



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:49 AM UTC

PDB ID : 6NMP / pdb_00006nmp
Title : SFX structure of oxidized cytochrome c oxidase at room temperature
Authors : Rousseau, D.L.; Yeh, S.-R.; Ishigami, I.
Deposited on : 2019-01-11
Resolution : 2.90 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

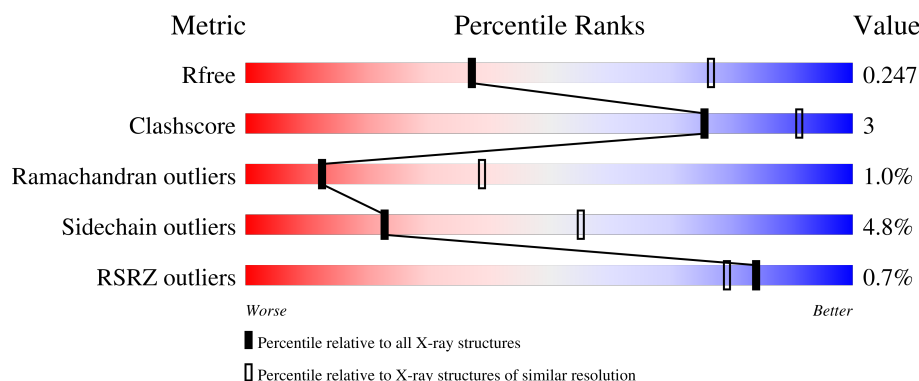
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



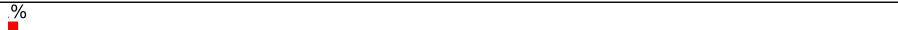
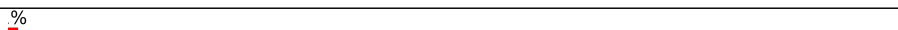
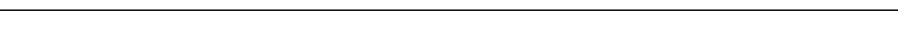
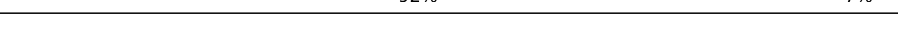
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	90% 9% .
1	N	514	87% 12% .
2	B	227	86% 13% .
2	O	227	88% 10% .
3	C	261	93% 6% .

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Mol	Chain	Length	Quality of chain
3	P	261	 90% 9% .
4	D	147	 90% 7% ..
4	Q	147	 2% 88% 10% .
5	E	109	 86% 10% .
5	R	109	 89% 7% .
6	F	98	 3% 90% 8% ..
6	S	98	 3% 89% 9% .
7	G	85	 5% 76% 16% 6% .
7	T	85	 7% 78% 16% . ..
8	H	85	 1% 80% 9% .. 7%
8	U	85	 1% 82% 9% . 7%
9	I	73	 1% 92% 8%
9	V	73	 1% 84% 16%
10	J	59	 92% 7% .
10	W	59	 75% 22% ..
11	K	56	 79% 9% 12%
11	X	56	 77% 9% . 12%
12	L	47	 89% 9% .
12	Y	47	 83% 13% ..
13	M	46	 80% 13% 7%
13	Z	46	 74% 20% 7%

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 31210 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	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

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

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

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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		

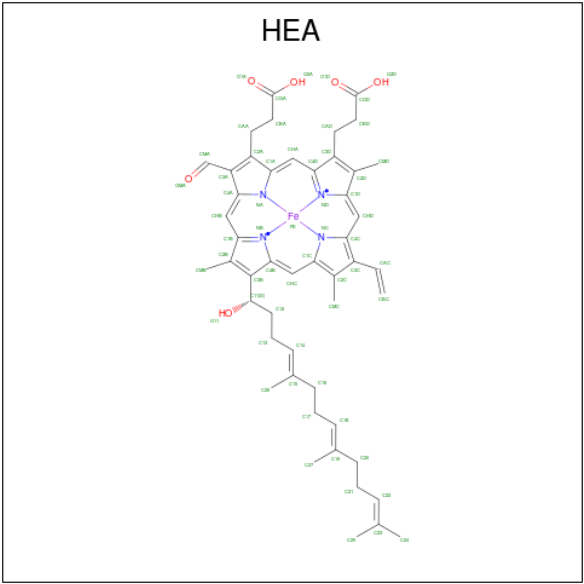
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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).

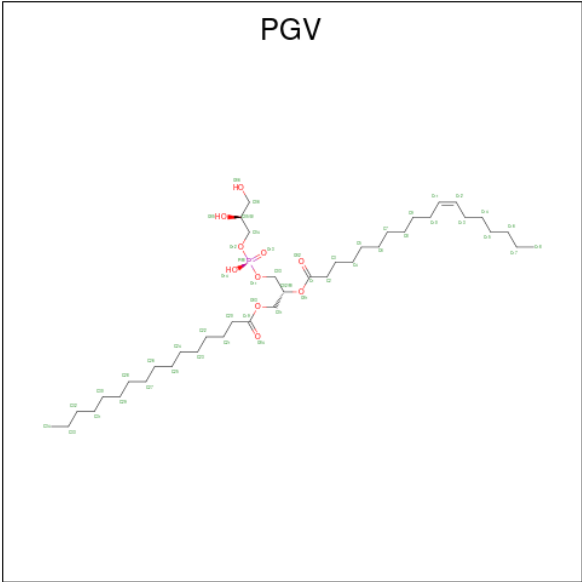
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



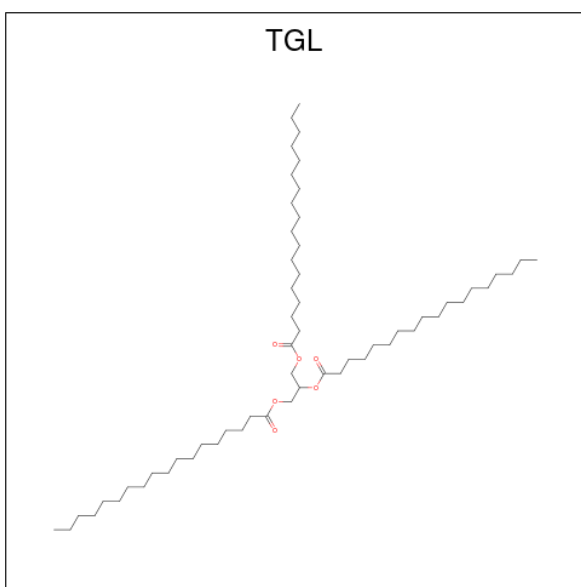
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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



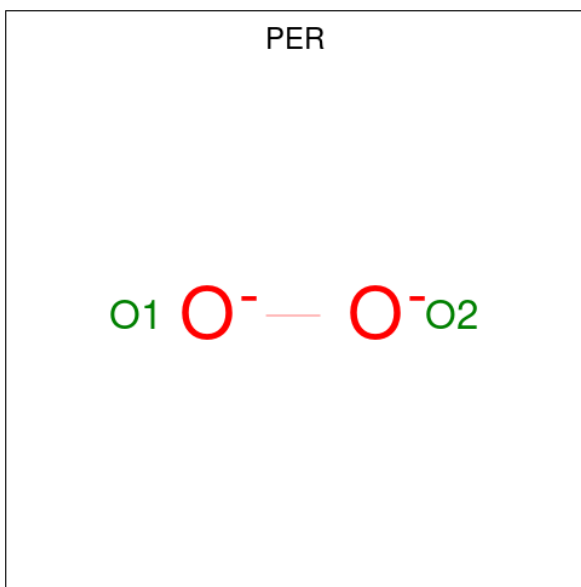
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



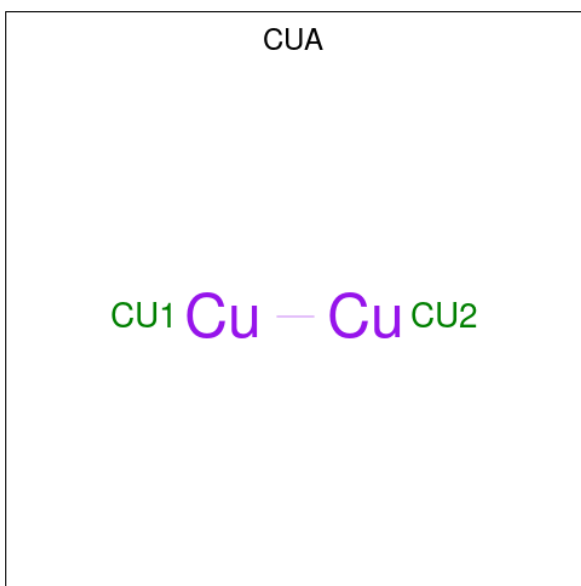
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	I	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	V	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

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



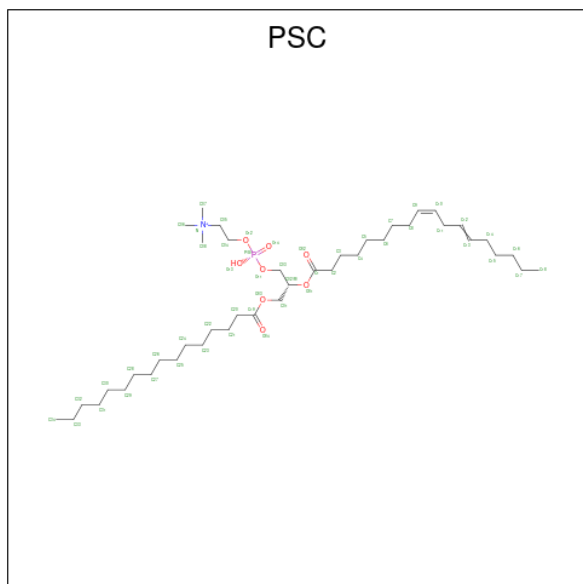
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	O	0	0
			2	2		
20	N	1	Total	O	0	0
			2	2		

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



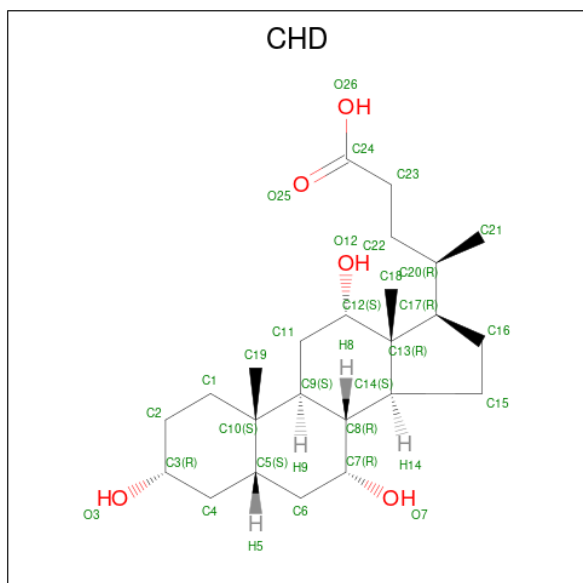
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- Molecule 22 is (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: $C_{42}H_{81}NO_8P$).



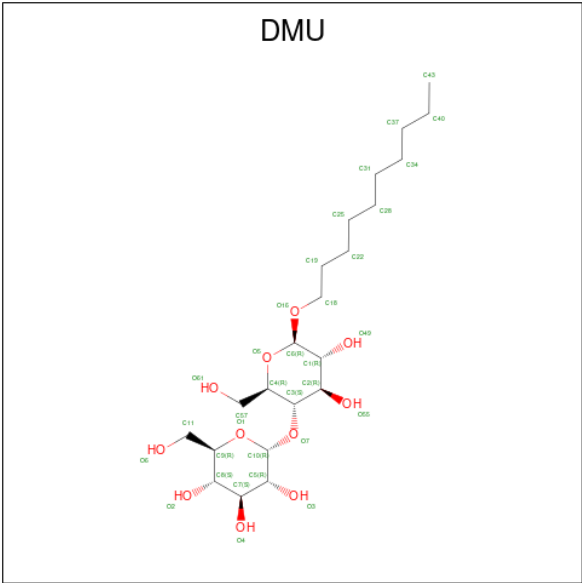
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: C₂₂H₄₂O₁₁).



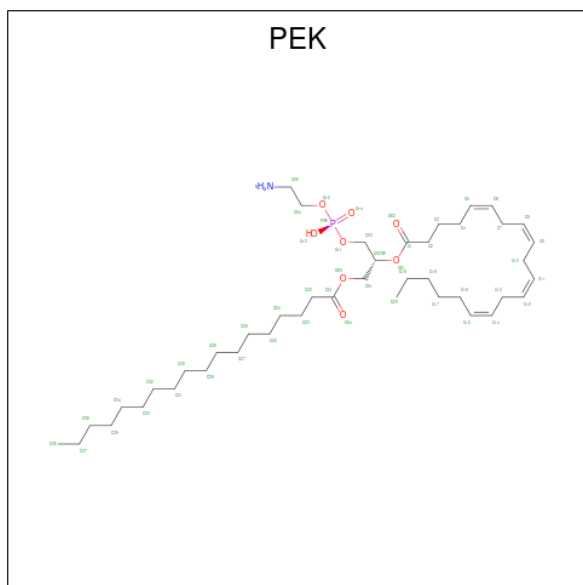
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	Q	1	Total	C	O	0	0
			33	22	11		

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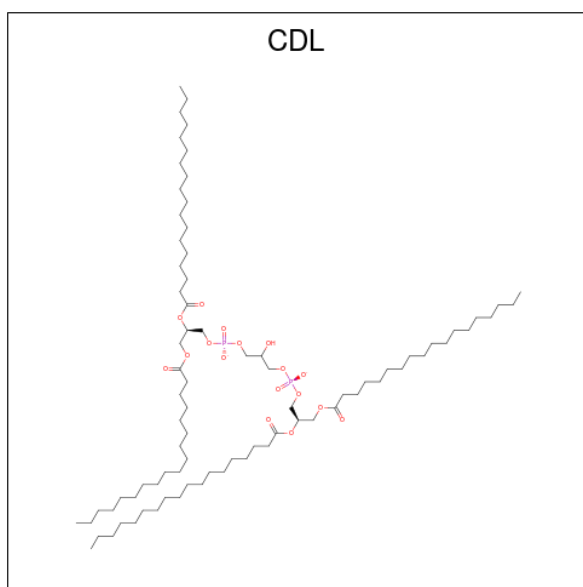
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	T	1	Total	C	O	0	0
			33	22	11		

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



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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	79	Total	O	0	0
			79	79		
28	B	55	Total	O	0	0
			55	55		
28	C	28	Total	O	0	0
			28	28		

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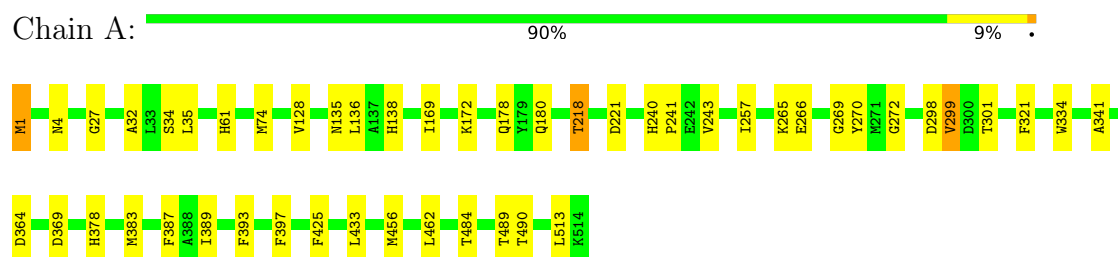
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	9	Total O 9 9	0	0
28	E	16	Total O 16 16	0	0
28	F	17	Total O 17 17	0	0
28	G	18	Total O 18 18	0	0
28	H	13	Total O 13 13	0	0
28	I	10	Total O 10 10	0	0
28	J	7	Total O 7 7	0	0
28	L	10	Total O 10 10	0	0
28	M	9	Total O 9 9	0	0
28	N	59	Total O 59 59	0	0
28	O	29	Total O 29 29	0	0
28	P	30	Total O 30 30	0	0
28	Q	19	Total O 19 19	0	0
28	R	14	Total O 14 14	0	0
28	S	7	Total O 7 7	0	0
28	T	14	Total O 14 14	0	0
28	U	11	Total O 11 11	0	0
28	V	12	Total O 12 12	0	0
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28	Y	4	Total O 4 4	0	0
28	Z	2	Total O 2 2	0	0

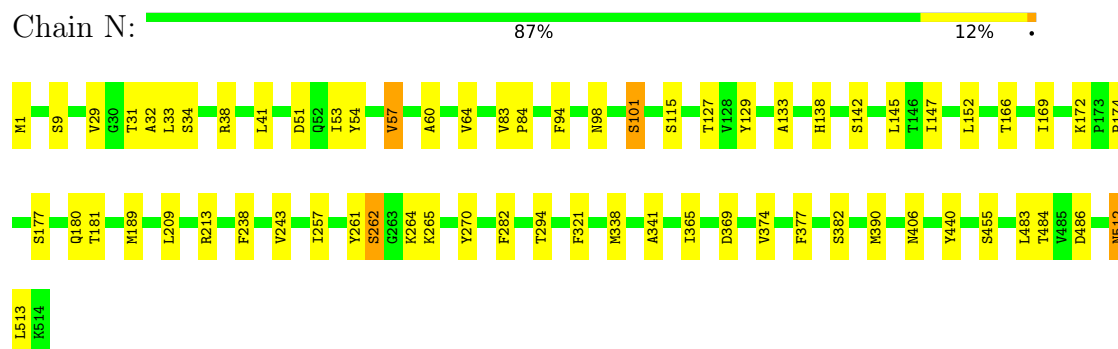
3 Residue-property plots

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

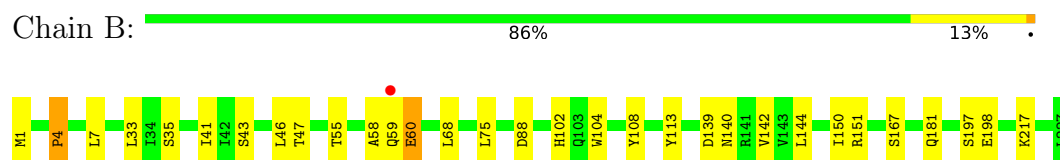
• Molecule 1: Cytochrome c oxidase subunit 1



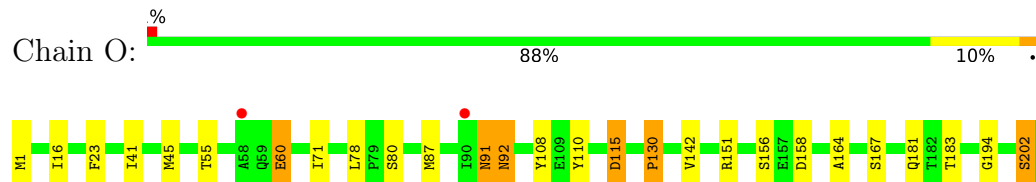
• Molecule 1: Cytochrome c oxidase subunit 1



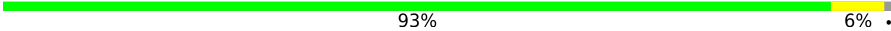
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:  93% 6% .



- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  90% 9% .



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

Chain D:  90% 7% ..



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

Chain Q:  88% 10% .



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

Chain E:  86% 10% .



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

Chain R:  89% 7% .

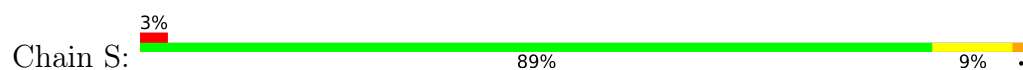


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

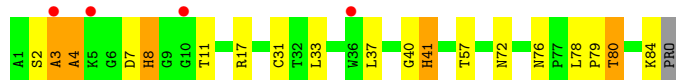
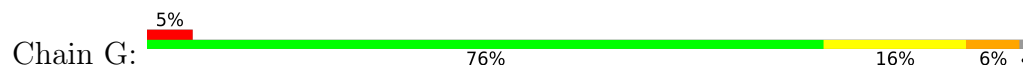
Chain F:  90% 8% ..



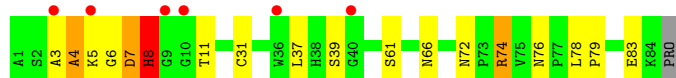
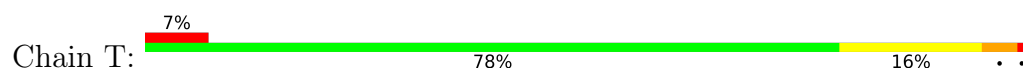
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



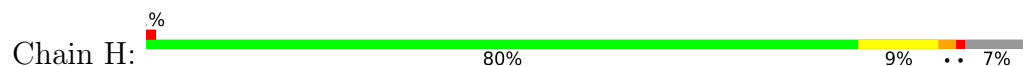
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



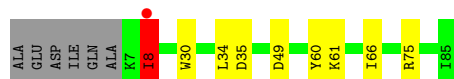
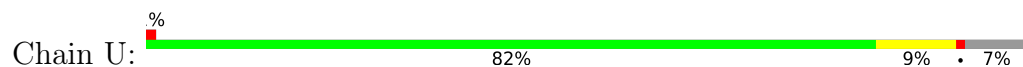
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



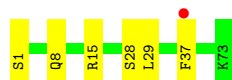
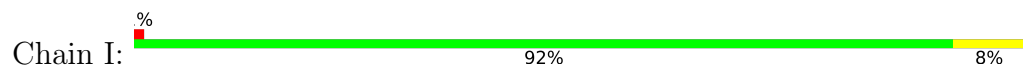
- Molecule 8: Cytochrome c oxidase subunit 6B1



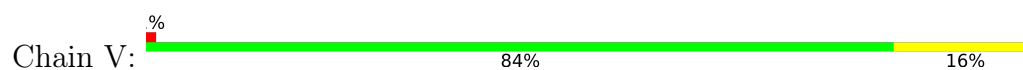
- Molecule 8: Cytochrome c oxidase subunit 6B1



- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 9: Cytochrome c oxidase subunit 6C



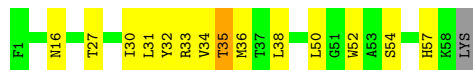
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain J:  92% 7%



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

Chain W:  75% 22%



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

Chain K:  79% 9% 12%



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

Chain X:  77% 9% 12%



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

Chain L:  89% 9%



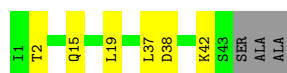
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain Y:  83% 13%

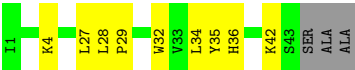


- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  80% 13% 7%



- 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	178.70Å 189.80Å 211.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 15.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (15.00-2.90) 99.2 (15.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.192 , 0.244 0.201 , 0.247	Depositor DCC
R_{free} test set	7805 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 91.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31210	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: PGV, PEK, SAC, CU, PER, PSC, TPO, DMU, MG, ZN, FME, NA, HEA, CHD, TGL, CUA, CDL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/4156	0.99	1/5678 (0.0%)
1	N	0.72	0/4156	1.00	1/5678 (0.0%)
2	B	0.74	1/1860 (0.1%)	0.97	0/2534
2	O	0.74	1/1860 (0.1%)	0.93	0/2534
3	C	0.71	0/2197	0.97	0/3005
3	P	0.69	0/2197	0.95	0/3005
4	D	0.66	0/1229	0.91	0/1658
4	Q	0.74	0/1229	0.99	1/1658 (0.1%)
5	E	0.69	0/871	0.93	0/1182
5	R	0.68	0/871	0.94	0/1182
6	F	0.78	0/765	0.99	0/1038
6	S	0.69	0/765	0.90	0/1038
7	G	0.81	0/690	0.92	0/937
7	T	0.80	0/690	0.96	0/937
8	H	0.76	0/682	0.97	0/921
8	U	0.74	0/682	0.98	0/921
9	I	0.74	0/605	0.98	0/802
9	V	0.73	0/605	1.03	0/802
10	J	0.68	0/471	1.04	0/636
10	W	0.71	0/471	1.06	0/636
11	K	0.77	0/398	0.99	0/546
11	X	0.70	0/398	0.93	0/546
12	L	0.72	0/393	0.91	0/526
12	Y	0.72	0/393	1.01	0/526
13	M	0.72	0/345	1.00	0/470
13	Z	0.67	0/345	1.02	0/470
All	All	0.73	2/29324 (0.0%)	0.97	3/39866 (0.0%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
6	S	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLU	C-O	6.18	1.31	1.23
2	O	158	ASP	CA-C	5.36	1.54	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	GLU	N-CA-C	6.60	114.07	108.13
4	Q	133	GLY	N-CA-C	5.24	119.47	112.77
1	N	169	ILE	CB-CA-C	-5.05	105.43	112.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	93	PRO	Peptide
6	S	94	HIS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	24	0
1	N	4027	0	4001	39	0
2	B	1824	0	1833	14	0
2	O	1824	0	1833	13	0
3	C	2110	0	2027	10	0
3	P	2110	0	2027	12	0
4	D	1195	0	1183	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	1195	0	1183	9	0
5	E	852	0	845	6	0
5	R	852	0	845	1	0
6	F	748	0	728	2	0
6	S	748	0	728	4	0
7	G	675	0	643	11	0
7	T	675	0	643	11	0
8	H	662	0	623	3	0
8	U	662	0	623	4	0
9	I	601	0	613	1	0
9	V	601	0	613	0	0
10	J	460	0	459	1	0
10	W	460	0	459	5	0
11	K	384	0	366	2	0
11	X	384	0	366	3	0
12	L	380	0	380	2	0
12	Y	380	0	380	4	0
13	M	335	0	352	1	0
13	Z	335	0	352	5	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	120	0	108	4	0
17	N	120	0	108	3	0
18	A	102	0	152	1	0
18	C	102	0	152	0	0
18	N	51	0	76	2	0
18	P	153	0	228	1	0
19	A	63	0	110	1	0
19	I	63	0	110	3	0
19	L	63	0	110	1	0
19	O	63	0	110	0	0
19	V	63	0	110	0	0
19	Y	63	0	110	2	0
20	A	2	0	0	1	0
20	N	2	0	0	1	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	O	52	0	80	4	0
23	B	29	0	39	0	0
23	C	58	0	78	1	0
23	J	29	0	39	0	0
23	O	29	0	39	1	0
23	P	58	0	78	0	0
23	W	29	0	39	2	0
24	C	33	0	42	0	0
24	M	33	0	42	0	0
24	Q	33	0	42	2	0
24	T	33	0	42	0	0
25	C	106	0	154	1	0
25	G	106	0	154	1	0
25	P	53	0	77	3	0
25	T	53	0	77	1	0
26	C	100	0	156	4	0
26	G	100	0	156	1	0
26	P	100	0	156	2	0
26	T	100	0	156	2	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	79	0	0	0	0
28	B	55	0	0	2	0
28	C	28	0	0	0	0
28	D	9	0	0	0	0
28	E	16	0	0	0	0
28	F	17	0	0	1	0
28	G	18	0	0	0	0
28	H	13	0	0	1	0
28	I	10	0	0	0	0
28	J	7	0	0	0	0
28	L	10	0	0	0	0
28	M	9	0	0	0	0
28	N	59	0	0	4	0
28	O	29	0	0	1	0
28	P	30	0	0	0	0
28	Q	19	0	0	3	0
28	R	14	0	0	0	0
28	S	7	0	0	0	0
28	T	14	0	0	0	0
28	U	11	0	0	0	0
28	V	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	W	4	0	0	1	0
28	Y	4	0	0	0	0
28	Z	2	0	0	0	0
All	All	31210	0	31316	185	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 3.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:607:PER:O1	20:N:607:PER:O2	1.61	1.19
20:A:609:PER:O1	20:A:609:PER:O2	1.61	1.18
7:T:31:CYS:SG	26:T:103:CDL:H532	2.20	0.81
8:H:10:ASN:HA	28:H:107:HOH:O	1.82	0.79
7:G:76:ASN:HD21	25:G:101:PEK:HN2	1.33	0.77
25:P:303:PEK:HN2	7:T:76:ASN:HD21	1.33	0.73
7:G:72:ASN:H	7:G:76:ASN:HD22	1.34	0.73
7:G:31:CYS:SG	26:G:102:CDL:H532	2.33	0.69
2:O:41:ILE:HD13	22:O:303:PSC:H342	1.74	0.68
2:O:115:ASP:OD1	8:U:61:LYS:NZ	2.30	0.65
2:B:41:ILE:HD13	22:B:302:PSC:H342	1.80	0.62
19:I:101:TGL:H363	19:I:101:TGL:H211	1.81	0.62
7:G:7:ASP:O	7:G:8:HIS:HB2	2.00	0.61
17:A:604:HEA:HBC1	17:A:604:HEA:HMC1	1.83	0.60
1:N:321:PHE:CD1	22:O:303:PSC:H341	2.36	0.60
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.40	0.56
25:P:303:PEK:C05	7:T:76:ASN:HD21	2.18	0.56
28:B:451:HOH:O	19:I:101:TGL:HG2	2.06	0.55
1:A:240:HIS:O	1:A:243:VAL:HG22	2.06	0.55
11:X:31:TYR:CD1	11:X:35:GLN:HG3	2.42	0.55
3:P:155:ASP:OD2	3:P:158:HIS:ND1	2.33	0.54
11:X:22:ALA:O	11:X:26:VAL:HG23	2.08	0.54
1:N:262:SER:HB2	28:N:706:HOH:O	2.08	0.54
4:Q:102:TYR:HB3	28:Q:311:HOH:O	2.07	0.53
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	1.90	0.53
12:Y:24:MET:HE1	19:Y:101:TGL:H162	1.91	0.53
3:C:55:TYR:CE1	26:C:306:CDL:H521	2.43	0.53
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.44	0.53
1:N:177:SER:H	1:N:180:GLN:HE21	1.57	0.52
10:W:31:LEU:O	10:W:35:THR:OG1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133:ALA:O	1:N:213:ARG:NH1	2.43	0.52
2:O:130:PRO:HA	4:Q:115:TRP:CZ2	2.45	0.52
2:B:151:ARG:HE	2:B:181:GLN:NE2	2.07	0.52
10:J:32:TYR:CE1	10:J:36:MET:HE3	2.45	0.52
2:O:164:ALA:O	2:O:194:GLY:HA3	2.10	0.52
2:O:108:TYR:CE2	2:O:142:VAL:HG21	2.45	0.52
3:C:149:HIS:HA	3:C:152:MET:HE3	1.92	0.51
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.46	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.46	0.51
4:Q:98:TRP:CZ3	24:Q:201:DMU:H16	2.46	0.51
1:N:127:THR:HB	1:N:129:TYR:CD1	2.46	0.51
2:B:33:LEU:HD12	9:I:28:SER:HB3	1.93	0.50
2:B:58:ALA:O	2:B:60:GLU:N	2.43	0.50
1:N:261:TYR:HB2	1:N:338:MET:HE2	1.92	0.50
7:T:3:ALA:O	7:T:4:ALA:HB2	2.11	0.50
1:N:264:LYS:HB2	28:N:706:HOH:O	2.11	0.50
23:W:101:CHD:C21	28:W:203:HOH:O	2.60	0.49
19:I:101:TGL:H102	19:I:101:TGL:H281	1.93	0.49
2:B:4:PRO:HB2	11:K:43:SER:HA	1.94	0.49
1:A:74:MET:HE2	1:A:389:ILE:HG13	1.95	0.49
7:G:7:ASP:O	7:G:8:HIS:CB	2.61	0.48
1:N:60:ALA:O	1:N:64:VAL:HG23	2.13	0.48
6:F:96:LEU:N	28:F:201:HOH:O	2.46	0.48
1:N:33:LEU:HD23	1:N:57:VAL:HG13	1.96	0.48
2:O:91:ASN:O	2:O:92:ASN:C	2.56	0.48
4:Q:76:ASN:O	4:Q:77:GLU:C	2.56	0.48
4:Q:76:ASN:ND2	11:X:11:ASP:OD1	2.47	0.48
1:A:383:MET:HA	1:A:387:PHE:CD1	2.49	0.48
5:E:49:ASP:OD1	5:E:92:THR:OG1	2.29	0.48
1:N:406:ASN:HD21	18:N:606:PGV:C2	2.27	0.48
1:N:51:ASP:HB2	2:O:202:SER:O	2.14	0.48
8:U:34:LEU:O	8:U:35:ASP:C	2.57	0.47
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.95	0.47
1:N:321:PHE:CE1	22:O:303:PSC:H341	2.48	0.47
2:O:151:ARG:CD	2:O:181:GLN:HE21	2.27	0.47
3:C:111:GLU:OE1	3:C:111:GLU:N	2.46	0.47
22:O:303:PSC:H343	22:O:303:PSC:H142	1.97	0.47
3:P:146:TRP:CE3	3:P:162:ALA:HB2	2.50	0.47
1:N:374:VAL:HA	1:N:377:PHE:CE2	2.49	0.47
1:A:135:ASN:HD21	7:G:57:THR:CB	2.27	0.46
17:N:604:HEA:HBC1	17:N:604:HEA:HMC3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:261:TYR:CB	1:N:338:MET:HE2	2.46	0.46
7:T:72:ASN:OD1	7:T:74:ARG:HB2	2.15	0.46
1:A:27:GLY:HA3	17:A:604:HEA:H271	1.97	0.46
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.50	0.46
1:A:393:PHE:O	1:A:397:PHE:HB2	2.15	0.46
1:N:53:ILE:O	1:N:57:VAL:HG23	2.16	0.46
17:N:605:HEA:HBC1	17:N:605:HEA:HMC3	1.97	0.46
7:T:7:ASP:O	7:T:8:HIS:HB2	2.16	0.46
26:C:306:CDL:HB32	26:C:306:CDL:CB2	2.45	0.45
1:N:147:ILE:HD11	1:N:209:LEU:HD23	1.98	0.45
7:T:66:ASN:HD21	7:T:79:PRO:HD2	1.81	0.45
19:A:608:TGL:H331	2:B:47:THR:HB	1.98	0.45
3:C:23:SER:CB	3:C:49:THR:OG1	2.64	0.45
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.99	0.45
17:A:604:HEA:HHB	17:A:604:HEA:OMA	2.17	0.45
10:W:33:ARG:HG2	23:W:101:CHD:H151	1.97	0.45
2:B:108:TYR:CE2	2:B:142:VAL:HG21	2.52	0.45
1:A:1:FME:HCN	1:A:4:ASN:HB2	1.97	0.45
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.99	0.45
7:G:3:ALA:O	7:G:4:ALA:HB2	2.16	0.45
1:N:98:ASN:O	1:N:101:SER:HB2	2.18	0.44
1:N:177:SER:H	1:N:180:GLN:NE2	2.14	0.44
1:N:390:MET:HE3	1:N:390:MET:HA	1.99	0.44
18:P:304:PGV:H182	26:P:306:CDL:H673	2.00	0.44
4:D:33:LEU:HA	4:D:37:GLN:HE21	1.82	0.44
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.53	0.44
2:B:144:LEU:HB3	2:B:150:ILE:CD1	2.48	0.44
1:N:181:THR:O	1:N:270:TYR:OH	2.32	0.44
7:G:40:GLY:O	7:G:41:HIS:C	2.61	0.44
25:P:303:PEK:C05	7:T:76:ASN:ND2	2.81	0.44
5:R:82:TYR:HB3	5:R:83:PRO:CD	2.47	0.44
7:T:3:ALA:O	7:T:4:ALA:CB	2.65	0.44
25:T:102:PEK:H383	26:T:103:CDL:H272	1.99	0.44
3:C:23:SER:HB2	3:C:49:THR:OG1	2.18	0.43
5:E:44:GLU:O	5:E:45:PRO:C	2.60	0.43
1:N:483:LEU:HG	13:Z:4:LYS:HG3	2.00	0.43
4:Q:109:HIS:CE1	28:Q:302:HOH:O	2.71	0.43
1:A:298:ASP:O	1:A:299:VAL:C	2.62	0.43
1:N:94:PHE:CZ	1:N:166:THR:HG21	2.53	0.43
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.48	0.43
1:N:406:ASN:HD21	18:N:606:PGV:H21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:64:GLU:O	6:S:65:ASP:HB2	2.17	0.43
1:A:269:GLY:O	1:A:270:TYR:C	2.62	0.43
1:N:440:TYR:HE1	2:O:204:HIS:CE1	2.37	0.43
2:B:7:LEU:HB3	28:B:451:HOH:O	2.18	0.43
5:E:90:ARG:HB3	5:E:91:PRO:HD3	2.01	0.43
1:A:321:PHE:CD1	22:B:302:PSC:H341	2.54	0.43
2:B:41:ILE:HG21	22:B:302:PSC:H342	2.00	0.43
1:A:364:ASP:OD1	17:A:605:HEA:O1A	2.36	0.43
3:C:103:HIS:HD1	23:C:303:CHD:C24	2.31	0.43
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.43
1:N:83:VAL:HB	1:N:84:PRO:HD3	2.01	0.43
1:A:269:GLY:O	1:A:272:GLY:N	2.51	0.43
1:A:298:ASP:O	1:A:301:THR:N	2.52	0.43
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.00	0.43
1:N:294:THR:HA	28:O:410:HOH:O	2.18	0.43
25:C:308:PEK:H382	7:T:3:ALA:HB1	2.00	0.42
1:N:174:PRO:HB2	6:S:35:ALA:HB2	2.01	0.42
3:C:63:ARG:HE	26:C:306:CDL:HA22	1.84	0.42
3:P:16:TRP:HA	3:P:19:THR:OG1	2.20	0.42
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.42
2:B:139:ASP:OD1	2:B:140:ASN:N	2.51	0.42
6:F:95:GLN:O	6:F:97:ALA:N	2.52	0.42
1:A:378:HIS:CG	1:A:425:PHE:CE1	3.07	0.42
8:H:8:ILE:O	8:H:8:ILE:HG23	2.20	0.42
1:N:127:THR:HB	1:N:129:TYR:CE1	2.54	0.42
1:N:41:LEU:HD11	1:N:54:TYR:OH	2.20	0.42
1:N:257:ILE:HG21	1:N:341:ALA:HB2	2.01	0.42
1:N:512:ASN:HD22	1:N:512:ASN:HA	1.68	0.42
3:P:68:GLN:HE21	3:P:70:HIS:CD2	2.38	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.19	0.42
4:D:46:ALA:O	5:E:56:ARG:NH1	2.47	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.19	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.44	0.42
26:P:306:CDL:CB2	26:P:306:CDL:HB32	2.49	0.42
23:O:302:CHD:H212	23:O:302:CHD:H12	2.02	0.41
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.33	0.41
6:S:95:GLN:O	6:S:97:ALA:N	2.53	0.41
3:P:16:TRP:N	3:P:17:PRO:CD	2.83	0.41
3:P:72:THR:HB	3:P:73:PRO:HD2	2.02	0.41
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.73	0.41
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:VAL:HG12	1:N:33:LEU:HD12	2.03	0.41
7:T:78:LEU:HB3	7:T:79:PRO:CD	2.50	0.41
12:Y:24:MET:HE1	19:Y:101:TGL:C16	2.50	0.41
18:A:606:PGV:H222	13:M:15:GLN:HE22	1.85	0.41
8:H:60:TYR:CD1	8:H:60:TYR:C	2.99	0.41
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.55	0.41
1:N:172:LYS:HB2	28:N:752:HOH:O	2.20	0.41
28:Q:311:HOH:O	13:Z:35:TYR:HA	2.21	0.41
26:C:306:CDL:HB32	26:C:306:CDL:HB21	2.02	0.41
3:P:204:HIS:O	3:P:208:VAL:HG23	2.20	0.41
4:Q:16:TYR:OH	4:Q:18:ASP:OD1	2.32	0.41
13:Z:32:TRP:O	13:Z:36:HIS:ND1	2.53	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.56	0.41
1:N:31:THR:O	1:N:34:SER:OG	2.29	0.41
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.03	0.41
1:N:365:ILE:HG13	2:O:87:MET:HE1	2.02	0.41
24:Q:201:DMU:H14	13:Z:27:LEU:HD22	2.02	0.41
8:U:8:ILE:O	8:U:8:ILE:HG23	2.21	0.41
10:W:32:TYR:CE1	10:W:36:MET:CE	3.04	0.41
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.40
12:L:11:ILE:CG2	19:L:101:TGL:H271	2.51	0.40
17:N:604:HEA:C2C	28:N:740:HOH:O	2.69	0.40
1:N:53:ILE:HD12	12:Y:43:GLN:HB3	2.03	0.40
1:A:218:THR:HG22	1:A:221:ASP:HB3	2.02	0.40
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.03	0.40
1:A:35:LEU:HD11	1:A:462:LEU:HB2	2.04	0.40
1:A:257:ILE:HG21	1:A:341:ALA:HB2	2.03	0.40
4:D:24:LEU:HD12	5:E:33:MET:HB2	2.03	0.40
1:N:145:LEU:HG	3:P:32:THR:HG21	2.04	0.40
1:A:169:ILE:O	1:A:172:LYS:NZ	2.55	0.40
1:A:456:MET:HG2	4:D:96:LEU:HD13	2.03	0.40
10:W:52:TRP:NE1	10:W:57:HIS:CE1	2.90	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%)	492 (96%)	19 (4%)	1 (0%)	43	72
1	N	512/514 (100%)	481 (94%)	30 (6%)	1 (0%)	43	72
2	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	14	41
2	O	225/227 (99%)	202 (90%)	19 (8%)	4 (2%)	6	25
3	C	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	30	59
3	P	257/261 (98%)	245 (95%)	11 (4%)	1 (0%)	30	59
4	D	142/147 (97%)	131 (92%)	11 (8%)	0	100	100
4	Q	142/147 (97%)	130 (92%)	12 (8%)	0	100	100
5	E	103/109 (94%)	95 (92%)	8 (8%)	0	100	100
5	R	103/109 (94%)	99 (96%)	4 (4%)	0	100	100
6	F	96/98 (98%)	83 (86%)	10 (10%)	3 (3%)	3	14
6	S	96/98 (98%)	82 (85%)	12 (12%)	2 (2%)	5	21
7	G	81/85 (95%)	64 (79%)	11 (14%)	6 (7%)	1	2
7	T	81/85 (95%)	62 (76%)	12 (15%)	7 (9%)	0	1
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	2	10
8	U	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	9	32
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	9	30
9	V	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	30
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	6	25
11	K	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	5	21
11	X	47/56 (84%)	40 (85%)	7 (15%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	39 (89%)	5 (11%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
All	All	3504/3614 (97%)	3236 (92%)	232 (7%)	36 (1%)	12	39

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	VAL
2	B	59	GLN
6	F	94	HIS
7	G	4	ALA
9	I	37	PHE
1	N	142	SER
7	T	4	ALA
7	T	7	ASP
7	T	37	LEU
2	B	60	GLU
3	C	128	GLU
6	F	96	LEU
7	G	8	HIS
7	G	41	HIS
8	H	47	GLY
2	O	60	GLU
7	T	5	LYS
7	T	8	HIS
8	U	8	ILE
9	V	37	PHE
10	W	16	ASN
7	G	3	ALA
8	H	10	ASN
11	K	7	PRO
2	O	130	PRO
2	O	202	SER
3	P	232	HIS
6	S	96	LEU
7	T	6	GLY
7	T	83	GLU
6	F	95	GLN
2	O	92	ASN
7	G	37	LEU
6	S	95	GLN
7	G	80	THR
8	H	8	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	40	73
1	N	426/426 (100%)	407 (96%)	19 (4%)	24	58
2	B	210/210 (100%)	199 (95%)	11 (5%)	21	52
2	O	210/210 (100%)	199 (95%)	11 (5%)	21	52
3	C	224/226 (99%)	222 (99%)	2 (1%)	70	90
3	P	224/226 (99%)	218 (97%)	6 (3%)	39	73
4	D	128/129 (99%)	122 (95%)	6 (5%)	23	56
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	69
5	E	92/95 (97%)	91 (99%)	1 (1%)	65	88
5	R	92/95 (97%)	86 (94%)	6 (6%)	15	44
6	F	81/81 (100%)	75 (93%)	6 (7%)	13	38
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	54
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	47
7	T	67/68 (98%)	63 (94%)	4 (6%)	17	47
8	H	71/75 (95%)	62 (87%)	9 (13%)	4	14
8	U	71/75 (95%)	66 (93%)	5 (7%)	14	40
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	52
9	V	57/57 (100%)	47 (82%)	10 (18%)	2	6
10	J	49/50 (98%)	47 (96%)	2 (4%)	27	61
10	W	49/50 (98%)	44 (90%)	5 (10%)	7	23
11	K	39/46 (85%)	37 (95%)	2 (5%)	21	53
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	53
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	53
12	Y	39/40 (98%)	34 (87%)	5 (13%)	4	14
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	12
13	Z	37/38 (97%)	35 (95%)	2 (5%)	20	51
All	All	3040/3082 (99%)	2893 (95%)	147 (5%)	23	55

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL

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Mol	Chain	Res	Type
1	A	136	LEU
1	A	138	HIS
1	A	178	GLN
1	A	180	GLN
1	A	218	THR
1	A	369	ASP
1	A	433	LEU
1	A	484	THR
1	A	489	THR
1	A	513	LEU
2	B	4	PRO
2	B	35	SER
2	B	43	SER
2	B	55	THR
2	B	68	LEU
2	B	75	LEU
2	B	88	ASP
2	B	113	TYR
2	B	167	SER
2	B	197	SER
2	B	217	LYS
3	C	159	MET
3	C	180	GLU
4	D	36	SER
4	D	43	LYS
4	D	51	LEU
4	D	107	ILE
4	D	114	GLU
4	D	143	ASN
5	E	70	VAL
6	F	33	ILE
6	F	44	GLU
6	F	48	LEU
6	F	53	THR
6	F	63	GLU
6	F	96	LEU
7	G	2	SER
7	G	33	LEU
7	G	80	THR
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS

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Mol	Chain	Res	Type
8	H	46	LYS
8	H	50	VAL
8	H	60	TYR
8	H	61	LYS
8	H	67	SER
8	H	75	ARG
8	H	85	ILE
9	I	8	GLN
9	I	15	ARG
9	I	29	LEU
10	J	27	THR
10	J	50	LEU
11	K	23	THR
11	K	49	THR
12	L	20	ARG
12	L	26	THR
13	M	2	THR
13	M	19	LEU
13	M	37	LEU
13	M	38	ASP
13	M	42	LYS
1	N	9	SER
1	N	38	ARG
1	N	57	VAL
1	N	101	SER
1	N	115	SER
1	N	138	HIS
1	N	152	LEU
1	N	189	MET
1	N	238	PHE
1	N	243	VAL
1	N	262	SER
1	N	265	LYS
1	N	369	ASP
1	N	382	SER
1	N	455	SER
1	N	484	THR
1	N	486	ASP
1	N	512	ASN
1	N	513	LEU
2	O	16	ILE
2	O	55	THR

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Mol	Chain	Res	Type
2	O	60	GLU
2	O	71	ILE
2	O	78	LEU
2	O	91	ASN
2	O	110	TYR
2	O	115	ASP
2	O	156	SER
2	O	167	SER
2	O	183	THR
3	P	14	SER
3	P	32	THR
3	P	127	LEU
3	P	159	MET
3	P	230	ASN
3	P	258	TRP
4	Q	17	VAL
4	Q	31	LYS
4	Q	143	ASN
4	Q	144	GLU
5	R	5	HIS
5	R	7	THR
5	R	70	VAL
5	R	79	LYS
5	R	80	GLU
5	R	109	VAL
6	S	12	GLN
6	S	53	THR
6	S	54	ASN
6	S	96	LEU
7	T	8	HIS
7	T	39	SER
7	T	61	SER
7	T	74	ARG
8	U	8	ILE
8	U	49	ASP
8	U	60	TYR
8	U	66	ILE
8	U	75	ARG
9	V	15	ARG
9	V	18	ARG
9	V	21	ILE
9	V	26	MET

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Mol	Chain	Res	Type
9	V	31	PHE
9	V	33	THR
9	V	36	LYS
9	V	52	ARG
9	V	61	GLU
9	V	68	ILE
10	W	27	THR
10	W	35	THR
10	W	38	LEU
10	W	50	LEU
10	W	54	SER
11	X	23	THR
11	X	26	VAL
12	Y	11	ILE
12	Y	17	ASN
12	Y	24	MET
12	Y	26	THR
12	Y	31	SER
13	Z	34	LEU
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	422	ASN
1	A	512	ASN
2	B	59	GLN
2	B	181	GLN
2	B	203	ASN
3	C	38	ASN
3	C	50	ASN
3	C	68	GLN
3	C	161	GLN
3	C	230	ASN
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
6	F	28	GLN
6	F	54	ASN
6	F	95	GLN

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Mol	Chain	Res	Type
7	G	76	ASN
8	H	22	ASN
8	H	23	GLN
11	K	35	GLN
13	M	15	GLN
1	N	4	ASN
1	N	180	GLN
1	N	496	ASN
1	N	512	ASN
2	O	10	GLN
2	O	140	ASN
2	O	181	GLN
3	P	12	ASN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN
4	Q	37	GLN
4	Q	76	ASN
4	Q	109	HIS
4	Q	119	GLN
5	R	78	HIS
5	R	94	ASN
6	S	88	HIS
7	T	8	HIS
7	T	34	ASN
7	T	66	ASN
7	T	67	HIS
7	T	76	ASN
8	U	31	GLN
8	U	37	HIS
10	W	13	GLN
10	W	21	HIS
10	W	29	ASN
11	X	15	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	FME	N	1	1	8,9,10	0.50	0	8,9,11	1.53	1 (12%)
2	FME	O	1	2	8,9,10	0.53	0	8,9,11	2.27	3 (37%)
7	TPO	T	11	7	8,10,11	1.14	1 (12%)	10,14,16	0.81	0
9	SAC	I	1	9	7,8,9	1.96	1 (14%)	7,9,11	1.63	2 (28%)
1	FME	A	1	1	8,9,10	0.59	0	8,9,11	1.63	2 (25%)
7	TPO	G	11	7	8,10,11	1.27	1 (12%)	10,14,16	0.91	1 (10%)
9	SAC	V	1	9	7,8,9	1.57	1 (14%)	7,9,11	1.49	2 (28%)
2	FME	B	1	2	8,9,10	0.67	0	8,9,11	2.30	3 (37%)

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	N	1	1	-	6/7/9/11	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-
7	TPO	G	11	7	-	2/9/11/13	-
9	SAC	V	1	9	-	5/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	CA-N	4.90	1.53	1.46
9	V	1	SAC	CA-N	3.94	1.52	1.46
7	G	11	TPO	P-OG1	2.39	1.63	1.59
7	T	11	TPO	P-OG1	2.26	1.63	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-5.03	115.08	122.82
2	O	1	FME	CA-N-CN	-4.89	115.30	122.82
1	A	1	FME	CA-N-CN	-3.28	117.78	122.82
2	O	1	FME	C-CA-N	2.99	115.28	109.50
2	B	1	FME	C-CA-N	2.94	115.18	109.50
1	N	1	FME	CA-N-CN	-2.77	118.56	122.82
9	I	1	SAC	OAC-C1A-C2A	-2.59	117.44	122.05
9	I	1	SAC	C-CA-N	2.53	114.38	109.50
9	V	1	SAC	C2A-C1A-N	2.41	120.11	116.12
1	A	1	FME	O-C-CA	-2.37	118.67	124.77
7	G	11	TPO	P-OG1-CB	-2.37	116.89	123.33
2	B	1	FME	O1-CN-N	-2.32	119.33	125.32
9	V	1	SAC	O-C-CA	-2.12	119.33	124.77
2	O	1	FME	O1-CN-N	-2.02	120.10	125.32

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-OG1
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-OG1
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	N-CA-CB-OG
9	I	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CB-CG-SD-CE
7	T	11	TPO	CB-OG1-P-O2P
9	I	1	SAC	C-CA-N-C1A
1	N	1	FME	CA-CB-CG-SD
1	N	1	FME	CB-CG-SD-CE
1	A	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	N	1	FME	C-CA-CB-CG
7	G	11	TPO	CB-OG1-P-O1P
1	N	1	FME	CB-CA-N-CN
7	T	11	TPO	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 8 are monoatomic - leaving 46 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	$\# Z > 2$
18	PGV	A	606	-	50,50,50	1.06	2 (4%)	53,56,56	1.11	5 (9%)
19	TGL	I	101	-	62,62,62	1.03	3 (4%)	65,65,65	1.34	8 (12%)
26	CDL	G	102	-	99,99,99	1.00	4 (4%)	105,111,111	0.91	6 (5%)
19	TGL	A	608	-	62,62,62	1.16	3 (4%)	65,65,65	0.89	4 (6%)
18	PGV	N	606	-	50,50,50	1.04	2 (4%)	53,56,56	1.07	3 (5%)
23	CHD	W	101	-	32,32,32	0.68	0	51,51,51	1.71	8 (15%)
17	HEA	A	604	1	67,67,67	2.39	27 (40%)	81,103,103	2.43	27 (33%)
22	PSC	B	302	-	51,51,51	1.09	3 (5%)	57,59,59	1.40	8 (14%)
25	PEK	G	101	-	52,52,52	0.90	2 (3%)	55,57,57	0.71	1 (1%)
20	PER	N	607	14,17	1,1,1	1.33	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	P	306	-	99,99,99	1.02	4 (4%)	105,111,111	1.14	6 (5%)
18	PGV	C	301	-	50,50,50	0.93	3 (6%)	53,56,56	0.73	0
18	PGV	P	301	-	50,50,50	0.93	2 (4%)	53,56,56	1.02	3 (5%)
18	PGV	P	305	-	50,50,50	1.18	2 (4%)	53,56,56	1.16	3 (5%)
20	PER	A	609	14,17	1,1,1	1.32	0	-		
18	PGV	A	607	-	50,50,50	1.12	2 (4%)	53,56,56	1.10	3 (5%)
17	HEA	A	605	20,1	67,67,67	2.46	28 (41%)	81,103,103	2.65	28 (34%)
18	PGV	C	305	-	50,50,50	1.01	2 (4%)	53,56,56	0.90	2 (3%)
23	CHD	C	307	-	32,32,32	0.67	0	51,51,51	1.49	6 (11%)
17	HEA	N	605	20,1	67,67,67	2.43	28 (41%)	81,103,103	2.48	29 (35%)
23	CHD	B	303	-	32,32,32	0.66	0	51,51,51	1.25	5 (9%)
19	TGL	O	304	-	62,62,62	1.04	3 (4%)	65,65,65	0.92	4 (6%)
24	DMU	Q	201	-	34,34,34	0.84	0	45,45,45	1.29	4 (8%)
23	CHD	C	303	-	32,32,32	0.57	0	51,51,51	1.03	2 (3%)
25	PEK	T	102	-	52,52,52	1.01	2 (3%)	55,57,57	0.86	2 (3%)
19	TGL	V	101	-	62,62,62	1.03	3 (4%)	65,65,65	0.97	6 (9%)
21	CUA	B	301	2	0,1,1	-	-	-		
25	PEK	G	103	-	52,52,52	1.03	2 (3%)	55,57,57	0.96	4 (7%)
22	PSC	O	303	-	51,51,51	1.05	2 (3%)	57,59,59	1.49	8 (14%)
25	PEK	C	304	-	52,52,52	1.00	2 (3%)	55,57,57	0.89	3 (5%)
21	CUA	O	301	2	0,1,1	-	-	-		
26	CDL	T	103	-	99,99,99	1.05	4 (4%)	105,111,111	0.93	6 (5%)
19	TGL	L	101	-	62,62,62	1.06	3 (4%)	65,65,65	0.78	3 (4%)
25	PEK	C	308	-	52,52,52	1.06	2 (3%)	55,57,57	1.03	3 (5%)
24	DMU	C	302	-	34,34,34	1.56	7 (20%)	45,45,45	1.86	9 (20%)
24	DMU	T	101	-	34,34,34	1.48	5 (14%)	45,45,45	1.54	9 (20%)
25	PEK	P	303	-	52,52,52	0.90	2 (3%)	55,57,57	0.74	2 (3%)
19	TGL	Y	101	-	62,62,62	1.08	3 (4%)	65,65,65	0.77	2 (3%)
23	CHD	O	302	-	32,32,32	0.64	0	51,51,51	1.42	8 (15%)
26	CDL	C	306	-	99,99,99	0.99	4 (4%)	105,111,111	1.11	8 (7%)
18	PGV	P	304	-	50,50,50	1.01	2 (4%)	53,56,56	0.92	4 (7%)
17	HEA	N	604	1	67,67,67	2.40	27 (40%)	81,103,103	2.42	26 (32%)
23	CHD	J	101	-	32,32,32	0.88	2 (6%)	51,51,51	2.23	17 (33%)
24	DMU	M	101	-	34,34,34	1.40	2 (5%)	45,45,45	1.24	4 (8%)
23	CHD	P	302	-	32,32,32	0.68	0	51,51,51	1.04	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	P	307	-	32,32,32	0.58	0	51,51,51	1.46	6 (11%)

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
18	PGV	A	606	-	-	32/55/55/55	-
19	TGL	I	101	-	-	38/65/65/65	-
26	CDL	G	102	-	-	42/110/110/110	-
19	TGL	A	608	-	-	33/65/65/65	-
18	PGV	N	606	-	-	33/55/55/55	-
23	CHD	W	101	-	-	7/9/74/74	0/4/4/4
17	HEA	A	604	1	-	9/36/76/76	-
22	PSC	B	302	-	-	25/55/55/55	-
25	PEK	G	101	-	-	21/56/56/56	-
26	CDL	P	306	-	-	69/110/110/110	-
18	PGV	C	301	-	-	18/55/55/55	-
18	PGV	P	301	-	-	16/55/55/55	-
18	PGV	P	305	-	-	29/55/55/55	-
18	PGV	A	607	-	-	25/55/55/55	-
23	CHD	C	307	-	-	4/9/74/74	0/4/4/4
17	HEA	A	605	20,1	-	7/36/76/76	-
18	PGV	C	305	-	-	25/55/55/55	-
17	HEA	N	605	20,1	-	8/36/76/76	-
23	CHD	B	303	-	-	6/9/74/74	0/4/4/4
19	TGL	O	304	-	-	41/65/65/65	-
24	DMU	Q	201	-	-	10/19/59/59	0/2/2/2
23	CHD	C	303	-	-	2/9/74/74	0/4/4/4
25	PEK	T	102	-	-	22/56/56/56	-
19	TGL	V	101	-	-	34/65/65/65	-
25	PEK	G	103	-	-	19/56/56/56	-
22	PSC	O	303	-	-	30/55/55/55	-
25	PEK	C	304	-	-	24/56/56/56	-
26	CDL	T	103	-	-	58/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	L	101	-	-	31/65/65/65	-
25	PEK	C	308	-	-	20/56/56/56	-
24	DMU	C	302	-	-	10/19/59/59	0/2/2/2
24	DMU	T	101	-	-	8/19/59/59	0/2/2/2
25	PEK	P	303	-	-	20/56/56/56	-
19	TGL	Y	101	-	-	28/65/65/65	-
23	CHD	O	302	-	-	4/9/74/74	0/4/4/4
26	CDL	C	306	-	-	61/110/110/110	-
18	PGV	P	304	-	-	14/55/55/55	-
17	HEA	N	604	1	-	10/36/76/76	-
23	CHD	J	101	-	-	5/9/74/74	0/4/4/4
24	DMU	M	101	-	-	9/19/59/59	0/2/2/2
23	CHD	P	302	-	-	2/9/74/74	0/4/4/4
23	CHD	P	307	-	-	5/9/74/74	0/4/4/4

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	101	DMU	O16-C6	6.88	1.51	1.40
17	N	605	HEA	FE-ND	5.72	2.12	1.94
17	A	605	HEA	FE-ND	5.48	2.11	1.94
17	N	604	HEA	C3B-C2B	5.45	1.47	1.34
17	A	605	HEA	C3B-C2B	5.40	1.47	1.34
17	A	604	HEA	C3B-C2B	5.37	1.46	1.34
17	A	605	HEA	CHC-C4B	5.25	1.49	1.38
17	A	604	HEA	FE-NB	5.24	2.11	1.94
18	A	607	PGV	O01-C1	5.18	1.48	1.34
17	N	605	HEA	C3B-C2B	5.16	1.46	1.34
17	N	604	HEA	FE-ND	5.13	2.10	1.94
17	N	604	HEA	FE-NB	5.11	2.10	1.94
17	A	605	HEA	FE-NC	5.08	2.11	1.95
18	P	305	PGV	O03-C19	5.06	1.48	1.33
18	P	305	PGV	O01-C1	5.05	1.48	1.34
25	C	304	PEK	O01-C1	5.01	1.48	1.34
26	P	306	CDL	OA6-CA5	5.00	1.48	1.34
18	N	606	PGV	O03-C19	4.95	1.47	1.33
17	N	604	HEA	FE-NA	4.88	2.11	1.95
18	A	606	PGV	O03-C19	4.88	1.47	1.33
25	T	102	PEK	O01-C1	4.87	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	605	HEA	FE-NA	4.84	2.11	1.95
17	A	604	HEA	FE-ND	4.80	2.09	1.94
19	A	608	TGL	OG2-CB1	4.78	1.47	1.34
26	P	306	CDL	OA8-CA7	4.77	1.47	1.33
25	C	308	PEK	O01-C1	4.77	1.47	1.34
22	B	302	PSC	O01-C1	4.75	1.47	1.34
17	N	604	HEA	C3D-C2D	4.74	1.47	1.36
26	C	306	CDL	OA6-CA5	4.73	1.47	1.34
17	N	605	HEA	CHB-C4A	4.72	1.47	1.38
19	A	608	TGL	OG3-CC1	4.71	1.47	1.33
17	A	604	HEA	CHD-C1D	4.70	1.47	1.38
17	N	605	HEA	CHA-C1A	4.69	1.47	1.38
22	O	303	PSC	O01-C1	4.69	1.47	1.34
25	G	103	PEK	O03-C21	4.65	1.46	1.33
19	V	101	TGL	OG2-CB1	4.63	1.47	1.34
26	T	103	CDL	OA6-CA5	4.61	1.47	1.34
17	A	605	HEA	CHB-C4A	4.59	1.47	1.38
19	Y	101	TGL	OG2-CB1	4.58	1.47	1.34
17	A	605	HEA	CHA-C1A	4.58	1.47	1.38
26	G	102	CDL	OB6-CB5	4.57	1.47	1.34
19	L	101	TGL	OG2-CB1	4.57	1.47	1.34
26	T	103	CDL	OB6-CB5	4.56	1.47	1.34
19	O	304	TGL	OG2-CB1	4.55	1.47	1.34
18	A	607	PGV	O03-C19	4.53	1.46	1.33
25	C	308	PEK	O03-C21	4.49	1.46	1.33
18	P	304	PGV	O03-C19	4.47	1.46	1.33
19	I	101	TGL	OG1-CA1	4.44	1.46	1.33
26	T	103	CDL	OB8-CB7	4.43	1.46	1.33
17	A	604	HEA	C3D-C2D	4.43	1.46	1.36
19	A	608	TGL	OG1-CA1	4.43	1.46	1.33
26	G	102	CDL	OB8-CB7	4.43	1.46	1.33
17	N	605	HEA	C3D-C2D	4.43	1.46	1.36
17	A	604	HEA	FE-NC	4.42	2.09	1.95
17	N	604	HEA	CHA-C1A	4.40	1.47	1.38
18	A	606	PGV	O01-C1	4.40	1.46	1.34
19	Y	101	TGL	OG3-CC1	4.40	1.46	1.33
26	G	102	CDL	OA8-CA7	4.40	1.46	1.33
18	P	304	PGV	O01-C1	4.40	1.46	1.34
18	C	305	PGV	O03-C19	4.39	1.46	1.33
17	N	605	HEA	FE-NC	4.35	2.09	1.95
17	N	604	HEA	CHD-C1D	4.35	1.47	1.38
26	C	306	CDL	OB6-CB5	4.35	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	103	CDL	OA8-CA7	4.34	1.46	1.33
19	I	101	TGL	OG2-CB1	4.33	1.46	1.34
19	O	304	TGL	OG1-CA1	4.32	1.45	1.33
17	A	605	HEA	C3D-C2D	4.32	1.46	1.36
17	N	605	HEA	CHB-C1B	4.30	1.49	1.39
25	T	102	PEK	O03-C21	4.30	1.45	1.33
17	A	604	HEA	CHD-C4C	4.28	1.49	1.39
19	L	101	TGL	OG3-CC1	4.26	1.45	1.33
18	C	301	PGV	O03-C19	4.26	1.45	1.33
17	A	604	HEA	CHB-C4A	4.25	1.46	1.38
17	A	604	HEA	CHC-C4B	4.24	1.47	1.38
25	P	303	PEK	O03-C21	4.24	1.45	1.33
22	B	302	PSC	O03-C19	4.23	1.45	1.33
26	G	102	CDL	OA6-CA5	4.22	1.46	1.34
25	G	103	PEK	O01-C1	4.21	1.46	1.34
17	N	604	HEA	CHB-C4A	4.20	1.46	1.38
26	P	306	CDL	OB8-CB7	4.19	1.45	1.33
17	N	604	HEA	C3A-C2A	4.19	1.46	1.37
17	A	604	HEA	FE-NA	4.19	2.09	1.95
19	Y	101	TGL	OG1-CA1	4.18	1.45	1.33
19	L	101	TGL	OG1-CA1	4.17	1.45	1.33
22	O	303	PSC	O03-C19	4.15	1.45	1.33
18	P	301	PGV	O03-C19	4.13	1.45	1.33
17	A	605	HEA	FE-NA	4.12	2.08	1.95
17	N	605	HEA	FE-NB	4.11	2.07	1.94
18	P	301	PGV	O01-C1	4.10	1.45	1.34
17	A	605	HEA	CHC-C1C	4.08	1.48	1.39
18	C	305	PGV	O01-C1	4.07	1.45	1.34
26	C	306	CDL	OB8-CB7	4.04	1.45	1.33
25	C	304	PEK	O03-C21	4.01	1.45	1.33
17	A	604	HEA	CHA-C1A	4.01	1.46	1.38
17	N	605	HEA	C4B-NB	-3.95	1.33	1.40
18	N	606	PGV	O01-C1	3.93	1.45	1.34
26	C	306	CDL	OA8-CA7	3.92	1.44	1.33
24	T	101	DMU	O1-C10	3.91	1.51	1.41
17	N	604	HEA	FE-NC	3.90	2.08	1.95
17	A	605	HEA	FE-NB	3.89	2.06	1.94
17	N	605	HEA	C3A-C2A	3.86	1.46	1.37
26	P	306	CDL	OB6-CB5	3.85	1.45	1.34
17	N	604	HEA	CHD-C4C	3.85	1.48	1.39
17	A	605	HEA	C3A-C2A	3.81	1.45	1.37
19	O	304	TGL	OG3-CC1	3.80	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	101	PEK	O01-C1	3.80	1.45	1.34
19	V	101	TGL	OG3-CC1	3.79	1.44	1.33
17	A	604	HEA	CHC-C1C	3.79	1.47	1.39
17	N	605	HEA	CHC-C4B	3.78	1.46	1.38
17	A	605	HEA	C4B-NB	-3.76	1.33	1.40
19	V	101	TGL	OG1-CA1	3.74	1.44	1.33
25	G	101	PEK	O03-C21	3.73	1.44	1.33
18	C	301	PGV	O01-C1	3.73	1.44	1.34
17	N	604	HEA	CHC-C1C	3.70	1.47	1.39
17	A	604	HEA	C4A-NA	-3.67	1.32	1.39
24	T	101	DMU	O16-C6	3.64	1.46	1.40
25	P	303	PEK	O01-C1	3.62	1.44	1.34
17	A	605	HEA	C1D-ND	-3.62	1.34	1.40
17	N	605	HEA	CHD-C1D	3.61	1.45	1.38
24	C	302	DMU	O7-C10	3.58	1.51	1.41
17	A	605	HEA	CHA-C4D	3.53	1.47	1.39
17	A	604	HEA	C4B-C3B	3.53	1.50	1.44
17	A	605	HEA	C4A-NA	-3.53	1.33	1.39
24	C	302	DMU	O7-C3	3.51	1.52	1.43
17	N	604	HEA	CHB-C1B	3.50	1.47	1.39
17	N	604	HEA	CHC-C4B	3.47	1.45	1.38
24	C	302	DMU	O16-C6	3.47	1.46	1.40
17	N	605	HEA	CHC-C1C	3.40	1.47	1.39
17	A	605	HEA	C1B-NB	-3.39	1.32	1.38
17	A	605	HEA	CHD-C1D	3.39	1.45	1.38
17	N	605	HEA	CHA-C4D	3.31	1.46	1.39
19	I	101	TGL	OG3-CC1	3.31	1.43	1.33
17	N	604	HEA	C11-C3B	-3.28	1.47	1.51
17	N	605	HEA	CHD-C4C	3.26	1.46	1.39
17	A	604	HEA	C1D-ND	-3.24	1.34	1.40
17	A	604	HEA	C3A-C2A	3.21	1.44	1.37
24	T	101	DMU	O7-C3	3.19	1.52	1.43
24	T	101	DMU	O7-C10	3.12	1.50	1.41
17	A	605	HEA	CHB-C1B	3.07	1.46	1.39
17	N	604	HEA	CHA-C4D	3.06	1.46	1.39
17	A	604	HEA	CHA-C4D	3.04	1.46	1.39
17	N	604	HEA	C1D-ND	-2.95	1.35	1.40
17	N	605	HEA	C1D-ND	-2.93	1.35	1.40
17	A	605	HEA	CHD-C4C	2.90	1.45	1.39
17	A	604	HEA	CHB-C1B	2.84	1.45	1.39
17	N	604	HEA	C4A-NA	-2.82	1.34	1.39
17	N	605	HEA	C4A-NA	-2.80	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	605	HEA	C1B-NB	-2.78	1.33	1.38
17	N	604	HEA	C4B-NB	-2.77	1.35	1.40
17	A	605	HEA	C1C-C2C	2.77	1.49	1.43
17	N	605	HEA	C1C-NC	-2.73	1.34	1.39
17	N	604	HEA	C1C-NC	-2.73	1.34	1.39
17	A	605	HEA	C4D-C3D	2.59	1.49	1.45
17	A	604	HEA	C1D-C2D	2.57	1.49	1.44
17	A	604	HEA	C1B-NB	-2.57	1.33	1.38
24	T	101	DMU	C10-C5	2.56	1.60	1.52
17	N	605	HEA	C4C-NC	-2.56	1.34	1.39
17	N	605	HEA	C1C-C2C	2.55	1.49	1.43
17	N	605	HEA	C1A-C2A	2.55	1.49	1.45
24	C	302	DMU	C8-C9	2.52	1.58	1.53
17	A	605	HEA	C4D-ND	-2.50	1.33	1.38
17	N	604	HEA	C1C-C2C	2.49	1.49	1.43
17	A	604	HEA	C4C-NC	-2.48	1.35	1.39
24	C	302	DMU	C10-C5	2.47	1.59	1.52
17	A	604	HEA	C1B-C2B	2.43	1.49	1.44
17	A	604	HEA	C4D-ND	-2.41	1.34	1.38
24	M	101	DMU	O5-C6	2.39	1.48	1.41
17	A	605	HEA	C1A-NA	-2.38	1.35	1.39
17	N	604	HEA	C4B-C3B	2.38	1.48	1.44
17	N	604	HEA	C4C-NC	-2.38	1.35	1.39
17	N	604	HEA	C1A-C2A	2.38	1.49	1.45
24	C	302	DMU	O1-C10	2.38	1.48	1.41
17	A	605	HEA	C1C-NC	-2.37	1.35	1.39
17	A	605	HEA	C4C-NC	-2.33	1.35	1.39
17	A	604	HEA	C1A-NA	-2.33	1.35	1.39
17	A	605	HEA	C11-C3B	-2.32	1.48	1.51
17	A	604	HEA	C4B-NB	-2.22	1.36	1.40
17	N	605	HEA	C4D-ND	-2.22	1.34	1.38
17	A	604	HEA	C1C-NC	-2.19	1.35	1.39
23	J	101	CHD	C20-C17	2.18	1.58	1.54
23	J	101	CHD	C23-C24	2.17	1.55	1.50
24	C	302	DMU	C2-C1	2.17	1.58	1.52
17	A	604	HEA	C11-C3B	-2.16	1.48	1.51
17	N	605	HEA	C3A-C4A	2.15	1.49	1.46
17	A	605	HEA	C4B-C3B	2.14	1.48	1.44
17	N	605	HEA	C11-C3B	-2.14	1.48	1.51
17	A	605	HEA	C1D-C2D	2.12	1.48	1.44
17	N	604	HEA	C4D-ND	-2.11	1.34	1.38
18	C	301	PGV	O01-C02	-2.09	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	302	PSC	C05-N	-2.07	1.45	1.51
17	N	604	HEA	C3C-C2C	2.01	1.47	1.41
17	N	605	HEA	C1A-NA	-2.01	1.35	1.39
17	N	604	HEA	C1B-C2B	2.00	1.48	1.44
17	N	605	HEA	C4B-C3B	2.00	1.48	1.44

All (298) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	604	HEA	C3A-C2A-C1A	-8.76	98.76	107.05
17	N	605	HEA	C3A-C2A-C1A	-7.59	99.86	107.05
17	A	605	HEA	C3C-C4C-NC	7.53	116.14	109.80
17	N	604	HEA	C2A-C1A-NA	7.48	117.54	110.32
17	A	605	HEA	C3A-C2A-C1A	-7.48	99.97	107.05
24	C	302	DMU	C10-O7-C3	7.22	135.09	117.98
17	A	604	HEA	C3A-C2A-C1A	-6.80	100.61	107.05
23	J	101	CHD	C6-C5-C10	6.76	119.86	112.66
17	N	605	HEA	C2A-C1A-NA	6.72	116.81	110.32
17	A	605	HEA	C3D-C4D-ND	6.70	116.82	110.35
17	A	605	HEA	C2D-C1D-ND	6.47	117.28	109.84
19	I	101	TGL	OG2-CB1-CB2	6.41	125.35	111.48
17	A	605	HEA	C2A-C1A-NA	6.41	116.51	110.32
17	N	605	HEA	C2D-C1D-ND	6.36	117.15	109.84
26	P	306	CDL	OA6-CA5-C11	6.34	125.19	111.48
17	A	604	HEA	C2B-C1B-NB	6.27	117.15	109.90
17	N	604	HEA	C3D-C4D-ND	6.20	116.34	110.35
17	N	605	HEA	C3D-C4D-ND	6.15	116.30	110.35
17	A	604	HEA	C3D-C4D-ND	5.63	115.80	110.35
17	A	604	HEA	C3B-C4B-NB	5.58	116.25	109.84
17	N	605	HEA	C3C-C4C-NC	5.54	114.47	109.80
17	A	604	HEA	C2A-C1A-NA	5.43	115.56	110.32
23	W	101	CHD	C22-C20-C17	5.34	121.39	110.33
18	P	305	PGV	O01-C1-C2	5.31	122.96	111.48
24	C	302	DMU	C18-O16-C6	5.29	122.72	113.68
17	A	604	HEA	C3C-C2C-C1C	-5.27	100.96	107.17
18	A	607	PGV	O01-C1-C2	5.24	122.81	111.48
17	N	605	HEA	C1D-C2D-C3D	-5.24	101.47	106.98
17	A	605	HEA	C2B-C1B-NB	5.05	115.75	109.90
22	O	303	PSC	C08-N-C06	-5.02	95.79	108.98
23	J	101	CHD	C22-C20-C17	4.84	120.36	110.33
17	A	605	HEA	C1D-C2D-C3D	-4.84	101.89	106.98
26	C	306	CDL	OA6-CA5-C11	4.83	121.94	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	O	303	PSC	C08-N-C07	-4.81	96.35	108.98
17	N	604	HEA	C2D-C1D-ND	4.72	115.27	109.84
25	C	308	PEK	O01-C1-C2	4.62	121.48	111.48
23	J	101	CHD	C9-C10-C5	4.61	114.92	108.51
24	Q	201	DMU	C18-O16-C6	4.59	121.52	113.68
24	T	101	DMU	C10-O1-C9	4.57	122.65	113.72
17	N	605	HEA	C3C-C2C-C1C	-4.56	101.79	107.17
17	A	604	HEA	C2D-C1D-ND	4.53	115.04	109.84
23	J	101	CHD	C10-C9-C8	4.46	116.81	111.84
17	N	604	HEA	C3B-C4B-NB	4.46	114.97	109.84
18	A	606	PGV	O01-C1-C2	4.40	120.99	111.48
17	A	604	HEA	C1D-C2D-C3D	-4.39	102.36	106.98
23	P	307	CHD	C1-C2-C3	4.36	116.25	110.48
23	P	307	CHD	C10-C9-C8	4.35	116.68	111.84
26	G	102	CDL	OB6-CB5-C51	4.34	120.87	111.48
23	C	307	CHD	C10-C9-C8	4.33	116.67	111.84
22	B	302	PSC	C08-N-C06	-4.33	97.60	108.98
22	O	303	PSC	C07-N-C06	4.33	120.35	108.98
26	T	103	CDL	OA6-CA5-C11	4.33	120.84	111.48
25	G	103	PEK	O01-C1-C2	4.32	120.82	111.48
17	N	604	HEA	C3C-C2C-C1C	-4.28	102.12	107.17
23	J	101	CHD	C5-C6-C7	4.27	119.48	114.40
17	A	605	HEA	C3C-C2C-C1C	-4.24	102.18	107.17
17	N	604	HEA	C3C-C4C-NC	4.24	113.37	109.80
17	A	604	HEA	CMD-C2D-C1D	4.11	131.45	125.03
17	A	605	HEA	C3B-C4B-NB	4.10	114.56	109.84
17	N	605	HEA	C3B-C4B-NB	4.09	114.54	109.84
26	P	306	CDL	OB6-CB5-C51	4.04	120.22	111.48
22	B	302	PSC	C08-N-C07	-3.98	98.51	108.98
18	P	305	PGV	O03-C19-C20	3.88	123.66	111.83
17	A	605	HEA	CMD-C2D-C1D	3.88	131.09	125.03
23	W	101	CHD	C17-C13-C14	-3.83	96.27	100.11
17	A	605	HEA	CAD-CBD-CGD	-3.81	103.57	113.67
24	M	101	DMU	O5-C6-O16	3.79	119.01	110.04
17	A	605	HEA	C1B-C2B-C3B	-3.79	102.41	106.80
23	J	101	CHD	C13-C17-C20	3.77	124.06	119.48
18	N	606	PGV	O01-C1-C2	3.77	119.63	111.48
17	A	604	HEA	CHA-C4D-C3D	-3.76	119.29	124.77
22	B	302	PSC	C07-N-C06	3.76	118.84	108.98
17	N	604	HEA	C1D-C2D-C3D	-3.74	103.05	106.98
17	N	604	HEA	C2B-C1B-NB	3.73	114.21	109.90
26	T	103	CDL	OB6-CB5-C51	3.70	119.50	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	102	PEK	O01-C1-C2	3.68	119.44	111.48
18	N	606	PGV	O03-C19-C20	3.67	123.04	111.83
18	A	606	PGV	O03-C19-C20	3.63	122.90	111.83
23	J	101	CHD	C6-C7-C8	3.62	115.45	111.50
17	A	605	HEA	C2C-C1C-NC	3.61	115.93	110.14
23	W	101	CHD	C16-C17-C20	3.59	117.61	112.18
18	A	607	PGV	O03-C19-C20	3.59	122.78	111.83
19	I	101	TGL	OG1-CA1-CA2	3.57	122.73	111.83
25	C	304	PEK	O01-C1-C2	3.53	119.13	111.48
17	A	605	HEA	C13-C12-C11	-3.50	108.80	114.39
17	A	604	HEA	C1B-C2B-C3B	-3.50	102.74	106.80
17	A	605	HEA	C4C-C3C-C2C	-3.50	102.95	107.30
17	A	604	HEA	CMB-C2B-C1B	3.48	130.47	125.03
17	A	604	HEA	C4B-C3B-C2B	-3.47	101.61	107.44
19	A	608	TGL	OG2-CB1-CB2	3.46	118.97	111.48
18	P	301	PGV	O01-C1-C2	3.46	118.96	111.48
22	B	302	PSC	O01-C1-C2	3.46	118.96	111.48
17	N	604	HEA	CHA-C4D-C3D	-3.44	119.76	124.77
19	V	101	TGL	OG2-CB1-CB2	3.43	118.90	111.48
17	N	605	HEA	CMD-C2D-C1D	3.41	130.37	125.03
17	N	604	HEA	CHA-C1A-C2A	-3.40	119.49	124.86
19	O	304	TGL	OG2-CB1-CB2	3.40	118.84	111.48
26	P	306	CDL	OA8-CA7-C31	3.39	122.18	111.83
24	T	101	DMU	C10-O7-C3	3.39	126.00	117.98
23	J	101	CHD	C19-C10-C1	-3.37	102.94	108.31
24	M	101	DMU	O5-C6-C1	-3.33	103.53	110.37
17	A	604	HEA	CAA-CBA-CGA	-3.33	104.83	113.67
17	A	605	HEA	C4D-C3D-C2D	-3.32	102.06	106.89
17	N	604	HEA	C4D-C3D-C2D	-3.29	102.11	106.89
23	C	307	CHD	C9-C10-C5	3.27	113.05	108.51
17	A	605	HEA	CAD-C3D-C4D	3.26	130.38	124.70
26	G	102	CDL	OA6-CA5-C11	3.26	118.53	111.48
26	T	103	CDL	OA8-CA7-C31	3.25	121.75	111.83
24	C	302	DMU	O7-C3-C4	3.24	117.97	109.48
26	G	102	CDL	OA8-CA7-C31	3.22	121.66	111.83
23	W	101	CHD	C14-C13-C12	3.20	110.34	107.42
17	A	604	HEA	CHC-C4B-NB	-3.20	120.41	124.37
26	C	306	CDL	OB6-CB5-C51	3.19	118.39	111.48
17	N	605	HEA	C4B-C3B-C2B	-3.19	102.08	107.44
23	C	307	CHD	C14-C8-C9	-3.18	105.31	109.75
26	C	306	CDL	OA8-CA7-C31	3.18	121.53	111.83
23	P	307	CHD	C11-C9-C8	-3.18	106.19	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C21-C20-C17	-3.16	108.14	112.88
17	N	605	HEA	CHA-C1A-C2A	-3.13	119.92	124.86
17	N	604	HEA	CAA-C2A-C1A	3.12	131.20	124.85
22	O	303	PSC	O03-C19-C20	3.10	121.28	111.83
17	A	605	HEA	CHA-C4D-C3D	-3.09	120.27	124.77
18	C	305	PGV	O01-C1-C2	3.09	118.16	111.48
19	V	101	TGL	CG2-OG2-CB1	3.07	125.15	117.80
23	O	302	CHD	C6-C5-C4	-3.07	107.72	111.23
23	O	302	CHD	C4-C3-C2	3.05	114.34	110.62
25	C	308	PEK	O01-C1-O02	-3.05	116.58	123.70
19	Y	101	TGL	OG2-CB1-CB2	3.05	118.08	111.48
17	N	604	HEA	OMA-CMA-C3A	-3.04	118.77	125.62
23	B	303	CHD	C6-C5-C4	-3.03	107.77	111.23
22	B	302	PSC	C08-N-C05	-3.03	97.88	109.91
17	N	605	HEA	C2C-C1C-NC	3.02	114.98	110.14
22	O	303	PSC	C08-N-C05	-3.00	97.97	109.91
17	N	605	HEA	CAA-C2A-C1A	3.00	130.96	124.85
17	A	604	HEA	OMA-CMA-C3A	-3.00	118.84	125.62
19	I	101	TGL	CG2-OG2-CB1	3.00	124.98	117.80
17	N	605	HEA	OMA-CMA-C3A	-3.00	118.85	125.62
17	A	605	HEA	CHA-C1A-C2A	-2.99	120.14	124.86
26	C	306	CDL	OA6-CA5-OA7	-2.99	116.72	123.70
17	N	605	HEA	C2B-C1B-NB	2.98	113.35	109.90
17	A	604	HEA	CHB-C1B-C2B	-2.98	120.32	125.03
19	A	608	TGL	OG3-CC1-CC2	2.98	120.93	111.83
23	B	303	CHD	C19-C10-C1	-2.97	103.58	108.31
17	N	605	HEA	CAD-CBD-CGD	-2.97	105.79	113.67
17	A	605	HEA	C4B-C3B-C2B	-2.97	102.45	107.44
17	A	604	HEA	C2C-C1C-NC	2.96	114.88	110.14
17	N	604	HEA	C4B-C3B-C2B	-2.96	102.47	107.44
24	Q	201	DMU	C7-C8-C9	2.92	115.52	110.23
17	N	604	HEA	CMB-C2B-C1B	2.91	129.58	125.03
23	C	307	CHD	C1-C2-C3	2.91	114.34	110.48
17	A	605	HEA	CMB-C2B-C1B	2.91	129.57	125.03
17	A	605	HEA	CAA-C2A-C1A	2.90	130.75	124.85
17	N	605	HEA	CHA-C4D-C3D	-2.90	120.54	124.77
26	T	103	CDL	OA8-CA7-OA9	-2.90	116.38	123.63
24	M	101	DMU	C22-C19-C18	-2.90	100.88	113.47
23	O	302	CHD	C19-C10-C1	-2.90	103.70	108.31
19	O	304	TGL	OG1-CA1-CA2	2.89	120.66	111.83
24	Q	201	DMU	O5-C6-O16	-2.86	103.28	110.04
23	W	101	CHD	C6-C7-C8	2.86	114.62	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	604	HEA	CAA-C2A-C1A	2.83	130.61	124.85
17	N	604	HEA	C12-C13-C14	-2.81	104.77	112.16
22	O	303	PSC	O01-C1-C2	2.81	117.56	111.48
17	A	605	HEA	CBD-CAD-C3D	2.79	120.23	112.53
23	P	302	CHD	C19-C10-C1	-2.78	103.88	108.31
17	A	605	HEA	C1D-ND-C4D	-2.78	101.91	105.21
25	T	102	PEK	O03-C21-C22	2.77	120.29	111.83
24	C	302	DMU	C6-C1-C2	2.76	115.82	110.01
23	J	101	CHD	C16-C17-C20	2.76	116.35	112.18
23	B	303	CHD	C1-C10-C9	2.75	115.61	111.34
17	N	605	HEA	CHB-C4A-NA	-2.75	121.46	124.45
17	A	605	HEA	CMC-C2C-C1C	2.74	129.60	125.42
17	N	605	HEA	C1D-ND-C4D	-2.72	101.98	105.21
17	A	604	HEA	C4D-C3D-C2D	-2.72	102.93	106.89
23	C	307	CHD	C11-C9-C8	-2.71	106.88	110.89
22	B	302	PSC	O03-C19-C20	2.71	120.09	111.83
17	A	605	HEA	CHD-C1D-C2D	-2.70	119.27	126.95
24	M	101	DMU	C18-O16-C6	-2.68	109.10	113.68
18	P	301	PGV	O03-C19-C20	2.67	119.98	111.83
17	N	604	HEA	CHB-C1B-C2B	-2.67	120.81	125.03
17	N	604	HEA	C1B-C2B-C3B	-2.66	103.72	106.80
24	C	302	DMU	C10-O1-C9	2.64	118.88	113.72
25	C	308	PEK	O03-C21-C22	2.63	119.86	111.83
23	J	101	CHD	C22-C23-C24	2.63	119.50	112.49
24	T	101	DMU	C18-O16-C6	2.63	118.17	113.68
24	T	101	DMU	C25-C22-C19	-2.61	101.15	114.37
17	N	605	HEA	C4C-C3C-C2C	-2.61	104.05	107.30
26	C	306	CDL	OA8-CA7-OA9	-2.61	117.10	123.63
17	N	605	HEA	C4D-C3D-C2D	-2.61	103.10	106.89
17	N	604	HEA	CMD-C2D-C1D	2.60	129.10	125.03
19	A	608	TGL	OG1-CA1-CA2	2.59	119.73	111.83
17	A	604	HEA	CAD-C3D-C4D	2.58	129.20	124.70
19	I	101	TGL	OG3-CC1-CC2	2.58	119.69	111.83
17	N	605	HEA	CMB-C2B-C1B	2.57	129.06	125.03
24	T	101	DMU	O1-C10-C5	2.57	115.66	110.37
17	N	605	HEA	CMC-C2C-C1C	2.57	129.34	125.42
23	C	303	CHD	C15-C14-C13	2.57	106.03	103.54
24	C	302	DMU	C1-C2-C3	2.57	115.51	109.68
25	G	103	PEK	O01-C1-O02	-2.56	117.72	123.70
19	V	101	TGL	OG2-CG2-CG3	2.56	117.53	108.34
24	C	302	DMU	O16-C18-C19	-2.56	100.69	109.37
19	O	304	TGL	OG3-CC1-CC2	2.56	119.63	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	304	PGV	O03-C19-O04	-2.55	117.24	123.63
23	J	101	CHD	C5-C4-C3	2.55	116.56	112.71
23	W	101	CHD	C4-C3-C2	2.54	113.72	110.62
25	C	304	PEK	O03-C21-C22	2.54	119.57	111.83
17	N	604	HEA	O11-C11-C3B	-2.52	106.64	111.26
18	P	304	PGV	O03-C19-C20	2.51	119.49	111.83
25	G	101	PEK	O01-C1-C2	2.51	116.91	111.48
17	A	604	HEA	C4B-NB-C1B	-2.51	102.24	105.21
26	C	306	CDL	OB8-CB7-C71	2.50	119.47	111.83
23	P	307	CHD	C2-C1-C10	2.50	116.97	112.74
23	J	101	CHD	C6-C5-C4	-2.50	108.37	111.23
25	P	303	PEK	O01-C1-C2	2.50	116.88	111.48
26	C	306	CDL	C52-C51-CB5	-2.49	104.58	113.69
22	B	302	PSC	C04-C05-N	-2.48	107.86	115.82
17	N	605	HEA	C1B-C2B-C3B	-2.48	103.93	106.80
24	T	101	DMU	C31-C28-C25	-2.48	101.85	114.37
18	A	607	PGV	O03-C19-O04	-2.47	117.44	123.63
19	I	101	TGL	OG2-CB1-OB1	-2.46	117.95	123.70
17	N	604	HEA	O2D-CGD-CBD	2.45	121.73	114.00
25	G	103	PEK	C01-O03-C21	2.45	126.06	117.12
24	T	101	DMU	O1-C9-C11	2.45	112.50	106.44
24	C	302	DMU	C2-C3-C4	-2.44	105.52	110.93
26	P	306	CDL	CB4-OB6-CB5	-2.44	111.96	117.80
24	T	101	DMU	C7-C8-C9	-2.43	105.82	110.23
17	A	605	HEA	OMA-CMA-C3A	-2.43	120.14	125.62
17	N	605	HEA	CAD-C3D-C4D	2.43	128.93	124.70
23	P	307	CHD	C14-C8-C9	-2.42	106.36	109.75
26	G	102	CDL	OA8-CA7-OA9	-2.42	117.58	123.63
17	N	605	HEA	CHB-C1B-C2B	-2.41	121.22	125.03
17	A	604	HEA	C3C-C4C-NC	2.41	111.83	109.80
22	B	302	PSC	C06-N-C05	2.40	119.46	109.91
23	C	303	CHD	C6-C5-C4	-2.40	108.49	111.23
17	N	604	HEA	C4C-C3C-C2C	-2.39	104.33	107.30
19	I	101	TGL	OG1-CA1-OA1	-2.39	117.65	123.63
26	G	102	CDL	OB8-CB7-C71	2.38	119.11	111.83
17	N	604	HEA	C2C-C1C-NC	2.38	113.96	110.14
26	T	103	CDL	OB8-CB7-C71	2.37	119.06	111.83
19	I	101	TGL	CG3-OG3-CC1	2.37	125.77	117.12
25	G	103	PEK	O03-C21-C22	2.36	119.04	111.83
24	T	101	DMU	O16-C18-C19	-2.36	101.37	109.37
23	O	302	CHD	C23-C22-C20	2.36	118.86	114.46
23	W	101	CHD	C9-C11-C12	-2.35	111.21	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	606	PGV	O01-C1-O02	-2.35	118.20	123.70
24	Q	201	DMU	C8-C7-C5	2.34	114.94	110.83
19	Y	101	TGL	OG3-CC1-CC2	2.34	118.96	111.83
18	C	305	PGV	O03-C19-C20	2.34	118.96	111.83
17	A	605	HEA	CHB-C1B-C2B	-2.34	121.34	125.03
18	P	304	PGV	O01-C1-C2	2.33	116.53	111.48
17	N	605	HEA	CHD-C1D-C2D	-2.31	120.38	126.95
18	N	606	PGV	O01-C1-O02	-2.31	118.31	123.70
23	P	302	CHD	C6-C5-C4	-2.31	108.59	111.23
23	J	101	CHD	C19-C10-C5	-2.30	106.59	110.44
26	C	306	CDL	OB8-CB7-OB9	-2.30	117.87	123.63
19	I	101	TGL	OG3-CC1-OC1	-2.30	117.88	123.63
23	O	302	CHD	C1-C10-C9	2.30	114.91	111.34
17	N	605	HEA	O2A-CGA-CBA	2.28	121.21	114.00
19	A	608	TGL	OG3-CC1-OC1	-2.28	117.94	123.63
17	A	604	HEA	CHC-C1C-C2C	-2.27	120.84	127.43
17	A	604	HEA	C26-C15-C16	2.26	119.15	115.23
23	O	302	CHD	C5-C4-C3	2.26	116.11	112.71
26	P	306	CDL	OA6-CA5-OA7	-2.25	118.44	123.70
22	O	303	PSC	O03-C19-O04	-2.25	118.00	123.63
26	T	103	CDL	OB8-CB7-OB9	-2.25	118.01	123.63
23	O	302	CHD	C6-C7-C8	2.24	113.95	111.50
19	V	101	TGL	OG1-CA1-CA2	2.23	118.62	111.83
18	P	301	PGV	O01-C1-O02	-2.22	118.51	123.70
17	N	604	HEA	CHC-C1C-C2C	-2.22	120.98	127.43
23	B	303	CHD	C22-C20-C17	2.21	114.91	110.33
22	O	303	PSC	C06-N-C05	2.21	118.69	109.91
19	L	101	TGL	OG3-CC1-CC2	2.20	118.55	111.83
23	P	302	CHD	C13-C17-C20	2.20	122.15	119.48
23	J	101	CHD	O26-C24-C23	2.20	120.95	114.00
25	C	304	PEK	C03-C02-C01	-2.19	106.67	111.78
23	O	302	CHD	O25-C24-C23	-2.19	116.14	123.09
18	A	606	PGV	O03-C19-O04	-2.19	118.14	123.63
25	P	303	PEK	O01-C1-O02	-2.18	118.60	123.70
26	G	102	CDL	OA6-CA5-OA7	-2.17	118.63	123.70
23	J	101	CHD	O12-C12-C11	-2.17	104.72	109.12
17	A	604	HEA	O2D-CGD-O1D	-2.16	117.79	123.33
24	C	302	DMU	O7-C10-C5	2.15	113.38	108.09
23	J	101	CHD	C1-C10-C5	2.14	110.81	107.75
17	A	604	HEA	CHA-C1A-C2A	-2.13	121.50	124.86
19	V	101	TGL	OG1-CA1-OA1	-2.13	118.31	123.63
23	P	307	CHD	C11-C12-C13	2.12	113.42	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	101	TGL	OG3-CC1-CC2	2.11	118.27	111.83
18	P	305	PGV	O01-C1-O02	-2.09	118.82	123.70
26	P	306	CDL	CA4-OA6-CA5	2.09	122.80	117.80
18	P	304	PGV	C02-O01-C1	2.09	122.80	117.80
23	C	307	CHD	C19-C10-C5	-2.08	106.95	110.44
19	L	101	TGL	OG3-CC1-OC1	-2.08	118.43	123.63
17	N	604	HEA	CAD-C3D-C4D	2.05	128.27	124.70
23	B	303	CHD	C16-C17-C20	2.05	115.28	112.18
18	A	606	PGV	C02-O01-C1	2.04	122.68	117.80
23	J	101	CHD	C18-C13-C12	-2.04	107.02	109.06
17	N	605	HEA	CBA-CAA-C2A	2.04	118.16	112.53
19	O	304	TGL	OG3-CC1-OC1	-2.03	118.56	123.63
19	L	101	TGL	OG2-CB1-CB2	2.01	115.82	111.48

There are no chirality outliers.

All (914) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C03-O11-P-O14
18	A	606	PGV	C04-O12-P-O11
18	A	606	PGV	C04-O12-P-O13
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
18	A	606	PGV	O02-C1-O01-C02
18	A	606	PGV	C2-C1-O01-C02
18	A	606	PGV	O04-C19-O03-C01
18	A	606	PGV	C20-C19-O03-C01
18	A	607	PGV	C04-C05-C06-O06
18	A	607	PGV	O05-C05-C06-O06
18	C	305	PGV	C04-C05-C06-O06
18	N	606	PGV	C03-O11-P-O12
18	N	606	PGV	C03-O11-P-O13
18	N	606	PGV	C03-O11-P-O14
18	N	606	PGV	C04-O12-P-O11
18	N	606	PGV	C04-O12-P-O13
18	N	606	PGV	C04-O12-P-O14
18	N	606	PGV	O02-C1-O01-C02
18	N	606	PGV	O04-C19-O03-C01
18	N	606	PGV	C20-C19-O03-C01
18	P	304	PGV	C04-C05-C06-O06
18	P	304	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
18	P	305	PGV	C03-O11-P-O12
18	P	305	PGV	C03-O11-P-O13
18	P	305	PGV	C05-C04-O12-P
18	P	305	PGV	C04-C05-C06-O06
18	P	305	PGV	C2-C1-O01-C02
19	I	101	TGL	OB1-CB1-OG2-CG2
19	V	101	TGL	OG1-CG1-CG2-OG2
22	B	302	PSC	C03-O11-P-O12
22	B	302	PSC	C03-O11-P-O13
22	B	302	PSC	C04-O12-P-O11
22	B	302	PSC	C04-O12-P-O13
22	B	302	PSC	C04-O12-P-O14
22	B	302	PSC	O12-C04-C05-N
22	O	303	PSC	C03-O11-P-O12
22	O	303	PSC	C03-O11-P-O13
22	O	303	PSC	C03-O11-P-O14
22	O	303	PSC	C04-O12-P-O11
22	O	303	PSC	C04-O12-P-O14
22	O	303	PSC	C9-C10-C11-C12
24	M	101	DMU	O5-C6-O16-C18
24	Q	201	DMU	C1-C6-O16-C18
24	Q	201	DMU	O5-C6-O16-C18
25	C	304	PEK	C03-O11-P-O13
25	C	304	PEK	C6-C7-C8-C9
25	C	308	PEK	C03-O11-P-O12
25	C	308	PEK	C03-O11-P-O13
25	C	308	PEK	O12-C04-C05-N
25	G	103	PEK	O12-C04-C05-N
25	G	103	PEK	C6-C7-C8-C9
25	T	102	PEK	C03-O11-P-O12
25	T	102	PEK	C04-O12-P-O11
25	T	102	PEK	C04-O12-P-O14
26	C	306	CDL	CA2-OA2-PA1-OA4
26	C	306	CDL	CA2-OA2-PA1-OA5
26	C	306	CDL	CA3-OA5-PA1-OA3
26	C	306	CDL	CA4-CA3-OA5-PA1
26	C	306	CDL	OA7-CA5-OA6-CA4
26	C	306	CDL	C11-CA5-OA6-CA4
26	G	102	CDL	C1-CB2-OB2-PB2
26	P	306	CDL	CB2-C1-CA2-OA2
26	P	306	CDL	CA2-OA2-PA1-OA4
26	P	306	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	CA3-OA5-PA1-OA2
26	P	306	CDL	CA3-OA5-PA1-OA3
26	P	306	CDL	CA3-OA5-PA1-OA4
26	P	306	CDL	OA7-CA5-OA6-CA4
26	P	306	CDL	C11-CA5-OA6-CA4
26	P	306	CDL	CB3-OB5-PB2-OB3
26	P	306	CDL	CB3-OB5-PB2-OB4
26	T	103	CDL	C11-CA5-OA6-CA4
26	T	103	CDL	C1-CB2-OB2-PB2
26	T	103	CDL	CB2-OB2-PB2-OB4
26	T	103	CDL	CB2-OB2-PB2-OB5
26	T	103	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	CB3-OB5-PB2-OB3
26	T	103	CDL	CB3-OB5-PB2-OB4
24	C	302	DMU	C4-C3-O7-C10
19	A	608	TGL	OC1-CC1-OG3-CG3
19	Y	101	TGL	OA1-CA1-OG1-CG1
25	C	308	PEK	O04-C21-O03-C01
26	T	103	CDL	OA9-CA7-OA8-CA6
24	T	101	DMU	C4-C3-O7-C10
18	P	305	PGV	O02-C1-O01-C02
26	T	103	CDL	OA7-CA5-OA6-CA4
19	A	608	TGL	CC2-CC1-OG3-CG3
26	P	306	CDL	C31-CA7-OA8-CA6
18	N	606	PGV	C2-C1-O01-C02
19	I	101	TGL	CB2-CB1-OG2-CG2
24	T	101	DMU	O5-C4-C57-O61
19	O	304	TGL	CC2-CC1-OG3-CG3
19	V	101	TGL	CA2-CA1-OG1-CG1
19	Y	101	TGL	CA2-CA1-OG1-CG1
22	B	302	PSC	C20-C19-O03-C01
22	O	303	PSC	C20-C19-O03-C01
25	C	308	PEK	C22-C21-O03-C01
26	T	103	CDL	C31-CA7-OA8-CA6
19	O	304	TGL	OC1-CC1-OG3-CG3
19	V	101	TGL	OA1-CA1-OG1-CG1
26	G	102	CDL	OA9-CA7-OA8-CA6
24	T	101	DMU	O6-C11-C9-C8
26	T	103	CDL	O1-C1-CA2-OA2
26	G	102	CDL	C31-CA7-OA8-CA6
26	G	102	CDL	C71-CB7-OB8-CB6
22	O	303	PSC	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	OA9-CA7-OA8-CA6
22	B	302	PSC	O04-C19-O03-C01
23	W	101	CHD	C17-C20-C22-C23
24	C	302	DMU	O5-C4-C57-O61
17	A	604	HEA	C15-C16-C17-C18
17	A	604	HEA	C19-C20-C21-C22
17	N	604	HEA	C15-C16-C17-C18
24	C	302	DMU	C3-C4-C57-O61
26	T	103	CDL	CB4-CB3-OB5-PB2
24	C	302	DMU	O6-C11-C9-O1
24	T	101	DMU	O6-C11-C9-O1
24	T	101	DMU	C3-C4-C57-O61
23	W	101	CHD	C21-C20-C22-C23
26	G	102	CDL	OB9-CB7-OB8-CB6
23	O	302	CHD	C17-C20-C22-C23
23	P	307	CHD	C17-C20-C22-C23
23	O	302	CHD	C21-C20-C22-C23
26	C	306	CDL	CB2-C1-CA2-OA2
19	L	101	TGL	CA2-CA1-OG1-CG1
25	G	101	PEK	C22-C21-O03-C01
19	O	304	TGL	CC2-CC3-CC4-CC5
23	C	307	CHD	C17-C20-C22-C23
23	J	101	CHD	C17-C20-C22-C23
24	Q	201	DMU	C3-C4-C57-O61
18	A	606	PGV	C19-C20-C21-C22
19	L	101	TGL	OA1-CA1-OG1-CG1
24	C	302	DMU	O6-C11-C9-C8
25	T	102	PEK	C2-C1-O01-C02
26	T	103	CDL	OB6-CB4-CB6-OB8
26	T	103	CDL	C71-CB7-OB8-CB6
23	J	101	CHD	C21-C20-C22-C23
23	P	307	CHD	C21-C20-C22-C23
18	P	305	PGV	O05-C05-C06-O06
26	P	306	CDL	CB7-C71-C72-C73
19	A	608	TGL	CA2-CA1-OG1-CG1
26	C	306	CDL	C19-C20-C21-C22
19	L	101	TGL	CC1-CC2-CC3-CC4
25	T	102	PEK	O02-C1-O01-C02
17	N	604	HEA	C19-C20-C21-C22
19	V	101	TGL	CA1-CA2-CA3-CA4
25	G	101	PEK	O04-C21-O03-C01
23	C	307	CHD	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
24	Q	201	DMU	O5-C4-C57-O61
18	N	606	PGV	C19-C20-C21-C22
19	O	304	TGL	CB1-CB2-CB3-CB4
25	P	303	PEK	C21-C22-C23-C24
26	C	306	CDL	CB7-C71-C72-C73
24	Q	201	DMU	O16-C18-C19-C22
18	N	606	PGV	O12-C04-C05-O05
26	C	306	CDL	O1-C1-CA2-OA2
26	P	306	CDL	O1-C1-CA2-OA2
18	A	607	PGV	C1-C2-C3-C4
19	Y	101	TGL	OB1-CB1-OG2-CG2
26	P	306	CDL	C16-C17-C18-C19
19	I	101	TGL	CC1-CC2-CC3-CC4
26	C	306	CDL	CB5-C51-C52-C53
19	Y	101	TGL	CB2-CB1-OG2-CG2
25	P	303	PEK	C2-C1-O01-C02
26	G	102	CDL	C11-CA5-OA6-CA4
26	P	306	CDL	C51-CB5-OB6-CB4
26	T	103	CDL	OB9-CB7-OB8-CB6
25	C	304	PEK	O02-C1-O01-C02
25	P	303	PEK	O02-C1-O01-C02
26	G	102	CDL	OA7-CA5-OA6-CA4
18	N	606	PGV	O12-C04-C05-C06
19	O	304	TGL	C20-C21-C22-C23
25	C	304	PEK	C2-C1-O01-C02
25	G	103	PEK	C2-C1-O01-C02
26	P	306	CDL	OB7-CB5-OB6-CB4
18	A	606	PGV	O12-C04-C05-O05
18	A	607	PGV	O12-C04-C05-O05
18	P	304	PGV	C20-C19-O03-C01
19	A	608	TGL	OA1-CA1-OG1-CG1
23	P	307	CHD	C20-C22-C23-C24
18	A	606	PGV	C04-C05-C06-O06
25	C	304	PEK	C1-C2-C3-C4
22	O	303	PSC	C04-C05-N-C06
23	J	101	CHD	C13-C17-C20-C22
19	I	101	TGL	CB3-CB4-CB5-CB6
26	C	306	CDL	C31-C32-C33-C34
26	T	103	CDL	C37-C38-C39-C40
19	Y	101	TGL	C10-C11-C12-C13
19	Y	101	TGL	CC2-CC3-CC4-CC5
22	B	302	PSC	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	I	101	TGL	CC3-CC4-CC5-CC6
19	L	101	TGL	CA3-CA4-CA5-CA6
22	O	303	PSC	C26-C27-C28-C29
24	Q	201	DMU	C22-C25-C28-C31
26	G	102	CDL	C36-C37-C38-C39
26	G	102	CDL	C52-C53-C54-C55
26	P	306	CDL	C15-C16-C17-C18
18	P	304	PGV	C7-C8-C9-C10
19	A	608	TGL	CC3-CC4-CC5-CC6
19	I	101	TGL	C17-C18-C19-C33
19	O	304	TGL	CA3-CA4-CA5-CA6
19	O	304	TGL	CC7-CC8-CC9-C15
19	Y	101	TGL	C21-C22-C23-C24
25	P	303	PEK	C34-C35-C36-C37
26	T	103	CDL	C41-C42-C43-C44
25	G	103	PEK	O02-C1-O01-C02
19	L	101	TGL	CA9-C20-C21-C22
26	C	306	CDL	C16-C17-C18-C19
18	C	305	PGV	C1-C2-C3-C4
18	C	305	PGV	C30-C31-C32-C33
26	P	306	CDL	C17-C18-C19-C20
25	G	103	PEK	C15-C16-C17-C18
23	W	101	CHD	C13-C17-C20-C22
19	O	304	TGL	C17-C18-C19-C33
25	G	101	PEK	C2-C1-O01-C02
18	P	305	PGV	C22-C23-C24-C25
22	B	302	PSC	C21-C22-C23-C24
18	P	301	PGV	C25-C26-C27-C28
25	P	303	PEK	C26-C27-C28-C29
26	C	306	CDL	C54-C55-C56-C57
25	C	304	PEK	C21-C22-C23-C24
25	C	308	PEK	C1-C2-C3-C4
18	A	607	PGV	C20-C21-C22-C23
19	L	101	TGL	CB7-CB8-CB9-C10
19	L	101	TGL	C23-C24-C25-C26
25	G	101	PEK	C34-C35-C36-C37
25	G	103	PEK	C16-C17-C18-C19
26	G	102	CDL	C63-C64-C65-C66
18	P	301	PGV	C5-C6-C7-C8
19	O	304	TGL	C11-C12-C13-C14
26	C	306	CDL	C38-C39-C40-C41
19	A	608	TGL	C17-C18-C19-C33

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Mol	Chain	Res	Type	Atoms
24	C	302	DMU	C19-C22-C25-C28
19	L	101	TGL	CC3-CC4-CC5-CC6
25	C	308	PEK	C27-C28-C29-C30
26	P	306	CDL	C13-C14-C15-C16
18	A	606	PGV	C2-C3-C4-C5
18	P	304	PGV	C30-C31-C32-C33
26	T	103	CDL	C21-C22-C23-C24
18	A	607	PGV	O12-C04-C05-C06
19	O	304	TGL	CA2-CA1-OG1-CG1
25	P	303	PEK	O03-C01-C02-C03
24	C	302	DMU	O16-C18-C19-C22
19	L	101	TGL	C17-C18-C19-C33
19	L	101	TGL	C22-C23-C24-C25
19	O	304	TGL	CA5-CA6-CA7-CA8
19	O	304	TGL	CC5-CC6-CC7-CC8
19	Y	101	TGL	CA1-CA2-CA3-CA4
18	C	301	PGV	C13-C14-C15-C16
19	O	304	TGL	C21-C22-C23-C24
19	Y	101	TGL	CC7-CC8-CC9-C15
24	T	101	DMU	C25-C28-C31-C34
25	G	103	PEK	C26-C27-C28-C29
26	P	306	CDL	C59-C60-C61-C62
26	P	306	CDL	C74-C75-C76-C77
18	P	304	PGV	O04-C19-O03-C01
18	C	301	PGV	C5-C6-C7-C8
25	T	102	PEK	C34-C35-C36-C37
26	C	306	CDL	C82-C83-C84-C85
19	I	101	TGL	CB5-CB6-CB7-CB8
26	P	306	CDL	C35-C36-C37-C38
26	P	306	CDL	C43-C44-C45-C46
18	A	607	PGV	C26-C27-C28-C29
19	O	304	TGL	CB9-C10-C11-C12
25	C	308	PEK	C33-C34-C35-C36
25	C	308	PEK	C34-C35-C36-C37
26	C	306	CDL	C18-C19-C20-C21
18	C	301	PGV	C21-C22-C23-C24
19	A	608	TGL	C19-C33-C34-C35
19	O	304	TGL	CB6-CB7-CB8-CB9
22	B	302	PSC	C13-C14-C15-C16
25	P	303	PEK	C22-C21-O03-C01
18	P	301	PGV	C7-C8-C9-C10
19	I	101	TGL	CC4-CC5-CC6-CC7

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Mol	Chain	Res	Type	Atoms
18	P	304	PGV	C20-C21-C22-C23
19	I	101	TGL	CB6-CB7-CB8-CB9
26	P	306	CDL	C73-C74-C75-C76
26	P	306	CDL	C34-C35-C36-C37
19	O	304	TGL	OA1-CA1-OG1-CG1
25	G	101	PEK	O02-C1-O01-C02
19	L	101	TGL	C12-C13-C14-C29
26	P	306	CDL	C71-C72-C73-C74
23	J	101	CHD	C13-C17-C20-C21
19	A	608	TGL	C15-C16-C17-C18
19	I	101	TGL	CA5-CA6-CA7-CA8
19	I	101	TGL	CC2-CC3-CC4-CC5
19	I	101	TGL	CA9-C20-C21-C22
25	C	308	PEK	C25-C26-C27-C28
18	C	305	PGV	C20-C19-O03-C01
19	A	608	TGL	CA9-C20-C21-C22
18	C	305	PGV	C22-C23-C24-C25
19	I	101	TGL	C13-C14-C29-C30
19	L	101	TGL	C21-C22-C23-C24
19	Y	101	TGL	C13-C14-C29-C30
25	G	101	PEK	C16-C17-C18-C19
18	P	305	PGV	C26-C27-C28-C29
19	O	304	TGL	C12-C13-C14-C29
26	C	306	CDL	C41-C42-C43-C44
26	G	102	CDL	C23-C24-C25-C26
18	A	607	PGV	C30-C31-C32-C33
19	A	608	TGL	CA6-CA7-CA8-CA9
19	I	101	TGL	C19-C33-C34-C35
19	A	608	TGL	CC2-CC3-CC4-CC5
19	I	101	TGL	C23-C24-C25-C26
26	G	102	CDL	C31-C32-C33-C34
26	P	306	CDL	C81-C82-C83-C84
19	V	101	TGL	CC2-CC3-CC4-CC5
23	W	101	CHD	C13-C17-C20-C21
19	A	608	TGL	CB2-CB1-OG2-CG2
25	C	308	PEK	C2-C1-O01-C02
26	T	103	CDL	C51-CB5-OB6-CB4
18	C	305	PGV	C19-C20-C21-C22
26	P	306	CDL	C79-C80-C81-C82
26	T	103	CDL	C39-C40-C41-C42
19	A	608	TGL	OB1-CB1-OG2-CG2
26	T	103	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	CB7-CB8-CB9-C10
26	G	102	CDL	C72-C73-C74-C75
18	A	607	PGV	C11-C10-C9-C8
18	A	607	PGV	C12-C13-C14-C15
24	M	101	DMU	C22-C25-C28-C31
18	P	304	PGV	C13-C14-C15-C16
19	V	101	TGL	CB5-CB6-CB7-CB8
22	O	303	PSC	C5-C6-C7-C8
26	C	306	CDL	C53-C54-C55-C56
26	C	306	CDL	C75-C76-C77-C78
19	V	101	TGL	CA5-CA6-CA7-CA8
23	W	101	CHD	C16-C17-C20-C21
19	A	608	TGL	CB5-CB6-CB7-CB8
26	C	306	CDL	C62-C63-C64-C65
18	A	607	PGV	C3-C4-C5-C6
18	N	606	PGV	C22-C23-C24-C25
19	O	304	TGL	C22-C23-C24-C25
22	O	303	PSC	C3-C4-C5-C6
26	C	306	CDL	C11-C12-C13-C14
26	T	103	CDL	C80-C81-C82-C83
18	A	606	PGV	C27-C28-C29-C30
22	O	303	PSC	C29-C30-C31-C32
18	A	606	PGV	C13-C14-C15-C16
19	A	608	TGL	C21-C20-CA9-CA8
18	P	305	PGV	O01-C02-C03-O11
18	C	301	PGV	C4-C5-C6-C7
26	G	102	CDL	C51-CB5-OB6-CB4
19	Y	101	TGL	CA9-C20-C21-C22
26	G	102	CDL	C55-C56-C57-C58
18	P	305	PGV	C12-C13-C14-C15
22	O	303	PSC	C6-C7-C8-C9
19	O	304	TGL	CC4-CC5-CC6-CC7
18	A	606	PGV	C24-C25-C26-C27
18	C	301	PGV	C23-C24-C25-C26
25	G	101	PEK	C26-C27-C28-C29
26	G	102	CDL	C21-C22-C23-C24
18	A	606	PGV	C30-C31-C32-C33
19	Y	101	TGL	CB4-CB5-CB6-CB7
26	G	102	CDL	C13-C14-C15-C16
18	P	304	PGV	C22-C23-C24-C25
19	O	304	TGL	CA7-CA8-CA9-C20
19	V	101	TGL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	302	DMU	C25-C28-C31-C34
25	G	101	PEK	C30-C31-C32-C33
26	C	306	CDL	C52-C53-C54-C55
18	A	607	PGV	C05-C04-O12-P
18	N	606	PGV	C02-C03-O11-P
23	J	101	CHD	C16-C17-C20-C21
25	G	103	PEK	C30-C31-C32-C33
25	C	308	PEK	O02-C1-O01-C02
18	A	606	PGV	O12-C04-C05-C06
26	P	306	CDL	C20-C21-C22-C23
22	O	303	PSC	C27-C28-C29-C30
19	A	608	TGL	CC7-CC8-CC9-C15
19	A	608	TGL	C12-C13-C14-C29
19	Y	101	TGL	CC3-CC4-CC5-CC6
18	C	305	PGV	O05-C05-C06-O06
18	C	305	PGV	O04-C19-O03-C01
18	N	606	PGV	C14-C15-C16-C17
19	V	101	TGL	C17-C18-C19-C33
19	Y	101	TGL	CC5-CC6-CC7-CC8
18	P	305	PGV	C11-C10-C9-C8
25	P	303	PEK	O04-C21-O03-C01
19	L	101	TGL	CC6-CC7-CC8-CC9
24	M	101	DMU	O16-C18-C19-C22
18	A	606	PGV	C01-C02-C03-O11
26	T	103	CDL	OA5-CA3-CA4-CA6
26	G	102	CDL	OB7-CB5-OB6-CB4
19	O	304	TGL	C15-C16-C17-C18
26	P	306	CDL	CB5-C51-C52-C53
18	A	607	PGV	C27-C28-C29-C30
19	A	608	TGL	CB9-C10-C11-C12
19	A	608	TGL	C13-C14-C29-C30
26	C	306	CDL	C59-C60-C61-C62
26	C	306	CDL	C36-C37-C38-C39
18	C	305	PGV	C28-C29-C30-C31
19	I	101	TGL	C11-C10-CB9-CB8
22	O	303	PSC	C2-C1-O01-C02
19	O	304	TGL	CC6-CC7-CC8-CC9
26	T	103	CDL	C20-C21-C22-C23
19	L	101	TGL	CC2-CC1-OG3-CG3
19	L	101	TGL	CC7-CC8-CC9-C15
18	N	606	PGV	O03-C01-C02-C03
19	A	608	TGL	CG1-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
22	B	302	PSC	O03-C01-C02-C03
26	C	306	CDL	CA3-CA4-CA6-OA8
26	T	103	CDL	CA3-CA4-CA6-OA8
26	T	103	CDL	CB3-CB4-CB6-OB8
26	C	306	CDL	C64-C65-C66-C67
18	C	305	PGV	C25-C26-C27-C28
25	C	304	PEK	C27-C28-C29-C30
18	C	305	PGV	C12-C13-C14-C15
18	A	607	PGV	C6-C7-C8-C9
18	A	607	PGV	C20-C19-O03-C01
19	Y	101	TGL	C17-C18-C19-C33
19	Y	101	TGL	C18-C19-C33-C34
26	P	306	CDL	C14-C15-C16-C17
18	C	301	PGV	C6-C7-C8-C9
18	C	301	PGV	C25-C26-C27-C28
19	I	101	TGL	C18-C19-C33-C34
26	C	306	CDL	C20-C21-C22-C23
19	V	101	TGL	C21-C22-C23-C24
19	O	304	TGL	CC9-C15-C16-C17
25	C	308	PEK	C30-C31-C32-C33
19	V	101	TGL	C16-C15-CC9-CC8
19	V	101	TGL	CC3-CC4-CC5-CC6
18	C	301	PGV	C7-C8-C9-C10
26	C	306	CDL	C15-C16-C17-C18
26	C	306	CDL	C61-C62-C63-C64
19	V	101	TGL	C11-C12-C13-C14
19	I	101	TGL	CA2-CA1-OG1-CG1
19	V	101	TGL	CC2-CC1-OG3-CG3
18	N	606	PGV	C03-C02-O01-C1
22	O	303	PSC	C01-C02-O01-C1
18	C	301	PGV	C29-C30-C31-C32
18	N	606	PGV	C4-C5-C6-C7
19	I	101	TGL	C24-C25-C26-C27
26	T	103	CDL	C23-C24-C25-C26
18	A	606	PGV	C11-C10-C9-C8
25	G	101	PEK	C15-C16-C17-C18
18	C	305	PGV	C20-C21-C22-C23
19	A	608	TGL	CB3-CB4-CB5-CB6
17	A	604	HEA	C2A-C3A-CMA-OMA
26	T	103	CDL	C82-C83-C84-C85
18	A	607	PGV	O01-C02-C03-O11
18	N	606	PGV	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	C16-C15-CC9-CC8
26	P	306	CDL	C36-C37-C38-C39
18	P	301	PGV	C2-C1-O01-C02
25	P	303	PEK	C25-C26-C27-C28
18	P	305	PGV	C4-C5-C6-C7
19	O	304	TGL	CA2-CA3-CA4-CA5
24	M	101	DMU	C25-C28-C31-C34
19	I	101	TGL	C22-C23-C24-C25
22	O	303	PSC	C23-C24-C25-C26
26	P	306	CDL	C42-C43-C44-C45
26	C	306	CDL	C76-C77-C78-C79
26	G	102	CDL	C61-C62-C63-C64
26	P	306	CDL	C19-C20-C21-C22
18	A	607	PGV	C15-C16-C17-C18
19	L	101	TGL	C11-C12-C13-C14
26	C	306	CDL	C79-C80-C81-C82
19	O	304	TGL	OG2-CG2-CG3-OG3
18	P	301	PGV	C31-C32-C33-C34
26	T	103	CDL	O1-C1-CB2-OB2
18	A	607	PGV	C22-C23-C24-C25
19	A	608	TGL	CC6-CC7-CC8-CC9
19	I	101	TGL	C21-C20-CA9-CA8
18	N	606	PGV	C25-C26-C27-C28
17	A	605	HEA	C3B-C11-C12-C13
18	A	607	PGV	O04-C19-O03-C01
26	T	103	CDL	C64-C65-C66-C67
18	A	606	PGV	C14-C15-C16-C17
18	P	301	PGV	C2-C3-C4-C5
26	P	306	CDL	C84-C85-C86-C87
25	C	308	PEK	C31-C32-C33-C34
19	V	101	TGL	C25-C26-C27-C28
26	G	102	CDL	C20-C21-C22-C23
26	P	306	CDL	C23-C24-C25-C26
19	A	608	TGL	CB1-CB2-CB3-CB4
25	T	102	PEK	C21-C22-C23-C24
18	P	305	PGV	C28-C29-C30-C31
25	C	304	PEK	C28-C29-C30-C31
19	I	101	TGL	CB2-CB3-CB4-CB5
18	A	606	PGV	C05-C04-O12-P
22	B	302	PSC	C02-C03-O11-P
19	O	304	TGL	CA4-CA5-CA6-CA7
25	C	304	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	P	303	PEK	C32-C33-C34-C35
25	T	102	PEK	C28-C29-C30-C31
18	C	305	PGV	C21-C22-C23-C24
25	G	101	PEK	C28-C29-C30-C31
24	M	101	DMU	C1-C6-O16-C18
18	P	305	PGV	C01-C02-C03-O11
25	C	304	PEK	C01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-CB6
18	N	606	PGV	C29-C30-C31-C32
22	O	303	PSC	C15-C16-C17-C18
18	C	301	PGV	C15-C16-C17-C18
19	Y	101	TGL	CB3-CB4-CB5-CB6
19	I	101	TGL	OA1-CA1-OG1-CG1
19	L	101	TGL	OC1-CC1-OG3-CG3
19	V	101	TGL	OC1-CC1-OG3-CG3
25	T	102	PEK	C35-C36-C37-C38
22	O	303	PSC	C22-C23-C24-C25
26	P	306	CDL	C11-C12-C13-C14
25	T	102	PEK	C25-C26-C27-C28
26	G	102	CDL	C44-C45-C46-C47
25	G	101	PEK	C23-C24-C25-C26
26	G	102	CDL	C62-C63-C64-C65
25	C	304	PEK	C30-C31-C32-C33
19	L	101	TGL	C29-C30-C31-C32
18	A	607	PGV	C24-C25-C26-C27
22	O	303	PSC	O02-C1-O01-C02
24	M	101	DMU	C3-C4-C57-O61
19	V	101	TGL	CA2-CA3-CA4-CA5
26	C	306	CDL	CA2-C1-CB2-OB2
23	B	303	CHD	C20-C22-C23-C24
18	A	606	PGV	O03-C01-C02-C03
19	O	304	TGL	CG1-CG2-CG3-OG3
19	V	101	TGL	OG1-CG1-CG2-CG3
25	G	101	PEK	O03-C01-C02-C03
26	C	306	CDL	CB3-CB4-CB6-OB8
26	G	102	CDL	CA3-CA4-CA6-OA8
26	P	306	CDL	CA3-CA4-CA6-OA8
26	P	306	CDL	CB3-CB4-CB6-OB8
26	P	306	CDL	C51-C52-C53-C54
26	T	103	CDL	C31-C32-C33-C34
26	P	306	CDL	C77-C78-C79-C80
26	C	306	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	CC5-CC6-CC7-CC8
25	P	303	PEK	C33-C34-C35-C36
19	A	608	TGL	C33-C34-C35-C36
25	C	304	PEK	C35-C36-C37-C38
24	Q	201	DMU	C25-C28-C31-C34
22	O	303	PSC	C21-C22-C23-C24
18	N	606	PGV	O01-C02-C03-O11
18	C	305	PGV	C11-C10-C9-C8
26	C	306	CDL	C1-CA2-OA2-PA1
26	C	306	CDL	C32-C33-C34-C35
18	P	305	PGV	C20-C21-C22-C23
26	G	102	CDL	C80-C81-C82-C83
18	N	606	PGV	O03-C01-C02-O01
19	A	608	TGL	OG2-CG2-CG3-OG3
22	B	302	PSC	O03-C01-C02-O01
25	G	101	PEK	O03-C01-C02-O01
26	G	102	CDL	OA6-CA4-CA6-OA8
25	C	304	PEK	C11-C12-C13-C14
25	C	304	PEK	C12-C13-C14-C15
25	C	308	PEK	C6-C7-C8-C9
25	P	303	PEK	C5-C6-C7-C8
25	P	303	PEK	C11-C10-C9-C8
25	P	303	PEK	C9-C10-C11-C12
25	T	102	PEK	C6-C7-C8-C9
25	T	102	PEK	C11-C12-C13-C14
25	T	102	PEK	C12-C13-C14-C15
19	I	101	TGL	CA3-CA4-CA5-CA6
26	T	103	CDL	C77-C78-C79-C80
18	N	606	PGV	C21-C22-C23-C24
19	V	101	TGL	CB3-CB4-CB5-CB6
26	C	306	CDL	C74-C75-C76-C77
26	P	306	CDL	C61-C62-C63-C64
22	B	302	PSC	C31-C32-C33-C34
26	C	306	CDL	C21-C22-C23-C24
26	G	102	CDL	C77-C78-C79-C80
18	C	305	PGV	C24-C25-C26-C27
26	G	102	CDL	C75-C76-C77-C78
18	P	305	PGV	C31-C32-C33-C34
25	G	101	PEK	C21-C22-C23-C24
18	A	607	PGV	C29-C30-C31-C32
18	A	606	PGV	C21-C22-C23-C24
19	L	101	TGL	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
24	Q	201	DMU	C19-C22-C25-C28
26	T	103	CDL	C44-C45-C46-C47
26	P	306	CDL	C64-C65-C66-C67
26	C	306	CDL	C31-CA7-OA8-CA6
19	A	608	TGL	C23-C24-C25-C26
26	P	306	CDL	C12-C11-CA5-OA6
18	C	301	PGV	C2-C3-C4-C5
26	G	102	CDL	C16-C17-C18-C19
26	T	103	CDL	CB2-C1-CA2-OA2
26	T	103	CDL	C56-C57-C58-C59
19	V	101	TGL	CA9-C20-C21-C22
26	T	103	CDL	C63-C64-C65-C66
22	O	303	PSC	C31-C32-C33-C34
26	T	103	CDL	C71-C72-C73-C74
25	P	303	PEK	C29-C30-C31-C32
18	A	607	PGV	C2-C3-C4-C5
18	P	301	PGV	O02-C1-O01-C02
22	O	303	PSC	C04-C05-N-C08
24	M	101	DMU	C34-C37-C40-C43
18	A	606	PGV	C03-C02-O01-C1
22	B	302	PSC	C01-C02-O01-C1
25	G	101	PEK	C2-C3-C4-C5
25	T	102	PEK	C15-C16-C17-C18
24	M	101	DMU	C19-C22-C25-C28
19	Y	101	TGL	CC9-C15-C16-C17
25	G	103	PEK	C34-C35-C36-C37
19	Y	101	TGL	C23-C24-C25-C26
22	B	302	PSC	C27-C28-C29-C30
25	C	304	PEK	O04-C21-O03-C01
25	C	308	PEK	C16-C17-C18-C19
25	C	304	PEK	O01-C02-C03-O11
19	V	101	TGL	C20-C21-C22-C23
22	O	303	PSC	O03-C01-C02-C03
19	L	101	TGL	C24-C25-C26-C27
22	B	302	PSC	C05-C04-O12-P
19	Y	101	TGL	C22-C23-C24-C25
22	O	303	PSC	C14-C15-C16-C17
18	P	301	PGV	O03-C01-C02-O01
26	C	306	CDL	OB6-CB4-CB6-OB8
26	P	306	CDL	OA6-CA4-CA6-OA8
26	P	306	CDL	OB6-CB4-CB6-OB8
26	T	103	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
22	B	302	PSC	C23-C24-C25-C26
18	A	606	PGV	C4-C5-C6-C7
26	P	306	CDL	C83-C84-C85-C86
25	C	304	PEK	C23-C24-C25-C26
18	N	606	PGV	C30-C31-C32-C33
18	P	305	PGV	C02-C03-O11-P
19	Y	101	TGL	CC4-CC5-CC6-CC7
26	T	103	CDL	C51-C52-C53-C54
26	T	103	CDL	CA2-C1-CB2-OB2
19	A	608	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	CA6-CA7-CA8-CA9
26	C	306	CDL	OA9-CA7-OA8-CA6
25	C	304	PEK	C24-C25-C26-C27
18	C	305	PGV	C23-C24-C25-C26
25	C	304	PEK	C22-C21-O03-C01
19	I	101	TGL	C21-C22-C23-C24
18	C	301	PGV	C31-C32-C33-C34
18	A	606	PGV	O05-C05-C06-O06
26	T	103	CDL	C74-C75-C76-C77
18	P	305	PGV	C24-C25-C26-C27
18	A	607	PGV	C01-C02-C03-O11
18	N	606	PGV	C01-C02-C03-O11
26	G	102	CDL	OB5-CB3-CB4-CB6
18	C	305	PGV	C2-C1-O01-C02
26	P	306	CDL	C75-C76-C77-C78
26	G	102	CDL	C11-C12-C13-C14
26	P	306	CDL	C40-C41-C42-C43
18	N	606	PGV	C05-C04-O12-P
24	Q	201	DMU	C34-C37-C40-C43
18	C	305	PGV	O02-C1-O01-C02
18	A	606	PGV	O01-C02-C03-O11
26	G	102	CDL	OB5-CB3-CB4-OB6
26	T	103	CDL	OA5-CA3-CA4-OA6
26	T	103	CDL	OB5-CB3-CB4-OB6
18	P	305	PGV	C5-C6-C7-C8
19	V	101	TGL	C15-C16-C17-C18
18	A	606	PGV	O03-C01-C02-O01
22	O	303	PSC	O03-C01-C02-O01
25	P	303	PEK	O03-C01-C02-O01
26	C	306	CDL	OA6-CA4-CA6-OA8
18	P	301	PGV	O03-C01-C02-C03
19	A	608	TGL	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
18	P	305	PGV	C19-C20-C21-C22
26	C	306	CDL	C81-C82-C83-C84
18	C	305	PGV	C31-C32-C33-C34
18	C	301	PGV	C9-C10-C11-C12
26	T	103	CDL	C52-C53-C54-C55
25	C	308	PEK	C29-C30-C31-C32
19	I	101	TGL	C16-C17-C18-C19
25	T	102	PEK	C29-C30-C31-C32
18	C	305	PGV	C04-O12-P-O11
18	C	305	PGV	C04-O12-P-O13
18	P	305	PGV	C03-O11-P-O14
22	O	303	PSC	C04-O12-P-O13
25	T	102	PEK	C03-O11-P-O14
25	T	102	PEK	C04-O12-P-O13
26	C	306	CDL	CB3-OB5-PB2-OB2
26	C	306	CDL	CB3-OB5-PB2-OB3
26	C	306	CDL	CB3-OB5-PB2-OB4
26	P	306	CDL	CB3-OB5-PB2-OB2
26	T	103	CDL	CA2-OA2-PA1-OA3
26	C	306	CDL	C78-C79-C80-C81
19	V	101	TGL	CA4-CA5-CA6-CA7
18	P	304	PGV	C02-C03-O11-P
26	P	306	CDL	CA4-CA3-OA5-PA1
19	V	101	TGL	CB7-CB8-CB9-C10
26	P	306	CDL	C52-C53-C54-C55
19	A	608	TGL	CG1-CG2-OG2-CB1
19	V	101	TGL	CG3-CG2-OG2-CB1
19	O	304	TGL	C18-C19-C33-C34
26	C	306	CDL	C84-C85-C86-C87
18	P	305	PGV	C15-C16-C17-C18
18	P	301	PGV	O03-C19-C20-C21
19	L	101	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	CB6-CB7-CB8-CB9
25	G	103	PEK	C35-C36-C37-C38
17	A	605	HEA	O11-C11-C12-C13
17	N	605	HEA	O11-C11-C12-C13
19	Y	101	TGL	C29-C30-C31-C32
19	O	304	TGL	OB1-CB1-OG2-CG2
25	T	102	PEK	C23-C24-C25-C26
26	G	102	CDL	C41-C42-C43-C44
26	T	103	CDL	C60-C61-C62-C63
19	I	101	TGL	CC7-CC8-CC9-C15

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Mol	Chain	Res	Type	Atoms
24	M	101	DMU	O5-C4-C57-O61
18	C	305	PGV	O03-C01-C02-C03
17	N	604	HEA	C3A-C2A-CAA-CBA
19	I	101	TGL	C15-C16-C17-C18
26	T	103	CDL	C17-C18-C19-C20
26	C	306	CDL	C63-C64-C65-C66
19	I	101	TGL	C29-C30-C31-C32
23	B	303	CHD	C13-C17-C20-C22
18	N	606	PGV	C3-C4-C5-C6
19	O	304	TGL	C19-C33-C34-C35
18	N	606	PGV	C13-C14-C15-C16
19	O	304	TGL	CA9-C20-C21-C22
19	V	101	TGL	CA3-CA4-CA5-CA6
26	C	306	CDL	C13-C14-C15-C16
18	C	301	PGV	C30-C31-C32-C33
19	A	608	TGL	C18-C19-C33-C34
26	C	306	CDL	O1-C1-CB2-OB2
17	N	604	HEA	C1A-C2A-CAA-CBA
25	T	102	PEK	C33-C34-C35-C36
19	I	101	TGL	CB1-CB2-CB3-CB4
23	B	303	CHD	C16-C17-C20-C22
26	C	306	CDL	C56-C57-C58-C59
25	C	304	PEK	C3-C4-C5-C6
26	P	306	CDL	C63-C64-C65-C66
18	A	607	PGV	C02-C03-O11-P
18	C	305	PGV	C02-C03-O11-P
19	I	101	TGL	C11-C12-C13-C14
25	P	303	PEK	C17-C18-C19-C20
26	C	306	CDL	C23-C24-C25-C26
17	A	605	HEA	CAA-CBA-CGA-O1A
26	G	102	CDL	C24-C25-C26-C27
17	A	605	HEA	CAD-CBD-CGD-O2D
26	C	306	CDL	C80-C81-C82-C83
25	C	308	PEK	C3-C4-C5-C6
19	V	101	TGL	CC5-CC6-CC7-CC8
26	G	102	CDL	C39-C40-C41-C42
18	P	304	PGV	C19-C20-C21-C22
26	P	306	CDL	C39-C40-C41-C42
19	O	304	TGL	CG1-CG2-OG2-CB1
26	P	306	CDL	CA3-CA4-OA6-CA5
26	P	306	CDL	C44-C45-C46-C47
18	P	305	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
17	A	605	HEA	CAA-CBA-CGA-O2A
26	T	103	CDL	C36-C37-C38-C39
26	C	306	CDL	C14-C15-C16-C17
19	Y	101	TGL	CC1-CC2-CC3-CC4
22	B	302	PSC	O01-C02-C03-O11
17	N	605	HEA	CAD-CBD-CGD-O2D
26	C	306	CDL	C43-C44-C45-C46
18	C	305	PGV	C05-C04-O12-P
26	G	102	CDL	CB4-CB3-OB5-PB2
18	P	304	PGV	C15-C16-C17-C18
17	N	605	HEA	CAA-CBA-CGA-O1A
23	W	101	CHD	C22-C23-C24-O26
25	P	303	PEK	C27-C28-C29-C30
26	C	306	CDL	C55-C56-C57-C58
26	G	102	CDL	C53-C54-C55-C56
18	A	606	PGV	C11-C12-C13-C14
22	B	302	PSC	C7-C8-C9-C10
18	C	305	PGV	C6-C7-C8-C9
19	Y	101	TGL	CB5-CB6-CB7-CB8
22	B	302	PSC	C9-C10-C11-C12
25	G	101	PEK	C5-C6-C7-C8
25	G	101	PEK	C11-C10-C9-C8
25	G	101	PEK	C9-C10-C11-C12
25	G	103	PEK	C32-C33-C34-C35
19	V	101	TGL	CA6-CA7-CA8-CA9
17	A	604	HEA	CAA-CBA-CGA-O1A
17	A	604	HEA	CAD-CBD-CGD-O1D
17	N	605	HEA	C26-C15-C16-C17
17	N	605	HEA	CAD-CBD-CGD-O1D
23	P	307	CHD	C22-C23-C24-O26
19	I	101	TGL	CC6-CC7-CC8-CC9
18	P	301	PGV	C22-C23-C24-C25
24	T	101	DMU	C31-C34-C37-C40
18	C	301	PGV	C26-C27-C28-C29
19	O	304	TGL	CC1-CC2-CC3-CC4
25	C	304	PEK	C29-C30-C31-C32
26	T	103	CDL	C72-C73-C74-C75
17	N	604	HEA	CAD-CBD-CGD-O1D
17	N	605	HEA	CAA-CBA-CGA-O2A
18	P	305	PGV	C20-C19-O03-C01
26	T	103	CDL	C16-C17-C18-C19
19	I	101	TGL	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
25	C	304	PEK	C16-C17-C18-C19
17	A	605	HEA	CAD-CBD-CGD-O1D
26	T	103	CDL	C1-CA2-OA2-PA1
23	B	303	CHD	C22-C23-C24-O25
25	G	103	PEK	C31-C32-C33-C34
26	P	306	CDL	C52-C51-CB5-OB6
25	G	103	PEK	C28-C29-C30-C31
23	P	302	CHD	C22-C23-C24-O26
25	C	304	PEK	C32-C33-C34-C35
19	V	101	TGL	CG2-CG3-OG3-CC1
17	A	604	HEA	CAD-CBD-CGD-O2D
23	C	307	CHD	C22-C23-C24-O26
26	P	306	CDL	C18-C19-C20-C21
26	P	306	CDL	C53-C54-C55-C56
18	C	301	PGV	C11-C12-C13-C14
25	G	101	PEK	C27-C28-C29-C30
23	O	302	CHD	C22-C23-C24-O25
23	O	302	CHD	C22-C23-C24-O26
17	A	604	HEA	C11-C12-C13-C14
23	C	303	CHD	C22-C23-C24-O26
26	P	306	CDL	OA5-CA3-CA4-CA6
17	A	604	HEA	CAA-CBA-CGA-O2A
17	N	604	HEA	CAA-CBA-CGA-O1A
17	N	605	HEA	C14-C15-C16-C17
18	P	305	PGV	C3-C4-C5-C6
19	Y	101	TGL	C21-C20-CA9-CA8
23	B	303	CHD	C13-C17-C20-C21
19	A	608	TGL	C16-C17-C18-C19
23	P	302	CHD	C22-C23-C24-O25
19	O	304	TGL	C24-C25-C26-C27
23	W	101	CHD	C22-C23-C24-O25
25	C	308	PEK	C32-C33-C34-C35
25	C	308	PEK	C22-C23-C24-C25
24	C	302	DMU	C18-C19-C22-C25
23	P	307	CHD	C22-C23-C24-O25
24	T	101	DMU	C22-C25-C28-C31
25	P	303	PEK	C22-C23-C24-C25
19	V	101	TGL	C21-C20-CA9-CA8
19	A	608	TGL	OG1-CA1-CA2-CA3
26	P	306	CDL	CA6-CA4-OA6-CA5
18	P	304	PGV	C11-C12-C13-C14
22	O	303	PSC	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	G	103	PEK	C14-C15-C16-C17
25	T	102	PEK	C3-C4-C5-C6
18	P	301	PGV	C12-C13-C14-C15
17	N	604	HEA	C2A-C3A-CMA-OMA
18	P	301	PGV	C9-C10-C11-C12
22	B	302	PSC	C12-C13-C14-C15
23	C	307	CHD	C22-C23-C24-O25
26	P	306	CDL	C1-CA2-OA2-PA1
23	C	303	CHD	C22-C23-C24-O25
25	P	303	PEK	C23-C24-C25-C26
18	P	304	PGV	C9-C10-C11-C12
26	P	306	CDL	C37-C38-C39-C40
26	C	306	CDL	C12-C13-C14-C15
17	N	605	HEA	C12-C13-C14-C15
19	V	101	TGL	CB6-CB7-CB8-CB9
19	O	304	TGL	OG3-CC1-CC2-CC3
19	O	304	TGL	CB2-CB1-OG2-CG2
18	C	301	PGV	C22-C23-C24-C25
18	N	606	PGV	C11-C12-C13-C14
25	G	103	PEK	C3-C4-C5-C6
26	T	103	CDL	C52-C51-CB5-OB6
17	N	604	HEA	CAD-CBD-CGD-O2D
25	G	103	PEK	O01-C1-C2-C3
19	A	608	TGL	C25-C26-C27-C28
22	B	302	PSC	C4-C5-C6-C7
19	I	101	TGL	C20-C21-C22-C23
17	A	604	HEA	C2C-C3C-CAC-CBC
17	A	605	HEA	C2C-C3C-CAC-CBC
17	N	604	HEA	C2C-C3C-CAC-CBC
19	I	101	TGL	OG1-CA1-CA2-CA3
18	P	301	PGV	C11-C12-C13-C14
18	P	301	PGV	C02-C03-O11-P
26	G	102	CDL	C32-C31-CA7-OA8
26	G	102	CDL	C82-C83-C84-C85
26	G	102	CDL	C43-C44-C45-C46
18	P	305	PGV	O01-C1-C2-C3
19	O	304	TGL	CB3-CB4-CB5-CB6
19	O	304	TGL	CA6-CA7-CA8-CA9
23	B	303	CHD	C22-C23-C24-O26
19	L	101	TGL	CA5-CA6-CA7-CA8
24	C	302	DMU	C5-C10-O7-C3
25	G	101	PEK	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	C21-C20-CA9-CA8
18	A	606	PGV	O01-C1-C2-C3
25	T	102	PEK	O01-C1-C2-C3
26	C	306	CDL	C83-C84-C85-C86
17	N	604	HEA	CAA-CBA-CGA-O2A
19	L	101	TGL	C25-C26-C27-C28
19	O	304	TGL	OG1-CA1-CA2-CA3
19	V	101	TGL	OG3-CC1-CC2-CC3
26	P	306	CDL	C54-C55-C56-C57
25	G	103	PEK	O03-C21-C22-C23
26	T	103	CDL	C15-C16-C17-C18
19	I	101	TGL	CB7-CB8-CB9-C10
19	Y	101	TGL	CA3-CA4-CA5-CA6
22	B	302	PSC	C2-C3-C4-C5
26	C	306	CDL	C39-C40-C41-C42
18	P	305	PGV	O02-C1-C2-C3
19	I	101	TGL	OA1-CA1-CA2-CA3
26	G	102	CDL	C32-C31-CA7-OA9
18	N	606	PGV	O01-C1-C2-C3
26	T	103	CDL	C75-C76-C77-C78
19	L	101	TGL	CC4-CC5-CC6-CC7
26	T	103	CDL	C38-C39-C40-C41
25	C	304	PEK	C22-C23-C24-C25
24	Q	201	DMU	C18-C19-C22-C25
19	L	101	TGL	OG3-CC1-CC2-CC3
26	T	103	CDL	C57-C58-C59-C60
18	C	301	PGV	C27-C28-C29-C30
18	P	305	PGV	C2-C3-C4-C5
18	P	301	PGV	C19-C20-C21-C22
26	P	306	CDL	C32-C33-C34-C35
26	P	306	CDL	C80-C81-C82-C83
19	O	304	TGL	OC1-CC1-CC2-CC3
25	G	103	PEK	O02-C1-C2-C3
26	T	103	CDL	C52-C51-CB5-OB7
19	V	101	TGL	OB1-CB1-OG2-CG2
25	T	102	PEK	O02-C1-C2-C3
19	Y	101	TGL	OG1-CA1-CA2-CA3
26	G	102	CDL	C81-C82-C83-C84
26	P	306	CDL	C60-C61-C62-C63
25	G	101	PEK	O02-C1-C2-C3
19	I	101	TGL	OG2-CB1-CB2-CB3
22	O	303	PSC	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	O	304	TGL	OA1-CA1-CA2-CA3
19	L	101	TGL	OC1-CC1-CC2-CC3
19	V	101	TGL	OC1-CC1-CC2-CC3
26	P	306	CDL	C12-C11-CA5-OA7
26	G	102	CDL	C52-C51-CB5-OB6
18	A	607	PGV	O01-C1-C2-C3
18	N	606	PGV	O02-C1-C2-C3
25	G	103	PEK	O04-C21-C22-C23

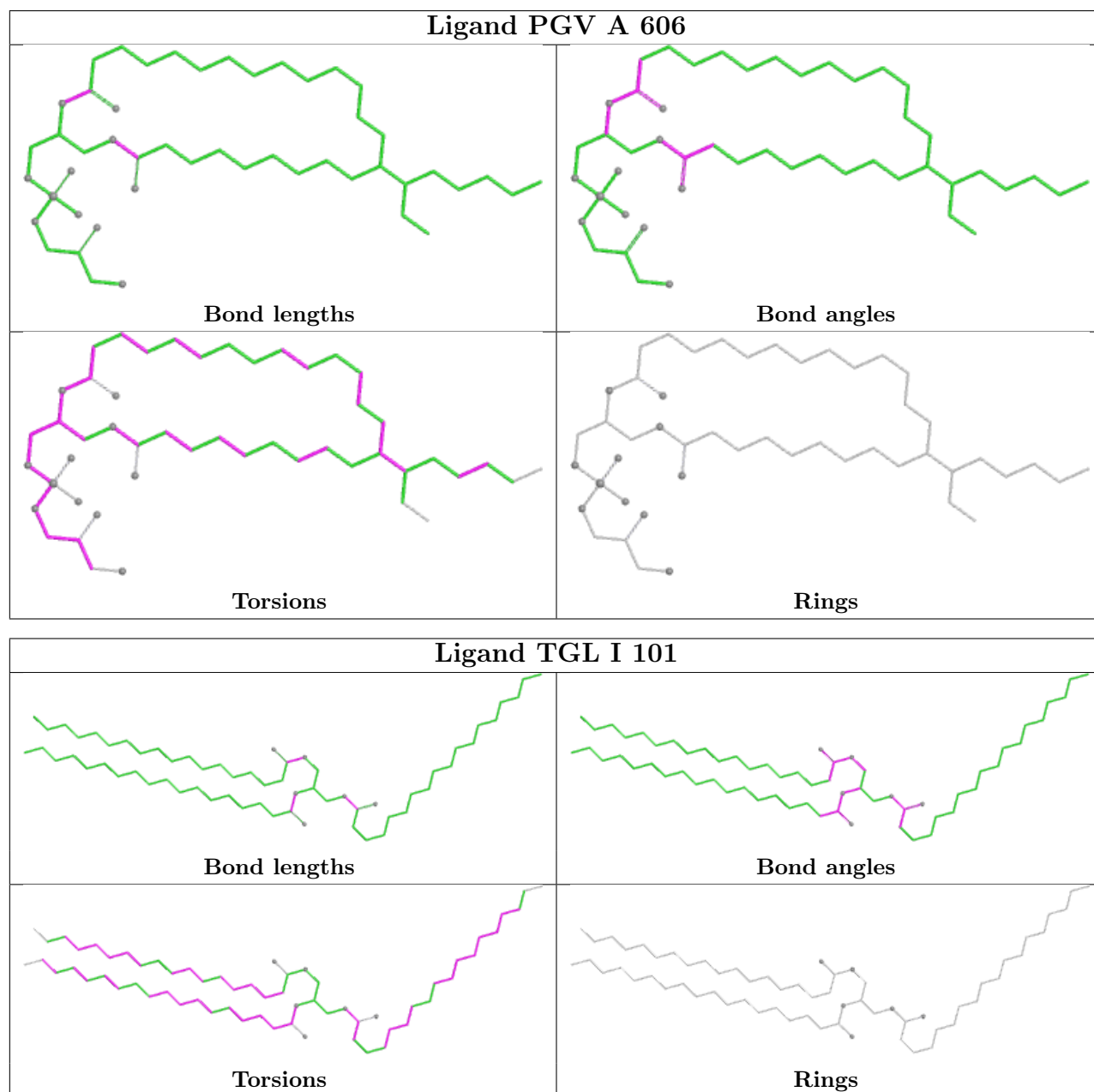
There are no ring outliers.

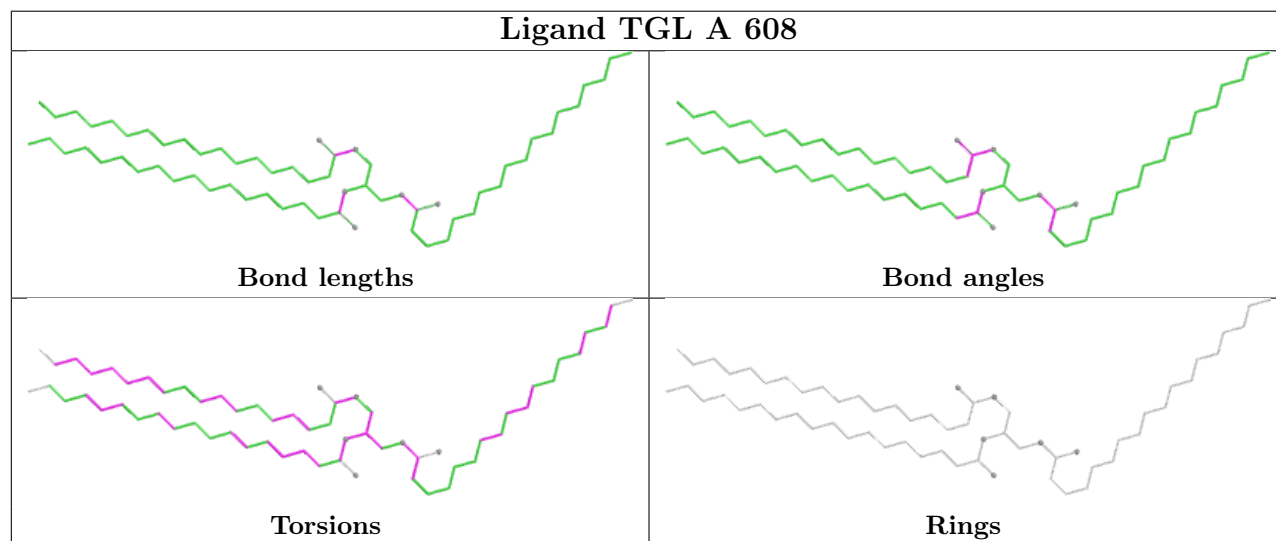
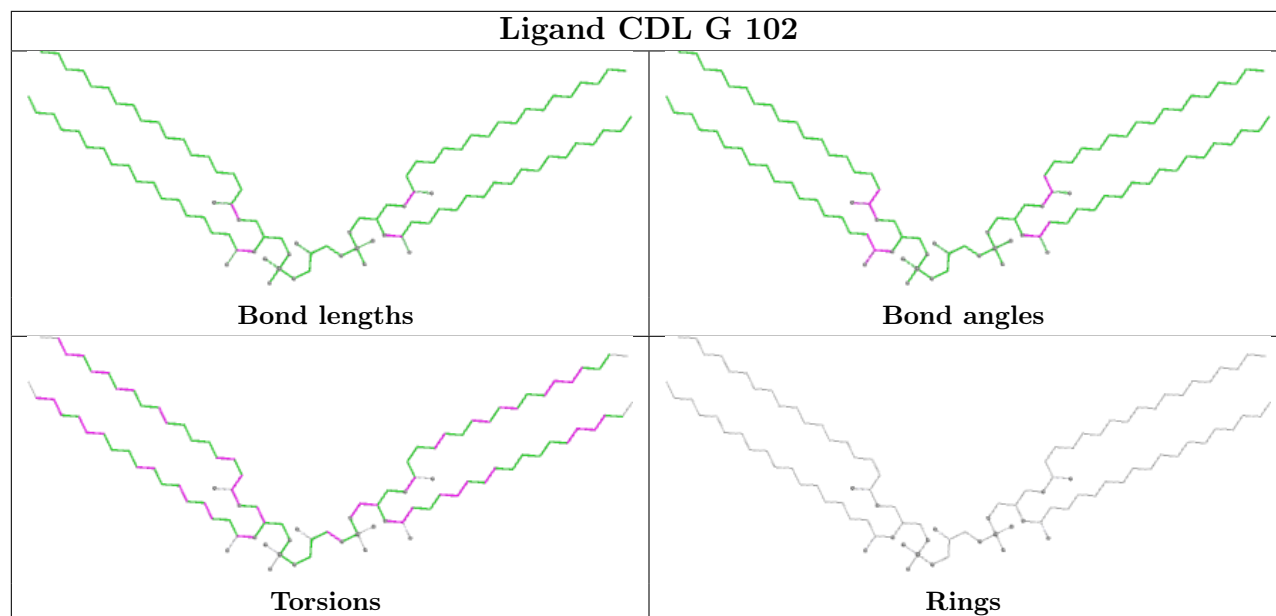
27 monomers are involved in 46 short contacts:

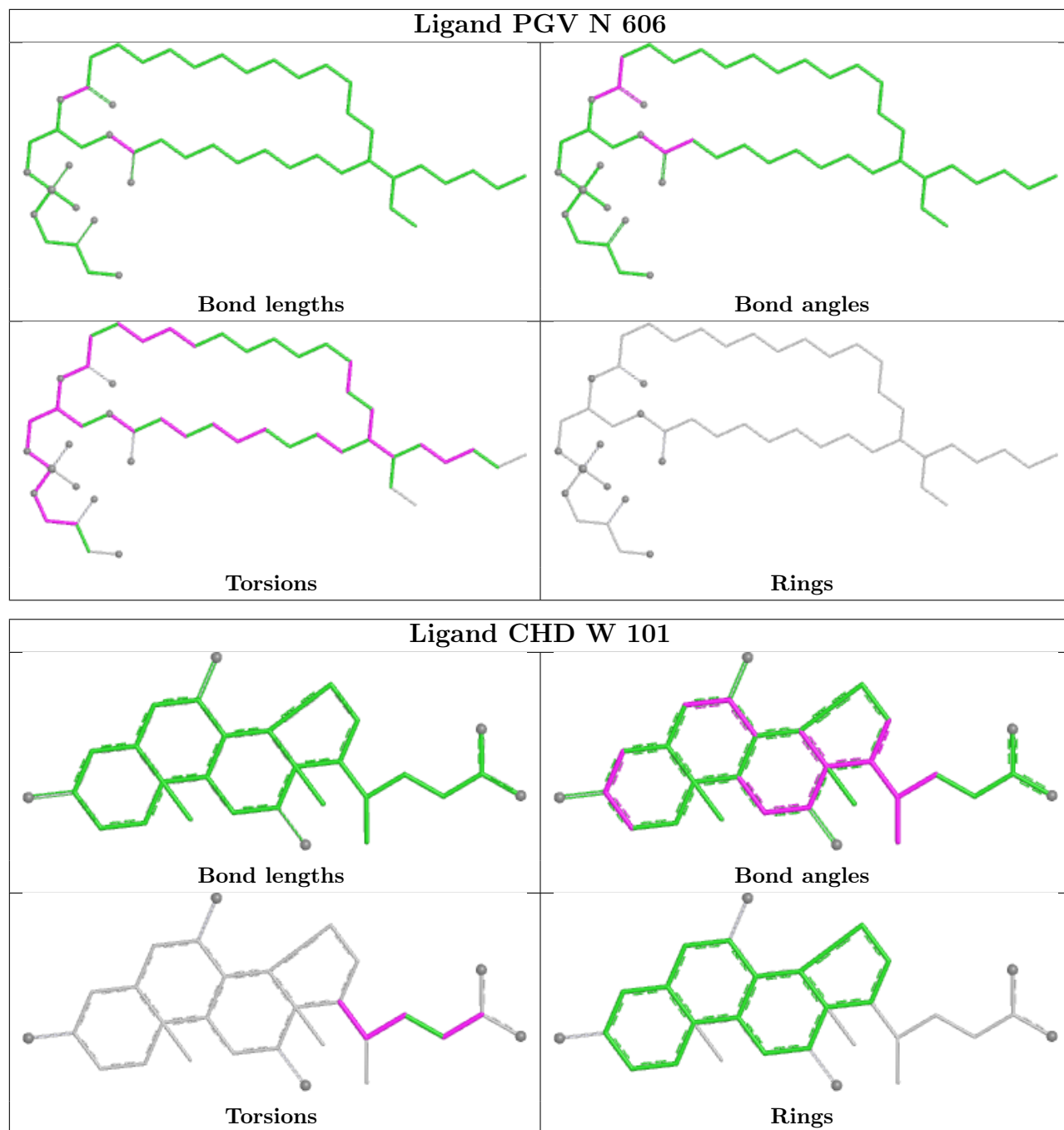
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	606	PGV	1	0
19	I	101	TGL	3	0
26	G	102	CDL	1	0
19	A	608	TGL	1	0
18	N	606	PGV	2	0
23	W	101	CHD	2	0
17	A	604	HEA	3	0
22	B	302	PSC	3	0
25	G	101	PEK	1	0
20	N	607	PER	1	0
26	P	306	CDL	2	0
20	A	609	PER	1	0
17	A	605	HEA	1	0
17	N	605	HEA	1	0
24	Q	201	DMU	2	0
23	C	303	CHD	1	0
25	T	102	PEK	1	0
22	O	303	PSC	4	0
26	T	103	CDL	2	0
19	L	101	TGL	1	0
25	C	308	PEK	1	0
25	P	303	PEK	3	0
19	Y	101	TGL	2	0
23	O	302	CHD	1	0
26	C	306	CDL	4	0
18	P	304	PGV	1	0
17	N	604	HEA	2	0

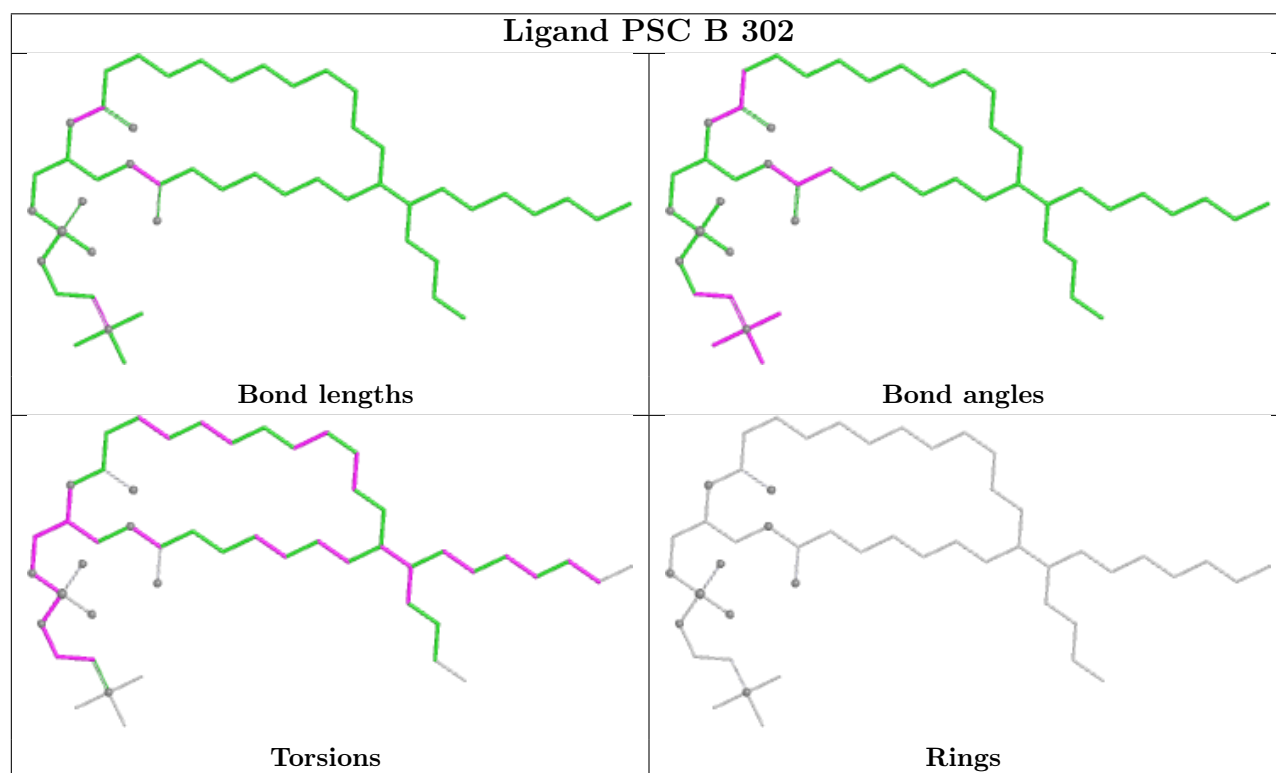
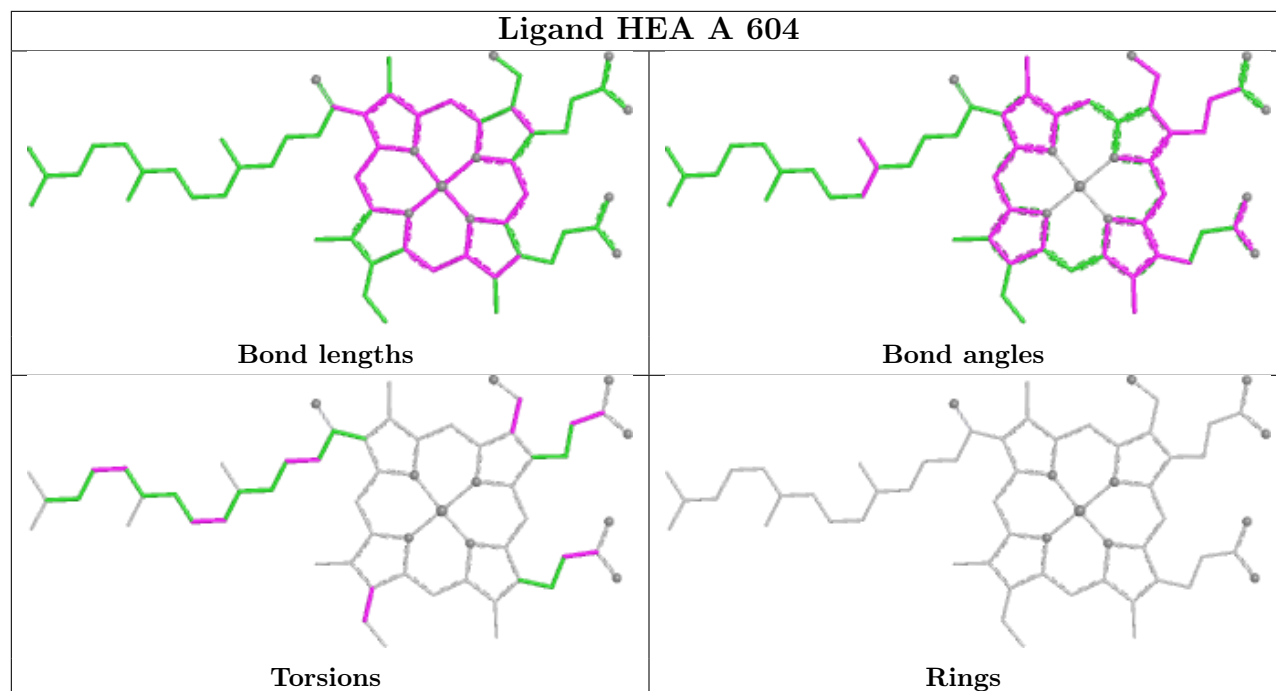
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

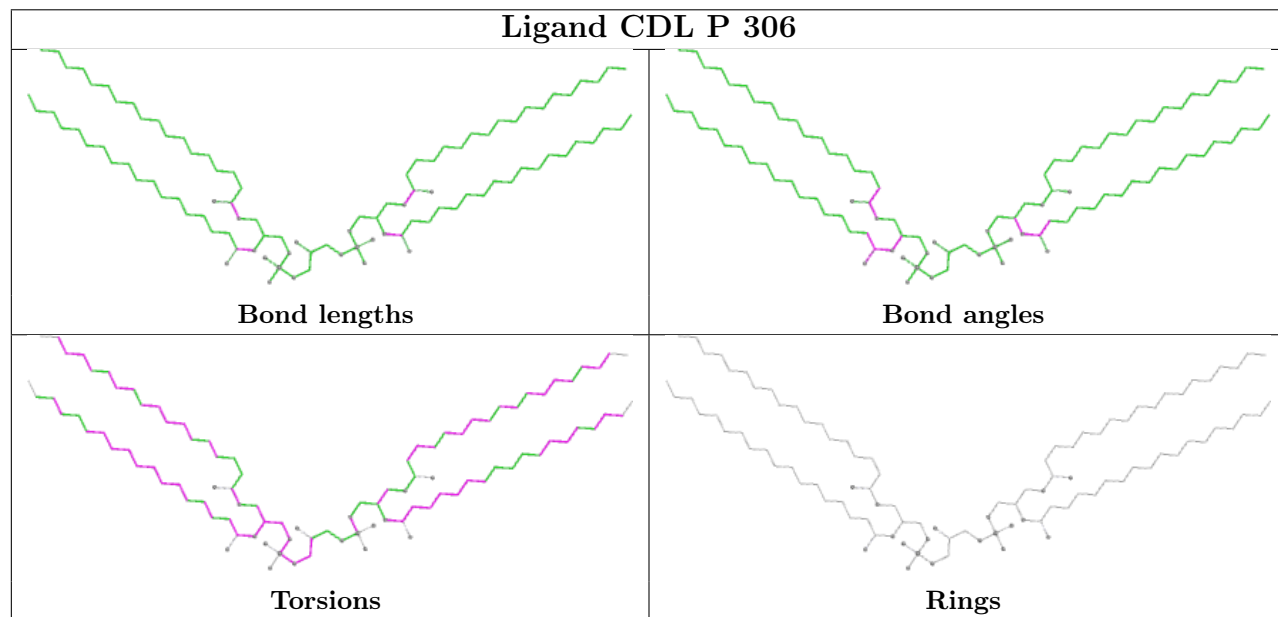
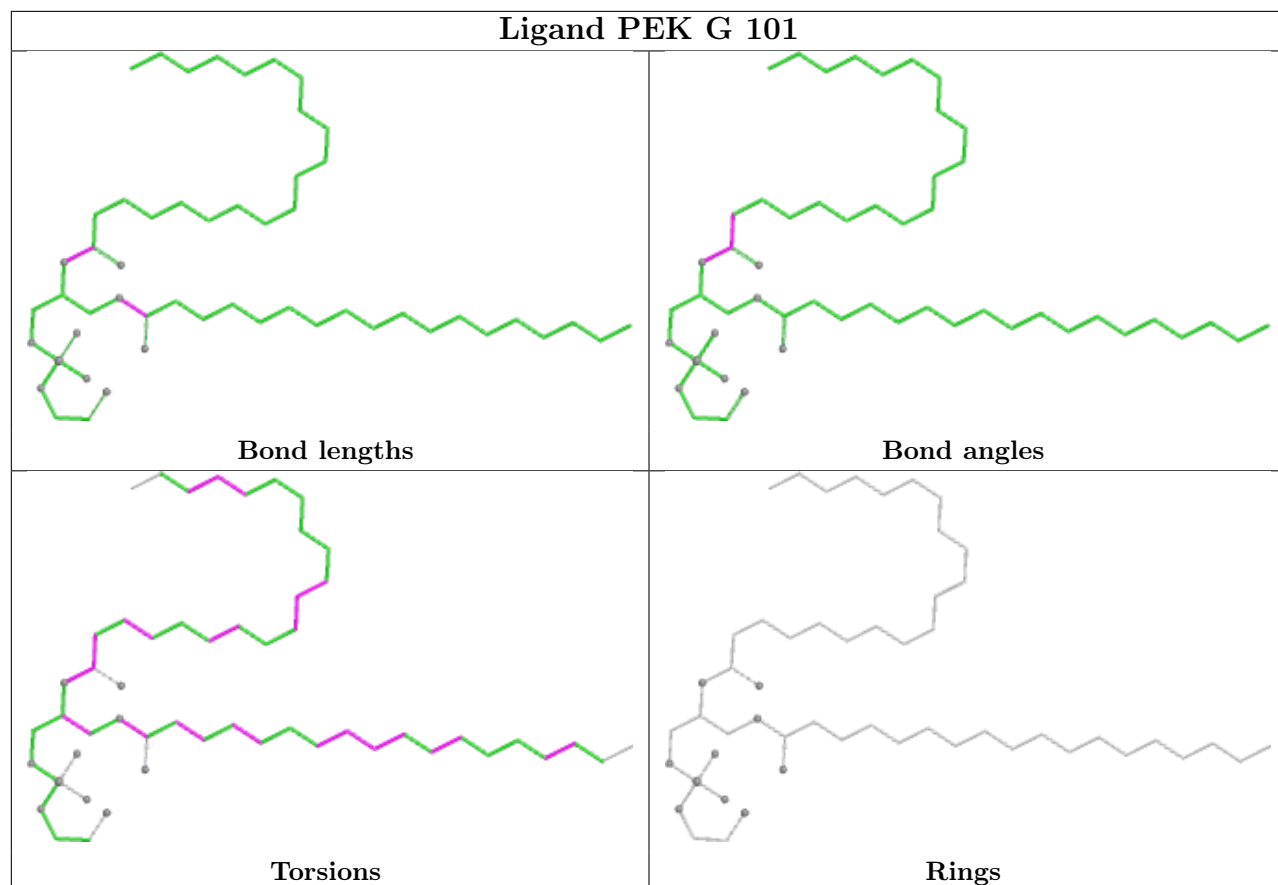
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

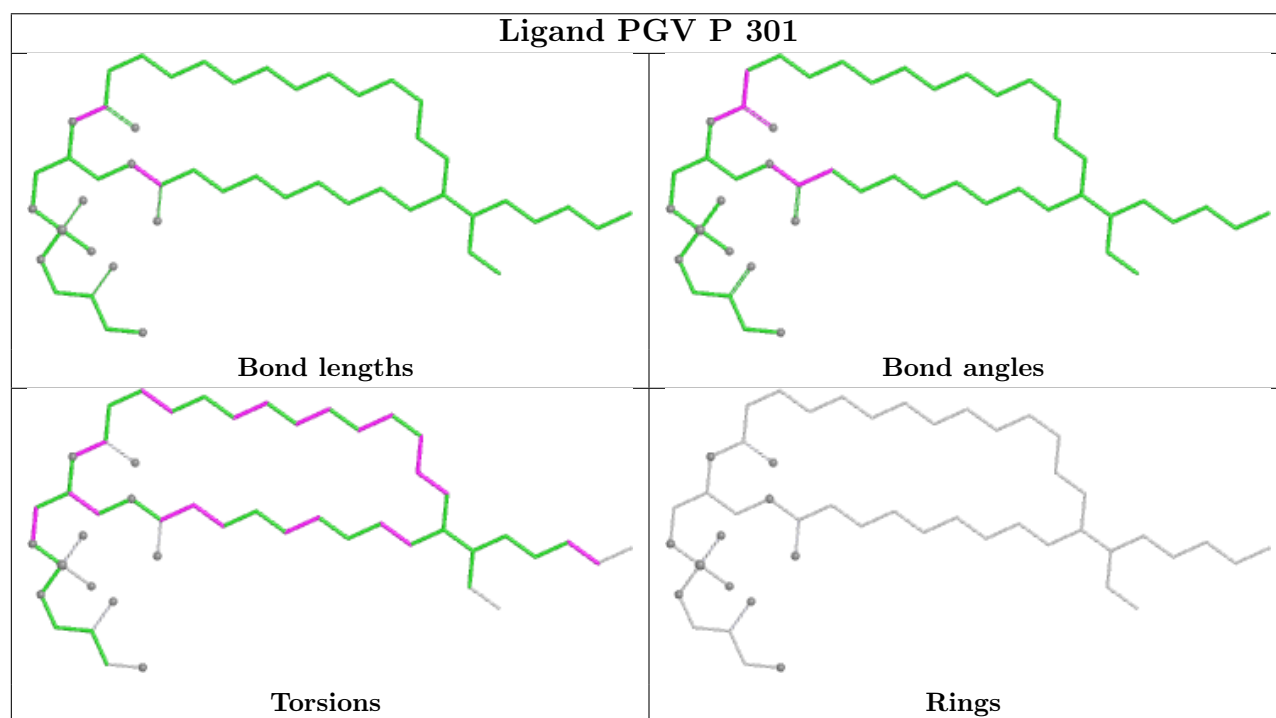
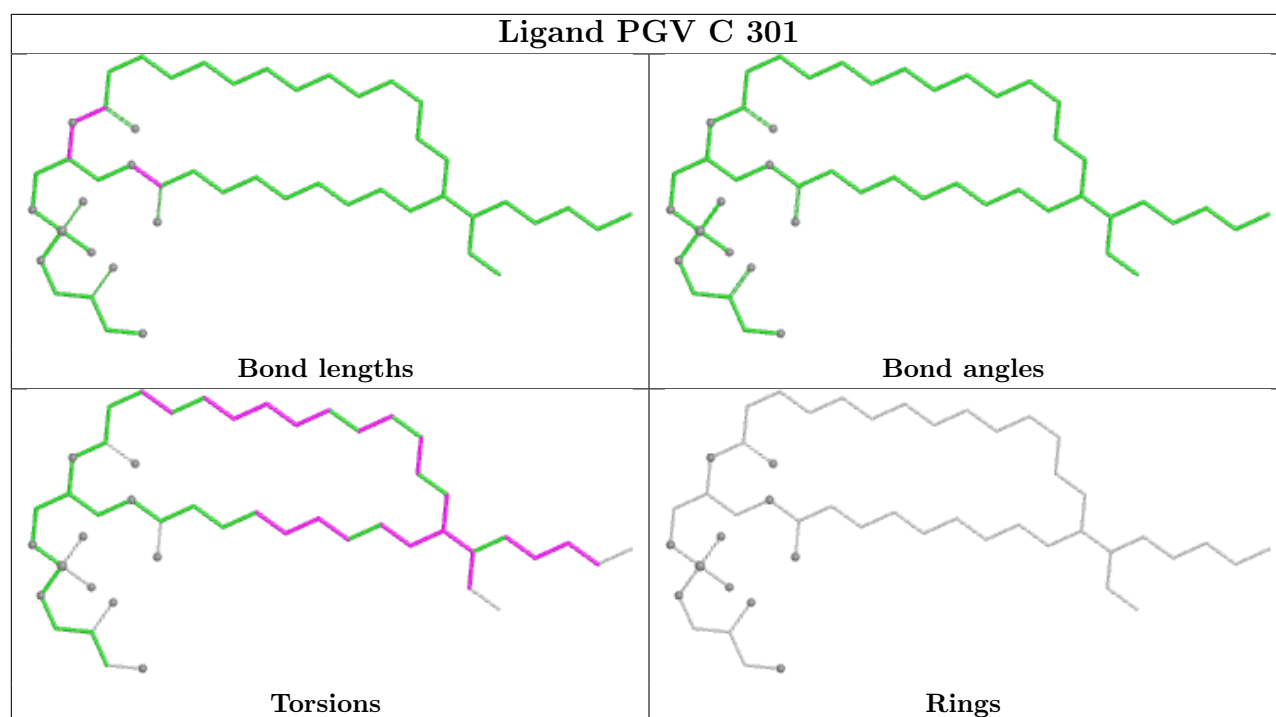


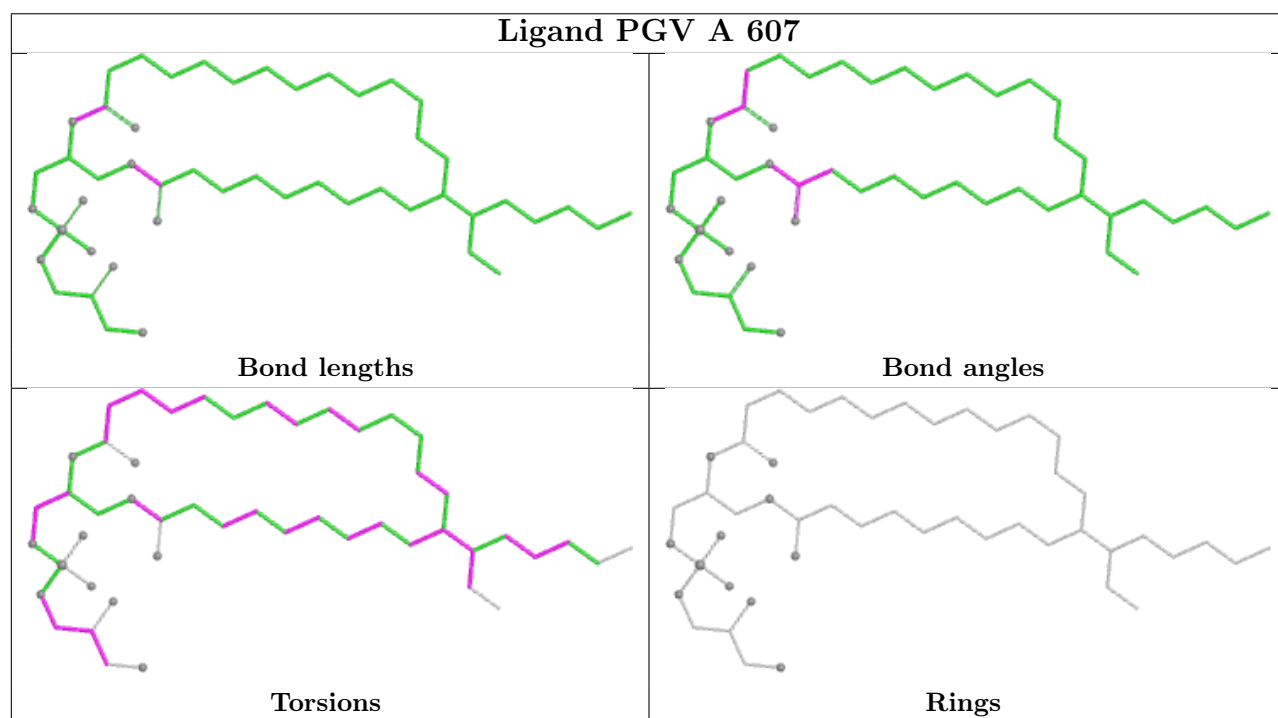
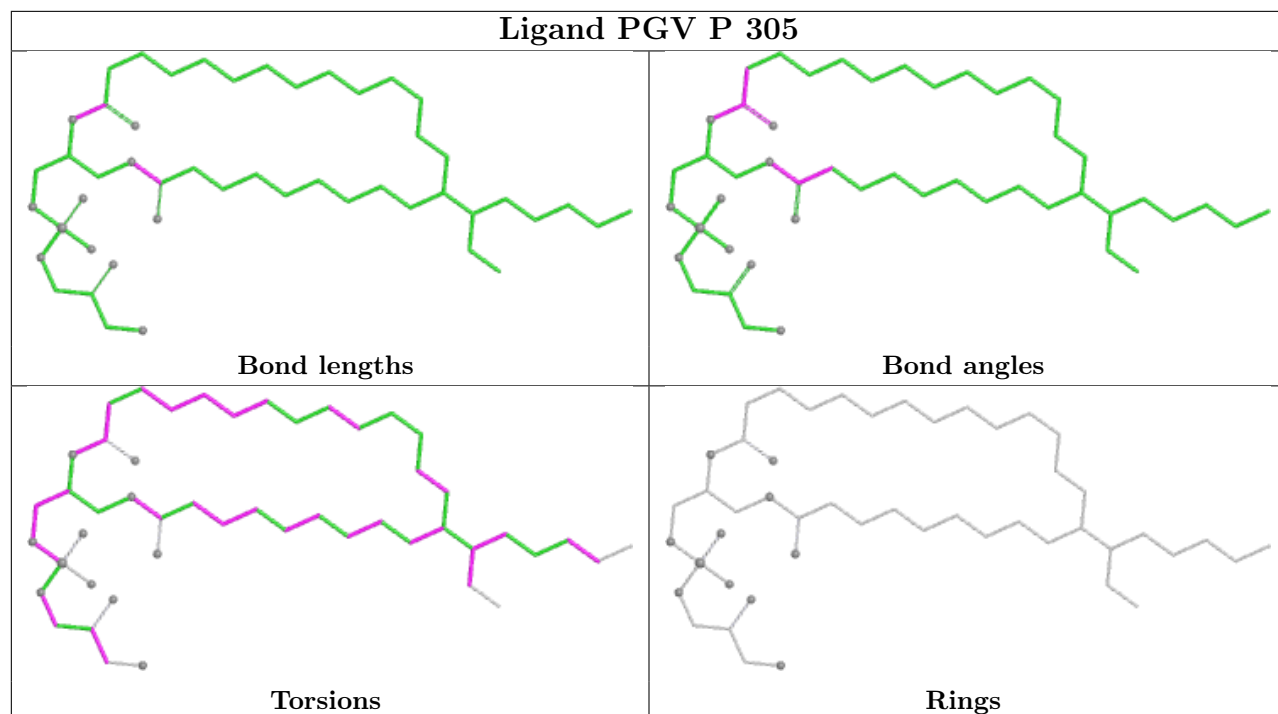


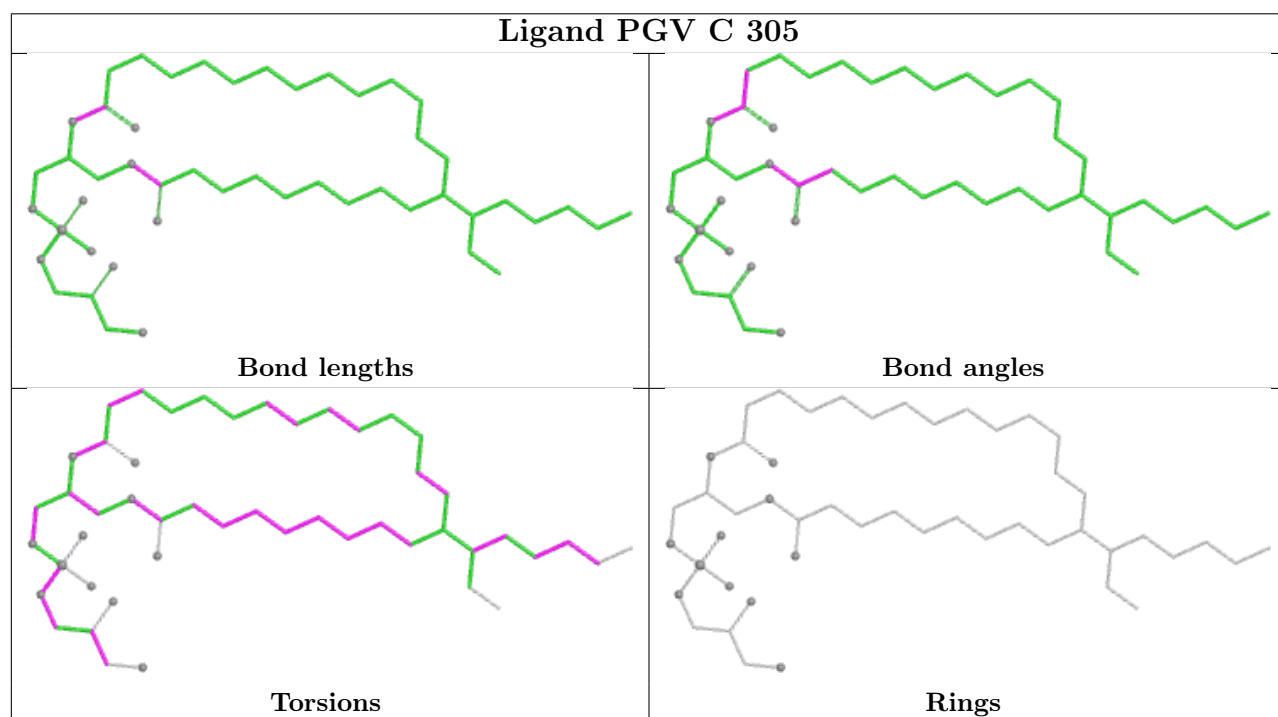
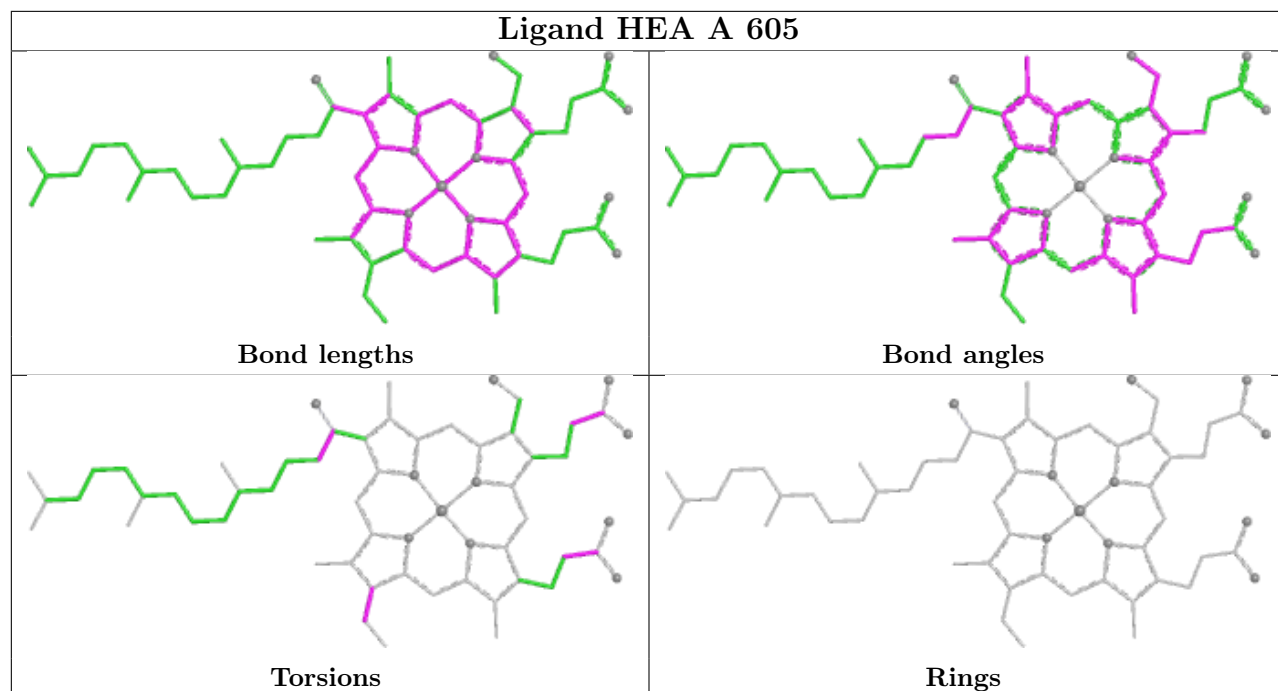


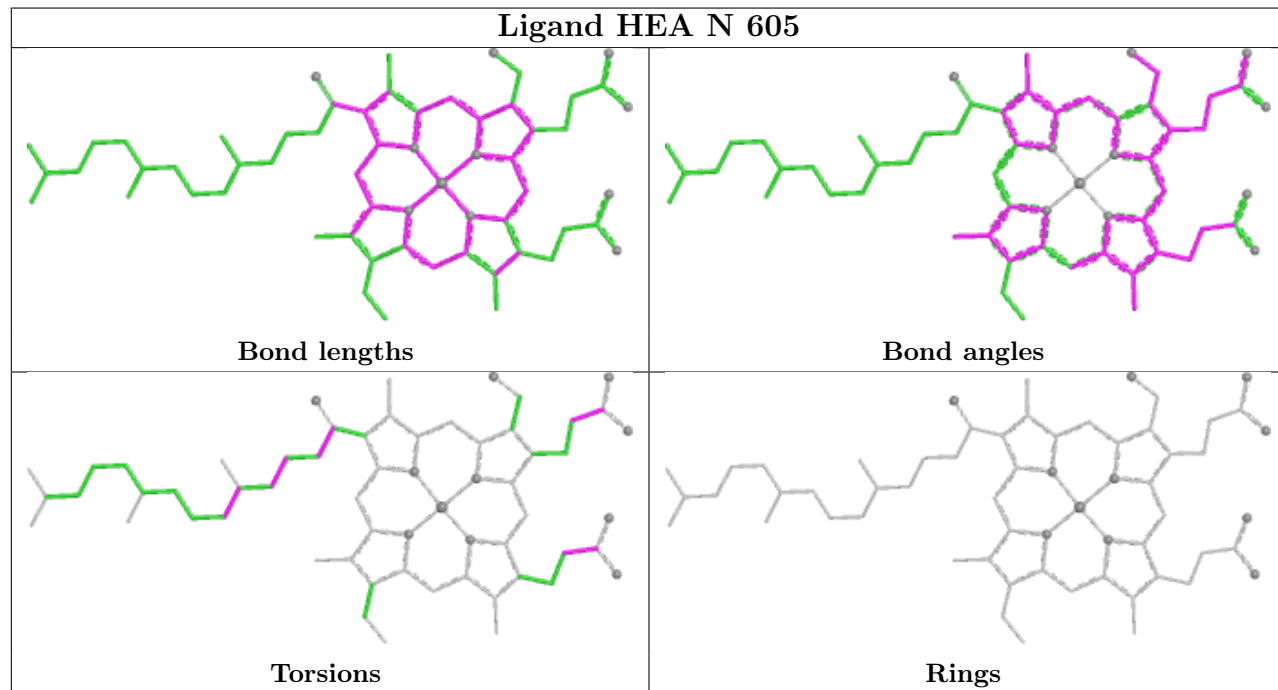
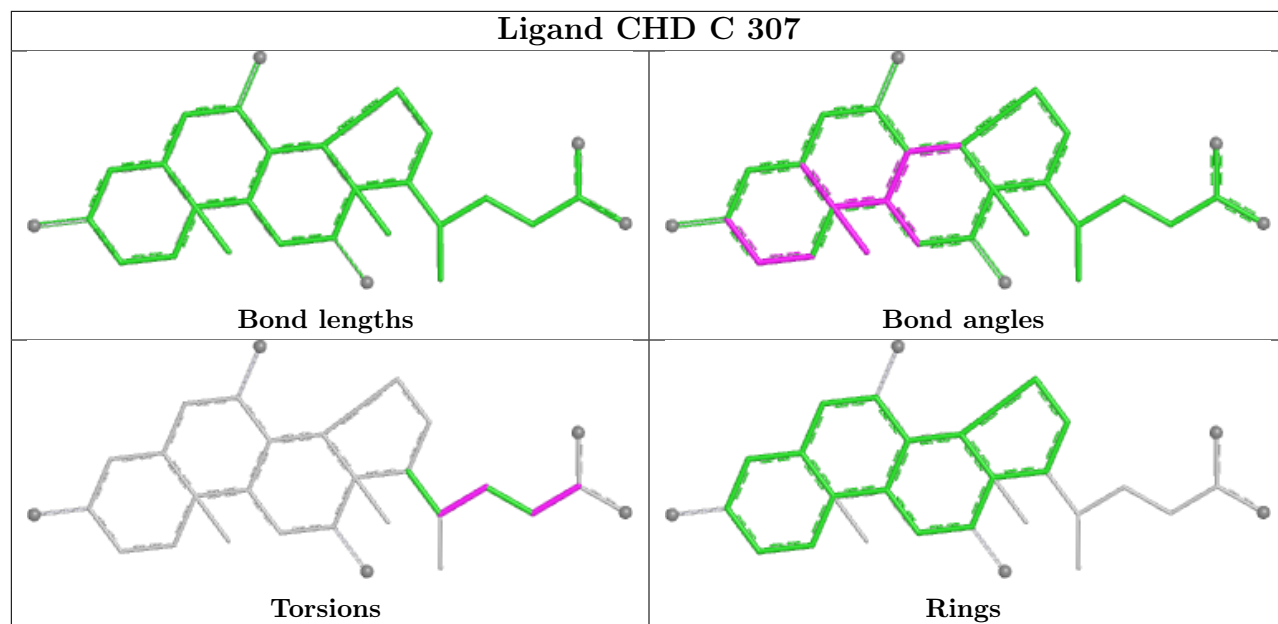


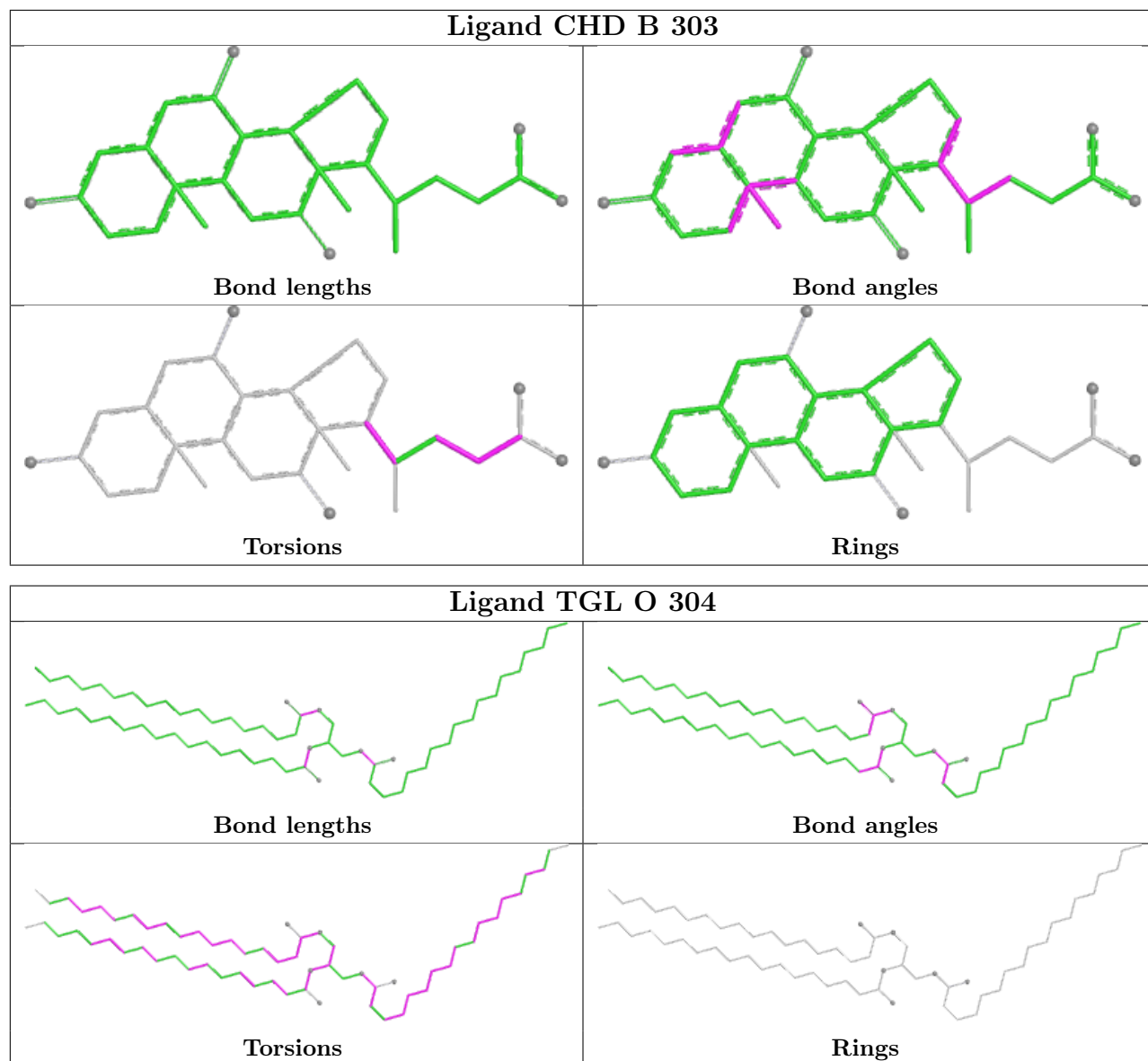


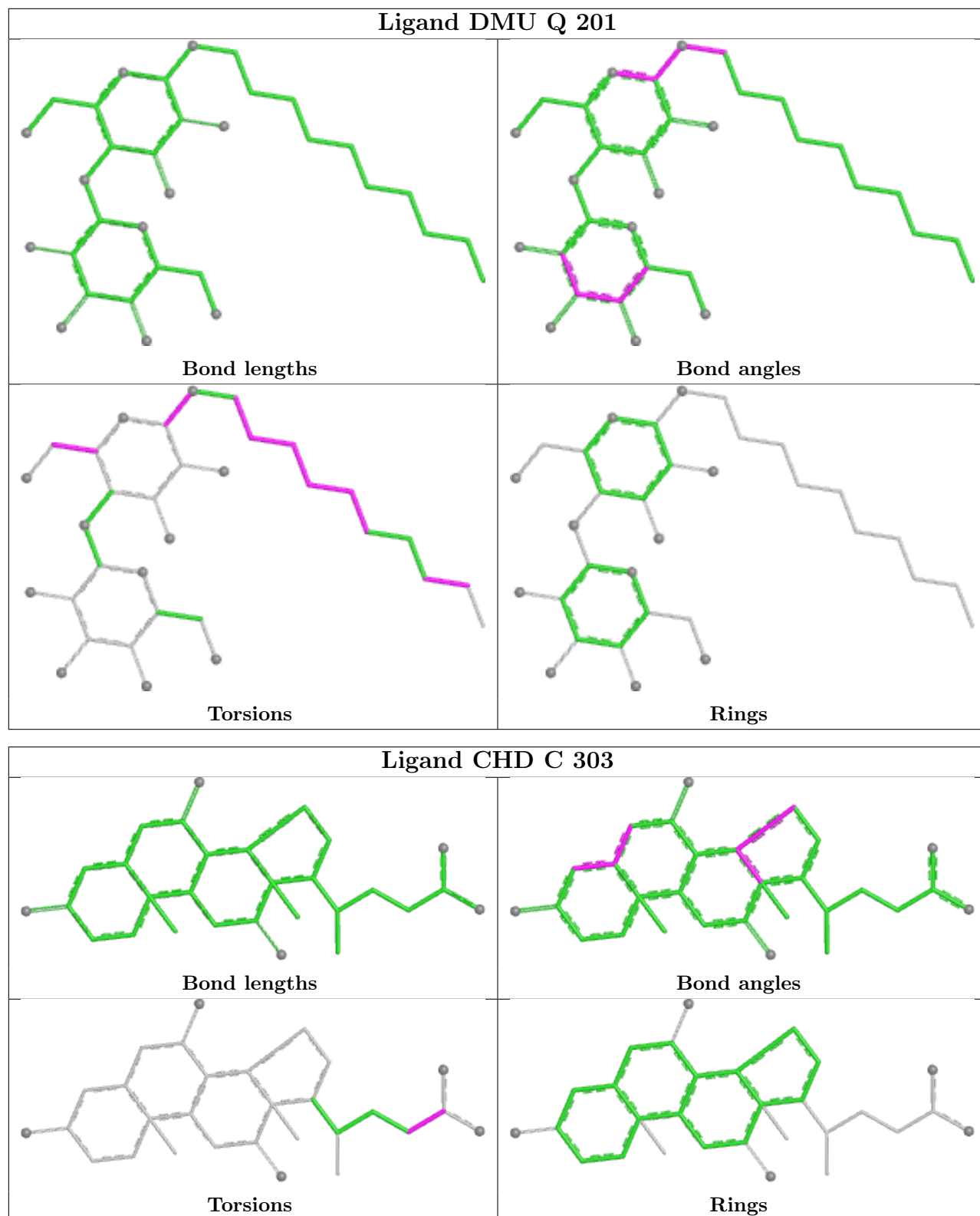


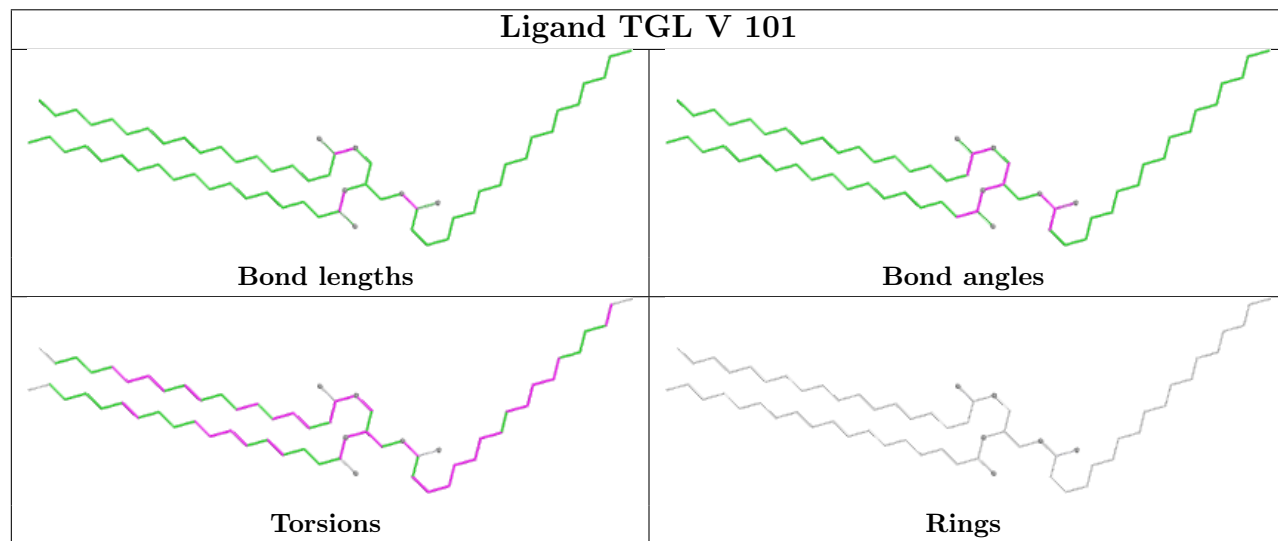
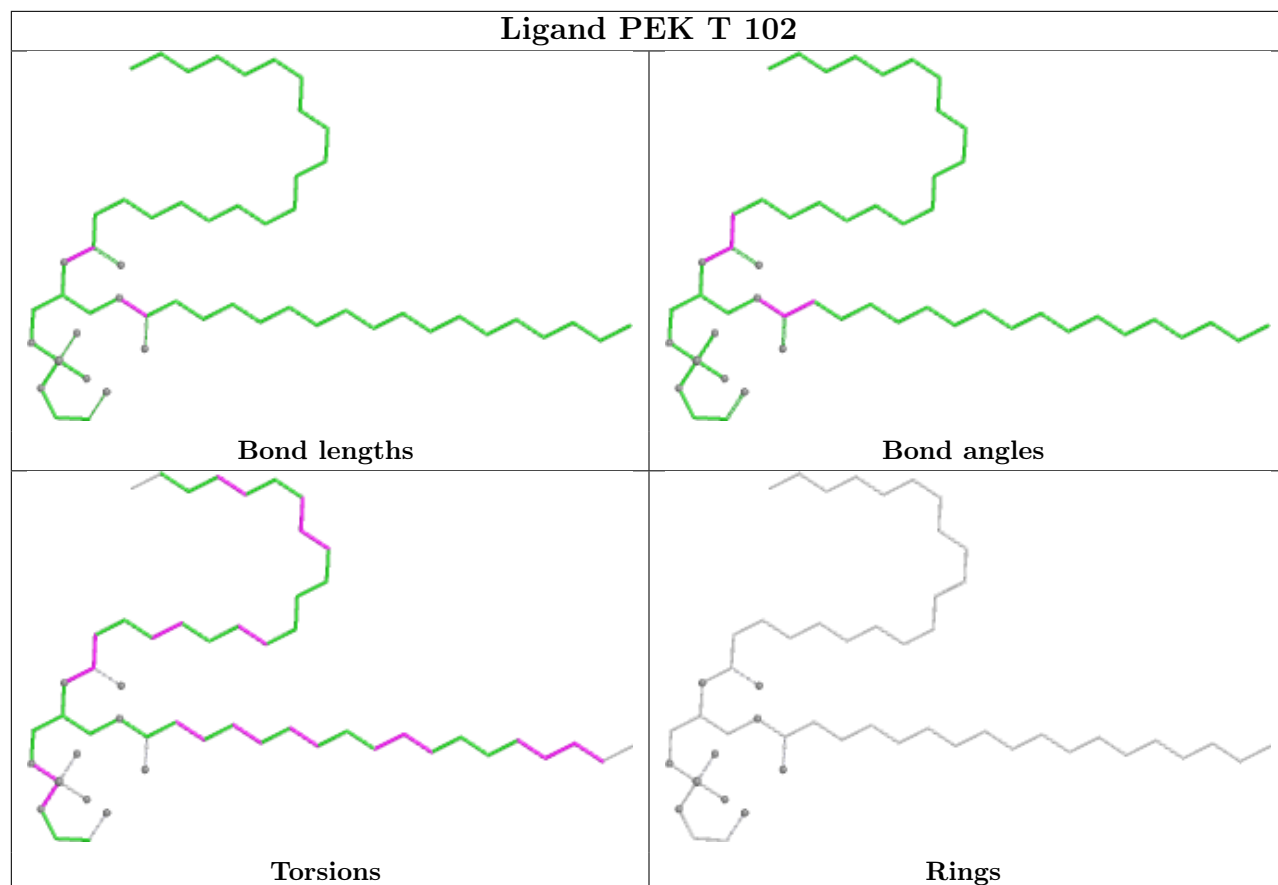


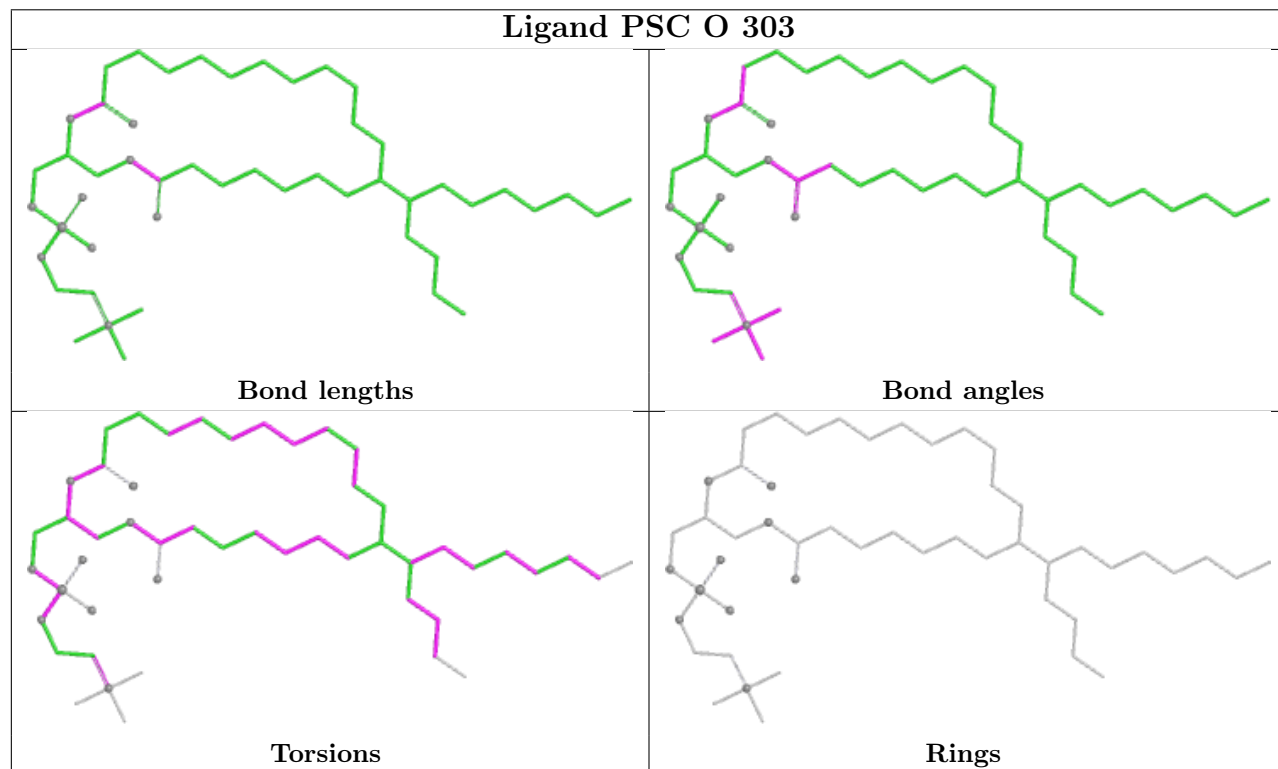
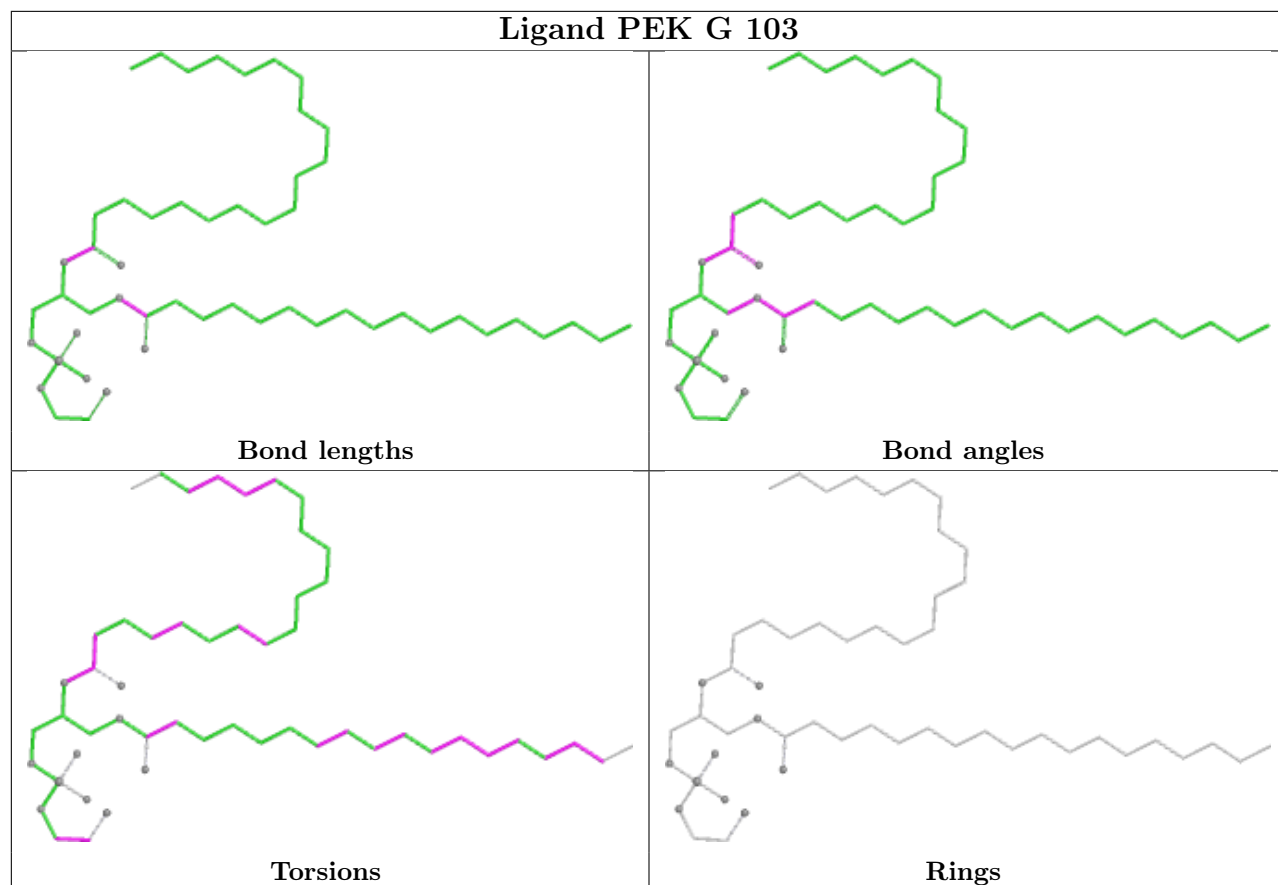


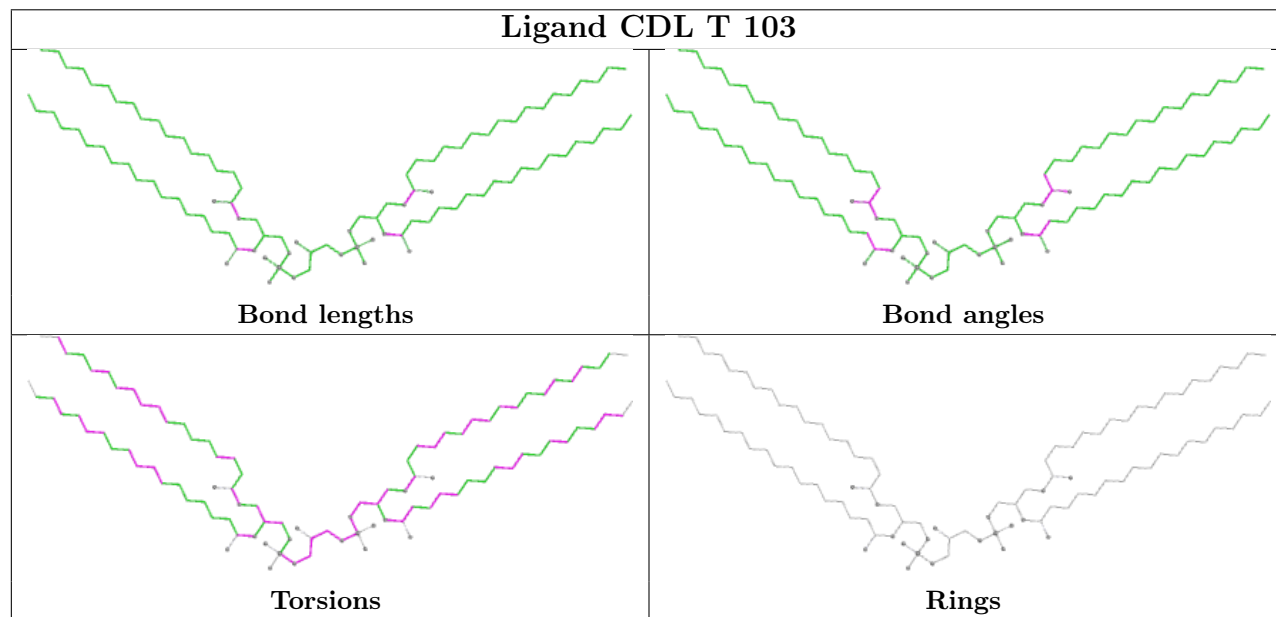
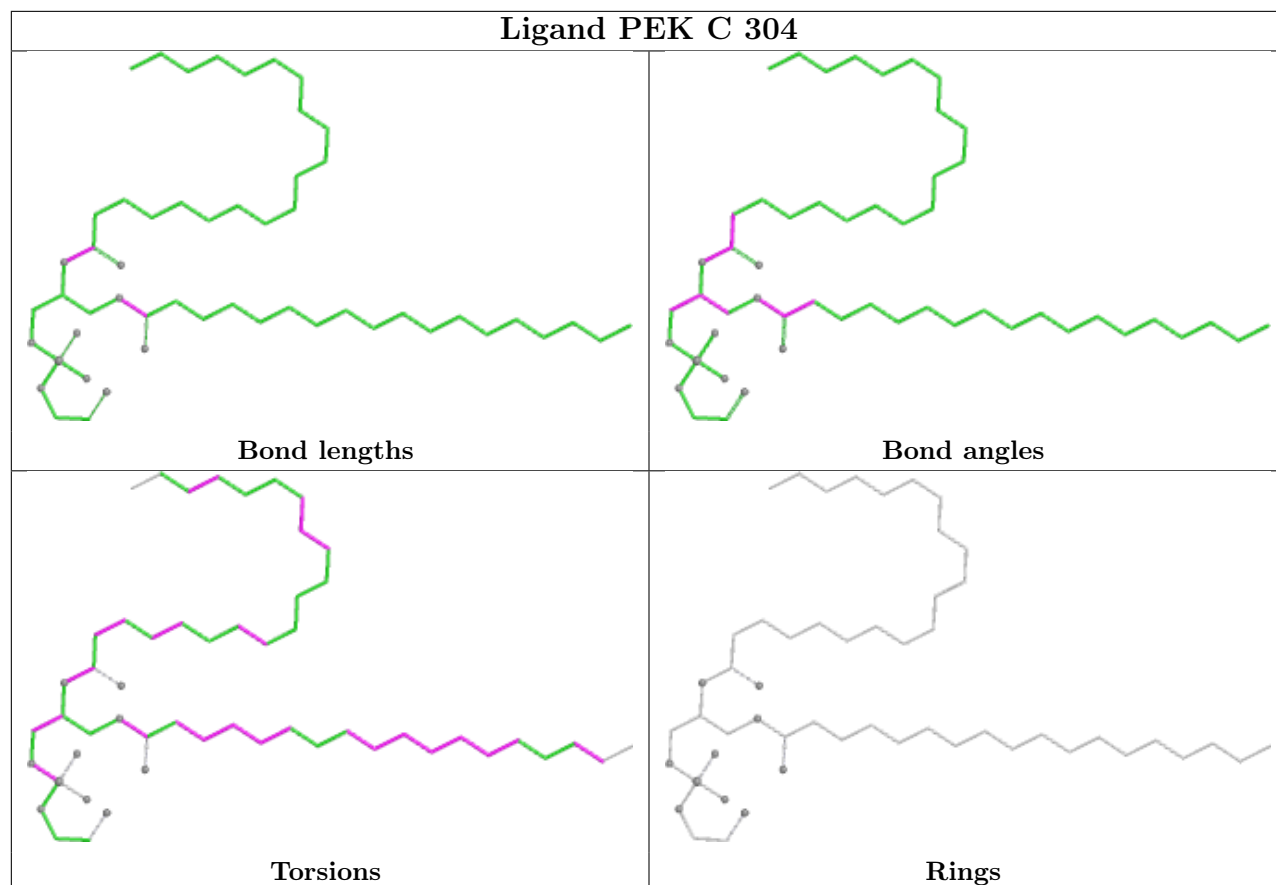


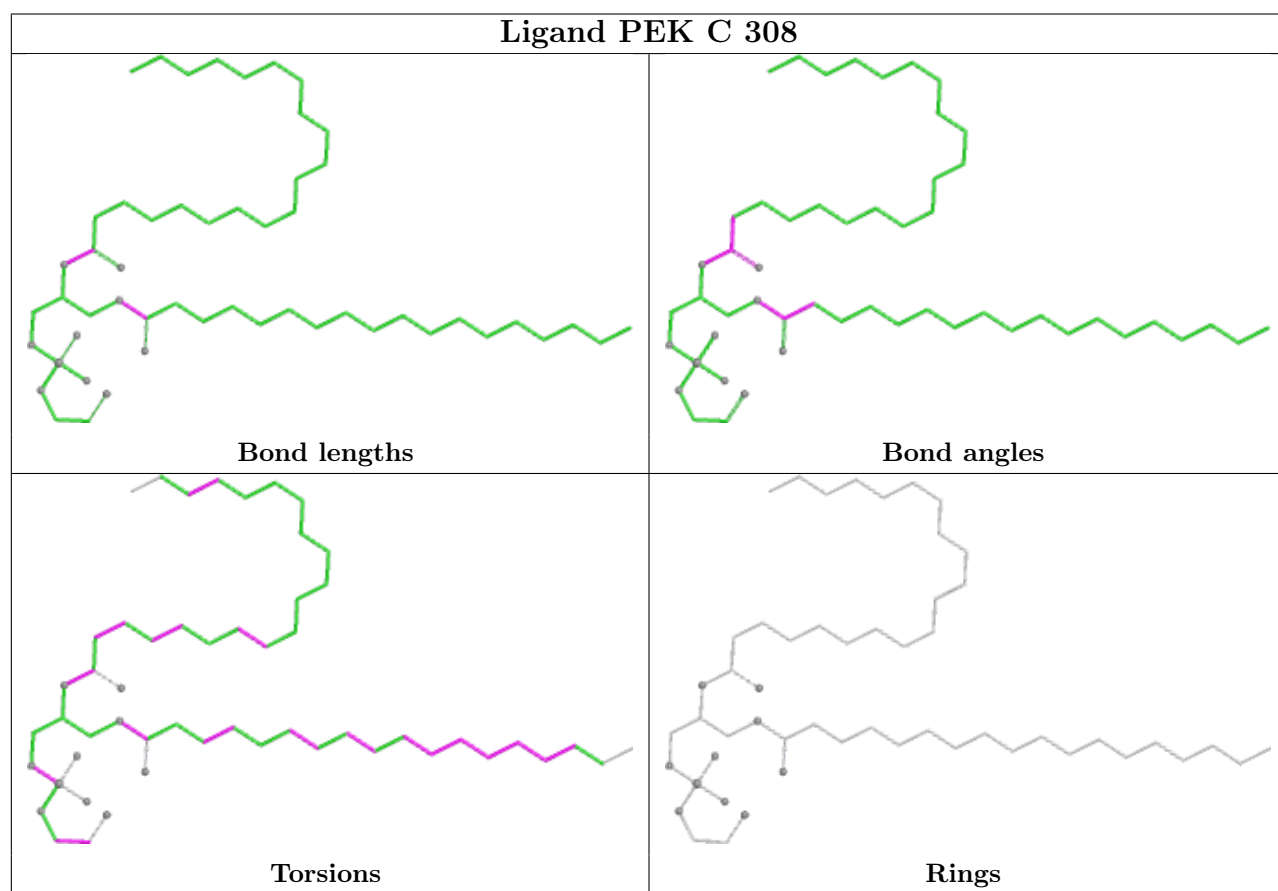
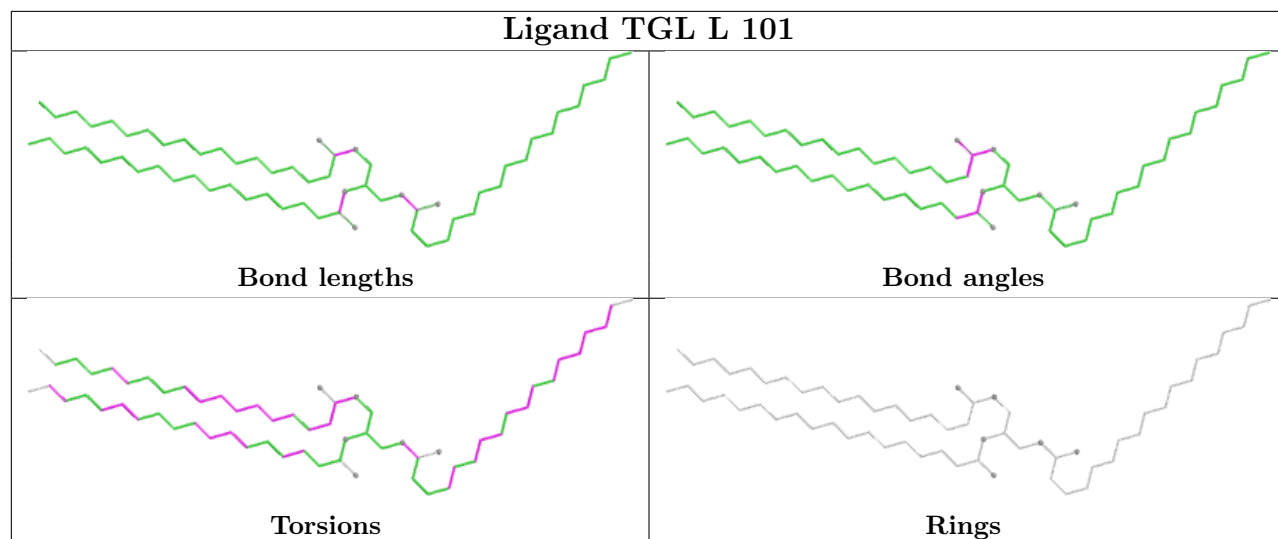


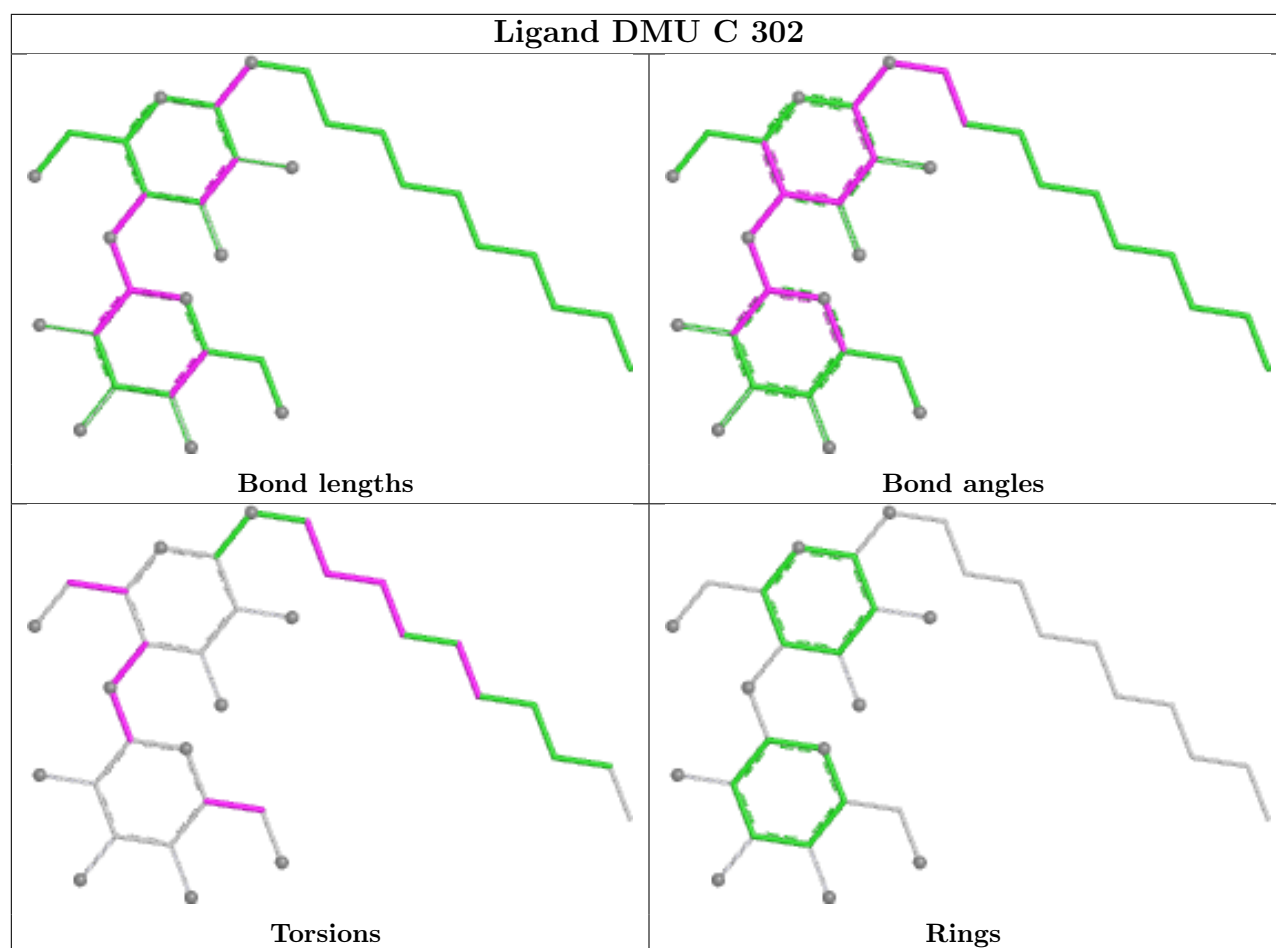


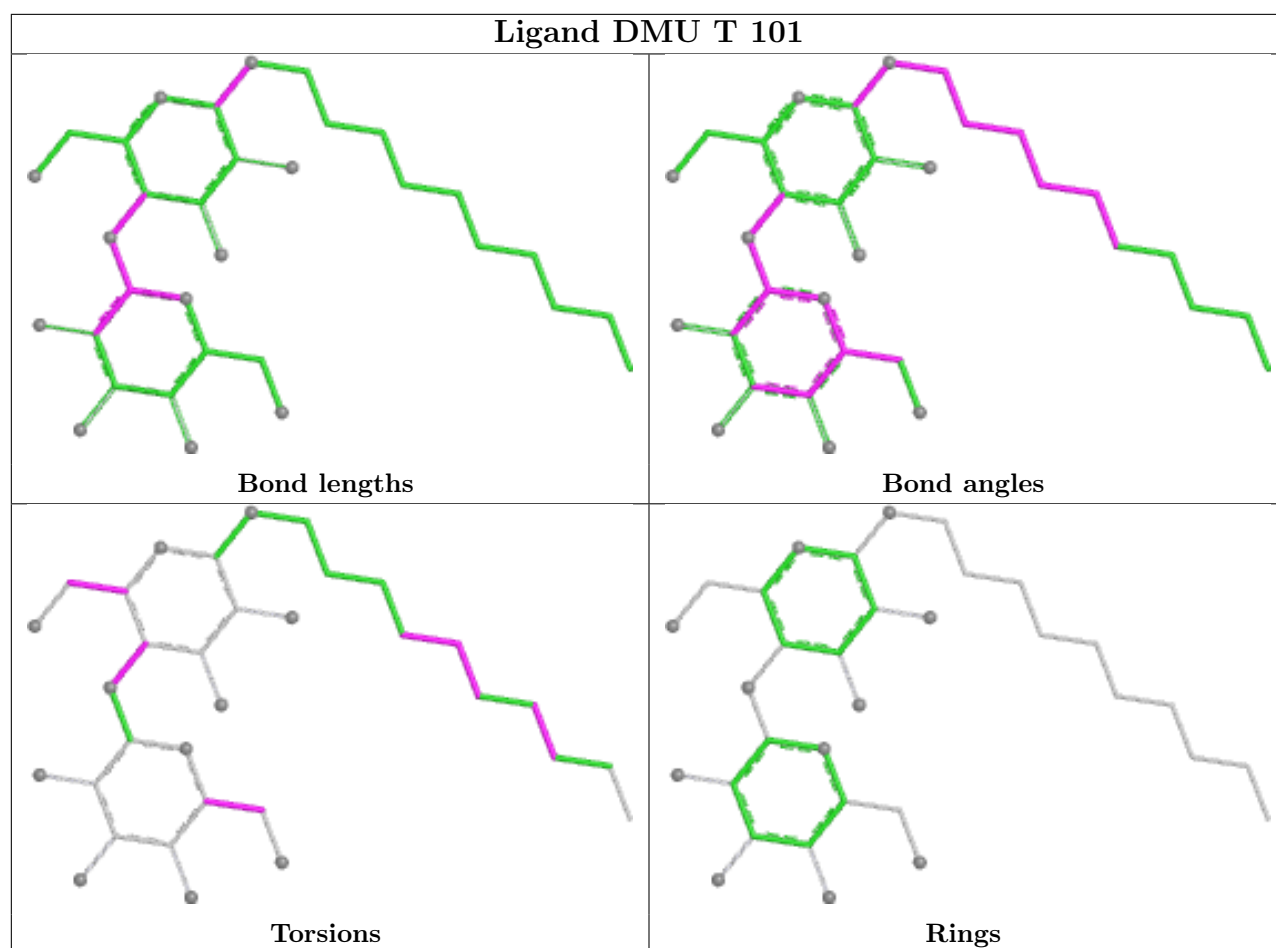


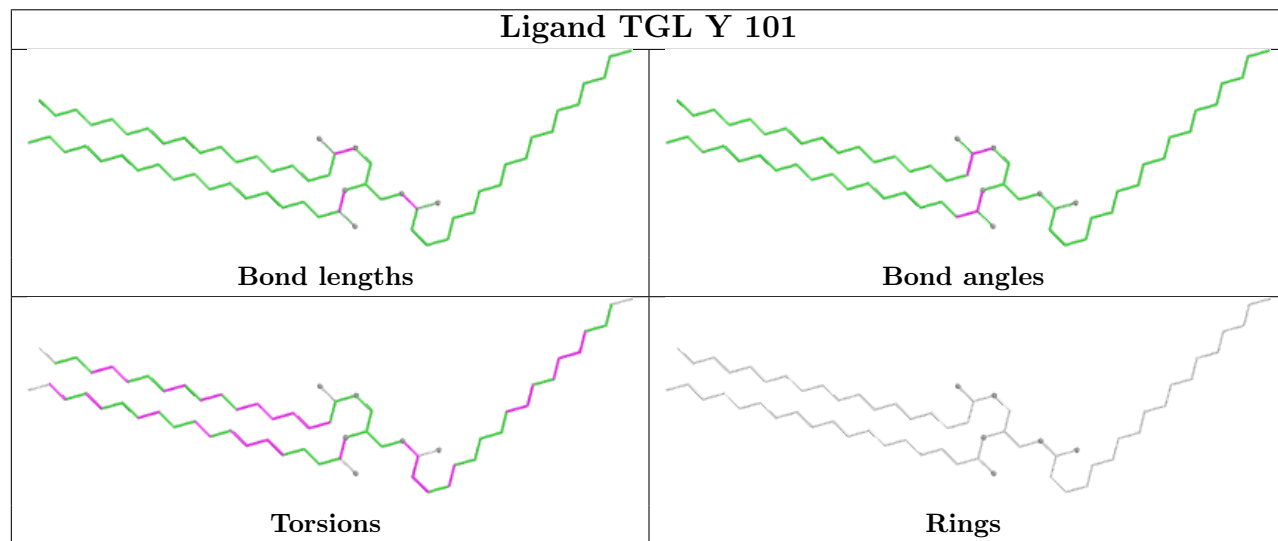
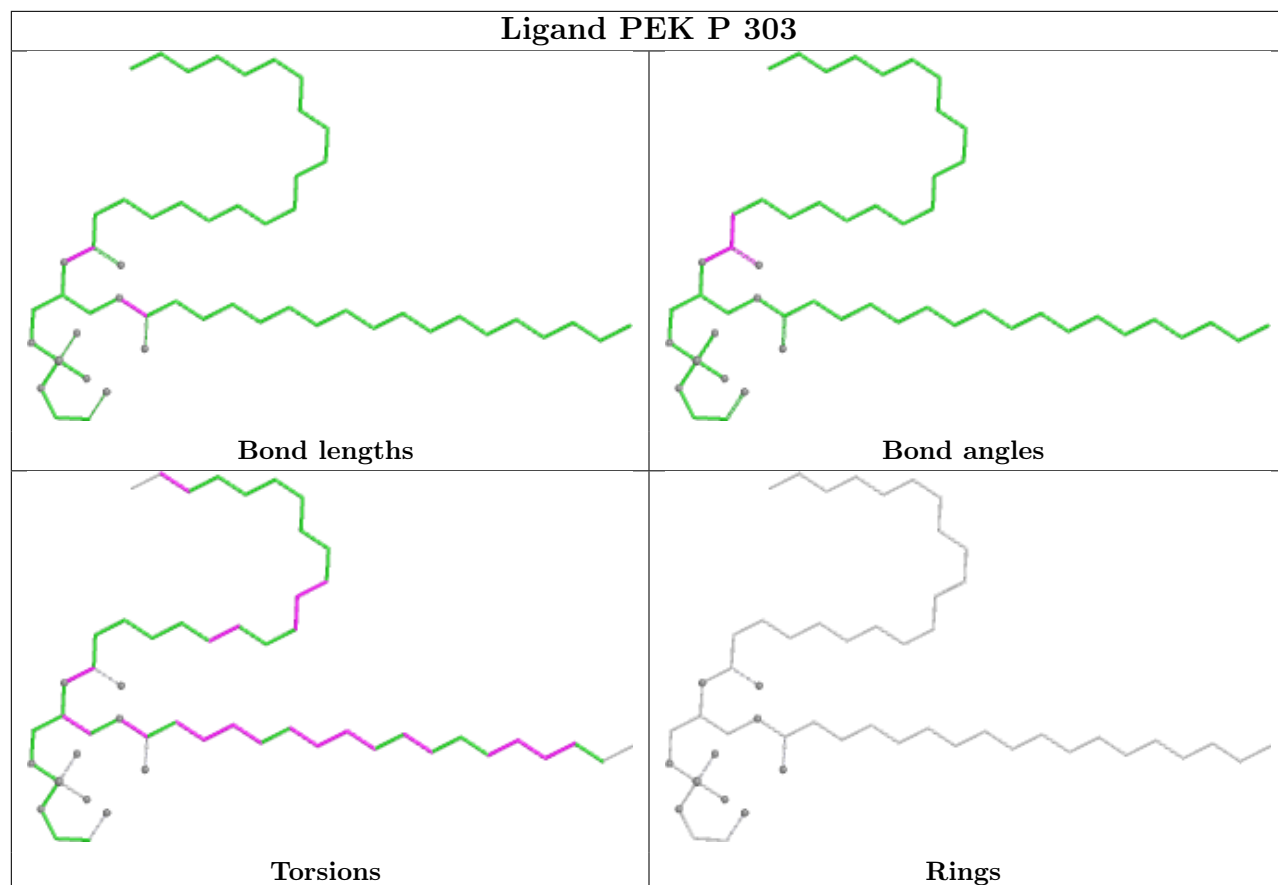


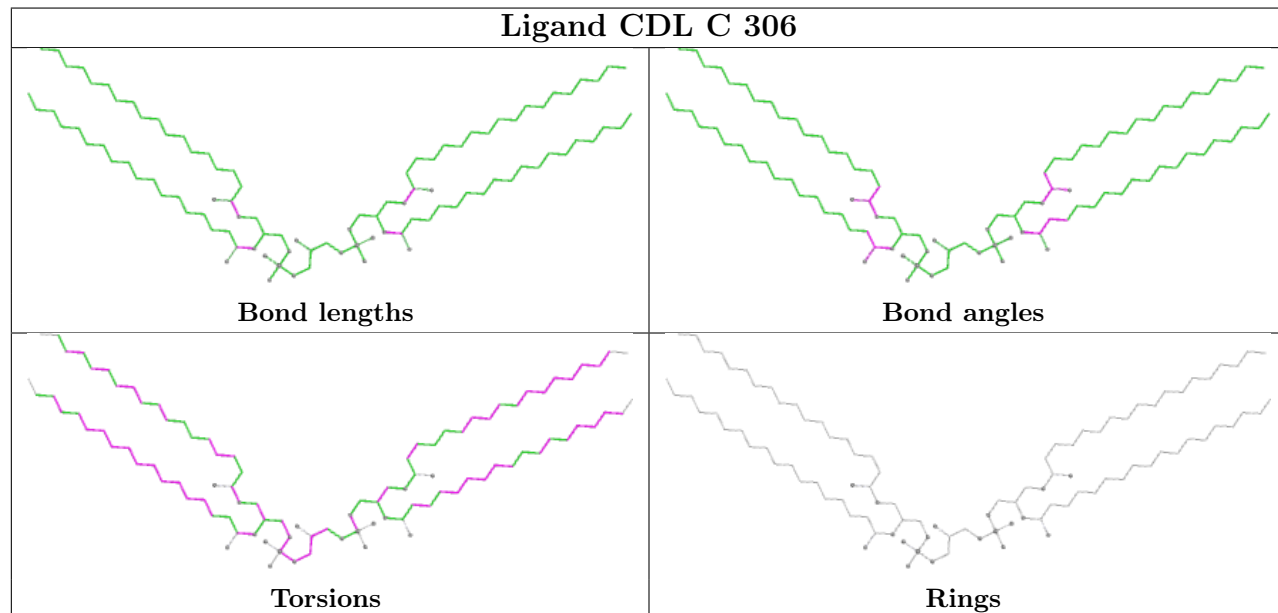
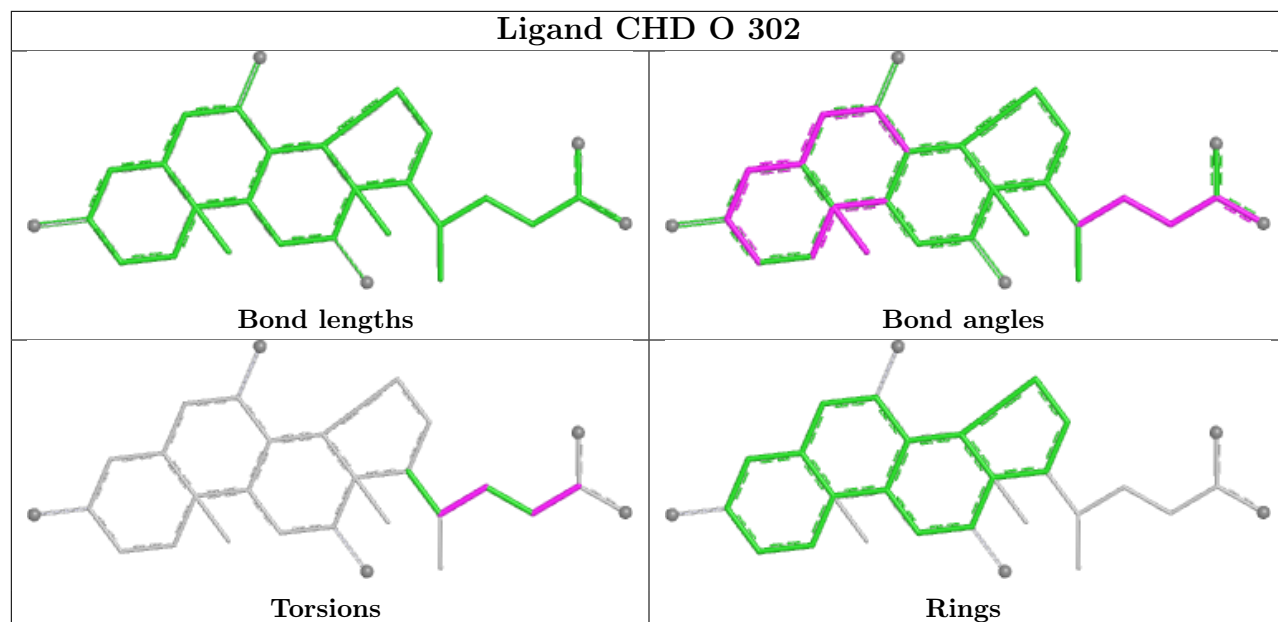


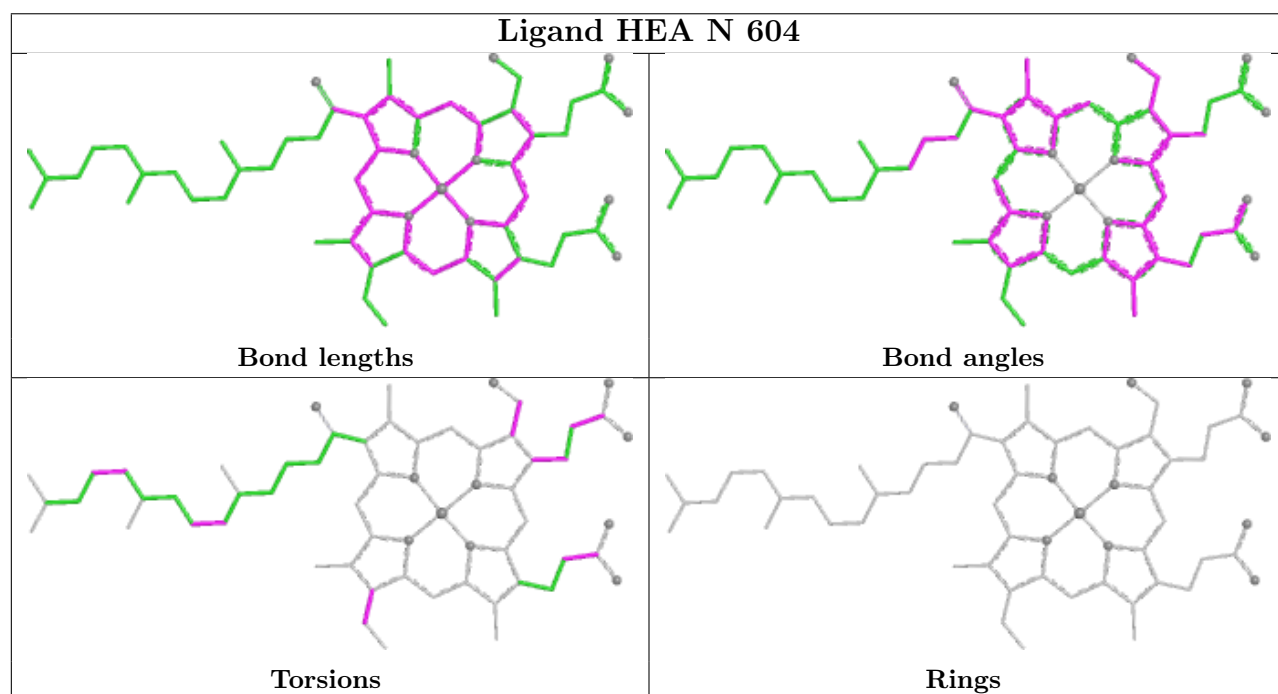
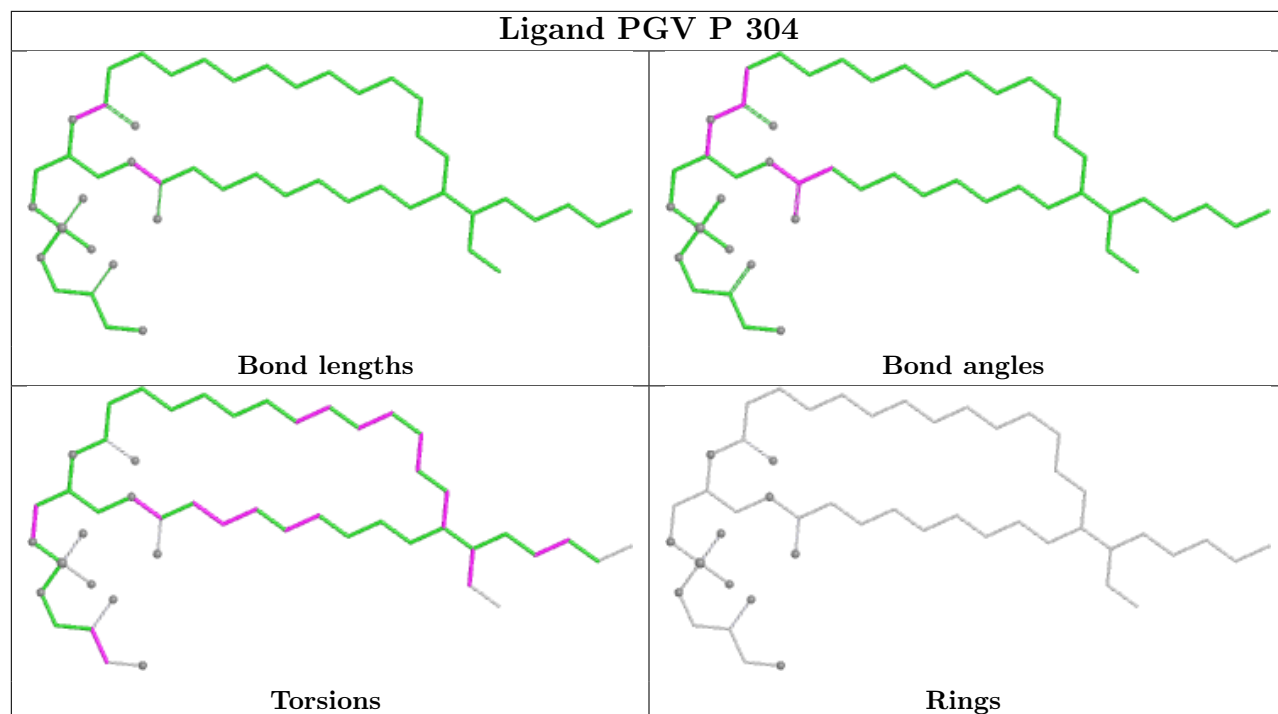




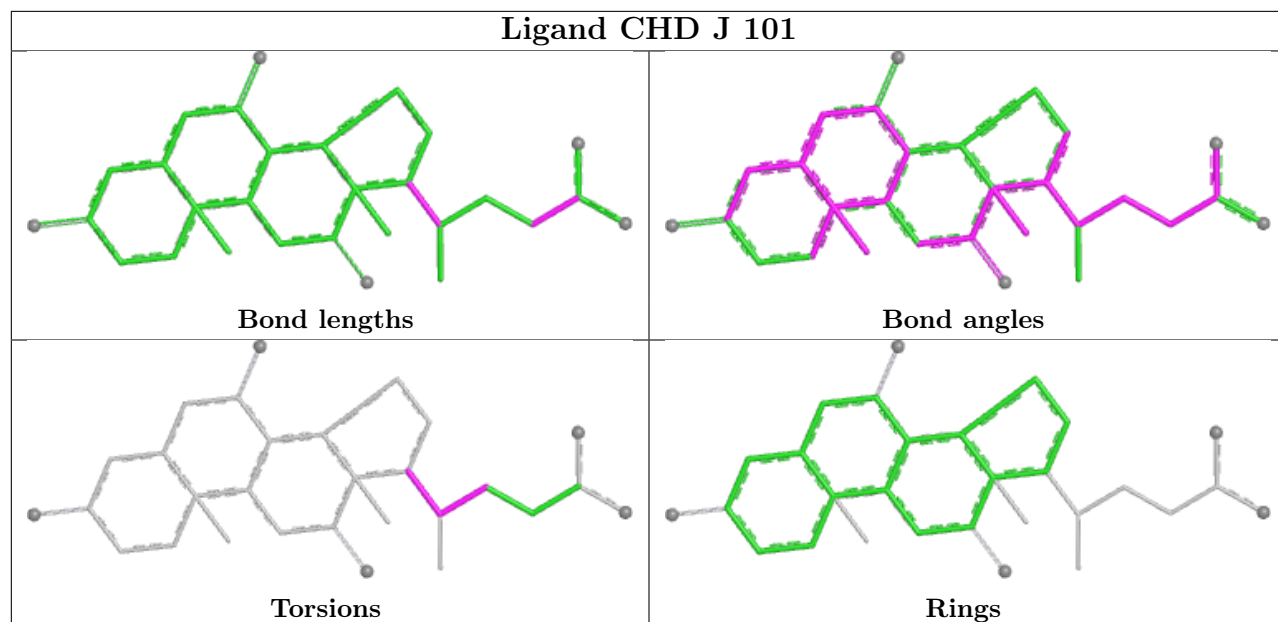




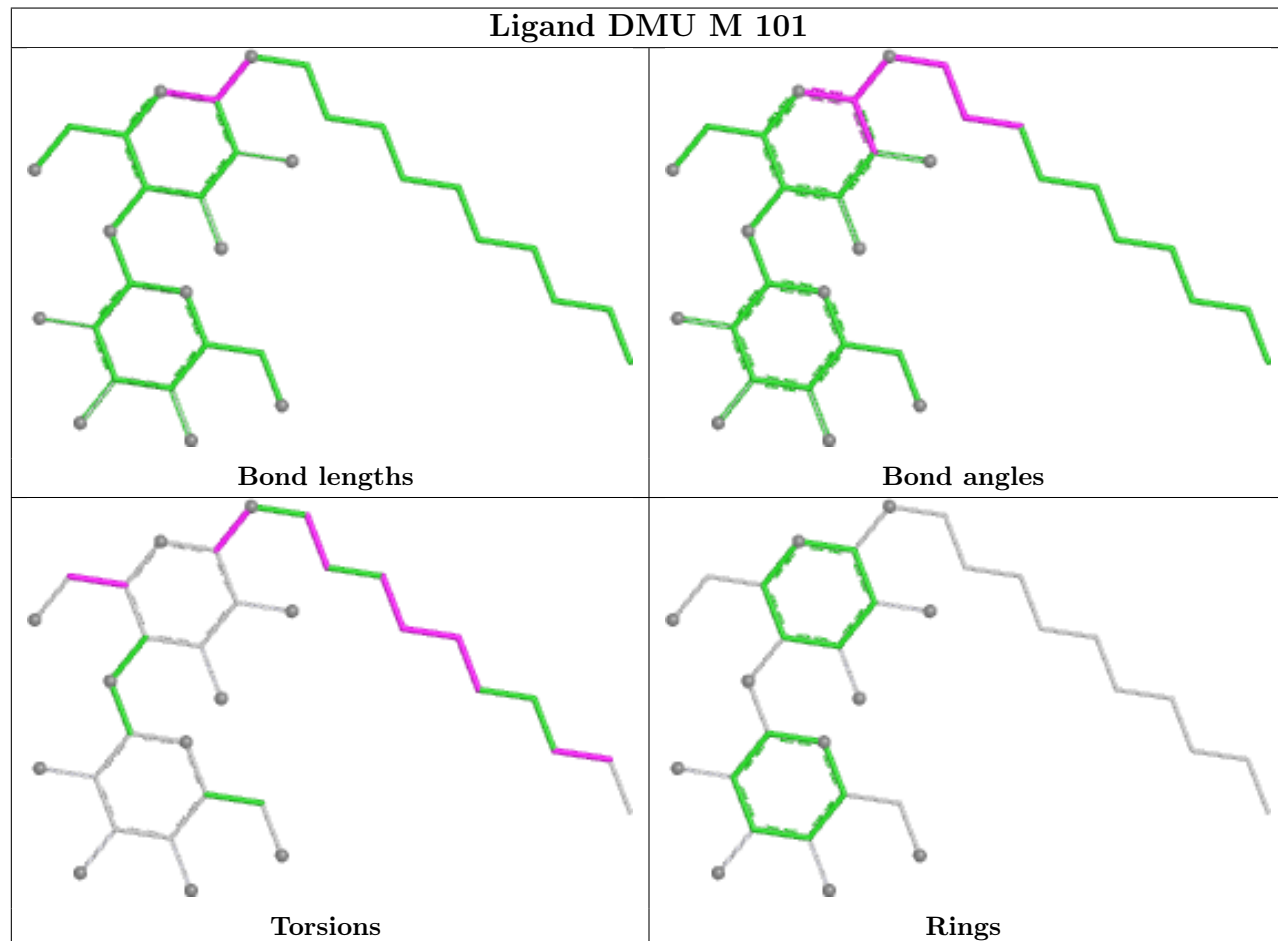


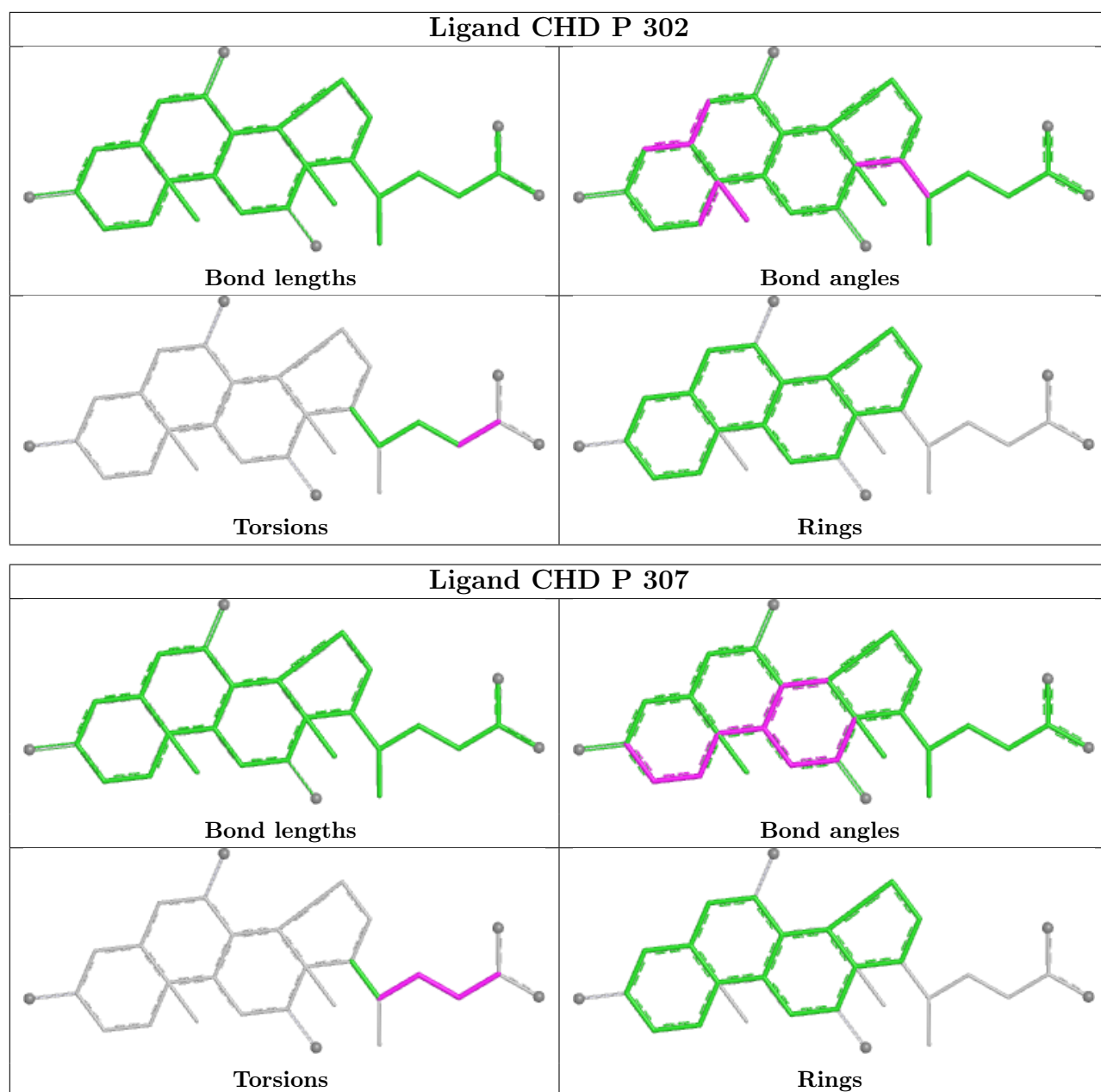


Ligand CHD J 101



Ligand DMU M 101





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%)	-1.00	0 100 100	31, 41, 54, 91	0
1	N	513/514 (99%)	-0.72	0 100 100	36, 55, 75, 108	0
2	B	226/227 (99%)	-0.81	1 (0%) 88 85	33, 50, 83, 128	0
2	O	226/227 (99%)	-0.52	2 (0%) 81 75	49, 68, 104, 155	0
3	C	259/261 (99%)	-0.90	0 100 100	34, 46, 65, 98	0
3	P	259/261 (99%)	-0.71	0 100 100	42, 57, 80, 124	0
4	D	144/147 (97%)	-0.83	0 100 100	39, 53, 80, 110	0
4	Q	144/147 (97%)	-0.27	3 (2%) 63 54	56, 83, 120, 202	0
5	E	105/109 (96%)	-0.87	0 100 100	39, 53, 84, 140	0
5	R	105/109 (96%)	-0.65	0 100 100	52, 69, 90, 134	0
6	F	98/98 (100%)	-0.51	3 (3%) 51 42	38, 56, 130, 154	0
6	S	98/98 (100%)	-0.37	3 (3%) 51 42	47, 68, 152, 176	0
7	G	83/85 (97%)	-0.27	4 (4%) 35 28	40, 59, 144, 161	0
7	T	83/85 (97%)	-0.18	6 (7%) 21 17	43, 72, 144, 163	0
8	H	79/85 (92%)	-0.60	1 (1%) 75 67	43, 60, 119, 135	0
8	U	79/85 (92%)	-0.33	1 (1%) 75 67	54, 75, 129, 157	0
9	I	72/73 (98%)	-0.49	1 (1%) 73 65	46, 63, 93, 114	0
9	V	72/73 (98%)	-0.15	1 (1%) 73 65	49, 79, 112, 127	0
10	J	58/59 (98%)	-0.58	0 100 100	44, 60, 104, 138	0
10	W	58/59 (98%)	-0.18	0 100 100	61, 79, 130, 151	0
11	K	49/56 (87%)	-0.68	0 100 100	47, 60, 81, 96	0
11	X	49/56 (87%)	-0.26	0 100 100	59, 80, 104, 123	0
12	L	46/47 (97%)	-0.73	0 100 100	40, 49, 75, 124	0
12	Y	46/47 (97%)	-0.25	0 100 100	58, 76, 102, 137	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	43/46 (93%)	-0.80	0 100 100	40, 48, 95, 139	0
13	Z	43/46 (93%)	-0.17	0 100 100	62, 74, 131, 153	0
All	All	3550/3614 (98%)	-0.66	26 (0%) 84 79	31, 56, 101, 202	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	S	1	ALA	7.3
4	Q	6	VAL	5.3
9	V	37	PHE	3.6
7	G	3	ALA	3.5
6	S	96	LEU	3.5
4	Q	5	VAL	3.4
2	O	58	ALA	3.3
7	T	36	TRP	3.3
2	B	59	GLN	3.2
2	O	90	ILE	2.9
7	G	10	GLY	2.7
7	T	10	GLY	2.7
8	U	8	ILE	2.6
6	F	96	LEU	2.6
6	S	94	HIS	2.6
6	F	94	HIS	2.5
7	G	5	LYS	2.5
7	G	36	TRP	2.4
9	I	37	PHE	2.4
7	T	5	LYS	2.4
7	T	3	ALA	2.4
6	F	1	ALA	2.4
8	H	8	ILE	2.2
7	T	9	GLY	2.1
4	Q	7	LYS	2.1
7	T	40	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	SAC	V	1	9/10	0.51	0.17	144,155,160,162	0
9	SAC	I	1	9/10	0.61	0.14	122,141,150,151	0
7	TPO	T	11	11/12	0.72	0.16	139,153,169,174	0
7	TPO	G	11	11/12	0.76	0.19	112,136,147,154	0
1	FME	N	1	10/11	0.82	0.14	86,103,121,132	0
1	FME	A	1	10/11	0.87	0.15	80,84,135,138	0
2	FME	O	1	10/11	0.94	0.09	60,73,78,88	0
2	FME	B	1	10/11	0.97	0.07	46,49,54,64	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
25	PEK	G	103	53/53	0.66	0.21	79,133,192,210	0
24	DMU	T	101	33/33	0.67	0.14	116,164,194,199	0
18	PGV	P	305	51/51	0.76	0.14	77,111,129,133	0
19	TGL	Y	101	63/63	0.79	0.16	76,102,153,164	0
18	PGV	N	606	51/51	0.79	0.14	59,100,150,166	0
25	PEK	C	308	53/53	0.79	0.18	71,111,178,196	0
19	TGL	O	304	63/63	0.79	0.15	89,112,126,138	0
23	CHD	W	101	29/29	0.80	0.14	105,123,144,151	0
25	PEK	C	304	53/53	0.80	0.14	75,104,180,197	0
23	CHD	J	101	29/29	0.82	0.14	82,94,112,120	0
18	PGV	A	607	51/51	0.82	0.13	76,107,130,136	0
25	PEK	T	102	53/53	0.82	0.13	73,108,155,162	0
19	TGL	A	608	63/63	0.83	0.13	57,92,112,120	0
26	CDL	C	306	100/100	0.83	0.14	60,109,150,157	0
26	CDL	G	102	100/100	0.83	0.15	78,128,168,200	0
26	CDL	P	306	100/100	0.83	0.13	66,112,142,143	0
26	CDL	T	103	100/100	0.83	0.15	76,113,183,211	0
18	PGV	A	606	51/51	0.84	0.14	57,108,156,190	0
19	TGL	I	101	63/63	0.85	0.13	44,91,123,136	0
19	TGL	L	101	63/63	0.85	0.16	58,93,123,133	0
24	DMU	C	302	33/33	0.85	0.13	112,136,174,194	0

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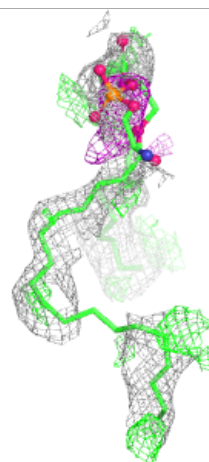
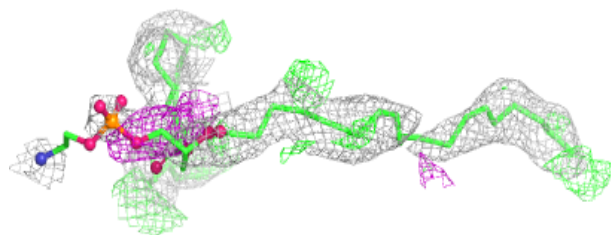
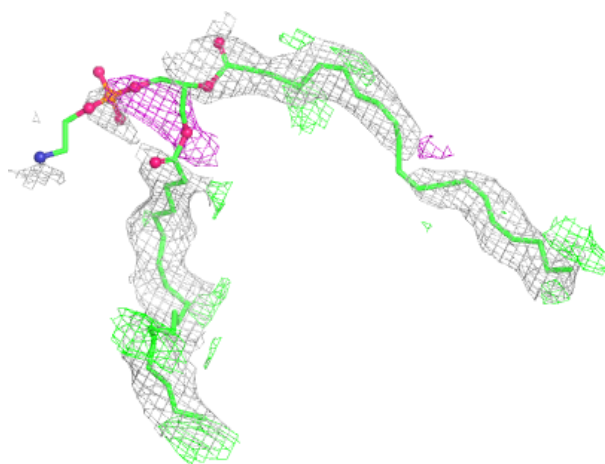
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	PSC	O	303	52/52	0.85	0.15	79,119,224,231	0
22	PSC	B	302	52/52	0.86	0.15	69,119,211,230	0
19	TGL	V	101	63/63	0.86	0.12	50,93,138,147	0
24	DMU	Q	201	33/33	0.88	0.11	86,103,119,123	0
16	NA	N	603	1/1	0.89	0.14	64,64,64,64	0
23	CHD	C	307	29/29	0.91	0.10	77,85,92,93	0
23	CHD	P	307	29/29	0.93	0.09	85,103,118,128	0
24	DMU	M	101	33/33	0.93	0.08	50,57,74,75	0
25	PEK	P	303	53/53	0.94	0.09	56,83,135,148	0
23	CHD	P	302	29/29	0.95	0.07	45,49,60,63	0
18	PGV	P	304	51/51	0.96	0.09	45,54,149,162	0
25	PEK	G	101	53/53	0.96	0.08	37,67,111,123	0
18	PGV	P	301	51/51	0.96	0.08	37,65,89,93	0
23	CHD	C	303	29/29	0.97	0.05	36,41,44,48	0
15	MG	A	602	1/1	0.97	0.04	38,38,38,38	0
17	HEA	N	604	60/60	0.97	0.07	45,52,71,75	0
23	CHD	O	302	29/29	0.97	0.05	41,46,52,54	0
18	PGV	C	301	51/51	0.97	0.07	35,61,86,95	0
18	PGV	C	305	51/51	0.97	0.07	37,51,97,105	0
23	CHD	B	303	29/29	0.97	0.06	41,44,57,69	0
16	NA	A	603	1/1	0.98	0.04	39,39,39,39	0
15	MG	N	602	1/1	0.98	0.06	46,46,46,46	0
17	HEA	A	604	60/60	0.98	0.06	33,39,78,81	0
17	HEA	A	605	60/60	0.99	0.05	28,34,47,55	0
17	HEA	N	605	60/60	0.99	0.05	39,43,47,52	0
20	PER	A	609	2/2	0.99	0.04	38,38,38,38	0
20	PER	N	607	2/2	0.99	0.06	50,50,50,53	0
21	CUA	B	301	2/2	0.99	0.03	42,42,42,43	0
21	CUA	O	301	2/2	0.99	0.03	62,62,62,62	0
14	CU	A	601	1/1	1.00	0.03	44,44,44,44	0
14	CU	N	601	1/1	1.00	0.04	58,58,58,58	0
27	ZN	F	101	1/1	1.00	0.01	54,54,54,54	0
27	ZN	S	101	1/1	1.00	0.01	65,65,65,65	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.

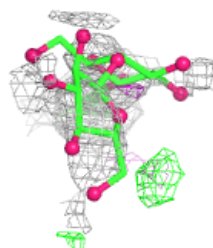
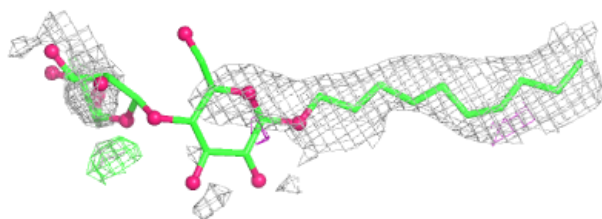
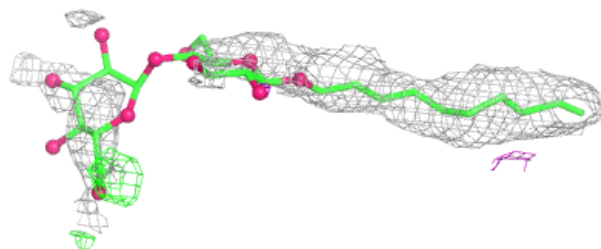
Electron density around PEK G 103:

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

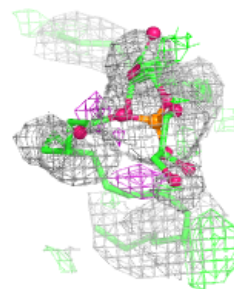
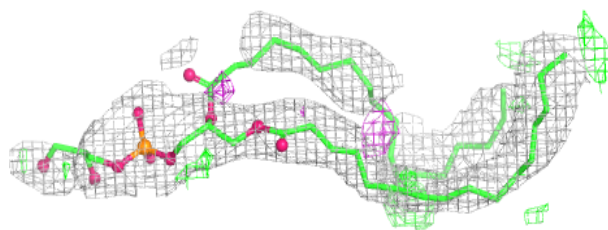
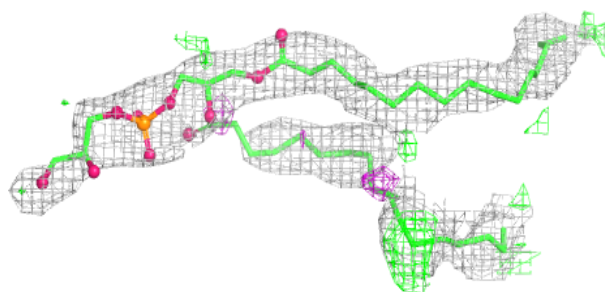


Electron density around DMU T 101:

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

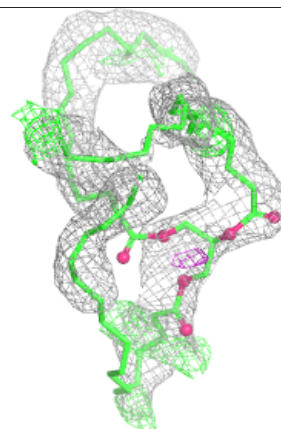
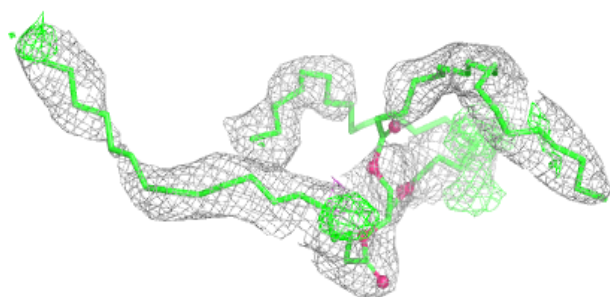
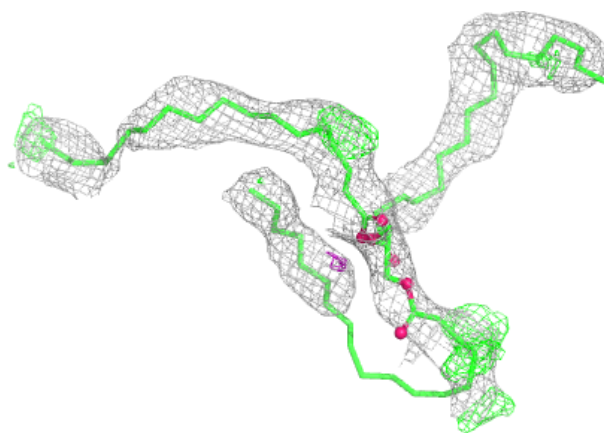
**Electron density around PGV P 305:**

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

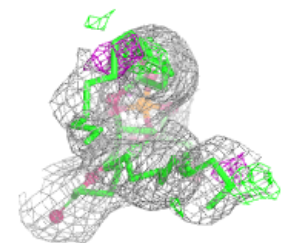
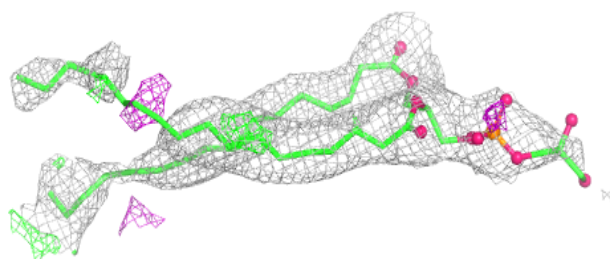
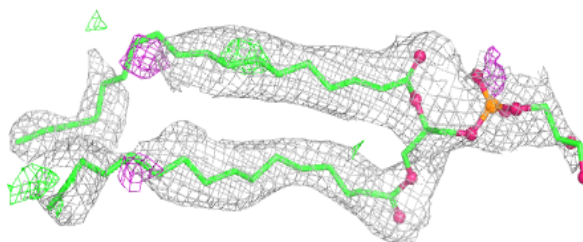


Electron density around TGL Y 101:

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

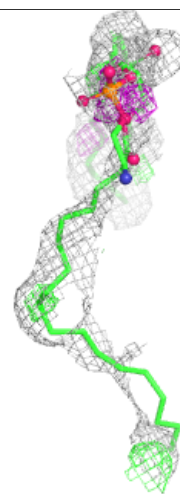
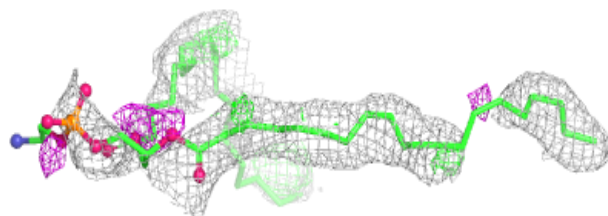
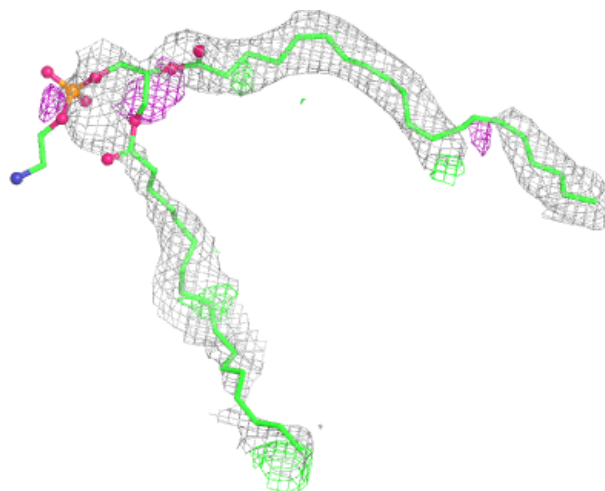
**Electron density around PGV N 606:**

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



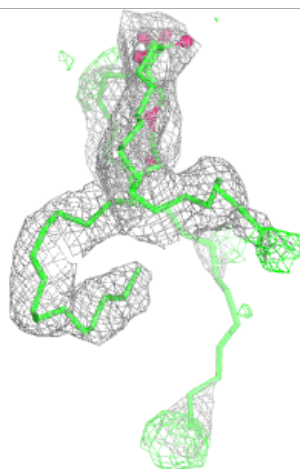
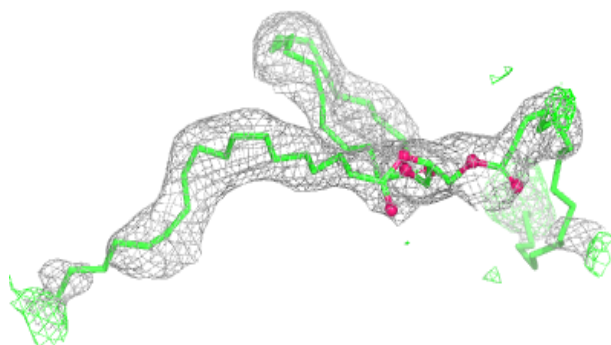
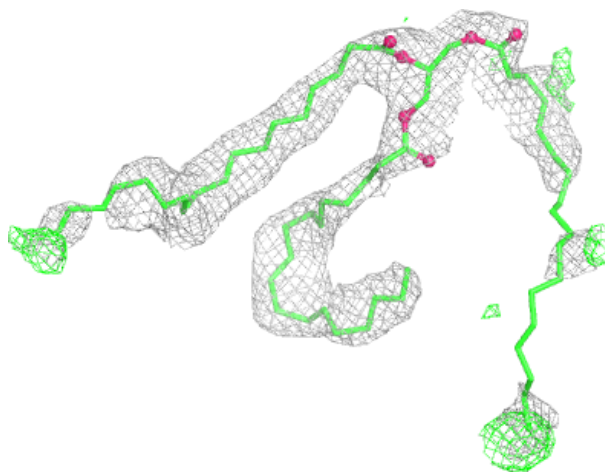
Electron density around PEK C 308:

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



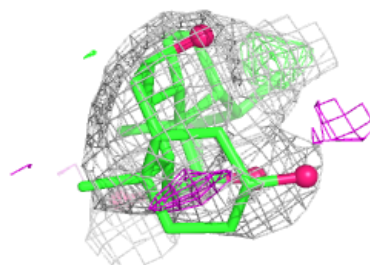
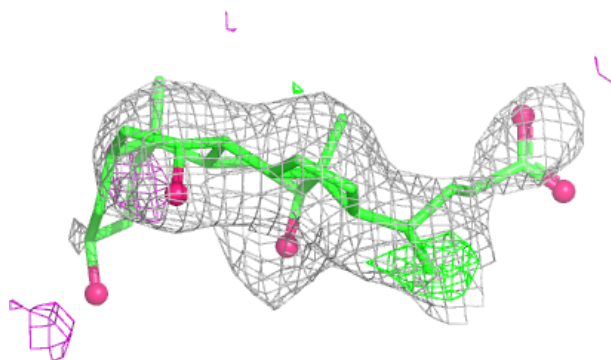
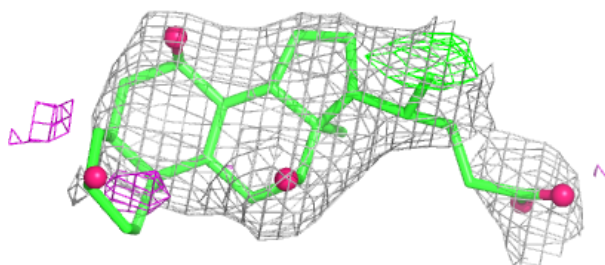
Electron density around TGL O 304:

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



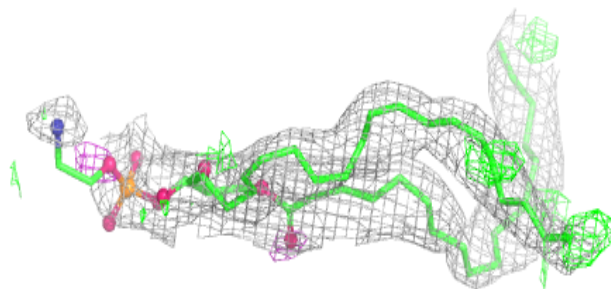
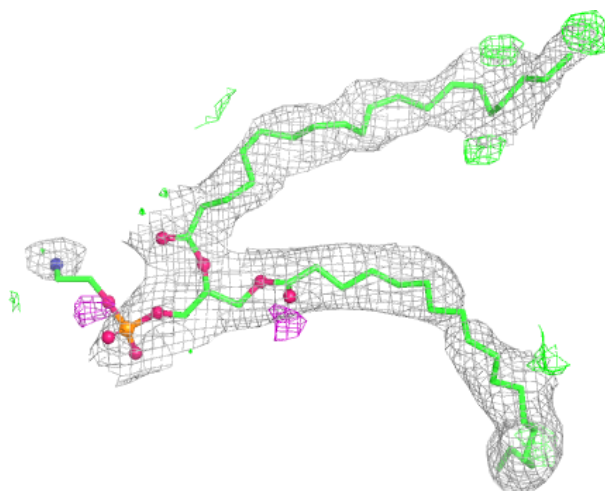
Electron density around CHD W 101:

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



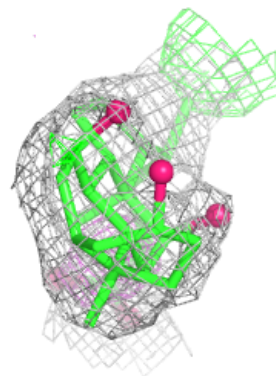
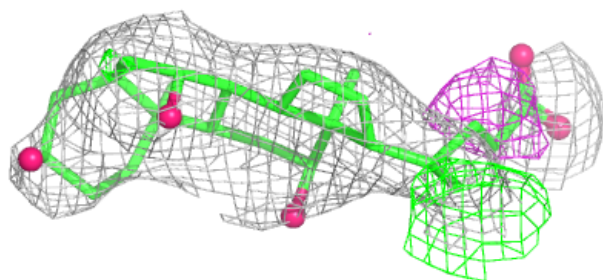
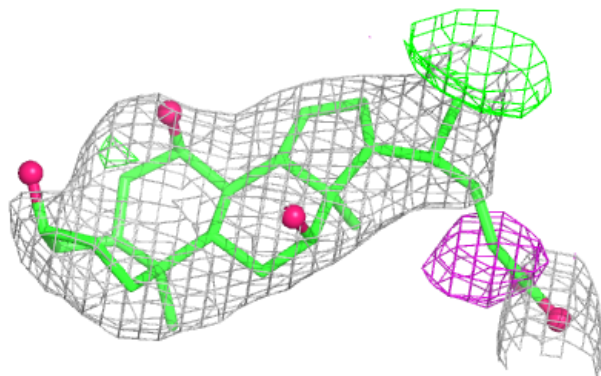
Electron density around PEK C 304:

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

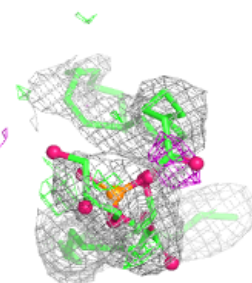
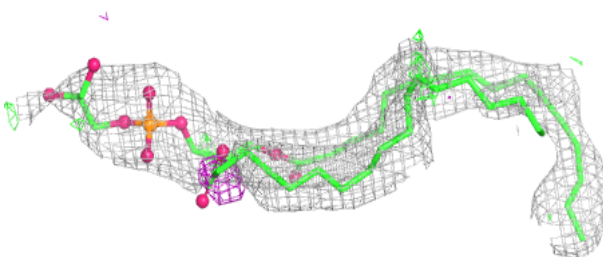
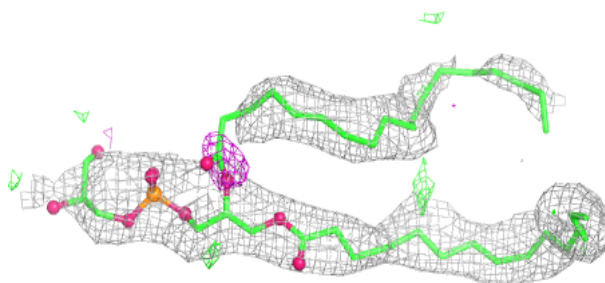


Electron density around CHD J 101:

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

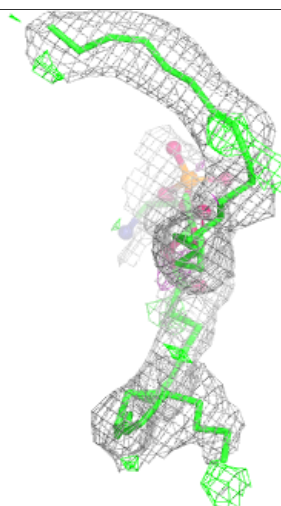
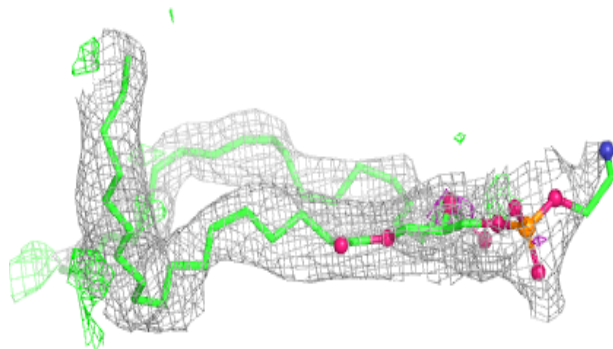
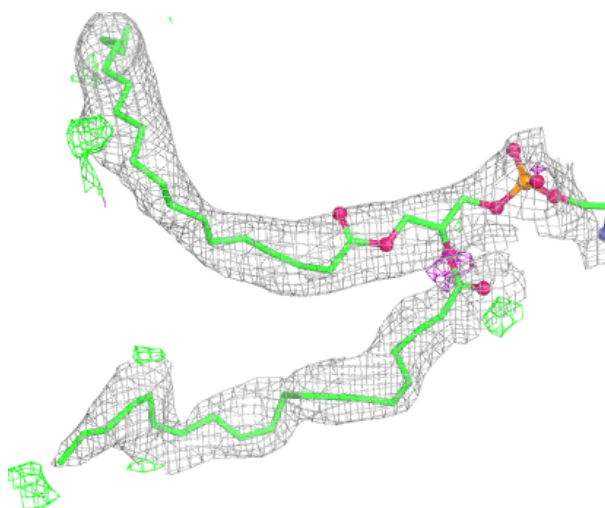
**Electron density around PGV A 607:**

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



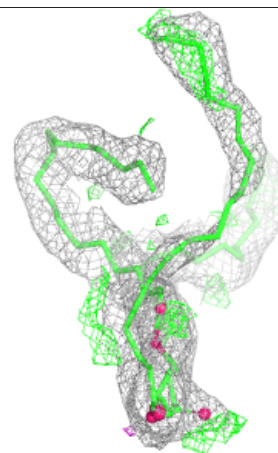
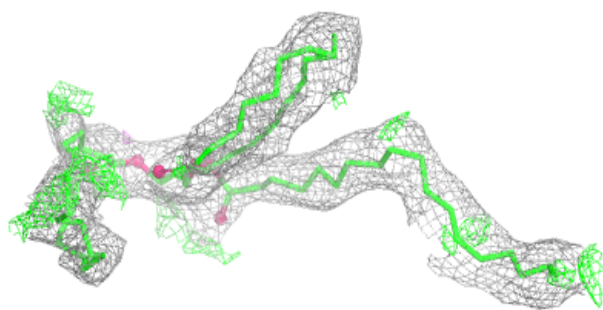
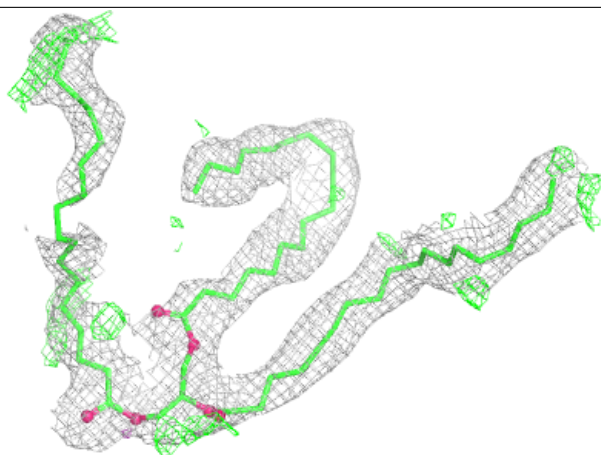
Electron density around PEK T 102:

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



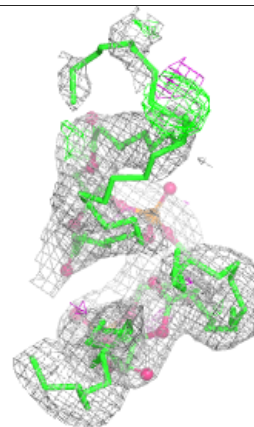
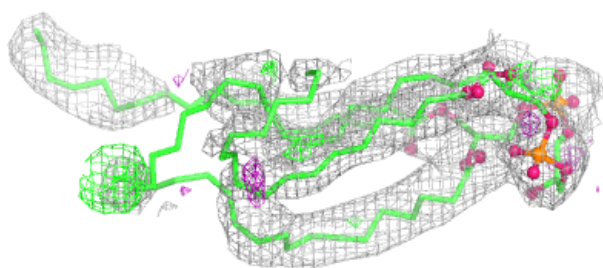
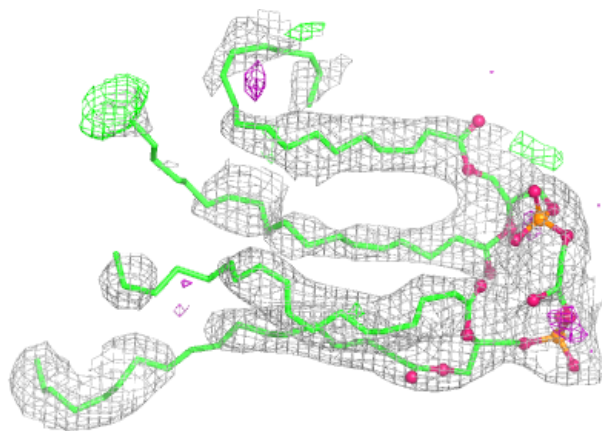
Electron density around TGL A 608:

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

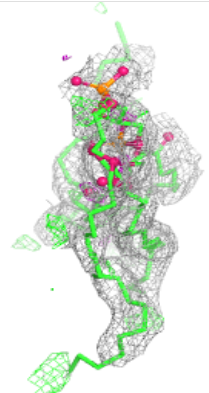
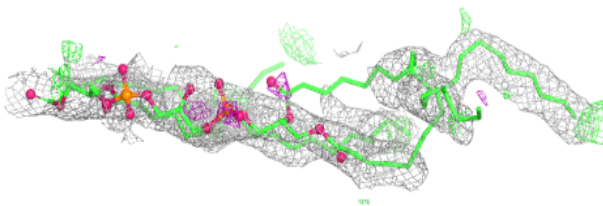
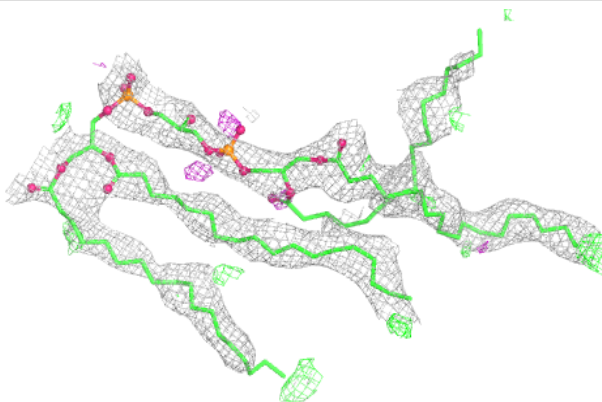


Electron density around CDL C 306:

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

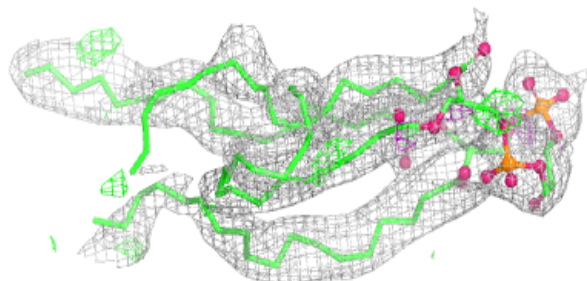
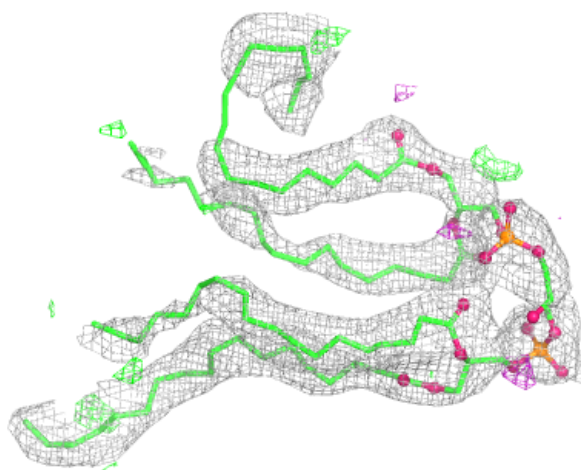
**Electron density around CDL G 102:**

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



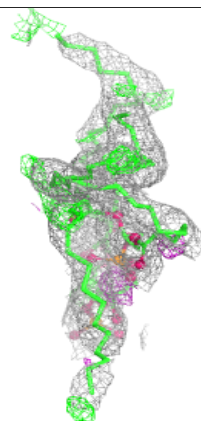
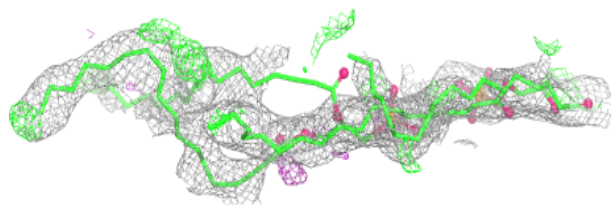
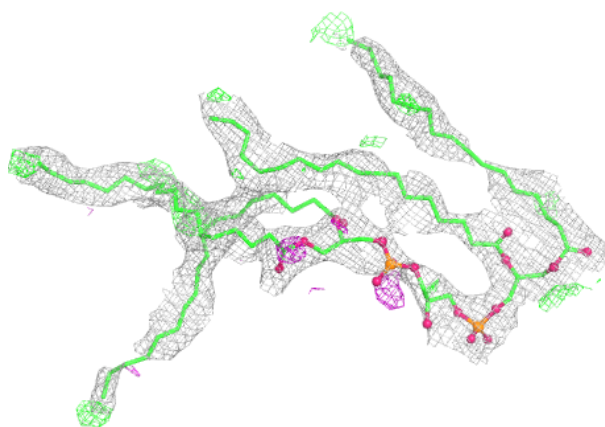
Electron density around CDL P 306:

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

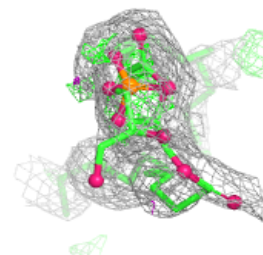
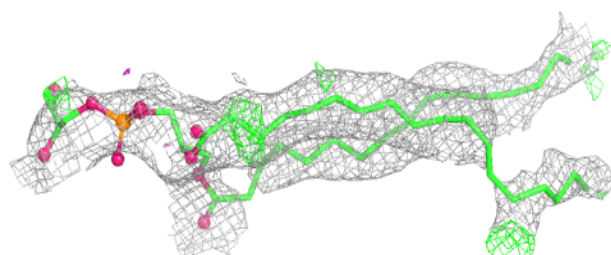
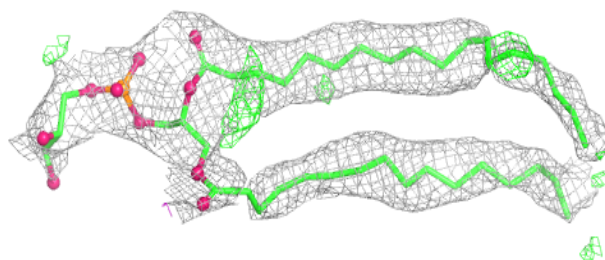


Electron density around CDL T 103:

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

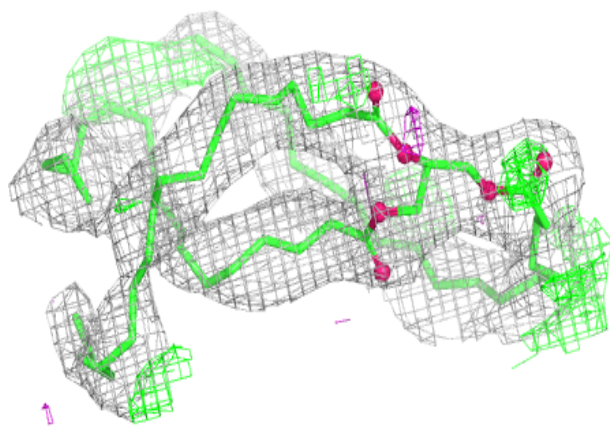
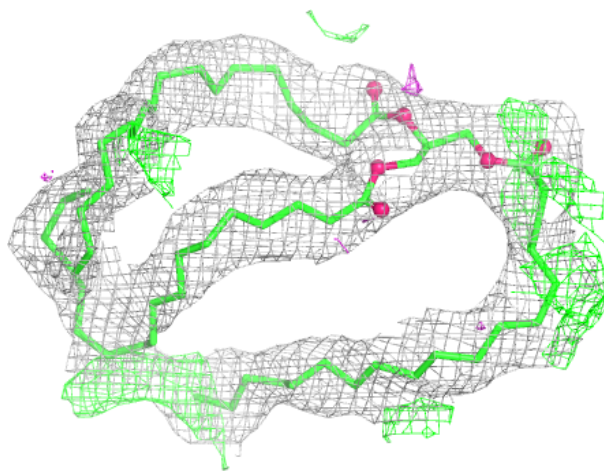
**Electron density around PGV A 606:**

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



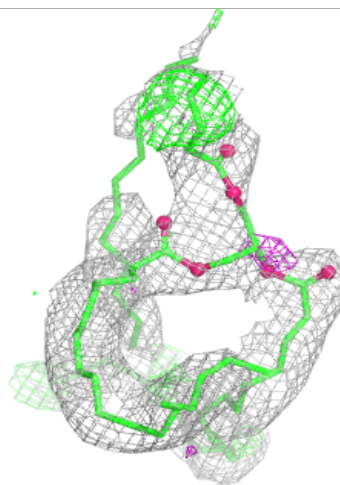
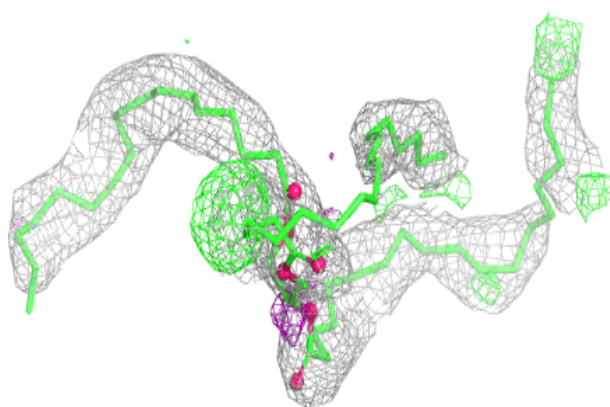
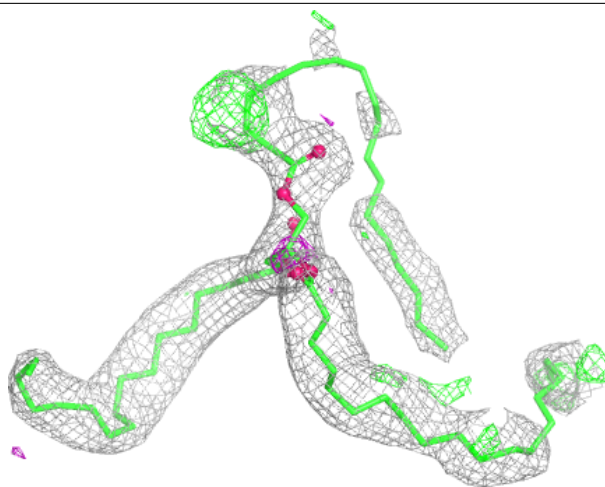
Electron density around TGL I 101:

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



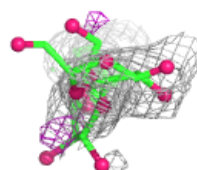
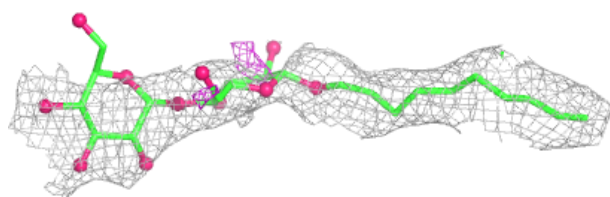
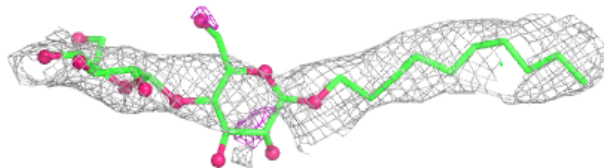
Electron density around TGL L 101:

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

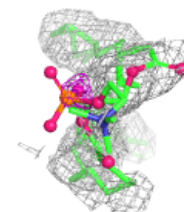
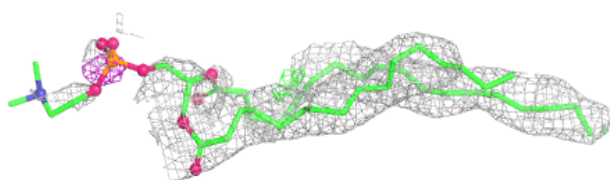
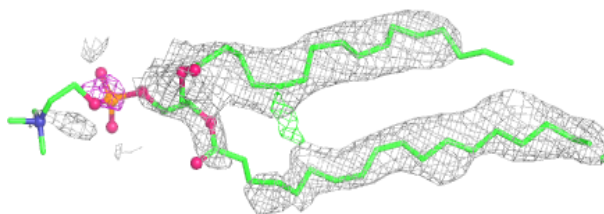


Electron density around DMU C 302:

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

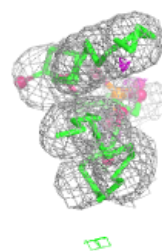
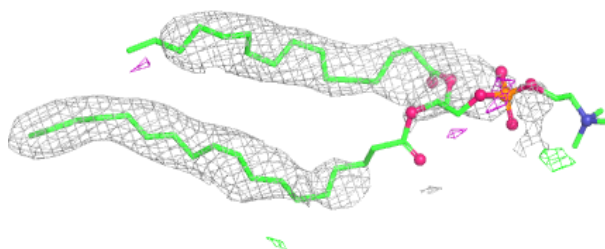
**Electron density around PSC O 303:**

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

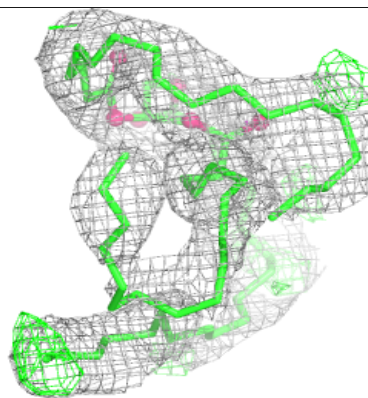
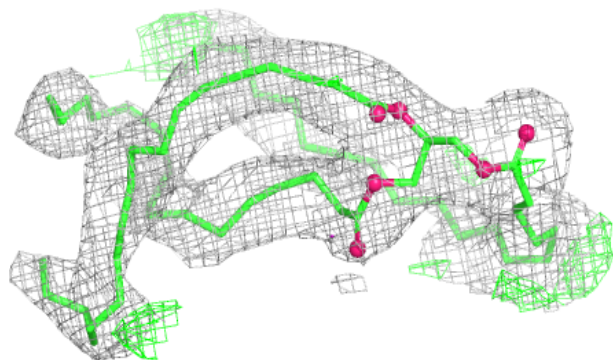
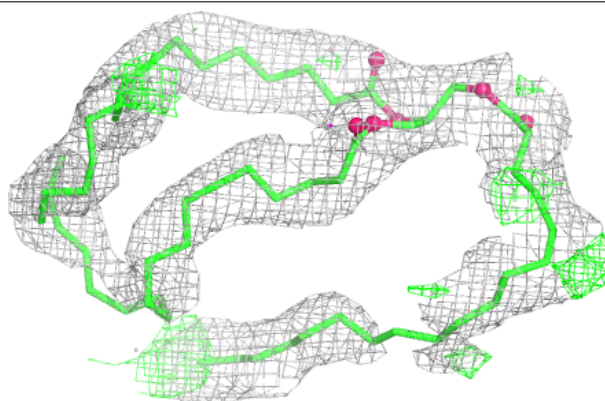


Electron density around PSC B 302:

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

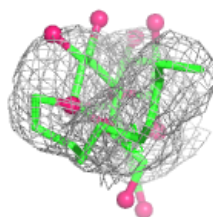
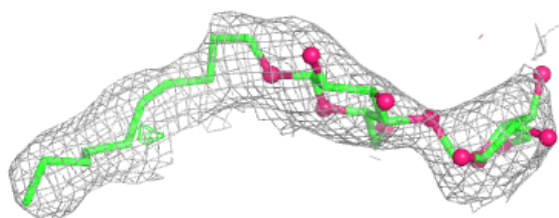
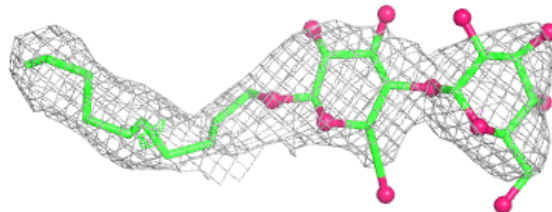
**Electron density around TGL V 101:**

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

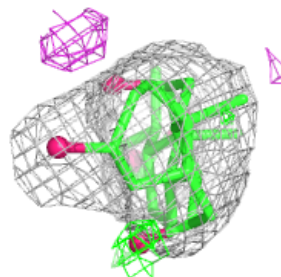
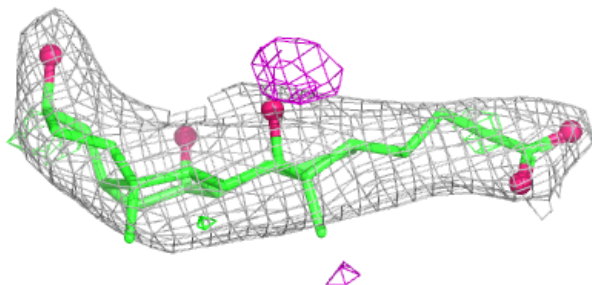
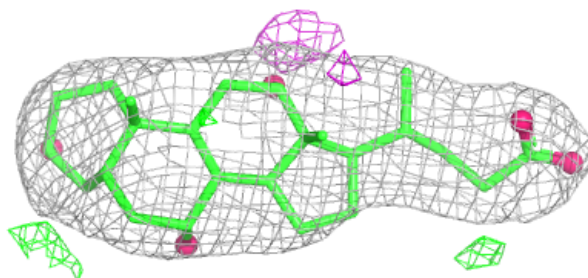


Electron density around DMU Q 201:

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

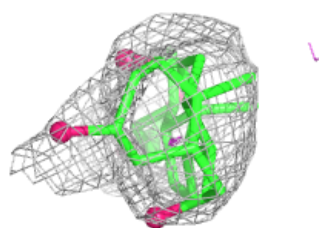
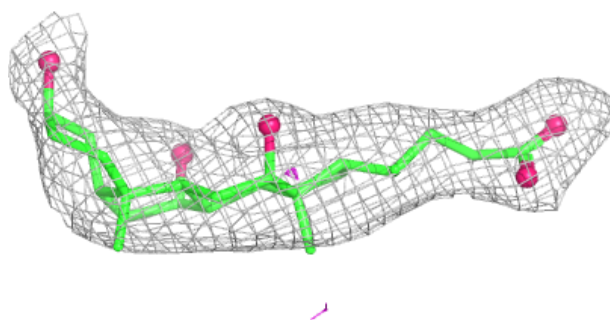
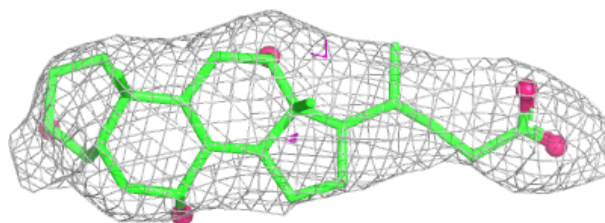
**Electron density around CHD C 307:**

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

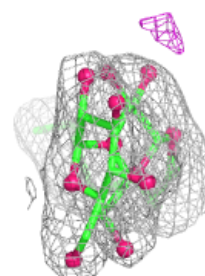
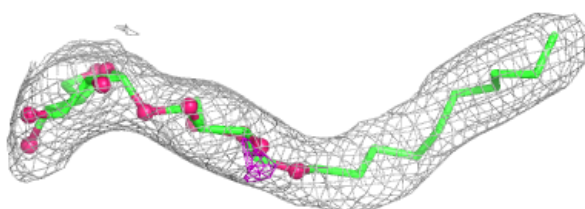
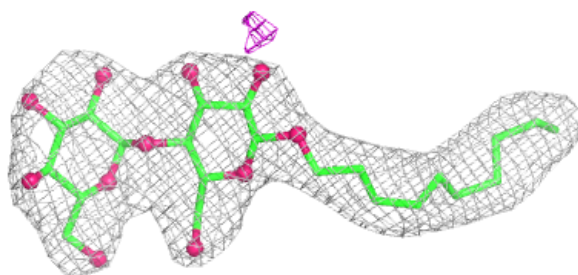


Electron density around CHD P 307:

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

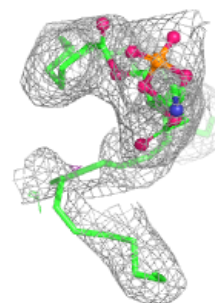
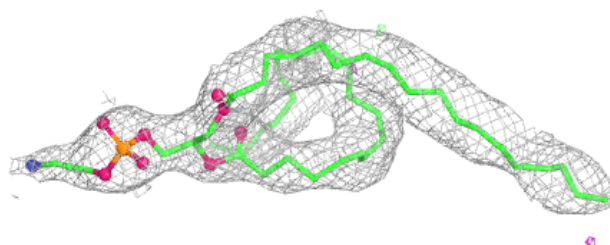
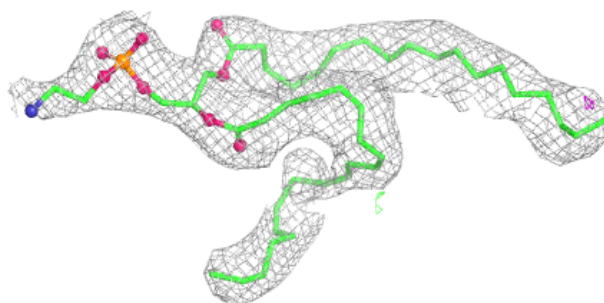
**Electron density around DMU M 101:**

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

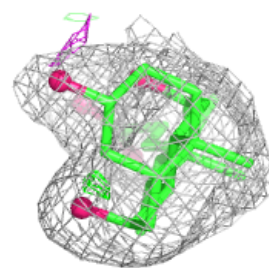
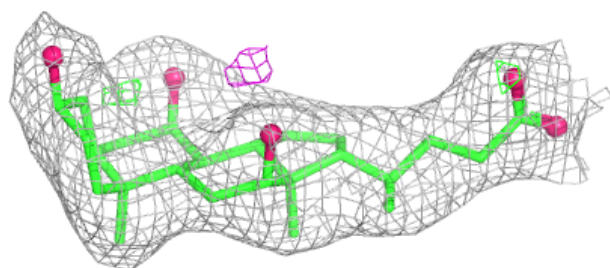
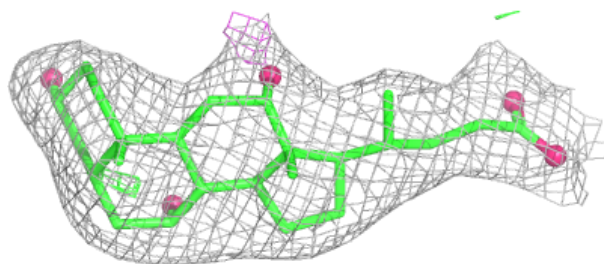


Electron density around PEK P 303:

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

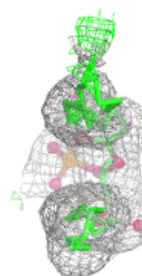
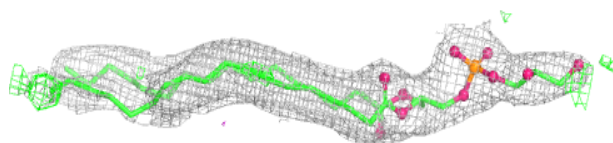
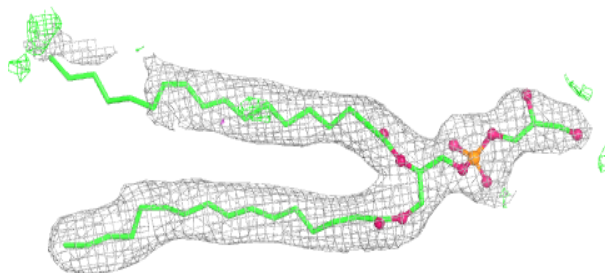
**Electron density around CHD P 302:**

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

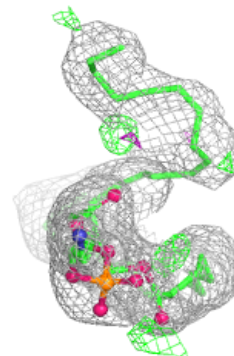
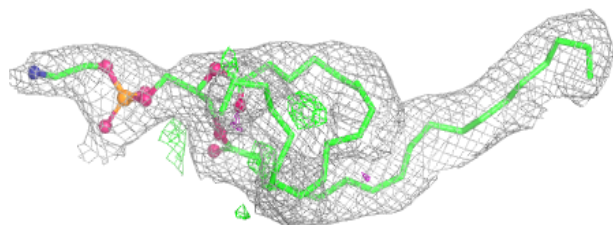
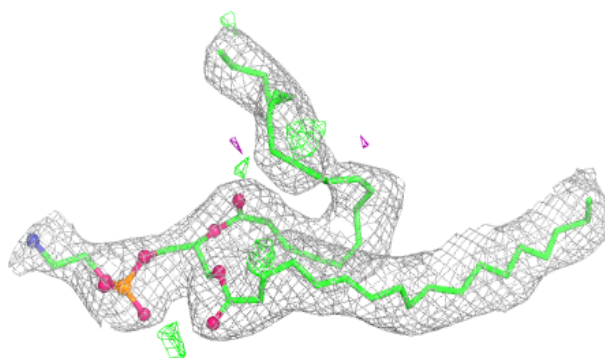


Electron density around PGV P 304:

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

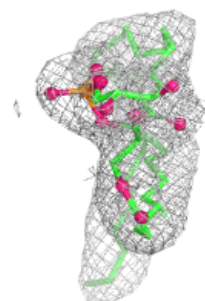
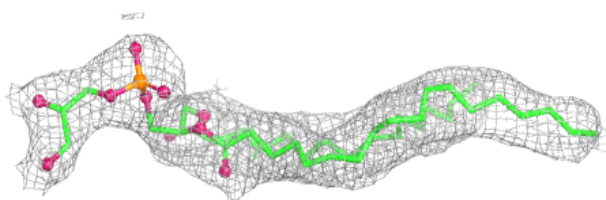
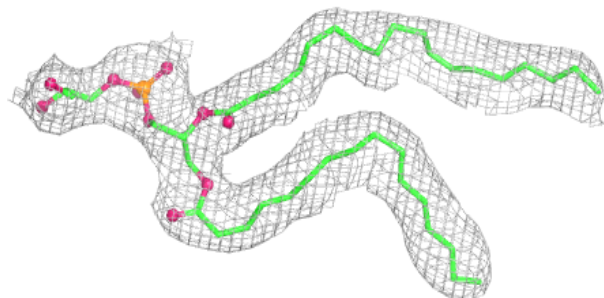
**Electron density around PEK G 101:**

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

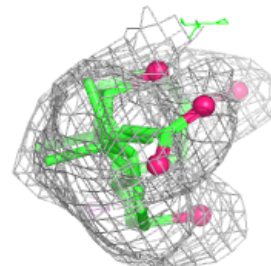
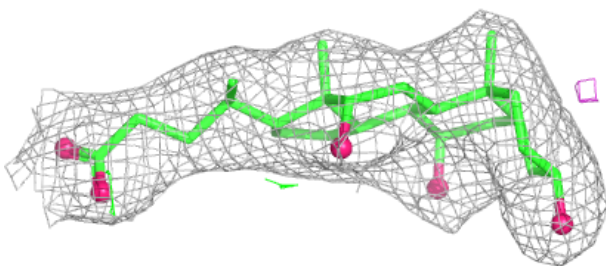
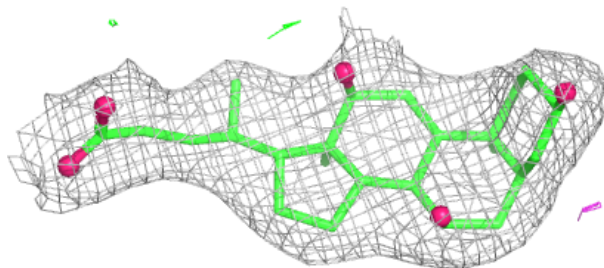


Electron density around PGV P 301:

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

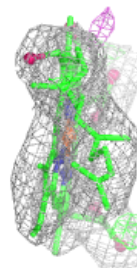
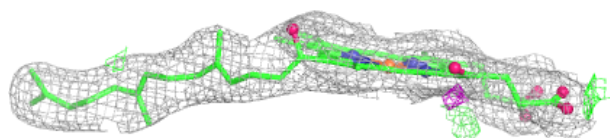
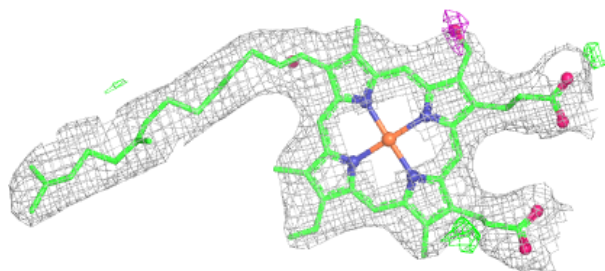
**Electron density around CHD C 303:**

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

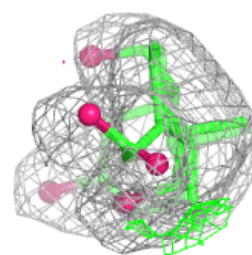
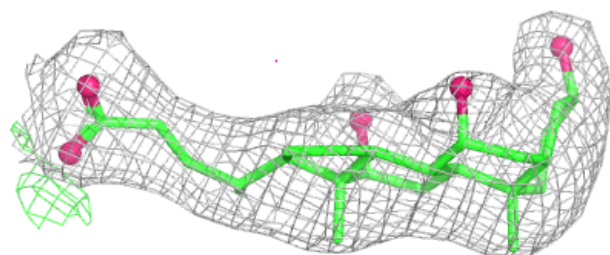
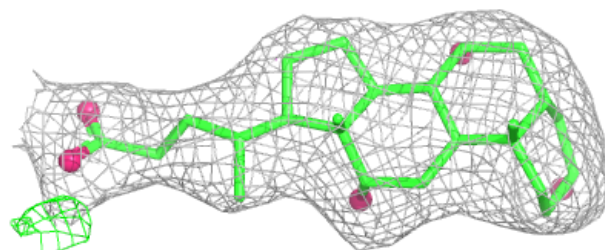


Electron density around HEA N 604:

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

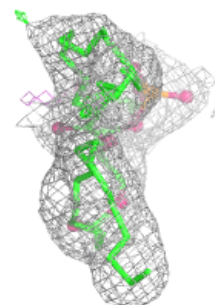
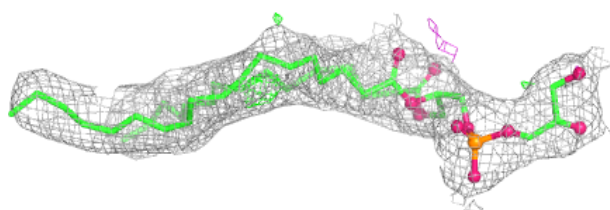
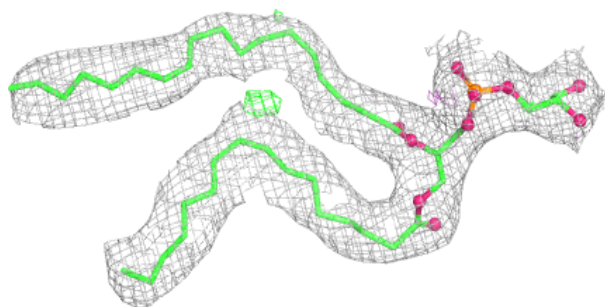
**Electron density around CHD O 302:**

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

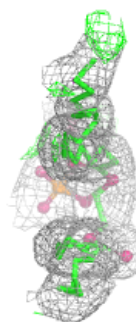
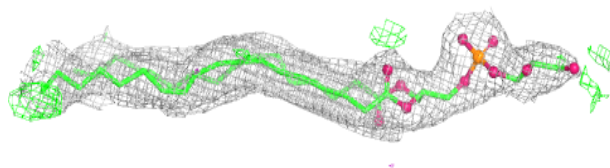
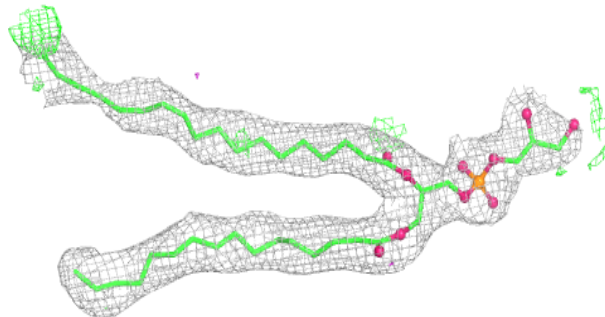


Electron density around PGV C 301:

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

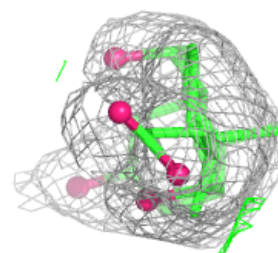
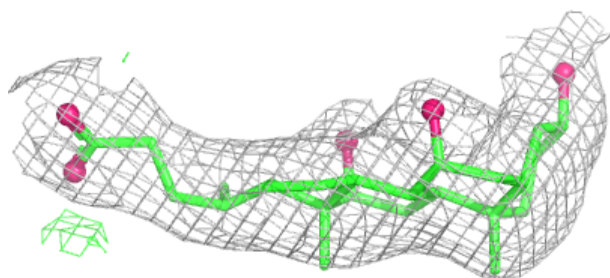
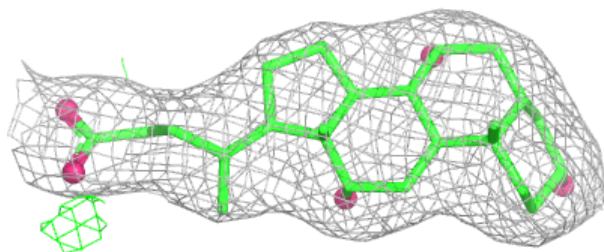
**Electron density around PGV C 305:**

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

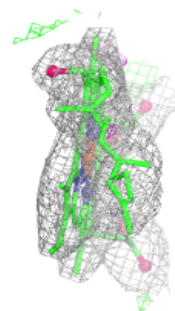
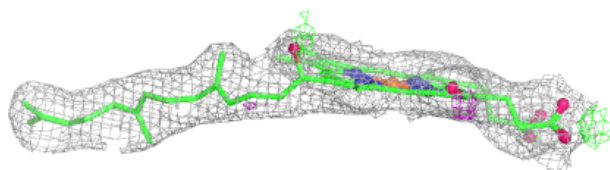
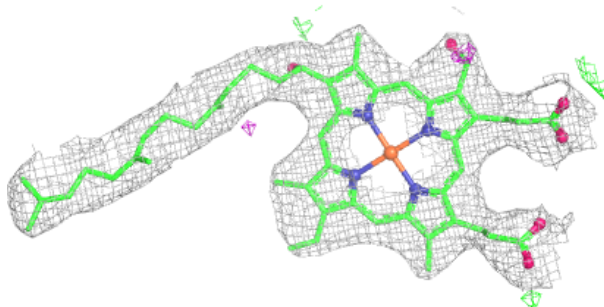


Electron density around CHD B 303:

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

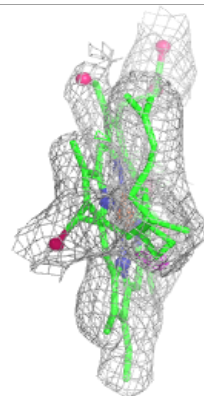
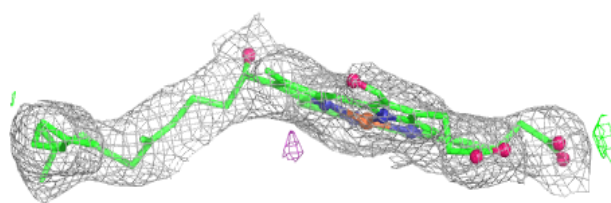
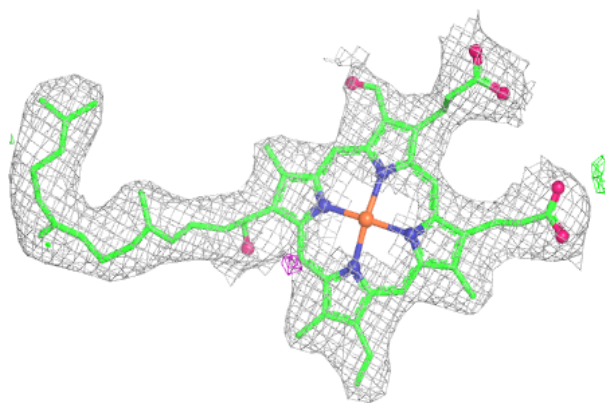
**Electron density around HEA A 604:**

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

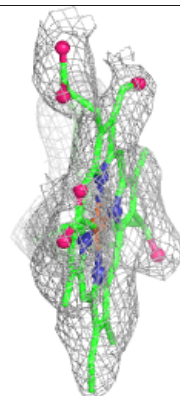
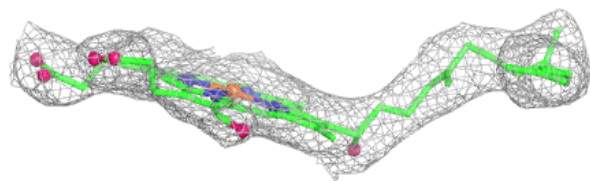
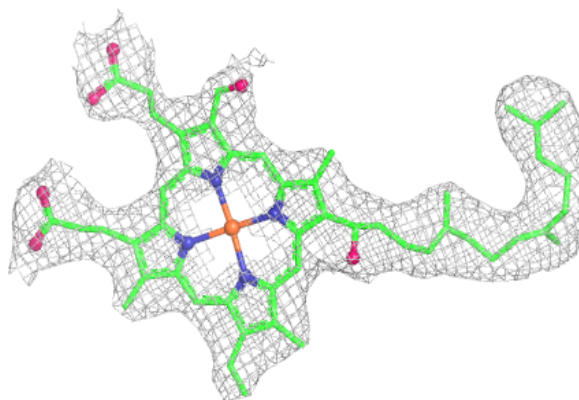


Electron density around HEA A 605:

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

**Electron density around HEA N 605:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.