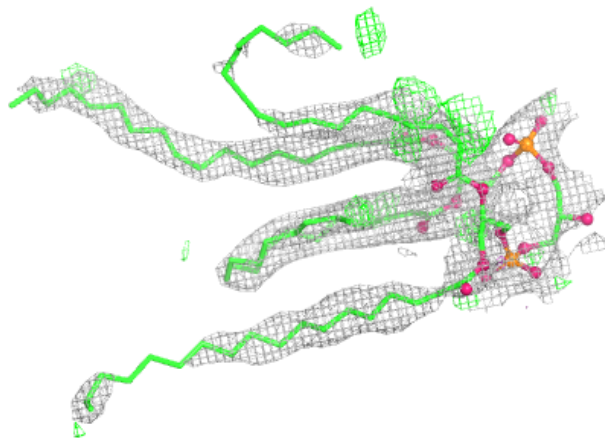
**Electron density around TGL Y 101:**

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



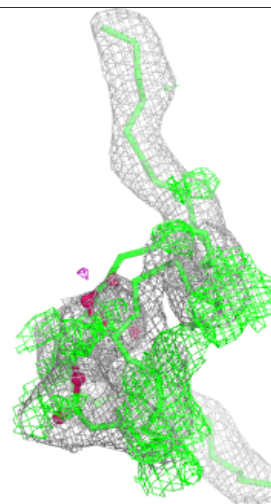
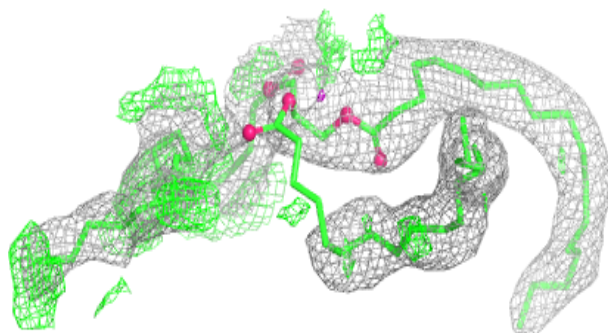
Electron density around CDL P 308:

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



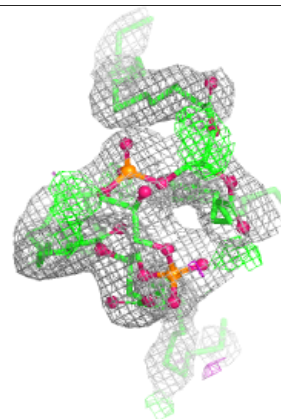
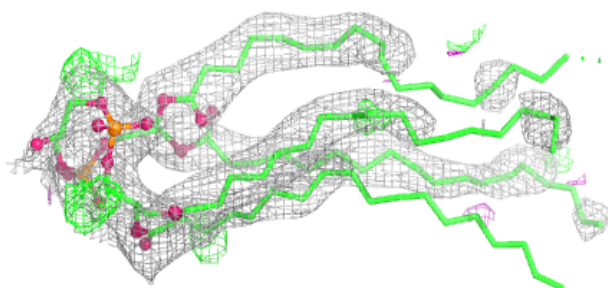
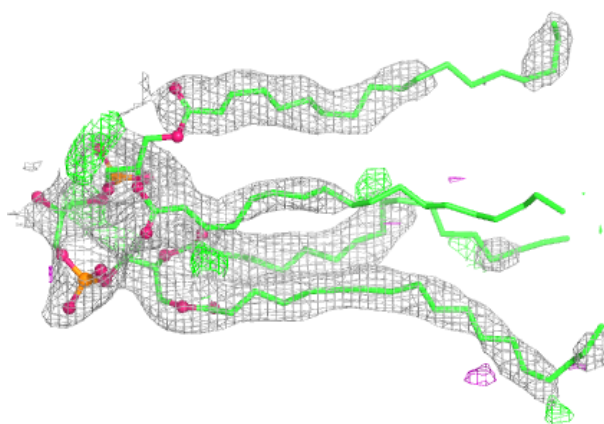
Electron density around TGL L 101:

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

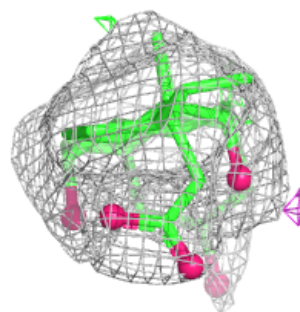
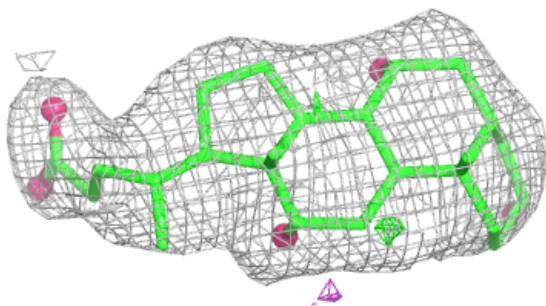
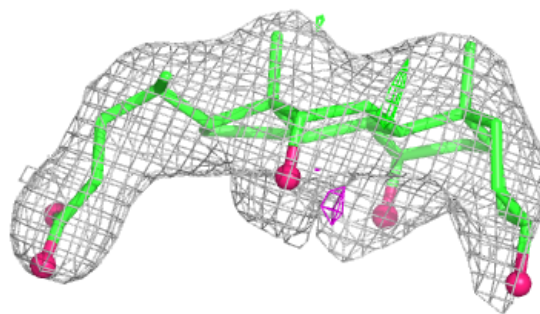


Electron density around CDL C 304:

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

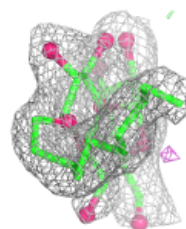
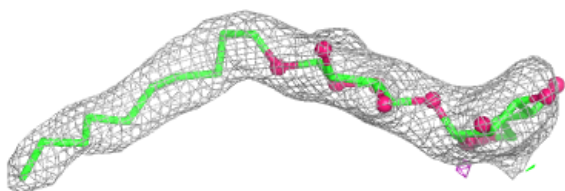
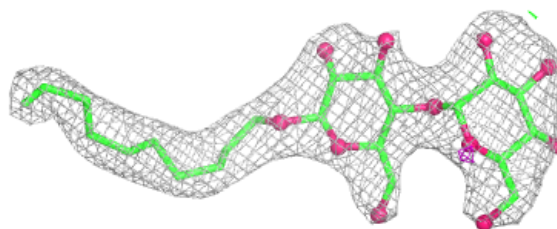
**Electron density around CHD J 101:**

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

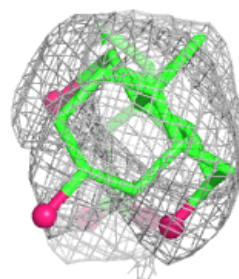
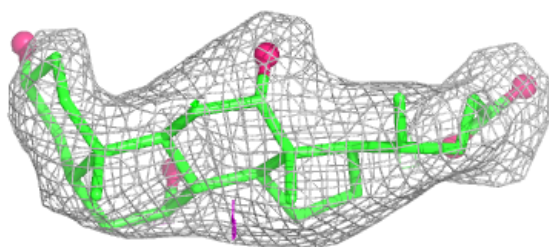
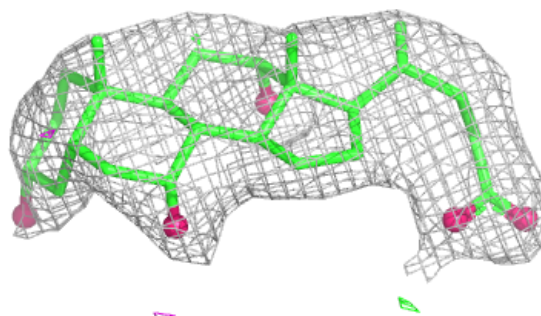


Electron density around DMU Q 206:

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

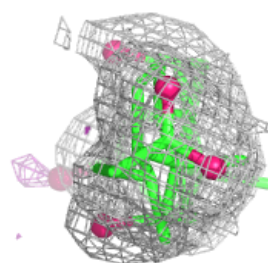
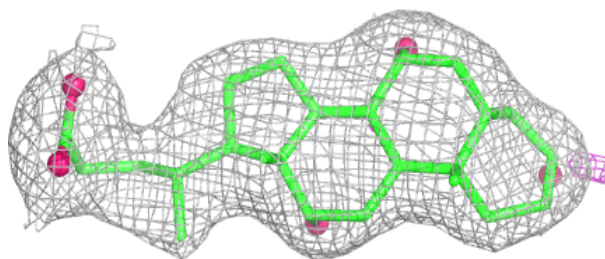
**Electron density around CHD W 302:**

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

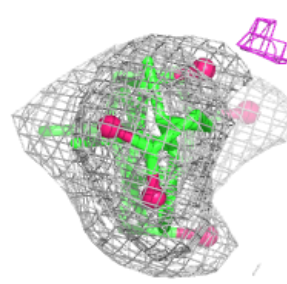
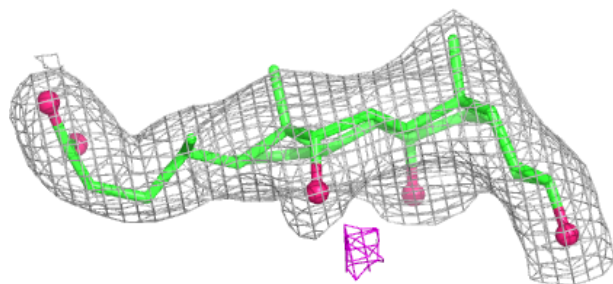
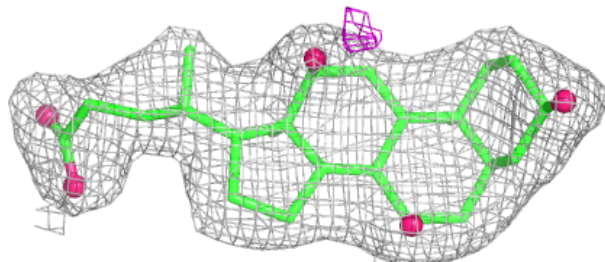


Electron density around CHD P 309:

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

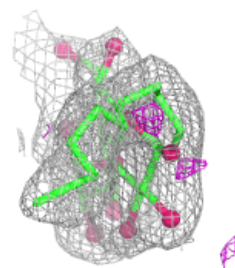
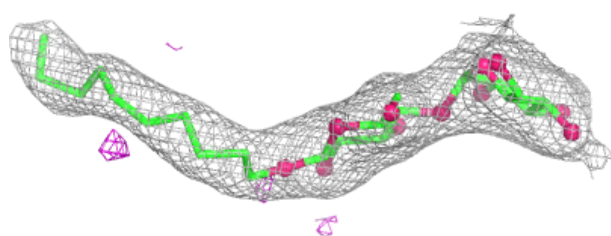
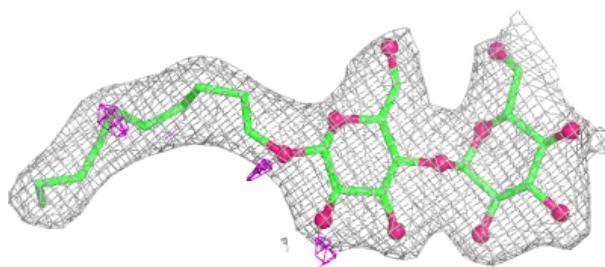
**Electron density around CHD C 305:**

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

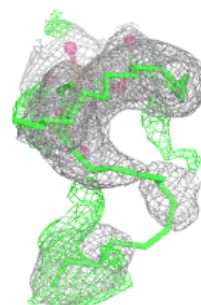
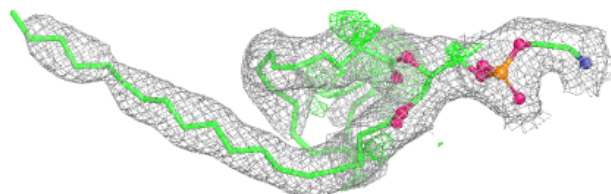
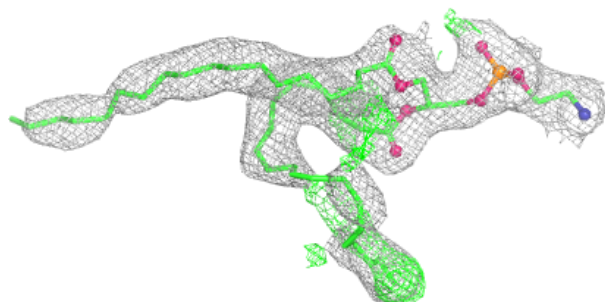


Electron density around DMU D 208:

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

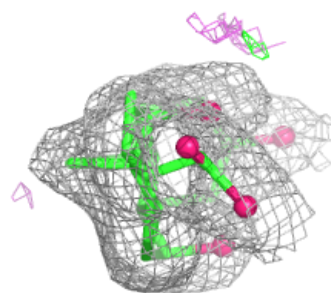
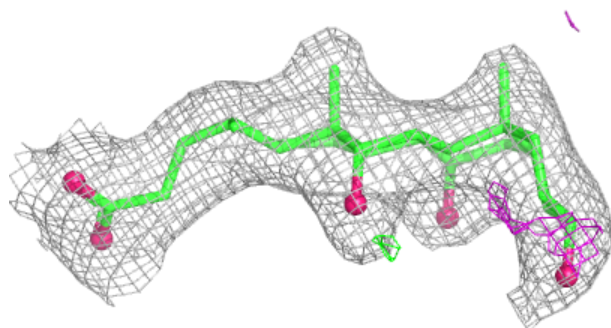
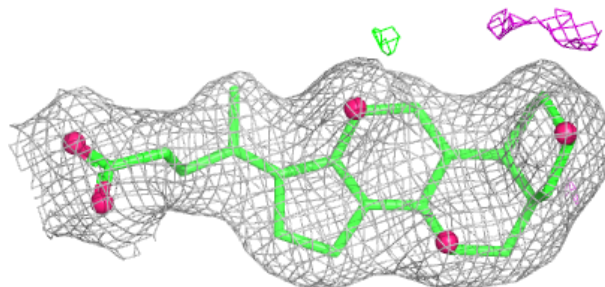
**Electron density around PEK T 102:**

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

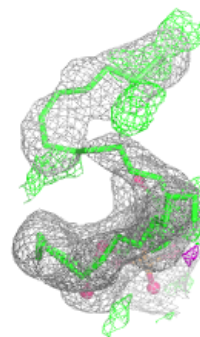
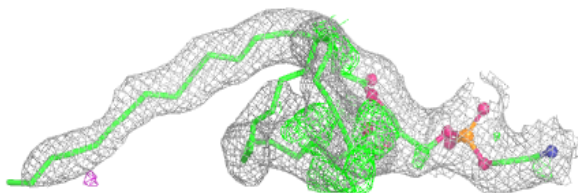
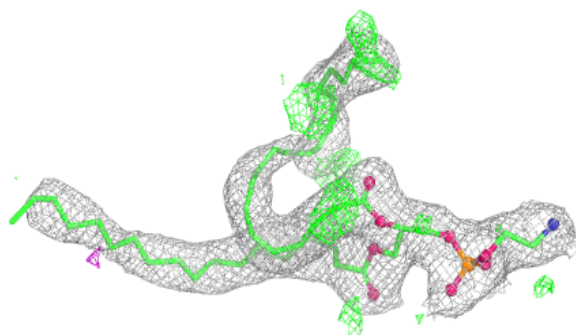


Electron density around CHD T 101:

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

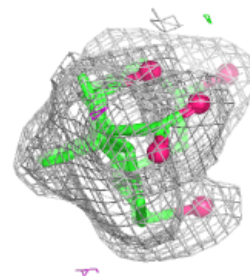
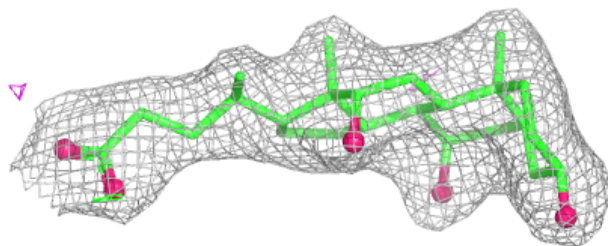
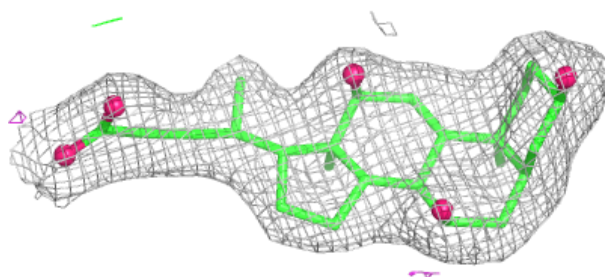
**Electron density around PEK G 102:**

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

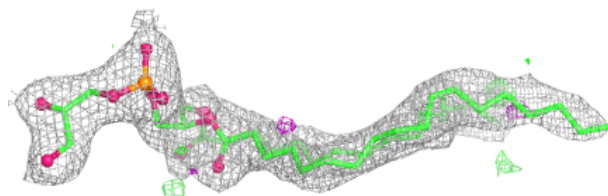
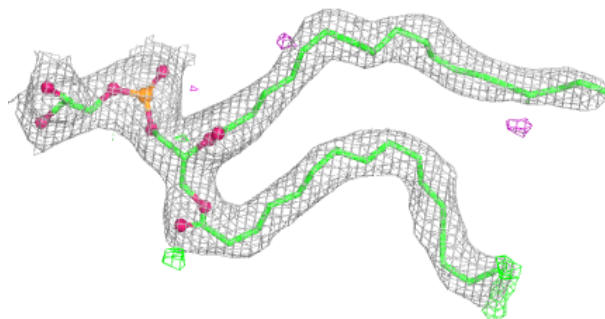


Electron density around CHD C 301:

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

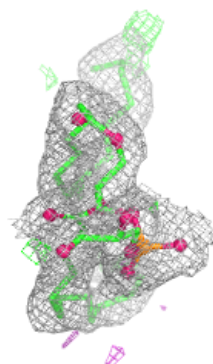
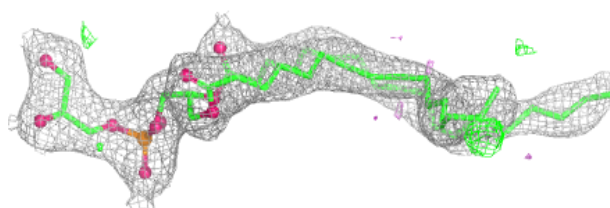
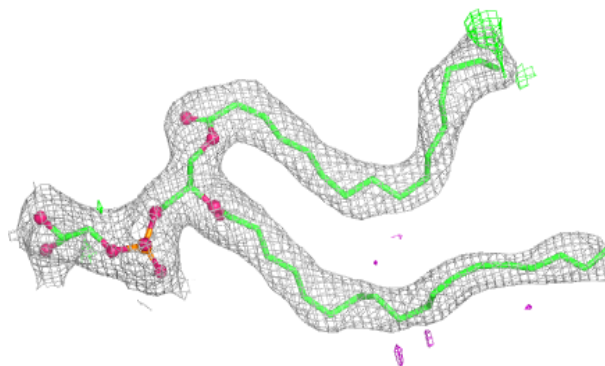
**Electron density around PGV P 302:**

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

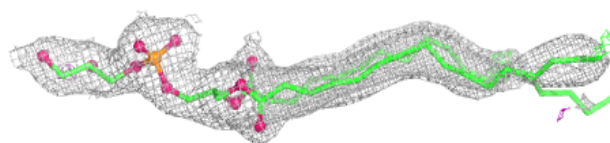
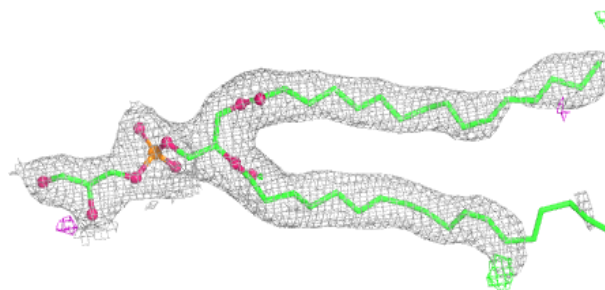


Electron density around PGV A 605:

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

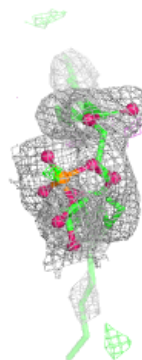
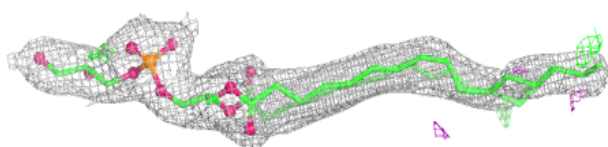
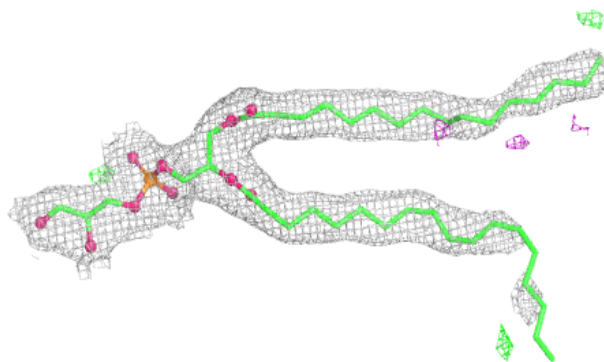
**Electron density around PGV C 302:**

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

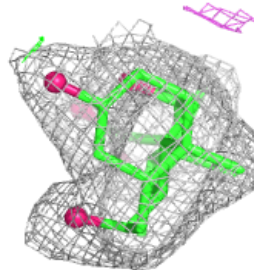
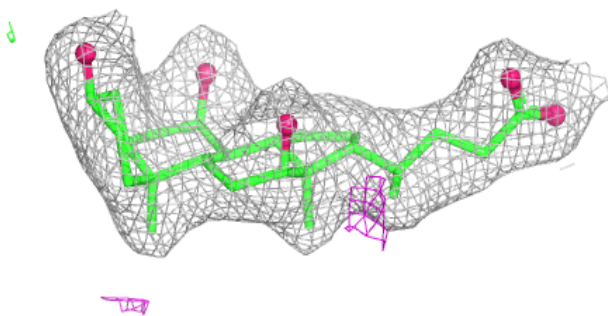
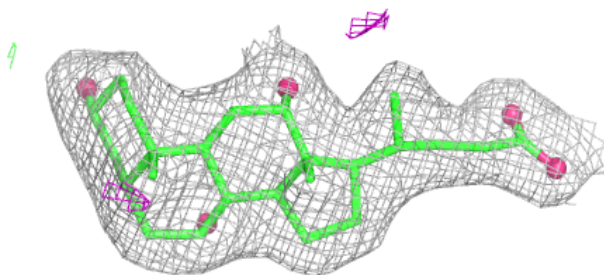


Electron density around PGV P 306:

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

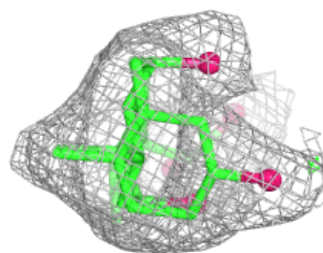
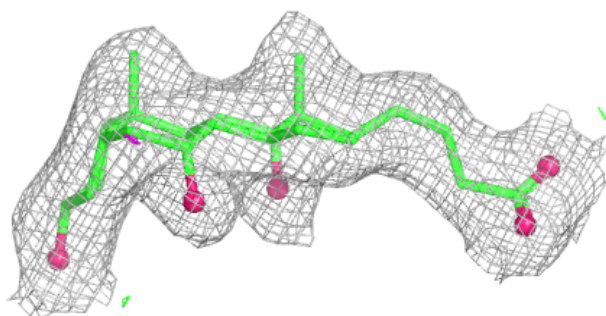
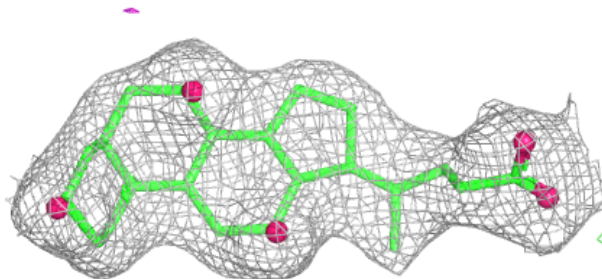
**Electron density around CHD P 304:**

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

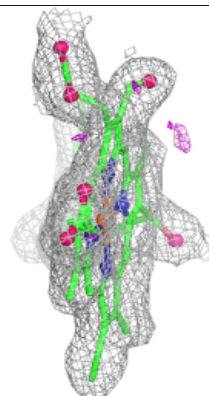
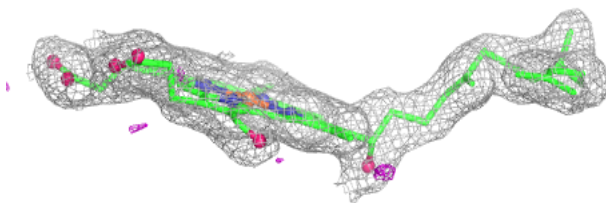
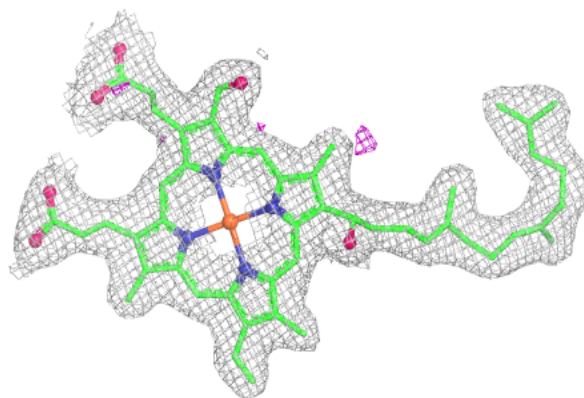


Electron density around CHD G 108:

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

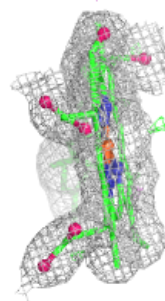
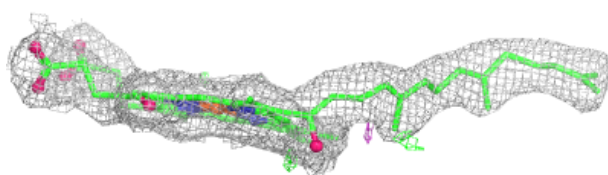
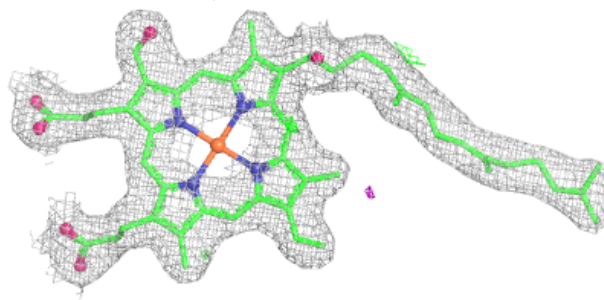
**Electron density around HEA A 606:**

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

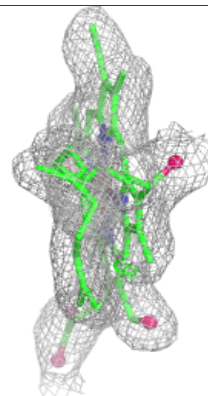
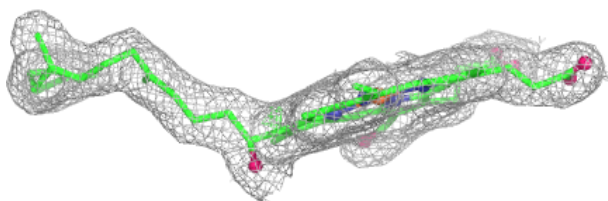
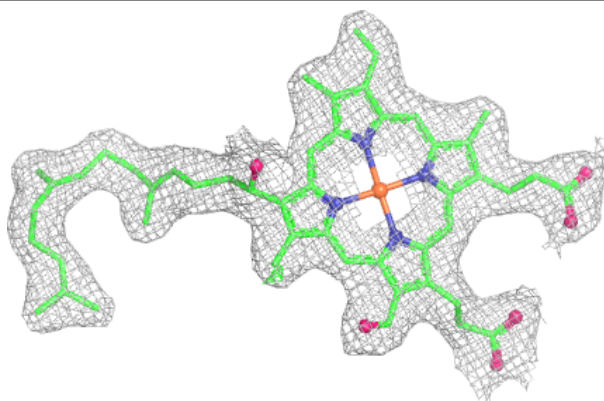


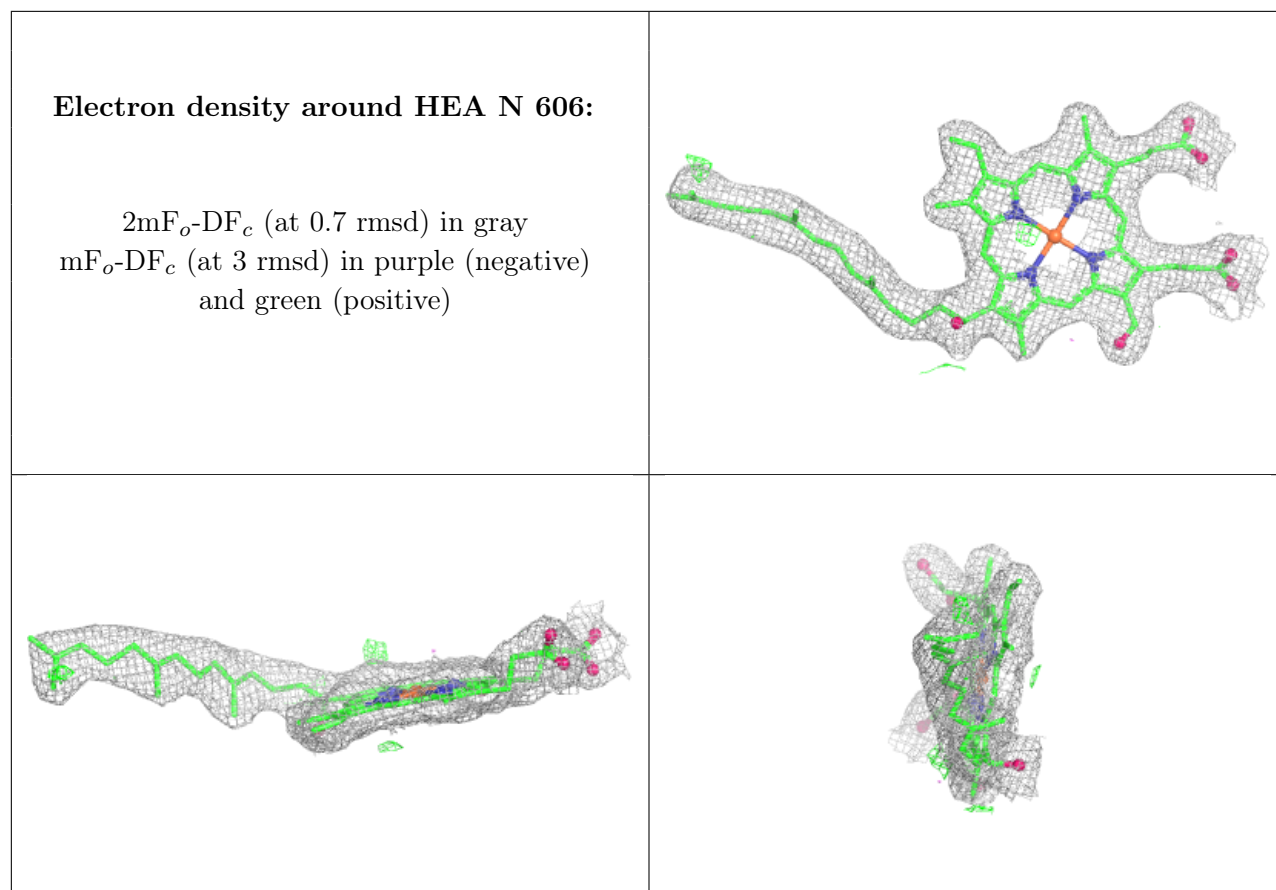
Electron density around HEA A 607:

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

**Electron density around HEA N 605:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.