



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 7TIE / pdb_00007tie
Title : Structure of oxidized bovine cytochrome c oxidase at 1.90 Angstrom resolution
obtained by synchrotron X-rays
Authors : Ishigami, I.; Rousseau, D.L.; Yeh, S.-R.
Deposited on : 2022-01-13
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

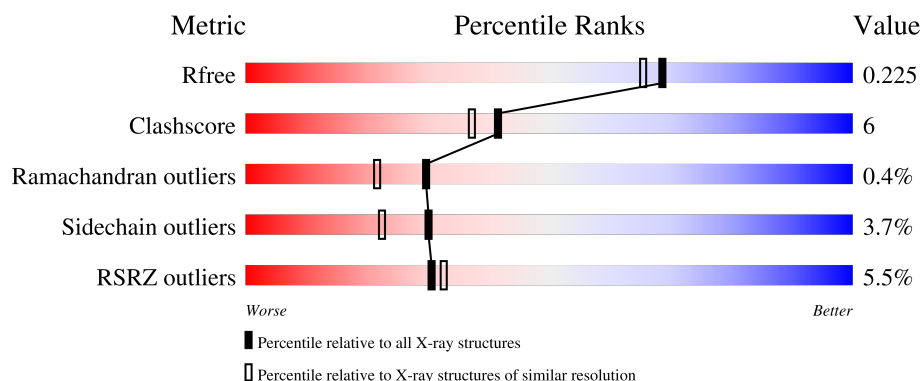
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	87% 13% .
1	N	514	91% 9% .
2	B	227	4% 85% 14% .
2	O	227	7% 84% 13% .
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	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 32913 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		

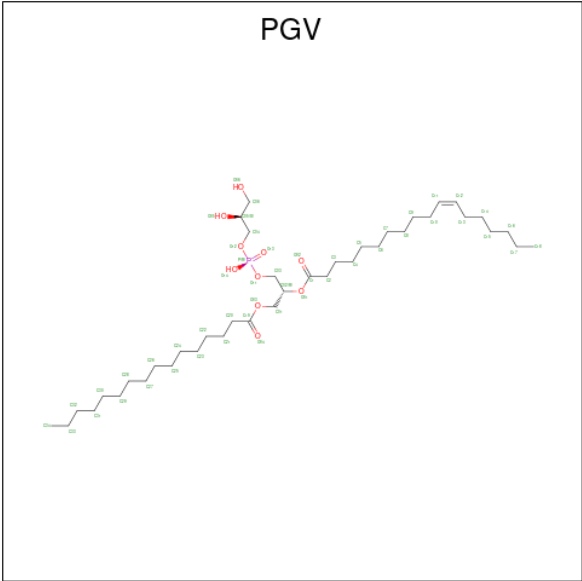
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

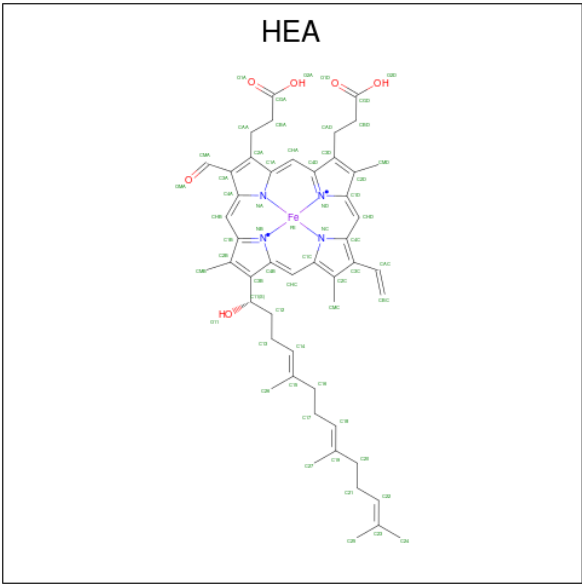
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- 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).



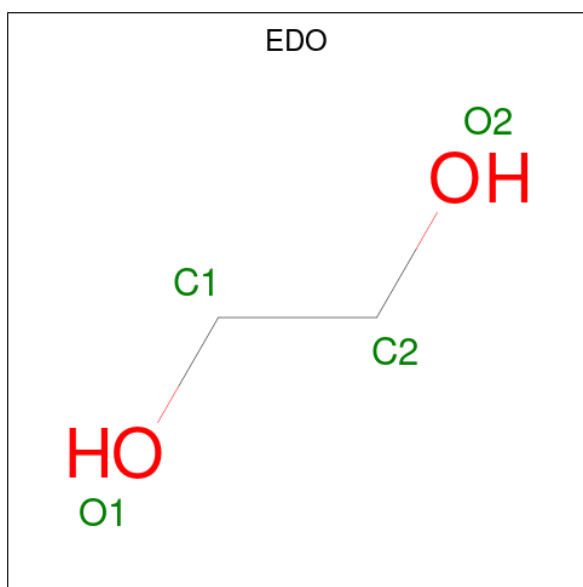
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	A	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	C	1	Total	C	O	P	0	0
			51	40	10	1		
17	M	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	N	1	Total	C	O	P	0	0
			51	40	10	1		
17	P	1	Total	C	O	P	0	0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

- 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	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		

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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	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	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	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 C O 4 2 2	0	0
19	F	1	Total C O 4 2 2	0	0
19	F	1	Total C O 4 2 2	0	0
19	F	1	Total C O 4 2 2	0	0
19	G	1	Total C O 4 2 2	0	0
19	G	1	Total C O 4 2 2	0	0
19	G	1	Total C O 4 2 2	0	0
19	G	1	Total C O 4 2 2	0	0
19	H	1	Total C O 4 2 2	0	0
19	I	1	Total C O 4 2 2	0	0
19	I	1	Total C O 4 2 2	0	0
19	J	1	Total C O 4 2 2	0	0
19	J	1	Total C O 4 2 2	0	0
19	K	1	Total C O 4 2 2	0	0
19	L	1	Total C O 4 2 2	0	0
19	L	1	Total C O 4 2 2	0	0
19	L	1	Total C O 4 2 2	0	0
19	M	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

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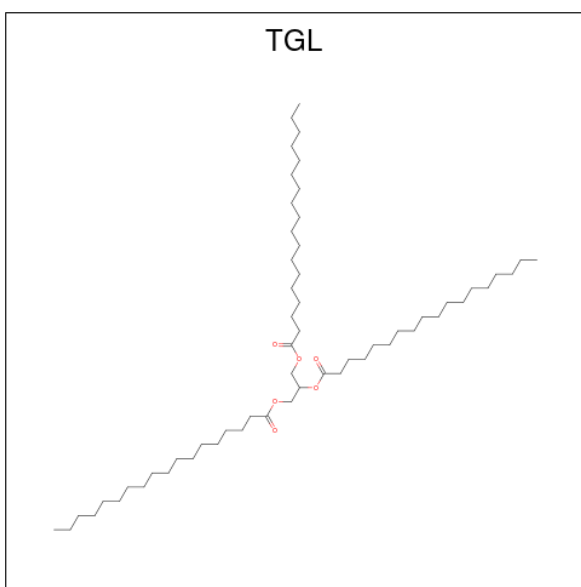
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	N	1	Total	C	O	0	0
			4	2	2		
19	O	1	Total	C	O	0	0
			4	2	2		
19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

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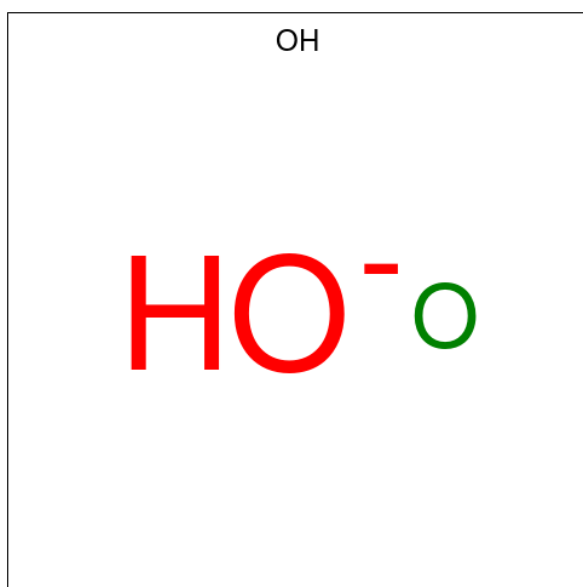
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	S	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	T	1	Total	C	O	0	0
			4	2	2		
19	U	1	Total	C	O	0	0
			4	2	2		
19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

- Molecule 20 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆) (labeled as "Ligand of Interest" by depositor).



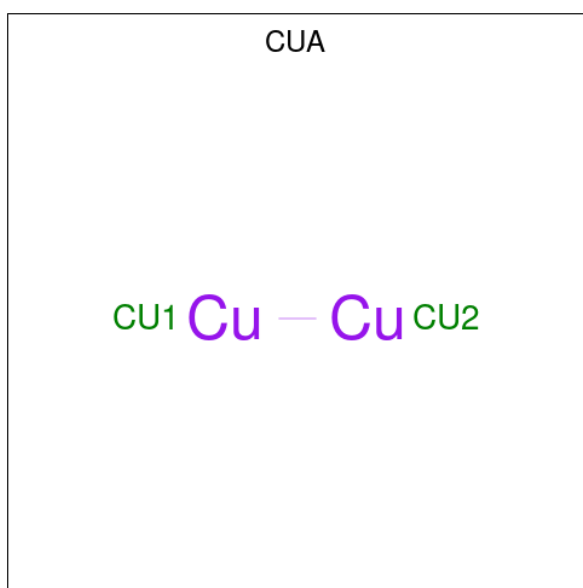
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	A	1	Total	C	O	0	0
			63	57	6		
20	D	1	Total	C	O	0	0
			63	57	6		
20	L	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		
20	N	1	Total	C	O	0	0
			63	57	6		

- Molecule 21 is HYDROXIDE ION (CCD ID: OH) (formula: HO).



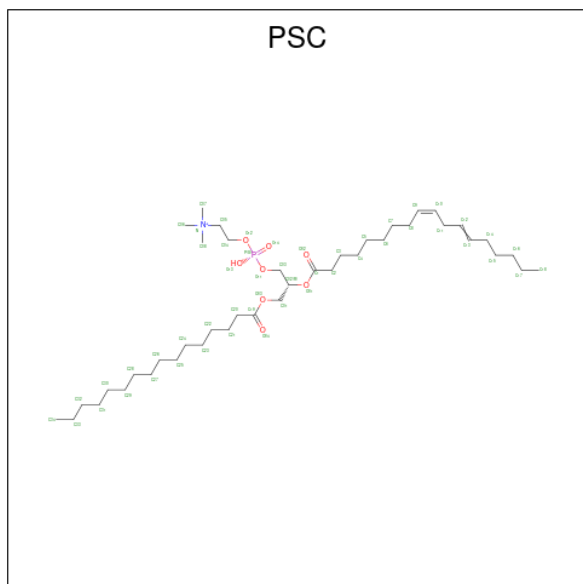
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
21	A	1	Total O 1 1	0	0
21	N	1	Total O 1 1	0	0

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



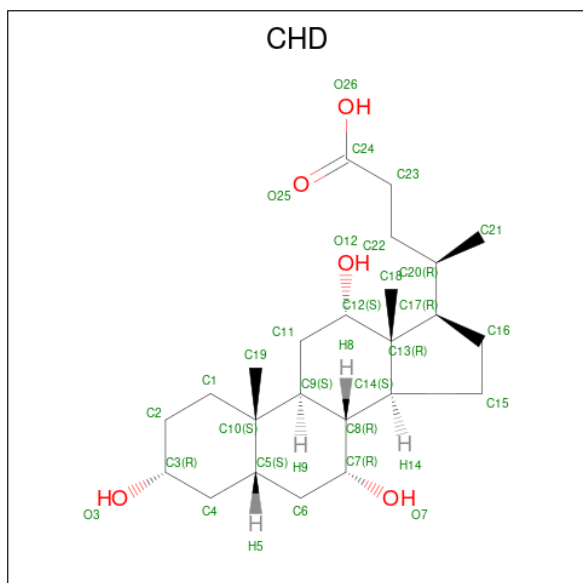
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total Cu 2 2	0	0
22	O	1	Total Cu 2 2	0	0

- 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: $C_{42}H_{81}NO_8P$).



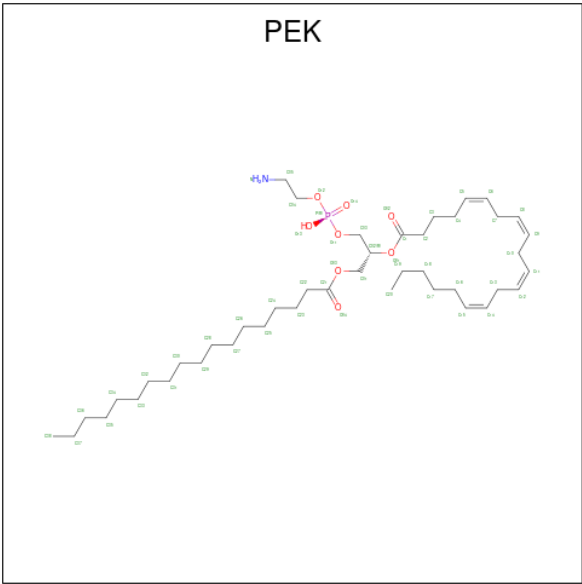
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



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

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



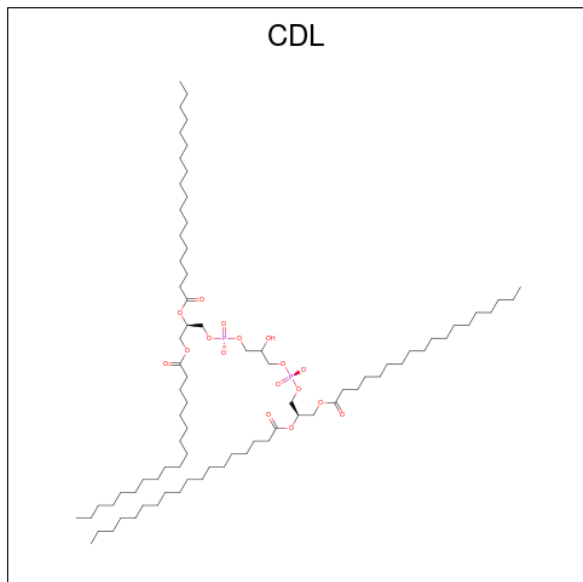
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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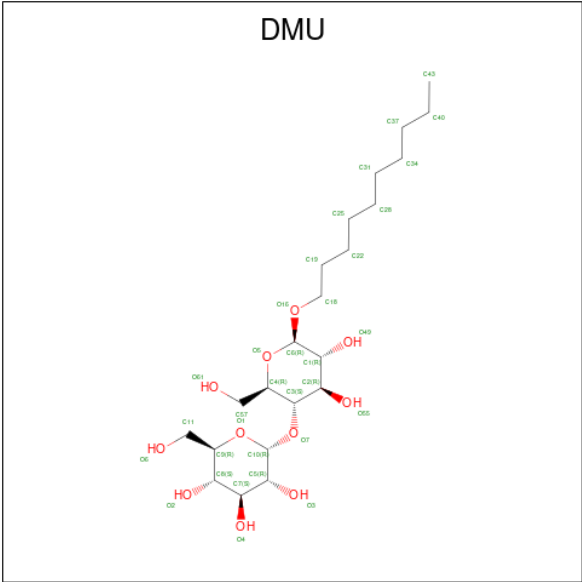
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



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

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

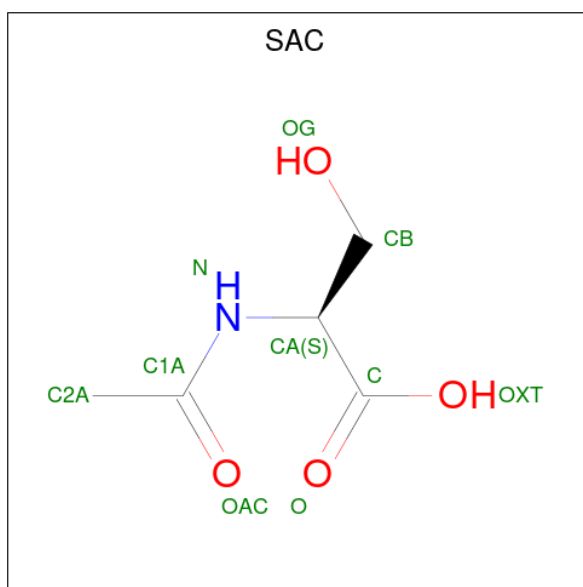


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	C	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	G	1	Total	C	O	0	0
			33	22	11		
27	M	1	Total	C	O	0	0
			33	22	11		
27	P	1	Total	C	O	0	0
			33	22	11		
27	Z	1	Total	C	O	0	0
			33	22	11		

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

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

- Molecule 29 is 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	215	Total	O	0	0
			215	215		
30	B	149	Total	O	0	0
			149	149		
30	C	111	Total	O	0	0
			111	111		
30	D	98	Total	O	0	0
			98	98		
30	E	81	Total	O	0	0
			81	81		
30	F	85	Total	O	0	0
			85	85		
30	G	45	Total	O	0	0
			45	45		
30	H	50	Total	O	0	0
			50	50		
30	I	31	Total	O	0	0
			31	31		
30	J	32	Total	O	0	0
			32	32		

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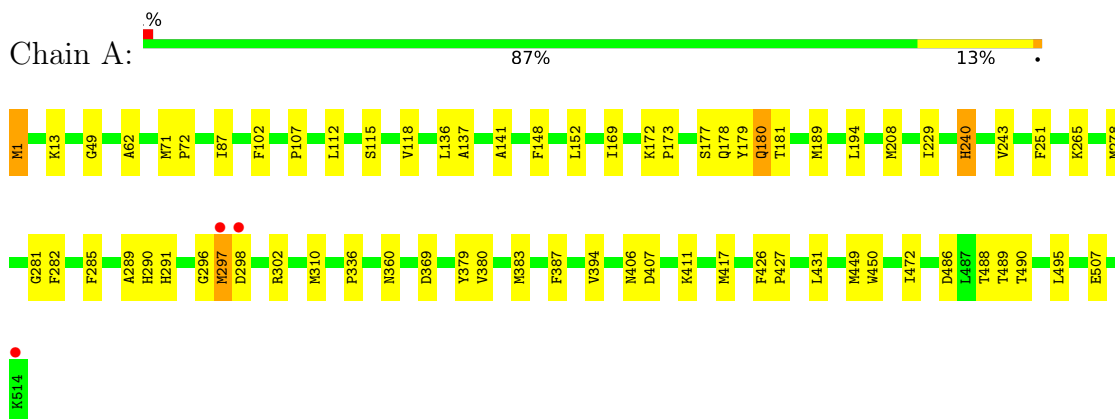
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	K	24	Total 24	O 24	0	0
30	L	24	Total 24	O 24	0	0
30	M	23	Total 23	O 23	0	0
30	N	184	Total 184	O 184	0	0
30	O	111	Total 111	O 111	0	0
30	P	96	Total 96	O 96	0	0
30	Q	59	Total 59	O 59	0	0
30	R	58	Total 58	O 58	0	0
30	S	73	Total 73	O 73	0	0
30	T	35	Total 35	O 35	0	0
30	U	47	Total 47	O 47	0	0
30	V	18	Total 18	O 18	0	0
30	W	18	Total 18	O 18	0	0
30	X	14	Total 14	O 14	0	0
30	Y	6	Total 6	O 6	0	0
30	Z	6	Total 6	O 6	0	0

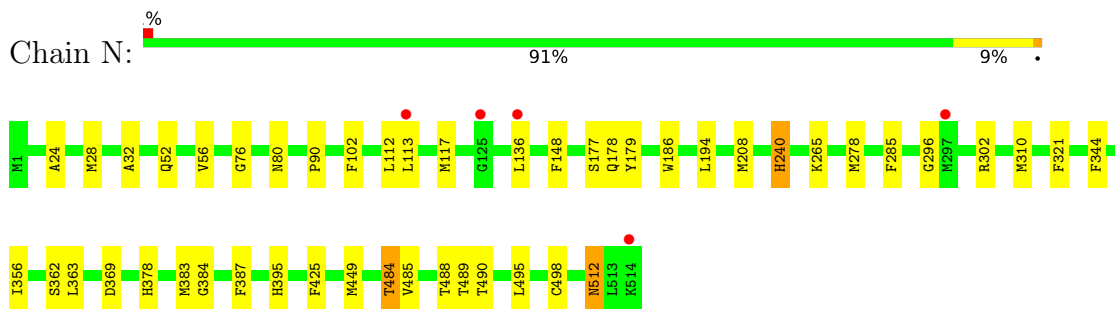
3 Residue-property plots [i](#)

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

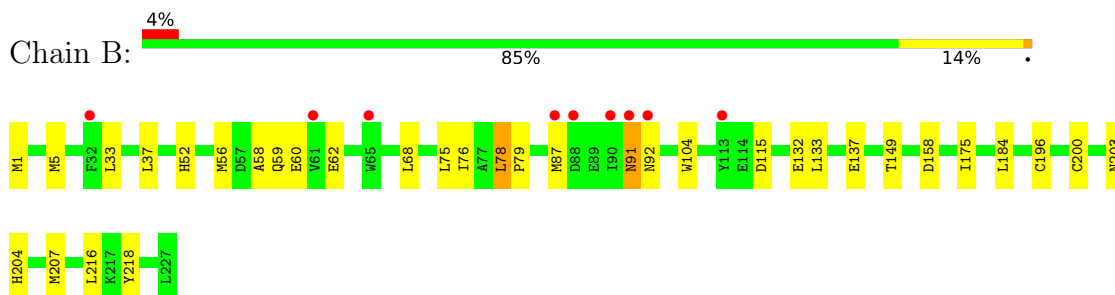
- Molecule 1: Cytochrome c oxidase subunit 1



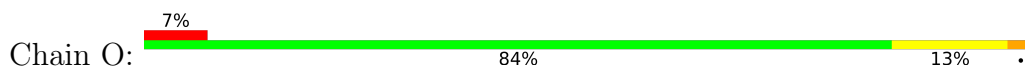
- Molecule 1: Cytochrome c oxidase subunit 1

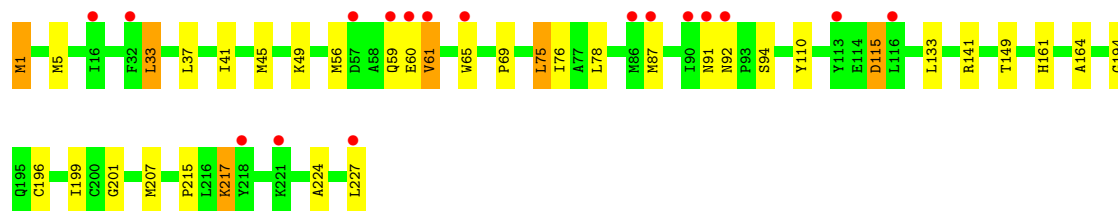


- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 2: Cytochrome c oxidase subunit 2





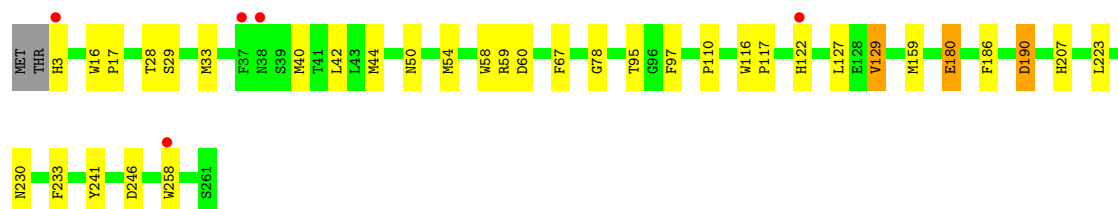
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 90% 9% .



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 86% 12% ..



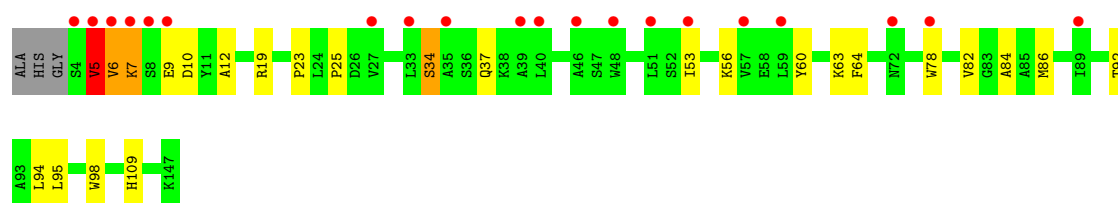
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 88% 7% ..



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

Chain Q: 81% 14% ...

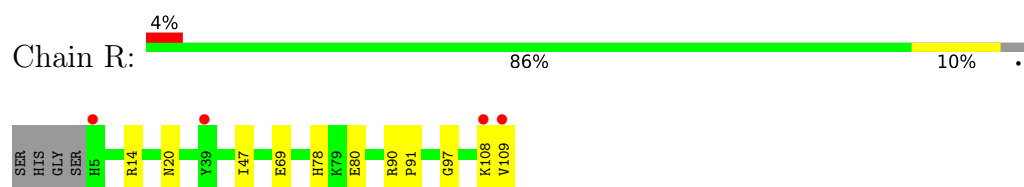


• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

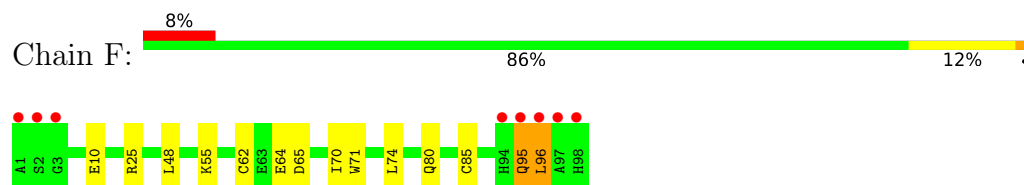
Chain E: 89% 6% ..



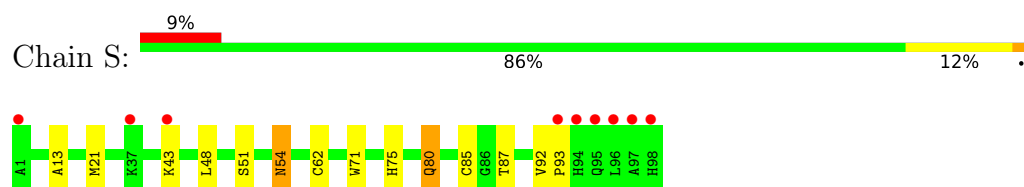
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



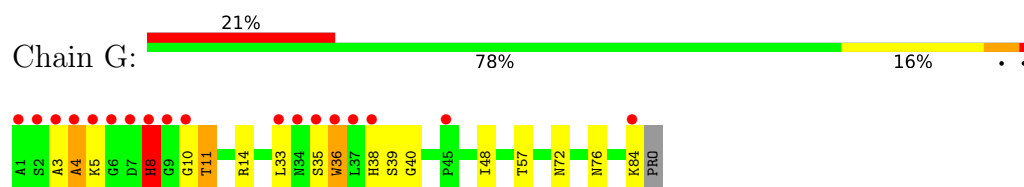
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



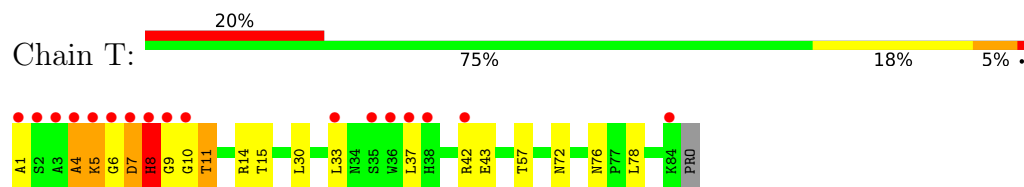
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



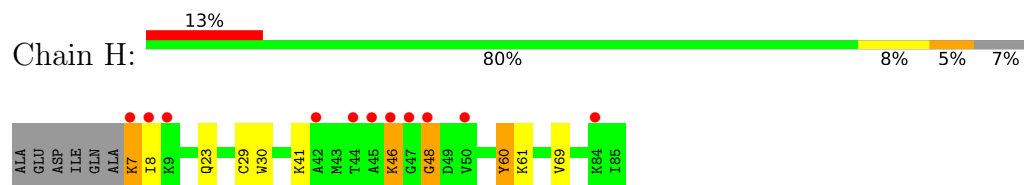
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



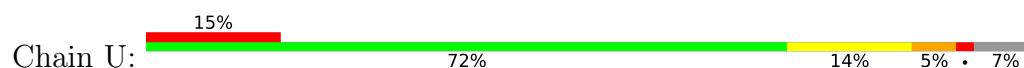
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

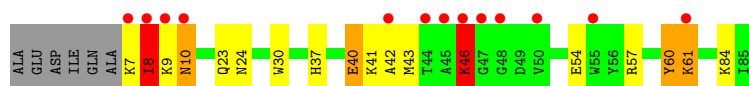


- Molecule 8: Cytochrome c oxidase subunit 6B1

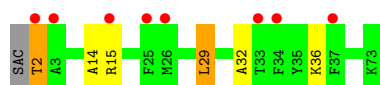
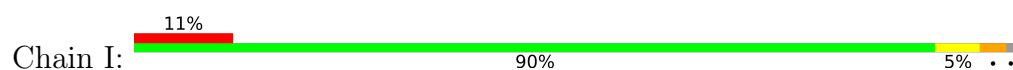


- Molecule 8: Cytochrome c oxidase subunit 6B1

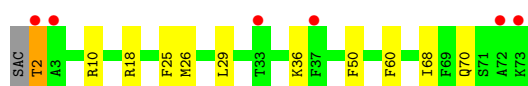
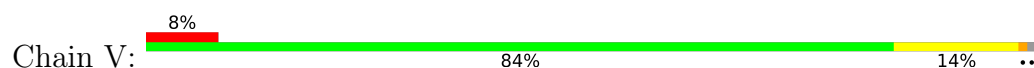




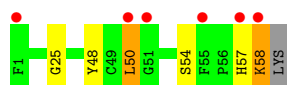
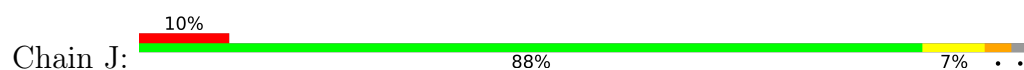
- Molecule 9: Cytochrome c oxidase subunit 6C



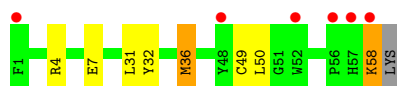
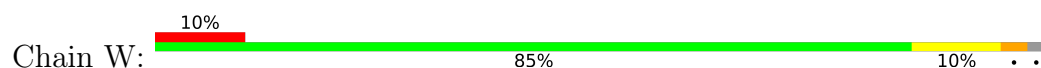
- Molecule 9: Cytochrome c oxidase subunit 6C



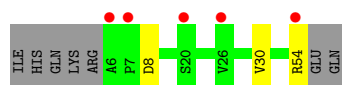
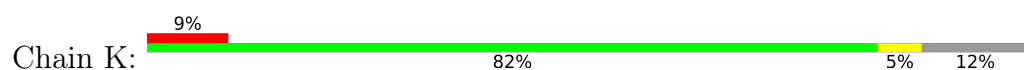
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



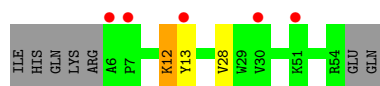
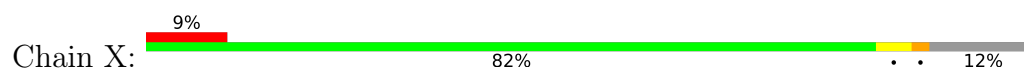
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



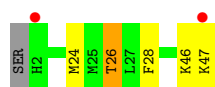
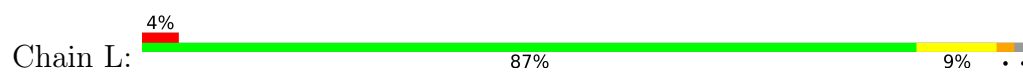
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



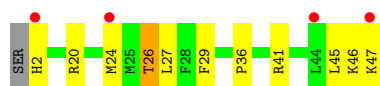
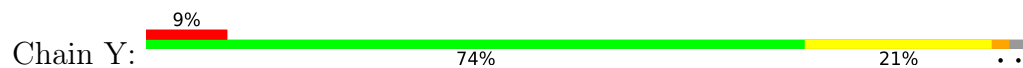
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



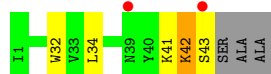
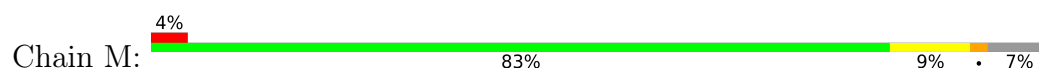
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



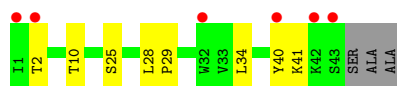
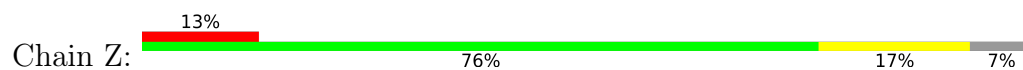
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



- 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	178.12Å 182.41Å 208.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 1.90 39.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.99-1.90) 99.8 (39.99-1.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.185 , 0.215 0.196 , 0.225	Depositor DCC
R_{free} test set	26755 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32913	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: CU, HEA, OH, PSC, CHD, NA, PGV, SAC, MG, PEK, CUA, CDL, EDO, TGL, DMU, TPO, ZN, 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	1.09	2/4156 (0.0%)	1.37	7/5678 (0.1%)
1	N	1.13	2/4156 (0.0%)	1.29	3/5678 (0.1%)
2	B	1.12	1/1860 (0.1%)	1.39	3/2534 (0.1%)
2	O	1.07	1/1860 (0.1%)	1.37	4/2534 (0.2%)
3	C	1.06	0/2197	1.28	1/3005 (0.0%)
3	P	1.13	3/2197 (0.1%)	1.24	2/3005 (0.1%)
4	D	1.11	0/1229	1.30	2/1658 (0.1%)
4	Q	1.09	0/1229	1.33	0/1658
5	E	1.07	0/871	1.38	3/1182 (0.3%)
5	R	1.04	0/871	1.43	3/1182 (0.3%)
6	F	1.12	0/765	1.32	2/1038 (0.2%)
6	S	1.13	0/765	1.25	0/1038
7	G	1.11	1/690 (0.1%)	1.36	4/937 (0.4%)
7	T	1.07	0/690	1.30	3/937 (0.3%)
8	H	1.07	0/682	1.44	2/921 (0.2%)
8	U	1.02	0/682	1.45	0/921
9	I	1.04	0/605	1.41	2/802 (0.2%)
9	V	1.02	0/605	1.48	0/802
10	J	0.99	0/471	1.37	4/636 (0.6%)
10	W	1.16	0/471	1.29	0/636
11	K	1.10	0/398	1.42	1/546 (0.2%)
11	X	1.08	0/398	1.40	0/546
12	L	1.00	0/393	1.41	1/526 (0.2%)
12	Y	1.09	0/393	1.38	0/526
13	M	1.09	0/345	1.45	0/470
13	Z	1.03	0/345	1.45	0/470
All	All	1.09	10/29324 (0.0%)	1.34	47/39866 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	161	HIS	CE1-NE2	6.47	1.39	1.32
1	A	240	HIS	CE1-NE2	5.99	1.38	1.32
1	N	395	HIS	CE1-NE2	5.82	1.38	1.32
3	P	78	GLY	C-O	5.75	1.30	1.23
3	P	60	ASP	C-O	5.69	1.30	1.24
1	A	49	GLY	C-O	5.50	1.30	1.23
3	P	190	ASP	C-O	5.50	1.30	1.23
1	N	90	PRO	C-O	-5.20	1.18	1.24
2	B	216	LEU	C-O	5.19	1.30	1.24
7	G	48	ILE	N-CA	5.17	1.49	1.45

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	240	HIS	CA-CB-CG	-10.56	103.24	113.80
2	O	92	ASN	CB-CA-C	10.03	121.31	110.17
1	A	240	HIS	CA-CB-CG	-9.45	104.35	113.80
2	B	92	ASN	CB-CA-C	7.12	118.08	110.17
1	N	102	PHE	CA-CB-CG	-7.02	106.78	113.80
1	A	102	PHE	CA-CB-CG	-6.49	107.31	113.80
3	P	122	HIS	CB-CA-C	6.25	117.15	110.65
5	R	78	HIS	CA-C-N	6.16	129.15	120.28
5	R	78	HIS	C-N-CA	6.16	129.15	120.28
5	E	17	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	240	HIS	N-CA-CB	6.00	117.50	110.42
8	H	41	LYS	CA-C-N	5.99	128.80	120.29
8	H	41	LYS	C-N-CA	5.99	128.80	120.29
3	P	233	PHE	CA-CB-CG	-5.92	107.88	113.80
7	G	57	THR	N-CA-C	-5.85	106.48	113.97
11	K	30	VAL	N-CA-C	-5.84	104.82	110.72
12	L	26	THR	CA-CB-OG1	-5.82	100.86	109.60
7	G	8	HIS	CA-CB-CG	5.75	119.55	113.80
1	A	360	ASN	CA-C-O	-5.67	114.86	120.98
2	B	158	ASP	CA-CB-CG	5.55	118.15	112.60
2	O	49	LYS	N-CA-C	-5.49	106.42	113.23
2	B	184	LEU	N-CA-CB	-5.42	101.43	110.80
9	I	32	ALA	CA-C-N	5.38	127.43	120.44
9	I	32	ALA	C-N-CA	5.38	127.43	120.44
7	T	57	THR	N-CA-C	-5.36	106.91	113.50
1	A	380	VAL	CA-C-O	-5.31	114.51	120.25
1	N	240	HIS	N-CA-CB	5.30	116.67	110.42
4	D	20	ARG	CG-CD-NE	-5.28	100.38	112.00
10	J	25	GLY	CA-C-N	5.25	127.57	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	25	GLY	C-N-CA	5.25	127.57	120.38
1	A	251	PHE	CA-CB-CG	5.20	119.00	113.80
2	O	201	GLY	CA-C-N	5.18	127.48	120.38
2	O	201	GLY	C-N-CA	5.18	127.48	120.38
1	A	486	ASP	CA-CB-CG	5.18	117.78	112.60
7	G	36	TRP	N-CA-C	-5.16	107.15	112.93
7	T	5	LYS	CB-CA-C	5.14	120.66	110.42
5	E	108	LYS	CA-C-N	5.13	130.94	121.70
5	E	108	LYS	C-N-CA	5.13	130.94	121.70
5	R	47	ILE	N-CA-C	-5.09	105.88	110.82
4	D	20	ARG	NE-CZ-NH1	-5.09	116.41	121.50
7	T	8	HIS	CA-CB-CG	5.07	118.87	113.80
7	G	40	GLY	CA-C-O	-5.07	117.02	121.58
6	F	96	LEU	CA-C-N	5.06	127.31	120.38
6	F	96	LEU	C-N-CA	5.06	127.31	120.38
10	J	48	TYR	CA-C-N	5.05	127.05	120.28
10	J	48	TYR	C-N-CA	5.05	127.05	120.28
3	C	80	ARG	CG-CD-NE	-5.01	100.98	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	54	0
1	N	4027	0	4001	44	0
2	B	1824	0	1833	23	0
2	O	1824	0	1833	27	0
3	C	2110	0	2027	19	0
3	P	2110	0	2027	21	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	18	0
5	E	852	0	845	4	0
5	R	852	0	845	7	0
6	F	748	0	728	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	748	0	728	9	0
7	G	675	0	644	20	0
7	T	675	0	644	22	0
8	H	662	0	623	9	0
8	U	662	0	623	17	0
9	I	592	0	604	8	0
9	V	592	0	604	10	0
10	J	460	0	459	4	0
10	W	460	0	459	7	0
11	K	384	0	366	4	0
11	X	384	0	366	2	0
12	L	380	0	380	4	0
12	Y	380	0	380	14	0
13	M	335	0	352	5	0
13	Z	335	0	352	10	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	51	0	76	4	0
17	C	102	0	152	7	0
17	M	51	0	76	6	0
17	N	102	0	152	16	0
17	P	102	0	152	2	0
18	A	120	0	108	5	0
18	N	120	0	108	6	0
19	A	44	0	66	8	0
19	B	32	0	48	2	0
19	C	20	0	30	1	0
19	D	16	0	24	0	0
19	E	20	0	30	0	0
19	F	24	0	36	0	0
19	G	16	0	24	0	0
19	H	4	0	6	1	0
19	I	8	0	12	0	0
19	J	8	0	12	0	0
19	K	4	0	6	0	0
19	L	12	0	18	0	0
19	M	4	0	6	0	0
19	N	48	0	72	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	O	8	0	12	0	0
19	P	16	0	24	0	0
19	Q	16	0	24	0	0
19	R	8	0	12	1	0
19	S	24	0	36	1	0
19	T	8	0	12	0	0
19	U	4	0	6	3	0
19	V	12	0	18	1	0
19	W	8	0	12	0	0
20	A	63	0	110	0	0
20	D	63	0	110	10	0
20	L	63	0	110	3	0
20	N	189	0	330	11	0
21	A	1	0	0	1	0
21	N	1	0	0	1	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	8	0
23	R	52	0	80	6	0
24	B	29	0	39	1	0
24	C	58	0	78	1	0
24	G	29	0	39	0	0
24	J	29	0	39	2	0
24	P	58	0	78	1	0
24	T	29	0	39	4	0
24	W	29	0	39	1	0
24	Y	29	0	39	4	0
25	C	106	0	154	4	0
25	G	53	0	77	7	0
25	P	159	0	231	10	0
26	C	200	0	312	4	0
26	P	200	0	312	13	0
27	C	33	0	42	0	0
27	G	66	0	84	0	0
27	M	33	0	42	0	0
27	P	33	0	42	0	0
27	Z	33	0	42	4	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	I	9	0	8	2	0
29	V	9	0	8	3	0
30	A	215	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	149	0	0	7	0
30	C	111	0	0	1	0
30	D	98	0	0	2	0
30	E	81	0	0	0	0
30	F	85	0	0	0	0
30	G	45	0	0	0	0
30	H	50	0	0	2	0
30	I	31	0	0	1	0
30	J	32	0	0	1	0
30	K	24	0	0	2	0
30	L	24	0	0	3	0
30	M	23	0	0	3	0
30	N	184	0	0	7	0
30	O	111	0	0	1	0
30	P	96	0	0	2	0
30	Q	59	0	0	3	0
30	R	58	0	0	4	0
30	S	73	0	0	1	0
30	T	35	0	0	1	0
30	U	47	0	0	5	0
30	V	18	0	0	0	0
30	W	18	0	0	0	0
30	X	14	0	0	0	0
30	Y	6	0	0	1	0
30	Z	6	0	0	0	0
All	All	32913	0	32024	407	0

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

All (407) 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)
3:P:44:MET:HG3	30:P:495:HOH:O	1.49	1.11
7:G:11:TPO:HA	7:G:11:TPO:O3P	1.51	1.05
1:N:484:THR:HG23	30:N:870:HOH:O	1.58	1.03
23:B:302:PSC:H42	9:I:14:ALA:HB2	1.35	1.01
1:A:177:SER:HB2	7:T:10:GLY:HA2	1.46	0.97
25:P:304:PEK:H71	25:P:304:PEK:H32	1.48	0.95
7:G:72:ASN:H	7:G:76:ASN:HD22	1.14	0.93
26:C:305:CDL:OA5	26:C:305:CDL:H1	1.68	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:302:PSC:H61	23:B:302:PSC:H21	1.54	0.90
21:A:619:OH:O	30:A:701:HOH:O	1.90	0.88
2:B:56:MET:HA	23:B:302:PSC:H221	1.57	0.87
2:B:52:HIS:ND1	23:B:302:PSC:H31	1.90	0.86
30:B:527:HOH:O	17:C:304:PGV:H041	1.79	0.82
21:N:623:OH:O	30:N:701:HOH:O	1.98	0.81
26:C:310:CDL:H382	30:O:496:HOH:O	1.79	0.81
17:N:622:PGV:H241	17:N:622:PGV:H011	1.63	0.81
23:B:302:PSC:H42	9:I:14:ALA:CB	2.12	0.80
17:N:622:PGV:O02	17:N:622:PGV:H52	1.81	0.79
7:T:1:ALA:O	30:T:1401:HOH:O	2.01	0.77
8:U:10:ASN:HA	30:U:1643:HOH:O	1.84	0.75
7:G:76:ASN:HD21	25:G:102:PEK:HN2	1.32	0.75
11:K:54:ARG:NH2	30:K:301:HOH:O	2.20	0.74
7:T:72:ASN:H	7:T:76:ASN:HD22	1.36	0.73
5:R:90:ARG:HD3	30:R:338:HOH:O	1.88	0.72
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.70	0.72
7:G:11:TPO:HG23	7:G:14:ARG:H	1.53	0.72
25:P:304:PEK:HN2	7:T:76:ASN:HD21	1.38	0.72
2:B:1:FME:HE2	2:B:133:LEU:HD13	1.72	0.72
6:S:75:HIS:H	6:S:80:GLN:HE22	1.34	0.71
4:D:78:TRP:N	20:D:201:TGL:HB32	2.05	0.71
9:V:2:THR:N	29:V:101:SAC:HG	1.88	0.71
2:O:217:LYS:H	2:O:217:LYS:CE	2.03	0.70
18:N:608:HEA:HBC1	18:N:608:HEA:HMC3	1.74	0.70
17:N:622:PGV:C1	17:N:622:PGV:C5	2.70	0.70
7:G:5:LYS:CD	1:N:278:MET:HB3	2.21	0.69
19:B:311:EDO:O1	30:B:401:HOH:O	2.09	0.69
7:G:72:ASN:H	7:G:76:ASN:ND2	1.89	0.69
20:N:618:TGL:HG2	20:N:618:TGL:HC22	1.74	0.68
25:P:305:PEK:H382	26:P:312:CDL:C25	2.24	0.67
1:A:310:MET:HE1	2:B:76:ILE:CG2	2.24	0.67
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.93	0.67
19:N:615:EDO:H11	30:N:776:HOH:O	1.96	0.66
7:T:11:TPO:HG23	7:T:14:ARG:H	1.59	0.66
2:B:1:FME:HE2	2:B:133:LEU:CD1	2.26	0.65
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.78	0.65
25:P:305:PEK:C38	26:P:312:CDL:H271	2.26	0.65
1:A:298:ASP:HB3	30:A:830:HOH:O	1.97	0.65
19:B:305:EDO:O2	30:B:402:HOH:O	2.15	0.64
1:N:488:THR:HB	1:N:495:LEU:HD13	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:90:ARG:CD	30:R:338:HOH:O	2.44	0.64
23:R:201:PSC:H32	30:R:353:HOH:O	1.97	0.64
30:A:702:HOH:O	20:D:201:TGL:HG11	1.97	0.63
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.63
3:C:161:GLN:HE22	25:C:302:PEK:H031	1.63	0.63
1:N:113:LEU:HB2	20:N:605:TGL:H323	1.81	0.63
17:A:604:PGV:H343	25:G:102:PEK:H371	1.81	0.62
2:O:56:MET:HA	23:R:201:PSC:H221	1.79	0.62
30:B:522:HOH:O	8:H:61:LYS:HE3	1.98	0.62
30:L:622:HOH:O	13:M:32:TRP:HH2	1.80	0.62
2:O:217:LYS:H	2:O:217:LYS:HE2	1.63	0.62
12:L:46:LYS:O	12:L:47:LYS:HD2	2.00	0.61
17:N:622:PGV:H241	17:N:622:PGV:C01	2.29	0.61
7:G:10:GLY:HA2	1:N:177:SER:HB2	1.82	0.61
17:N:622:PGV:O02	17:N:622:PGV:C5	2.49	0.61
4:D:78:TRP:HA	20:D:201:TGL:HB52	1.82	0.61
3:P:33:MET:HE2	10:W:49:CYS:SG	2.41	0.60
25:P:305:PEK:H382	26:P:312:CDL:H251	1.84	0.60
1:A:169:ILE:CD1	1:A:189:MET:HE1	2.32	0.60
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.02	0.60
11:K:54:ARG:HG3	11:K:54:ARG:NH1	2.17	0.60
4:D:77:GLU:HB3	20:D:201:TGL:HB31	1.84	0.59
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.01	0.59
6:S:85:CYS:SG	6:S:87:THR:HG23	2.43	0.58
7:G:3:ALA:O	7:G:4:ALA:HB2	2.04	0.58
1:A:194:LEU:CD2	7:T:4:ALA:HB1	2.33	0.58
4:D:78:TRP:H	20:D:201:TGL:HB32	1.67	0.58
20:L:502:TGL:HC82	20:L:502:TGL:H363	1.85	0.58
7:G:8:HIS:HB2	1:N:179:TYR:OH	2.04	0.58
1:A:289:ALA:HB1	1:A:297:MET:HE1	1.85	0.58
8:H:46:LYS:NZ	30:H:201:HOH:O	2.36	0.58
17:N:622:PGV:C1	17:N:622:PGV:C6	2.81	0.58
1:N:512:ASN:C	1:N:512:ASN:HD22	2.10	0.58
30:A:735:HOH:O	3:C:77:LYS:HE3	2.03	0.57
17:N:622:PGV:O12	17:N:622:PGV:H02	2.04	0.57
8:U:54:GLU:OE2	8:U:57:ARG:NH2	2.33	0.57
19:N:612:EDO:H12	30:N:743:HOH:O	2.04	0.57
17:N:622:PGV:H52	17:N:622:PGV:C1	2.34	0.57
1:A:297:MET:CG	1:A:302:ARG:HG3	2.34	0.57
2:B:52:HIS:ND1	23:B:302:PSC:C3	2.66	0.57
4:Q:6:VAL:HG12	4:Q:6:VAL:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:24:ASN:HD21	19:U:1501:EDO:C1	2.17	0.57
1:N:28:MET:HE3	12:Y:29:PHE:CD1	2.40	0.57
1:N:310:MET:HE1	2:O:76:ILE:CG2	2.34	0.56
25:P:304:PEK:H71	25:P:304:PEK:C3	2.30	0.56
1:N:310:MET:HE1	2:O:76:ILE:HG21	1.87	0.56
20:N:618:TGL:HB42	4:Q:78:TRP:HA	1.88	0.56
30:A:891:HOH:O	20:D:201:TGL:HC82	2.05	0.56
12:L:28:PHE:CD1	20:L:502:TGL:HA32	2.39	0.56
9:V:25:PHE:HD2	9:V:26:MET:CE	2.19	0.56
1:A:87:ILE:O	1:A:173:PRO:HD3	2.06	0.56
2:B:87:MET:HE2	30:B:404:HOH:O	2.06	0.56
1:A:336:PRO:HB2	1:A:394:VAL:HG11	1.86	0.56
20:N:618:TGL:HB22	30:Q:1742:HOH:O	2.06	0.55
20:N:605:TGL:HC42	12:Y:20:ARG:HH12	1.72	0.55
2:O:217:LYS:H	2:O:217:LYS:HE3	1.71	0.55
23:R:201:PSC:C1	23:R:201:PSC:H232	2.36	0.55
17:N:622:PGV:H011	17:N:622:PGV:C24	2.35	0.55
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.88	0.55
4:Q:5:VAL:O	4:Q:7:LYS:N	2.40	0.55
18:N:608:HEA:HHC	18:N:608:HEA:H122	1.88	0.55
7:G:35:SER:O	7:G:39:SER:HB3	2.06	0.54
9:V:25:PHE:CD2	9:V:26:MET:CE	2.90	0.54
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.37	0.54
19:A:614:EDO:H21	2:B:58:ALA:HB3	1.87	0.54
7:G:8:HIS:ND1	7:G:8:HIS:N	2.55	0.54
10:J:57:HIS:HA	30:J:228:HOH:O	2.06	0.54
2:O:227:LEU:C	2:O:227:LEU:HD12	2.32	0.54
17:C:304:PGV:H72	17:C:304:PGV:H22	1.89	0.54
23:R:201:PSC:C08	9:V:10:ARG:HH21	2.21	0.54
8:U:54:GLU:HA	8:U:54:GLU:OE1	2.07	0.54
1:A:169:ILE:HD11	1:A:189:MET:HE1	1.89	0.54
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.54
1:A:281:GLY:C	7:T:4:ALA:HB3	2.33	0.54
1:N:449:MET:SD	2:O:5:MET:HG2	2.48	0.54
7:G:4:ALA:CB	1:N:285:PHE:CE2	2.91	0.54
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.90	0.54
19:C:312:EDO:H22	10:J:50:LEU:HB2	1.90	0.53
2:B:1:FME:CE	2:B:133:LEU:CD1	2.86	0.53
7:T:11:TPO:O1P	7:T:11:TPO:HA	2.07	0.53
30:A:735:HOH:O	3:C:77:LYS:CE	2.54	0.53
8:U:24:ASN:HD21	19:U:1501:EDO:H11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:141:ARG:H	9:V:70:GLN:NE2	2.06	0.53
24:C:301:CHD:H212	24:C:301:CHD:H183	1.90	0.53
1:N:136:LEU:HD12	30:N:852:HOH:O	2.09	0.52
25:P:305:PEK:H383	26:P:312:CDL:H271	1.90	0.52
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.90	0.52
7:G:4:ALA:HB2	1:N:285:PHE:CE2	2.44	0.52
1:N:310:MET:HE3	1:N:356:ILE:HG23	1.91	0.52
17:N:622:PGV:H151	4:Q:84:ALA:HB2	1.90	0.52
9:V:25:PHE:CD2	9:V:26:MET:HE2	2.44	0.52
6:F:95:GLN:N	6:F:95:GLN:HE21	2.07	0.52
12:Y:41:ARG:HH12	24:Y:101:CHD:C18	2.22	0.52
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.91	0.52
1:N:113:LEU:HD13	20:N:605:TGL:H311	1.92	0.52
7:G:11:TPO:O3P	7:G:11:TPO:CA	2.43	0.52
1:N:24:ALA:HB2	18:N:608:HEA:H253	1.90	0.52
10:W:36:MET:HE3	10:W:36:MET:HA	1.92	0.52
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.46	0.51
17:C:304:PGV:C18	7:T:1:ALA:HB2	2.41	0.51
17:C:304:PGV:H262	7:T:1:ALA:N	2.25	0.51
17:A:604:PGV:H343	25:G:102:PEK:C37	2.39	0.51
9:I:2:THR:OG1	29:I:101:SAC:H2A1	2.10	0.51
8:H:7:LYS:O	8:H:7:LYS:HD3	2.11	0.51
1:A:1:FME:HE3	1:A:1:FME:HA	1.92	0.51
6:F:64:GLU:O	6:F:65:ASP:HB2	2.09	0.51
1:N:302:ARG:NH1	30:N:706:HOH:O	2.44	0.51
17:N:622:PGV:C01	17:N:622:PGV:C24	2.88	0.51
8:U:10:ASN:CA	30:U:1643:HOH:O	2.52	0.51
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.26	0.51
2:O:91:ASN:HB2	2:O:149:THR:HG21	1.91	0.51
23:B:302:PSC:H42	9:I:14:ALA:CA	2.41	0.51
25:P:304:PEK:H101	25:P:304:PEK:H31	1.93	0.51
4:D:19:ARG:HD3	4:D:21:ASP:OD1	2.10	0.50
1:N:383:MET:O	1:N:387:PHE:HB2	2.12	0.50
4:D:23:PRO:HB3	5:E:70:VAL:CG2	2.42	0.50
19:N:612:EDO:C1	30:N:743:HOH:O	2.58	0.50
6:S:92:VAL:O	6:S:92:VAL:HG23	2.11	0.50
3:P:246:ASP:HB2	30:P:484:HOH:O	2.11	0.50
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.75	0.50
1:A:472:ILE:HG21	20:L:502:TGL:H202	1.92	0.50
1:A:406:ASN:HD21	17:M:101:PGV:H71	1.76	0.50
4:D:4:SER:HA	30:D:363:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:201:PSC:H011	23:R:201:PSC:H211	1.94	0.49
1:A:507:GLU:OE1	19:A:616:EDO:O1	2.22	0.49
2:B:1:FME:CE	2:B:133:LEU:HD11	2.42	0.49
1:N:76:GLY:O	1:N:80:ASN:HB2	2.12	0.49
13:M:42:LYS:O	13:M:43:SER:HB2	2.12	0.49
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.95	0.49
1:A:417:MET:CE	18:A:606:HEA:H263	2.42	0.49
11:K:54:ARG:HG3	11:K:54:ARG:HH11	1.77	0.49
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.46	0.49
1:N:208:MET:HE2	3:P:97:PHE:CD1	2.48	0.49
4:D:77:GLU:HB3	20:D:201:TGL:CB3	2.43	0.49
25:G:102:PEK:C12	25:G:102:PEK:H162	2.43	0.49
4:Q:5:VAL:HG13	4:Q:10:ASP:OD1	2.13	0.49
8:U:42:ALA:O	8:U:46:LYS:HB2	2.12	0.49
11:X:12:LYS:HB3	11:X:13:TYR:CD2	2.47	0.49
2:B:218:TYR:OH	30:B:403:HOH:O	2.19	0.49
2:O:33:LEU:O	2:O:37:LEU:HD23	2.12	0.49
1:A:297:MET:SD	1:A:302:ARG:HG2	2.53	0.48
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.11	0.48
8:U:41:LYS:O	8:U:42:ALA:C	2.56	0.48
2:O:41:ILE:O	2:O:45:MET:HG2	2.13	0.48
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.96	0.48
1:A:177:SER:H	1:A:180:GLN:HE21	1.62	0.48
7:G:5:LYS:HG2	1:N:278:MET:O	2.13	0.48
9:I:2:THR:N	29:I:101:SAC:H	2.11	0.48
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
11:K:8:ASP:HB2	30:K:309:HOH:O	2.14	0.48
10:W:32:TYR:CZ	10:W:36:MET:HG3	2.48	0.48
3:C:161:GLN:NE2	25:C:302:PEK:H031	2.29	0.48
17:M:101:PGV:H062	30:M:219:HOH:O	2.13	0.48
1:A:179:TYR:OH	7:T:8:HIS:HB3	2.14	0.48
2:B:1:FME:HE1	2:B:133:LEU:HD11	1.95	0.48
3:P:258:TRP:CD1	26:P:312:CDL:H781	2.49	0.48
7:G:4:ALA:CB	1:N:285:PHE:CD2	2.96	0.47
2:O:141:ARG:H	9:V:70:GLN:HE22	1.60	0.47
3:P:54:MET:HE1	17:P:306:PGV:H131	1.94	0.47
4:Q:92:THR:O	4:Q:95:LEU:HB2	2.13	0.47
1:A:240:HIS:C	1:A:240:HIS:CD2	2.93	0.47
1:N:112:LEU:HD23	1:N:112:LEU:C	2.39	0.47
1:N:240:HIS:C	1:N:240:HIS:CD2	2.91	0.47
12:Y:41:ARG:NH1	30:Y:201:HOH:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:TYR:CD1	8:H:60:TYR:C	2.93	0.47
1:A:383:MET:O	1:A:387:PHE:HB2	2.15	0.47
4:D:78:TRP:CA	20:D:201:TGL:HB52	2.45	0.47
3:P:95:THR:HG21	17:P:307:PGV:H302	1.97	0.47
26:P:308:CDL:OA5	26:P:308:CDL:H1	2.14	0.47
7:T:15:THR:HG21	24:T:1302:CHD:H213	1.95	0.47
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.47
8:U:40:GLU:OE2	30:U:1601:HOH:O	2.20	0.47
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.96	0.47
3:P:40:MET:O	3:P:44:MET:HG2	2.14	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE2	2.50	0.46
8:U:8:ILE:O	8:U:8:ILE:CG2	2.62	0.46
1:A:411:LYS:NZ	30:A:702:HOH:O	2.48	0.46
17:M:101:PGV:H042	30:M:219:HOH:O	2.16	0.46
26:P:312:CDL:H872	26:P:312:CDL:H811	1.97	0.46
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.50	0.46
3:C:168:THR:HG22	25:C:302:PEK:H132	1.98	0.46
13:Z:28:LEU:HD23	27:Z:101:DMU:C18	2.45	0.46
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.79	0.46
26:P:312:CDL:OB7	26:P:312:CDL:CB6	2.62	0.46
9:V:50:PHE:O	19:V:103:EDO:H21	2.16	0.46
1:A:118:VAL:HG11	1:A:141:ALA:HB3	1.97	0.46
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.51	0.46
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.99	0.46
4:Q:98:TRP:CE2	27:Z:101:DMU:H11	2.51	0.46
4:D:29:HIS:HD2	4:D:61:ARG:O	1.99	0.46
7:G:4:ALA:HB1	1:N:194:LEU:CD2	2.45	0.45
9:V:2:THR:N	29:V:101:SAC:OG	2.48	0.45
13:Z:28:LEU:HD23	27:Z:101:DMU:H7	1.99	0.45
1:A:379:TYR:O	1:A:383:MET:HB2	2.17	0.45
20:D:201:TGL:HG11	20:D:201:TGL:HB42	1.98	0.45
2:O:60:GLU:HG2	2:O:61:VAL:N	2.30	0.45
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.97	0.45
18:N:608:HEA:HBC1	18:N:608:HEA:CMC	2.43	0.45
24:W:302:CHD:H17	24:W:302:CHD:H232	1.81	0.45
4:D:23:PRO:CB	5:E:70:VAL:HG21	2.47	0.45
1:N:321:PHE:HB3	2:O:65:TRP:CE2	2.51	0.45
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.15	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
3:P:67:PHE:CE2	26:P:308:CDL:HB22	2.51	0.45
8:U:60:TYR:CD1	8:U:60:TYR:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:O	1:A:115:SER:HB3	2.16	0.45
7:T:6:GLY:O	7:T:7:ASP:C	2.60	0.45
19:S:106:EDO:H22	30:S:264:HOH:O	2.16	0.45
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.99	0.45
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.98	0.45
10:J:54:SER:O	12:L:46:LYS:HE2	2.16	0.45
4:D:147:LYS:CE	4:D:147:LYS:HA	2.47	0.45
30:L:622:HOH:O	13:M:32:TRP:CH2	2.56	0.45
17:N:622:PGV:O02	17:N:622:PGV:H61	2.16	0.45
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.99	0.44
3:C:210:ILE:HG21	17:C:303:PGV:H282	1.98	0.44
9:I:36:LYS:NZ	30:I:203:HOH:O	2.45	0.44
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.99	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.44
2:O:199:ILE:HG23	2:O:199:ILE:O	2.18	0.44
1:A:297:MET:HG3	1:A:302:ARG:HG3	1.98	0.44
24:J:101:CHD:H12	24:J:101:CHD:H212	1.98	0.44
19:A:615:EDO:H21	6:F:70:ILE:HD12	1.99	0.44
1:A:407:ASP:OD2	19:A:610:EDO:O1	2.32	0.44
20:N:618:TGL:HG31	20:N:618:TGL:CC3	2.47	0.44
6:S:54:ASN:HD22	6:S:54:ASN:C	2.26	0.44
2:B:200:CYS:SG	2:B:204:HIS:HA	2.58	0.44
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.44
7:T:9:GLY:HA2	24:T:1302:CHD:C11	2.48	0.44
1:A:489:THR:HA	6:F:71:TRP:O	2.18	0.44
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.52	0.44
12:Y:41:ARG:HH12	24:Y:101:CHD:H182	1.81	0.44
1:A:194:LEU:HD21	7:T:4:ALA:HB1	2.00	0.44
18:A:606:HEA:HBC1	18:A:606:HEA:HMC3	1.99	0.44
8:H:69:VAL:HG11	19:H:101:EDO:C1	2.48	0.44
3:P:59:ARG:HA	26:P:308:CDL:H512	1.98	0.44
4:Q:109:HIS:HD2	30:Q:1737:HOH:O	2.00	0.44
8:U:24:ASN:HD21	19:U:1501:EDO:H12	1.82	0.44
20:D:201:TGL:HG32	20:D:201:TGL:HC52	1.99	0.43
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.91	0.43
2:O:215:PRO:HD3	9:V:60:PHE:CD1	2.53	0.43
1:A:278:MET:HE1	7:T:8:HIS:CD2	2.53	0.43
17:N:622:PGV:H212	13:Z:10:THR:H	1.83	0.43
8:U:10:ASN:CB	30:U:1643:HOH:O	2.65	0.43
19:A:618:EDO:H12	13:M:41:LYS:HG3	2.00	0.43
2:B:115:ASP:HB2	30:H:223:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:52:GLN:O	1:N:56:VAL:HG23	2.18	0.43
1:N:498:CYS:H	4:Q:7:LYS:HE2	1.82	0.43
19:A:618:EDO:C1	13:M:41:LYS:HG3	2.48	0.43
3:C:76:GLN:O	3:C:80:ARG:HG3	2.17	0.43
3:C:246:ASP:HB2	30:C:483:HOH:O	2.18	0.43
20:N:605:TGL:HC42	12:Y:24:MET:SD	2.57	0.43
26:P:312:CDL:HB32	26:P:312:CDL:H151	1.99	0.43
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.07	0.43
2:O:115:ASP:OD1	8:U:61:LYS:HE3	2.19	0.43
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.99	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.43
3:P:54:MET:HB3	3:P:58:TRP:CZ3	2.54	0.43
17:M:101:PGV:C04	30:M:219:HOH:O	2.67	0.43
19:N:611:EDO:O2	4:Q:7:LYS:NZ	2.50	0.43
12:Y:45:LEU:HD13	24:Y:101:CHD:H5	2.00	0.43
12:L:24:MET:HG3	30:L:619:HOH:O	2.19	0.43
3:P:129:VAL:HG22	3:P:180:GLU:CD	2.43	0.43
1:A:62:ALA:HB2	18:A:606:HEA:HBD1	2.01	0.43
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.00	0.43
7:T:9:GLY:HA2	24:T:1302:CHD:H112	2.00	0.43
8:U:37:HIS:HE1	30:U:1608:HOH:O	2.02	0.43
24:B:303:CHD:H12	24:B:303:CHD:H212	2.01	0.43
25:P:305:PEK:H02	25:P:305:PEK:H6	2.01	0.43
25:G:102:PEK:C12	25:G:102:PEK:C16	2.97	0.42
8:H:46:LYS:C	8:H:48:GLY:H	2.27	0.42
26:P:312:CDL:O1	26:P:312:CDL:H873	2.18	0.42
30:B:522:HOH:O	8:H:61:LYS:CE	2.62	0.42
4:Q:60:TYR:OH	5:R:69:GLU:OE1	2.37	0.42
10:W:32:TYR:CE1	10:W:36:MET:HG3	2.54	0.42
18:N:607:HEA:HBC1	18:N:607:HEA:CMC	2.49	0.42
18:A:605:HEA:HBC1	18:A:605:HEA:CMC	2.49	0.42
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.55	0.42
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.19	0.42
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.01	0.42
17:N:622:PGV:C1	17:N:622:PGV:H61	2.50	0.42
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.34	0.42
4:Q:12:ALA:O	6:S:75:HIS:NE2	2.51	0.42
1:A:488:THR:HB	1:A:495:LEU:HD13	2.02	0.42
17:N:622:PGV:O02	17:N:622:PGV:C6	2.68	0.42
10:W:4:ARG:HD2	10:W:7:GLU:OE2	2.20	0.42
1:A:229:ILE:HD11	2:B:175:ILE:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:MET:SD	2:B:5:MET:HG2	2.60	0.42
7:G:4:ALA:HB2	1:N:285:PHE:CD2	2.55	0.42
1:N:344:PHE:CD1	1:N:344:PHE:C	2.98	0.42
4:D:60:TYR:OH	5:E:69:GLU:OE1	2.38	0.42
26:P:312:CDL:OB7	26:P:312:CDL:HB62	2.20	0.42
7:T:8:HIS:O	24:T:1302:CHD:H212	2.20	0.41
17:C:304:PGV:H72	17:C:304:PGV:C2	2.48	0.41
20:N:618:TGL:HB31	30:Q:1742:HOH:O	2.19	0.41
2:O:1:FME:HE1	2:O:133:LEU:CD2	2.50	0.41
17:A:604:PGV:H183	25:G:102:PEK:H341	2.01	0.41
3:C:59:ARG:HA	26:C:305:CDL:H512	2.02	0.41
4:D:48:TRP:O	4:D:51:LEU:HB2	2.20	0.41
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.90	0.41
26:C:310:CDL:H671	26:C:310:CDL:HA31	2.01	0.41
9:I:36:LYS:HD3	9:I:36:LYS:HA	1.90	0.41
2:O:61:VAL:HG23	23:R:201:PSC:C8	2.51	0.41
25:P:301:PEK:H5	25:P:301:PEK:H241	2.03	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
2:B:91:ASN:HB2	2:B:149:THR:HG21	2.03	0.41
24:J:101:CHD:H213	24:J:101:CHD:H232	1.98	0.41
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.20	0.41
1:A:148:PHE:HB3	3:C:28:THR:HB	2.02	0.41
1:A:243:VAL:HB	18:A:605:HEA:C3C	2.50	0.41
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.51	0.41
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.95	0.41
3:C:248:VAL:HG22	25:C:314:PEK:H8	2.02	0.41
10:J:57:HIS:O	10:J:58:LYS:C	2.63	0.41
1:A:13:LYS:HD3	19:A:612:EDO:H22	2.01	0.41
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.85	0.41
17:C:304:PGV:H172	7:T:1:ALA:HB2	2.03	0.41
7:G:8:HIS:HB3	1:N:186:TRP:HH2	1.86	0.41
17:M:101:PGV:C4	17:M:101:PGV:H02	2.51	0.41
17:N:622:PGV:C18	17:N:622:PGV:H343	2.49	0.41
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.03	0.41
24:P:303:CHD:H212	24:P:303:CHD:H12	2.01	0.41
10:W:58:LYS:HE3	10:W:58:LYS:N	2.36	0.41
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.55	0.41
17:A:604:PGV:C34	25:G:102:PEK:C37	2.99	0.41
18:N:608:HEA:H211	18:N:608:HEA:H271	1.88	0.41
2:O:65:TRP:O	2:O:69:PRO:HG2	2.21	0.41
2:O:75:LEU:HD12	2:O:75:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:90:ARG:HD2	30:R:338:HOH:O	2.16	0.41
1:A:137:ALA:O	19:A:611:EDO:H21	2.21	0.41
20:N:605:TGL:CC4	12:Y:24:MET:SD	3.09	0.41
4:Q:56:LYS:NZ	5:R:97:GLY:O	2.53	0.41
5:R:20:ASN:HD21	19:R:203:EDO:H12	1.86	0.41
6:S:13:ALA:CB	6:S:21:MET:HE1	2.51	0.41
3:P:186:PHE:HA	3:P:190:ASP:OD2	2.21	0.40
1:A:172:LYS:HD2	1:A:181:THR:HG22	2.04	0.40
1:A:426:PHE:N	1:A:427:PRO:CD	2.84	0.40
23:B:302:PSC:H222	23:B:302:PSC:H012	2.03	0.40
17:M:101:PGV:O11	17:M:101:PGV:H31	2.21	0.40
1:N:113:LEU:HB2	20:N:605:TGL:C32	2.50	0.40
7:T:6:GLY:O	7:T:8:HIS:N	2.55	0.40
29:V:101:SAC:HA	29:V:101:SAC:H2A1	1.75	0.40
12:Y:45:LEU:CD1	24:Y:101:CHD:H7	2.51	0.40
13:Z:28:LEU:HA	27:Z:101:DMU:H7	2.03	0.40
1:A:169:ILE:HD13	1:A:189:MET:HE1	2.04	0.40
4:D:109:HIS:HD2	30:D:340:HOH:O	2.03	0.40
1:N:148:PHE:HB3	3:P:28:THR:HB	2.02	0.40
1:N:362:SER:HA	2:O:87:MET:HE1	2.04	0.40
1:N:378:HIS:CG	1:N:425:PHE:CE1	3.10	0.40
6:S:51:SER:O	6:S:93:PRO:HA	2.22	0.40
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.04	0.40
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.40
9:I:29:LEU:HD12	9:I:29:LEU:HA	1.85	0.40
3:P:16:TRP:N	3:P:17:PRO:CD	2.85	0.40
3:P:223:LEU:HD23	3:P:223:LEU:HA	1.89	0.40
4:Q:94:LEU:HD23	11:X:28:VAL:HG21	2.02	0.40
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.56	0.40
2:O:224:ALA:O	2:O:227:LEU:HG	2.22	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%)	497 (97%)	15 (3%)	0	100	100
1	N	512/514 (100%)	499 (98%)	12 (2%)	1 (0%)	43	36
2	B	225/227 (99%)	220 (98%)	5 (2%)	0	100	100
2	O	225/227 (99%)	218 (97%)	7 (3%)	0	100	100
3	C	257/261 (98%)	253 (98%)	4 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	134 (94%)	4 (3%)	4 (3%)	4	0
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
6	S	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
7	G	81/85 (95%)	74 (91%)	6 (7%)	1 (1%)	10	4
7	T	81/85 (95%)	69 (85%)	9 (11%)	3 (4%)	2	0
8	H	77/85 (91%)	72 (94%)	4 (5%)	1 (1%)	9	3
8	U	77/85 (91%)	68 (88%)	6 (8%)	3 (4%)	2	0
9	I	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
9	V	70/73 (96%)	69 (99%)	1 (1%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	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%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	41 (93%)	3 (7%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3502/3614 (97%)	3393 (97%)	96 (3%)	13 (0%)	30	22

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
4	Q	6	VAL
4	Q	7	LYS
7	T	7	ASP
8	U	8	ILE
8	U	46	LYS
7	T	4	ALA
4	Q	34	SER
8	H	48	GLY
7	T	5	LYS
8	U	43	MET
1	N	384	GLY
4	Q	5	VAL

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%)	420 (99%)	6 (1%)	59	59
1	N	426/426 (100%)	420 (99%)	6 (1%)	59	59
2	B	210/210 (100%)	202 (96%)	8 (4%)	29	21
2	O	210/210 (100%)	201 (96%)	9 (4%)	26	18
3	C	224/226 (99%)	219 (98%)	5 (2%)	45	42
3	P	224/226 (99%)	218 (97%)	6 (3%)	39	34
4	D	128/129 (99%)	125 (98%)	3 (2%)	44	40
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	29
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	26
5	R	92/95 (97%)	88 (96%)	4 (4%)	26	18
6	F	81/81 (100%)	77 (95%)	4 (5%)	22	14
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	14
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	6
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	71/75 (95%)	66 (93%)	5 (7%)	14	7
8	U	71/75 (95%)	62 (87%)	9 (13%)	4	1
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	12
9	V	57/57 (100%)	52 (91%)	5 (9%)	9	4
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	19
10	W	49/50 (98%)	46 (94%)	3 (6%)	17	9
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	35
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	35
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	1
13	M	37/38 (97%)	35 (95%)	2 (5%)	20	12
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	12
All	All	3040/3082 (99%)	2928 (96%)	112 (4%)	30	22

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	152	LEU
1	A	178	GLN
1	A	180	GLN
1	A	297	MET
1	A	369	ASP
2	B	33	LEU
2	B	37	LEU
2	B	59	GLN
2	B	60	GLU
2	B	68	LEU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
3	C	127	LEU
3	C	144	ILE
3	C	159	MET
3	C	180	GLU
3	C	230	ASN
4	D	4	SER
4	D	51	LEU

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Mol	Chain	Res	Type
4	D	147	LYS
5	E	70	VAL
5	E	93	LEU
5	E	104	LEU
6	F	48	LEU
6	F	80	GLN
6	F	95	GLN
6	F	96	LEU
7	G	8	HIS
7	G	33	LEU
7	G	36	TRP
7	G	38	HIS
7	G	84	LYS
8	H	7	LYS
8	H	8	ILE
8	H	29	CYS
8	H	46	LYS
8	H	60	TYR
9	I	2	THR
9	I	15	ARG
9	I	29	LEU
10	J	50	LEU
10	J	58	LYS
12	L	26	THR
13	M	34	LEU
13	M	42	LYS
1	N	117	MET
1	N	178	GLN
1	N	369	ASP
1	N	484	THR
1	N	485	VAL
1	N	512	ASN
2	O	33	LEU
2	O	59	GLN
2	O	61	VAL
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	217	LYS
3	P	3	HIS

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Mol	Chain	Res	Type
3	P	127	LEU
3	P	129	VAL
3	P	159	MET
3	P	180	GLU
3	P	230	ASN
4	Q	5	VAL
4	Q	9	GLU
4	Q	19	ARG
4	Q	53	ILE
5	R	14	ARG
5	R	80	GLU
5	R	108	LYS
5	R	109	VAL
6	S	43	LYS
6	S	48	LEU
6	S	54	ASN
6	S	80	GLN
7	T	8	HIS
7	T	30	LEU
7	T	33	LEU
7	T	37	LEU
7	T	42	ARG
7	T	43	GLU
7	T	78	LEU
8	U	7	LYS
8	U	8	ILE
8	U	9	LYS
8	U	10	ASN
8	U	40	GLU
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
8	U	84	LYS
9	V	2	THR
9	V	18	ARG
9	V	29	LEU
9	V	36	LYS
9	V	68	ILE
10	W	36	MET
10	W	50	LEU
10	W	58	LYS
11	X	12	LYS

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Mol	Chain	Res	Type
12	Y	2	HIS
12	Y	26	THR
12	Y	27	LEU
12	Y	46	LYS
12	Y	47	LYS
13	Z	34	LEU
13	Z	41	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	43	GLN
1	A	178	GLN
1	A	180	GLN
1	A	422	ASN
2	B	59	GLN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	32	ASN
4	D	109	HIS
4	D	119	GLN
5	E	94	ASN
6	F	95	GLN
7	G	34	ASN
7	G	76	ASN
10	J	13	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	55	ASN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	232	GLN
1	N	422	ASN
1	N	512	ASN
2	O	10	GLN

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Mol	Chain	Res	Type
2	O	181	GLN
3	P	50	ASN
3	P	68	GLN
3	P	149	HIS
4	Q	37	GLN
4	Q	109	HIS
4	Q	119	GLN
5	R	20	ASN
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
8	U	10	ASN
8	U	31	GLN
8	U	32	ASN
9	V	8	GLN
11	X	35	GLN
13	Z	15	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	$\# Z > 2$
1	FME	A	1	1	8,9,10	0.52	0	8,9,11	0.95	1 (12%)
7	TPO	T	11	7	8,10,11	1.59	1 (12%)	10,14,16	1.26	1 (10%)
7	TPO	G	11	7	8,10,11	1.56	1 (12%)	10,14,16	1.04	1 (10%)
1	FME	N	1	1	8,9,10	0.42	0	8,9,11	0.96	0
2	FME	O	1	2	8,9,10	0.82	1 (12%)	8,9,11	1.11	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	0.67	0	8,9,11	1.09	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
1	FME	A	1	1	-	0/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
7	TPO	G	11	7	-	5/9/11/13	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
2	FME	B	1	2	-	4/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	11	TPO	P-OG1	3.98	1.66	1.59
7	G	11	TPO	P-OG1	3.78	1.66	1.59
2	O	1	FME	CG-SD	-2.17	1.70	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	P-OG1-CB	3.10	131.76	123.33
7	G	11	TPO	O-C-CA	-2.29	118.87	124.77
2	O	1	FME	CG-CB-CA	-2.19	106.18	112.87
1	A	1	FME	O-C-CA	-2.03	119.55	124.77

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	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
7	G	11	TPO	CA-CB-OG1-P

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

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
7	T	11	TPO	2	0
7	G	11	TPO	3	0
2	O	1	FME	2	0
2	B	1	FME	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 8 are monoatomic and 2 are modelled with single atom - leaving 141 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	$\# Z > 2$
17	PGV	P	306	-	50,50,50	0.50	0	53,56,56	0.56	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	I	103	-	3,3,3	0.46	0	2,2,2	0.21	0
27	DMU	G	101	-	34,34,34	2.16	6 (17%)	45,45,45	2.00	11 (24%)
19	EDO	G	108	-	3,3,3	0.07	0	2,2,2	0.15	0
19	EDO	T	1301	-	3,3,3	0.36	0	2,2,2	0.11	0
19	EDO	F	702	-	3,3,3	0.28	0	2,2,2	0.11	0
19	EDO	A	612	-	3,3,3	0.28	0	2,2,2	0.22	0
19	EDO	G	105	-	3,3,3	0.09	0	2,2,2	0.22	0
26	CDL	C	305	-	99,99,99	0.39	0	105,111,111	0.70	4 (3%)
17	PGV	P	307	-	50,50,50	0.35	0	53,56,56	0.44	0
19	EDO	R	202	-	3,3,3	0.16	0	2,2,2	0.15	0
19	EDO	S	106	-	3,3,3	0.20	0	2,2,2	0.26	0
18	HEA	N	607	1	67,67,67	2.17	24 (35%)	81,103,103	2.34	28 (34%)
19	EDO	L	501	-	3,3,3	0.16	0	2,2,2	0.20	0
19	EDO	N	611	-	3,3,3	0.23	0	2,2,2	0.23	0
19	EDO	W	303	-	3,3,3	0.10	0	2,2,2	0.11	0
19	EDO	N	613	-	3,3,3	0.21	0	2,2,2	0.06	0
19	EDO	R	203	-	3,3,3	0.01	0	2,2,2	0.04	0
20	TGL	N	604	-	62,62,62	0.34	0	65,65,65	0.60	1 (1%)
19	EDO	B	304	-	3,3,3	0.27	0	2,2,2	0.25	0
19	EDO	E	202	-	3,3,3	0.17	0	2,2,2	0.27	0
19	EDO	A	614	-	3,3,3	0.04	0	2,2,2	0.19	0
27	DMU	M	102	-	34,34,34	1.64	5 (14%)	45,45,45	1.69	9 (20%)
17	PGV	M	101	-	50,50,50	0.48	0	53,56,56	0.80	2 (3%)
26	CDL	C	310	-	99,99,99	0.39	0	105,111,111	0.43	0
19	EDO	B	311	-	3,3,3	0.08	0	2,2,2	0.18	0
19	EDO	A	607	-	3,3,3	0.40	0	2,2,2	0.53	0
24	CHD	P	303	-	32,32,32	0.67	1 (3%)	51,51,51	0.71	0
19	EDO	V	103	-	3,3,3	0.10	0	2,2,2	0.11	0
19	EDO	G	103	-	3,3,3	0.39	0	2,2,2	0.48	0
24	CHD	G	107	-	32,32,32	0.66	0	51,51,51	0.75	0
25	PEK	P	301	-	52,52,52	0.36	0	55,57,57	0.60	1 (1%)
19	EDO	S	105	-	3,3,3	0.15	0	2,2,2	0.21	0
19	EDO	A	615	-	3,3,3	0.10	0	2,2,2	0.14	0
19	EDO	C	312	-	3,3,3	0.68	0	2,2,2	0.81	0
19	EDO	K	201	-	3,3,3	0.09	0	2,2,2	0.11	0
19	EDO	F	701	-	3,3,3	0.23	0	2,2,2	0.45	0
24	CHD	P	309	-	32,32,32	0.66	0	51,51,51	1.08	3 (5%)
19	EDO	C	308	-	3,3,3	0.13	0	2,2,2	0.14	0
29	SAC	V	101	-	7,8,9	0.55	0	7,9,11	1.46	1 (14%)
19	EDO	D	202	-	3,3,3	0.18	0	2,2,2	0.23	0
19	EDO	A	618	-	3,3,3	0.27	0	2,2,2	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	PGV	A	604	-	50,50,50	0.58	1 (2%)	53,56,56	0.71	1 (1%)
24	CHD	J	101	-	32,32,32	0.64	1 (3%)	51,51,51	0.96	2 (3%)
18	HEA	A	606	1	67,67,67	2.09	20 (29%)	81,103,103	2.63	36 (44%)
19	EDO	J	102	-	3,3,3	0.15	0	2,2,2	0.14	0
19	EDO	N	612	-	3,3,3	0.38	0	2,2,2	0.59	0
19	EDO	Q	1601	-	3,3,3	0.11	0	2,2,2	0.12	0
19	EDO	F	704	-	3,3,3	0.10	0	2,2,2	0.32	0
19	EDO	N	610	-	3,3,3	0.42	0	2,2,2	0.11	0
19	EDO	O	302	-	3,3,3	0.02	0	2,2,2	0.16	0
25	PEK	P	304	-	52,52,52	0.43	0	55,57,57	0.90	4 (7%)
27	DMU	C	311	-	34,34,34	1.90	8 (23%)	45,45,45	2.16	14 (31%)
19	EDO	D	205	-	3,3,3	0.09	0	2,2,2	0.23	0
19	EDO	N	621	-	3,3,3	0.30	0	2,2,2	0.43	0
17	PGV	C	304	-	50,50,50	0.51	0	53,56,56	0.66	0
19	EDO	T	1303	-	3,3,3	0.31	0	2,2,2	0.08	0
17	PGV	N	606	-	50,50,50	0.51	0	53,56,56	0.68	1 (1%)
19	EDO	B	306	-	3,3,3	0.35	0	2,2,2	0.20	0
19	EDO	B	305	-	3,3,3	0.32	0	2,2,2	0.05	0
19	EDO	Q	1604	-	3,3,3	0.30	0	2,2,2	0.35	0
19	EDO	N	619	-	3,3,3	0.12	0	2,2,2	0.05	0
23	PSC	B	302	-	51,51,51	0.52	0	57,59,59	0.58	0
19	EDO	P	310	-	3,3,3	0.07	0	2,2,2	0.12	0
19	EDO	P	311	-	3,3,3	0.09	0	2,2,2	0.17	0
19	EDO	N	614	-	3,3,3	0.13	0	2,2,2	0.48	0
19	EDO	A	617	-	3,3,3	0.31	0	2,2,2	0.48	0
19	EDO	N	617	-	3,3,3	0.22	0	2,2,2	0.26	0
19	EDO	E	205	-	3,3,3	0.04	0	2,2,2	0.33	0
19	EDO	B	307	-	3,3,3	0.27	0	2,2,2	0.24	0
19	EDO	A	608	-	3,3,3	0.33	0	2,2,2	0.13	0
25	PEK	G	102	-	52,52,52	0.48	0	55,57,57	0.65	0
29	SAC	I	101	-	7,8,9	0.64	0	7,9,11	0.97	1 (14%)
17	PGV	C	303	-	50,50,50	0.42	0	53,56,56	0.54	0
19	EDO	L	503	-	3,3,3	0.09	0	2,2,2	0.05	0
19	EDO	A	609	-	3,3,3	0.36	0	2,2,2	0.17	0
19	EDO	E	203	-	3,3,3	0.15	0	2,2,2	0.10	0
20	TGL	N	618	-	62,62,62	0.31	0	65,65,65	0.40	0
19	EDO	B	309	-	3,3,3	0.15	0	2,2,2	0.26	0
22	CUA	B	301	2	0,1,1	-	-	-	-	-
27	DMU	G	104	-	34,34,34	1.70	7 (20%)	45,45,45	1.78	15 (33%)
19	EDO	S	102	-	3,3,3	0.46	0	2,2,2	0.28	0
19	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	EDO	W	301	-	3,3,3	0.09	0	2,2,2	0.05	0
27	DMU	P	302	-	34,34,34	0.90	3 (8%)	45,45,45	1.67	9 (20%)
19	EDO	V	104	-	3,3,3	0.56	0	2,2,2	0.72	0
19	EDO	J	103	-	3,3,3	0.41	0	2,2,2	0.24	0
24	CHD	C	306	-	32,32,32	0.62	0	51,51,51	0.76	1 (1%)
19	EDO	S	104	-	3,3,3	0.22	0	2,2,2	0.16	0
19	EDO	F	705	-	3,3,3	0.35	0	2,2,2	0.32	0
19	EDO	U	1501	-	3,3,3	0.30	0	2,2,2	0.32	0
19	EDO	S	107	-	3,3,3	0.09	0	2,2,2	0.62	0
19	EDO	B	308	-	3,3,3	0.29	0	2,2,2	0.25	0
19	EDO	O	303	-	3,3,3	0.36	0	2,2,2	0.04	0
20	TGL	N	605	-	62,62,62	0.39	0	65,65,65	0.50	1 (1%)
23	PSC	R	201	-	51,51,51	0.41	0	57,59,59	0.51	0
19	EDO	N	620	-	3,3,3	0.26	0	2,2,2	0.27	0
19	EDO	C	313	-	3,3,3	0.36	0	2,2,2	0.13	0
19	EDO	P	313	-	3,3,3	0.56	0	2,2,2	0.52	0
19	EDO	I	102	-	3,3,3	0.07	0	2,2,2	0.07	0
19	EDO	L	504	-	3,3,3	0.11	0	2,2,2	0.27	0
19	EDO	G	106	-	3,3,3	0.22	0	2,2,2	0.22	0
19	EDO	V	102	-	3,3,3	0.11	0	2,2,2	0.34	0
20	TGL	L	502	-	62,62,62	0.42	0	65,65,65	0.38	0
26	CDL	P	308	-	99,99,99	0.38	0	105,111,111	0.50	1 (0%)
27	DMU	Z	101	-	34,34,34	0.98	2 (5%)	45,45,45	1.47	9 (20%)
25	PEK	C	314	-	52,52,52	0.41	0	55,57,57	0.60	0
25	PEK	C	302	-	52,52,52	0.43	0	55,57,57	0.55	1 (1%)
19	EDO	D	203	-	3,3,3	0.13	0	2,2,2	0.07	0
24	CHD	B	303	-	32,32,32	0.57	0	51,51,51	0.90	2 (3%)
19	EDO	N	609	-	3,3,3	0.15	0	2,2,2	0.44	0
24	CHD	Y	101	-	32,32,32	0.71	0	51,51,51	1.22	6 (11%)
19	EDO	A	610	-	3,3,3	0.12	0	2,2,2	0.10	0
26	CDL	P	312	-	99,99,99	0.36	0	105,111,111	0.42	0
19	EDO	M	103	-	3,3,3	0.11	0	2,2,2	0.25	0
25	PEK	P	305	-	52,52,52	0.42	0	55,57,57	0.48	0
19	EDO	D	204	-	3,3,3	0.20	0	2,2,2	0.22	0
19	EDO	Q	1603	-	3,3,3	0.15	0	2,2,2	0.17	0
19	EDO	C	309	-	3,3,3	0.12	0	2,2,2	0.20	0
20	TGL	D	201	-	62,62,62	0.37	0	65,65,65	0.38	0
18	HEA	A	605	1	67,67,67	1.99	23 (34%)	81,103,103	2.43	29 (35%)
19	EDO	F	707	-	3,3,3	0.12	0	2,2,2	0.07	0
19	EDO	F	706	-	3,3,3	0.31	0	2,2,2	0.12	0
19	EDO	S	103	-	3,3,3	0.39	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHD	T	1302	-	32,32,32	0.64	0	51,51,51	0.99	2 (3%)
19	EDO	Q	1602	-	3,3,3	0.17	0	2,2,2	0.14	0
19	EDO	A	611	-	3,3,3	0.33	0	2,2,2	0.24	0
19	EDO	P	314	-	3,3,3	0.05	0	2,2,2	0.19	0
20	TGL	A	613	-	62,62,62	0.44	0	65,65,65	0.79	1 (1%)
18	HEA	N	608	1	67,67,67	2.29	24 (35%)	81,103,103	2.48	32 (39%)
19	EDO	A	616	-	3,3,3	0.11	0	2,2,2	0.38	0
19	EDO	C	307	-	3,3,3	0.46	0	2,2,2	0.43	0
24	CHD	W	302	-	32,32,32	0.60	0	51,51,51	0.70	1 (1%)
19	EDO	H	101	-	3,3,3	0.39	0	2,2,2	0.09	0
19	EDO	N	615	-	3,3,3	0.63	0	2,2,2	0.57	0
17	PGV	N	622	-	50,50,50	0.44	0	53,56,56	0.54	0
24	CHD	C	301	-	32,32,32	0.70	0	51,51,51	0.82	1 (1%)
19	EDO	B	310	-	3,3,3	0.08	0	2,2,2	0.14	0
22	CUA	O	301	2	0,1,1	-	-	-	-	-
19	EDO	E	204	-	3,3,3	0.10	0	2,2,2	0.05	0
19	EDO	N	616	-	3,3,3	0.16	0	2,2,2	0.23	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
17	PGV	P	306	-	-	15/55/55/55	-
19	EDO	I	103	-	-	0/1/1/1	-
27	DMU	G	101	-	-	13/19/59/59	0/2/2/2
19	EDO	G	108	-	-	1/1/1/1	-
19	EDO	T	1301	-	-	1/1/1/1	-
19	EDO	F	702	-	-	1/1/1/1	-
19	EDO	A	612	-	-	0/1/1/1	-
19	EDO	G	105	-	-	1/1/1/1	-
26	CDL	C	305	-	-	66/110/110/110	-
17	PGV	P	307	-	-	30/55/55/55	-
19	EDO	R	202	-	-	0/1/1/1	-
19	EDO	S	106	-	-	1/1/1/1	-
18	HEA	N	607	1	-	5/36/76/76	-
19	EDO	L	501	-	-	1/1/1/1	-
19	EDO	N	611	-	-	0/1/1/1	-
19	EDO	W	303	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	N	613	-	-	1/1/1/1	-
19	EDO	R	203	-	-	1/1/1/1	-
20	TGL	N	604	-	-	29/65/65/65	-
19	EDO	B	304	-	-	0/1/1/1	-
19	EDO	E	202	-	-	1/1/1/1	-
19	EDO	A	614	-	-	0/1/1/1	-
27	DMU	M	102	-	-	7/19/59/59	0/2/2/2
17	PGV	M	101	-	-	39/55/55/55	-
26	CDL	C	310	-	-	52/110/110/110	-
19	EDO	B	311	-	-	1/1/1/1	-
19	EDO	A	607	-	-	0/1/1/1	-
24	CHD	P	303	-	-	2/9/74/74	0/4/4/4
19	EDO	V	103	-	-	1/1/1/1	-
19	EDO	G	103	-	-	0/1/1/1	-
24	CHD	G	107	-	-	3/9/74/74	0/4/4/4
25	PEK	P	301	-	-	32/56/56/56	-
19	EDO	S	105	-	-	1/1/1/1	-
19	EDO	A	615	-	-	0/1/1/1	-
19	EDO	C	312	-	-	0/1/1/1	-
19	EDO	K	201	-	-	1/1/1/1	-
19	EDO	F	701	-	-	1/1/1/1	-
24	CHD	P	309	-	-	2/9/74/74	0/4/4/4
19	EDO	C	308	-	-	0/1/1/1	-
29	SAC	V	101	-	-	2/7/8/10	-
19	EDO	D	202	-	-	1/1/1/1	-
19	EDO	A	618	-	-	0/1/1/1	-
17	PGV	A	604	-	-	14/55/55/55	-
24	CHD	J	101	-	-	3/9/74/74	0/4/4/4
18	HEA	A	606	1	-	2/36/76/76	-
19	EDO	J	102	-	-	0/1/1/1	-
19	EDO	N	612	-	-	1/1/1/1	-
19	EDO	Q	1601	-	-	1/1/1/1	-
19	EDO	F	704	-	-	0/1/1/1	-
19	EDO	N	610	-	-	0/1/1/1	-
19	EDO	O	302	-	-	1/1/1/1	-
25	PEK	P	304	-	-	18/56/56/56	-
27	DMU	C	311	-	-	7/19/59/59	0/2/2/2
19	EDO	D	205	-	-	0/1/1/1	-
19	EDO	N	621	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	PGV	C	304	-	-	29/55/55/55	-
19	EDO	T	1303	-	-	1/1/1/1	-
17	PGV	N	606	-	-	9/55/55/55	-
19	EDO	B	306	-	-	0/1/1/1	-
19	EDO	B	305	-	-	0/1/1/1	-
19	EDO	Q	1604	-	-	1/1/1/1	-
19	EDO	N	619	-	-	1/1/1/1	-
23	PSC	B	302	-	-	28/55/55/55	-
19	EDO	P	310	-	-	1/1/1/1	-
19	EDO	P	311	-	-	1/1/1/1	-
19	EDO	N	614	-	-	1/1/1/1	-
19	EDO	A	617	-	-	0/1/1/1	-
19	EDO	N	617	-	-	1/1/1/1	-
19	EDO	E	205	-	-	1/1/1/1	-
19	EDO	B	307	-	-	1/1/1/1	-
19	EDO	A	608	-	-	0/1/1/1	-
25	PEK	G	102	-	-	21/56/56/56	-
29	SAC	I	101	-	-	5/7/8/10	-
17	PGV	C	303	-	-	15/55/55/55	-
19	EDO	L	503	-	-	1/1/1/1	-
19	EDO	A	609	-	-	0/1/1/1	-
19	EDO	E	203	-	-	1/1/1/1	-
20	TGL	N	618	-	-	36/65/65/65	-
19	EDO	B	309	-	-	1/1/1/1	-
27	DMU	G	104	-	-	11/19/59/59	0/2/2/2
19	EDO	S	102	-	-	1/1/1/1	-
19	EDO	E	201	-	-	1/1/1/1	-
19	EDO	W	301	-	-	0/1/1/1	-
27	DMU	P	302	-	-	9/19/59/59	0/2/2/2
19	EDO	V	104	-	-	0/1/1/1	-
19	EDO	J	103	-	-	0/1/1/1	-
24	CHD	C	306	-	-	2/9/74/74	0/4/4/4
19	EDO	S	104	-	-	0/1/1/1	-
19	EDO	F	705	-	-	0/1/1/1	-
19	EDO	U	1501	-	-	1/1/1/1	-
19	EDO	S	107	-	-	0/1/1/1	-
19	EDO	B	308	-	-	1/1/1/1	-
19	EDO	O	303	-	-	0/1/1/1	-
20	TGL	N	605	-	-	34/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSC	R	201	-	-	33/55/55/55	-
19	EDO	N	620	-	-	1/1/1/1	-
19	EDO	C	313	-	-	1/1/1/1	-
19	EDO	P	313	-	-	0/1/1/1	-
19	EDO	I	102	-	-	1/1/1/1	-
19	EDO	L	504	-	-	0/1/1/1	-
19	EDO	G	106	-	-	1/1/1/1	-
19	EDO	V	102	-	-	1/1/1/1	-
20	TGL	L	502	-	-	38/65/65/65	-
26	CDL	P	308	-	-	59/110/110/110	-
27	DMU	Z	101	-	-	8/19/59/59	0/2/2/2
25	PEK	C	314	-	-	30/56/56/56	-
25	PEK	C	302	-	-	27/56/56/56	-
19	EDO	D	203	-	-	0/1/1/1	-
24	CHD	B	303	-	-	2/9/74/74	0/4/4/4
19	EDO	N	609	-	-	1/1/1/1	-
24	CHD	Y	101	-	-	9/9/74/74	0/4/4/4
19	EDO	A	610	-	-	1/1/1/1	-
26	CDL	P	312	-	-	52/110/110/110	-
19	EDO	M	103	-	-	1/1/1/1	-
25	PEK	P	305	-	-	30/56/56/56	-
19	EDO	D	204	-	-	0/1/1/1	-
19	EDO	Q	1603	-	-	1/1/1/1	-
19	EDO	C	309	-	-	1/1/1/1	-
20	TGL	D	201	-	-	30/65/65/65	-
18	HEA	A	605	1	-	5/36/76/76	-
19	EDO	F	707	-	-	0/1/1/1	-
19	EDO	F	706	-	-	0/1/1/1	-
19	EDO	S	103	-	-	1/1/1/1	-
24	CHD	T	1302	-	-	6/9/74/74	0/4/4/4
19	EDO	Q	1602	-	-	0/1/1/1	-
19	EDO	A	611	-	-	1/1/1/1	-
19	EDO	P	314	-	-	0/1/1/1	-
20	TGL	A	613	-	-	37/65/65/65	-
18	HEA	N	608	1	-	4/36/76/76	-
19	EDO	A	616	-	-	1/1/1/1	-
19	EDO	C	307	-	-	1/1/1/1	-
24	CHD	W	302	-	-	1/9/74/74	0/4/4/4
19	EDO	H	101	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EDO	N	615	-	-	0/1/1/1	-
17	PGV	N	622	-	-	25/55/55/55	-
24	CHD	C	301	-	-	1/9/74/74	0/4/4/4
19	EDO	B	310	-	-	1/1/1/1	-
19	EDO	E	204	-	-	1/1/1/1	-
19	EDO	N	616	-	-	1/1/1/1	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	G	101	DMU	O16-C6	9.12	1.55	1.40
27	C	311	DMU	O16-C6	6.95	1.51	1.40
27	M	102	DMU	O16-C6	6.59	1.51	1.40
18	N	608	HEA	FE-ND	5.76	2.12	1.94
18	N	608	HEA	C1D-ND	-5.38	1.31	1.40
18	N	607	HEA	C11-C3B	-5.37	1.44	1.51
18	A	606	HEA	C4A-NA	-5.20	1.29	1.39
27	G	104	DMU	O16-C6	4.95	1.48	1.40
18	N	608	HEA	C4B-NB	-4.76	1.32	1.40
18	A	606	HEA	C4C-NC	-4.74	1.30	1.39
18	N	607	HEA	CHA-C1A	4.61	1.47	1.38
18	N	607	HEA	FE-ND	4.55	2.08	1.94
18	N	607	HEA	FE-NB	4.52	2.08	1.94
18	A	605	HEA	C3B-C2B	4.46	1.44	1.34
18	A	606	HEA	FE-NC	4.45	2.09	1.95
18	N	608	HEA	FE-NB	4.44	2.08	1.94
18	N	608	HEA	C3B-C2B	4.40	1.44	1.34
18	A	606	HEA	C3D-C2D	4.37	1.46	1.36
18	N	608	HEA	C3A-C2A	4.37	1.47	1.37
18	A	605	HEA	C3D-C2D	4.27	1.46	1.36
18	N	608	HEA	C11-C3B	-4.27	1.46	1.51
18	A	606	HEA	C1D-ND	-4.26	1.32	1.40
18	N	607	HEA	C3B-C2B	4.22	1.44	1.34
18	A	606	HEA	CHA-C1A	4.17	1.46	1.38
18	N	607	HEA	C1D-ND	-4.17	1.33	1.40
18	A	605	HEA	C4A-NA	-4.07	1.32	1.39
27	C	311	DMU	O7-C10	4.07	1.53	1.41
18	N	608	HEA	CHA-C1A	4.00	1.46	1.38
18	N	607	HEA	C4B-NB	-3.97	1.33	1.40
18	N	607	HEA	C3A-C2A	3.93	1.46	1.37
18	A	605	HEA	FE-NA	3.87	2.07	1.95
18	A	606	HEA	FE-NA	3.84	2.07	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	CHD-C1D	3.83	1.46	1.38
18	N	608	HEA	C3D-C2D	3.81	1.45	1.36
18	N	607	HEA	CHB-C4A	3.79	1.45	1.38
18	A	605	HEA	C1A-NA	-3.75	1.32	1.39
18	N	608	HEA	C1B-NB	-3.71	1.31	1.38
18	A	605	HEA	C4C-NC	-3.60	1.32	1.39
27	G	104	DMU	O1-C10	3.56	1.51	1.41
18	A	606	HEA	C3B-C2B	3.54	1.42	1.34
18	A	606	HEA	C1A-NA	-3.52	1.33	1.39
18	N	608	HEA	C4B-C3B	3.51	1.50	1.44
18	A	605	HEA	CHA-C1A	3.49	1.45	1.38
18	A	606	HEA	C3A-C2A	3.47	1.45	1.37
18	A	605	HEA	CHB-C1B	3.44	1.47	1.39
27	C	311	DMU	C3-C4	3.39	1.62	1.52
18	A	605	HEA	C1D-ND	-3.37	1.34	1.40
18	N	608	HEA	CHD-C4C	3.37	1.47	1.39
18	N	608	HEA	C4D-ND	-3.35	1.32	1.38
18	A	605	HEA	FE-NC	3.27	2.06	1.95
18	A	605	HEA	C3A-C2A	3.23	1.44	1.37
18	N	608	HEA	C1C-NC	-3.23	1.33	1.39
18	A	606	HEA	C1B-NB	-3.16	1.32	1.38
18	A	605	HEA	CHD-C1D	3.14	1.44	1.38
18	N	607	HEA	C1B-NB	-3.14	1.32	1.38
27	G	104	DMU	C2-C1	3.10	1.60	1.52
18	A	606	HEA	C4B-NB	-3.03	1.35	1.40
27	C	311	DMU	O1-C10	2.97	1.49	1.41
18	A	605	HEA	C1B-NB	-2.97	1.33	1.38
27	G	104	DMU	C2-C3	2.96	1.60	1.52
18	N	608	HEA	C4A-NA	-2.95	1.34	1.39
18	N	607	HEA	CHC-C1C	2.94	1.46	1.39
18	N	607	HEA	CHD-C4C	2.94	1.46	1.39
18	A	605	HEA	CHB-C4A	2.94	1.44	1.38
27	M	102	DMU	C6-C1	-2.92	1.43	1.52
27	M	102	DMU	O1-C9	2.88	1.51	1.44
18	N	607	HEA	C4D-C3D	2.87	1.49	1.45
27	G	104	DMU	O1-C9	2.87	1.51	1.44
18	N	607	HEA	C1C-NC	-2.86	1.34	1.39
18	N	608	HEA	CHB-C1B	2.86	1.45	1.39
27	G	104	DMU	O5-C6	2.85	1.49	1.41
18	A	606	HEA	CHD-C1D	2.84	1.44	1.38
18	N	607	HEA	C1D-C2D	2.84	1.50	1.44
18	A	605	HEA	CHC-C1C	2.83	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	606	HEA	CHB-C4A	2.80	1.43	1.38
27	Z	101	DMU	O1-C10	2.79	1.49	1.41
18	N	608	HEA	CHC-C1C	2.79	1.45	1.39
18	N	608	HEA	CHD-C1D	2.77	1.44	1.38
27	G	101	DMU	C2-C1	2.74	1.59	1.52
18	A	605	HEA	FE-ND	2.73	2.03	1.94
18	N	608	HEA	CHB-C4A	2.67	1.43	1.38
27	C	311	DMU	O5-C4	2.63	1.50	1.44
18	N	607	HEA	CHC-C4B	2.62	1.43	1.38
18	N	608	HEA	FE-NC	2.60	2.03	1.95
27	C	311	DMU	O1-C9	2.59	1.50	1.44
27	Z	101	DMU	O1-C9	2.59	1.50	1.44
18	N	608	HEA	CHA-C4D	2.58	1.45	1.39
27	G	101	DMU	O7-C10	2.58	1.49	1.41
27	G	101	DMU	C7-C5	2.51	1.58	1.52
18	A	606	HEA	C1C-C2C	2.50	1.49	1.43
18	A	605	HEA	CHC-C4B	2.50	1.43	1.38
18	A	605	HEA	C1C-NC	-2.48	1.34	1.39
18	A	605	HEA	C4B-C3B	2.44	1.49	1.44
24	J	101	CHD	O26-C24	-2.41	1.22	1.30
27	P	302	DMU	O1-C10	2.40	1.48	1.41
18	A	606	HEA	CHC-C4B	2.39	1.43	1.38
27	P	302	DMU	O55-C2	2.39	1.48	1.43
18	A	606	HEA	FE-NB	2.38	2.02	1.94
27	C	311	DMU	O5-C6	2.37	1.47	1.41
27	M	102	DMU	O5-C6	2.37	1.47	1.41
27	G	101	DMU	O5-C6	2.35	1.47	1.41
18	N	607	HEA	C4D-ND	-2.32	1.34	1.38
18	N	607	HEA	CHA-C4D	2.31	1.44	1.39
27	G	101	DMU	C8-C7	2.29	1.58	1.52
18	N	608	HEA	C1C-C2C	2.29	1.48	1.43
18	A	605	HEA	C1C-C2C	2.29	1.48	1.43
18	A	605	HEA	C11-C3B	-2.29	1.48	1.51
18	A	606	HEA	CHB-C1B	2.27	1.44	1.39
18	N	607	HEA	C4C-NC	-2.27	1.35	1.39
27	P	302	DMU	O16-C6	2.26	1.44	1.40
27	G	104	DMU	O7-C10	2.25	1.48	1.41
24	P	303	CHD	O26-C24	-2.24	1.23	1.30
18	A	605	HEA	FE-NB	2.24	2.01	1.94
18	N	607	HEA	CHB-C1B	2.22	1.44	1.39
18	N	607	HEA	C4B-C3B	2.16	1.48	1.44
18	N	608	HEA	C1B-C2B	2.12	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	607	HEA	C18-C19	2.10	1.37	1.33
27	C	311	DMU	O7-C3	2.09	1.49	1.43
18	N	607	HEA	C3D-C2D	2.08	1.41	1.36
27	M	102	DMU	O7-C10	2.07	1.47	1.41
18	A	606	HEA	FE-ND	2.05	2.01	1.94
18	A	606	HEA	C1C-NC	-2.03	1.35	1.39
18	A	605	HEA	C4D-ND	-2.03	1.34	1.38
17	A	604	PGV	C20-C19	2.01	1.56	1.50
18	N	608	HEA	CHC-C4B	2.00	1.42	1.38

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	C	311	DMU	C18-O16-C6	8.02	127.38	113.68
18	A	606	HEA	C3D-C4D-ND	7.48	117.58	110.35
27	G	101	DMU	C18-O16-C6	7.43	126.37	113.68
18	A	606	HEA	C3A-C2A-C1A	-6.46	100.93	107.05
27	P	302	DMU	C6-O5-C4	6.22	125.87	113.72
18	N	608	HEA	C3D-C4D-ND	6.18	116.33	110.35
18	A	605	HEA	C2D-C1D-ND	6.13	116.88	109.84
18	N	607	HEA	C2D-C1D-ND	6.08	116.83	109.84
18	N	608	HEA	C3B-C4B-NB	5.93	116.65	109.84
27	M	102	DMU	C18-O16-C6	-5.84	103.71	113.68
18	A	605	HEA	C3A-C2A-C1A	-5.81	101.55	107.05
18	A	606	HEA	C3C-C2C-C1C	-5.75	100.39	107.17
18	N	608	HEA	C2B-C1B-NB	5.69	116.48	109.90
18	N	607	HEA	CAD-CBD-CGD	-5.64	98.70	113.67
18	A	605	HEA	C2B-C1B-NB	5.57	116.34	109.90
18	A	606	HEA	C2D-C1D-ND	5.53	116.20	109.84
18	N	608	HEA	C3C-C4C-NC	5.46	114.40	109.80
27	C	311	DMU	O1-C9-C11	5.42	119.86	106.44
18	N	607	HEA	C2B-C1B-NB	5.40	116.14	109.90
18	N	608	HEA	C3A-C2A-C1A	-5.35	101.99	107.05
18	A	605	HEA	C3D-C4D-ND	5.32	115.49	110.35
18	N	607	HEA	C3C-C4C-NC	5.25	114.22	109.80
18	A	606	HEA	C2B-C1B-NB	5.25	115.97	109.90
18	A	606	HEA	C3B-C4B-NB	5.19	115.80	109.84
18	N	608	HEA	C13-C12-C11	-5.18	106.11	114.39
20	A	613	TGL	OG2-CB1-CB2	5.10	122.51	111.48
18	A	606	HEA	C3C-C4C-NC	5.05	114.06	109.80
18	A	605	HEA	C1D-C2D-C3D	-5.05	101.67	106.98
18	A	605	HEA	C3C-C2C-C1C	-5.02	101.25	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	607	HEA	C1D-C2D-C3D	-5.02	101.70	106.98
18	A	605	HEA	C3C-C4C-NC	4.94	113.96	109.80
18	A	605	HEA	C3B-C4B-NB	4.90	115.47	109.84
18	A	606	HEA	CHA-C4D-C3D	-4.85	117.71	124.77
18	N	607	HEA	C3D-C4D-ND	4.82	115.01	110.35
27	M	102	DMU	O16-C6-C1	4.69	115.39	108.27
18	A	606	HEA	C2A-C1A-NA	4.64	114.80	110.32
27	C	311	DMU	O5-C6-O16	4.61	120.93	110.04
18	A	606	HEA	C13-C12-C11	-4.58	107.07	114.39
18	N	607	HEA	C3B-C4B-NB	4.53	115.05	109.84
18	N	608	HEA	C2A-C1A-NA	4.48	114.65	110.32
18	A	606	HEA	C1D-C2D-C3D	-4.37	102.38	106.98
18	N	608	HEA	C2D-C1D-ND	4.35	114.84	109.84
18	N	608	HEA	C3C-C2C-C1C	-4.26	102.14	107.17
18	N	608	HEA	CAA-CBA-CGA	-4.15	102.66	113.67
18	N	607	HEA	C3C-C2C-C1C	-4.12	102.31	107.17
18	N	607	HEA	C1B-C2B-C3B	-4.02	102.14	106.80
18	N	608	HEA	C4D-C3D-C2D	-3.99	101.08	106.89
18	N	608	HEA	CMC-C2C-C1C	3.97	131.46	125.42
18	N	607	HEA	C3A-C2A-C1A	-3.97	103.29	107.05
18	A	605	HEA	CMB-C2B-C1B	3.97	131.23	125.03
27	G	101	DMU	C8-C7-C5	3.96	117.79	110.83
18	A	605	HEA	C2A-C1A-NA	3.96	114.14	110.32
18	N	608	HEA	C4B-C3B-C2B	-3.93	100.83	107.44
27	G	104	DMU	C1-C2-C3	3.92	118.58	109.68
18	N	608	HEA	CHB-C1B-C2B	-3.91	118.86	125.03
18	A	605	HEA	CMD-C2D-C1D	3.90	131.13	125.03
18	N	607	HEA	C2A-C1A-NA	3.89	114.08	110.32
17	M	101	PGV	O01-C1-C2	3.89	119.89	111.48
20	N	604	TGL	OG2-CB1-CB2	3.87	119.84	111.48
27	G	101	DMU	O16-C6-C1	3.76	113.98	108.27
27	Z	101	DMU	C18-O16-C6	3.58	119.80	113.68
27	G	101	DMU	C1-C2-C3	3.58	117.81	109.68
27	G	104	DMU	O5-C6-O16	3.57	118.48	110.04
27	G	101	DMU	C6-C1-C2	3.51	117.39	110.01
27	G	104	DMU	O1-C9-C11	3.50	115.12	106.44
27	M	102	DMU	C28-C25-C22	-3.50	96.70	114.37
18	N	608	HEA	C2C-C1C-NC	3.48	115.72	110.14
24	P	309	CHD	C1-C2-C3	3.48	115.09	110.48
18	A	605	HEA	C4B-C3B-C2B	-3.46	101.63	107.44
18	A	605	HEA	CHA-C4D-C3D	-3.44	119.76	124.77
27	G	104	DMU	C10-O1-C9	3.42	120.41	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	V	101	SAC	O-C-CA	-3.37	116.10	124.77
18	N	608	HEA	C1B-C2B-C3B	-3.36	102.91	106.80
18	A	606	HEA	CHC-C4B-NB	-3.35	120.22	124.37
18	N	607	HEA	CMC-C2C-C1C	3.35	130.51	125.42
18	A	606	HEA	C4D-C3D-C2D	-3.34	102.03	106.89
18	A	606	HEA	CAA-CBA-CGA	-3.34	104.81	113.67
18	N	607	HEA	CHC-C1C-C2C	-3.32	117.80	127.43
18	N	607	HEA	C2C-C1C-NC	3.27	115.38	110.14
18	A	606	HEA	C4B-C3B-C2B	-3.26	101.96	107.44
18	N	607	HEA	CHB-C1B-C2B	-3.26	119.89	125.03
27	G	101	DMU	O5-C6-O16	3.23	117.67	110.04
18	A	606	HEA	C2C-C1C-NC	3.23	115.31	110.14
18	A	605	HEA	C2C-C1C-NC	3.22	115.31	110.14
18	N	608	HEA	C1D-C2D-C3D	-3.22	103.60	106.98
18	A	605	HEA	CHA-C1A-C2A	-3.17	119.86	124.86
18	A	606	HEA	C1D-ND-C4D	-3.13	101.50	105.21
27	G	101	DMU	C7-C8-C9	3.12	115.90	110.23
18	N	607	HEA	CHA-C4D-C3D	-3.09	120.26	124.77
27	Z	101	DMU	C10-O1-C9	3.07	119.72	113.72
27	C	311	DMU	O5-C4-C3	3.01	115.94	109.72
18	A	606	HEA	C27-C19-C20	3.01	120.45	115.23
24	Y	101	CHD	C13-C14-C8	3.00	118.52	114.72
18	A	605	HEA	CMB-C2B-C3B	-2.99	124.50	130.28
18	A	605	HEA	CAA-C2A-C1A	2.98	130.92	124.85
26	C	305	CDL	OA6-CA5-C11	2.92	117.81	111.48
18	A	605	HEA	CAD-C3D-C4D	2.90	129.75	124.70
18	A	606	HEA	C21-C20-C19	2.90	122.80	113.19
18	A	605	HEA	CAD-CBD-CGD	-2.90	105.98	113.67
20	N	605	TGL	OG2-CB1-CB2	2.88	117.70	111.48
26	C	305	CDL	OB2-PB2-OB3	2.86	120.29	108.94
18	N	607	HEA	CAA-C2A-C1A	2.83	130.61	124.85
18	A	605	HEA	CHD-C1D-C2D	-2.79	119.01	126.95
24	C	301	CHD	C6-C7-C8	2.79	114.55	111.50
27	G	104	DMU	O7-C10-O1	2.79	118.03	110.69
18	N	608	HEA	C4C-C3C-C2C	-2.77	103.85	107.30
25	P	304	PEK	O11-P-O14	-2.76	98.00	108.94
27	C	311	DMU	O7-C10-O1	2.75	117.93	110.69
18	A	606	HEA	CAD-C3D-C4D	2.72	129.45	124.70
18	A	606	HEA	CMD-C2D-C1D	2.71	129.26	125.03
27	Z	101	DMU	O1-C9-C11	2.70	113.14	106.44
25	P	304	PEK	O01-C1-C2	-2.69	105.67	111.48
18	N	608	HEA	CHA-C1A-C2A	-2.68	120.64	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	606	PGV	O12-P-O13	2.66	119.49	108.94
18	A	606	HEA	C25-C23-C22	-2.66	114.67	122.66
18	A	606	HEA	O11-C11-C3B	-2.65	106.39	111.26
18	A	605	HEA	CHB-C1B-C2B	-2.64	120.85	125.03
18	A	606	HEA	CMB-C2B-C1B	2.62	129.13	125.03
18	N	607	HEA	C4B-C3B-C2B	-2.62	103.03	107.44
18	N	608	HEA	CHC-C1C-C2C	-2.61	119.84	127.43
27	C	311	DMU	C11-C9-C8	-2.61	106.60	113.02
18	N	608	HEA	O2D-CGD-O1D	-2.61	116.63	123.33
24	Y	101	CHD	C17-C13-C14	-2.60	97.51	100.11
24	Y	101	CHD	C18-C13-C14	2.60	115.27	111.20
18	A	606	HEA	CHD-C1D-C2D	-2.57	119.64	126.95
27	G	104	DMU	O49-C1-C6	-2.57	103.95	110.08
24	B	303	CHD	C17-C13-C14	2.56	102.69	100.11
24	Y	101	CHD	C17-C13-C12	2.56	119.97	117.67
27	P	302	DMU	C37-C34-C31	-2.56	101.44	114.37
27	P	302	DMU	C7-C8-C9	-2.55	105.60	110.23
18	N	607	HEA	CMD-C2D-C1D	2.55	129.02	125.03
18	A	605	HEA	C1D-ND-C4D	-2.54	102.20	105.21
27	Z	101	DMU	C6-O5-C4	-2.52	108.80	113.72
18	A	606	HEA	C1B-C2B-C3B	-2.52	103.88	106.80
18	N	607	HEA	OMA-CMA-C3A	-2.51	119.97	125.62
27	G	104	DMU	C31-C28-C25	-2.51	101.70	114.37
18	A	606	HEA	CHA-C1A-C2A	-2.51	120.91	124.86
18	N	608	HEA	C27-C19-C20	2.50	119.56	115.23
18	A	606	HEA	CAA-C2A-C1A	2.49	129.92	124.85
24	J	101	CHD	C5-C4-C3	2.48	116.45	112.71
18	N	607	HEA	CMB-C2B-C1B	2.46	128.88	125.03
27	G	101	DMU	O5-C4-C57	2.45	112.52	106.44
24	P	309	CHD	C2-C1-C10	2.45	116.87	112.74
25	P	304	PEK	O02-C1-C2	2.44	133.34	123.78
27	C	311	DMU	C6-O5-C4	2.44	118.48	113.72
27	C	311	DMU	C25-C22-C19	-2.44	102.04	114.37
27	M	102	DMU	C10-O1-C9	2.44	118.48	113.72
18	N	607	HEA	C1D-ND-C4D	-2.44	102.32	105.21
18	N	608	HEA	CHC-C4B-NB	-2.43	121.36	124.37
18	N	608	HEA	C4A-C3A-C2A	-2.42	104.71	106.81
18	A	606	HEA	C4B-NB-C1B	-2.42	102.35	105.21
18	N	607	HEA	C4A-C3A-C2A	-2.40	104.73	106.81
24	T	1302	CHD	C17-C13-C14	2.40	102.52	100.11
18	N	608	HEA	CHA-C4D-C3D	-2.39	121.28	124.77
18	A	605	HEA	C1B-C2B-C3B	-2.39	104.03	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	101	CHD	C18-C13-C12	-2.38	106.67	109.06
27	P	302	DMU	O1-C9-C11	2.38	112.34	106.44
27	M	102	DMU	O49-C1-C6	-2.38	104.41	110.08
17	P	306	PGV	O14-P-O13	2.36	123.42	112.44
27	Z	101	DMU	O5-C6-O16	-2.36	104.47	110.04
25	P	304	PEK	O13-P-O14	2.36	123.40	112.44
18	N	607	HEA	CHD-C4C-NC	2.35	128.12	123.86
18	A	605	HEA	C4D-C3D-C2D	-2.34	103.49	106.89
18	A	606	HEA	C4A-C3A-C2A	-2.33	104.80	106.81
25	P	301	PEK	O01-C1-C2	2.32	116.49	111.48
27	Z	101	DMU	C34-C31-C28	-2.31	102.70	114.37
24	B	303	CHD	C16-C17-C13	-2.30	101.31	103.54
17	M	101	PGV	O01-C1-O02	-2.30	118.32	123.70
18	A	605	HEA	C4B-NB-C1B	-2.30	102.48	105.21
27	M	102	DMU	O5-C4-C3	-2.29	104.99	109.72
27	C	311	DMU	C31-C28-C25	-2.28	102.84	114.37
27	Z	101	DMU	C11-C9-C8	-2.26	107.47	113.02
18	N	607	HEA	CHD-C4C-C3C	-2.26	117.57	127.37
27	G	104	DMU	C6-O5-C4	-2.25	109.32	113.72
18	A	606	HEA	CHB-C1B-C2B	-2.24	121.49	125.03
18	A	605	HEA	CAA-CBA-CGA	-2.23	107.75	113.67
18	N	607	HEA	C13-C12-C11	-2.23	110.84	114.39
27	P	302	DMU	O55-C2-C3	2.23	115.64	109.94
18	A	606	HEA	O11-C11-C12	2.21	115.00	109.14
27	C	311	DMU	O5-C6-C1	-2.20	105.84	110.37
27	G	104	DMU	C25-C22-C19	-2.20	103.27	114.37
27	C	311	DMU	C8-C7-C5	-2.18	107.00	110.83
27	G	104	DMU	O16-C18-C19	-2.18	101.97	109.37
18	N	608	HEA	CAD-CBD-CGD	-2.16	107.93	113.67
18	A	606	HEA	O2D-CGD-CBD	2.16	120.81	114.00
27	P	302	DMU	C8-C7-C5	-2.15	107.05	110.83
18	N	608	HEA	CAA-C2A-C1A	2.15	129.22	124.85
18	N	608	HEA	CAD-C3D-C4D	2.14	128.43	124.70
18	A	606	HEA	CMC-C2C-C3C	2.14	131.58	126.55
18	N	607	HEA	CHD-C1D-C2D	-2.14	120.87	126.95
27	C	311	DMU	C6-C1-C2	-2.14	105.52	110.01
27	M	102	DMU	C34-C31-C28	-2.14	103.57	114.37
27	G	104	DMU	C10-C5-C7	2.13	114.50	110.01
27	Z	101	DMU	O16-C6-C1	2.13	111.51	108.27
26	C	305	CDL	OB6-CB5-C51	2.13	116.09	111.48
24	C	306	CHD	C18-C13-C14	2.13	114.54	111.20
25	C	302	PEK	O01-C1-C2	2.12	116.08	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	608	HEA	C13-C14-C15	-2.12	122.77	127.62
26	C	305	CDL	OB4-PB2-OB2	-2.12	97.95	107.57
18	N	607	HEA	C20-C19-C18	-2.12	116.42	121.17
18	N	608	HEA	CHA-C4D-ND	-2.11	122.15	124.42
17	A	604	PGV	O03-C19-C20	2.10	118.25	111.83
24	P	309	CHD	C18-C13-C12	-2.10	106.96	109.06
27	P	302	DMU	C31-C28-C25	-2.09	103.78	114.37
27	P	302	DMU	O4-C7-C8	2.09	115.31	110.38
26	P	308	CDL	OB6-CB5-OB7	-2.09	118.82	123.70
18	A	605	HEA	CMC-C2C-C1C	2.09	128.60	125.42
27	Z	101	DMU	C8-C7-C5	-2.07	107.20	110.83
27	C	311	DMU	C10-O7-C3	-2.06	113.09	117.98
27	G	104	DMU	C6-C1-C2	2.06	114.34	110.01
18	A	605	HEA	O2A-CGA-CBA	2.06	120.51	114.00
27	G	104	DMU	C37-C34-C31	-2.06	103.97	114.37
18	N	608	HEA	O2A-CGA-O1A	-2.06	118.04	123.33
27	G	104	DMU	O5-C4-C57	2.05	111.53	106.44
27	P	302	DMU	O5-C4-C3	2.05	113.97	109.72
18	A	606	HEA	CHC-C1C-C2C	-2.05	121.47	127.43
18	A	606	HEA	O2D-CGD-O1D	-2.05	118.06	123.33
27	G	101	DMU	C28-C25-C22	-2.05	104.01	114.37
27	G	101	DMU	C31-C28-C25	-2.04	104.06	114.37
27	G	104	DMU	C28-C25-C22	-2.04	104.06	114.37
18	N	608	HEA	C21-C22-C23	-2.04	120.85	127.64
18	A	605	HEA	C13-C12-C11	-2.03	111.14	114.39
27	M	102	DMU	O1-C9-C11	2.03	111.48	106.44
27	C	311	DMU	O7-C10-C5	2.03	113.08	108.09
24	T	1302	CHD	O25-C24-C23	-2.03	116.66	123.09
27	G	101	DMU	C10-C5-C7	2.03	114.27	110.01
27	M	102	DMU	O49-C1-C2	-2.02	105.61	110.38
29	I	101	SAC	O-C-CA	-2.02	119.58	124.77
24	Y	101	CHD	C10-C9-C8	2.01	114.08	111.84
24	J	101	CHD	C13-C17-C20	-2.01	117.05	119.48
24	W	302	CHD	C9-C8-C7	2.00	114.38	111.86

There are no chirality outliers.

All (991) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	C	304	PGV	C03-O11-P-O12
17	C	304	PGV	C03-O11-P-O14
17	C	304	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
17	C	304	PGV	C04-O12-P-O13
17	C	304	PGV	C04-O12-P-O14
17	M	101	PGV	O03-C01-C02-O01
17	M	101	PGV	C02-C03-O11-P
17	M	101	PGV	O02-C1-O01-C02
17	M	101	PGV	C2-C1-O01-C02
17	N	622	PGV	C04-O12-P-O13
17	N	622	PGV	C02-C03-O11-P
17	N	622	PGV	O02-C1-O01-C02
17	N	622	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-O12-P-O13
17	P	307	PGV	C04-C05-C06-O06
18	A	606	HEA	C19-C20-C21-C22
18	N	607	HEA	C2A-C3A-CMA-OMA
18	N	608	HEA	C2A-C3A-CMA-OMA
20	D	201	TGL	CB2-CB1-OG2-CG2
20	D	201	TGL	OB1-CB1-OG2-CG2
20	L	502	TGL	CB2-CB1-OG2-CG2
20	N	605	TGL	OB1-CB1-OG2-CG2
20	N	618	TGL	CC2-CC1-OG3-CG3
20	N	618	TGL	OC1-CC1-OG3-CG3
23	B	302	PSC	C03-O11-P-O12
23	B	302	PSC	C03-O11-P-O13
23	B	302	PSC	C04-O12-P-O11
23	B	302	PSC	C04-O12-P-O13
23	B	302	PSC	C04-O12-P-O14
23	R	201	PSC	C03-O11-P-O14
23	R	201	PSC	C04-O12-P-O11
23	R	201	PSC	O12-C04-C05-N
25	C	302	PEK	C03-O11-P-O12
25	C	302	PEK	C03-O11-P-O13
25	C	302	PEK	O12-C04-C05-N
25	C	314	PEK	C03-O11-P-O12
25	C	314	PEK	C03-O11-P-O13
25	C	314	PEK	C03-O11-P-O14
25	C	314	PEK	C04-O12-P-O11
25	C	314	PEK	O12-C04-C05-N
25	C	314	PEK	C9-C10-C11-C12
25	G	102	PEK	C6-C7-C8-C9
25	G	102	PEK	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
25	P	301	PEK	C03-O11-P-O14
25	P	301	PEK	C04-O12-P-O14
25	P	301	PEK	O02-C1-O01-C02
25	P	305	PEK	C03-O11-P-O12
25	P	305	PEK	C03-O11-P-O14
25	P	305	PEK	O02-C1-O01-C02
25	P	305	PEK	C11-C12-C13-C14
26	C	305	CDL	C1-CA2-OA2-PA1
26	C	305	CDL	CA3-OA5-PA1-OA2
26	C	305	CDL	OA7-CA5-OA6-CA4
26	C	305	CDL	C11-CA5-OA6-CA4
26	C	310	CDL	CA2-OA2-PA1-OA4
26	C	310	CDL	CA2-OA2-PA1-OA5
26	C	310	CDL	CA3-OA5-PA1-OA3
26	C	310	CDL	C11-CA5-OA6-CA4
26	C	310	CDL	CB2-OB2-PB2-OB4
26	C	310	CDL	CB2-OB2-PB2-OB5
26	C	310	CDL	CB3-OB5-PB2-OB2
26	C	310	CDL	CB3-OB5-PB2-OB4
26	P	308	CDL	CB2-C1-CA2-OA2
26	P	308	CDL	C1-CA2-OA2-PA1
26	P	308	CDL	CA3-OA5-PA1-OA2
26	P	308	CDL	CA3-OA5-PA1-OA4
26	P	312	CDL	CB2-OB2-PB2-OB4
26	P	312	CDL	CB2-OB2-PB2-OB5
26	P	312	CDL	CB3-OB5-PB2-OB2
26	P	312	CDL	CB3-OB5-PB2-OB4
26	P	312	CDL	CB6-CB4-OB6-CB5
27	G	101	DMU	C1-C6-O16-C18
27	G	104	DMU	O5-C6-O16-C18
27	M	102	DMU	O5-C6-O16-C18
29	I	101	SAC	C2A-C1A-N-CA
29	I	101	SAC	OAC-C1A-N-CA
29	I	101	SAC	O-C-CA-CB
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	OAC-C1A-N-CA
23	R	201	PSC	O04-C19-O03-C01
23	R	201	PSC	C20-C19-O03-C01
27	G	104	DMU	O1-C10-O7-C3
17	N	622	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
26	P	308	CDL	OA9-CA7-OA8-CA6
20	L	502	TGL	OB1-CB1-OG2-CG2
23	B	302	PSC	O02-C1-O01-C02
26	C	310	CDL	OA7-CA5-OA6-CA4
17	N	622	PGV	C20-C19-O03-C01
27	G	104	DMU	O6-C11-C9-O1
20	N	605	TGL	CB2-CB1-OG2-CG2
23	B	302	PSC	C2-C1-O01-C02
25	P	301	PEK	C2-C1-O01-C02
25	P	305	PEK	C2-C1-O01-C02
24	T	1302	CHD	C21-C20-C22-C23
20	D	201	TGL	OC1-CC1-OG3-CG3
18	N	608	HEA	C27-C19-C20-C21
18	N	608	HEA	C18-C19-C20-C21
27	C	311	DMU	C5-C10-O7-C3
20	A	613	TGL	CC2-CC1-OG3-CG3
20	D	201	TGL	CC2-CC1-OG3-CG3
20	N	604	TGL	CC2-CC1-OG3-CG3
23	B	302	PSC	C20-C19-O03-C01
26	P	308	CDL	C31-CA7-OA8-CA6
20	N	604	TGL	OC1-CC1-OG3-CG3
17	C	304	PGV	O12-C04-C05-O05
26	C	310	CDL	O1-C1-CB2-OB2
26	P	308	CDL	O1-C1-CA2-OA2
26	P	312	CDL	C71-CB7-OB8-CB6
26	P	312	CDL	OB9-CB7-OB8-CB6
27	G	104	DMU	O6-C11-C9-C8
26	C	305	CDL	C51-CB5-OB6-CB4
23	B	302	PSC	O04-C19-O03-C01
27	G	101	DMU	O5-C4-C57-O61
17	M	101	PGV	C05-C04-O12-P
27	G	104	DMU	O5-C4-C57-O61
27	C	311	DMU	O1-C10-O7-C3
20	A	613	TGL	OC1-CC1-OG3-CG3
27	Z	101	DMU	O5-C6-O16-C18
17	M	101	PGV	C1-C2-C3-C4
27	G	101	DMU	O6-C11-C9-O1
24	T	1302	CHD	C17-C20-C22-C23
24	Y	101	CHD	C17-C20-C22-C23
26	P	312	CDL	OA9-CA7-OA8-CA6
17	C	304	PGV	O12-C04-C05-C06
17	M	101	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
26	C	310	CDL	CA2-C1-CB2-OB2
20	A	613	TGL	CA2-CA1-OG1-CG1
20	L	502	TGL	CC2-CC1-OG3-CG3
20	N	605	TGL	CA2-CA1-OG1-CG1
25	P	305	PEK	C22-C21-O03-C01
26	C	310	CDL	C71-CB7-OB8-CB6
26	P	312	CDL	C31-CA7-OA8-CA6
26	C	305	CDL	C82-C83-C84-C85
20	D	201	TGL	C14-C29-C30-C31
25	C	302	PEK	C23-C24-C25-C26
27	G	101	DMU	C3-C4-C57-O61
27	G	104	DMU	C3-C4-C57-O61
27	Z	101	DMU	C1-C6-O16-C18
24	Y	101	CHD	C21-C20-C22-C23
26	P	312	CDL	O1-C1-CA2-OA2
25	C	302	PEK	C1-C2-C3-C4
20	N	605	TGL	OA1-CA1-OG1-CG1
17	M	101	PGV	C20-C19-O03-C01
17	P	307	PGV	O05-C05-C06-O06
20	A	613	TGL	CA1-CA2-CA3-CA4
20	N	605	TGL	CA1-CA2-CA3-CA4
26	P	312	CDL	CA5-C11-C12-C13
27	G	101	DMU	O6-C11-C9-C8
26	C	305	CDL	CB7-C71-C72-C73
26	C	310	CDL	CA5-C11-C12-C13
27	P	302	DMU	C3-C4-C57-O61
23	R	201	PSC	C04-C05-N-C07
17	N	622	PGV	C19-C20-C21-C22
20	N	605	TGL	CC1-CC2-CC3-CC4
20	N	618	TGL	CC1-CC2-CC3-CC4
25	P	301	PEK	C1-C2-C3-C4
26	C	310	CDL	CA7-C31-C32-C33
20	L	502	TGL	OC1-CC1-OG3-CG3
25	P	305	PEK	O04-C21-O03-C01
17	N	622	PGV	C1-C2-C3-C4
20	N	618	TGL	CB1-CB2-CB3-CB4
25	G	102	PEK	C1-C2-C3-C4
20	A	613	TGL	OA1-CA1-OG1-CG1
20	L	502	TGL	C16-C15-CC9-CC8
23	B	302	PSC	C23-C24-C25-C26
17	M	101	PGV	O12-C04-C05-O05
26	C	305	CDL	O1-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
25	C	302	PEK	C22-C21-O03-C01
26	C	310	CDL	OB9-CB7-OB8-CB6
27	M	102	DMU	O6-C11-C9-C8
17	P	307	PGV	C1-C2-C3-C4
20	D	201	TGL	CC1-CC2-CC3-CC4
20	N	604	TGL	CB1-CB2-CB3-CB4
20	L	502	TGL	CC2-CC3-CC4-CC5
25	P	301	PEK	C13-C14-C15-C16
27	P	302	DMU	O16-C18-C19-C22
27	Z	101	DMU	O16-C18-C19-C22
27	M	102	DMU	O6-C11-C9-O1
20	A	613	TGL	CA5-CA6-CA7-CA8
20	D	201	TGL	C16-C17-C18-C19
26	C	305	CDL	OB7-CB5-OB6-CB4
26	C	305	CDL	CB2-C1-CA2-OA2
26	P	308	CDL	CA2-C1-CB2-OB2
20	N	605	TGL	C20-C21-C22-C23
27	Z	101	DMU	O6-C11-C9-O1
26	C	305	CDL	C31-CA7-OA8-CA6
20	A	613	TGL	CB2-CB1-OG2-CG2
25	C	314	PEK	C7-C8-C9-C10
25	P	304	PEK	C7-C8-C9-C10
25	P	305	PEK	C7-C8-C9-C10
25	C	302	PEK	O04-C21-O03-C01
24	J	101	CHD	C20-C22-C23-C24
24	W	302	CHD	C20-C22-C23-C24
23	B	302	PSC	C1-C2-C3-C4
20	L	502	TGL	C17-C18-C19-C33
17	C	303	PGV	C12-C13-C14-C15
17	M	101	PGV	O04-C19-O03-C01
27	G	101	DMU	C18-C19-C22-C25
27	G	104	DMU	C18-C19-C22-C25
27	M	102	DMU	C18-C19-C22-C25
17	M	101	PGV	C5-C6-C7-C8
17	N	622	PGV	C14-C15-C16-C17
20	A	613	TGL	C21-C22-C23-C24
27	G	101	DMU	O16-C18-C19-C22
17	M	101	PGV	C2-C3-C4-C5
20	D	201	TGL	CC4-CC5-CC6-CC7
20	D	201	TGL	C19-C33-C34-C35
20	N	605	TGL	C24-C25-C26-C27
25	C	314	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	G	102	PEK	C24-C25-C26-C27
25	P	301	PEK	C23-C24-C25-C26
26	C	310	CDL	C12-C13-C14-C15
26	P	308	CDL	C36-C37-C38-C39
26	P	308	CDL	C55-C56-C57-C58
25	C	302	PEK	C13-C14-C15-C16
25	C	314	PEK	C13-C14-C15-C16
25	P	301	PEK	C7-C8-C9-C10
17	A	604	PGV	C5-C6-C7-C8
20	D	201	TGL	C18-C19-C33-C34
20	N	605	TGL	C13-C14-C29-C30
20	N	618	TGL	CB2-CB3-CB4-CB5
20	N	618	TGL	C11-C12-C13-C14
26	C	305	CDL	C52-C53-C54-C55
26	C	305	CDL	C59-C60-C61-C62
26	C	310	CDL	C38-C39-C40-C41
26	P	312	CDL	C33-C34-C35-C36
25	C	314	PEK	C22-C21-O03-C01
25	P	301	PEK	C22-C21-O03-C01
17	M	101	PGV	C20-C21-C22-C23
20	A	613	TGL	CA3-CA4-CA5-CA6
20	D	201	TGL	CB4-CB5-CB6-CB7
20	L	502	TGL	CB6-CB7-CB8-CB9
23	R	201	PSC	C3-C4-C5-C6
25	C	302	PEK	C28-C29-C30-C31
25	G	102	PEK	C22-C23-C24-C25
26	C	310	CDL	C73-C74-C75-C76
26	P	308	CDL	C56-C57-C58-C59
20	A	613	TGL	OB1-CB1-OG2-CG2
27	Z	101	DMU	C19-C18-O16-C6
17	N	622	PGV	C3-C4-C5-C6
20	L	502	TGL	CC9-C15-C16-C17
20	N	605	TGL	C10-C11-C12-C13
26	C	305	CDL	C37-C38-C39-C40
26	P	312	CDL	C36-C37-C38-C39
26	P	312	CDL	C80-C81-C82-C83
23	R	201	PSC	C19-C20-C21-C22
20	N	618	TGL	CA4-CA5-CA6-CA7
26	C	310	CDL	C55-C56-C57-C58
20	D	201	TGL	CA6-CA7-CA8-CA9
25	C	314	PEK	C2-C1-O01-C02
17	M	101	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
20	N	618	TGL	CC9-C15-C16-C17
27	G	104	DMU	O16-C18-C19-C22
20	A	613	TGL	C24-C25-C26-C27
20	N	605	TGL	CB7-CB8-CB9-C10
23	B	302	PSC	C20-C21-C22-C23
17	C	303	PGV	C28-C29-C30-C31
17	N	606	PGV	C6-C7-C8-C9
17	P	307	PGV	C25-C26-C27-C28
20	N	605	TGL	CA9-C20-C21-C22
26	C	310	CDL	C75-C76-C77-C78
26	P	308	CDL	C61-C62-C63-C64
26	C	305	CDL	OA9-CA7-OA8-CA6
17	A	604	PGV	C6-C7-C8-C9
17	C	304	PGV	C6-C7-C8-C9
20	D	201	TGL	CA9-C20-C21-C22
26	C	310	CDL	C13-C14-C15-C16
26	P	312	CDL	C74-C75-C76-C77
27	M	102	DMU	C31-C34-C37-C40
23	R	201	PSC	C1-C2-C3-C4
17	P	306	PGV	C7-C8-C9-C10
17	P	306	PGV	C25-C26-C27-C28
20	A	613	TGL	C12-C13-C14-C29
20	A	613	TGL	C18-C19-C33-C34
20	N	618	TGL	C23-C24-C25-C26
26	C	310	CDL	C57-C58-C59-C60
20	N	605	TGL	CC2-CC3-CC4-CC5
26	P	312	CDL	C43-C44-C45-C46
17	M	101	PGV	C22-C23-C24-C25
17	N	622	PGV	C4-C5-C6-C7
17	P	307	PGV	C24-C25-C26-C27
20	A	613	TGL	C16-C15-CC9-CC8
20	D	201	TGL	CA3-CA4-CA5-CA6
20	N	605	TGL	C11-C12-C13-C14
25	P	305	PEK	C23-C24-C25-C26
26	C	305	CDL	C23-C24-C25-C26
26	C	305	CDL	C36-C37-C38-C39
25	P	305	PEK	C21-C22-C23-C24
17	P	307	PGV	C22-C23-C24-C25
20	A	613	TGL	C11-C12-C13-C14
20	N	604	TGL	C22-C23-C24-C25
20	N	605	TGL	CB9-C10-C11-C12
20	N	618	TGL	C13-C14-C29-C30

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Mol	Chain	Res	Type	Atoms
26	P	308	CDL	C22-C23-C24-C25
17	N	606	PGV	C7-C8-C9-C10
20	L	502	TGL	CB2-CB3-CB4-CB5
26	C	305	CDL	C43-C44-C45-C46
26	C	305	CDL	C76-C77-C78-C79
26	P	308	CDL	C77-C78-C79-C80
19	A	610	EDO	O1-C1-C2-O2
19	B	310	EDO	O1-C1-C2-O2
19	B	311	EDO	O1-C1-C2-O2
19	F	702	EDO	O1-C1-C2-O2
19	G	106	EDO	O1-C1-C2-O2
19	G	108	EDO	O1-C1-C2-O2
19	N	617	EDO	O1-C1-C2-O2
19	Q	1604	EDO	O1-C1-C2-O2
19	T	1301	EDO	O1-C1-C2-O2
26	P	308	CDL	C83-C84-C85-C86
20	L	502	TGL	CA9-C20-C21-C22
20	N	618	TGL	C20-C21-C22-C23
25	P	301	PEK	C33-C34-C35-C36
25	P	305	PEK	C30-C31-C32-C33
26	C	305	CDL	C21-C22-C23-C24
20	A	613	TGL	CC4-CC5-CC6-CC7
24	Y	101	CHD	C13-C17-C20-C22
17	P	306	PGV	C6-C7-C8-C9
20	D	201	TGL	CC7-CC8-CC9-C15
23	B	302	PSC	C4-C5-C6-C7
26	P	308	CDL	C43-C44-C45-C46
17	M	101	PGV	C3-C4-C5-C6
20	L	502	TGL	C24-C25-C26-C27
23	B	302	PSC	C22-C23-C24-C25
26	P	308	CDL	CA7-C31-C32-C33
26	P	312	CDL	CA7-C31-C32-C33
20	L	502	TGL	C16-C17-C18-C19
20	N	618	TGL	C24-C25-C26-C27
25	P	305	PEK	C28-C29-C30-C31
20	A	613	TGL	CA4-CA5-CA6-CA7
20	N	604	TGL	CA5-CA6-CA7-CA8
20	N	618	TGL	C16-C17-C18-C19
26	C	305	CDL	C16-C17-C18-C19
26	P	308	CDL	C52-C53-C54-C55
26	P	312	CDL	C11-C12-C13-C14
20	N	618	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
25	C	314	PEK	O02-C1-O01-C02
26	P	308	CDL	C39-C40-C41-C42
17	N	622	PGV	C26-C27-C28-C29
20	A	613	TGL	CC7-CC8-CC9-C15
20	L	502	TGL	CB7-CB8-CB9-C10
20	L	502	TGL	C14-C29-C30-C31
20	N	605	TGL	C18-C19-C33-C34
25	G	102	PEK	C23-C24-C25-C26
26	P	308	CDL	C78-C79-C80-C81
26	P	312	CDL	C35-C36-C37-C38
17	C	303	PGV	C24-C25-C26-C27
26	C	305	CDL	C41-C42-C43-C44
17	A	604	PGV	C30-C31-C32-C33
17	C	304	PGV	C20-C21-C22-C23
17	M	101	PGV	C23-C24-C25-C26
17	N	606	PGV	C5-C6-C7-C8
20	N	604	TGL	C10-C11-C12-C13
25	P	305	PEK	C16-C17-C18-C19
26	P	308	CDL	C19-C20-C21-C22
26	P	312	CDL	C12-C13-C14-C15
27	G	101	DMU	O5-C6-O16-C18
26	C	310	CDL	C78-C79-C80-C81
27	C	311	DMU	O5-C4-C57-O61
17	C	304	PGV	C22-C23-C24-C25
17	P	306	PGV	C22-C23-C24-C25
17	C	304	PGV	C24-C25-C26-C27
17	M	101	PGV	C27-C28-C29-C30
20	N	618	TGL	CB4-CB5-CB6-CB7
23	R	201	PSC	C25-C26-C27-C28
25	P	304	PEK	C24-C25-C26-C27
17	C	304	PGV	C2-C1-O01-C02
20	N	618	TGL	CB2-CB1-OG2-CG2
26	P	308	CDL	C51-CB5-OB6-CB4
20	A	613	TGL	C33-C34-C35-C36
17	C	304	PGV	O02-C1-O01-C02
17	A	604	PGV	C4-C5-C6-C7
20	L	502	TGL	CC6-CC7-CC8-CC9
25	P	304	PEK	C25-C26-C27-C28
26	C	305	CDL	C56-C57-C58-C59
17	M	101	PGV	C26-C27-C28-C29
17	A	604	PGV	C19-C20-C21-C22
17	M	101	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	N	604	TGL	CB3-CB4-CB5-CB6
25	P	301	PEK	C4-C5-C6-C7
17	C	303	PGV	C27-C28-C29-C30
26	P	312	CDL	C22-C23-C24-C25
23	R	201	PSC	C04-C05-N-C06
23	R	201	PSC	C04-C05-N-C08
20	N	605	TGL	CB2-CB3-CB4-CB5
26	C	305	CDL	C63-C64-C65-C66
20	N	604	TGL	C11-C12-C13-C14
20	L	502	TGL	C18-C19-C33-C34
17	P	307	PGV	C4-C5-C6-C7
20	N	604	TGL	C20-C21-C22-C23
20	N	618	TGL	C17-C18-C19-C33
26	P	312	CDL	C18-C19-C20-C21
20	N	605	TGL	CA3-CA4-CA5-CA6
26	P	312	CDL	C40-C41-C42-C43
17	M	101	PGV	C6-C7-C8-C9
17	C	304	PGV	C30-C31-C32-C33
26	C	305	CDL	CB5-C51-C52-C53
20	N	604	TGL	CA9-C20-C21-C22
20	N	618	TGL	CC5-CC6-CC7-CC8
26	C	310	CDL	C52-C53-C54-C55
17	N	606	PGV	C12-C13-C14-C15
25	C	302	PEK	C2-C3-C4-C5
25	P	301	PEK	C2-C3-C4-C5
17	N	622	PGV	C21-C22-C23-C24
25	P	301	PEK	C34-C35-C36-C37
26	C	305	CDL	C11-C12-C13-C14
20	D	201	TGL	OA1-CA1-OG1-CG1
17	M	101	PGV	C24-C25-C26-C27
23	R	201	PSC	C27-C28-C29-C30
26	C	305	CDL	C22-C23-C24-C25
26	C	305	CDL	C38-C39-C40-C41
20	N	605	TGL	CB5-CB6-CB7-CB8
26	P	308	CDL	C12-C13-C14-C15
26	P	312	CDL	C60-C61-C62-C63
17	P	306	PGV	C11-C12-C13-C14
25	C	302	PEK	C31-C32-C33-C34
26	C	310	CDL	C77-C78-C79-C80
26	C	305	CDL	CA2-C1-CB2-OB2
20	A	613	TGL	CA9-C20-C21-C22
20	N	618	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
25	P	301	PEK	C25-C26-C27-C28
24	Y	101	CHD	C20-C22-C23-C24
20	D	201	TGL	CA2-CA1-OG1-CG1
26	P	312	CDL	C78-C79-C80-C81
23	R	201	PSC	C22-C23-C24-C25
26	C	305	CDL	C61-C62-C63-C64
24	J	101	CHD	C17-C20-C22-C23
20	N	605	TGL	C17-C18-C19-C33
25	P	301	PEK	O04-C21-O03-C01
26	C	305	CDL	C83-C84-C85-C86
26	C	310	CDL	C34-C35-C36-C37
25	P	301	PEK	C28-C29-C30-C31
24	Y	101	CHD	C13-C17-C20-C21
25	G	102	PEK	C31-C32-C33-C34
20	A	613	TGL	CC9-C15-C16-C17
25	C	314	PEK	O04-C21-O03-C01
20	L	502	TGL	C12-C13-C14-C29
20	N	604	TGL	CC7-CC8-CC9-C15
25	C	314	PEK	C27-C28-C29-C30
25	P	305	PEK	C27-C28-C29-C30
17	M	101	PGV	C01-C02-C03-O11
17	P	307	PGV	C01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-CA6
26	P	308	CDL	OB7-CB5-OB6-CB4
20	A	613	TGL	CB4-CB5-CB6-CB7
20	D	201	TGL	C23-C24-C25-C26
26	P	312	CDL	C34-C35-C36-C37
24	Y	101	CHD	C16-C17-C20-C21
20	N	604	TGL	CA1-CA2-CA3-CA4
27	G	101	DMU	C31-C34-C37-C40
23	R	201	PSC	C2-C3-C4-C5
25	C	302	PEK	C25-C26-C27-C28
26	C	305	CDL	C81-C82-C83-C84
27	C	311	DMU	C1-C6-O16-C18
17	M	101	PGV	O03-C01-C02-C03
26	C	305	CDL	CA3-CA4-CA6-OA8
26	C	305	CDL	CB3-CB4-CB6-OB8
17	A	604	PGV	C12-C13-C14-C15
23	R	201	PSC	C13-C14-C15-C16
25	P	304	PEK	C15-C16-C17-C18
20	N	618	TGL	CC3-CC4-CC5-CC6
20	L	502	TGL	CB9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	G	101	DMU	C28-C31-C34-C37
19	B	308	EDO	O1-C1-C2-O2
19	C	313	EDO	O1-C1-C2-O2
19	N	620	EDO	O1-C1-C2-O2
19	P	310	EDO	O1-C1-C2-O2
19	V	103	EDO	O1-C1-C2-O2
19	W	303	EDO	O1-C1-C2-O2
25	C	302	PEK	C24-C25-C26-C27
20	N	604	TGL	CB4-CB5-CB6-CB7
25	P	305	PEK	C24-C25-C26-C27
26	P	308	CDL	C59-C60-C61-C62
17	A	604	PGV	C7-C8-C9-C10
20	A	613	TGL	CB5-CB6-CB7-CB8
25	P	304	PEK	C34-C35-C36-C37
20	N	605	TGL	C14-C29-C30-C31
25	G	102	PEK	C25-C26-C27-C28
26	C	305	CDL	C60-C61-C62-C63
26	C	305	CDL	C14-C15-C16-C17
26	P	312	CDL	C31-C32-C33-C34
23	B	302	PSC	C6-C7-C8-C9
25	P	305	PEK	C2-C3-C4-C5
17	C	304	PGV	C23-C24-C25-C26
18	A	605	HEA	C2A-C3A-CMA-OMA
18	A	606	HEA	C2A-C3A-CMA-OMA
25	P	304	PEK	C4-C5-C6-C7
25	C	302	PEK	C14-C15-C16-C17
25	P	301	PEK	C14-C15-C16-C17
26	P	312	CDL	C20-C21-C22-C23
27	Z	101	DMU	C19-C22-C25-C28
26	P	312	CDL	CB2-C1-CA2-OA2
17	N	622	PGV	O01-C02-C03-O11
26	P	312	CDL	OB5-CB3-CB4-OB6
20	N	604	TGL	CB2-CB1-OG2-CG2
25	P	301	PEK	C22-C23-C24-C25
27	P	302	DMU	O5-C4-C57-O61
20	L	502	TGL	C21-C22-C23-C24
20	N	618	TGL	CB7-CB8-CB9-C10
26	C	310	CDL	C44-C45-C46-C47
26	C	305	CDL	C80-C81-C82-C83
17	N	622	PGV	C6-C7-C8-C9
17	P	306	PGV	C27-C28-C29-C30
17	P	307	PGV	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	D	201	TGL	C12-C13-C14-C29
17	C	304	PGV	C31-C32-C33-C34
25	G	102	PEK	C35-C36-C37-C38
20	N	604	TGL	C21-C22-C23-C24
26	P	308	CDL	C72-C73-C74-C75
17	C	304	PGV	O03-C01-C02-O01
26	P	308	CDL	OB6-CB4-CB6-OB8
20	D	201	TGL	C15-C16-C17-C18
20	N	605	TGL	C22-C23-C24-C25
25	P	301	PEK	C29-C30-C31-C32
24	Y	101	CHD	C16-C17-C20-C22
20	N	605	TGL	C33-C34-C35-C36
20	N	604	TGL	C29-C30-C31-C32
20	N	618	TGL	C29-C30-C31-C32
25	P	305	PEK	C35-C36-C37-C38
20	L	502	TGL	C11-C12-C13-C14
25	C	314	PEK	C24-C25-C26-C27
20	N	604	TGL	C12-C13-C14-C29
20	N	605	TGL	C21-C22-C23-C24
25	P	305	PEK	C17-C18-C19-C20
20	N	605	TGL	C29-C30-C31-C32
25	C	302	PEK	C10-C11-C12-C13
25	C	302	PEK	C35-C36-C37-C38
20	N	604	TGL	CA2-CA1-OG1-CG1
17	N	606	PGV	C19-C20-C21-C22
17	P	306	PGV	C19-C20-C21-C22
25	G	102	PEK	C28-C29-C30-C31
25	P	305	PEK	C3-C4-C5-C6
20	N	604	TGL	CB5-CB6-CB7-CB8
27	M	102	DMU	C25-C28-C31-C34
27	Z	101	DMU	C18-C19-C22-C25
26	C	305	CDL	C44-C45-C46-C47
17	P	307	PGV	C27-C28-C29-C30
26	C	305	CDL	C18-C19-C20-C21
26	P	308	CDL	C57-C58-C59-C60
27	G	104	DMU	C1-C6-O16-C18
17	A	604	PGV	C29-C30-C31-C32
17	C	304	PGV	C5-C6-C7-C8
20	L	502	TGL	C22-C23-C24-C25
26	P	312	CDL	C24-C25-C26-C27
20	N	604	TGL	C15-C16-C17-C18
26	P	308	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
17	M	101	PGV	C4-C5-C6-C7
25	C	314	PEK	C17-C18-C19-C20
27	G	101	DMU	C34-C37-C40-C43
25	G	102	PEK	C4-C5-C6-C7
25	P	301	PEK	C35-C36-C37-C38
26	C	310	CDL	C22-C23-C24-C25
26	P	308	CDL	C37-C38-C39-C40
26	P	312	CDL	C23-C24-C25-C26
17	C	303	PGV	C22-C23-C24-C25
26	P	308	CDL	C64-C65-C66-C67
25	P	301	PEK	C16-C17-C18-C19
20	L	502	TGL	CG1-CG2-CG3-OG3
23	B	302	PSC	O03-C01-C02-C03
25	C	302	PEK	O03-C01-C02-C03
26	C	310	CDL	CB3-CB4-CB6-OB8
26	P	308	CDL	CB3-CB4-CB6-OB8
25	P	301	PEK	C17-C18-C19-C20
17	C	304	PGV	C7-C8-C9-C10
26	P	312	CDL	C56-C57-C58-C59
19	L	503	EDO	O1-C1-C2-O2
25	C	314	PEK	C16-C17-C18-C19
25	C	314	PEK	C35-C36-C37-C38
17	M	101	PGV	O01-C02-C03-O11
26	C	310	CDL	OB5-CB3-CB4-OB6
26	P	308	CDL	OB5-CB3-CB4-OB6
25	P	305	PEK	C15-C16-C17-C18
17	N	606	PGV	C29-C30-C31-C32
17	N	622	PGV	C27-C28-C29-C30
26	C	310	CDL	C31-C32-C33-C34
17	P	307	PGV	C28-C29-C30-C31
25	C	314	PEK	C30-C31-C32-C33
26	P	312	CDL	C83-C84-C85-C86
25	C	302	PEK	O03-C01-C02-O01
26	C	305	CDL	OA6-CA4-CA6-OA8
26	C	310	CDL	OB6-CB4-CB6-OB8
23	B	302	PSC	C9-C10-C11-C12
23	B	302	PSC	C10-C11-C12-C13
23	R	201	PSC	C9-C10-C11-C12
23	R	201	PSC	C10-C11-C12-C13
25	C	302	PEK	C6-C7-C8-C9
25	C	302	PEK	C11-C10-C9-C8
25	C	302	PEK	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	C	314	PEK	C5-C6-C7-C8
25	C	314	PEK	C6-C7-C8-C9
25	C	314	PEK	C12-C13-C14-C15
25	P	301	PEK	C5-C6-C7-C8
25	P	301	PEK	C9-C10-C11-C12
25	P	301	PEK	C11-C12-C13-C14
25	P	304	PEK	C9-C10-C11-C12
25	P	305	PEK	C5-C6-C7-C8
25	P	305	PEK	C12-C13-C14-C15
27	P	302	DMU	O6-C11-C9-C8
17	C	304	PGV	C2-C3-C4-C5
17	C	303	PGV	C7-C8-C9-C10
25	C	314	PEK	C1-C2-C3-C4
20	N	604	TGL	CC6-CC7-CC8-CC9
26	C	305	CDL	C77-C78-C79-C80
17	C	304	PGV	C11-C10-C9-C8
25	C	314	PEK	C28-C29-C30-C31
26	C	310	CDL	C71-C72-C73-C74
17	M	101	PGV	C21-C22-C23-C24
25	G	102	PEK	C3-C4-C5-C6
20	L	502	TGL	CC7-CC8-CC9-C15
26	C	310	CDL	C61-C62-C63-C64
25	P	305	PEK	C33-C34-C35-C36
26	C	305	CDL	C15-C16-C17-C18
20	N	618	TGL	CA3-CA4-CA5-CA6
26	P	308	CDL	C11-C12-C13-C14
20	D	201	TGL	CB2-CB3-CB4-CB5
26	C	310	CDL	C60-C61-C62-C63
20	N	605	TGL	CA6-CA7-CA8-CA9
26	P	308	CDL	OB5-CB3-CB4-CB6
25	P	301	PEK	C02-C03-O11-P
17	A	604	PGV	C13-C14-C15-C16
26	C	305	CDL	C40-C41-C42-C43
20	N	604	TGL	C19-C33-C34-C35
17	P	307	PGV	C13-C14-C15-C16
25	G	102	PEK	C7-C8-C9-C10
17	C	304	PGV	C4-C5-C6-C7
20	N	605	TGL	CC4-CC5-CC6-CC7
27	C	311	DMU	C34-C37-C40-C43
24	G	107	CHD	C17-C20-C22-C23
27	G	101	DMU	C19-C22-C25-C28
23	R	201	PSC	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
23	B	302	PSC	C31-C32-C33-C34
20	N	604	TGL	OA1-CA1-OG1-CG1
23	R	201	PSC	C24-C25-C26-C27
25	P	304	PEK	C3-C4-C5-C6
17	M	101	PGV	C12-C13-C14-C15
25	P	305	PEK	C31-C32-C33-C34
26	P	308	CDL	O1-C1-CB2-OB2
25	C	314	PEK	O01-C02-C03-O11
26	C	305	CDL	OB5-CB3-CB4-OB6
20	N	618	TGL	CB6-CB7-CB8-CB9
20	A	613	TGL	C25-C26-C27-C28
27	G	104	DMU	C31-C34-C37-C40
20	N	618	TGL	OG1-CG1-CG2-CG3
25	C	302	PEK	C05-C04-O12-P
27	P	302	DMU	C2-C3-O7-C10
19	R	203	EDO	O1-C1-C2-O2
20	L	502	TGL	OG2-CG2-CG3-OG3
26	P	308	CDL	C80-C81-C82-C83
26	C	310	CDL	C72-C73-C74-C75
17	C	304	PGV	C29-C30-C31-C32
20	L	502	TGL	C11-C10-CB9-CB8
25	P	305	PEK	C25-C26-C27-C28
26	C	305	CDL	C51-C52-C53-C54
26	C	310	CDL	C21-C22-C23-C24
20	L	502	TGL	CB1-CB2-CB3-CB4
17	P	306	PGV	C23-C24-C25-C26
26	P	308	CDL	C74-C75-C76-C77
20	D	201	TGL	C21-C20-CA9-CA8
26	C	305	CDL	C62-C63-C64-C65
26	P	308	CDL	C16-C17-C18-C19
26	P	312	CDL	C62-C63-C64-C65
23	B	302	PSC	O12-C04-C05-N
26	C	310	CDL	C11-C12-C13-C14
20	N	604	TGL	C13-C14-C29-C30
26	C	310	CDL	O1-C1-CA2-OA2
23	B	302	PSC	C24-C25-C26-C27
26	P	308	CDL	C17-C18-C19-C20
17	M	101	PGV	C11-C10-C9-C8
25	P	304	PEK	C30-C31-C32-C33
17	M	101	PGV	C19-C20-C21-C22
20	N	618	TGL	C11-C10-CB9-CB8
26	C	305	CDL	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	N	604	TGL	OB1-CB1-OG2-CG2
27	C	311	DMU	C19-C18-O16-C6
26	P	308	CDL	C21-C22-C23-C24
20	N	618	TGL	C21-C20-CA9-CA8
26	C	310	CDL	C56-C57-C58-C59
17	N	622	PGV	C01-C02-C03-O11
25	C	314	PEK	C01-C02-C03-O11
26	P	312	CDL	OB5-CB3-CB4-CB6
20	N	618	TGL	CA6-CA7-CA8-CA9
17	C	304	PGV	C27-C28-C29-C30
26	P	312	CDL	C81-C82-C83-C84
26	P	312	CDL	C84-C85-C86-C87
20	D	201	TGL	C22-C23-C24-C25
27	M	102	DMU	C34-C37-C40-C43
17	N	606	PGV	C23-C24-C25-C26
26	P	312	CDL	C57-C58-C59-C60
26	C	305	CDL	C74-C75-C76-C77
26	P	308	CDL	C20-C21-C22-C23
17	C	304	PGV	C02-C03-O11-P
26	P	308	CDL	C1-CB2-OB2-PB2
26	P	312	CDL	C73-C74-C75-C76
17	P	307	PGV	O01-C02-C03-O11
26	C	305	CDL	OA5-CA3-CA4-OA6
25	G	102	PEK	C2-C1-O01-C02
20	N	605	TGL	C25-C26-C27-C28
23	B	302	PSC	C5-C6-C7-C8
26	P	308	CDL	C81-C82-C83-C84
18	N	608	HEA	C4A-C3A-CMA-OMA
27	Z	101	DMU	C22-C25-C28-C31
17	C	304	PGV	C25-C26-C27-C28
23	R	201	PSC	O03-C01-C02-O01
26	C	305	CDL	OB6-CB4-CB6-OB8
26	P	312	CDL	C42-C43-C44-C45
17	P	306	PGV	C10-C11-C12-C13
17	C	303	PGV	C13-C14-C15-C16
26	C	310	CDL	C63-C64-C65-C66
17	C	304	PGV	O03-C01-C02-C03
20	D	201	TGL	OG1-CG1-CG2-CG3
20	D	201	TGL	CG1-CG2-CG3-OG3
26	P	312	CDL	CA3-CA4-CA6-OA8
17	M	101	PGV	C30-C31-C32-C33
25	P	301	PEK	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	P	305	PEK	C1-C2-C3-C4
20	L	502	TGL	CA2-CA3-CA4-CA5
20	D	201	TGL	CC9-C15-C16-C17
17	C	303	PGV	C11-C12-C13-C14
23	R	201	PSC	C7-C8-C9-C10
19	B	309	EDO	O1-C1-C2-O2
19	M	103	EDO	O1-C1-C2-O2
17	M	101	PGV	C7-C8-C9-C10
17	M	101	PGV	C03-O11-P-O13
17	N	622	PGV	C04-O12-P-O11
17	N	622	PGV	C04-O12-P-O14
17	P	307	PGV	C03-O11-P-O14
17	P	307	PGV	C04-O12-P-O11
17	P	307	PGV	C04-O12-P-O14
23	R	201	PSC	C04-O12-P-O14
25	C	314	PEK	C04-O12-P-O14
25	G	102	PEK	O12-C04-C05-N
25	P	301	PEK	C03-O11-P-O12
25	P	301	PEK	C03-O11-P-O13
26	C	305	CDL	CA3-OA5-PA1-OA3
26	C	305	CDL	CB2-OB2-PB2-OB3
26	C	310	CDL	CB3-OB5-PB2-OB3
26	P	308	CDL	CB2-OB2-PB2-OB3
26	P	308	CDL	CB2-OB2-PB2-OB4
26	P	308	CDL	CB2-OB2-PB2-OB5
26	P	312	CDL	CB2-OB2-PB2-OB3
27	P	302	DMU	C4-C3-O7-C10
17	C	303	PGV	C02-C03-O11-P
17	P	306	PGV	C02-C03-O11-P
17	P	307	PGV	C05-C04-O12-P
26	C	305	CDL	CA4-CA3-OA5-PA1
26	P	312	CDL	CA4-CA3-OA5-PA1
17	P	306	PGV	C1-C2-C3-C4
20	L	502	TGL	C19-C33-C34-C35
26	P	308	CDL	C62-C63-C64-C65
20	A	613	TGL	CA6-CA7-CA8-CA9
17	N	622	PGV	C03-C02-O01-C1
25	C	302	PEK	C03-C02-O01-C1
25	P	305	PEK	C03-C02-O01-C1
17	P	306	PGV	C21-C22-C23-C24
27	P	302	DMU	C34-C37-C40-C43
25	P	304	PEK	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	N	605	TGL	C16-C17-C18-C19
26	C	305	CDL	C17-C18-C19-C20
26	P	312	CDL	C71-C72-C73-C74
20	N	604	TGL	CC5-CC6-CC7-CC8
17	C	304	PGV	C9-C10-C11-C12
26	P	312	CDL	C63-C64-C65-C66
27	G	101	DMU	C25-C28-C31-C34
23	R	201	PSC	C26-C27-C28-C29
26	P	308	CDL	C44-C45-C46-C47
17	P	307	PGV	C15-C16-C17-C18
26	P	308	CDL	C63-C64-C65-C66
26	P	312	CDL	C1-CA2-OA2-PA1
20	D	201	TGL	OG1-CG1-CG2-OG2
23	B	302	PSC	O03-C01-C02-O01
17	N	606	PGV	O03-C19-C20-C21
26	C	305	CDL	C42-C43-C44-C45
26	C	310	CDL	C83-C84-C85-C86
20	A	613	TGL	C16-C17-C18-C19
20	D	201	TGL	C13-C14-C29-C30
17	M	101	PGV	C10-C11-C12-C13
20	A	613	TGL	CC2-CC3-CC4-CC5
20	N	605	TGL	CC7-CC8-CC9-C15
23	R	201	PSC	C4-C5-C6-C7
26	C	305	CDL	C57-C58-C59-C60
25	P	304	PEK	C2-C3-C4-C5
17	A	604	PGV	O03-C19-C20-C21
20	A	613	TGL	C11-C10-CB9-CB8
25	G	102	PEK	C17-C18-C19-C20
25	P	301	PEK	O03-C21-C22-C23
17	P	306	PGV	C9-C10-C11-C12
25	P	304	PEK	O03-C21-C22-C23
19	A	611	EDO	O1-C1-C2-O2
19	G	105	EDO	O1-C1-C2-O2
19	K	201	EDO	O1-C1-C2-O2
19	N	621	EDO	O1-C1-C2-O2
19	Q	1603	EDO	O1-C1-C2-O2
19	V	102	EDO	O1-C1-C2-O2
17	A	604	PGV	C26-C27-C28-C29
27	P	302	DMU	C19-C18-O16-C6
20	A	613	TGL	C21-C20-CA9-CA8
17	C	304	PGV	C1-C2-C3-C4
26	C	305	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
27	C	311	DMU	C31-C34-C37-C40
25	C	314	PEK	C10-C11-C12-C13
17	N	622	PGV	C7-C8-C9-C10
20	A	613	TGL	CC3-CC4-CC5-CC6
20	A	613	TGL	C29-C30-C31-C32
26	C	310	CDL	C19-C20-C21-C22
17	C	303	PGV	C29-C30-C31-C32
20	L	502	TGL	CA4-CA5-CA6-CA7
20	L	502	TGL	CC3-CC4-CC5-CC6
25	P	304	PEK	C14-C15-C16-C17
20	A	613	TGL	CC6-CC7-CC8-CC9
26	P	308	CDL	CA4-CA3-OA5-PA1
17	N	622	PGV	C13-C14-C15-C16
26	P	312	CDL	C16-C17-C18-C19
23	B	302	PSC	C14-C15-C16-C17
26	C	310	CDL	CB5-C51-C52-C53
17	P	306	PGV	C15-C16-C17-C18
26	C	305	CDL	C20-C21-C22-C23
26	C	305	CDL	C35-C36-C37-C38
26	C	310	CDL	C84-C85-C86-C87
20	N	618	TGL	CG1-CG2-OG2-CB1
20	N	605	TGL	C16-C15-CC9-CC8
24	P	309	CHD	C22-C23-C24-O25
26	P	312	CDL	C61-C62-C63-C64
19	B	307	EDO	O1-C1-C2-O2
19	C	307	EDO	O1-C1-C2-O2
19	E	201	EDO	O1-C1-C2-O2
19	P	311	EDO	O1-C1-C2-O2
23	R	201	PSC	C15-C16-C17-C18
24	G	107	CHD	C22-C23-C24-O26
24	T	1302	CHD	C22-C23-C24-O26
26	C	305	CDL	O1-C1-CB2-OB2
17	N	606	PGV	C9-C10-C11-C12
20	N	618	TGL	CC7-CC8-CC9-C15
26	P	312	CDL	C59-C60-C61-C62
24	B	303	CHD	C22-C23-C24-O25
26	C	305	CDL	C34-C35-C36-C37
26	C	305	CDL	OB5-CB3-CB4-CB6
25	P	305	PEK	C32-C33-C34-C35
18	A	605	HEA	CAD-CBD-CGD-O1D
18	A	605	HEA	CAD-CBD-CGD-O2D
23	B	302	PSC	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	P	301	PEK	C30-C31-C32-C33
20	L	502	TGL	OG1-CG1-CG2-OG2
17	P	307	PGV	C21-C22-C23-C24
25	C	302	PEK	C30-C31-C32-C33
25	C	314	PEK	C34-C35-C36-C37
26	C	305	CDL	C79-C80-C81-C82
26	C	310	CDL	C74-C75-C76-C77
25	P	301	PEK	C6-C7-C8-C9
25	P	305	PEK	C9-C10-C11-C12
26	C	310	CDL	C51-C52-C53-C54
26	P	308	CDL	C58-C59-C60-C61
24	C	306	CHD	C22-C23-C24-O25
20	N	604	TGL	C11-C10-CB9-CB8
17	C	303	PGV	C31-C32-C33-C34
20	D	201	TGL	C24-C25-C26-C27
23	R	201	PSC	C28-C29-C30-C31
20	A	613	TGL	CB9-C10-C11-C12
26	C	305	CDL	C64-C65-C66-C67
24	Y	101	CHD	C22-C23-C24-O25
24	B	303	CHD	C22-C23-C24-O26
24	G	107	CHD	C22-C23-C24-O25
24	P	309	CHD	C22-C23-C24-O26
23	R	201	PSC	C30-C31-C32-C33
27	P	302	DMU	O6-C11-C9-O1
26	P	312	CDL	C32-C31-CA7-OA8
25	P	304	PEK	C28-C29-C30-C31
17	C	303	PGV	C20-C21-C22-C23
20	N	604	TGL	C24-C25-C26-C27
25	P	304	PEK	C22-C23-C24-C25
18	A	605	HEA	CAA-CBA-CGA-O1A
27	G	104	DMU	C5-C10-O7-C3
20	N	618	TGL	CB5-CB6-CB7-CB8
20	L	502	TGL	CC4-CC5-CC6-CC7
19	A	616	EDO	O1-C1-C2-O2
19	C	309	EDO	O1-C1-C2-O2
19	E	202	EDO	O1-C1-C2-O2
19	E	204	EDO	O1-C1-C2-O2
19	E	205	EDO	O1-C1-C2-O2
19	I	102	EDO	O1-C1-C2-O2
19	N	609	EDO	O1-C1-C2-O2
19	N	614	EDO	O1-C1-C2-O2
19	S	106	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
24	T	1302	CHD	C22-C23-C24-O25
18	A	605	HEA	CAA-CBA-CGA-O2A
17	A	604	PGV	C31-C32-C33-C34
17	P	306	PGV	C26-C27-C28-C29
26	C	310	CDL	OB5-CB3-CB4-CB6
26	C	305	CDL	C58-C59-C60-C61
17	P	307	PGV	O03-C01-C02-O01
20	N	618	TGL	OG1-CG1-CG2-OG2
26	C	310	CDL	OA6-CA4-CA6-OA8
17	N	622	PGV	C25-C26-C27-C28
17	P	307	PGV	C26-C27-C28-C29
20	A	613	TGL	CB2-CB3-CB4-CB5
17	M	101	PGV	C29-C30-C31-C32
25	C	302	PEK	O03-C21-C22-C23
24	Y	101	CHD	C22-C23-C24-O26
20	L	502	TGL	C13-C14-C29-C30
20	A	613	TGL	CB3-CB4-CB5-CB6
20	N	618	TGL	CG3-CG2-OG2-CB1
25	C	302	PEK	C01-C02-O01-C1
25	P	305	PEK	C01-C02-O01-C1
26	C	310	CDL	CA3-CA4-OA6-CA5
17	N	622	PGV	C11-C12-C13-C14
20	D	201	TGL	OG2-CB1-CB2-CB3
20	N	605	TGL	C23-C24-C25-C26
25	G	102	PEK	C29-C30-C31-C32
26	P	312	CDL	C13-C14-C15-C16
18	N	607	HEA	CAD-CBD-CGD-O2D
26	P	308	CDL	C75-C76-C77-C78
23	R	201	PSC	O03-C01-C02-C03
17	P	307	PGV	O04-C19-O03-C01
26	P	308	CDL	C24-C25-C26-C27
24	C	301	CHD	C22-C23-C24-O25
17	P	307	PGV	C20-C21-C22-C23
23	B	302	PSC	C27-C28-C29-C30
25	C	302	PEK	C3-C4-C5-C6
23	R	201	PSC	C05-C04-O12-P
23	B	302	PSC	C25-C26-C27-C28
20	L	502	TGL	C23-C24-C25-C26
24	P	303	CHD	C22-C23-C24-O25
19	D	202	EDO	O1-C1-C2-O2
19	E	203	EDO	O1-C1-C2-O2
19	N	612	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
19	N	616	EDO	O1-C1-C2-O2
19	N	619	EDO	O1-C1-C2-O2
19	Q	1601	EDO	O1-C1-C2-O2
19	S	102	EDO	O1-C1-C2-O2
19	S	103	EDO	O1-C1-C2-O2
19	S	105	EDO	O1-C1-C2-O2
19	T	1303	EDO	O1-C1-C2-O2
19	U	1501	EDO	O1-C1-C2-O2
26	P	308	CDL	OA6-CA4-CA6-OA8
18	N	607	HEA	CAD-CBD-CGD-O1D
17	A	604	PGV	C9-C10-C11-C12
25	C	314	PEK	C14-C15-C16-C17
20	N	618	TGL	OG3-CC1-CC2-CC3
24	T	1302	CHD	C16-C17-C20-C22
20	A	613	TGL	C13-C14-C29-C30
17	A	604	PGV	C27-C28-C29-C30
18	N	607	HEA	CAA-CBA-CGA-O2A
25	P	304	PEK	C17-C18-C19-C20
20	L	502	TGL	CA3-CA4-CA5-CA6
20	N	605	TGL	CA7-CA8-CA9-C20
25	P	304	PEK	C35-C36-C37-C38
17	M	101	PGV	O03-C19-C20-C21
25	G	102	PEK	O01-C1-C2-C3
24	J	101	CHD	C22-C23-C24-O25
24	P	303	CHD	C22-C23-C24-O26
17	M	101	PGV	C15-C16-C17-C18
20	N	605	TGL	CB3-CB4-CB5-CB6
20	L	502	TGL	OG1-CG1-CG2-CG3
23	B	302	PSC	C26-C27-C28-C29
20	N	618	TGL	CA1-CA2-CA3-CA4
17	P	307	PGV	O01-C1-C2-C3
25	G	102	PEK	C26-C27-C28-C29
24	T	1302	CHD	C20-C22-C23-C24
19	F	701	EDO	O1-C1-C2-O2
19	L	501	EDO	O1-C1-C2-O2
19	O	302	EDO	O1-C1-C2-O2
23	R	201	PSC	O03-C19-C20-C21
20	N	604	TGL	CC1-CC2-CC3-CC4
17	C	303	PGV	C05-C04-O12-P
17	P	307	PGV	C02-C03-O11-P
24	C	306	CHD	C22-C23-C24-O26
18	N	607	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	P	308	CDL	C71-CB7-OB8-CB6
17	C	303	PGV	C23-C24-C25-C26
26	P	308	CDL	OB9-CB7-OB8-CB6
25	G	102	PEK	O03-C21-C22-C23
17	P	307	PGV	C23-C24-C25-C26
23	R	201	PSC	O02-C1-O01-C02
17	N	622	PGV	O12-C04-C05-C06
17	M	101	PGV	O04-C19-C20-C21
20	L	502	TGL	OG3-CC1-CC2-CC3
26	P	308	CDL	CA3-CA4-CA6-OA8
26	C	310	CDL	C81-C82-C83-C84
26	P	308	CDL	C53-C54-C55-C56
17	P	307	PGV	O02-C1-C2-C3
25	P	304	PEK	O01-C1-C2-C3
20	N	618	TGL	OC1-CC1-CC2-CC3
25	G	102	PEK	O02-C1-C2-C3
20	A	613	TGL	OG1-CA1-CA2-CA3
19	H	101	EDO	O1-C1-C2-O2
19	N	613	EDO	O1-C1-C2-O2
17	C	303	PGV	C1-C2-C3-C4
17	M	101	PGV	C9-C10-C11-C12
23	R	201	PSC	O04-C19-C20-C21

There are no ring outliers.

55 monomers are involved in 159 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	P	306	PGV	1	0
19	A	612	EDO	1	0
26	C	305	CDL	2	0
17	P	307	PGV	1	0
19	S	106	EDO	1	0
18	N	607	HEA	1	0
19	N	611	EDO	1	0
19	R	203	EDO	1	0
19	A	614	EDO	1	0
17	M	101	PGV	6	0
26	C	310	CDL	2	0
19	B	311	EDO	1	0
24	P	303	CHD	1	0
19	V	103	EDO	1	0
25	P	301	PEK	1	0

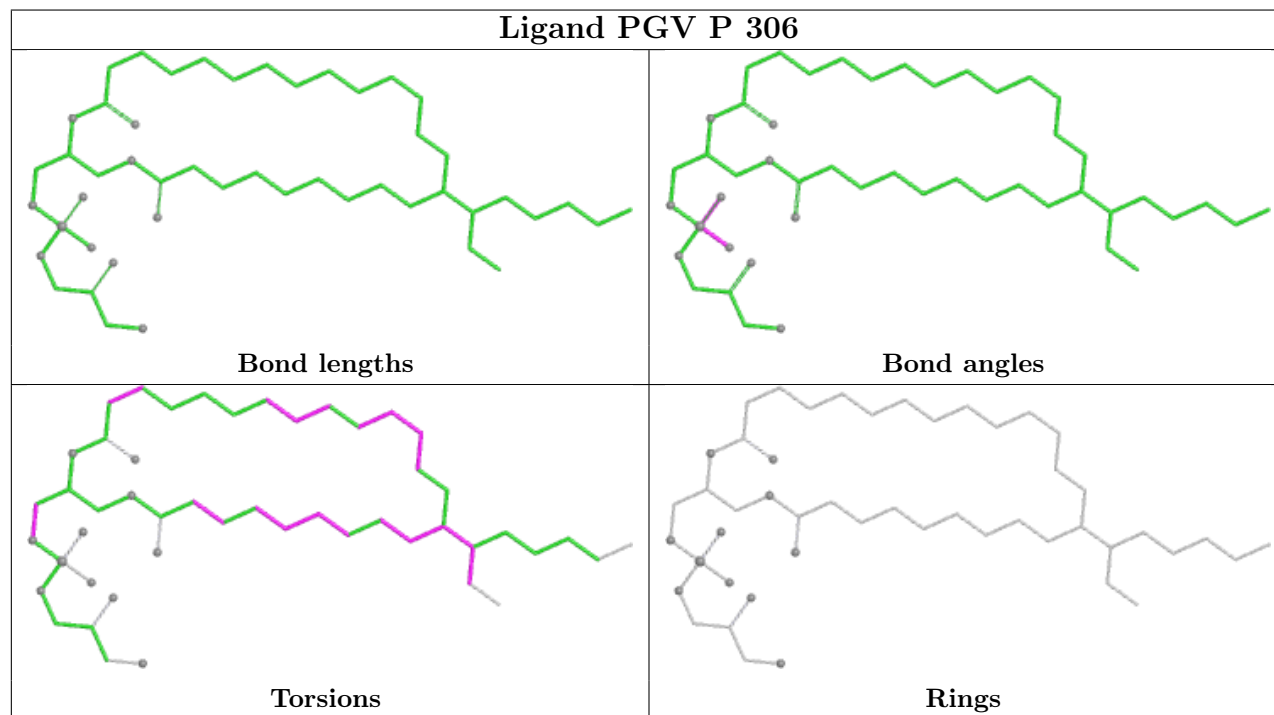
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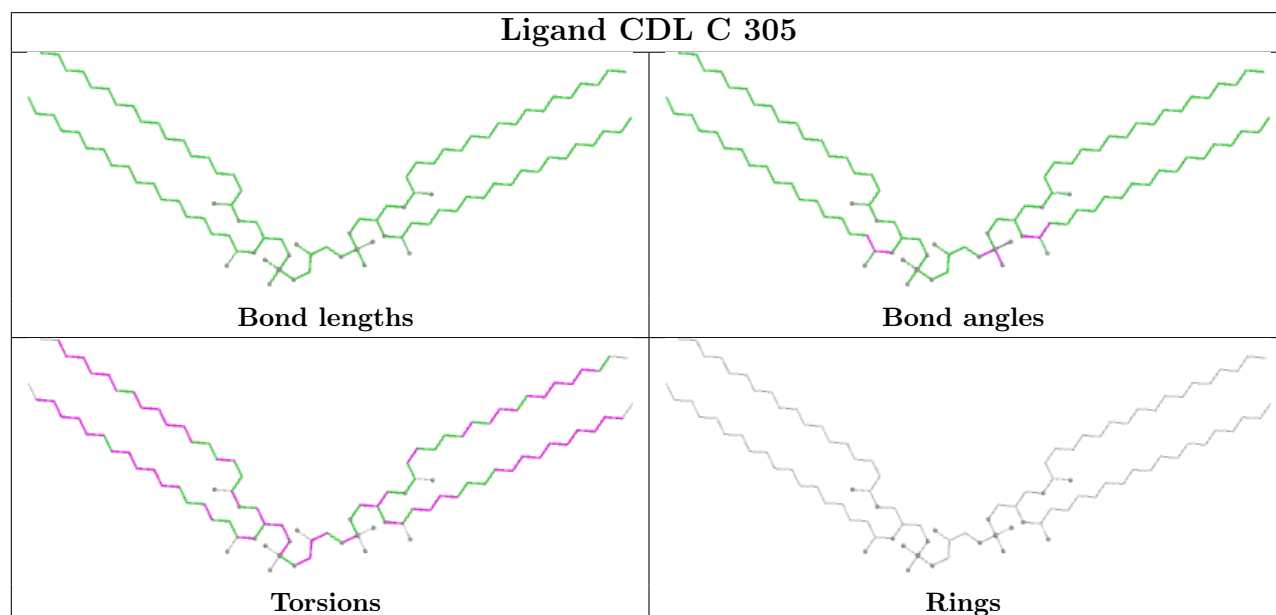
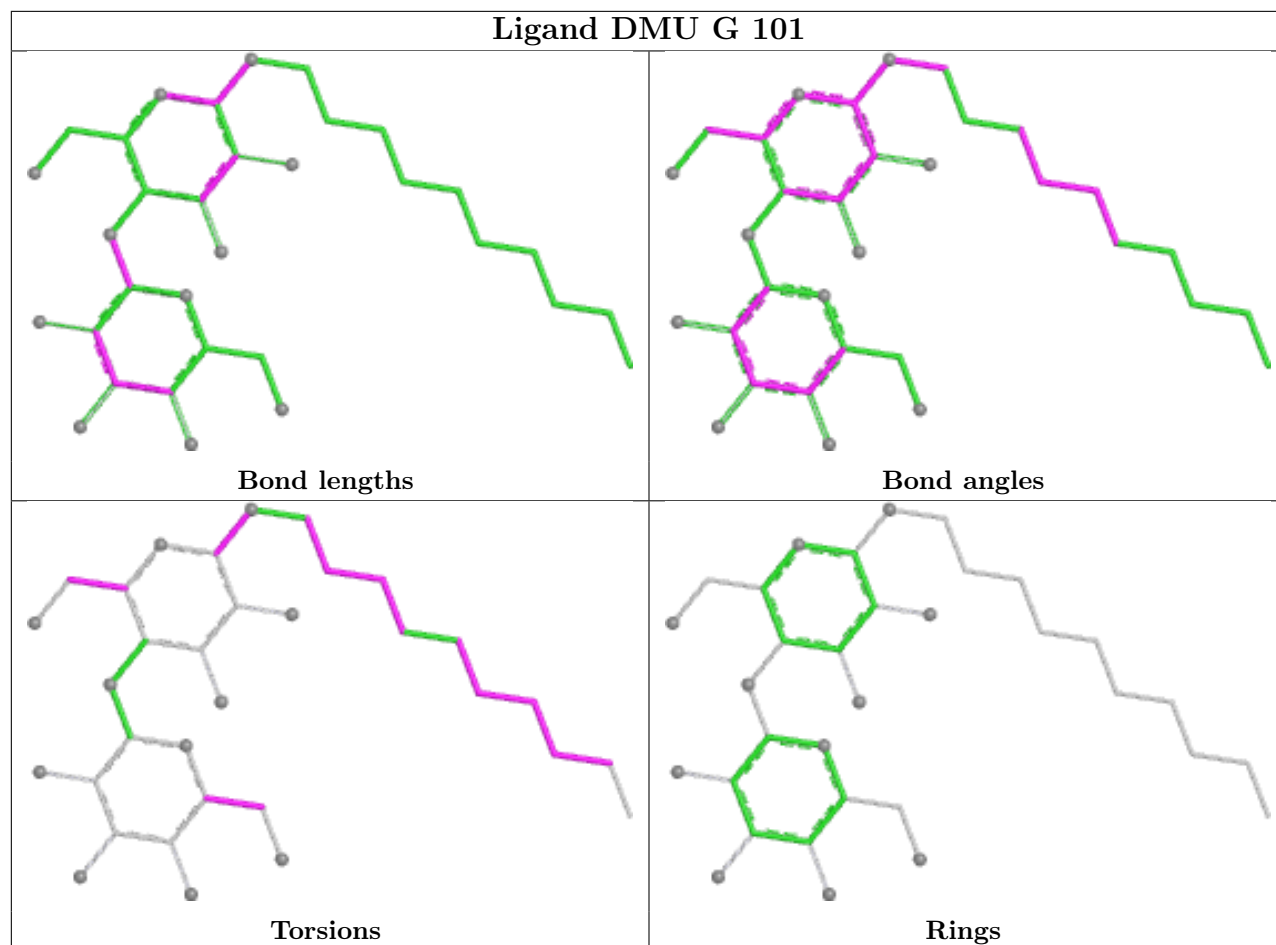
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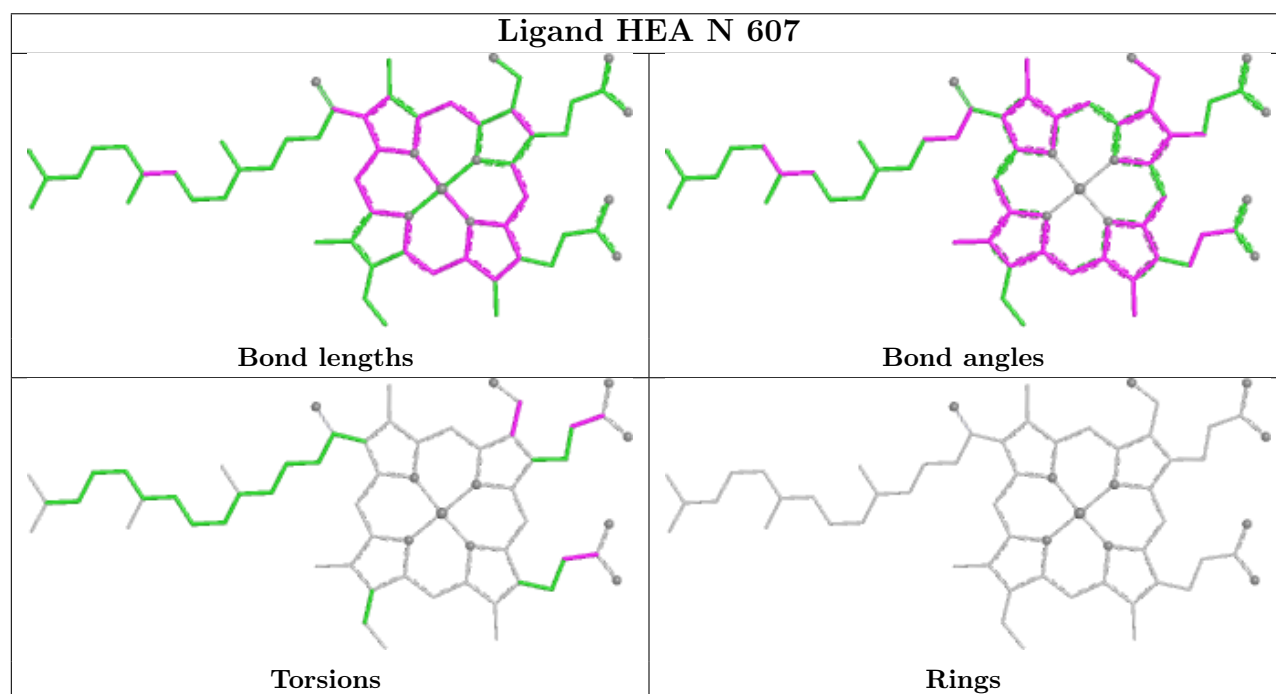
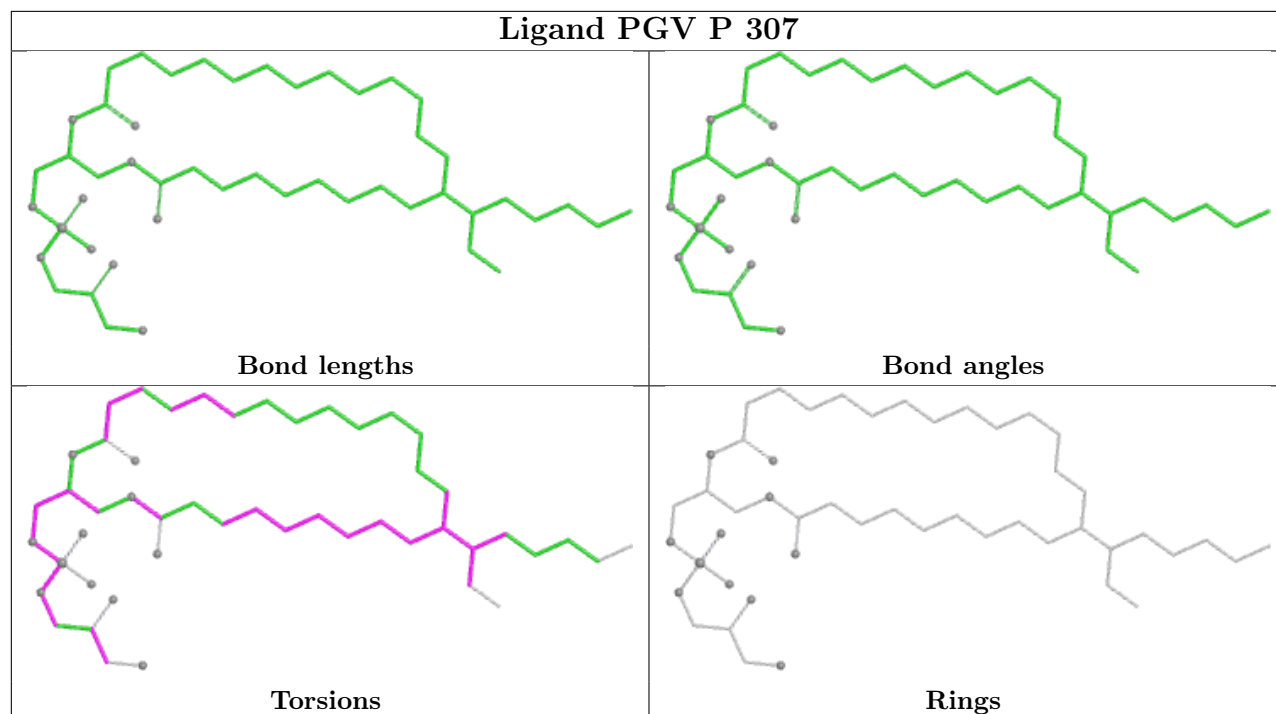
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	615	EDO	1	0
19	C	312	EDO	1	0
29	V	101	SAC	3	0
19	A	618	EDO	2	0
17	A	604	PGV	4	0
24	J	101	CHD	2	0
18	A	606	HEA	3	0
19	N	612	EDO	2	0
25	P	304	PEK	4	0
17	C	304	PGV	6	0
19	B	305	EDO	1	0
23	B	302	PSC	8	0
25	G	102	PEK	7	0
29	I	101	SAC	2	0
17	C	303	PGV	1	0
20	N	618	TGL	5	0
19	U	1501	EDO	3	0
20	N	605	TGL	6	0
23	R	201	PSC	6	0
20	L	502	TGL	3	0
26	P	308	CDL	3	0
27	Z	101	DMU	4	0
25	C	314	PEK	1	0
25	C	302	PEK	3	0
24	B	303	CHD	1	0
24	Y	101	CHD	4	0
19	A	610	EDO	1	0
26	P	312	CDL	10	0
25	P	305	PEK	5	0
20	D	201	TGL	10	0
18	A	605	HEA	2	0
24	T	1302	CHD	4	0
19	A	611	EDO	1	0
18	N	608	HEA	5	0
19	A	616	EDO	1	0
24	W	302	CHD	1	0
19	H	101	EDO	1	0
19	N	615	EDO	1	0
17	N	622	PGV	16	0
24	C	301	CHD	1	0

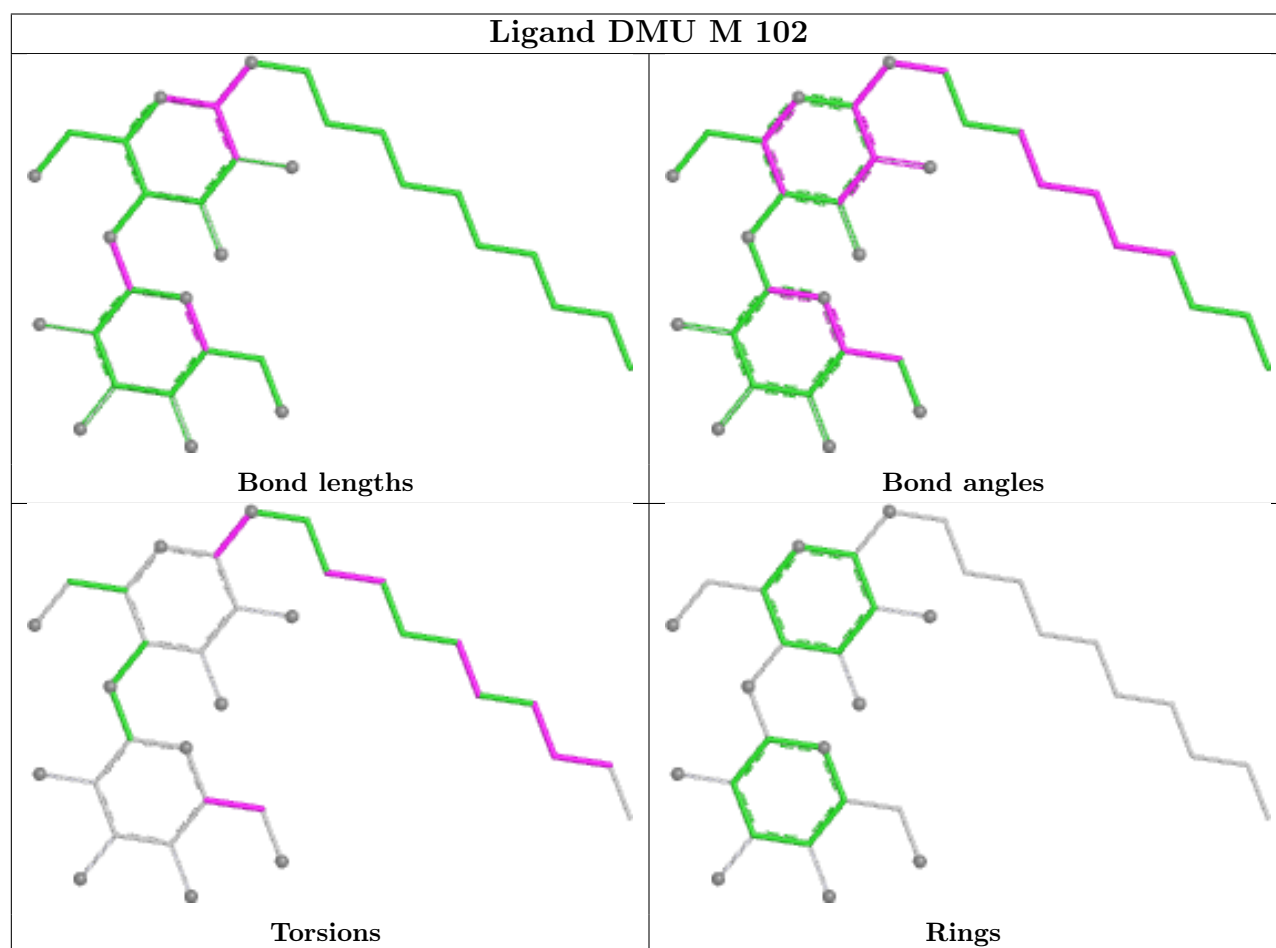
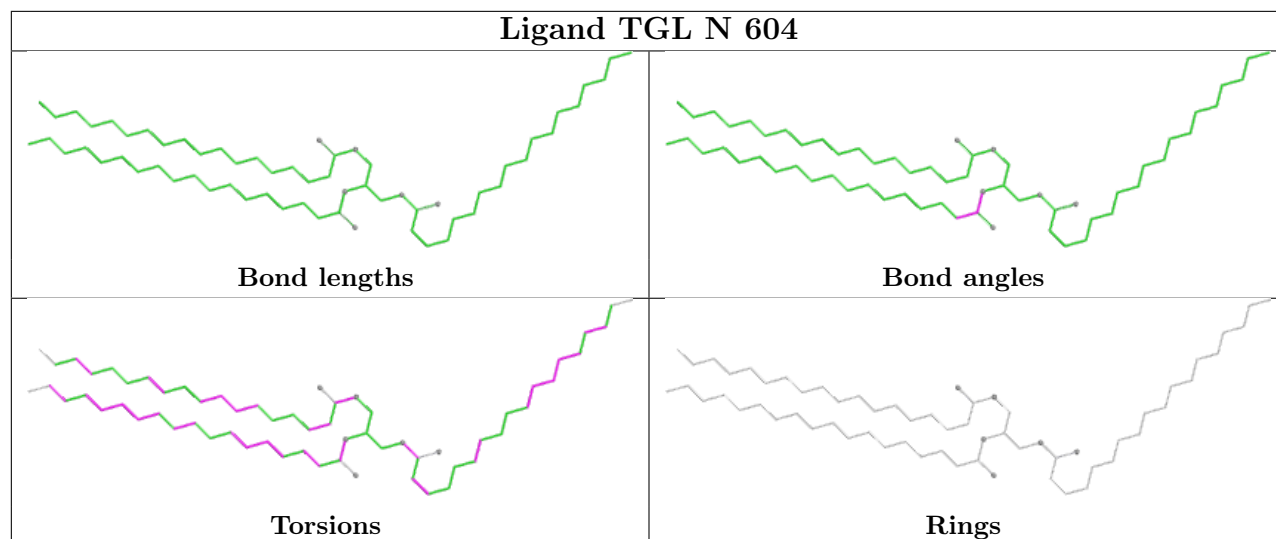
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

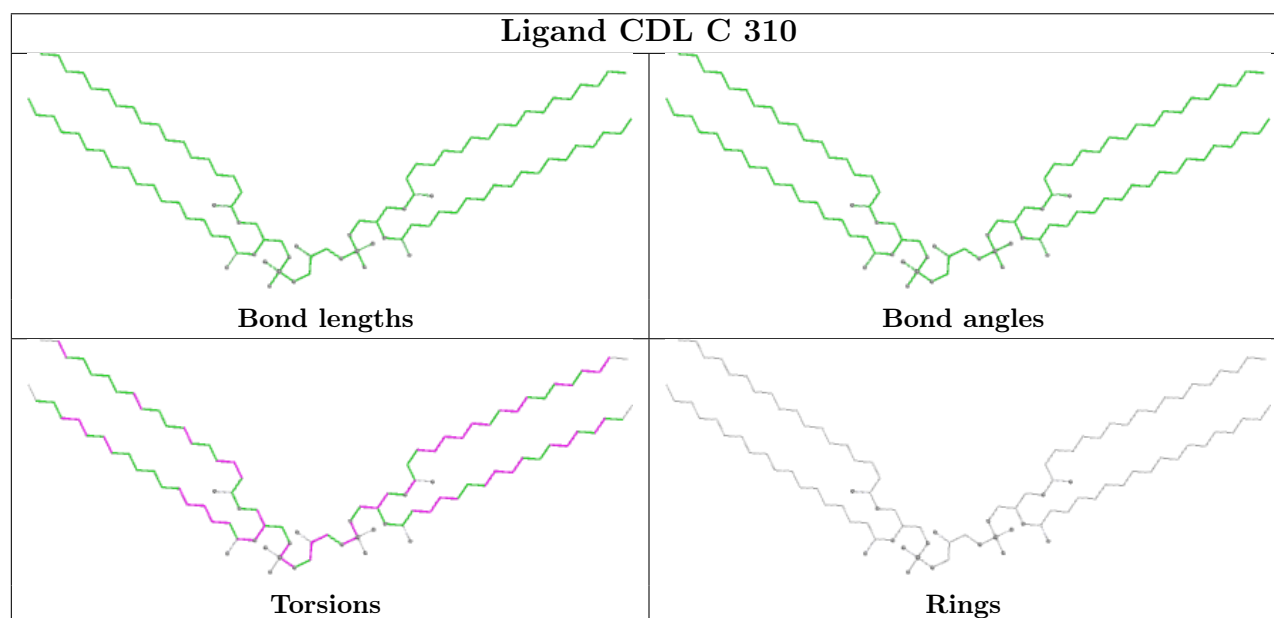
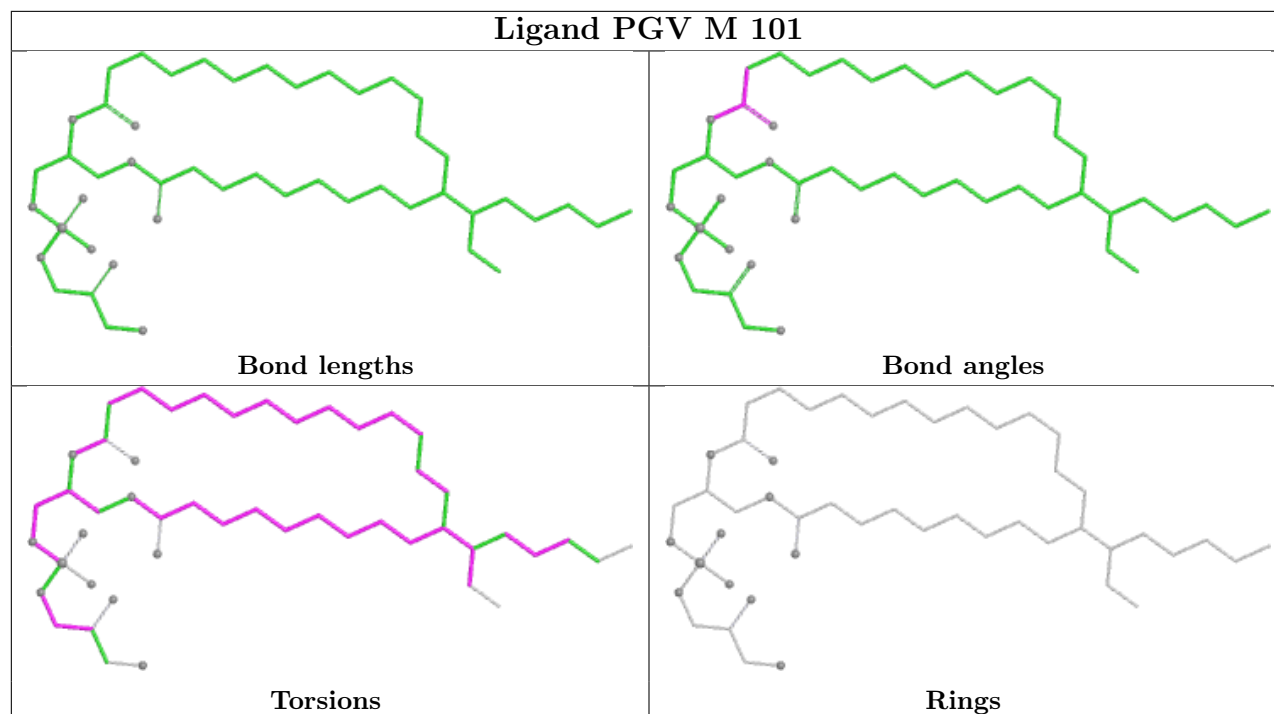
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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

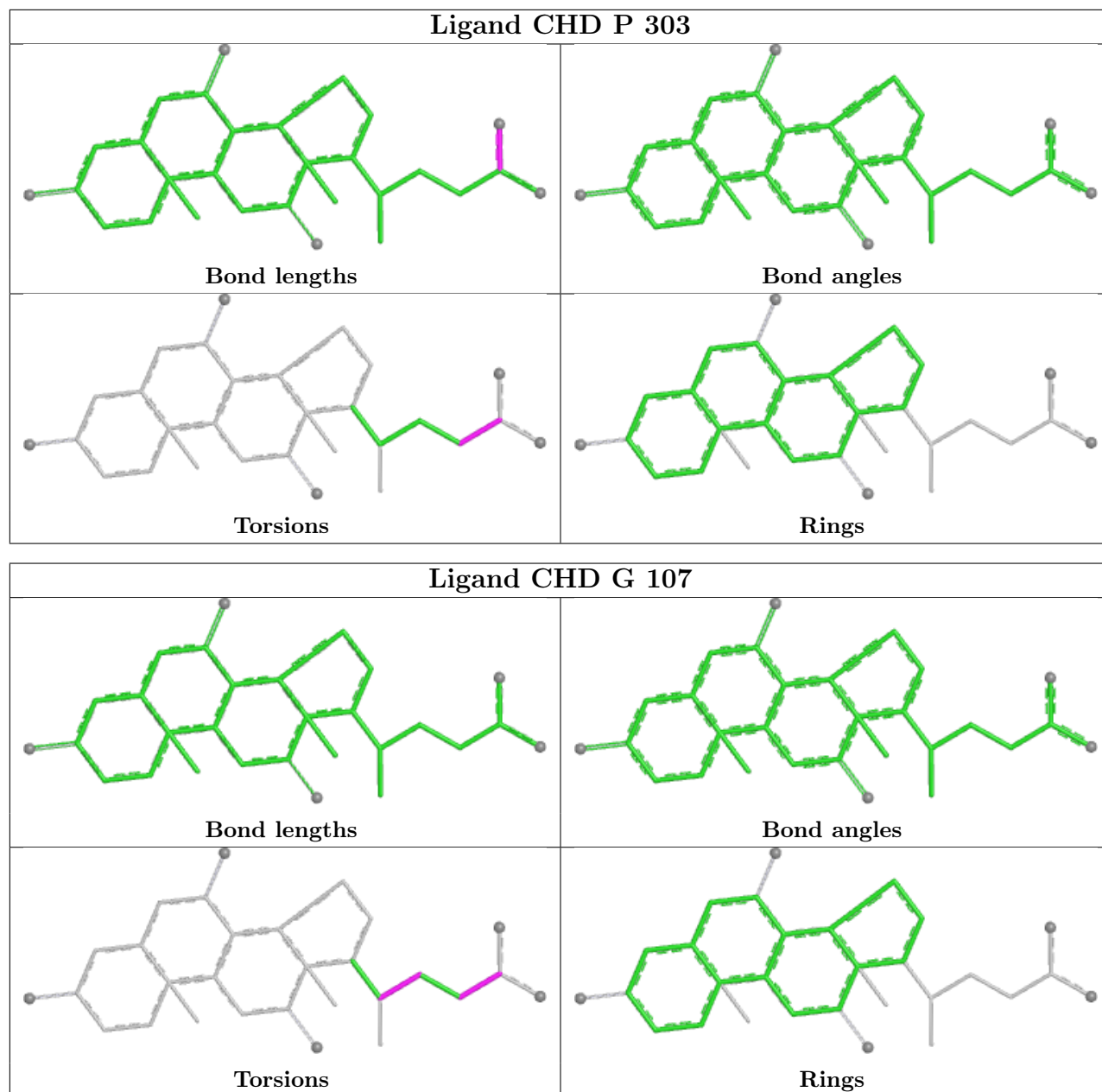




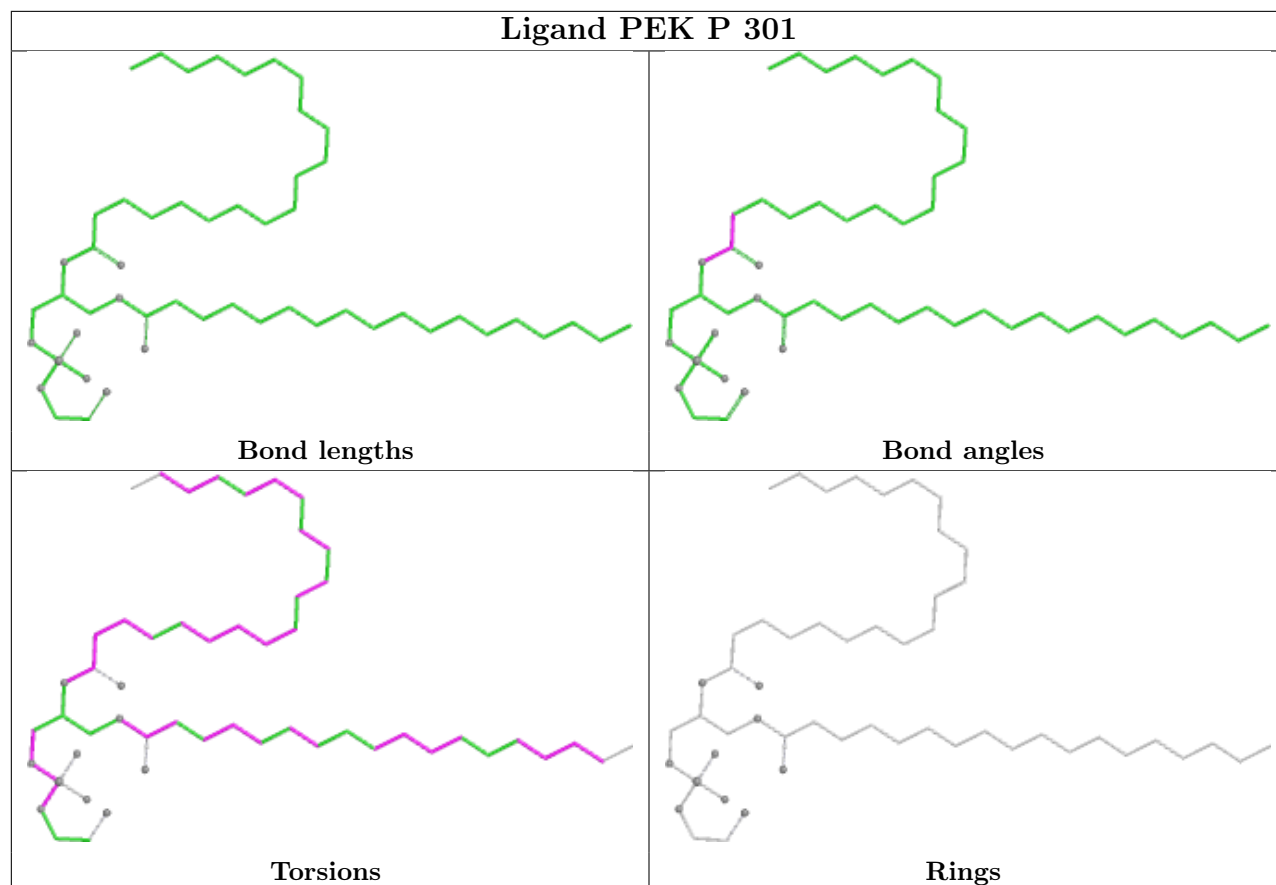




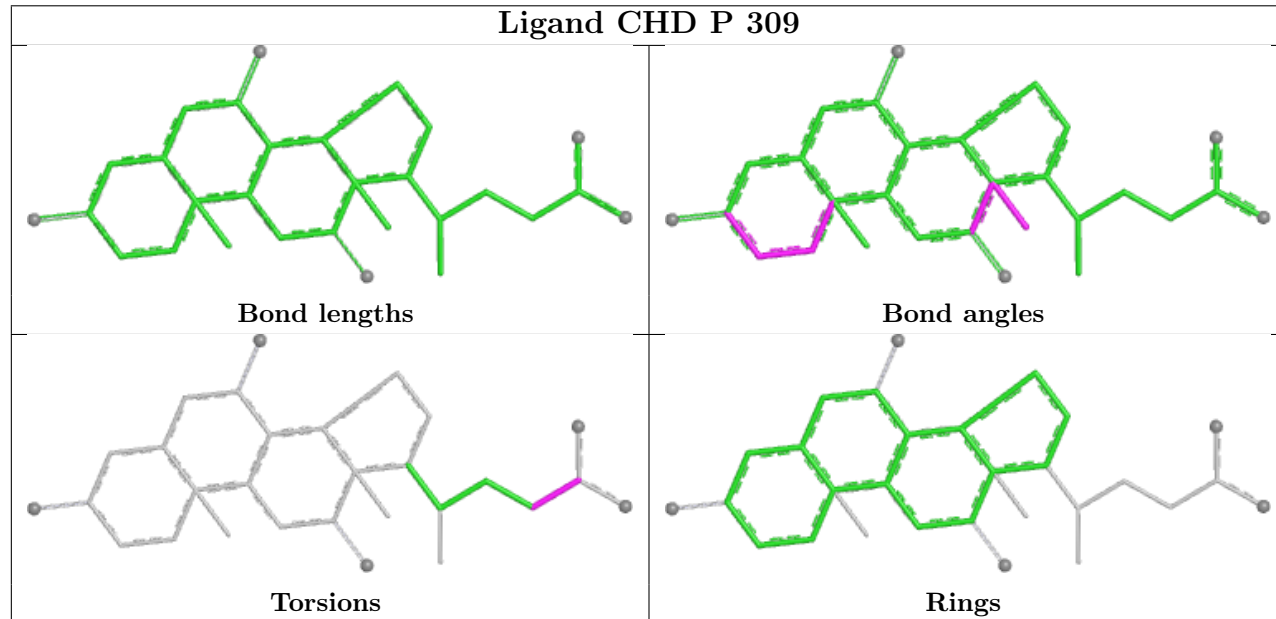


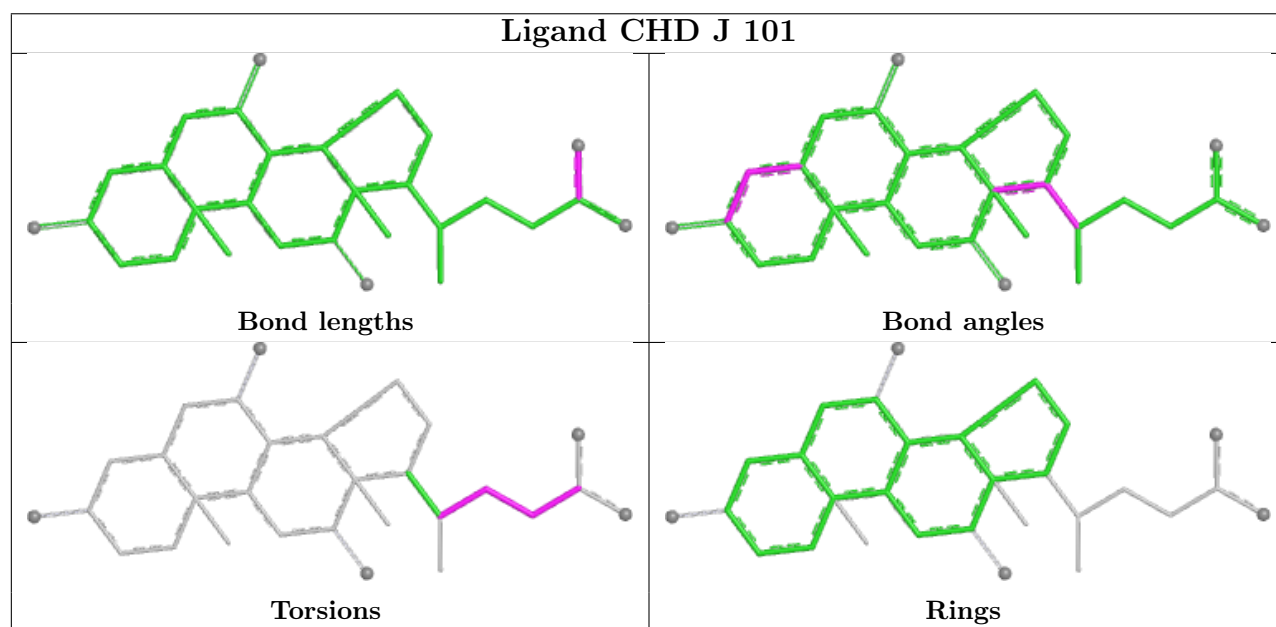
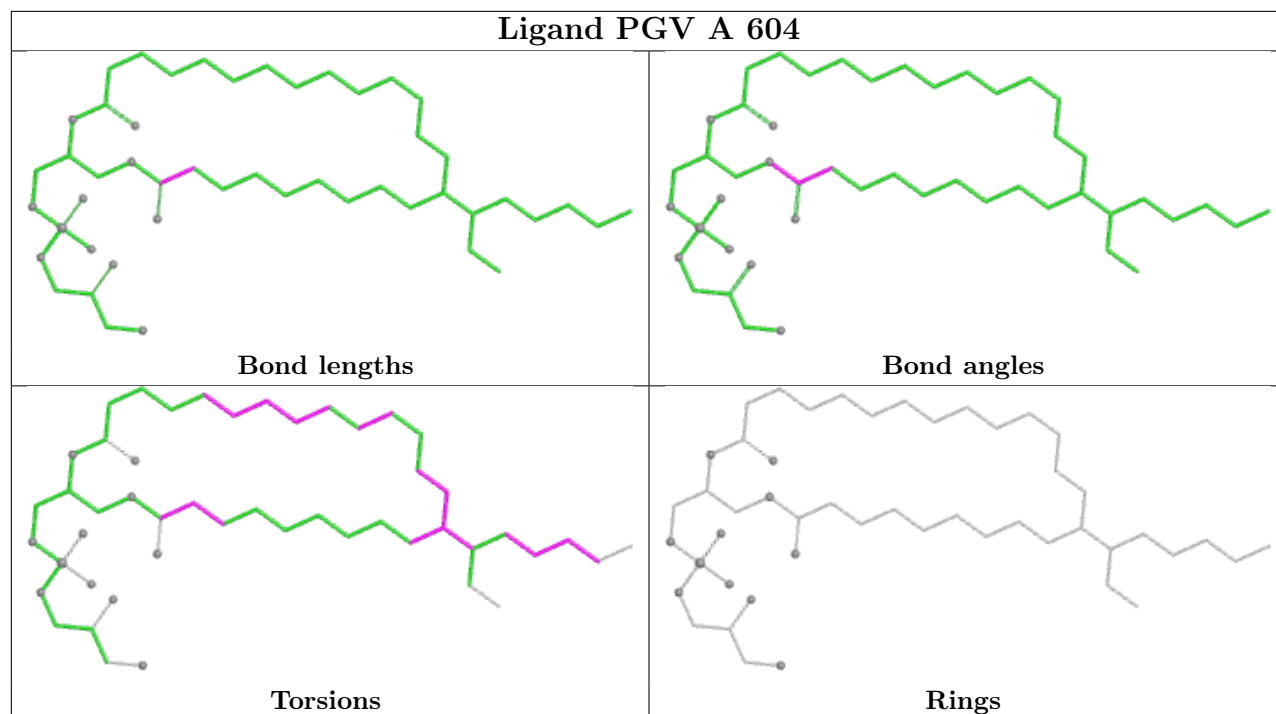


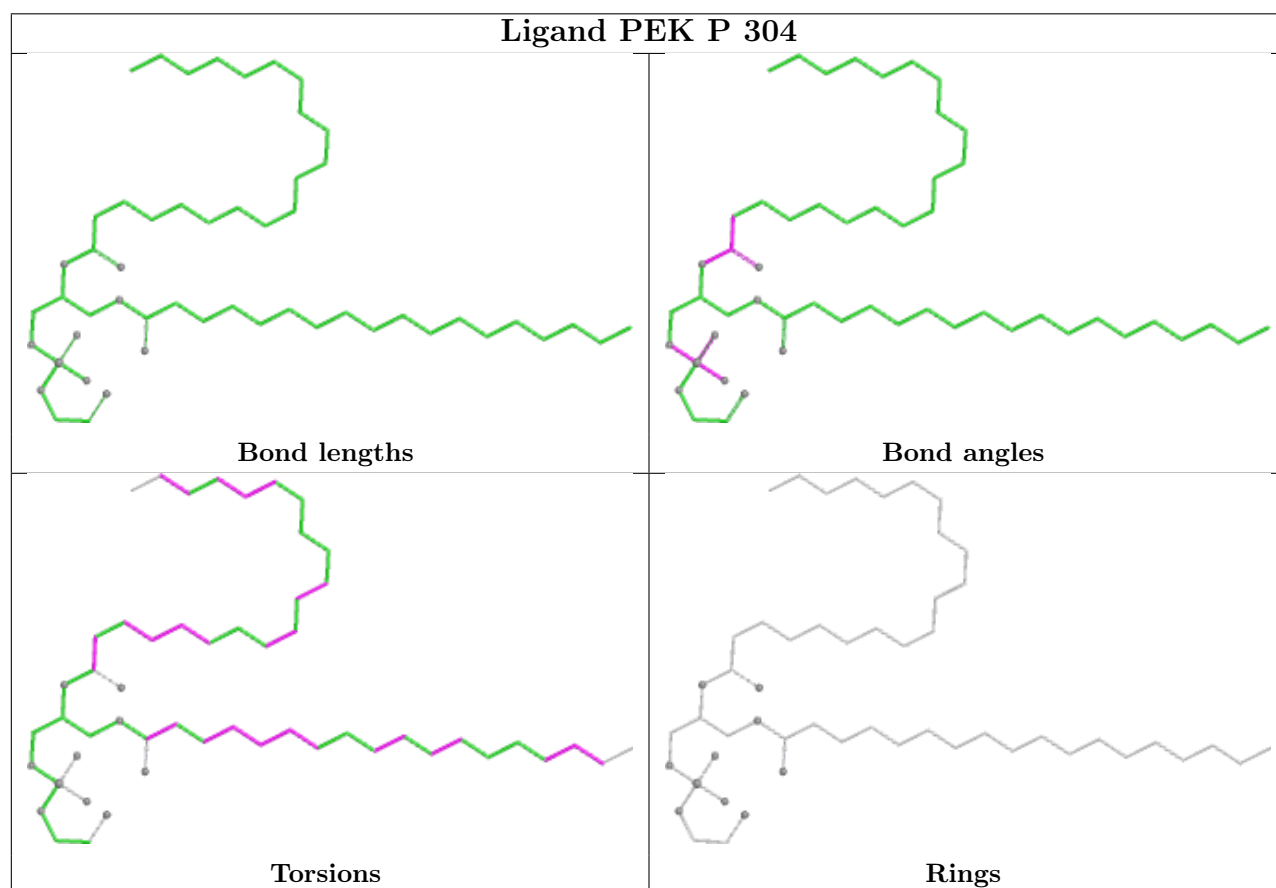
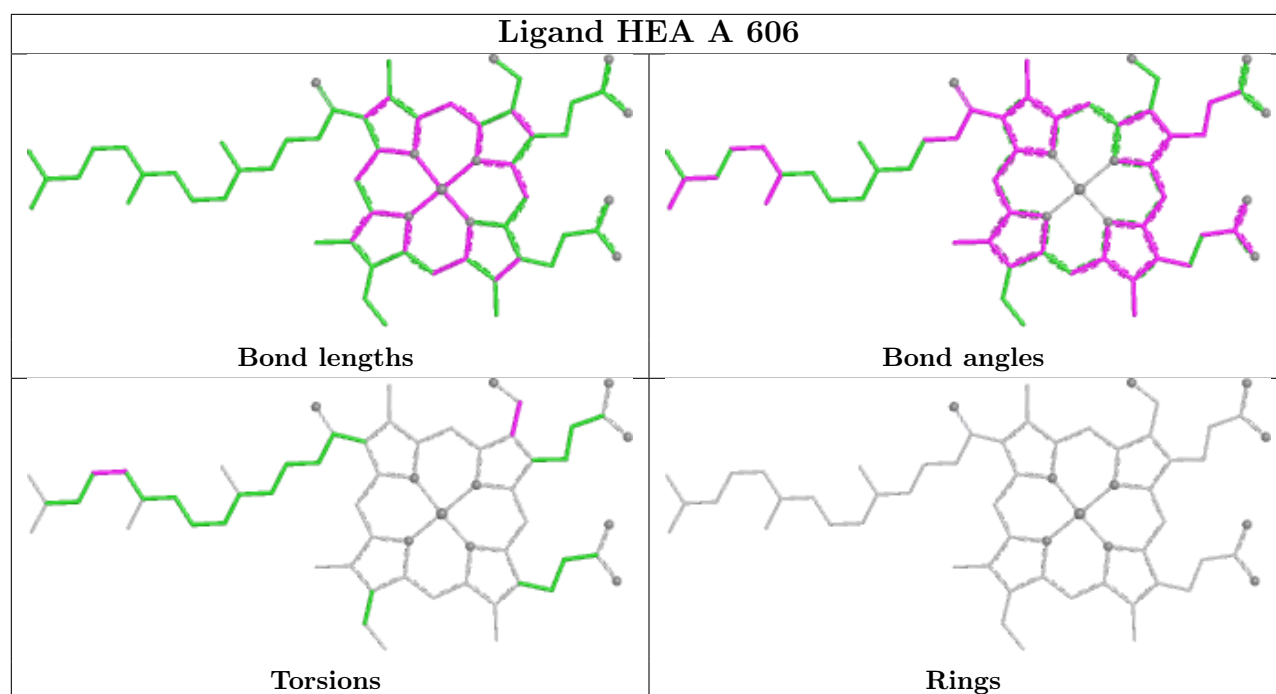
Ligand PEK P 301

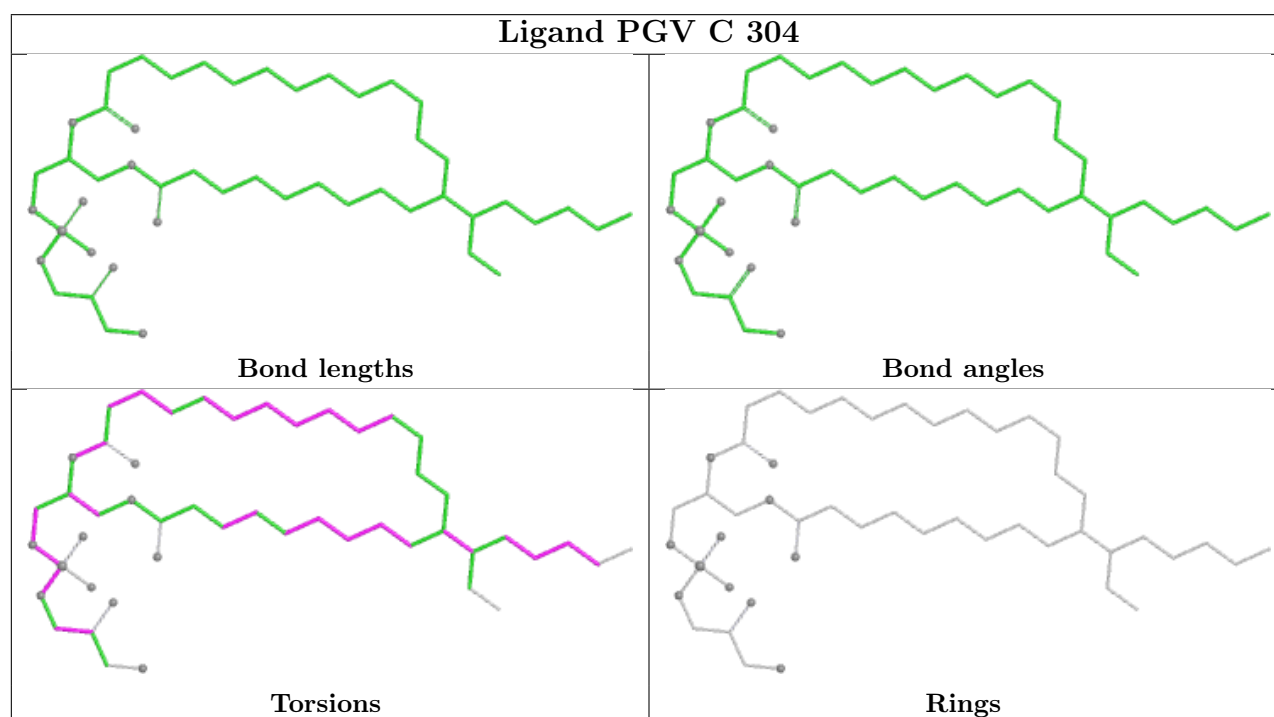
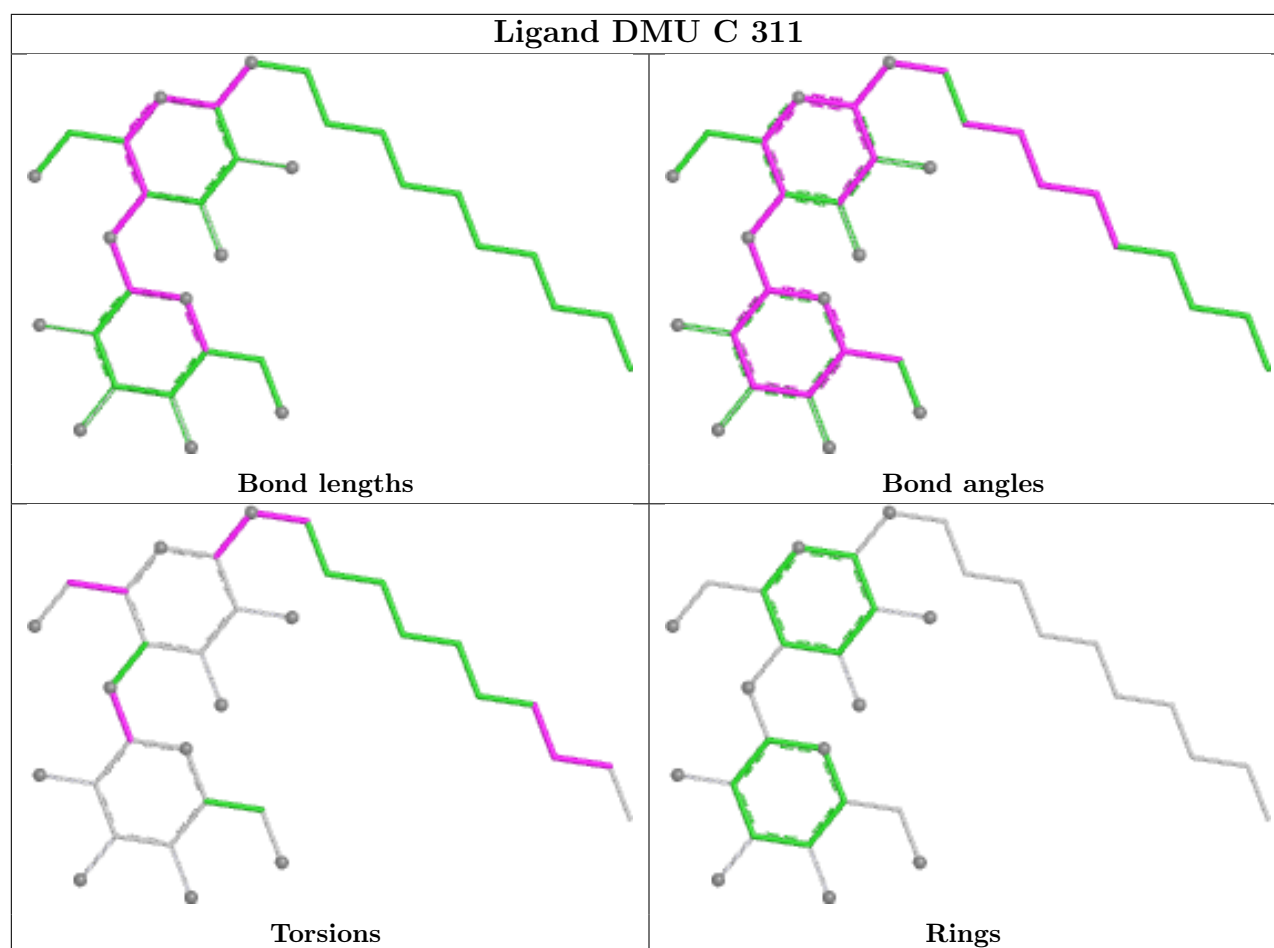


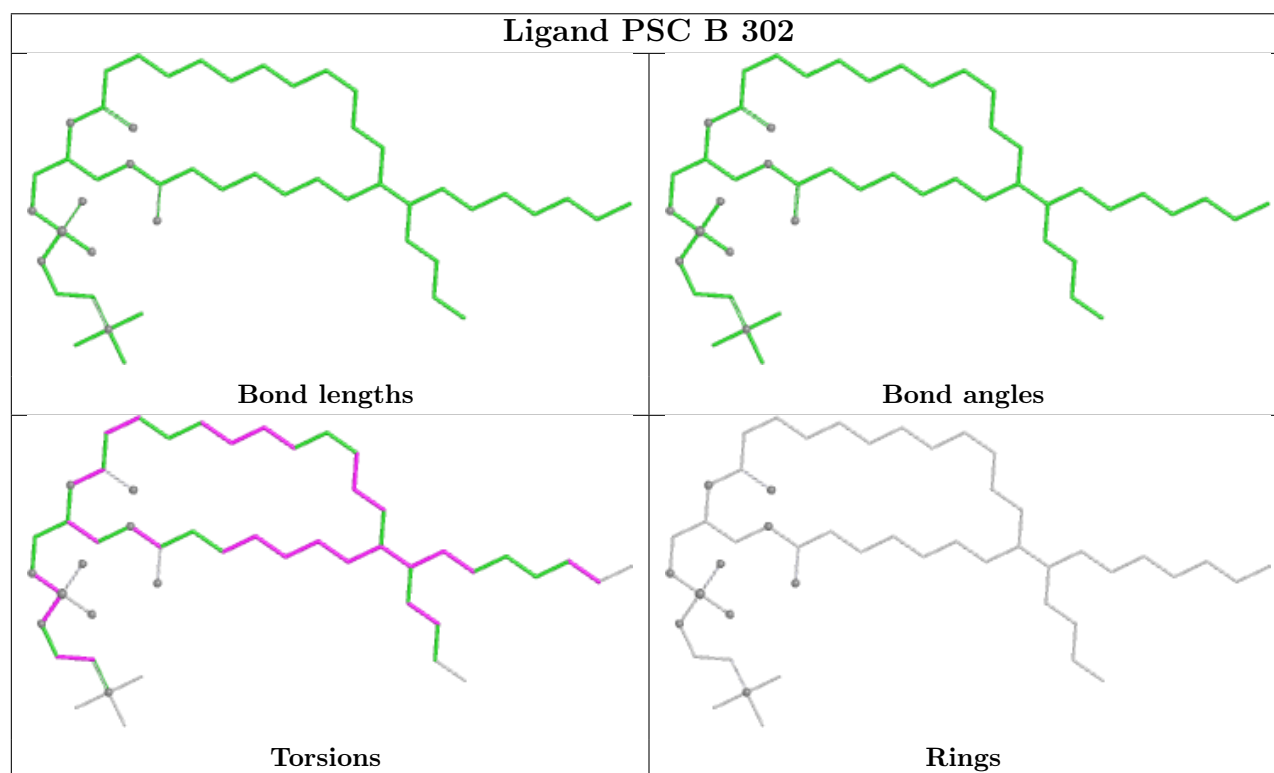
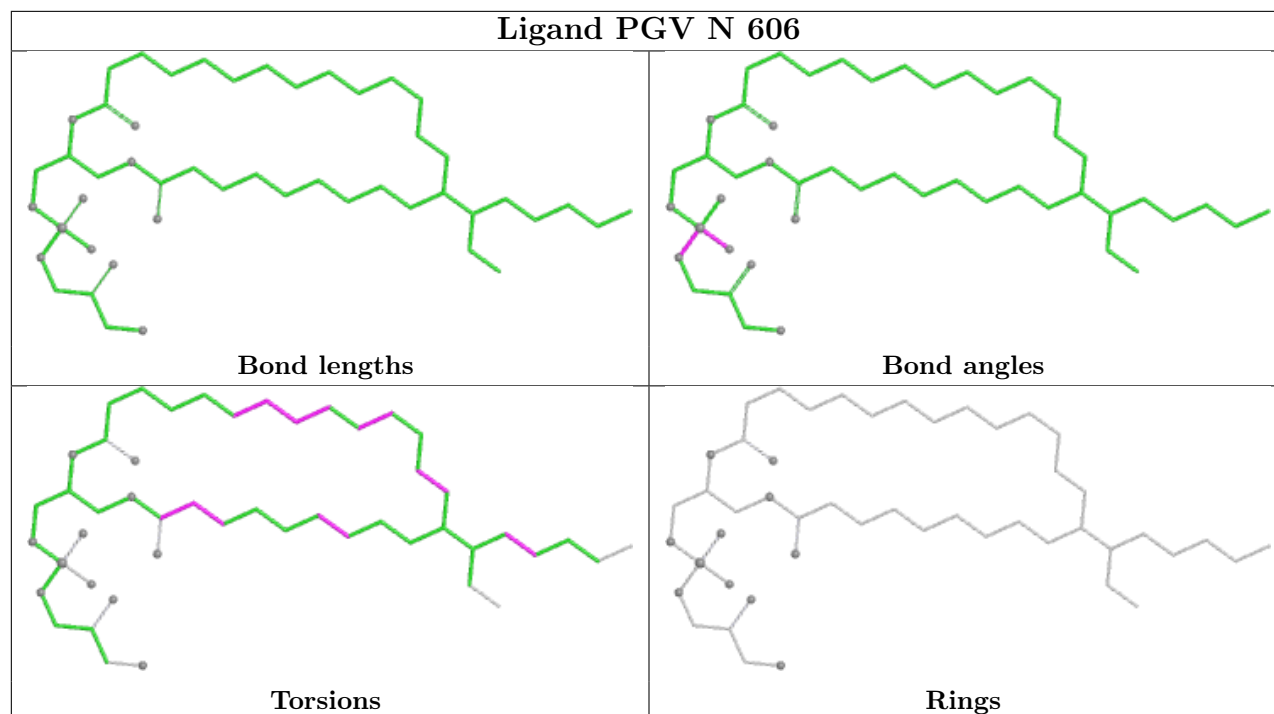
Ligand CHD P 309

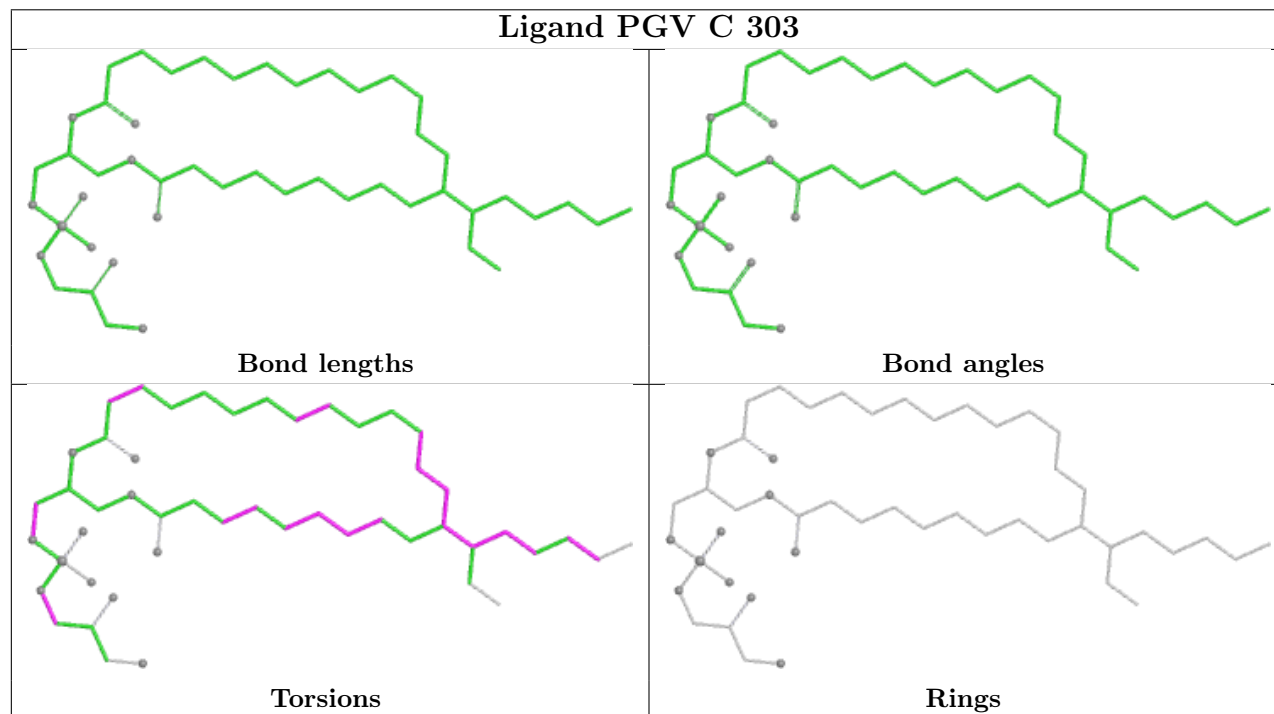
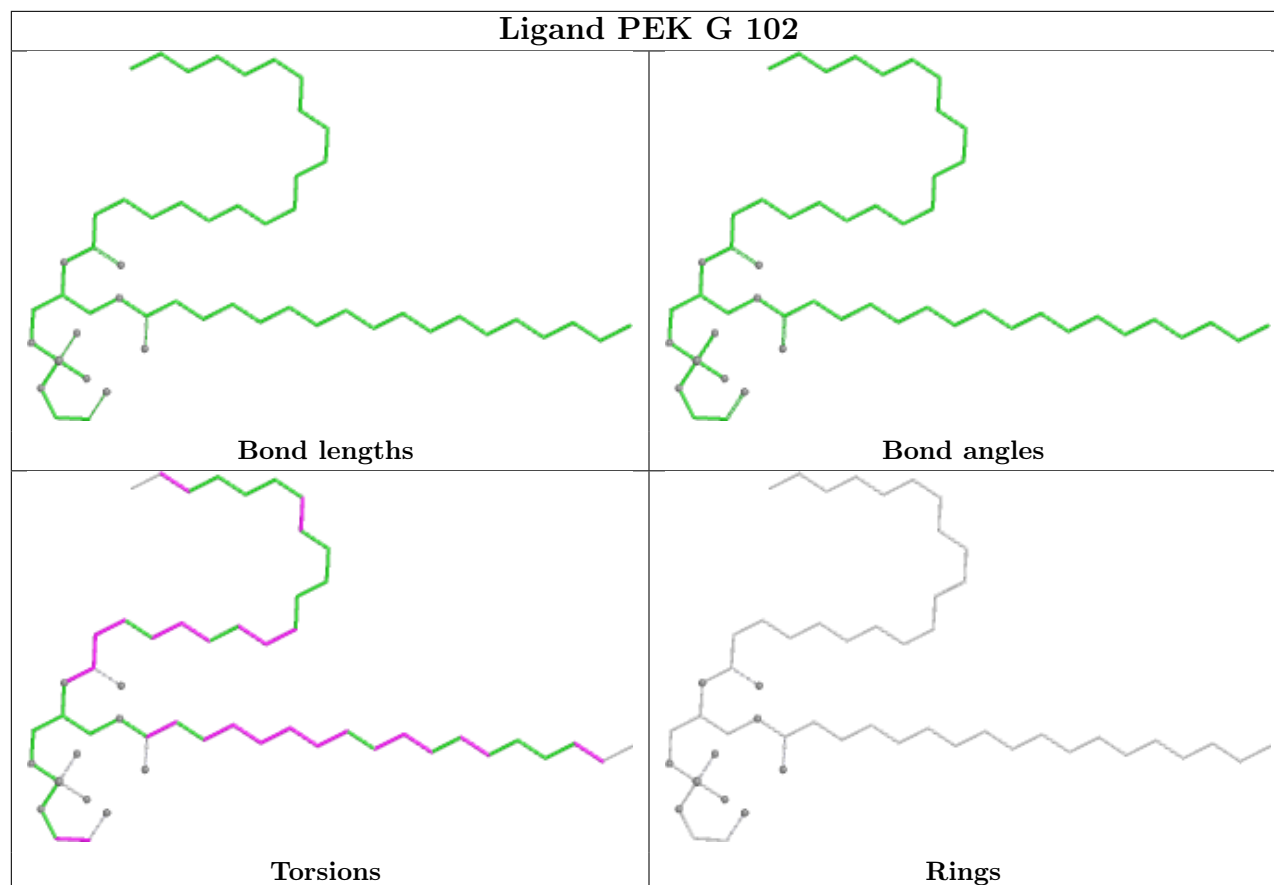


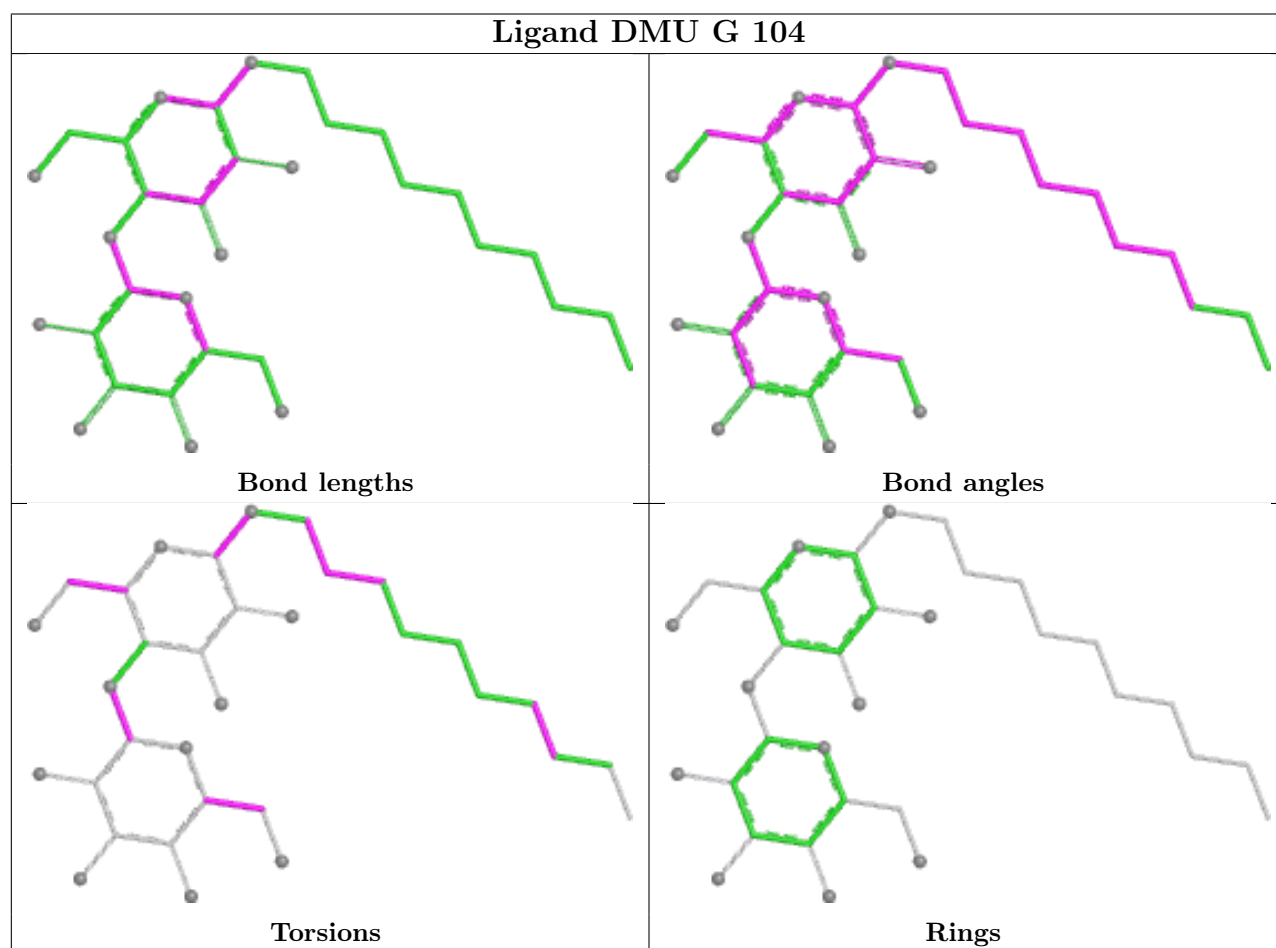
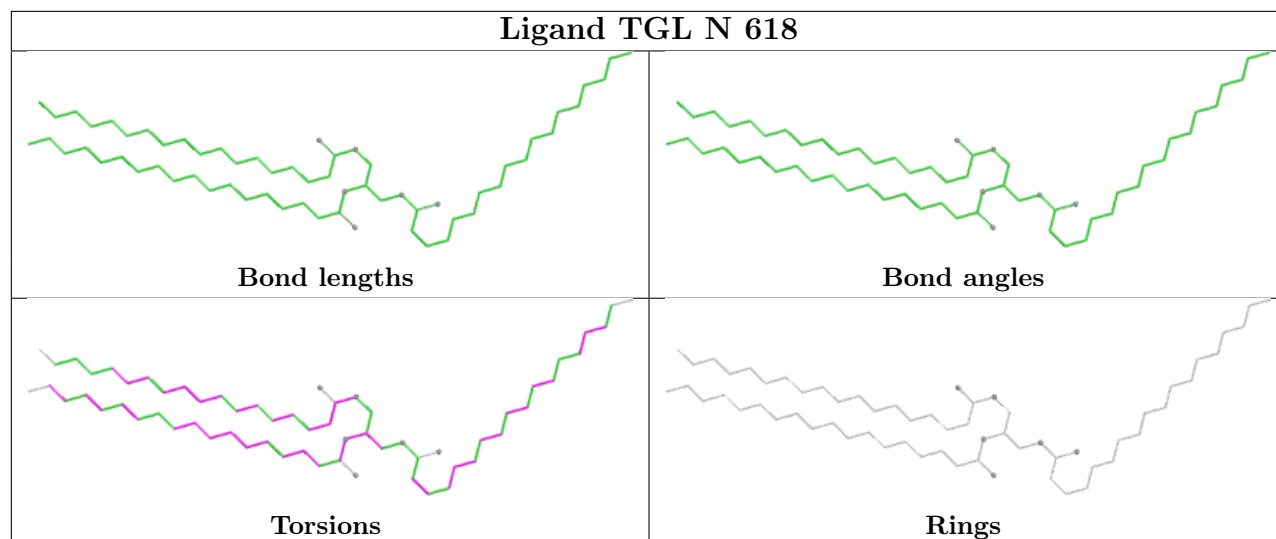


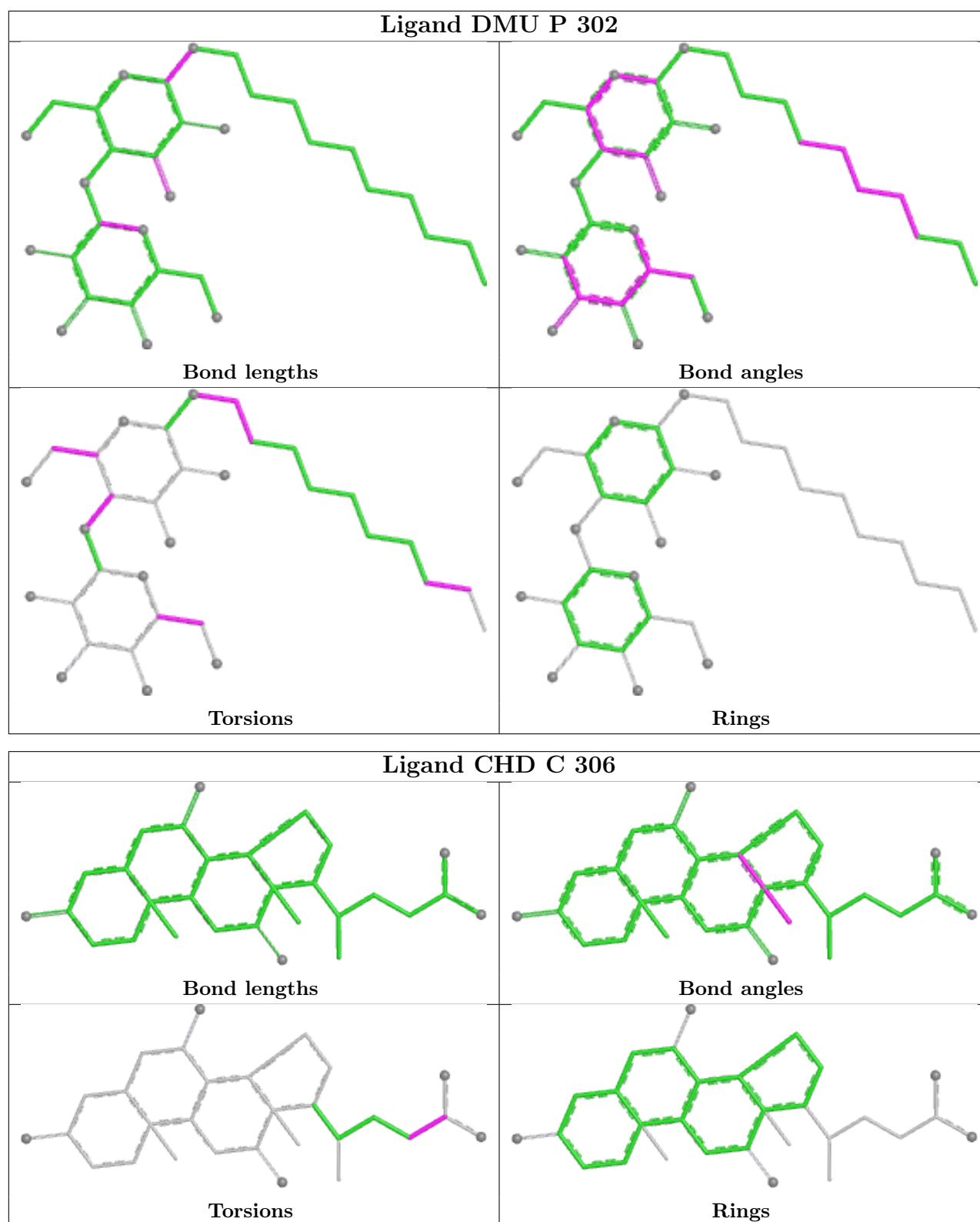


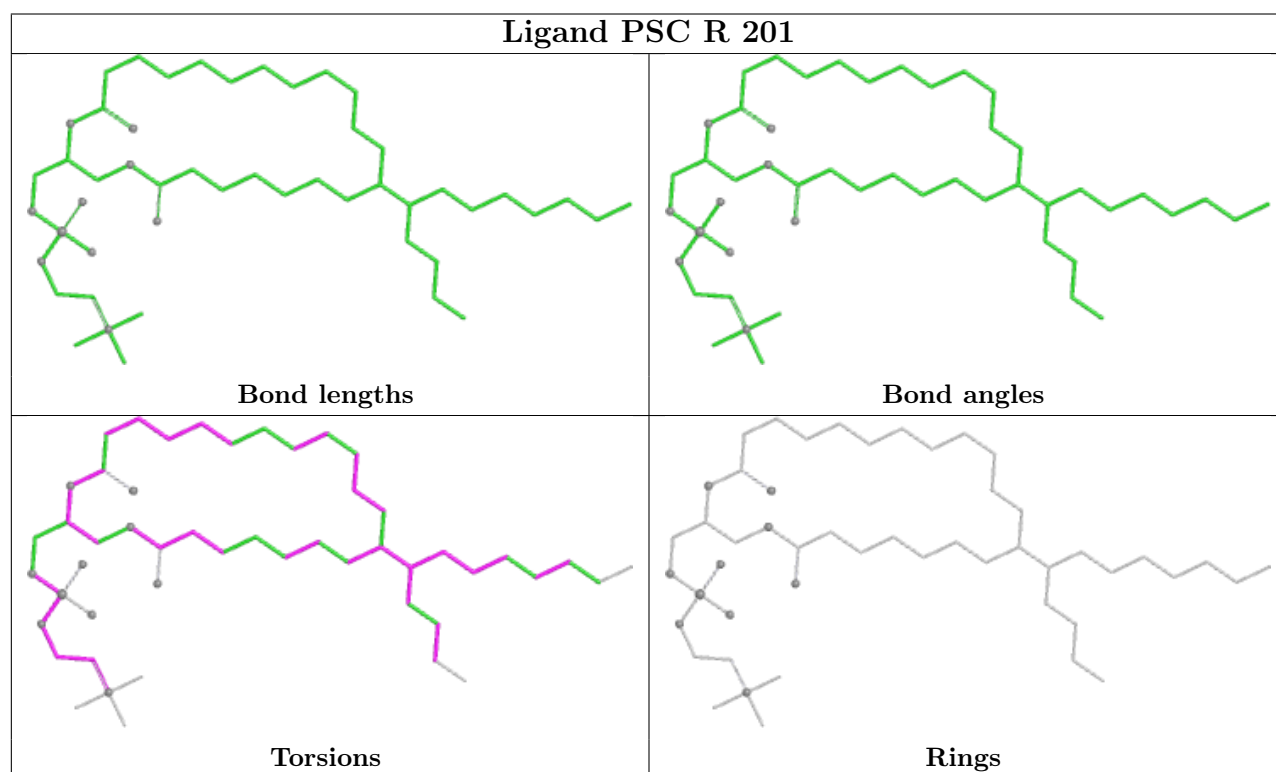
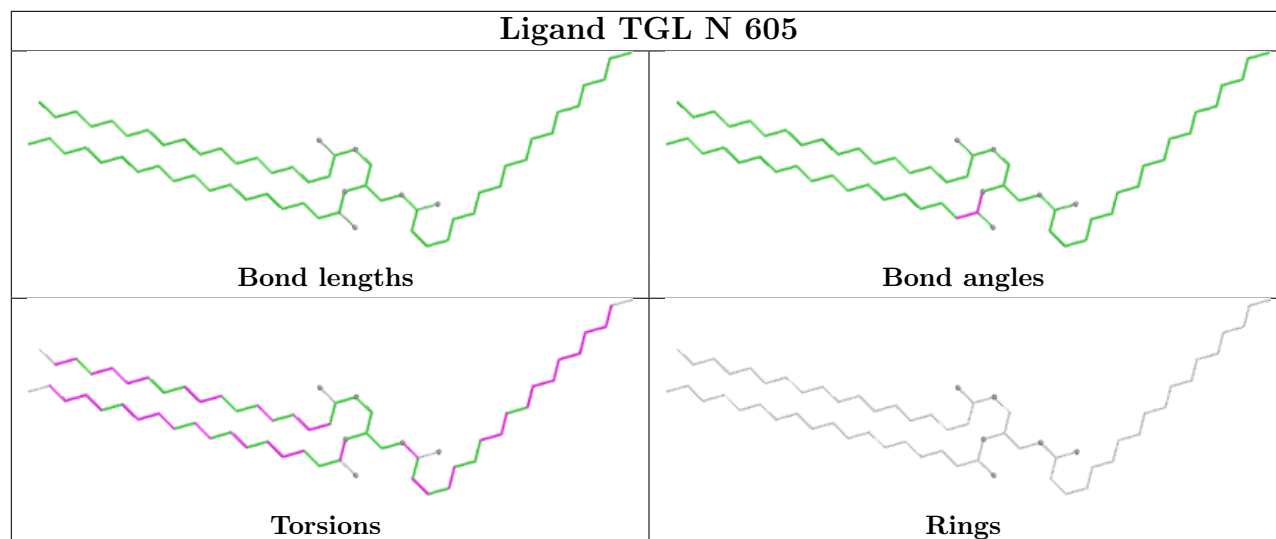


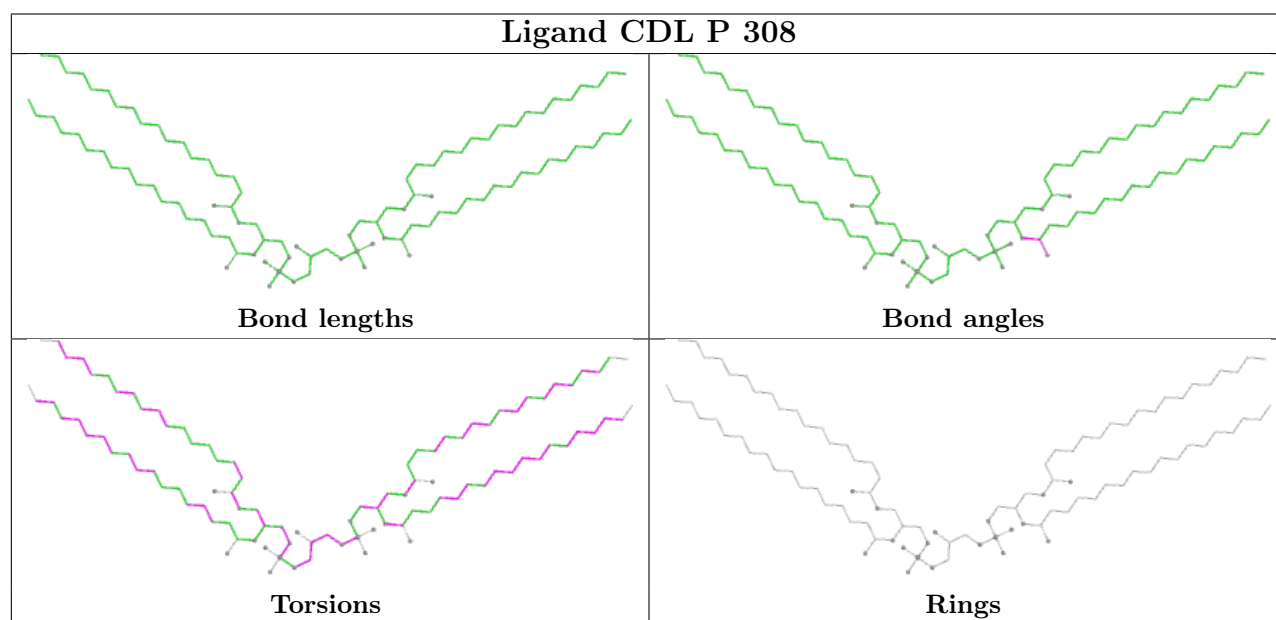
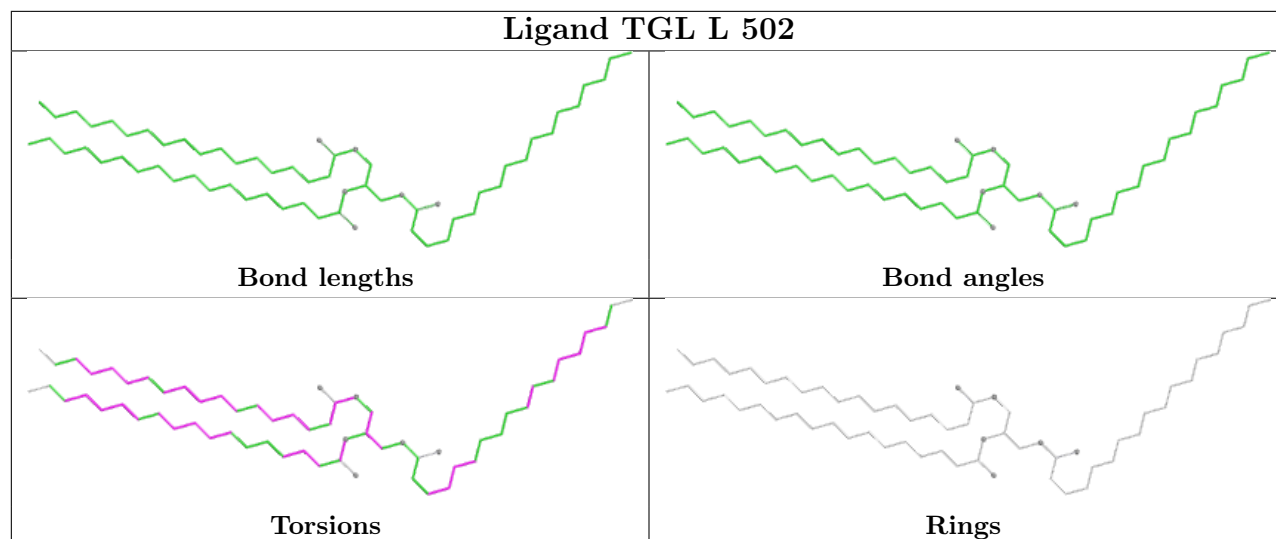


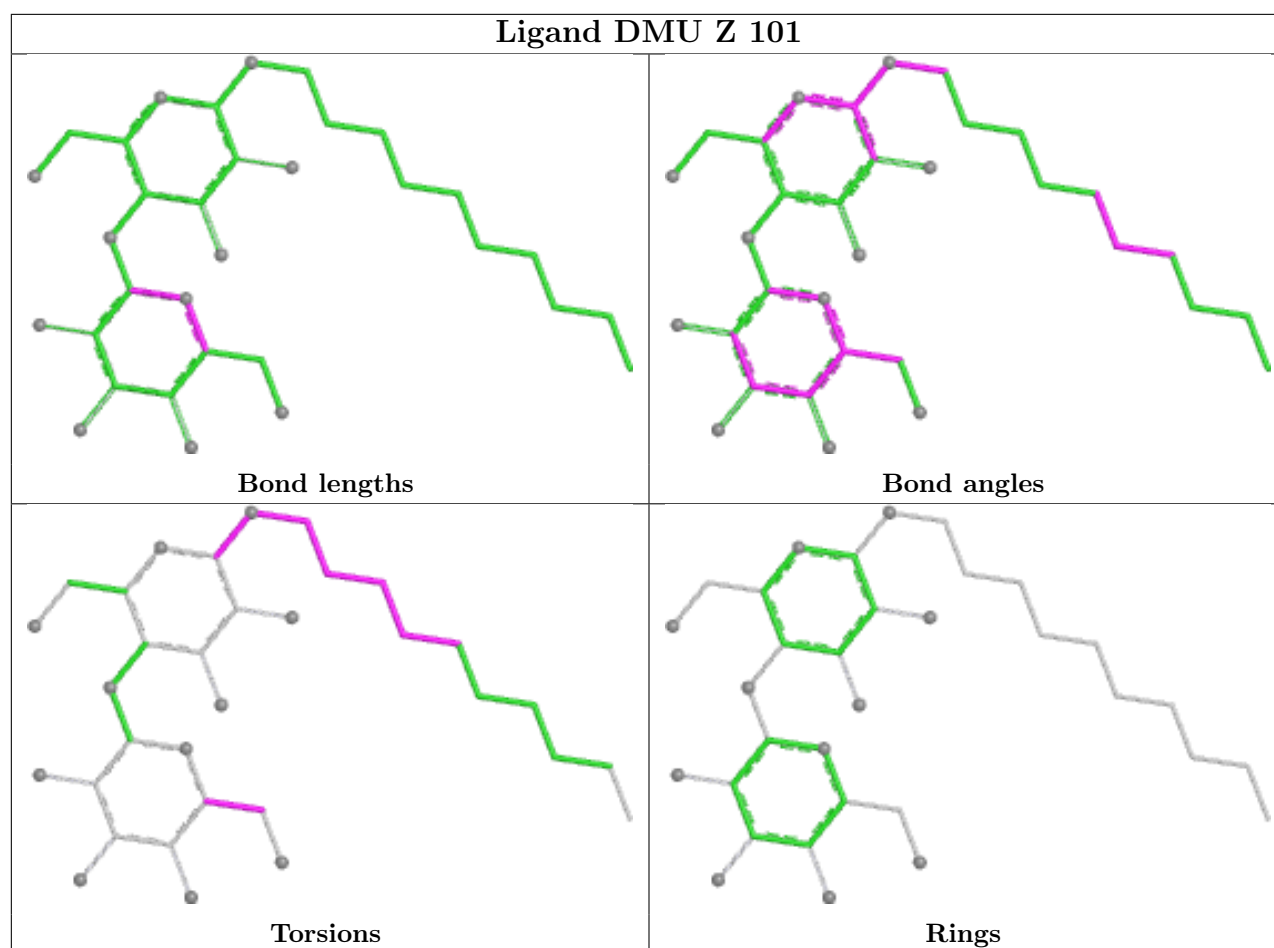




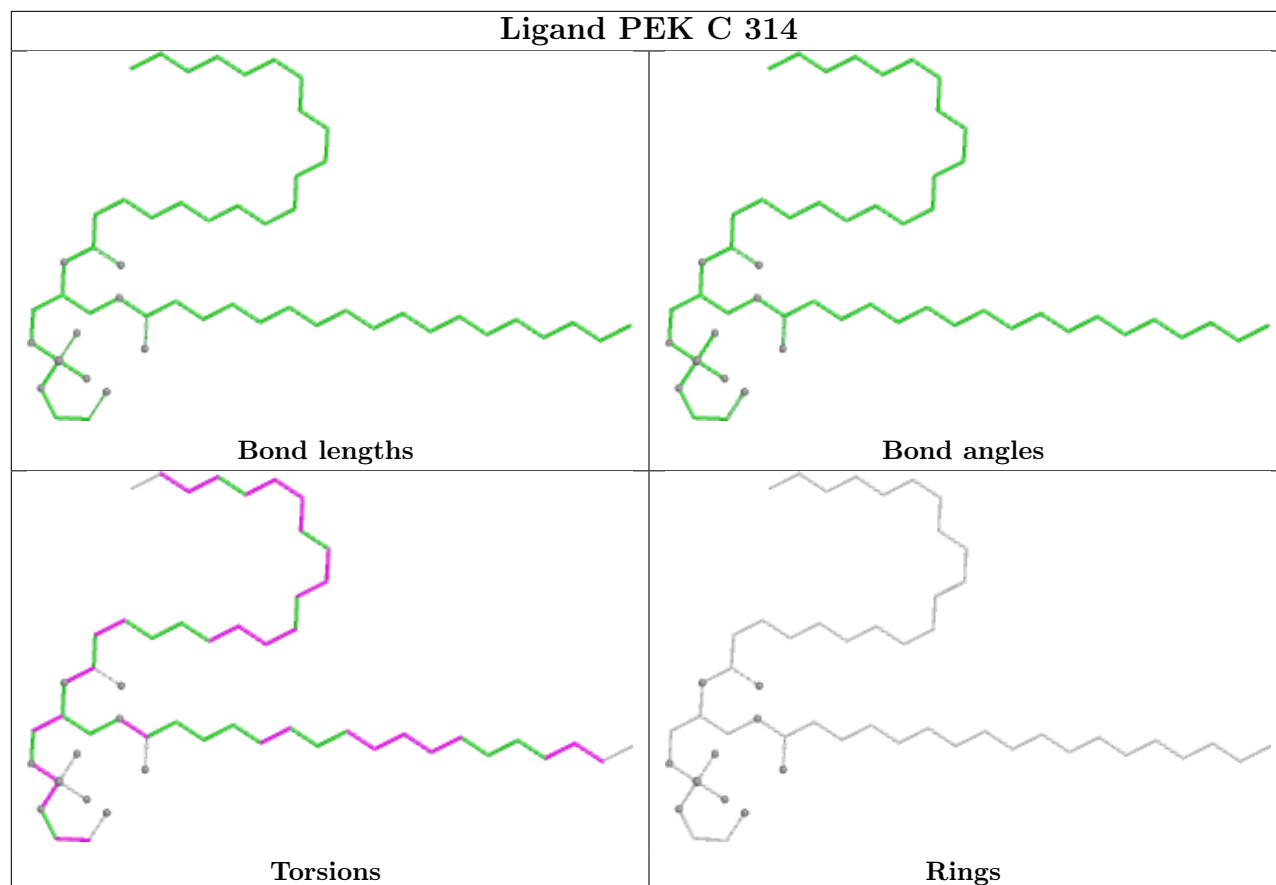




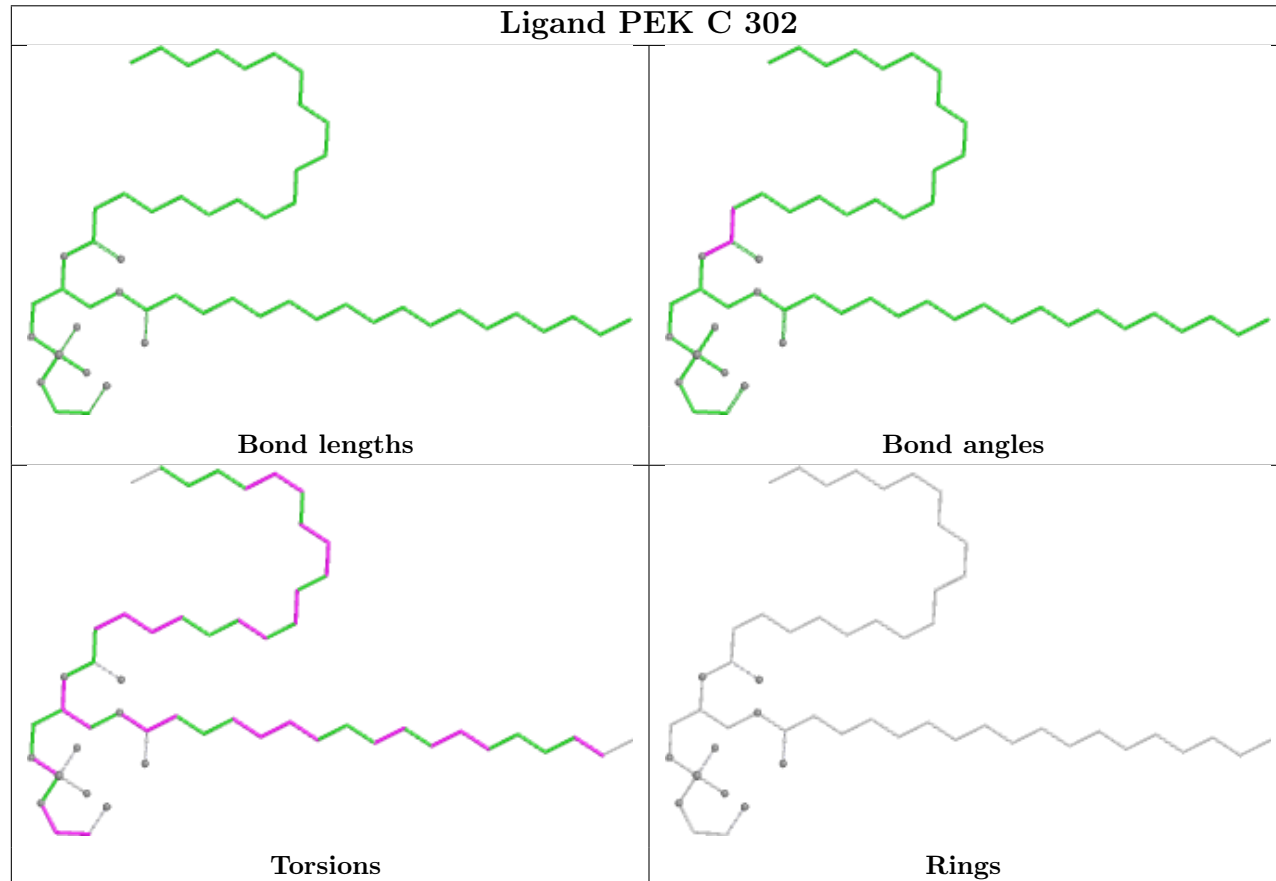


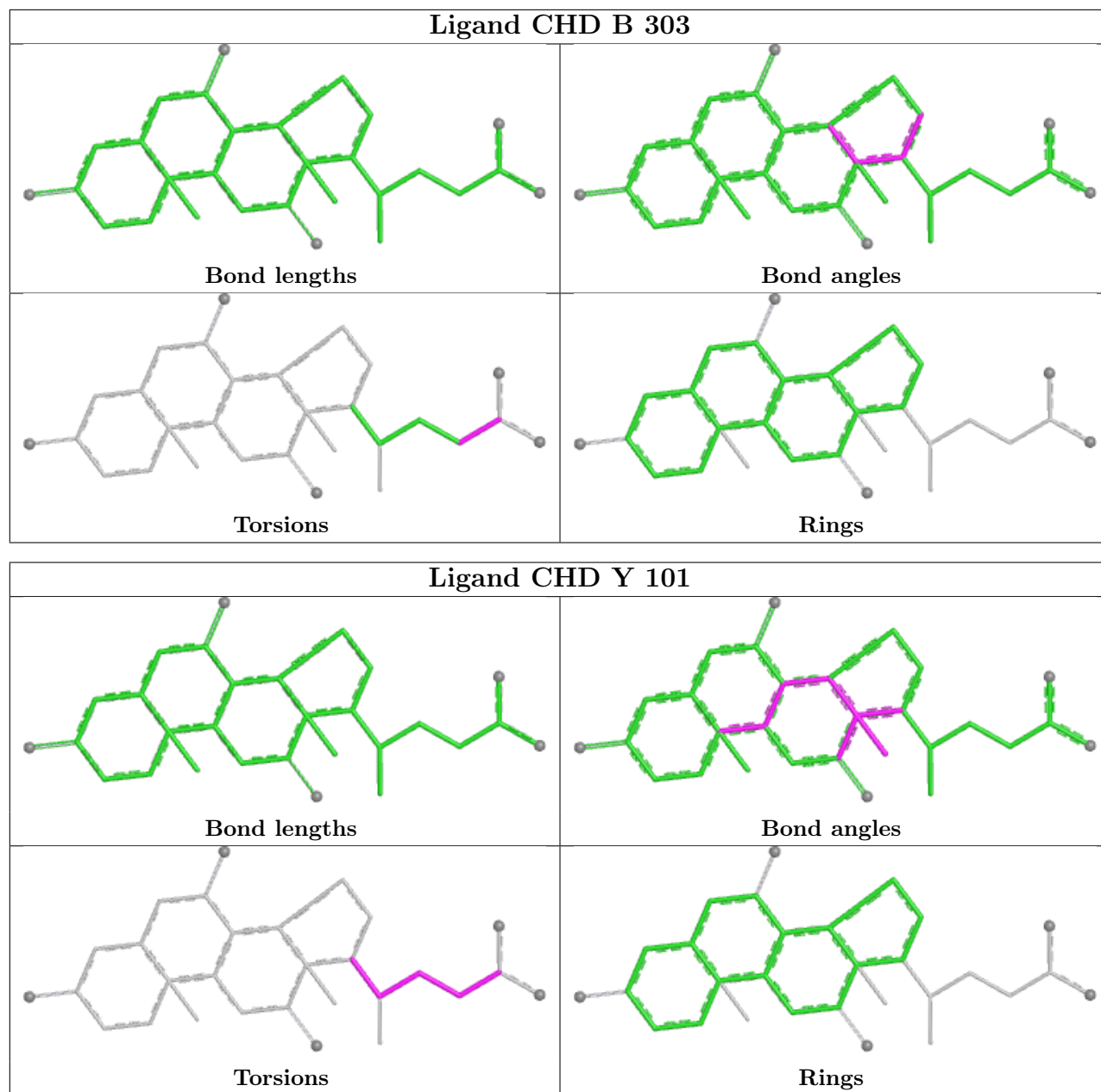


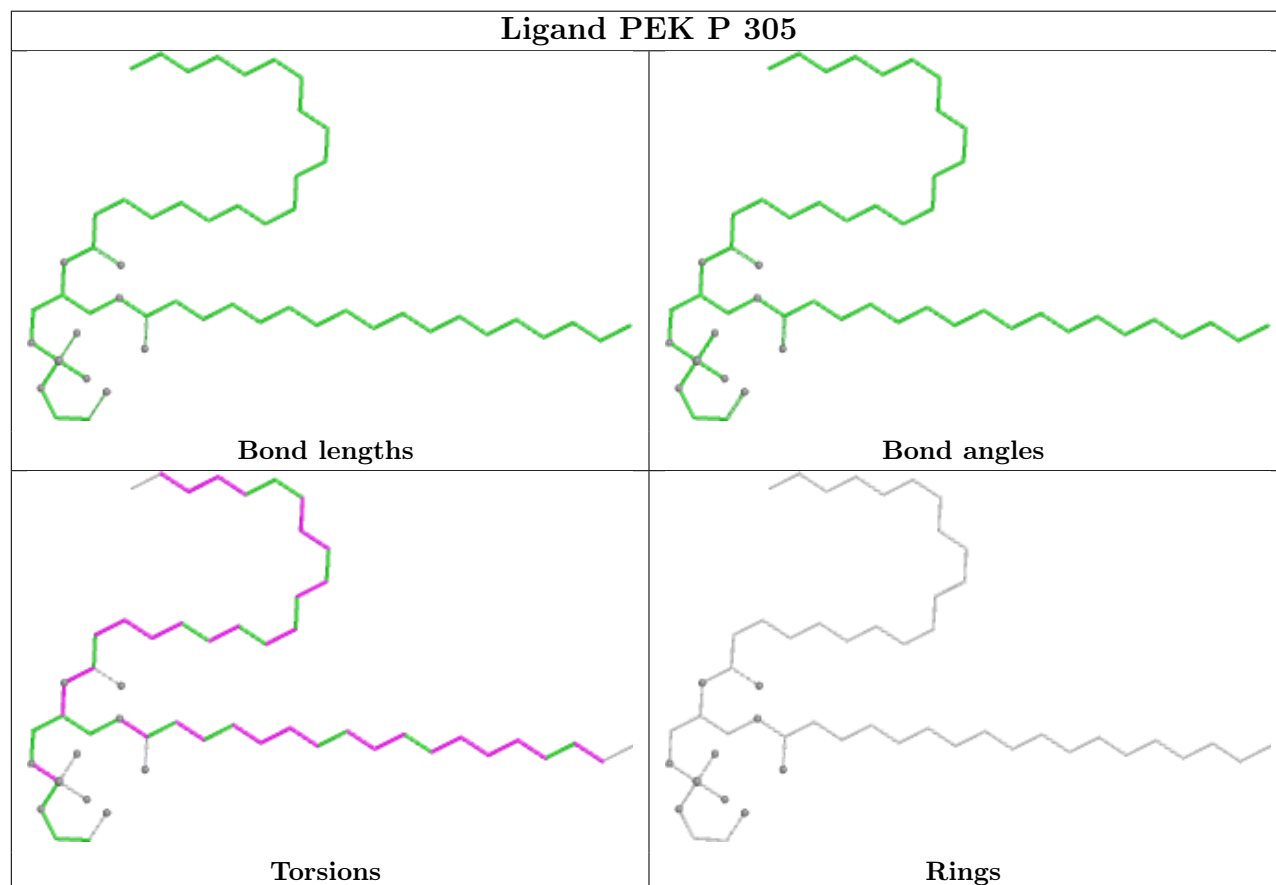
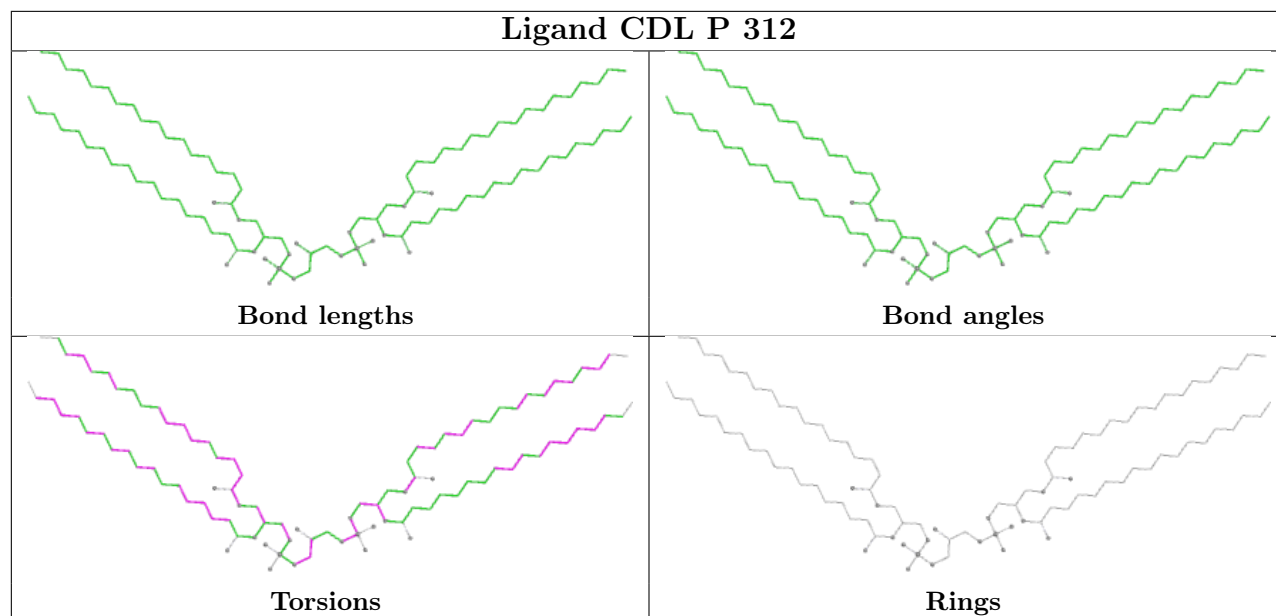
Ligand PEK C 314

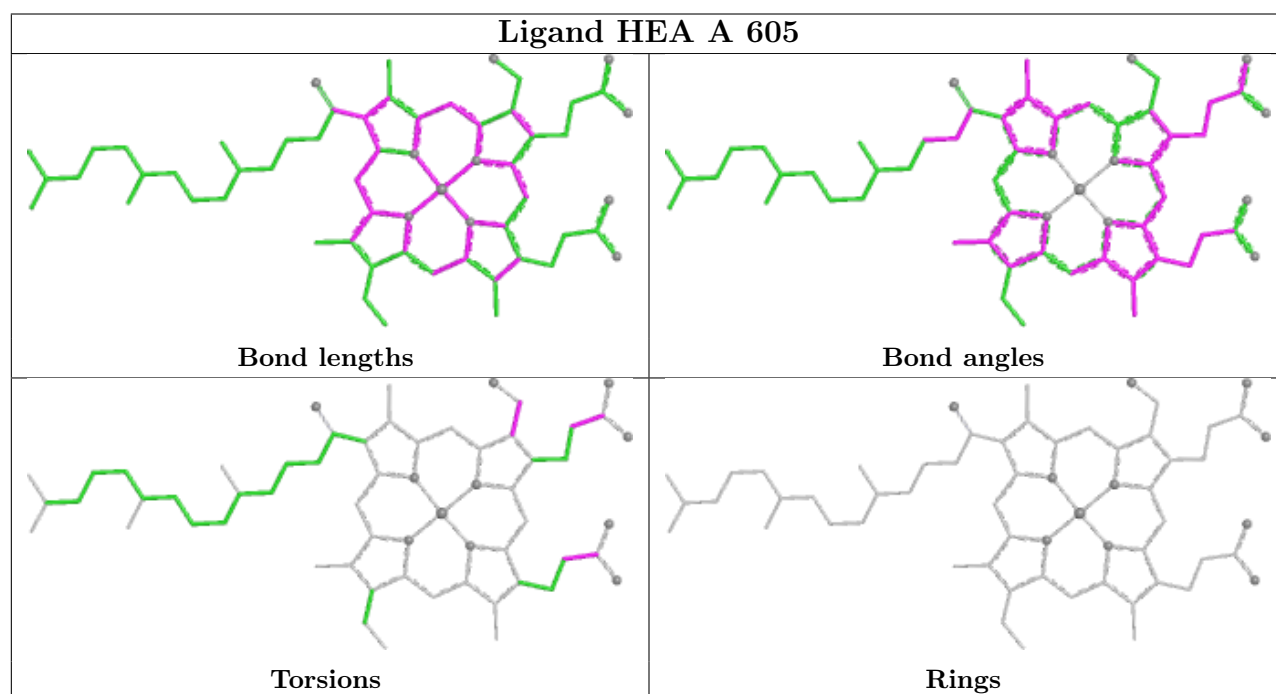
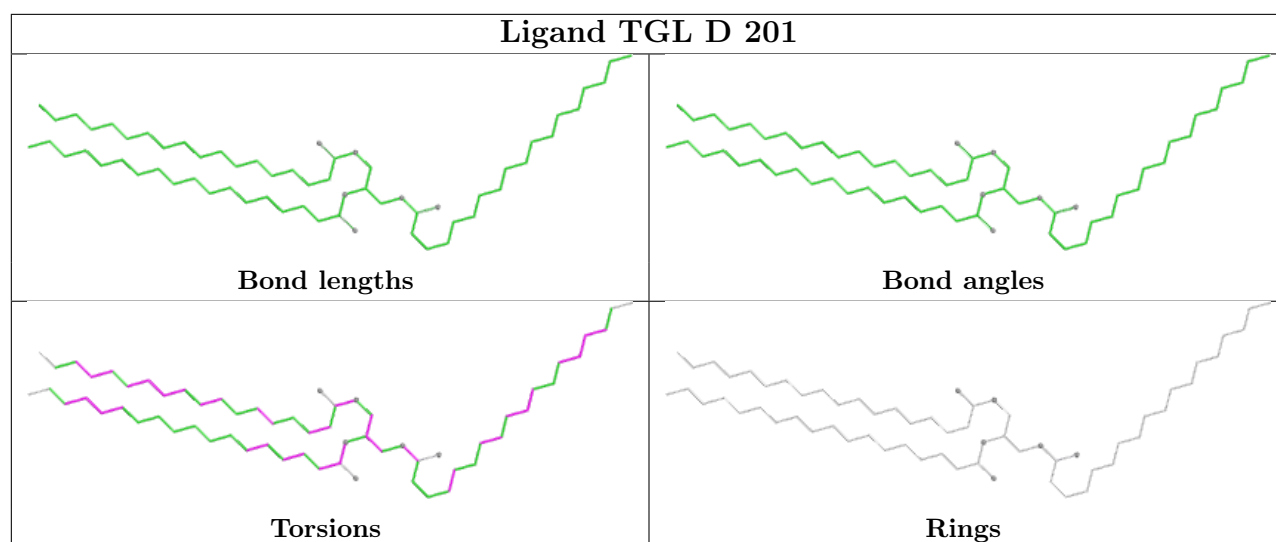


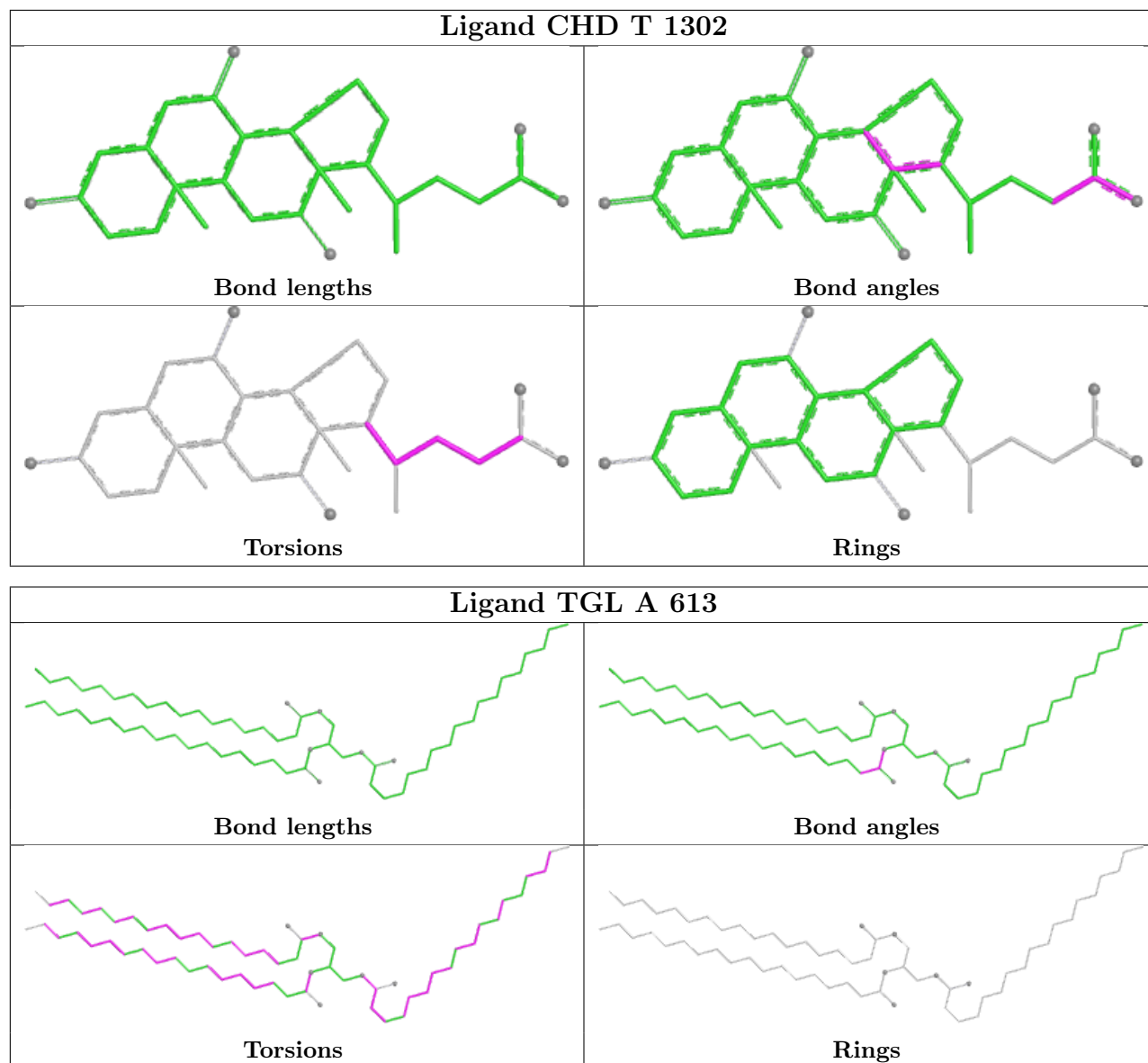
Ligand PEK C 302

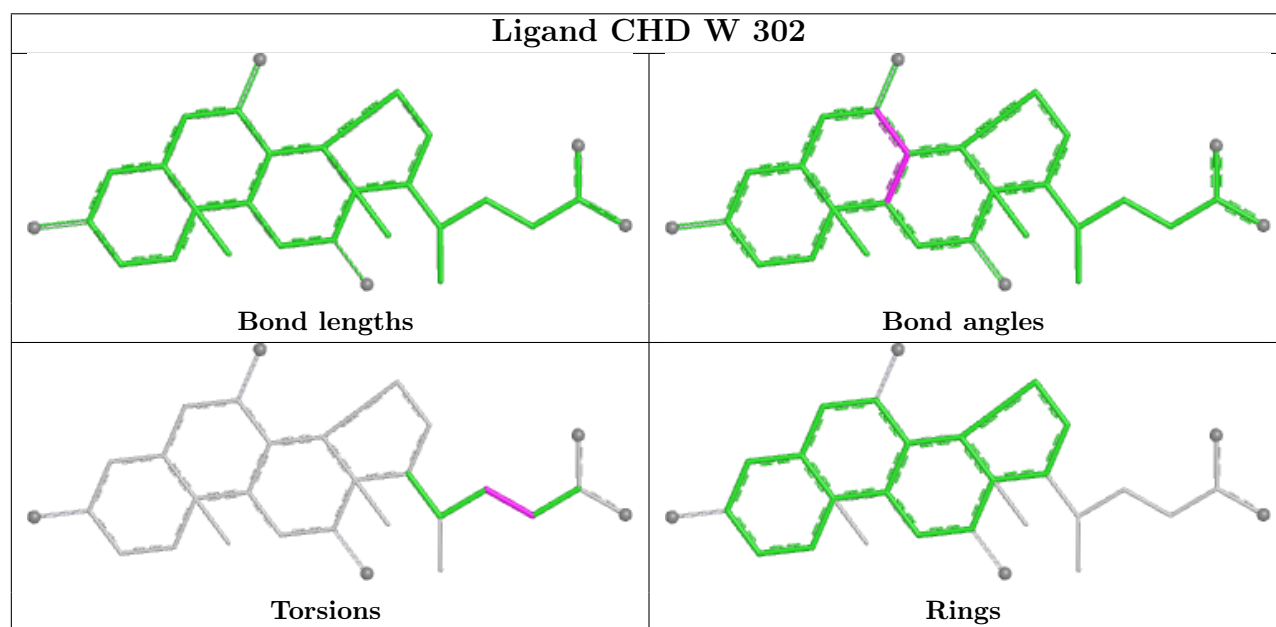
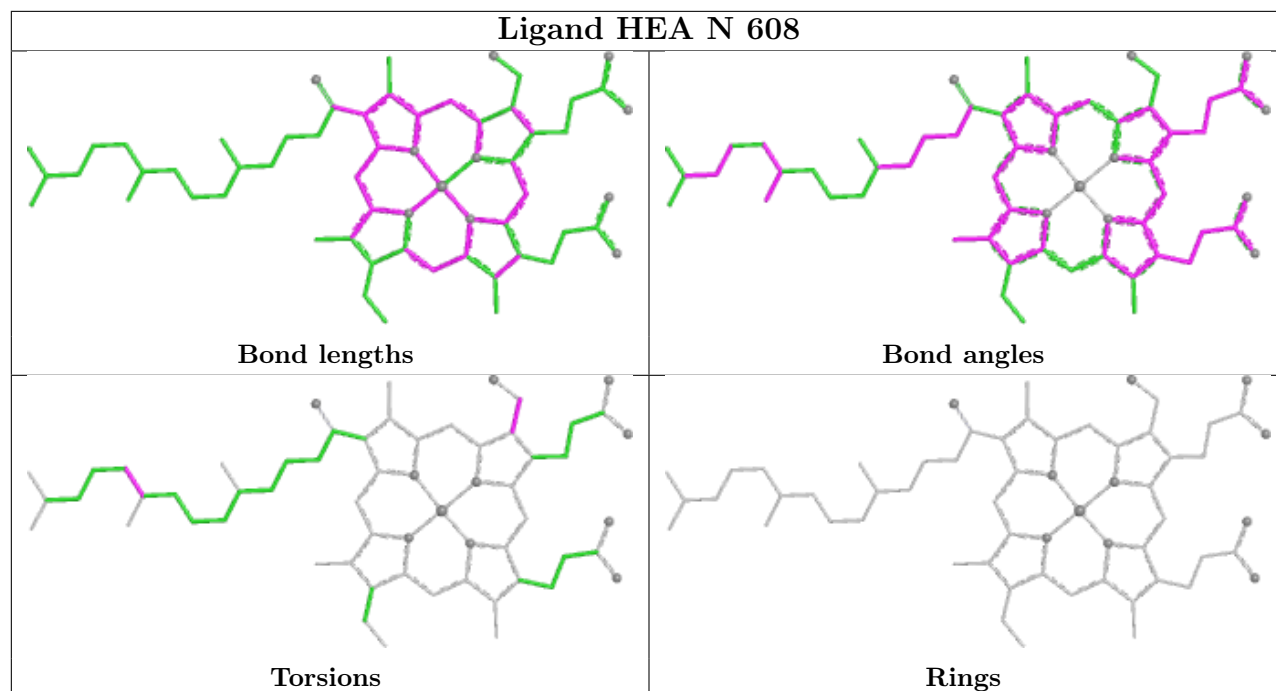


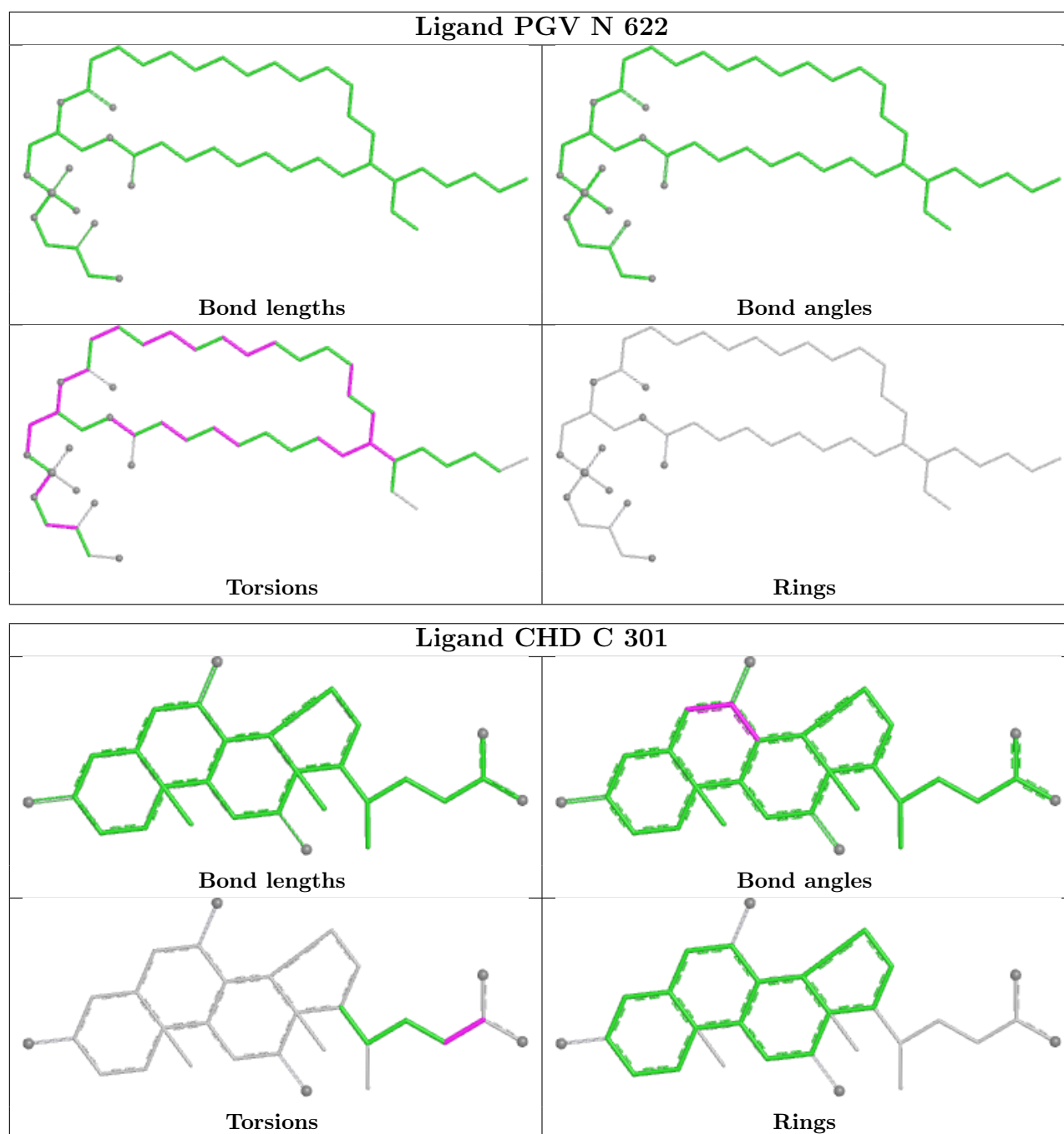












5.7 Other polymers [i](#)

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%)	-0.34	3 (0%) 85 87	23, 29, 37, 72	0
1	N	513/514 (99%)	0.07	5 (0%) 79 82	28, 35, 46, 77	0
2	B	226/227 (99%)	0.12	9 (3%) 42 45	25, 35, 57, 78	0
2	O	226/227 (99%)	0.49	17 (7%) 20 21	33, 43, 70, 90	0
3	C	259/261 (99%)	-0.14	1 (0%) 88 90	27, 33, 45, 81	0
3	P	259/261 (99%)	0.04	5 (1%) 66 70	29, 37, 51, 84	0
4	D	144/147 (97%)	0.16	3 (2%) 63 67	32, 39, 54, 80	0
4	Q	144/147 (97%)	1.21	20 (13%) 6 6	41, 55, 81, 164	0
5	E	105/109 (96%)	0.28	2 (1%) 66 70	34, 42, 67, 120	0
5	R	105/109 (96%)	0.73	4 (3%) 44 47	39, 51, 69, 119	0
6	F	98/98 (100%)	0.48	8 (8%) 17 18	30, 40, 82, 140	0
6	S	98/98 (100%)	0.64	9 (9%) 14 15	32, 44, 81, 118	0
7	G	83/85 (97%)	1.14	18 (21%) 2 2	31, 40, 110, 119	0
7	T	83/85 (97%)	1.26	17 (20%) 2 2	32, 46, 108, 117	0
8	H	79/85 (92%)	0.79	11 (13%) 6 6	31, 43, 92, 105	0
8	U	79/85 (92%)	0.98	13 (16%) 4 4	40, 49, 104, 130	0
9	I	72/73 (98%)	0.63	8 (11%) 10 11	32, 48, 69, 83	0
9	V	72/73 (98%)	0.89	6 (8%) 17 18	38, 54, 77, 100	0
10	J	58/59 (98%)	0.58	6 (10%) 12 12	33, 44, 71, 119	0
10	W	58/59 (98%)	0.96	6 (10%) 12 12	39, 50, 77, 122	0
11	K	49/56 (87%)	0.79	5 (10%) 12 12	32, 42, 59, 81	0
11	X	49/56 (87%)	1.10	5 (10%) 12 12	47, 54, 74, 111	0
12	L	46/47 (97%)	0.19	2 (4%) 40 42	30, 36, 57, 99	0
12	Y	46/47 (97%)	0.77	4 (8%) 16 17	39, 47, 75, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	0.38	2 (4%) 36 39	33, 36, 64, 99	0
13	Z	43/46 (93%)	0.92	6 (13%) 6 6	43, 50, 76, 112	0
All	All	3550/3614 (98%)	0.31	195 (5%) 30 32	23, 39, 71, 164	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	10.9
7	G	3	ALA	10.5
4	Q	5	VAL	9.4
7	T	3	ALA	8.5
7	G	5	LYS	8.2
6	F	97	ALA	7.6
6	F	96	LEU	7.4
8	U	8	ILE	7.2
7	T	1	ALA	6.8
7	G	1	ALA	6.7
7	G	36	TRP	6.2
6	S	96	LEU	6.1
4	Q	4	SER	6.1
7	G	2	SER	6.1
8	H	45	ALA	6.1
7	T	36	TRP	6.0
7	G	4	ALA	5.9
9	I	37	PHE	5.8
11	X	6	ALA	5.7
7	T	5	LYS	5.7
7	T	8	HIS	5.5
7	T	10	GLY	5.3
7	T	33	LEU	5.2
3	C	3	HIS	4.9
5	R	109	VAL	4.9
6	S	1	ALA	4.9
9	V	37	PHE	4.8
2	O	90	ILE	4.7
7	T	6	GLY	4.7
7	G	7	ASP	4.6
7	T	7	ASP	4.6
3	P	3	HIS	4.6
8	U	45	ALA	4.5
8	H	7	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
9	V	2	THR	4.5
7	T	37	LEU	4.5
7	G	9	GLY	4.4
10	W	52	TRP	4.4
12	L	2	HIS	4.4
8	H	47	GLY	4.3
2	B	90	ILE	4.2
7	G	37	LEU	4.2
7	T	4	ALA	4.1
5	E	109	VAL	4.1
8	H	48	GLY	4.0
7	G	8	HIS	4.0
7	T	2	SER	4.0
6	S	98	HIS	4.0
8	H	8	ILE	4.0
4	Q	7	LYS	3.9
6	F	2	SER	3.9
8	H	44	THR	3.9
6	S	94	HIS	3.9
10	J	1	PHE	3.9
6	S	95	GLN	3.8
7	G	10	GLY	3.8
9	V	3	ALA	3.7
2	O	113	TYR	3.6
6	S	93	PRO	3.6
1	A	298	ASP	3.6
4	Q	72	ASN	3.6
6	F	1	ALA	3.5
4	Q	8	SER	3.5
8	U	44	THR	3.5
11	K	6	ALA	3.4
10	W	1	PHE	3.4
6	S	97	ALA	3.3
12	Y	2	HIS	3.3
4	Q	48	TRP	3.3
7	G	6	GLY	3.3
7	T	84	LYS	3.3
10	W	58	LYS	3.3
10	W	48	TYR	3.2
4	Q	33	LEU	3.2
11	K	7	PRO	3.2
4	Q	46	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
2	O	227	LEU	3.2
2	O	59	GLN	3.2
2	B	113	TYR	3.1
4	Q	40	LEU	3.0
7	T	42	ARG	3.0
13	M	43	SER	3.0
6	F	98	HIS	3.0
6	F	3	GLY	3.0
7	G	84	LYS	3.0
12	Y	47	LYS	3.0
10	J	58	LYS	3.0
4	Q	35	ALA	3.0
4	Q	53	ILE	3.0
1	A	514	LYS	2.9
9	V	33	THR	2.9
4	D	4	SER	2.9
1	N	297	MET	2.9
10	J	55	PHE	2.9
5	E	5	HIS	2.9
8	U	9	LYS	2.9
2	O	57	ASP	2.9
8	H	50	VAL	2.9
7	G	38	HIS	2.9
10	J	50	LEU	2.8
2	B	65	TRP	2.8
11	X	7	PRO	2.8
11	X	13	TYR	2.8
8	U	48	GLY	2.7
2	B	87	MET	2.7
8	H	42	ALA	2.7
9	I	25	PHE	2.7
4	Q	51	LEU	2.7
7	T	38	HIS	2.7
9	I	34	PHE	2.6
11	K	26	VAL	2.6
9	I	2	THR	2.6
13	Z	43	SER	2.6
8	U	47	GLY	2.6
2	B	61	VAL	2.6
9	V	72	ALA	2.6
10	W	56	PRO	2.6
8	H	46	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	P	122	HIS	2.5
13	Z	32	TRP	2.5
8	U	7	LYS	2.5
9	V	73	LYS	2.5
5	R	5	HIS	2.5
2	O	218	TYR	2.5
2	O	116	LEU	2.5
7	G	35	SER	2.5
8	U	50	VAL	2.5
7	G	33	LEU	2.5
8	U	10	ASN	2.5
4	D	19	ARG	2.5
11	K	20	SER	2.5
1	N	125	GLY	2.4
1	N	136	LEU	2.4
12	Y	24	MET	2.4
12	L	47	LYS	2.4
3	P	258	TRP	2.4
2	O	87	MET	2.4
1	N	514	LYS	2.4
4	Q	57	VAL	2.4
8	U	55	TRP	2.4
2	B	91	ASN	2.4
2	B	92	ASN	2.4
5	R	108	LYS	2.4
8	U	42	ALA	2.4
6	F	95	GLN	2.4
2	O	92	ASN	2.4
7	G	34	ASN	2.4
4	Q	59	LEU	2.3
2	B	32	PHE	2.3
9	I	26	MET	2.3
6	S	43	LYS	2.3
11	K	54	ARG	2.3
1	N	113	LEU	2.3
4	D	51	LEU	2.3
5	R	39	TYR	2.3
13	Z	1	ILE	2.3
8	H	9	LYS	2.3
8	U	46	LYS	2.3
11	X	51	LYS	2.3
2	O	65	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
7	T	35	SER	2.3
2	O	61	VAL	2.3
2	O	60	GLU	2.2
6	F	94	HIS	2.2
13	Z	42	LYS	2.2
7	T	9	GLY	2.2
13	Z	40	TYR	2.2
1	A	297	MET	2.2
4	Q	9	GLU	2.2
4	Q	27	VAL	2.2
2	B	88	ASP	2.2
4	Q	39	ALA	2.2
2	O	221	LYS	2.2
10	J	57	HIS	2.1
3	P	37	PHE	2.1
2	O	16	ILE	2.1
11	X	30	VAL	2.1
10	J	51	GLY	2.1
2	O	86	MET	2.1
13	Z	2	THR	2.1
6	S	37	LYS	2.1
8	U	61	LYS	2.1
13	M	39	ASN	2.1
2	O	32	PHE	2.1
9	I	15	ARG	2.1
4	Q	78	TRP	2.1
12	Y	44	LEU	2.1
9	I	3	ALA	2.1
10	W	57	HIS	2.0
8	H	84	LYS	2.0
4	Q	89	ILE	2.0
9	I	33	THR	2.0
2	O	91	ASN	2.0
3	P	38	ASN	2.0
7	G	45	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	TPO	G	11	11/12	0.67	0.22	45,80,126,126	0
7	TPO	T	11	11/12	0.70	0.19	42,81,138,146	0
1	FME	A	1	10/11	0.91	0.14	43,47,72,89	0
1	FME	N	1	10/11	0.95	0.12	51,56,89,89	0
2	FME	O	1	10/11	0.96	0.10	37,42,53,65	0
2	FME	B	1	10/11	0.97	0.09	31,34,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CHD	Y	101	29/29	0.59	0.28	91,127,145,177	0
29	SAC	V	101	9/10	0.59	0.18	95,103,113,114	0
24	CHD	T	1302	29/29	0.61	0.31	97,136,151,152	0
29	SAC	I	101	9/10	0.65	0.21	81,96,103,109	0
27	DMU	G	101	33/33	0.67	0.23	79,121,140,147	0
23	PSC	B	302	52/52	0.71	0.27	47,82,154,167	0
26	CDL	C	310	100/100	0.72	0.31	65,91,146,163	0
25	PEK	C	314	53/53	0.74	0.28	59,83,139,159	0
25	PEK	C	302	53/53	0.75	0.27	65,84,142,176	0
19	EDO	A	618	4/4	0.75	0.24	58,69,77,79	0
17	PGV	C	304	51/51	0.75	0.28	43,82,124,144	0
17	PGV	N	622	51/51	0.76	0.27	54,89,159,169	0
19	EDO	A	610	4/4	0.76	0.26	56,65,66,69	0
25	PEK	P	301	53/53	0.77	0.24	55,83,136,152	0
19	EDO	N	614	4/4	0.78	0.25	55,67,68,76	0
20	TGL	A	613	63/63	0.78	0.30	51,74,117,120	0
19	EDO	G	105	4/4	0.78	0.20	75,75,80,101	0
27	DMU	P	302	33/33	0.79	0.16	59,101,117,119	0
26	CDL	P	312	100/100	0.79	0.28	68,96,141,163	0
23	PSC	R	201	52/52	0.79	0.27	44,100,157,168	0
17	PGV	P	307	51/51	0.80	0.27	64,96,123,143	0
25	PEK	P	305	53/53	0.80	0.26	52,87,152,165	0
17	PGV	M	101	51/51	0.80	0.26	48,92,149,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	TGL	N	604	63/63	0.80	0.28	58,83,114,119	0
27	DMU	G	104	33/33	0.81	0.20	64,106,127,137	0
19	EDO	N	615	4/4	0.81	0.24	55,59,61,74	0
19	EDO	F	702	4/4	0.81	0.21	57,69,73,86	0
20	TGL	D	201	63/63	0.81	0.26	49,79,97,114	0
19	EDO	R	203	4/4	0.82	0.20	64,68,71,77	0
19	EDO	T	1301	4/4	0.82	0.21	56,59,64,66	0
19	EDO	W	303	4/4	0.82	0.15	90,96,96,99	0
19	EDO	L	504	4/4	0.82	0.17	55,63,64,66	0
27	DMU	C	311	33/33	0.82	0.16	60,85,105,107	0
19	EDO	B	307	4/4	0.83	0.23	58,67,71,76	0
19	EDO	Q	1604	4/4	0.83	0.24	59,70,72,89	0
19	EDO	N	612	4/4	0.83	0.22	59,63,65,74	0
19	EDO	J	102	4/4	0.83	0.15	73,74,74,78	0
26	CDL	P	308	100/100	0.84	0.23	48,88,121,129	0
19	EDO	U	1501	4/4	0.84	0.19	57,60,62,68	0
19	EDO	H	101	4/4	0.85	0.16	66,68,68,77	0
19	EDO	D	202	4/4	0.85	0.15	60,61,70,75	0
26	CDL	C	305	100/100	0.85	0.23	45,82,118,125	0
20	TGL	N	618	63/63	0.85	0.24	64,82,103,110	0
19	EDO	B	310	4/4	0.86	0.20	55,64,65,74	0
20	TGL	N	605	63/63	0.86	0.23	52,72,118,136	0
19	EDO	D	205	4/4	0.86	0.16	60,70,70,78	0
19	EDO	V	103	4/4	0.86	0.17	75,79,82,83	0
19	EDO	B	311	4/4	0.86	0.16	65,71,77,89	0
19	EDO	S	103	4/4	0.86	0.20	53,66,68,69	0
19	EDO	S	104	4/4	0.86	0.16	52,55,59,61	0
19	EDO	G	108	4/4	0.87	0.19	90,90,94,98	0
27	DMU	Z	101	33/33	0.87	0.14	58,69,87,94	0
19	EDO	Q	1603	4/4	0.87	0.16	72,72,77,81	0
20	TGL	L	502	63/63	0.87	0.21	45,65,91,99	0
19	EDO	G	106	4/4	0.88	0.17	65,65,65,69	0
19	EDO	L	503	4/4	0.88	0.15	58,63,64,71	0
19	EDO	S	106	4/4	0.88	0.16	65,68,69,75	0
19	EDO	I	102	4/4	0.88	0.15	74,76,76,80	0
19	EDO	B	308	4/4	0.89	0.18	50,57,66,69	0
19	EDO	V	104	4/4	0.89	0.18	51,65,68,72	0
19	EDO	P	314	4/4	0.89	0.18	70,71,74,81	0
19	EDO	E	203	4/4	0.89	0.15	63,70,73,77	0
19	EDO	A	611	4/4	0.89	0.18	49,55,61,69	0
24	CHD	J	101	29/29	0.89	0.12	56,70,84,95	0
24	CHD	P	309	29/29	0.89	0.12	51,60,67,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	J	103	4/4	0.89	0.13	57,60,62,63	0
19	EDO	E	204	4/4	0.90	0.18	72,74,78,81	0
19	EDO	S	105	4/4	0.90	0.15	44,58,64,69	0
19	EDO	C	312	4/4	0.90	0.17	52,55,57,62	0
19	EDO	C	313	4/4	0.90	0.14	58,60,62,71	0
19	EDO	A	614	4/4	0.90	0.17	42,59,61,65	0
19	EDO	V	102	4/4	0.90	0.20	69,70,71,77	0
19	EDO	B	305	4/4	0.90	0.18	50,57,64,68	0
19	EDO	A	616	4/4	0.90	0.16	53,61,63,72	0
19	EDO	N	613	4/4	0.90	0.18	65,67,75,77	0
19	EDO	N	621	4/4	0.91	0.15	57,60,61,70	0
19	EDO	O	302	4/4	0.91	0.15	62,71,72,86	0
19	EDO	P	311	4/4	0.91	0.15	55,68,74,84	0
19	EDO	C	308	4/4	0.91	0.15	71,72,73,76	0
24	CHD	W	302	29/29	0.91	0.12	61,76,89,94	0
19	EDO	C	309	4/4	0.91	0.14	73,74,77,78	0
19	EDO	N	620	4/4	0.91	0.15	45,56,59,69	0
19	EDO	A	609	4/4	0.92	0.14	34,36,42,43	0
19	EDO	P	310	4/4	0.92	0.13	73,73,73,75	0
19	EDO	F	704	4/4	0.92	0.15	56,56,59,63	0
19	EDO	I	103	4/4	0.92	0.16	58,60,62,67	0
19	EDO	B	309	4/4	0.92	0.16	62,68,69,74	0
19	EDO	A	612	4/4	0.92	0.17	55,56,59,61	0
19	EDO	L	501	4/4	0.92	0.13	49,62,63,65	0
19	EDO	A	617	4/4	0.92	0.16	56,59,61,63	0
19	EDO	W	301	4/4	0.92	0.19	55,71,76,82	0
24	CHD	C	306	29/29	0.92	0.11	46,55,60,61	0
19	EDO	N	616	4/4	0.93	0.14	47,55,60,62	0
19	EDO	D	204	4/4	0.93	0.16	63,65,71,78	0
19	EDO	R	202	4/4	0.93	0.10	49,50,51,51	0
19	EDO	M	103	4/4	0.93	0.14	65,68,69,69	0
19	EDO	A	615	4/4	0.93	0.18	50,56,58,64	0
19	EDO	O	303	4/4	0.93	0.15	39,40,42,43	0
19	EDO	D	203	4/4	0.93	0.11	53,62,67,70	0
19	EDO	F	706	4/4	0.93	0.10	39,43,48,49	0
27	DMU	M	102	33/33	0.93	0.10	43,52,65,81	0
19	EDO	S	107	4/4	0.93	0.13	49,54,60,61	0
19	EDO	P	313	4/4	0.93	0.11	37,46,48,53	0
19	EDO	F	707	4/4	0.93	0.16	49,61,64,65	0
25	PEK	P	304	53/53	0.93	0.17	36,57,87,100	0
25	PEK	G	102	53/53	0.94	0.14	31,53,79,97	0
19	EDO	Q	1602	4/4	0.94	0.14	70,73,76,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
19	EDO	K	201	4/4	0.94	0.12	61,64,65,71	0
19	EDO	Q	1601	4/4	0.94	0.12	44,57,57,59	0
17	PGV	N	606	51/51	0.95	0.14	31,50,77,82	0
19	EDO	E	205	4/4	0.95	0.13	56,62,65,65	0
19	EDO	A	607	4/4	0.95	0.12	42,48,54,55	0
19	EDO	C	307	4/4	0.95	0.10	39,42,46,47	0
19	EDO	N	617	4/4	0.95	0.14	44,61,71,80	0
19	EDO	N	619	4/4	0.95	0.12	48,52,56,61	0
19	EDO	N	611	4/4	0.95	0.13	51,52,53,54	0
17	PGV	A	604	51/51	0.95	0.12	26,42,71,76	0
19	EDO	E	202	4/4	0.96	0.09	43,47,52,53	0
19	EDO	N	609	4/4	0.96	0.09	36,37,38,41	0
19	EDO	B	306	4/4	0.96	0.08	37,42,49,51	0
17	PGV	P	306	51/51	0.96	0.12	29,45,86,96	0
19	EDO	A	608	4/4	0.96	0.08	28,28,28,29	0
19	EDO	E	201	4/4	0.96	0.09	47,48,49,50	0
19	EDO	T	1303	4/4	0.96	0.10	36,40,43,44	0
24	CHD	C	301	29/29	0.96	0.07	29,33,39,42	0
17	PGV	C	303	51/51	0.97	0.12	26,39,103,112	0
24	CHD	P	303	29/29	0.97	0.06	33,36,42,43	0
19	EDO	S	102	4/4	0.97	0.08	31,32,33,36	0
19	EDO	F	701	4/4	0.97	0.08	38,39,41,42	0
24	CHD	B	303	29/29	0.97	0.07	30,34,41,46	0
19	EDO	N	610	4/4	0.97	0.08	36,40,43,43	0
15	MG	N	602	1/1	0.97	0.05	35,35,35,35	0
24	CHD	G	107	29/29	0.97	0.06	31,35,39,42	0
18	HEA	N	608	60/60	0.98	0.08	27,33,49,63	0
16	NA	N	603	1/1	0.98	0.05	40,40,40,40	0
19	EDO	G	103	4/4	0.98	0.06	33,34,41,43	0
18	HEA	N	607	60/60	0.98	0.06	25,29,36,43	0
19	EDO	B	304	4/4	0.98	0.08	27,29,30,34	0
19	EDO	F	705	4/4	0.98	0.09	28,30,30,31	0
15	MG	A	602	1/1	0.99	0.03	28,28,28,28	0
18	HEA	A	605	60/60	0.99	0.05	21,26,32,37	0
21	OH	A	619	1/1	0.99	0.08	24,24,24,24	0
21	OH	N	623	1/1	0.99	0.10	31,31,31,31	0
22	CUA	O	301	2/2	0.99	0.02	34,34,34,35	0
28	ZN	F	703	1/1	0.99	0.04	34,34,34,34	0
18	HEA	A	606	60/60	0.99	0.07	20,26,54,64	0
16	NA	A	603	1/1	0.99	0.08	25,25,25,25	0
22	CUA	B	301	2/2	1.00	0.01	26,26,26,26	0
28	ZN	S	101	1/1	1.00	0.02	38,38,38,38	0

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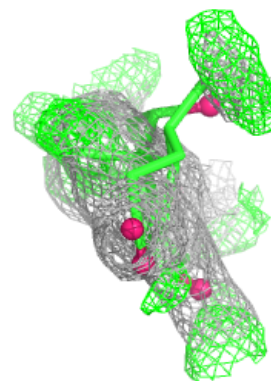
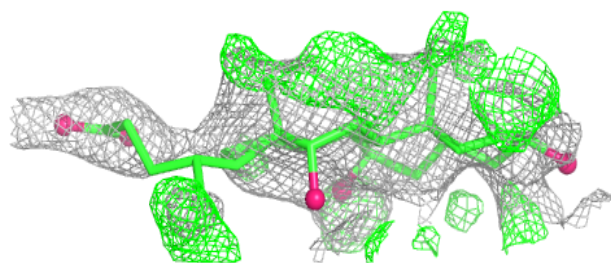
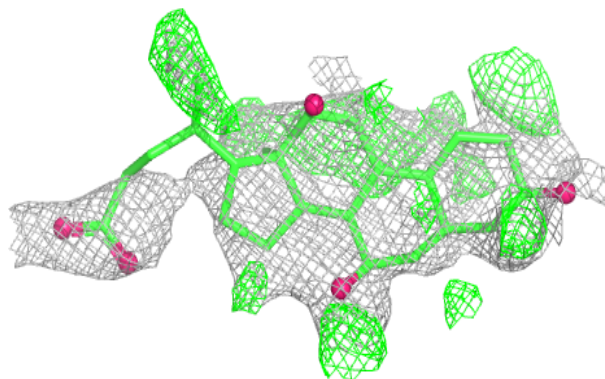
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	CU	N	601	1/1	1.00	0.02	34,34,34,34	0
14	CU	A	601	1/1	1.00	0.01	28,28,28,28	0

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

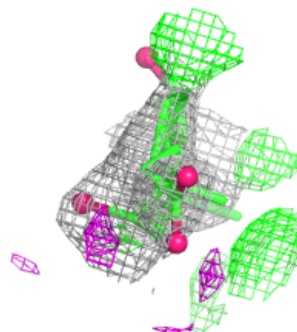
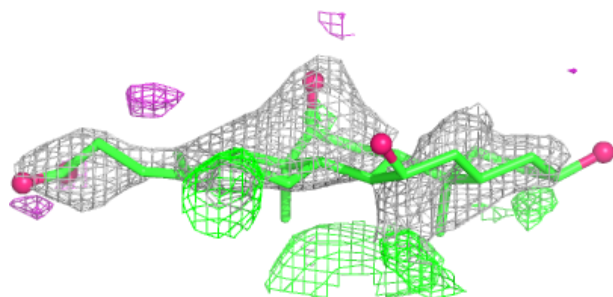
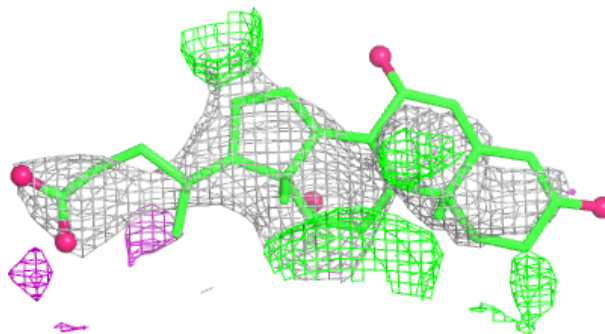
Electron density around CHD Y 101:

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

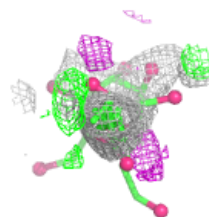
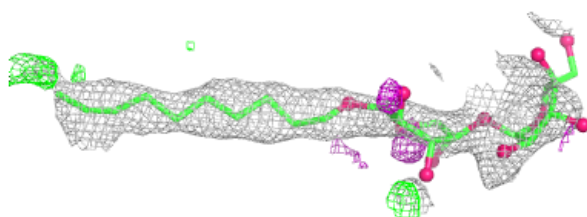
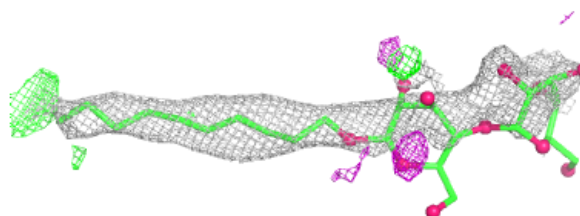


Electron density around CHD T 1302:

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

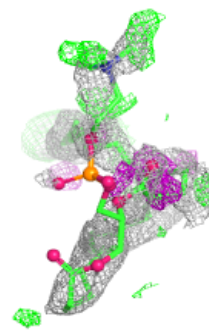
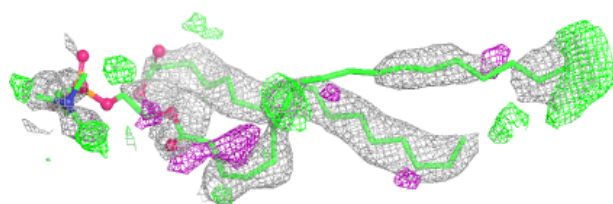
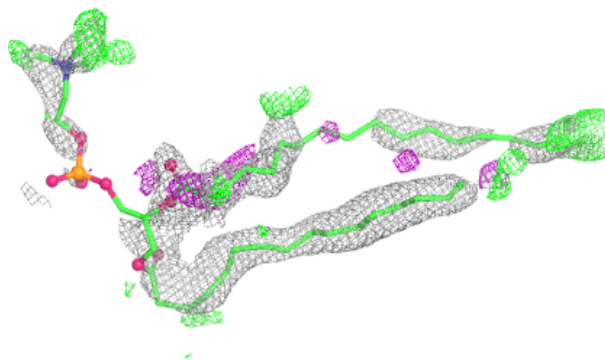
**Electron density around DMU G 101:**

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

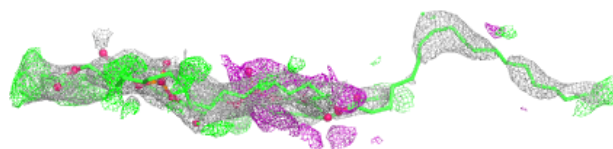
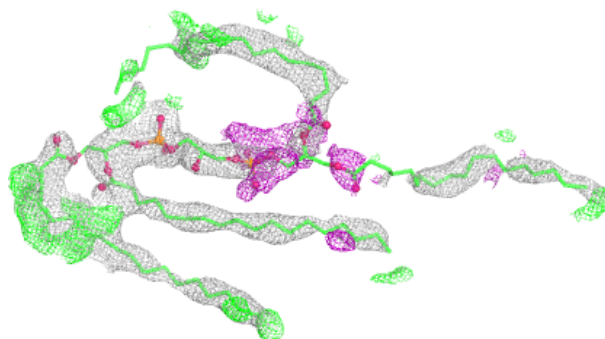


Electron density around PSC B 302:

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

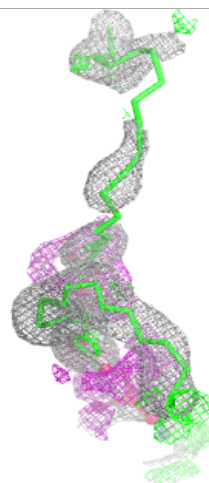
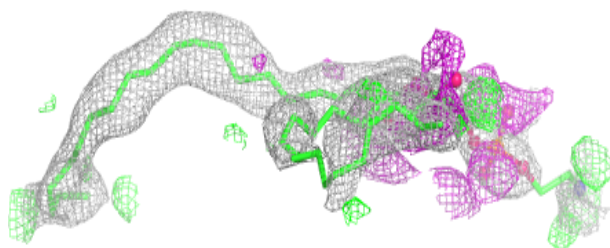
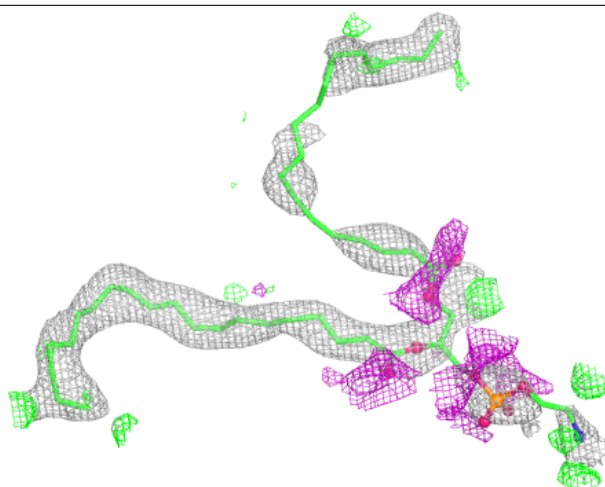
**Electron density around CDL C 310:**

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



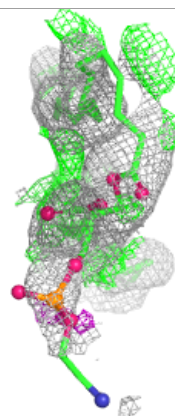
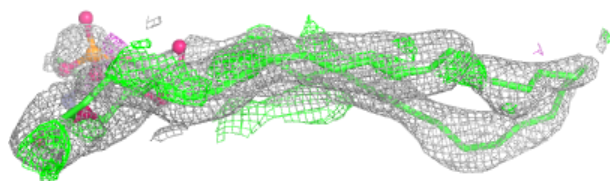
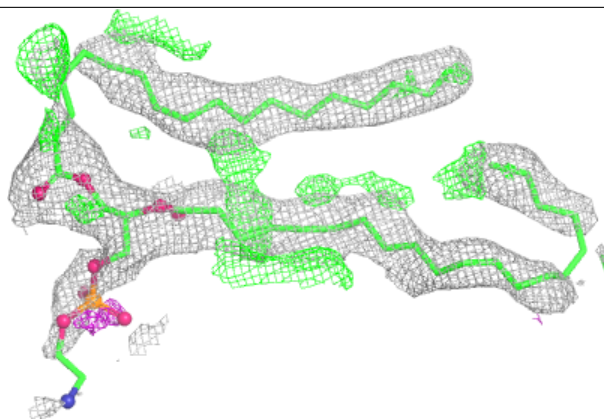
Electron density around PEK C 314:

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

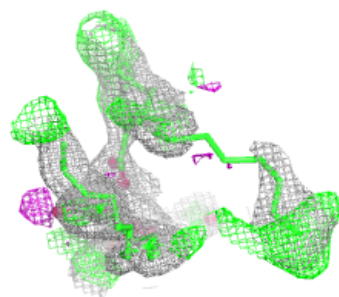
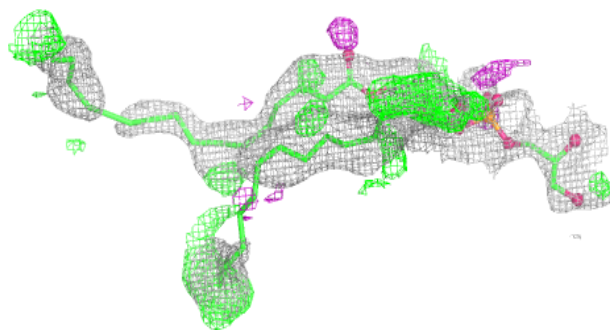
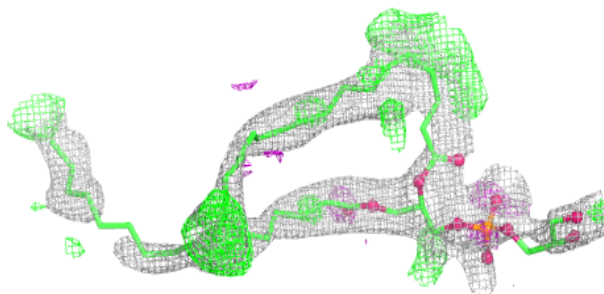


Electron density around PEK C 302:

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

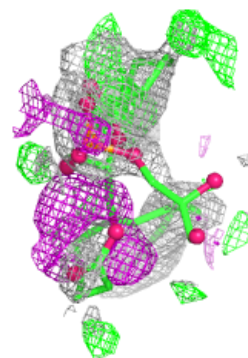
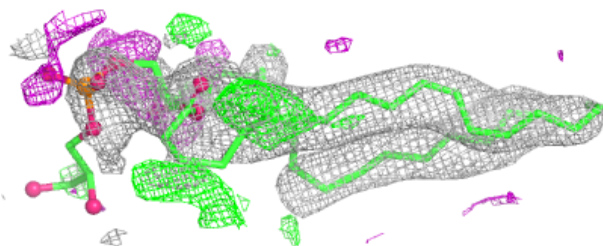
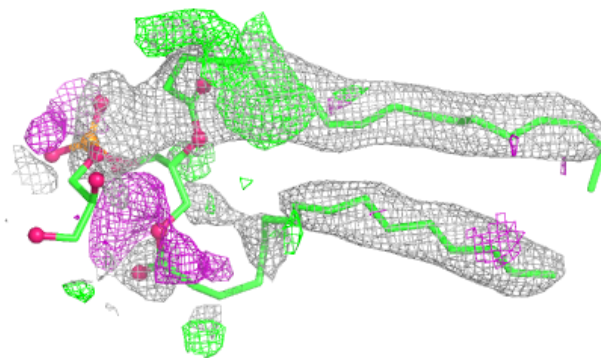
**Electron density around PGV C 304:**

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

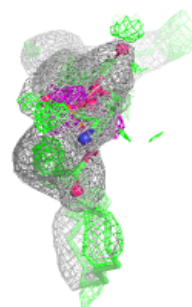
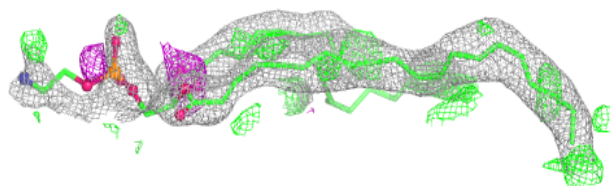
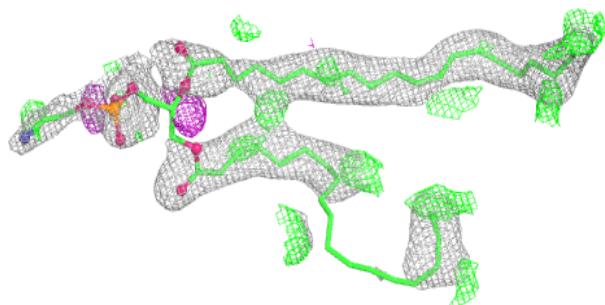


Electron density around PGV N 622:

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

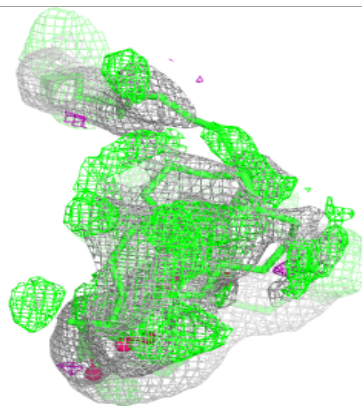
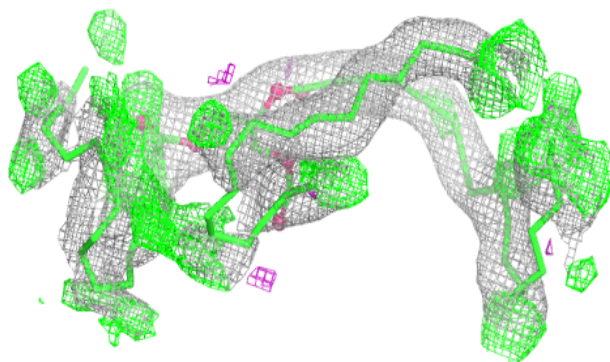
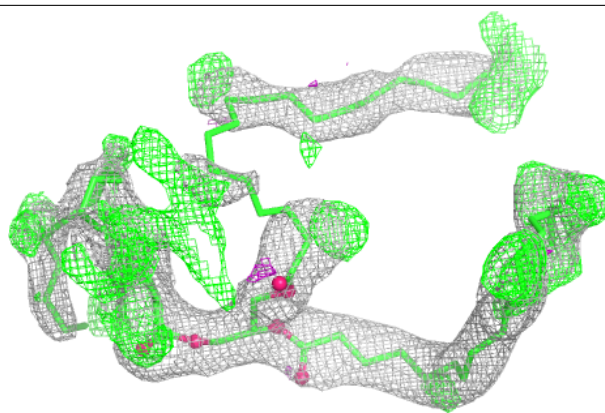
**Electron density around PEK P 301:**

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

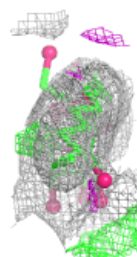
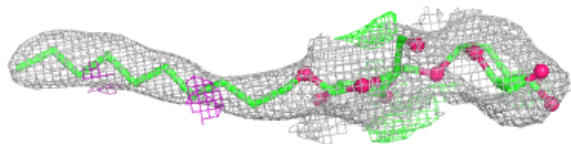
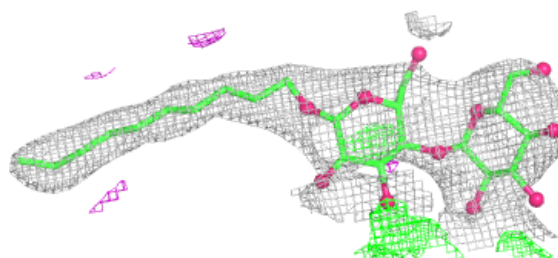


Electron density around TGL A 613:

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

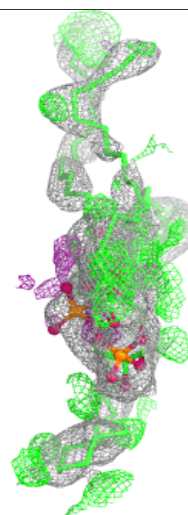
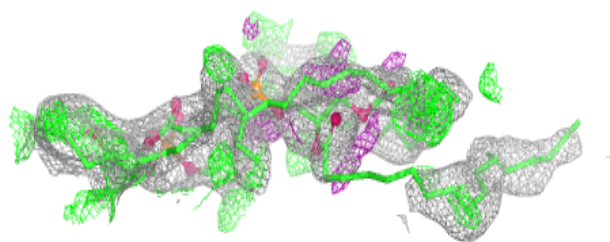
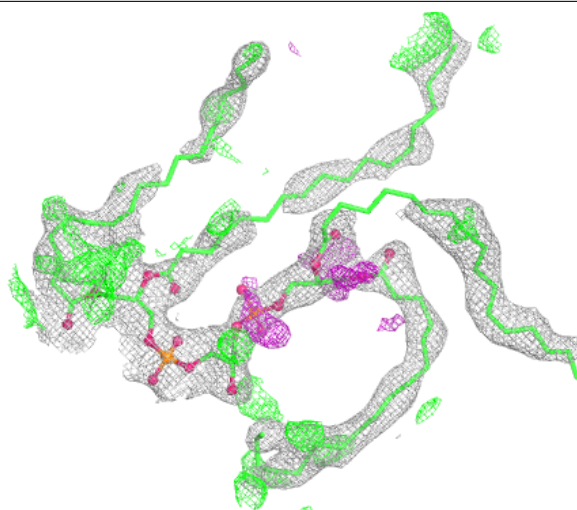
**Electron density around DMU P 302:**

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



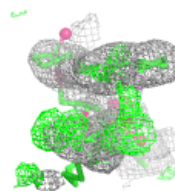
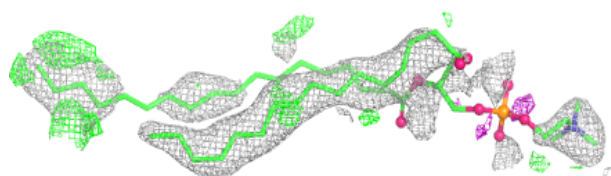
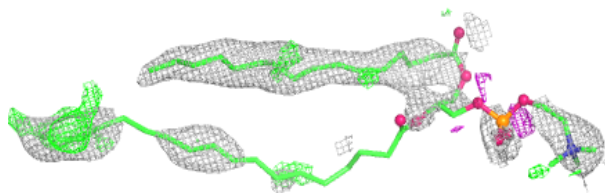
Electron density around CDL P 312:

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

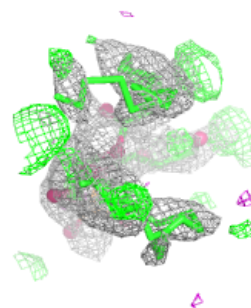
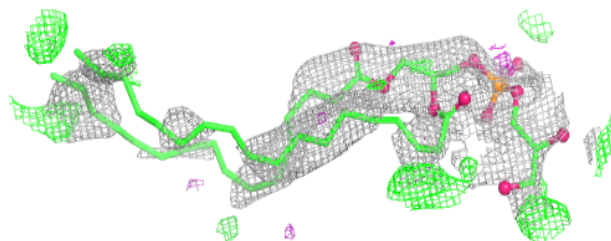
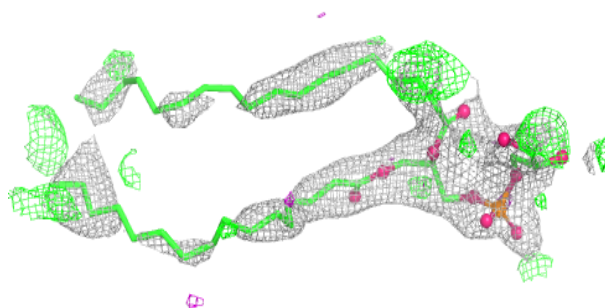


Electron density around PSC R 201:

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

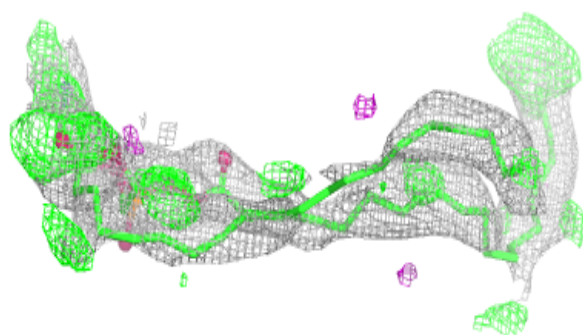
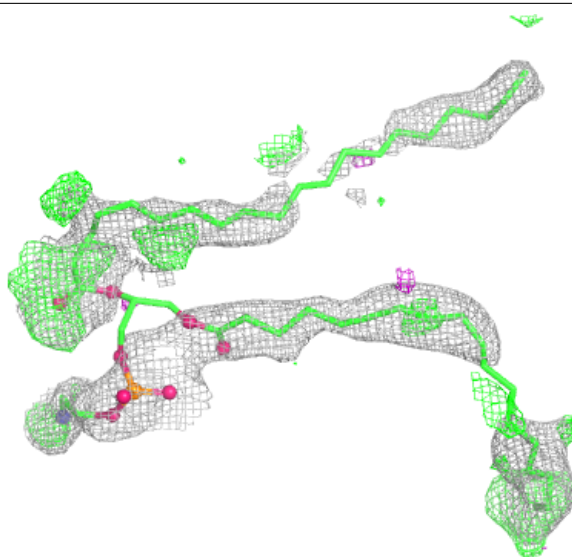
**Electron density around PGV P 307:**

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



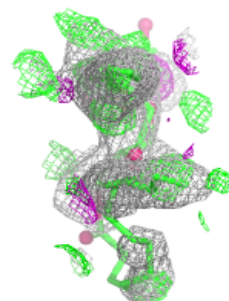
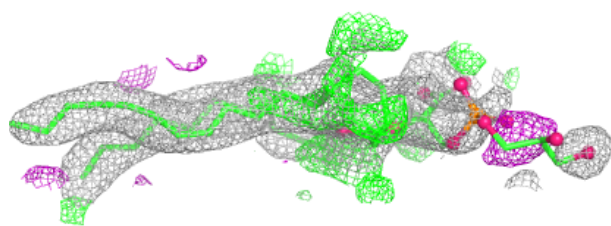
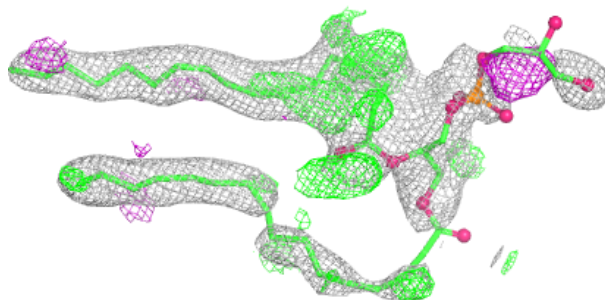
Electron density around PEK P 305:

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

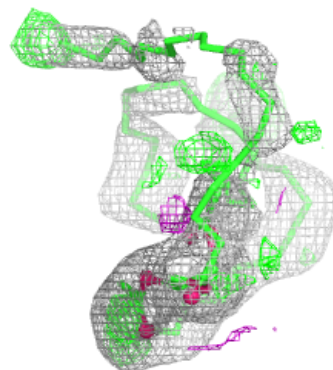
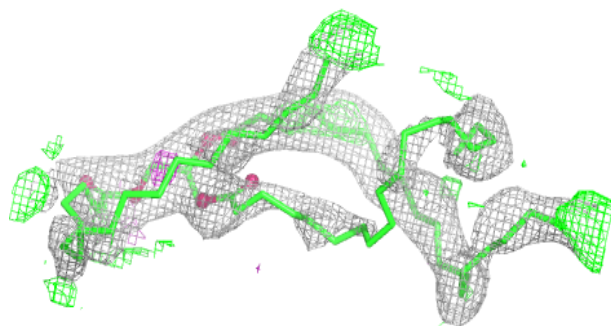
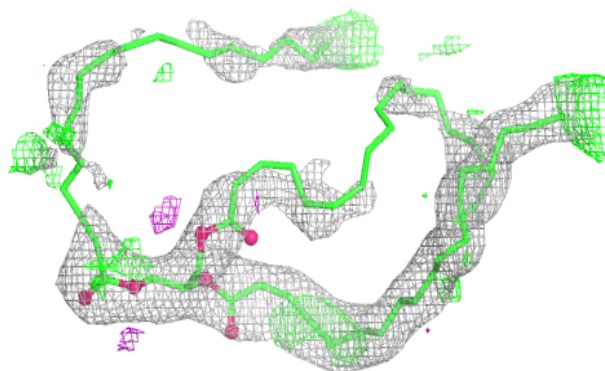


Electron density around PGV M 101:

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

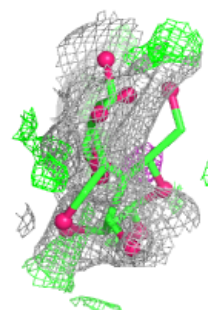
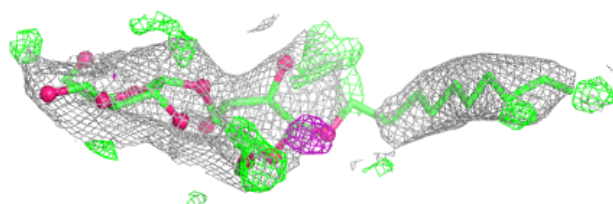
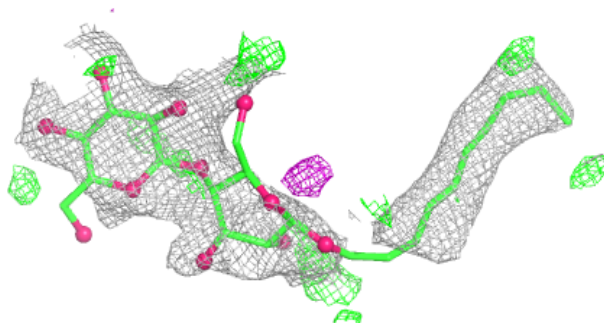
**Electron density around TGL N 604:**

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



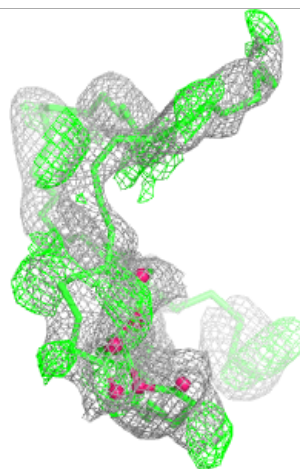
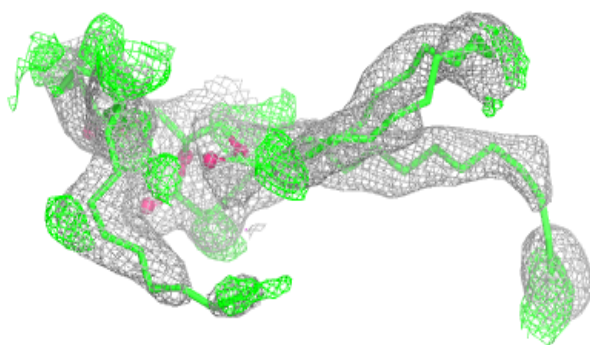
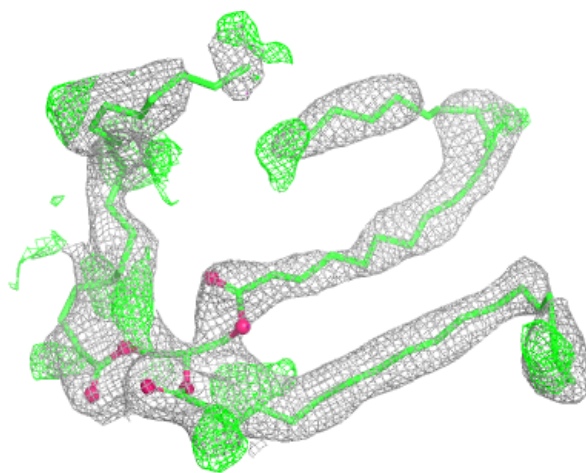
Electron density around DMU G 104:

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



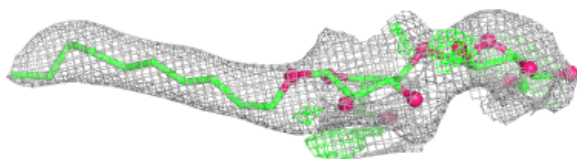
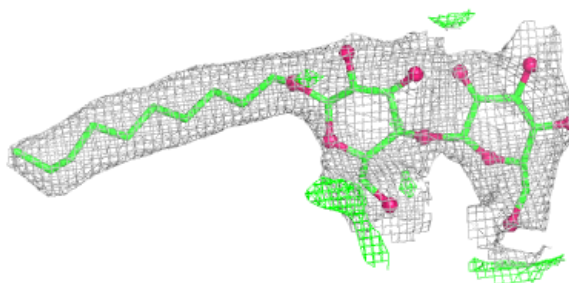
Electron density around TGL D 201:

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

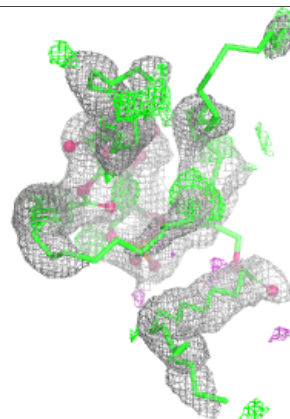
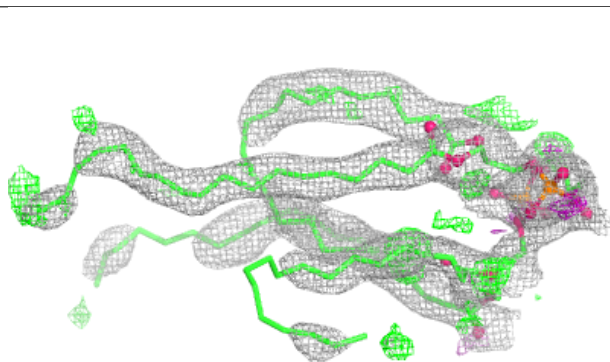
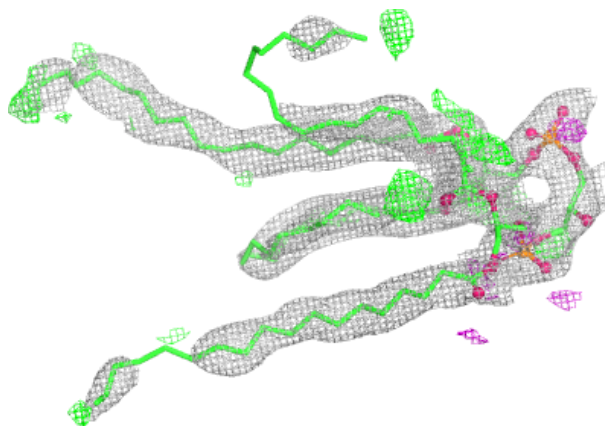


Electron density around DMU C 311:

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

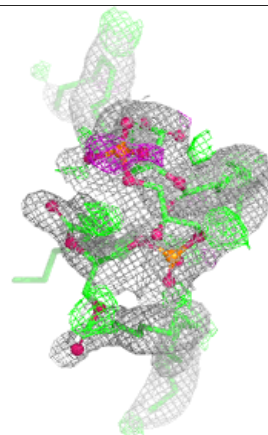
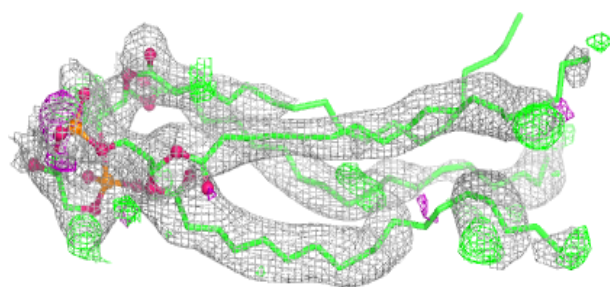
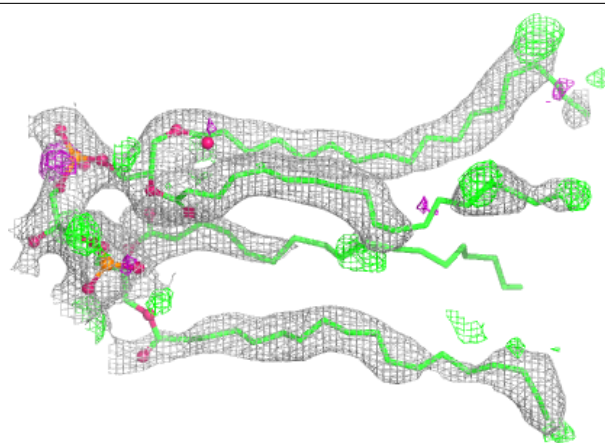
**Electron density around CDL P 308:**

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

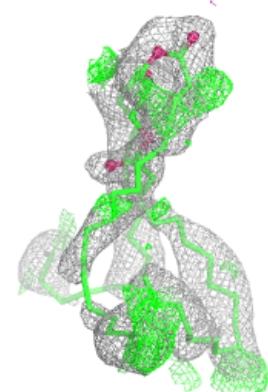
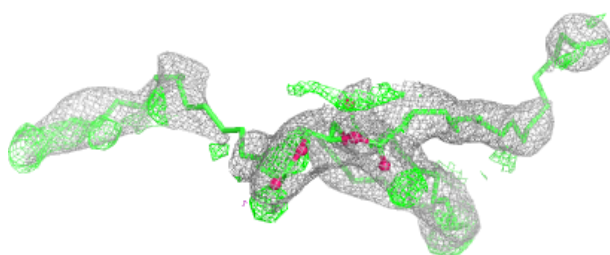
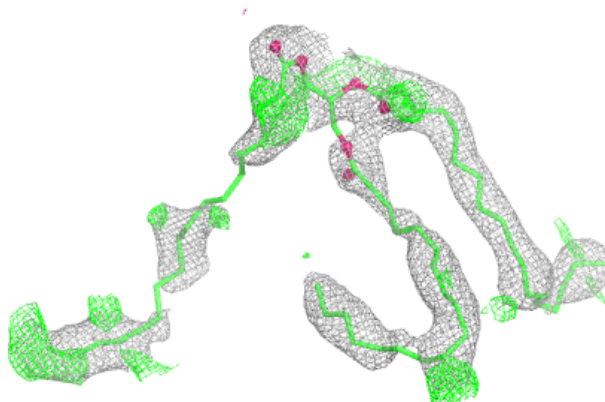


Electron density around CDL C 305:

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

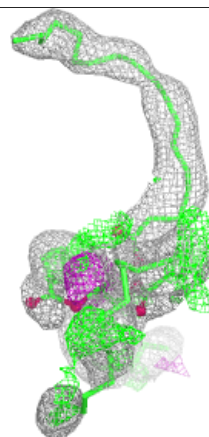
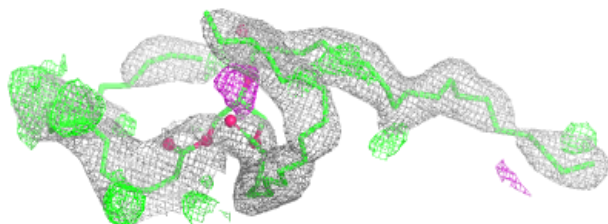
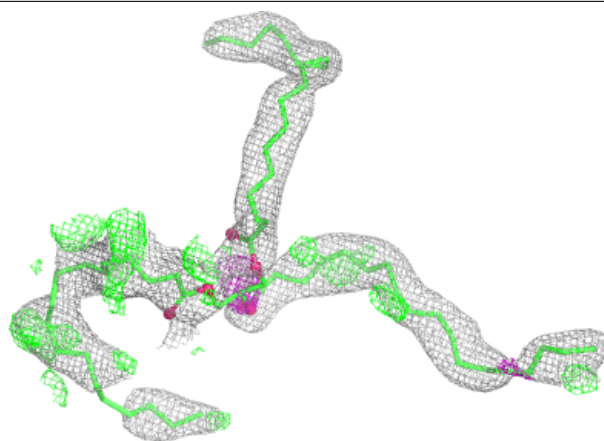
**Electron density around TGL N 618:**

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



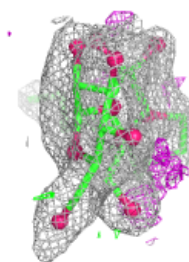
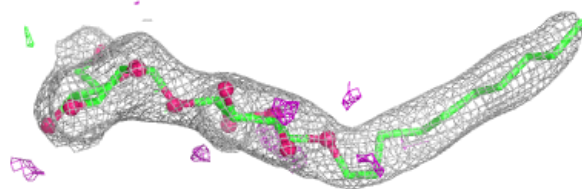
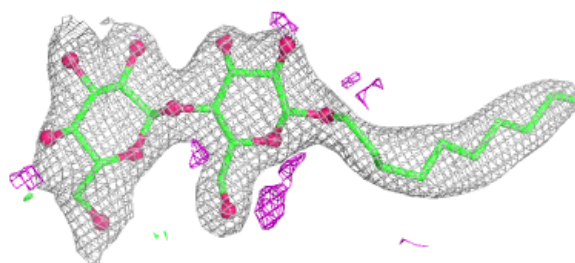
Electron density around TGL N 605:

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



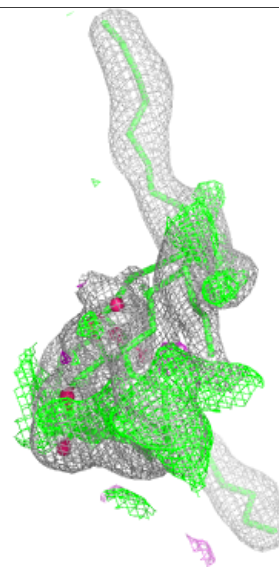
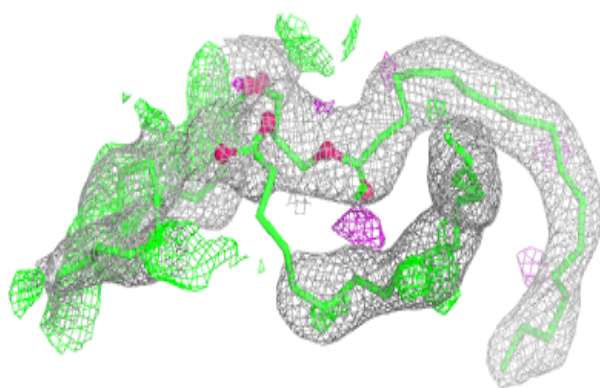
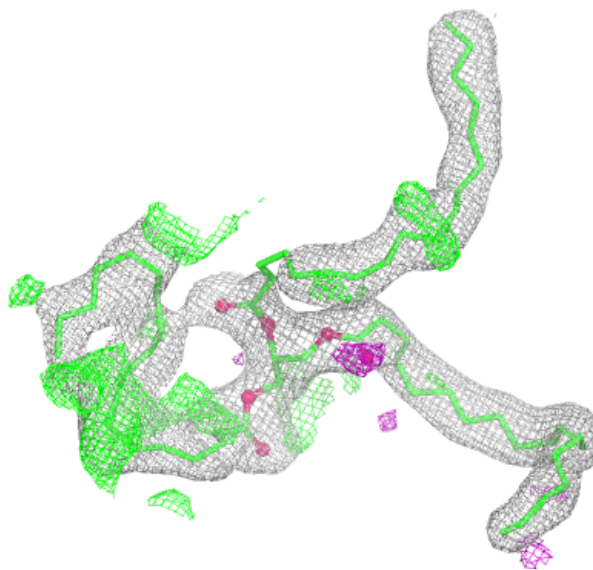
Electron density around DMU Z 101:

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



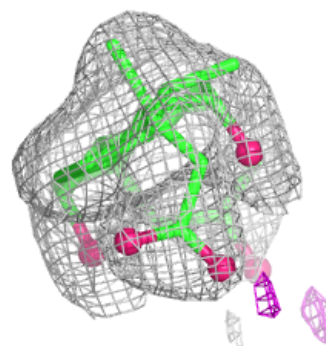
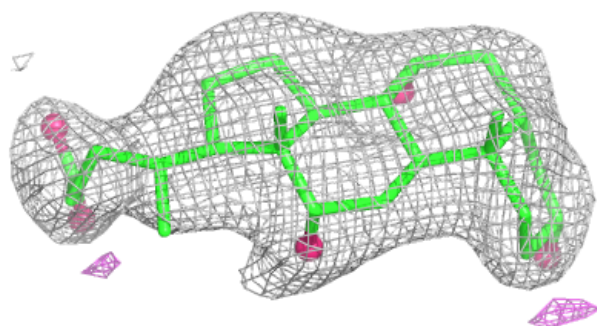
Electron density around TGL L 502:

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

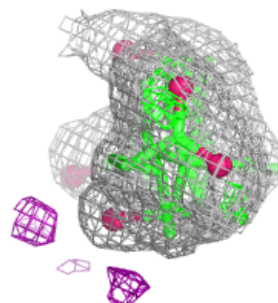
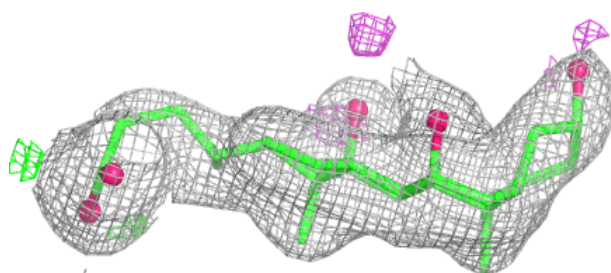
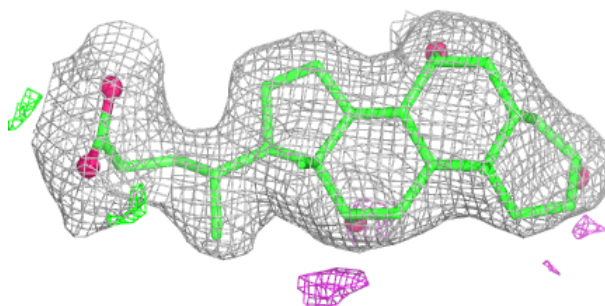


Electron density around CHD J 101:

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

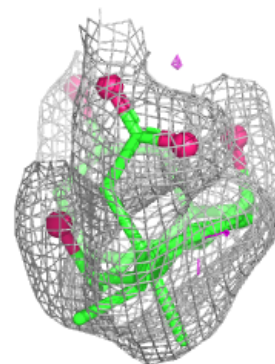
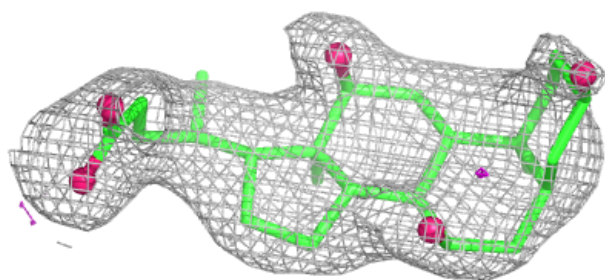
**Electron density around CHD P 309:**

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

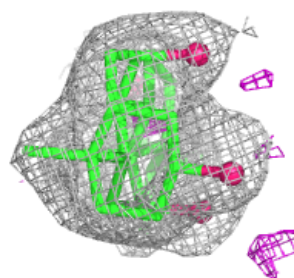
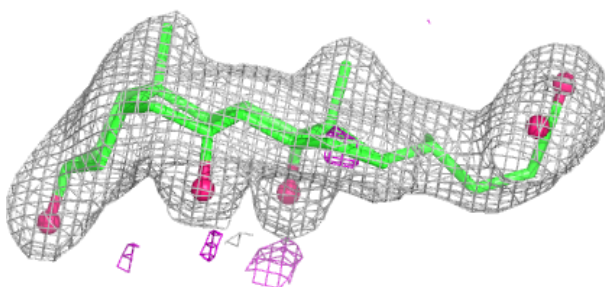
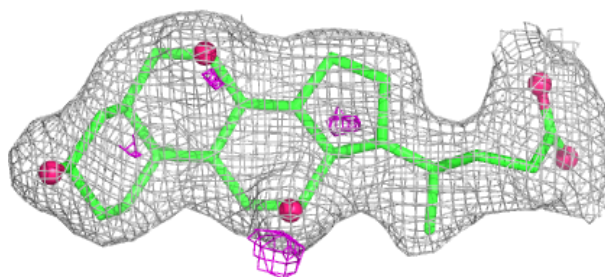


Electron density around CHD W 302:

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

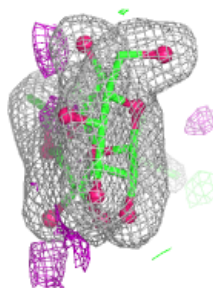
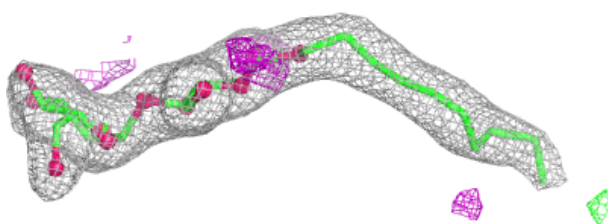
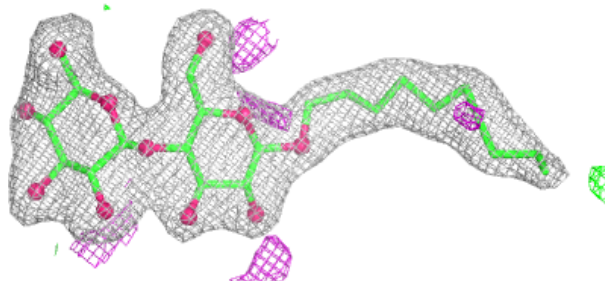
**Electron density around CHD C 306:**

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

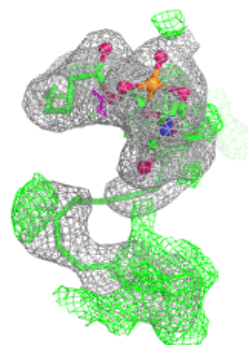
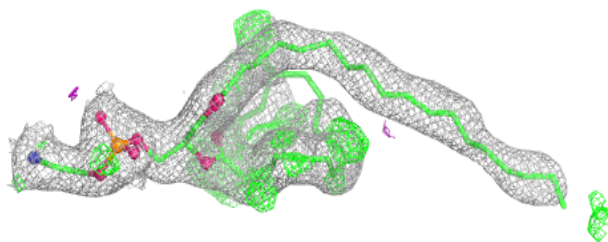
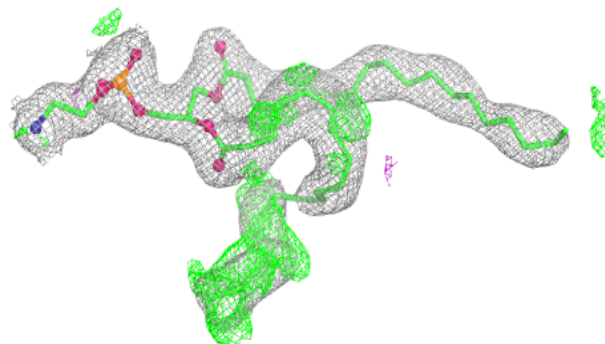


Electron density around DMU M 102:

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

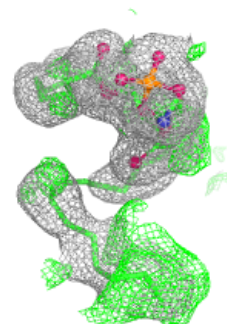
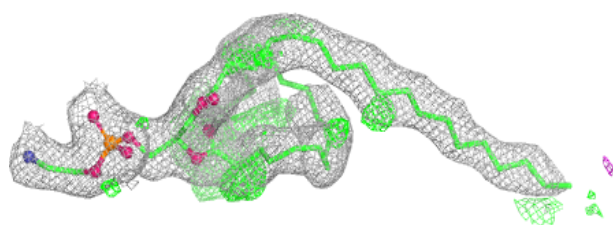
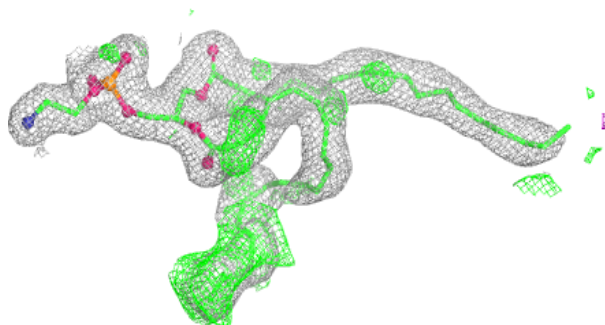
**Electron density around PEK P 304:**

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

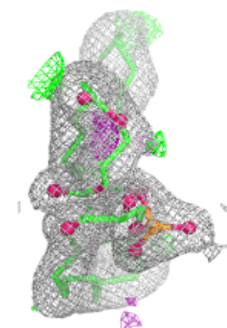
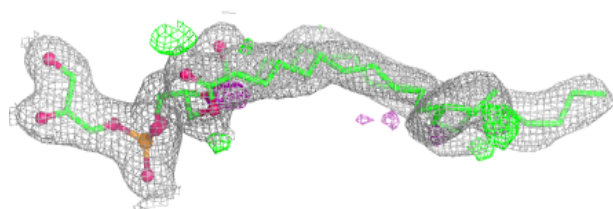
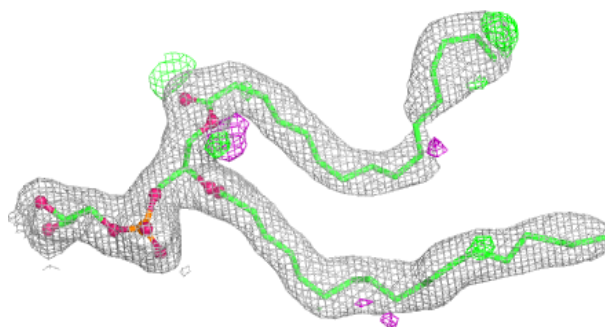


Electron density around PEK G 102:

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

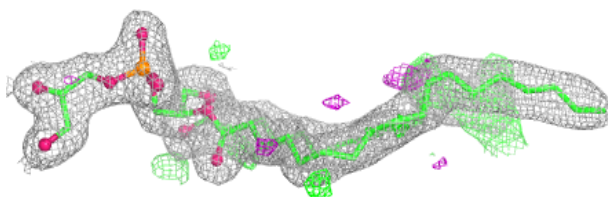
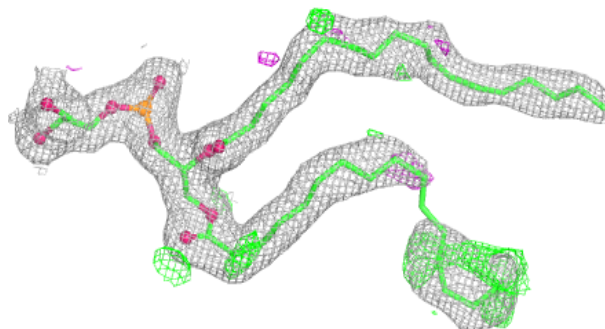
**Electron density around PGV N 606:**

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

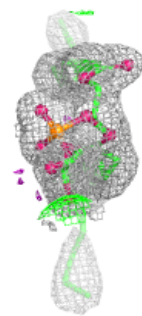
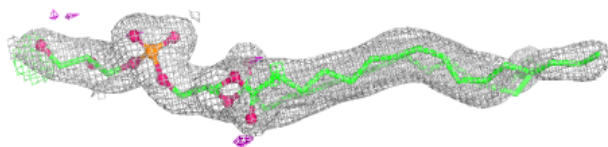
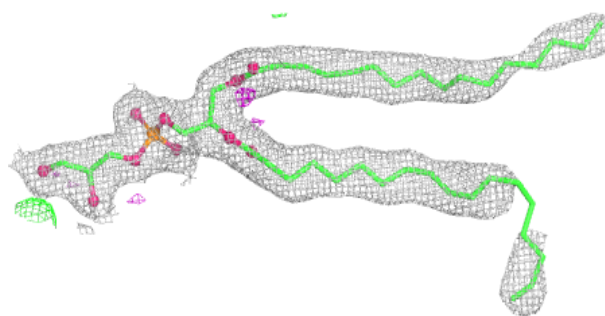


Electron density around PGV A 604:

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

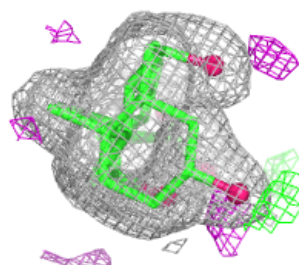
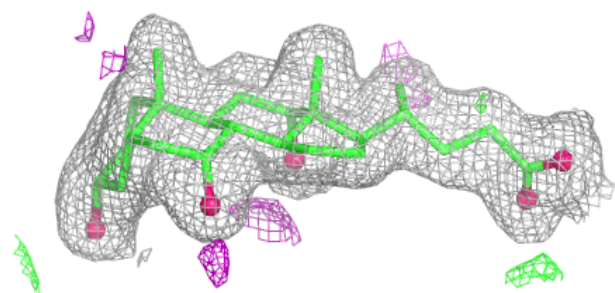
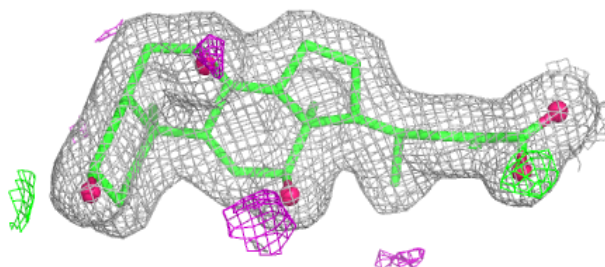
**Electron density around PGV P 306:**

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

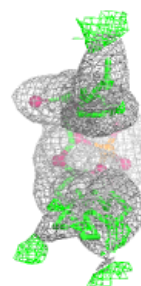
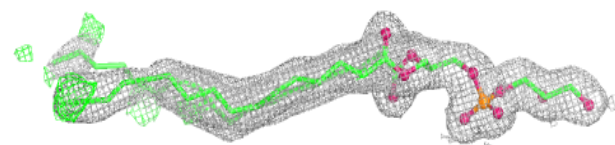
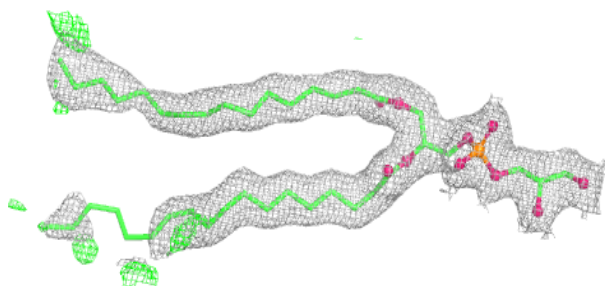


Electron density around CHD C 301:

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

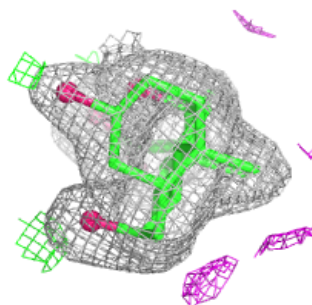
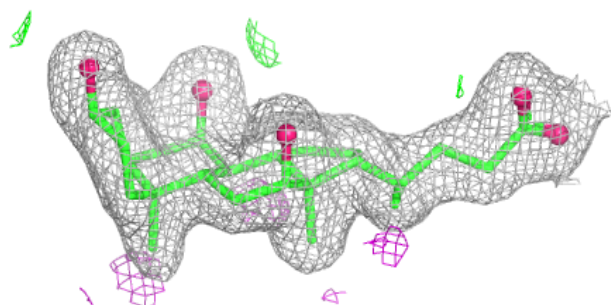
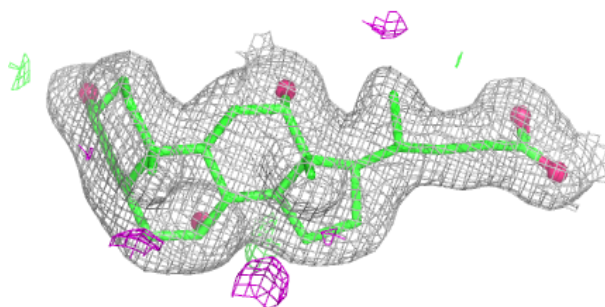
**Electron density around PGV C 303:**

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

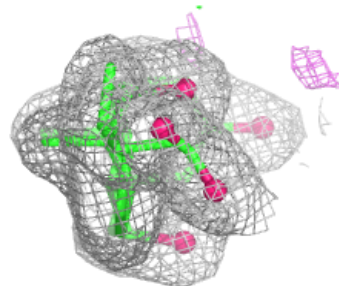
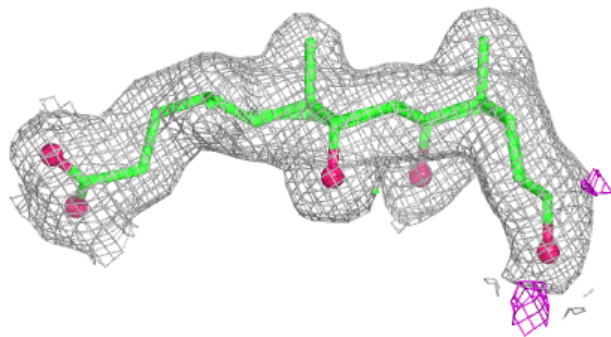
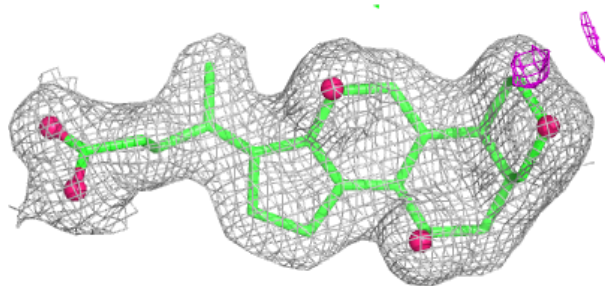


Electron density around CHD P 303:

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

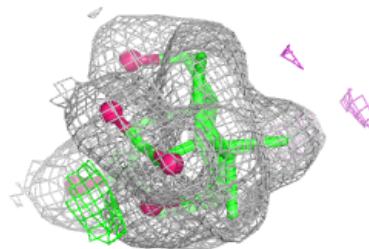
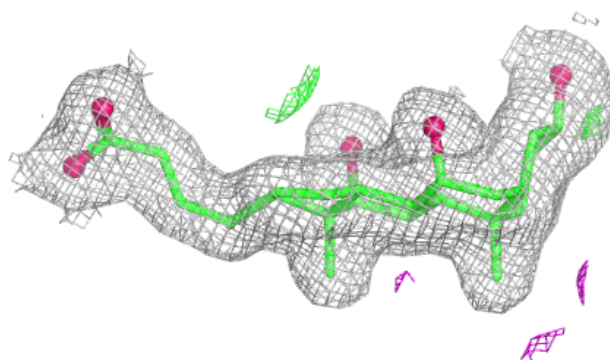
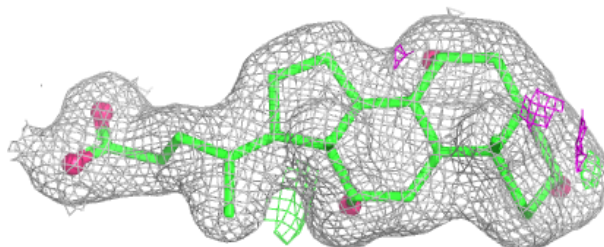
**Electron density around CHD B 303:**

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

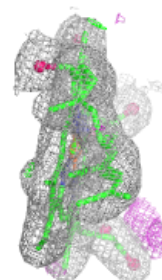
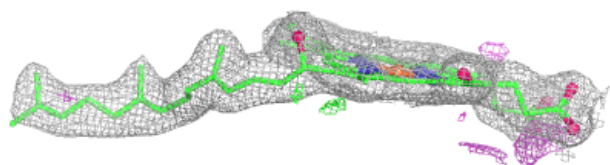
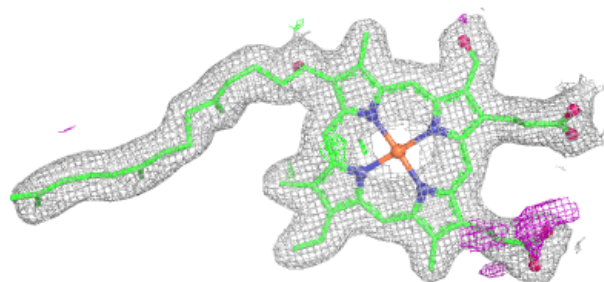


Electron density around CHD G 107:

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

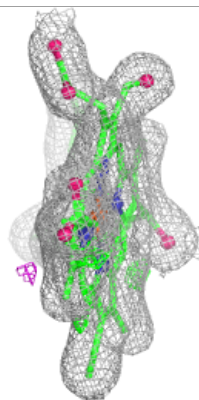
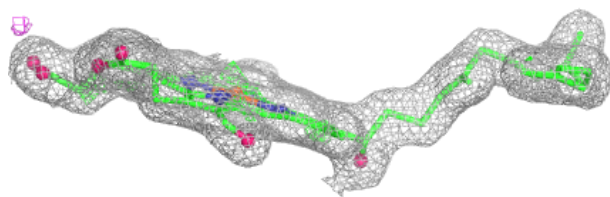
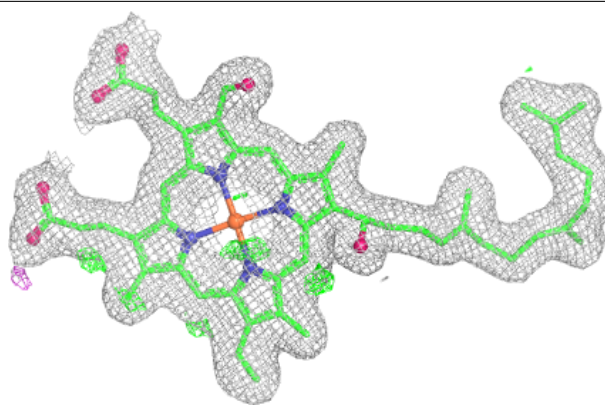
**Electron density around HEA N 608:**

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

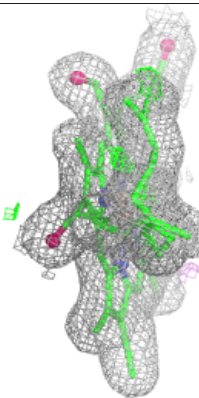
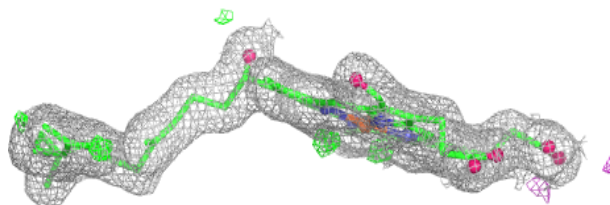
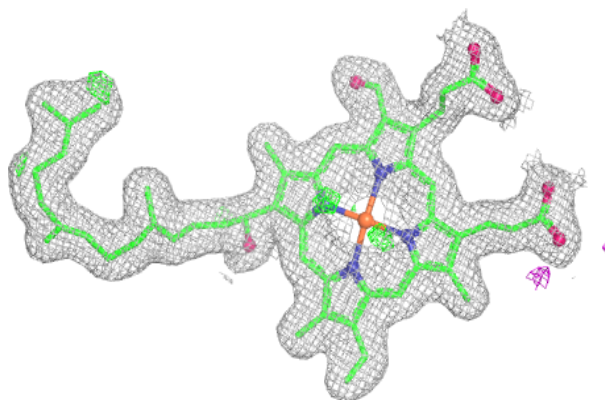


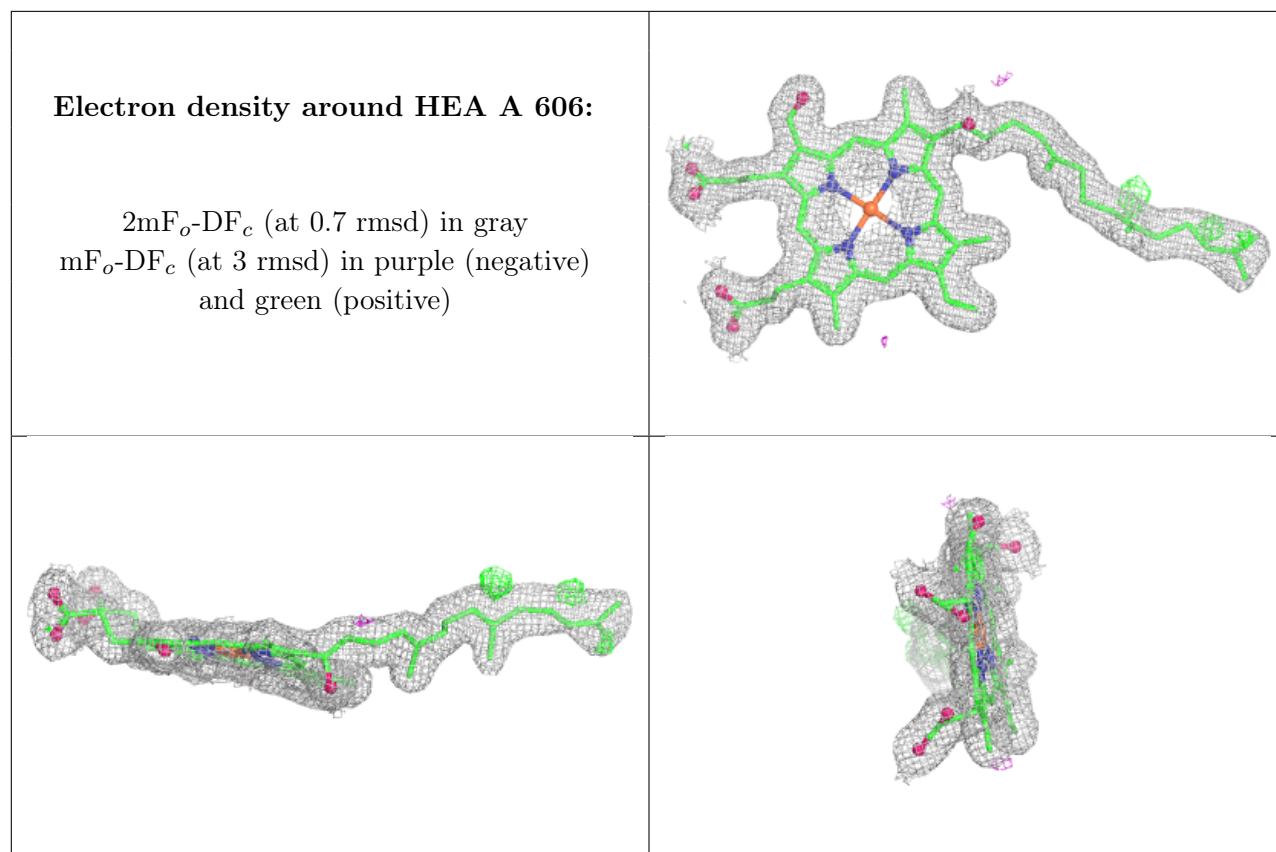
Electron density around HEA N 607:

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

**Electron density around HEA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.