



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:44 pm BST

PDB ID : 6NMP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

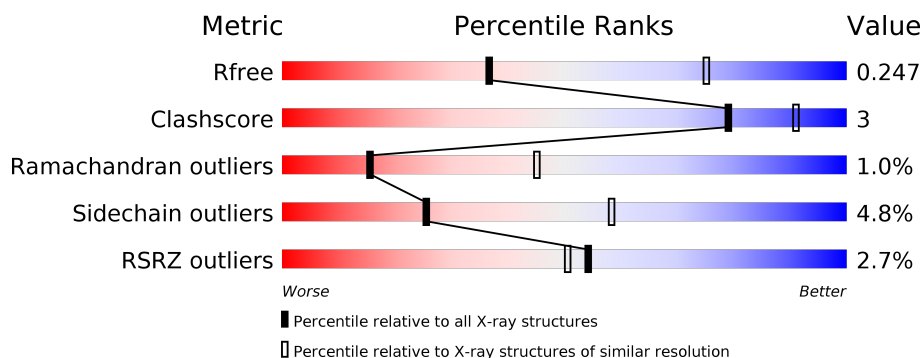
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 on 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	<div> <div>91%</div> <div>9%</div> </div>
1	N	514	<div> <div>89%</div> <div>11%</div> <div>.</div> </div>
2	B	227	<div> <div>%</div> <div>86%</div> <div>13%</div> </div>
2	O	227	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
3	C	261	<div> <div>94%</div> <div>5%</div> <div>.</div> </div>
3	P	261	<div> <div>90%</div> <div>8%</div> <div>.</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	A	604	X	-	-	-
17	HEA	A	605	X	-	-	-
17	HEA	N	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	HEA	N	605	X	-	-	-
24	DMU	T	101	-	-	-	X
25	PEK	G	103	-	-	-	X
7	TPO	G	11	-	-	-	X
7	TPO	T	11	-	-	-	X
9	SAC	I	1	-	-	-	X
9	SAC	V	1	-	-	-	X

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 (three-letter code: 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		

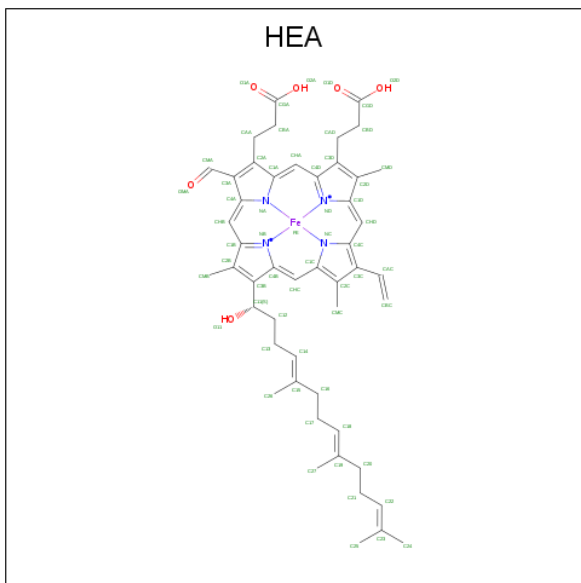
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: NA) (formula: Na).

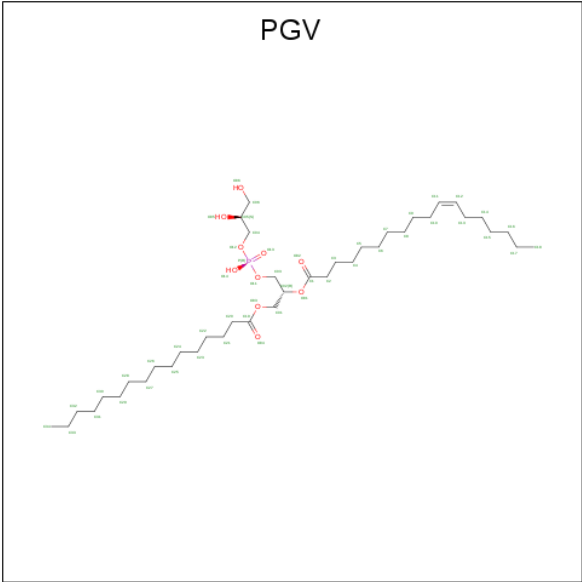
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



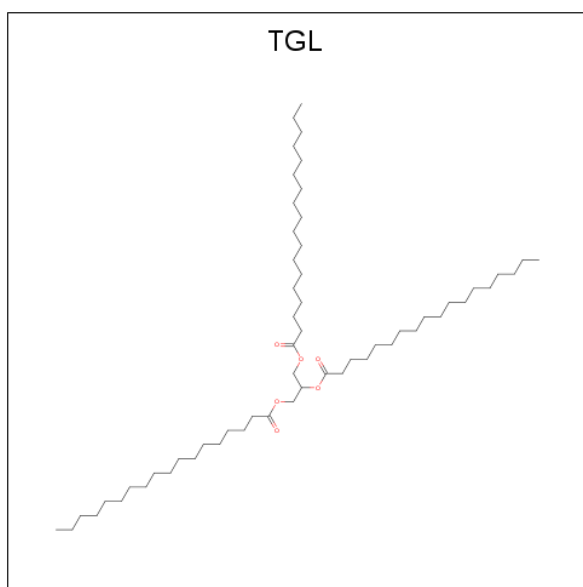
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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



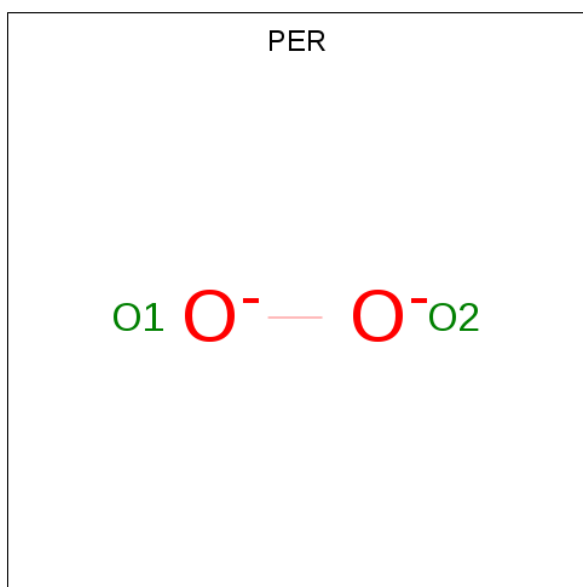
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	A	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	C	1	Total	C	O	P	0	0
			51	40	10	1		
18	N	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0
			51	40	10	1		
18	P	1	Total	C	O	P	0	0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

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



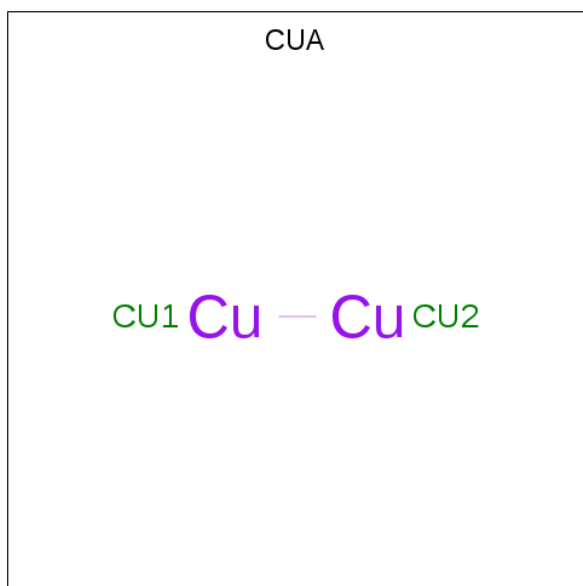
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	I	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	V	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is PEROXIDE ION (three-letter code: PER) (formula: O₂).



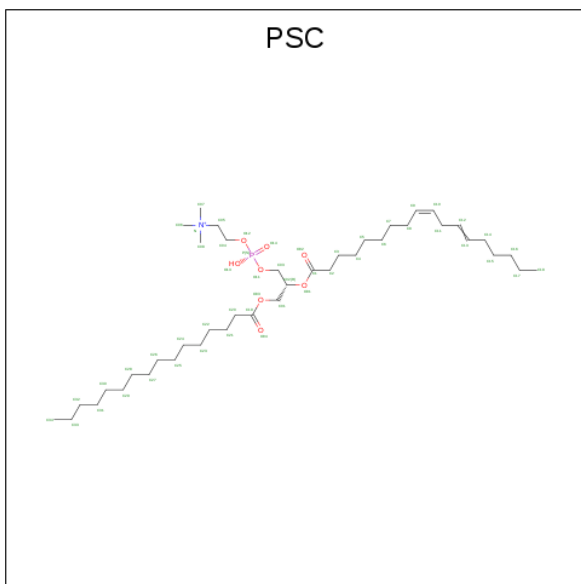
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	O	0	0
			2	2		
20	N	1	Total	O	0	0
			2	2		

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



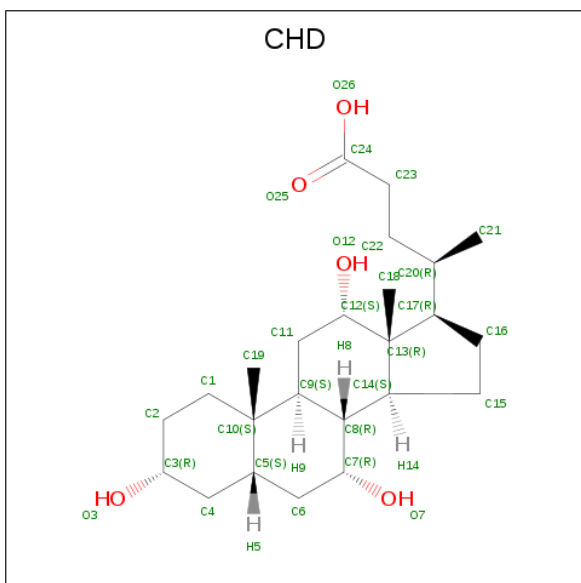
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

- 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 (three-letter code: PSC) (formula: $C_{42}H_{81}NO_8P$).



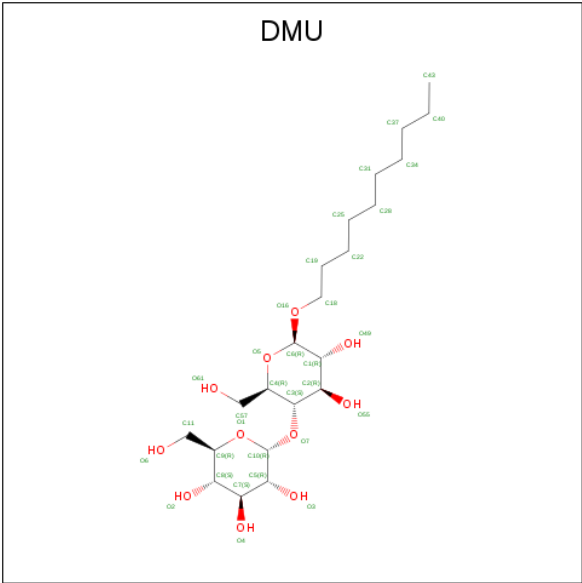
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (three-letter code: 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 (three-letter code: DMU) (formula: C₂₂H₄₂O₁₁).



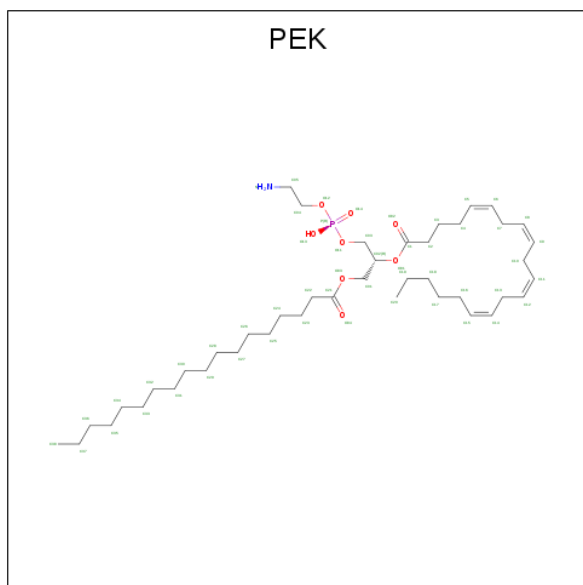
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	Q	1	Total	C	O	0	0
			33	22	11		

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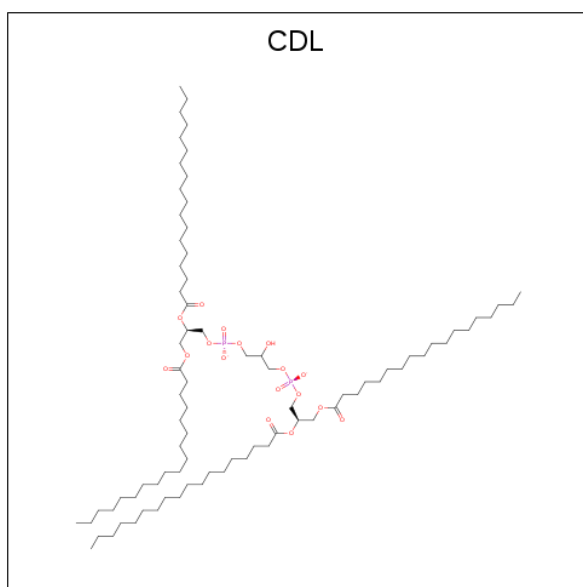
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	T	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: 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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	S	1	Total	Zn	0	0
			1	1		
27	F	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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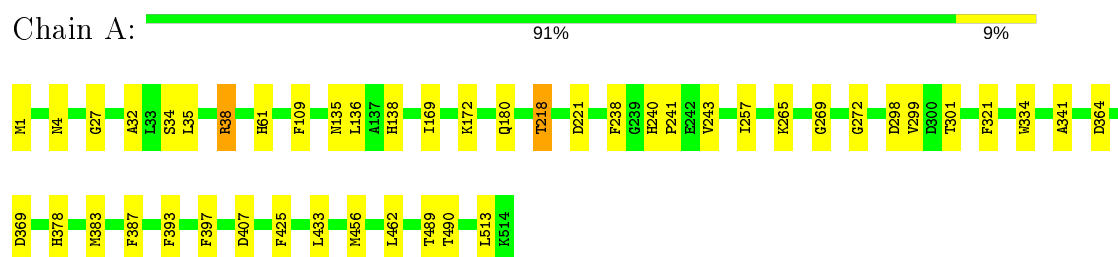
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	D	9	Total O 9 9	0	0
28	E	16	Total O 16 16	0	0
28	F	17	Total O 17 17	0	0
28	G	18	Total O 18 18	0	0
28	H	13	Total O 13 13	0	0
28	I	10	Total O 10 10	0	0
28	J	7	Total O 7 7	0	0
28	L	10	Total O 10 10	0	0
28	M	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
28	W	4	Total O 4 4	0	0
28	Y	4	Total O 4 4	0	0
28	Z	2	Total O 2 2	0	0

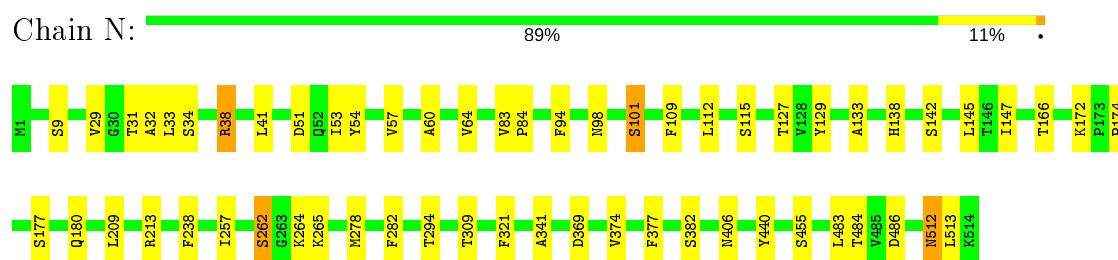
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

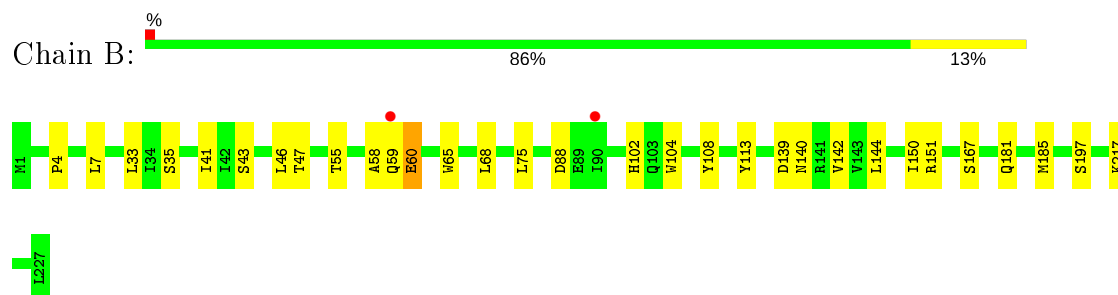
• Molecule 1: Cytochrome c oxidase subunit 1



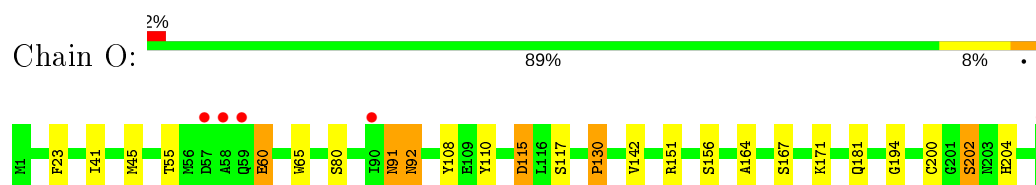
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3

Chain C:  94% 5%




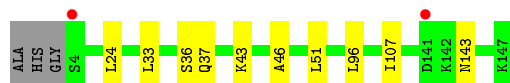
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  90% 8%




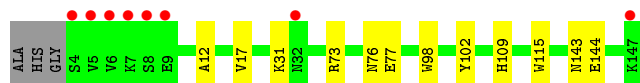
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D:  91% 7%




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

Chain Q:  90% 8%




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

Chain E:  86% 10%




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

Chain R:  90% 6%

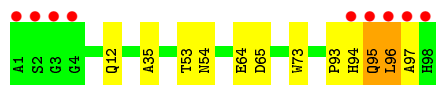
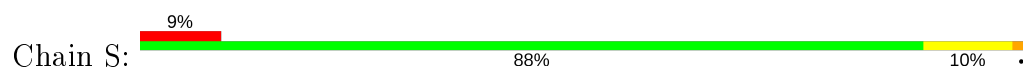


- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

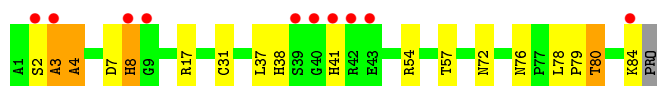
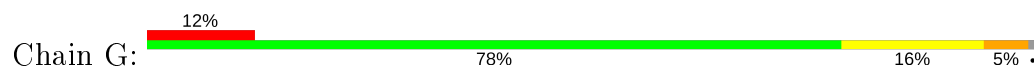
Chain F:  91% 7%



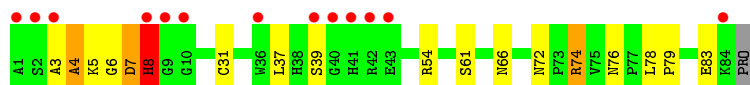
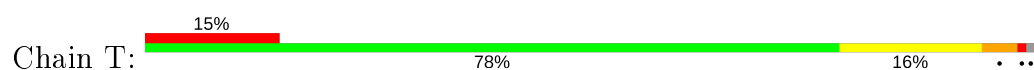
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



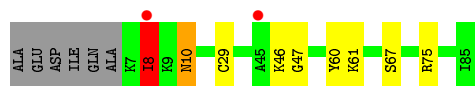
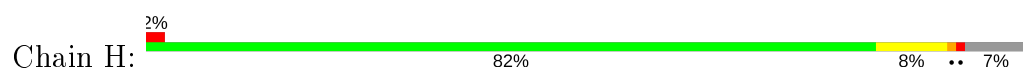
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



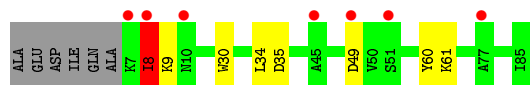
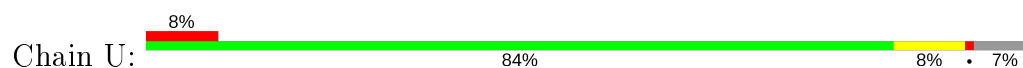
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



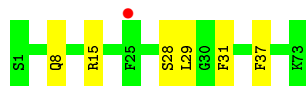
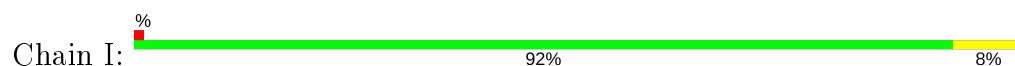
- Molecule 8: Cytochrome c oxidase subunit 6B1



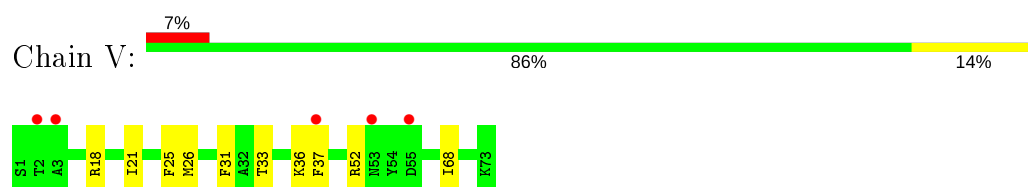
- Molecule 8: Cytochrome c oxidase subunit 6B1



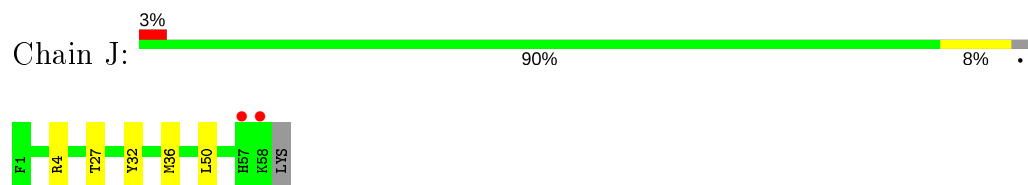
- Molecule 9: Cytochrome c oxidase subunit 6C



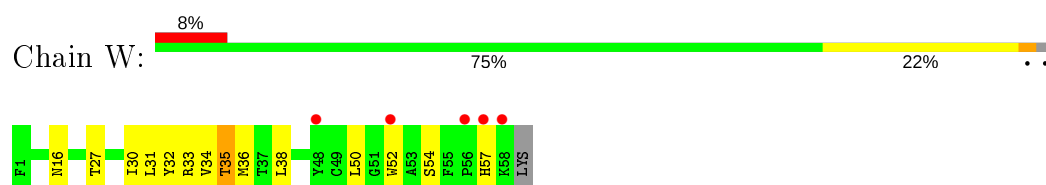
- Molecule 9: Cytochrome c oxidase subunit 6C



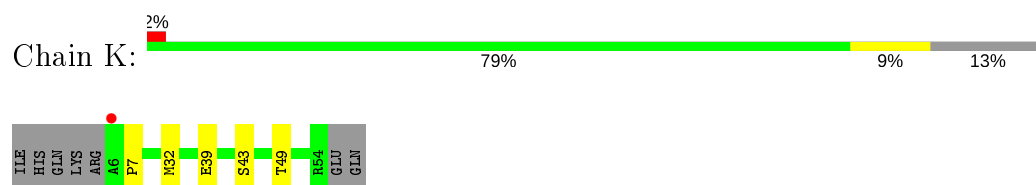
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



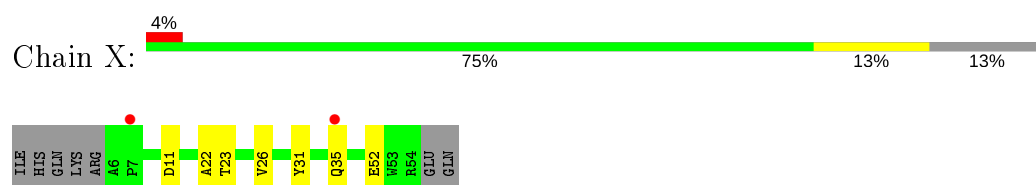
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



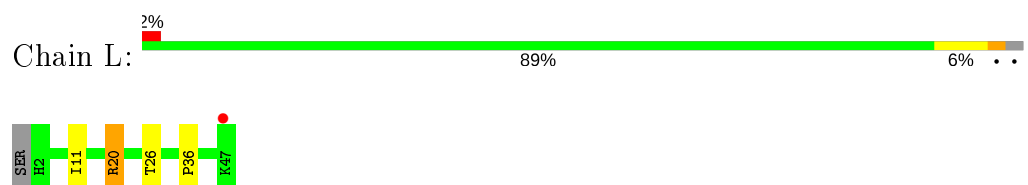
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



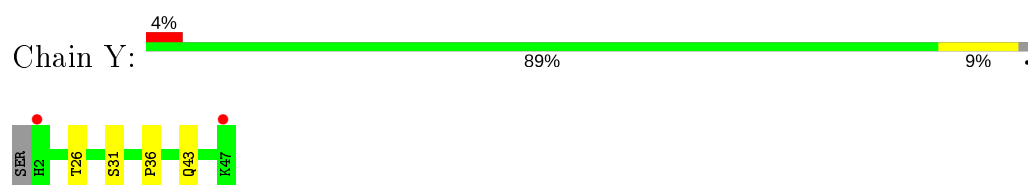
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial




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



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



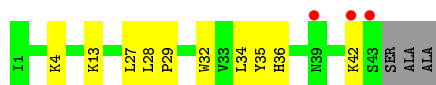
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

Chain M:  4% 83% 11% 7%



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

Chain Z:  7% 72% 22% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	178.70 Å 189.80 Å 211.30 Å 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) 100.0 (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 2.91 Å)	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)	0.30 , 67.4	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: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, PER, PGV, SAC, DMU, CUA, NA, FME, CU, HEA

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	0.53	0/4156	0.69	1/5678 (0.0%)
1	N	0.52	0/4156	0.65	1/5678 (0.0%)
2	B	0.52	0/1860	0.75	0/2534
2	O	0.51	0/1860	0.69	0/2534
3	C	0.52	0/2197	0.64	0/3005
3	P	0.51	0/2197	0.62	0/3005
4	D	0.48	0/1229	0.65	0/1658
4	Q	0.51	0/1229	0.65	0/1658
5	E	0.46	0/871	0.65	0/1182
5	R	0.46	0/871	0.65	0/1182
6	F	0.55	0/765	0.75	0/1038
6	S	0.49	0/765	0.70	0/1038
7	G	0.55	0/690	0.71	0/937
7	T	0.57	0/690	0.73	0/937
8	H	0.51	0/682	0.73	0/921
8	U	0.54	0/682	0.70	0/921
9	I	0.57	0/605	0.78	0/802
9	V	0.58	0/605	0.78	0/802
10	J	0.50	0/471	0.69	0/636
10	W	0.54	0/471	0.68	0/636
11	K	0.56	0/398	0.67	0/546
11	X	0.50	0/398	0.62	0/546
12	L	0.54	0/393	0.67	2/526 (0.4%)
12	Y	0.53	0/393	0.70	0/526
13	M	0.50	0/345	0.66	0/470
13	Z	0.49	0/345	0.63	0/470
All	All	0.52	0/29324	0.68	4/39866 (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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	N	38	ARG	NE-CZ-NH1	5.90	123.25	120.30
12	L	20	ARG	NE-CZ-NH1	5.50	123.05	120.30
12	L	20	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	21	0
1	N	4027	0	4001	35	0
2	B	1824	0	1833	14	0
2	O	1824	0	1833	12	0
3	C	2110	0	2027	9	0
3	P	2110	0	2027	11	0
4	D	1195	0	1183	5	0
4	Q	1195	0	1183	8	0
5	E	852	0	845	5	0
5	R	852	0	845	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	748	0	728	2	0
6	S	748	0	728	4	0
7	G	675	0	643	10	0
7	T	675	0	643	12	0
8	H	662	0	623	2	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	2	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	5	0
17	N	120	0	108	4	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	0	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
22	O	52	0	80	4	0
23	B	29	0	39	0	0
23	C	58	0	78	1	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31210	0	31316	172	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 (172) 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:O2	20:N:607:PER:O1	1.61	1.19
20:A:609:PER:O2	20:A:609:PER:O1	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
17:A:604:HEA:HMC1	17:A:604:HEA:HBC1	1.66	0.77
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
17:N:605:HEA:HBC1	17:N:605:HEA:HMC1	1.76	0.68
2:O:115:ASP:OD1	8:U:61:LYS:NZ	2.30	0.65
17:N:604:HEA:HBC1	17:N:604:HEA:HMC1	1.79	0.63
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
1:N:321:PHE:CD1	22:O:303:PSC:H341	2.36	0.60
17:A:605:HEA:HBC1	17:A:605:HEA:HMC1	1.84	0.58
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ARG:HE	2:B:181:GLN:NE2	2.07	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
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:58:ALA:O	2:B:60:GLU:N	2.43	0.50
2:B:33:LEU:HD12	9:I:28:SER:HB3	1.93	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:N:309:THR:CG2	17:N:605:HEA:HMB2	2.43	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
10:J:32:TYR:CE1	10:J:36:MET:HE3	2.48	0.48
1:N:33:LEU:HD23	1:N:57:VAL:HG13	1.96	0.48
4:Q:76:ASN:ND2	11:X:11:ASP:OD1	2.47	0.48
10:W:31:LEU:O	10:W:35:THR:OG1	2.28	0.48
1:A:383:MET:HA	1:A:387:PHE:CD1	2.49	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
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.95	0.47
5:E:49:ASP:OD1	5:E:92:THR:OG1	2.29	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:H142	22:O:303:PSC:H343	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
7:T:31:CYS:HG	26:T:103:CDL:H532	1.79	0.47
1:A:135:ASN:HD21	7:G:57:THR:CB	2.27	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
7:T:7:ASP:O	7:T:8:HIS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:O:91:ASN:O	2:O:92:ASN:C	2.56	0.44
5:R:82:TYR:HB3	5:R:83:PRO:CD	2.47	0.44
25:T:102:PEK:H383	26:T:103:CDL:H272	1.99	0.44
7:T:3:ALA:O	7:T:4:ALA:CB	2.65	0.44
25:P:303:PEK:C05	7:T:76:ASN:ND2	2.81	0.44
3:C:23:SER:HB2	3:C:49:THR:OG1	2.18	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
4:Q:76:ASN:O	4:Q:77:GLU:C	2.56	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
6:S:64:GLU:O	6:S:65:ASP:HB2	2.17	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
8:U:34:LEU:O	8:U:35:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:ILE:HG21	1:N:341:ALA:HB2	2.01	0.42
1:N:41:LEU:HD11	1:N:54:TYR:OH	2.20	0.42
1:N:512:ASN:HA	1:N:512:ASN:HD22	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
26:P:306:CDL:CB2	26:P:306:CDL:HB32	2.49	0.42
23:O:302:CHD:H12	23:O:302:CHD:H212	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:207:HIS:CD2	3:P:241:TYR:OH	2.73	0.41
3:P:72:THR:HB	3:P:73:PRO:HD2	2.02	0.41
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.55	0.41
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
18:A:606:PGV:H222	13:M:15:GLN:HE22	1.85	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
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
24:Q:201:DMU:H14	13:Z:27:LEU:HD22	2.02	0.41
1:N:31:THR:O	1:N:34:SER:OG	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:8:ILE:HG23	8:U:8:ILE:O	2.21	0.41
10:W:32:TYR:CE1	10:W:36:MET:CE	3.04	0.41
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	2.03	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:257:ILE:HG21	1:A:341:ALA:HB2	2.03	0.40
1:A:35:LEU:HD11	1:A:462:LEU:HB2	2.04	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%)	47	78
1	N	512/514 (100%)	481 (94%)	30 (6%)	1 (0%)	47	78
2	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	17	48
2	O	225/227 (99%)	202 (90%)	19 (8%)	4 (2%)	8	29
3	C	257/261 (98%)	248 (96%)	8 (3%)	1 (0%)	34	66
3	P	257/261 (98%)	245 (95%)	11 (4%)	1 (0%)	34	66
4	D	142/147 (97%)	131 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	4	16
6	S	96/98 (98%)	82 (85%)	12 (12%)	2 (2%)	7	26
7	G	81/85 (95%)	64 (79%)	11 (14%)	6 (7%)	1	2
7	T	81/85 (95%)	62 (76%)	12 (15%)	7 (9%)	1	2
8	H	77/85 (91%)	70 (91%)	4 (5%)	3 (4%)	3	12
8	U	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	12	37
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	36
9	V	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11	36
10	J	56/59 (95%)	56 (100%)	0	0	100	100
10	W	56/59 (95%)	51 (91%)	4 (7%)	1 (2%)	8	29
11	K	47/56 (84%)	41 (87%)	5 (11%)	1 (2%)	7	26
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%)	15	45

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

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Mol	Chain	Res	Type
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%)	414 (97%)	12 (3%)	43	76
1	N	426/426 (100%)	408 (96%)	18 (4%)	30	63
2	B	210/210 (100%)	198 (94%)	12 (6%)	20	51
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	55
3	C	224/226 (99%)	221 (99%)	3 (1%)	69	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	77
4	D	128/129 (99%)	124 (97%)	4 (3%)	40	74
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	66
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	72
5	R	92/95 (97%)	87 (95%)	5 (5%)	22	54
6	F	81/81 (100%)	76 (94%)	5 (6%)	18	47
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	47
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	37
7	T	67/68 (98%)	62 (92%)	5 (8%)	13	37
8	H	71/75 (95%)	64 (90%)	7 (10%)	8	24
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	52
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	41
9	V	57/57 (100%)	48 (84%)	9 (16%)	2	8
10	J	49/50 (98%)	46 (94%)	3 (6%)	18	48
10	W	49/50 (98%)	44 (90%)	5 (10%)	7	22
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	56
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	56
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	56
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	56
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	20
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	33
All	All	3040/3082 (99%)	2894 (95%)	146 (5%)	25	58

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	136	LEU
1	A	138	HIS
1	A	180	GLN
1	A	218	THR
1	A	238	PHE
1	A	369	ASP
1	A	407	ASP

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Mol	Chain	Res	Type
1	A	433	LEU
1	A	489	THR
1	A	513	LEU
2	B	35	SER
2	B	43	SER
2	B	55	THR
2	B	65	TRP
2	B	68	LEU
2	B	75	LEU
2	B	88	ASP
2	B	113	TYR
2	B	167	SER
2	B	185	MET
2	B	197	SER
2	B	217	LYS
3	C	159	MET
3	C	179	SER
3	C	230	ASN
4	D	36	SER
4	D	43	LYS
4	D	51	LEU
4	D	143	ASN
5	E	31	LYS
5	E	70	VAL
5	E	107	ASP
6	F	33	ILE
6	F	44	GLU
6	F	53	THR
6	F	63	GLU
6	F	96	LEU
7	G	2	SER
7	G	38	HIS
7	G	54	ARG
7	G	80	THR
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	46	LYS
8	H	60	TYR
8	H	61	LYS
8	H	67	SER
8	H	75	ARG

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Mol	Chain	Res	Type
9	I	8	GLN
9	I	15	ARG
9	I	29	LEU
9	I	31	PHE
10	J	4	ARG
10	J	27	THR
10	J	50	LEU
11	K	32	MET
11	K	49	THR
12	L	20	ARG
12	L	26	THR
13	M	2	THR
13	M	19	LEU
13	M	38	ASP
13	M	42	LYS
1	N	9	SER
1	N	38	ARG
1	N	101	SER
1	N	109	PHE
1	N	112	LEU
1	N	115	SER
1	N	138	HIS
1	N	238	PHE
1	N	262	SER
1	N	265	LYS
1	N	278	MET
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	55	THR
2	O	60	GLU
2	O	65	TRP
2	O	91	ASN
2	O	110	TYR
2	O	115	ASP
2	O	117	SER
2	O	156	SER
2	O	167	SER

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Mol	Chain	Res	Type
2	O	171	LYS
2	O	200	CYS
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	73	ARG
4	Q	143	ASN
4	Q	144	GLU
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	93	PRO
6	S	96	LEU
7	T	8	HIS
7	T	39	SER
7	T	54	ARG
7	T	61	SER
7	T	74	ARG
8	U	8	ILE
8	U	9	LYS
8	U	49	ASP
8	U	60	TYR
9	V	18	ARG
9	V	21	ILE
9	V	25	PHE
9	V	26	MET
9	V	31	PHE
9	V	33	THR
9	V	36	LYS
9	V	52	ARG
9	V	68	ILE
10	W	27	THR

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Mol	Chain	Res	Type
10	W	35	THR
10	W	38	LEU
10	W	50	LEU
10	W	54	SER
11	X	23	THR
11	X	52	GLU
12	Y	26	THR
12	Y	31	SER
13	Z	13	LYS
13	Z	34	LEU
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	512	ASN
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	68	GLN
3	C	70	HIS
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
6	F	95	GLN
7	G	76	ASN
1	N	180	GLN
1	N	491	ASN
1	N	512	ASN
2	O	10	GLN
2	O	181	GLN
2	O	203	ASN
3	P	12	ASN
3	P	68	GLN
3	P	161	GLN
4	Q	37	GLN
4	Q	76	ASN
5	R	78	HIS
5	R	94	ASN
6	S	54	ASN

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Mol	Chain	Res	Type
7	T	66	ASN
7	T	67	HIS
7	T	76	ASN
8	U	31	GLN
8	U	37	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
9	SAC	V	1	9	7,8,9	1.67	1 (14%)	8,9,11	1.67	3 (37%)
7	TPO	G	11	7	8,10,11	1.24	1 (12%)	10,14,16	0.83	1 (10%)
2	FME	O	1	2	8,9,10	0.52	0	7,9,11	2.42	2 (28%)
7	TPO	T	11	7	8,10,11	1.11	1 (12%)	10,14,16	0.76	0
9	SAC	I	1	9	7,8,9	2.06	1 (14%)	8,9,11	2.15	3 (37%)
1	FME	A	1	1	8,9,10	0.56	0	7,9,11	1.75	2 (28%)
1	FME	N	1	1	8,9,10	0.49	0	7,9,11	1.54	1 (14%)
2	FME	B	1	2	8,9,10	0.64	0	7,9,11	2.47	3 (42%)

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
9	SAC	V	1	9	-	5/7/8/10	-
7	TPO	G	11	7	-	2/9/11/13	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
9	SAC	I	1	9	-	4/7/8/10	-
1	FME	A	1	1	-	4/7/9/11	-
1	FME	N	1	1	-	6/7/9/11	-
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	5.21	1.53	1.46
9	V	1	SAC	CA-N	4.22	1.52	1.46
7	G	11	TPO	P-OG1	2.33	1.63	1.59
7	T	11	TPO	P-OG1	2.21	1.63	1.59

All (15) 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
9	I	1	SAC	CA-N-C1A	4.22	130.93	123.15
1	A	1	FME	CA-N-CN	-3.28	117.78	122.82
2	O	1	FME	C-CA-N	3.07	115.28	109.73
2	B	1	FME	C-CA-N	3.02	115.18	109.73
1	N	1	FME	CA-N-CN	-2.77	118.56	122.82
9	I	1	SAC	C-CA-N	2.57	114.38	109.73
9	V	1	SAC	CA-N-C1A	2.54	127.84	123.15
9	I	1	SAC	OAC-C1A-C2A	-2.48	117.44	122.06
9	V	1	SAC	C2A-C1A-N	2.37	120.11	116.10
1	A	1	FME	O-C-CA	-2.33	118.67	124.78
2	B	1	FME	O1-CN-N	-2.26	119.33	125.27
7	G	11	TPO	P-OG1-CB	-2.09	116.89	123.21
9	V	1	SAC	O-C-CA	-2.08	119.33	124.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	V	1	SAC	C2A-C1A-N-CA

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Mol	Chain	Res	Type	Atoms
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
9	V	1	SAC	N-CA-CB-OG
9	V	1	SAC	C-CA-CB-OG
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	CB-OG1-P-O1P
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	CB-OG1-P-O2P
9	I	1	SAC	CB-CA-N-C1A
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
1	A	1	FME	CB-CG-SD-CE
1	N	1	FME	CB-CG-SD-CE
1	N	1	FME	CA-CB-CG-SD
9	I	1	SAC	C-CA-N-C1A
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P
7	T	11	TPO	O-C-CA-CB
1	N	1	FME	CB-CA-N-CN

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 carbohydrates 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$
25	PEK	C	304	-	52,52,52	1.00	2 (3%)	55,57,57	0.88	3 (5%)
24	DMU	C	302	-	34,34,34	1.56	7 (20%)	45,45,45	1.82	9 (20%)
23	CHD	B	303	-	29,32,32	0.60	0	48,51,51	1.25	6 (12%)
25	PEK	P	303	-	52,52,52	0.90	2 (3%)	55,57,57	0.73	2 (3%)
18	PGV	P	301	-	50,50,50	0.93	2 (4%)	53,56,56	1.00	3 (5%)
19	TGL	I	101	-	62,62,62	1.02	3 (4%)	65,65,65	1.33	8 (12%)
18	PGV	N	606	-	50,50,50	1.04	2 (4%)	53,56,56	1.05	3 (5%)
26	CDL	P	306	-	99,99,99	1.02	4 (4%)	105,111,111	1.12	6 (5%)
23	CHD	P	307	-	29,32,32	0.48	0	48,51,51	1.50	6 (12%)
20	PER	N	607	14,17	0,1,1	0.00	-	-		
25	PEK	T	102	-	52,52,52	1.01	2 (3%)	55,57,57	0.86	2 (3%)
20	PER	A	609	14,17	0,1,1	0.00	-	-		
19	TGL	Y	101	-	62,62,62	1.07	3 (4%)	65,65,65	0.76	2 (3%)
26	CDL	C	306	-	99,99,99	0.98	4 (4%)	105,111,111	1.10	8 (7%)
24	DMU	T	101	-	34,34,34	1.48	5 (14%)	45,45,45	1.52	9 (20%)
23	CHD	O	302	-	29,32,32	0.58	0	48,51,51	1.44	7 (14%)
18	PGV	A	606	-	50,50,50	1.06	2 (4%)	53,56,56	1.10	4 (7%)
24	DMU	Q	201	-	34,34,34	0.85	0	45,45,45	1.28	4 (8%)
26	CDL	T	103	-	99,99,99	1.05	4 (4%)	105,111,111	0.92	6 (5%)
18	PGV	A	607	-	50,50,50	1.11	2 (4%)	53,56,56	1.09	3 (5%)
18	PGV	C	301	-	50,50,50	0.92	2 (4%)	53,56,56	0.72	0
24	DMU	M	101	-	34,34,34	1.38	2 (5%)	45,45,45	1.24	4 (8%)
18	PGV	C	305	-	50,50,50	1.01	2 (4%)	53,56,56	0.89	2 (3%)
18	PGV	P	305	-	50,50,50	1.17	2 (4%)	53,56,56	1.14	3 (5%)
25	PEK	G	103	-	52,52,52	1.03	2 (3%)	55,57,57	0.94	4 (7%)
23	CHD	C	307	-	29,32,32	0.58	0	48,51,51	1.55	8 (16%)
22	PSC	B	302	-	51,51,51	1.09	2 (3%)	57,59,59	1.39	8 (14%)
19	TGL	O	304	-	62,62,62	1.03	3 (4%)	65,65,65	0.91	3 (4%)
25	PEK	G	101	-	52,52,52	0.89	2 (3%)	55,57,57	0.70	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	G	102	-	99,99,99	1.00	4 (4%)	105,111,111	0.90	6 (5%)
19	TGL	A	608	-	62,62,62	1.15	3 (4%)	65,65,65	0.88	4 (6%)
23	CHD	P	302	-	29,32,32	0.60	0	48,51,51	1.05	3 (6%)
23	CHD	C	303	-	29,32,32	0.48	0	48,51,51	1.04	2 (4%)
19	TGL	L	101	-	62,62,62	1.05	3 (4%)	65,65,65	0.77	3 (4%)
21	CUA	O	301	2	0,1,1	0.00	-	-		
19	TGL	V	101	-	62,62,62	1.02	3 (4%)	65,65,65	0.95	6 (9%)
23	CHD	W	101	-	29,32,32	0.58	0	48,51,51	1.76	9 (18%)
17	HEA	A	604	1	44,67,67	1.72	9 (20%)	37,103,103	2.18	8 (21%)
17	HEA	N	605	1,20	44,67,67	1.76	11 (25%)	37,103,103	2.05	8 (21%)
25	PEK	C	308	-	52,52,52	1.06	2 (3%)	55,57,57	1.02	3 (5%)
23	CHD	J	101	-	29,32,32	0.70	1 (3%)	48,51,51	2.28	16 (33%)
18	PGV	P	304	-	50,50,50	1.00	2 (4%)	53,56,56	0.91	4 (7%)
17	HEA	N	604	1	44,67,67	1.94	10 (22%)	37,103,103	1.93	7 (18%)
22	PSC	O	303	-	51,51,51	1.05	2 (3%)	57,59,59	1.50	8 (14%)
17	HEA	A	605	1,20	44,67,67	1.75	9 (20%)	37,103,103	2.35	7 (18%)
21	CUA	B	301	2	0,1,1	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	C	304	-	-	27/56/56/56	-
24	DMU	C	302	-	-	10/19/59/59	0/2/2/2
23	CHD	B	303	-	-	4/7/74/74	0/4/4/4
25	PEK	P	303	-	-	22/56/56/56	-
18	PGV	P	301	-	-	16/55/55/55	-
19	TGL	I	101	-	-	39/65/65/65	-
18	PGV	N	606	-	-	32/55/55/55	-
26	CDL	P	306	-	-	68/110/110/110	-
23	CHD	P	307	-	-	3/7/74/74	0/4/4/4
25	PEK	T	102	-	-	22/56/56/56	-
19	TGL	Y	101	-	-	29/65/65/65	-
26	CDL	C	306	-	-	62/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	DMU	T	101	-	-	8/19/59/59	0/2/2/2
23	CHD	O	302	-	-	2/7/74/74	0/4/4/4
18	PGV	A	606	-	-	33/55/55/55	-
24	DMU	Q	201	-	-	11/19/59/59	0/2/2/2
26	CDL	T	103	-	-	58/110/110/110	-
18	PGV	A	607	-	-	25/55/55/55	-
18	PGV	C	301	-	-	18/55/55/55	-
24	DMU	M	101	-	-	9/19/59/59	0/2/2/2
18	PGV	C	305	-	-	26/55/55/55	-
18	PGV	P	305	-	-	31/55/55/55	-
25	PEK	G	103	-	-	22/56/56/56	-
23	CHD	C	307	-	-	3/7/74/74	0/4/4/4
22	PSC	B	302	-	-	25/55/55/55	-
19	TGL	O	304	-	-	41/65/65/65	-
25	PEK	G	101	-	-	22/56/56/56	-
26	CDL	G	102	-	-	45/110/110/110	-
19	TGL	A	608	-	-	33/65/65/65	-
23	CHD	P	302	-	-	0/7/74/74	0/4/4/4
23	CHD	C	303	-	-	0/7/74/74	0/4/4/4
19	TGL	L	101	-	-	31/65/65/65	-
19	TGL	V	101	-	-	34/65/65/65	-
23	CHD	W	101	-	-	5/7/74/74	0/4/4/4
17	HEA	A	604	1	3/3/7/16	3/24/76/76	-
17	HEA	N	605	1,20	3/3/7/16	4/24/76/76	-
25	PEK	C	308	-	-	22/56/56/56	-
23	CHD	J	101	-	-	5/7/74/74	0/4/4/4
18	PGV	P	304	-	-	14/55/55/55	-
17	HEA	N	604	1	3/3/7/16	2/24/76/76	-
17	HEA	A	605	1,20	3/3/7/16	2/24/76/76	-
22	PSC	O	303	-	-	30/55/55/55	-

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	604	HEA	C3B-C11	-7.12	1.47	1.52
24	M	101	DMU	O16-C6	6.70	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	605	HEA	C3B-C11	-5.60	1.48	1.52
17	N	604	HEA	C3C-C2C	5.46	1.47	1.40
17	A	604	HEA	C3B-C11	-5.36	1.48	1.52
17	N	605	HEA	C3B-C11	-5.32	1.48	1.52
18	A	607	PGV	O01-C1	5.19	1.48	1.34
18	P	305	PGV	O01-C1	5.05	1.48	1.34
18	P	305	PGV	O03-C19	5.04	1.48	1.33
25	C	304	PEK	O01-C1	5.02	1.48	1.34
26	P	306	CDL	OA6-CA5	5.00	1.48	1.34
18	N	606	PGV	O03-C19	4.93	1.47	1.33
25	T	102	PEK	O01-C1	4.88	1.48	1.34
18	A	606	PGV	O03-C19	4.87	1.47	1.33
19	A	608	TGL	OG2-CB1	4.78	1.47	1.34
25	C	308	PEK	O01-C1	4.77	1.47	1.34
26	P	306	CDL	OA8-CA7	4.76	1.47	1.33
17	N	605	HEA	C3C-C2C	4.76	1.47	1.40
22	B	302	PSC	O01-C1	4.75	1.47	1.34
26	C	306	CDL	OA6-CA5	4.73	1.47	1.34
19	A	608	TGL	OG3-CC1	4.70	1.47	1.33
22	O	303	PSC	O01-C1	4.69	1.47	1.34
25	G	103	PEK	O03-C21	4.64	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	604	HEA	C3C-C2C	4.61	1.46	1.40
17	N	604	HEA	C3A-C2A	4.59	1.46	1.40
19	Y	101	TGL	OG2-CB1	4.58	1.47	1.34
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	4.52	1.46	1.33
25	C	308	PEK	O03-C21	4.48	1.46	1.33
18	P	304	PGV	O03-C19	4.46	1.46	1.33
19	I	101	TGL	OG1-CA1	4.43	1.46	1.33
26	T	103	CDL	OB8-CB7	4.42	1.46	1.33
19	A	608	TGL	OG1-CA1	4.42	1.46	1.33
26	G	102	CDL	OB8-CB7	4.42	1.46	1.33
17	A	605	HEA	C3C-C2C	4.41	1.46	1.40
18	A	606	PGV	O01-C1	4.40	1.46	1.34
18	P	304	PGV	O01-C1	4.39	1.46	1.34
19	Y	101	TGL	OG3-CC1	4.39	1.46	1.33
26	G	102	CDL	OA8-CA7	4.39	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	305	PGV	O03-C19	4.38	1.46	1.33
26	C	306	CDL	OB6-CB5	4.35	1.46	1.34
26	T	103	CDL	OA8-CA7	4.33	1.46	1.33
19	I	101	TGL	OG2-CB1	4.33	1.46	1.34
19	O	304	TGL	OG1-CA1	4.31	1.45	1.33
25	T	102	PEK	O03-C21	4.29	1.45	1.33
19	L	101	TGL	OG3-CC1	4.25	1.45	1.33
18	C	301	PGV	O03-C19	4.25	1.45	1.33
25	P	303	PEK	O03-C21	4.23	1.45	1.33
22	B	302	PSC	O03-C19	4.22	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
26	P	306	CDL	OB8-CB7	4.18	1.45	1.33
19	Y	101	TGL	OG1-CA1	4.17	1.45	1.33
19	L	101	TGL	OG1-CA1	4.16	1.45	1.33
22	O	303	PSC	O03-C19	4.14	1.45	1.33
18	P	301	PGV	O03-C19	4.12	1.45	1.33
18	P	301	PGV	O01-C1	4.10	1.45	1.34
18	C	305	PGV	O01-C1	4.07	1.45	1.34
17	N	605	HEA	C3A-C2A	4.05	1.46	1.40
26	C	306	CDL	OB8-CB7	4.03	1.45	1.33
25	C	304	PEK	O03-C21	4.01	1.45	1.33
17	A	605	HEA	C3A-C2A	3.96	1.45	1.40
24	T	101	DMU	O1-C10	3.95	1.51	1.41
18	N	606	PGV	O01-C1	3.93	1.45	1.34
26	C	306	CDL	OA8-CA7	3.92	1.44	1.33
26	P	306	CDL	OB6-CB5	3.85	1.45	1.34
19	O	304	TGL	OG3-CC1	3.79	1.44	1.33
25	G	101	PEK	O01-C1	3.79	1.45	1.34
19	V	101	TGL	OG3-CC1	3.79	1.44	1.33
19	V	101	TGL	OG1-CA1	3.73	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	A	604	HEA	C4B-C3B	3.70	1.50	1.42
25	P	303	PEK	O01-C1	3.62	1.44	1.34
24	C	302	DMU	O7-C10	3.59	1.51	1.41
24	T	101	DMU	O16-C6	3.56	1.46	1.40
24	C	302	DMU	O7-C3	3.43	1.52	1.43
24	C	302	DMU	O16-C6	3.39	1.46	1.40
19	I	101	TGL	OG3-CC1	3.30	1.43	1.33
17	A	604	HEA	C1D-C2D	3.17	1.49	1.42
17	N	604	HEA	C3D-C2D	3.15	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	605	HEA	C1A-C2A	3.14	1.49	1.42
24	T	101	DMU	O7-C10	3.12	1.50	1.41
24	T	101	DMU	O7-C3	3.12	1.52	1.43
17	N	604	HEA	C1A-C2A	3.01	1.49	1.42
17	A	604	HEA	C3A-C2A	2.95	1.44	1.40
17	A	604	HEA	C3D-C2D	2.92	1.46	1.37
17	N	605	HEA	C3D-C2D	2.92	1.46	1.37
17	A	604	HEA	C4C-CHD	2.89	1.49	1.41
17	N	605	HEA	C1B-CHB	2.88	1.49	1.41
17	A	605	HEA	C3D-C2D	2.84	1.46	1.37
17	N	604	HEA	C4B-C3B	2.81	1.48	1.42
17	A	605	HEA	C1D-C2D	2.76	1.48	1.42
17	A	605	HEA	C1C-CHC	2.73	1.48	1.41
17	N	605	HEA	C1D-C2D	2.62	1.48	1.42
17	A	605	HEA	C4B-C3B	2.62	1.48	1.42
24	T	101	DMU	C10-C5	2.61	1.60	1.52
24	C	302	DMU	C8-C9	2.55	1.58	1.53
17	N	604	HEA	C4C-CHD	2.54	1.48	1.41
24	C	302	DMU	C10-C5	2.52	1.59	1.52
17	N	604	HEA	C1D-C2D	2.52	1.48	1.42
17	N	605	HEA	C4B-C3B	2.51	1.48	1.42
17	A	604	HEA	C1C-CHC	2.49	1.47	1.41
17	A	605	HEA	C1A-C2A	2.44	1.48	1.42
17	N	604	HEA	C1C-CHC	2.42	1.47	1.41
24	M	101	DMU	O5-C6	2.41	1.48	1.41
24	C	302	DMU	O1-C10	2.40	1.48	1.41
17	A	605	HEA	C4D-CHA	2.25	1.47	1.41
17	N	604	HEA	C1B-CHB	2.22	1.47	1.41
24	C	302	DMU	C2-C1	2.22	1.58	1.52
17	N	605	HEA	C1C-CHC	2.17	1.47	1.41
23	J	101	CHD	C20-C17	2.13	1.58	1.54
17	A	604	HEA	CAA-C2A	-2.08	1.48	1.52
17	N	605	HEA	C4C-CHD	2.07	1.46	1.41
17	N	605	HEA	C4D-CHA	2.06	1.46	1.41

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	604	HEA	C4B-C3B-C2B	-7.52	101.61	106.87
24	C	302	DMU	C10-O7-C3	6.92	135.09	117.96
17	N	605	HEA	C4B-C3B-C2B	-6.85	102.08	106.87
23	J	101	CHD	C6-C5-C10	6.78	119.86	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	605	HEA	C1B-C2B-C3B	-6.59	102.41	107.00
19	I	101	TGL	OG2-CB1-CB2	6.42	125.35	111.50
26	P	306	CDL	OA6-CA5-C11	6.35	125.19	111.50
17	A	605	HEA	C4B-C3B-C2B	-6.32	102.45	106.87
17	N	604	HEA	C4B-C3B-C2B	-6.30	102.47	106.87
17	A	604	HEA	C1B-C2B-C3B	-6.12	102.74	107.00
17	A	605	HEA	CAD-CBD-CGD	-5.43	103.57	112.67
23	W	101	CHD	C22-C20-C17	5.38	121.39	110.28
17	A	605	HEA	C3C-C4C-NC	5.36	116.14	109.21
24	C	302	DMU	C18-O16-C6	5.35	122.72	113.84
18	P	305	PGV	O01-C1-C2	5.32	122.96	111.50
18	A	607	PGV	O01-C1-C2	5.25	122.81	111.50
22	O	303	PSC	C08-N-C06	-5.13	95.79	108.97
22	O	303	PSC	C08-N-C07	-4.91	96.35	108.97
23	J	101	CHD	C22-C20-C17	4.88	120.36	110.28
26	C	306	CDL	OA6-CA5-C11	4.84	121.94	111.50
17	N	604	HEA	C1B-C2B-C3B	-4.72	103.72	107.00
17	A	604	HEA	CAA-CBA-CGA	-4.67	104.83	112.67
23	J	101	CHD	C10-C9-C8	4.65	116.81	111.82
24	Q	201	DMU	C18-O16-C6	4.63	121.52	113.84
25	C	308	PEK	O01-C1-C2	4.63	121.48	111.50
24	T	101	DMU	C10-O1-C9	4.57	122.65	113.69
23	J	101	CHD	C5-C6-C7	4.55	119.48	114.46
23	P	307	CHD	C10-C9-C8	4.53	116.68	111.82
23	C	307	CHD	C10-C9-C8	4.51	116.67	111.82
23	J	101	CHD	C9-C10-C5	4.51	114.92	108.58
23	P	307	CHD	C1-C2-C3	4.51	116.25	110.47
22	O	303	PSC	C07-N-C06	4.42	120.35	108.97
22	B	302	PSC	C08-N-C06	-4.42	97.60	108.97
17	N	605	HEA	C1B-C2B-C3B	-4.41	103.93	107.00
18	A	606	PGV	O01-C1-C2	4.40	120.99	111.50
26	G	102	CDL	OB6-CB5-C51	4.35	120.87	111.50
26	T	103	CDL	OA6-CA5-C11	4.33	120.84	111.50
25	G	103	PEK	O01-C1-C2	4.32	120.82	111.50
17	A	605	HEA	CBD-CAD-C3D	4.20	120.23	112.49
17	N	605	HEA	CAD-CBD-CGD	-4.10	105.79	112.67
22	B	302	PSC	C08-N-C07	-4.07	98.51	108.97
17	N	605	HEA	C3C-C4C-NC	4.06	114.47	109.21
26	P	306	CDL	OB6-CB5-C51	4.05	120.22	111.50
22	B	302	PSC	C07-N-C06	3.84	118.84	108.97
23	J	101	CHD	C13-C17-C20	3.82	124.06	119.50
24	M	101	DMU	O5-C6-O16	3.82	119.01	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	101	CHD	C17-C13-C14	-3.79	96.27	100.09
18	N	606	PGV	O01-C1-C2	3.77	119.63	111.50
18	P	305	PGV	O03-C19-C20	3.74	123.66	111.91
23	J	101	CHD	C6-C7-C8	3.72	115.45	111.48
26	T	103	CDL	OB6-CB5-C51	3.71	119.50	111.50
17	A	605	HEA	C13-C12-C11	-3.70	108.80	114.35
25	T	102	PEK	O01-C1-C2	3.69	119.44	111.50
18	N	606	PGV	O03-C19-C20	3.55	123.04	111.91
25	C	304	PEK	O01-C1-C2	3.54	119.13	111.50
23	W	101	CHD	C16-C17-C20	3.53	117.61	112.15
18	A	606	PGV	O03-C19-C20	3.50	122.90	111.91
18	A	607	PGV	O03-C19-C20	3.47	122.78	111.91
19	A	608	TGL	OG2-CB1-CB2	3.46	118.97	111.50
18	P	301	PGV	O01-C1-C2	3.46	118.96	111.50
22	B	302	PSC	O01-C1-C2	3.46	118.96	111.50
19	I	101	TGL	OG1-CA1-CA2	3.45	122.73	111.91
19	V	101	TGL	OG2-CB1-CB2	3.43	118.90	111.50
19	O	304	TGL	OG2-CB1-CB2	3.40	118.84	111.50
23	J	101	CHD	C19-C10-C1	-3.30	102.94	108.26
26	P	306	CDL	OA8-CA7-C31	3.27	122.18	111.91
26	G	102	CDL	OA6-CA5-C11	3.26	118.53	111.50
24	T	101	DMU	C10-O7-C3	3.25	126.00	117.96
24	M	101	DMU	O5-C6-C1	-3.22	103.53	110.35
17	N	604	HEA	C3C-C4C-NC	3.21	113.37	109.21
23	C	307	CHD	C14-C8-C9	-3.21	105.31	109.71
23	P	307	CHD	C11-C9-C8	-3.20	106.19	110.88
26	C	306	CDL	OB6-CB5-C51	3.20	118.39	111.50
23	C	307	CHD	C9-C10-C5	3.18	113.05	108.58
23	O	302	CHD	C4-C3-C2	3.18	114.34	110.55
17	A	604	HEA	CMC-C2C-C3C	3.17	130.62	124.68
23	W	101	CHD	C14-C13-C12	3.15	110.34	107.40
26	T	103	CDL	OA8-CA7-C31	3.13	121.75	111.91
23	W	101	CHD	C21-C20-C17	-3.12	108.14	112.92
24	C	302	DMU	O7-C3-C4	3.11	117.97	109.45
26	G	102	CDL	OA8-CA7-C31	3.11	121.66	111.91
18	C	305	PGV	O01-C1-C2	3.09	118.16	111.50
17	N	605	HEA	CBA-CAA-C2A	3.09	118.16	112.48
23	O	302	CHD	C23-C22-C20	3.07	118.86	114.72
26	C	306	CDL	OA8-CA7-C31	3.07	121.53	111.91
19	Y	101	TGL	OG2-CB1-CB2	3.05	118.08	111.50
17	N	604	HEA	CMC-C2C-C3C	3.04	130.36	124.68
23	C	307	CHD	C1-C2-C3	3.02	114.34	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	302	CHD	C6-C5-C4	-3.01	107.72	111.19
19	V	101	TGL	CG2-OG2-CB1	2.99	125.15	117.79
22	O	303	PSC	O03-C19-C20	2.99	121.28	111.91
23	B	303	CHD	C6-C5-C4	-2.97	107.77	111.19
24	Q	201	DMU	C7-C8-C9	2.96	115.52	110.24
25	C	308	PEK	O01-C1-O02	-2.95	116.58	123.70
23	W	101	CHD	C6-C7-C8	2.94	114.62	111.48
22	B	302	PSC	C08-N-C05	-2.94	97.88	109.92
19	I	101	TGL	CG2-OG2-CB1	2.92	124.98	117.79
22	O	303	PSC	C08-N-C05	-2.92	97.97	109.92
23	B	303	CHD	C19-C10-C1	-2.91	103.58	108.26
26	C	306	CDL	OA6-CA5-OA7	-2.89	116.72	123.70
19	A	608	TGL	OG3-CC1-CC2	2.87	120.93	111.91
26	T	103	CDL	OA8-CA7-OA9	-2.86	116.38	123.59
24	M	101	DMU	C18-O16-C6	-2.86	109.10	113.84
24	M	101	DMU	C22-C19-C18	-2.84	100.88	113.49
23	O	302	CHD	C19-C10-C1	-2.83	103.70	108.26
17	N	604	HEA	C12-C13-C14	-2.83	104.77	112.23
24	Q	201	DMU	O5-C6-O16	-2.83	103.28	109.97
17	N	604	HEA	OMA-CMA-C3A	-2.82	118.77	124.91
22	O	303	PSC	O01-C1-C2	2.81	117.56	111.50
24	C	302	DMU	C6-C1-C2	2.80	115.82	110.00
19	O	304	TGL	OG1-CA1-CA2	2.79	120.66	111.91
17	A	604	HEA	OMA-CMA-C3A	-2.78	118.84	124.91
17	N	605	HEA	OMA-CMA-C3A	-2.78	118.85	124.91
23	J	101	CHD	C22-C23-C24	2.75	119.50	113.59
23	C	307	CHD	C11-C9-C8	-2.73	106.88	110.88
23	P	302	CHD	C19-C10-C1	-2.72	103.88	108.26
23	J	101	CHD	C16-C17-C20	2.72	116.35	112.15
23	B	303	CHD	C1-C10-C9	2.71	115.61	111.35
17	N	604	HEA	CBD-CAD-C3D	-2.67	107.56	112.49
25	T	102	PEK	O03-C21-C22	2.67	120.29	111.91
23	W	101	CHD	C4-C3-C2	2.65	113.72	110.55
24	C	302	DMU	C10-O1-C9	2.65	118.88	113.69
24	T	101	DMU	C25-C22-C19	-2.61	101.15	114.42
22	B	302	PSC	O03-C19-C20	2.61	120.09	111.91
24	T	101	DMU	C18-O16-C6	2.61	118.17	113.84
23	J	101	CHD	C5-C4-C3	2.59	116.56	112.76
26	C	306	CDL	OA8-CA7-OA9	-2.57	117.10	123.59
18	P	301	PGV	O03-C19-C20	2.57	119.98	111.91
24	C	302	DMU	C1-C2-C3	2.55	115.51	109.68
23	C	307	CHD	C22-C23-C24	-2.55	108.12	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	308	PEK	O03-C21-C22	2.53	119.86	111.91
24	C	302	DMU	O16-C18-C19	-2.53	100.69	109.56
23	C	303	CHD	C15-C14-C13	2.53	106.03	103.55
19	V	101	TGL	OG2-CG2-CG3	2.52	117.53	108.40
18	P	304	PGV	O03-C19-O04	-2.52	117.24	123.59
25	G	101	PEK	O01-C1-C2	2.51	116.91	111.50
24	T	101	DMU	O1-C10-C5	2.51	115.66	110.35
25	P	303	PEK	O01-C1-C2	2.50	116.88	111.50
19	A	608	TGL	OG1-CA1-CA2	2.49	119.73	111.91
26	C	306	CDL	C52-C51-CB5	-2.49	104.58	113.62
19	I	101	TGL	OG3-CC1-CC2	2.48	119.69	111.91
24	T	101	DMU	C31-C28-C25	-2.48	101.85	114.42
24	T	101	DMU	C7-C8-C9	-2.48	105.82	110.24
25	G	103	PEK	O01-C1-O02	-2.48	117.72	123.70
19	O	304	TGL	OG3-CC1-CC2	2.46	119.63	111.91
23	J	101	CHD	C6-C5-C4	-2.45	108.37	111.19
25	C	304	PEK	O03-C21-C22	2.44	119.57	111.91
23	P	307	CHD	C2-C1-C10	2.44	116.97	112.78
23	P	307	CHD	C14-C8-C9	-2.44	106.36	109.71
24	T	101	DMU	O1-C9-C11	2.44	112.50	106.44
17	A	604	HEA	CBD-CAD-C3D	-2.44	107.99	112.49
18	A	607	PGV	O03-C19-O04	-2.44	117.44	123.59
18	P	304	PGV	O03-C19-C20	2.42	119.49	111.91
25	G	103	PEK	C01-O03-C21	2.41	126.06	117.12
26	C	306	CDL	OB8-CB7-C71	2.41	119.47	111.91
26	G	102	CDL	OA8-CA7-OA9	-2.38	117.58	123.59
19	I	101	TGL	OG2-CB1-OB1	-2.38	117.95	123.70
22	B	302	PSC	C04-C05-N	-2.37	107.86	115.78
26	P	306	CDL	CB4-OB6-CB5	-2.37	111.96	117.79
24	Q	201	DMU	C8-C7-C5	2.36	114.94	110.82
24	C	302	DMU	C2-C3-C4	-2.36	105.52	110.93
19	I	101	TGL	OG1-CA1-OA1	-2.35	117.65	123.59
23	C	303	CHD	C6-C5-C4	-2.35	108.49	111.19
24	T	101	DMU	O16-C18-C19	-2.34	101.37	109.56
23	W	101	CHD	C9-C11-C12	-2.34	111.21	114.30
19	I	101	TGL	CG3-OG3-CC1	2.34	125.77	117.12
22	B	302	PSC	C06-N-C05	2.33	119.46	109.92
18	P	304	PGV	O01-C1-C2	2.33	116.53	111.50
23	O	302	CHD	C6-C7-C8	2.31	113.95	111.48
17	A	604	HEA	C26-C15-C16	2.31	119.15	115.27
26	G	102	CDL	OB8-CB7-C71	2.29	119.11	111.91
23	O	302	CHD	C5-C4-C3	2.28	116.11	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	103	CDL	OB8-CB7-C71	2.28	119.06	111.91
18	A	606	PGV	O01-C1-O02	-2.28	118.20	123.70
25	G	103	PEK	O03-C21-C22	2.27	119.04	111.91
26	C	306	CDL	OB8-CB7-OB9	-2.27	117.87	123.59
19	I	101	TGL	OG3-CC1-OC1	-2.26	117.88	123.59
23	O	302	CHD	C1-C10-C9	2.26	114.91	111.35
23	P	302	CHD	C6-C5-C4	-2.26	108.59	111.19
19	Y	101	TGL	OG3-CC1-CC2	2.25	118.96	111.91
18	C	305	PGV	O03-C19-C20	2.25	118.96	111.91
17	N	605	HEA	CMC-C2C-C3C	2.24	128.87	124.68
19	A	608	TGL	OG3-CC1-OC1	-2.24	117.94	123.59
23	B	303	CHD	C22-C20-C17	2.24	114.91	110.28
23	W	101	CHD	C23-C22-C20	-2.23	111.72	114.72
18	N	606	PGV	O01-C1-O02	-2.23	118.31	123.70
23	J	101	CHD	C19-C10-C5	-2.23	106.59	110.36
23	P	302	CHD	C13-C17-C20	2.23	122.15	119.50
22	O	303	PSC	O03-C19-O04	-2.22	118.00	123.59
26	T	103	CDL	OB8-CB7-OB9	-2.21	118.01	123.59
17	A	605	HEA	OMA-CMA-C3A	-2.19	120.14	124.91
23	B	303	CHD	C23-C22-C20	2.19	117.67	114.72
26	P	306	CDL	OA6-CA5-OA7	-2.18	118.44	123.70
23	J	101	CHD	O12-C12-C11	-2.16	104.72	109.12
25	C	304	PEK	C03-C02-C01	-2.16	106.67	111.79
18	A	606	PGV	O03-C19-O04	-2.16	118.14	123.59
18	P	301	PGV	O01-C1-O02	-2.15	118.51	123.70
22	O	303	PSC	C06-N-C05	2.14	118.69	109.92
19	V	101	TGL	OG1-CA1-CA2	2.14	118.62	111.91
23	P	307	CHD	C11-C12-C13	2.12	113.42	111.24
19	L	101	TGL	OG3-CC1-CC2	2.12	118.55	111.91
25	P	303	PEK	O01-C1-O02	-2.11	118.60	123.70
26	G	102	CDL	OA6-CA5-OA7	-2.10	118.63	123.70
19	V	101	TGL	OG1-CA1-OA1	-2.09	118.31	123.59
17	N	605	HEA	C20-C19-C18	-2.09	116.89	121.12
23	C	307	CHD	C9-C8-C7	2.08	114.36	111.88
23	J	101	CHD	C1-C10-C5	2.06	110.81	107.77
19	L	101	TGL	OG3-CC1-OC1	-2.05	118.43	123.59
24	C	302	DMU	O7-C10-C5	2.04	113.38	108.10
26	P	306	CDL	CA4-OA6-CA5	2.03	122.80	117.79
18	P	304	PGV	C02-O01-C1	2.03	122.80	117.79
19	V	101	TGL	OG3-CC1-CC2	2.03	118.27	111.91
17	A	604	HEA	C3C-C4C-NC	2.02	111.83	109.21
23	B	303	CHD	C16-C17-C20	2.02	115.28	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	305	PGV	O01-C1-O02	-2.02	118.82	123.70
23	J	101	CHD	C18-C13-C12	-2.01	107.02	109.07
23	C	307	CHD	C19-C10-C5	-2.01	106.95	110.36
19	L	101	TGL	OG2-CB1-CB2	2.00	115.82	111.50

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
17	A	604	HEA	ND
17	A	604	HEA	NA
17	A	604	HEA	NB
17	N	605	HEA	ND
17	N	605	HEA	NA
17	N	605	HEA	NB
17	N	604	HEA	ND
17	N	604	HEA	NA
17	N	604	HEA	NB
17	A	605	HEA	ND
17	A	605	HEA	NA
17	A	605	HEA	NB

All (898) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	C	304	PEK	C03-O11-P-O13
25	C	304	PEK	C6-C7-C8-C9
19	I	101	TGL	OB1-CB1-OG2-CG2
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
26	P	306	CDL	CB2-C1-CA2-OA2
26	P	306	CDL	CA2-OA2-PA1-OA5
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

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C11-CA5-OA6-CA4
26	P	306	CDL	CB3-OB5-PB2-OB3
26	P	306	CDL	CB3-OB5-PB2-OB4
23	P	307	CHD	C20-C22-C23-C24
25	T	102	PEK	C04-O12-P-O14
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
18	A	606	PGV	C03-O11-P-O12
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	C04-C05-C06-O06
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
24	Q	201	DMU	C1-C6-O16-C18
24	Q	201	DMU	O5-C6-O16-C18
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	CB3-OB5-PB2-OB2
26	T	103	CDL	CB3-OB5-PB2-OB3
26	T	103	CDL	CB3-OB5-PB2-OB4
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	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
25	G	103	PEK	O12-C04-C05-N
25	G	103	PEK	C6-C7-C8-C9
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
26	G	102	CDL	C1-CB2-OB2-PB2
19	V	101	TGL	OG1-CG1-CG2-OG2

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Mol	Chain	Res	Type	Atoms
25	C	308	PEK	C03-O11-P-O13
25	C	308	PEK	O12-C04-C05-N
18	P	304	PGV	C04-C05-C06-O06
18	P	304	PGV	O05-C05-C06-O06
22	O	303	PSC	C03-O11-P-O13
22	O	303	PSC	C03-O11-P-O14
22	O	303	PSC	C04-O12-P-O14
22	O	303	PSC	C9-C10-C11-C12
17	A	605	HEA	C3B-C11-C12-C13
17	A	605	HEA	O11-C11-C12-C13
24	M	101	DMU	O5-C6-O16-C18
24	C	302	DMU	C4-C3-O7-C10
19	Y	101	TGL	OA1-CA1-OG1-CG1
26	T	103	CDL	OA9-CA7-OA8-CA6
19	A	608	TGL	OC1-CC1-OG3-CG3
25	C	308	PEK	O04-C21-O03-C01
24	T	101	DMU	C4-C3-O7-C10
26	T	103	CDL	OA7-CA5-OA6-CA4
18	P	305	PGV	O02-C1-O01-C02
26	P	306	CDL	C31-CA7-OA8-CA6
19	A	608	TGL	CC2-CC1-OG3-CG3
19	I	101	TGL	CB2-CB1-OG2-CG2
18	N	606	PGV	C2-C1-O01-C02
24	T	101	DMU	O5-C4-C57-O61
19	Y	101	TGL	CA2-CA1-OG1-CG1
26	T	103	CDL	C31-CA7-OA8-CA6
22	B	302	PSC	C20-C19-O03-C01
19	O	304	TGL	CC2-CC1-OG3-CG3
19	V	101	TGL	CA2-CA1-OG1-CG1
25	C	308	PEK	C22-C21-O03-C01
22	O	303	PSC	C20-C19-O03-C01
24	T	101	DMU	O6-C11-C9-C8
19	O	304	TGL	OC1-CC1-OG3-CG3
26	G	102	CDL	OA9-CA7-OA8-CA6
19	V	101	TGL	OA1-CA1-OG1-CG1
26	T	103	CDL	O1-C1-CA2-OA2
26	G	102	CDL	C31-CA7-OA8-CA6
26	G	102	CDL	C71-CB7-OB8-CB6
26	P	306	CDL	OA9-CA7-OA8-CA6
22	O	303	PSC	O04-C19-O03-C01
24	C	302	DMU	O5-C4-C57-O61
22	B	302	PSC	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
24	C	302	DMU	O6-C11-C9-O1
23	W	101	CHD	C17-C20-C22-C23
24	T	101	DMU	O6-C11-C9-O1
24	C	302	DMU	C3-C4-C57-O61
26	T	103	CDL	CB4-CB3-OB5-PB2
24	T	101	DMU	C3-C4-C57-O61
19	O	304	TGL	CC2-CC3-CC4-CC5
23	W	101	CHD	C21-C20-C22-C23
26	G	102	CDL	OB9-CB7-OB8-CB6
17	A	604	HEA	C15-C16-C17-C18
17	A	604	HEA	C19-C20-C21-C22
17	N	604	HEA	C15-C16-C17-C18
23	P	307	CHD	C17-C20-C22-C23
23	O	302	CHD	C17-C20-C22-C23
24	Q	201	DMU	C3-C4-C57-O61
26	C	306	CDL	CB2-C1-CA2-OA2
23	O	302	CHD	C21-C20-C22-C23
25	G	101	PEK	C22-C21-O03-C01
19	L	101	TGL	CA2-CA1-OG1-CG1
23	J	101	CHD	C17-C20-C22-C23
23	C	307	CHD	C17-C20-C22-C23
26	C	306	CDL	C19-C20-C21-C22
23	J	101	CHD	C21-C20-C22-C23
23	P	307	CHD	C21-C20-C22-C23
18	A	606	PGV	C19-C20-C21-C22
26	T	103	CDL	OB6-CB4-CB6-OB8
25	T	102	PEK	C2-C1-O01-C02
23	J	101	CHD	C13-C17-C20-C22
19	L	101	TGL	OA1-CA1-OG1-CG1
26	P	306	CDL	C16-C17-C18-C19
24	C	302	DMU	O6-C11-C9-C8
26	T	103	CDL	C71-CB7-OB8-CB6
26	P	306	CDL	CB7-C71-C72-C73
19	L	101	TGL	CC1-CC2-CC3-CC4
19	V	101	TGL	CA1-CA2-CA3-CA4
23	J	101	CHD	C13-C17-C20-C21
18	P	305	PGV	O05-C05-C06-O06
23	W	101	CHD	C13-C17-C20-C22
25	P	303	PEK	C21-C22-C23-C24
19	I	101	TGL	CC1-CC2-CC3-CC4
18	N	606	PGV	C19-C20-C21-C22
26	C	306	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
19	O	304	TGL	CB1-CB2-CB3-CB4
19	A	608	TGL	CA2-CA1-OG1-CG1
25	T	102	PEK	O02-C1-O01-C02
23	C	307	CHD	C21-C20-C22-C23
24	Q	201	DMU	O16-C18-C19-C22
18	A	607	PGV	C1-C2-C3-C4
19	O	304	TGL	C20-C21-C22-C23
23	W	101	CHD	C13-C17-C20-C21
25	G	101	PEK	O04-C21-O03-C01
24	Q	201	DMU	O5-C4-C57-O61
17	N	604	HEA	C19-C20-C21-C22
26	C	306	CDL	CB5-C51-C52-C53
18	N	606	PGV	O12-C04-C05-O05
26	P	306	CDL	O1-C1-CA2-OA2
26	C	306	CDL	O1-C1-CA2-OA2
19	Y	101	TGL	OB1-CB1-OG2-CG2
23	W	101	CHD	C16-C17-C20-C21
26	T	103	CDL	OB9-CB7-OB8-CB6
25	P	303	PEK	C2-C1-O01-C02
26	P	306	CDL	C51-CB5-OB6-CB4
19	Y	101	TGL	CB2-CB1-OG2-CG2
26	G	102	CDL	C11-CA5-OA6-CA4
26	P	306	CDL	CB3-OB5-PB2-OB2
25	T	102	PEK	C03-O11-P-O12
25	T	102	PEK	C04-O12-P-O11
26	C	306	CDL	CA2-OA2-PA1-OA5
26	C	306	CDL	CB3-OB5-PB2-OB2
18	A	606	PGV	C04-O12-P-O11
26	T	103	CDL	CB2-OB2-PB2-OB5
22	B	302	PSC	C03-O11-P-O12
25	C	308	PEK	C03-O11-P-O12
22	O	303	PSC	C03-O11-P-O12
22	O	303	PSC	C04-O12-P-O11
23	J	101	CHD	C16-C17-C20-C21
25	C	304	PEK	C1-C2-C3-C4
18	N	606	PGV	O12-C04-C05-C06
25	C	304	PEK	O02-C1-O01-C02
25	P	303	PEK	O02-C1-O01-C02
26	G	102	CDL	OA7-CA5-OA6-CA4
25	G	103	PEK	C15-C16-C17-C18
26	P	306	CDL	C15-C16-C17-C18
22	O	303	PSC	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	C	304	PEK	C2-C1-O01-C02
25	G	103	PEK	C2-C1-O01-C02
25	P	303	PEK	C34-C35-C36-C37
19	I	101	TGL	CB3-CB4-CB5-CB6
19	Y	101	TGL	C10-C11-C12-C13
19	Y	101	TGL	CC2-CC3-CC4-CC5
26	C	306	CDL	C31-C32-C33-C34
24	Q	201	DMU	C22-C25-C28-C31
26	T	103	CDL	C37-C38-C39-C40
22	B	302	PSC	C29-C30-C31-C32
19	O	304	TGL	CA3-CA4-CA5-CA6
26	G	102	CDL	C36-C37-C38-C39
18	P	304	PGV	C7-C8-C9-C10
19	I	101	TGL	C17-C18-C19-C33
26	P	306	CDL	C17-C18-C19-C20
26	T	103	CDL	C41-C42-C43-C44
19	O	304	TGL	CC7-CC8-CC9-C15
19	A	608	TGL	CC3-CC4-CC5-CC6
19	L	101	TGL	CA3-CA4-CA5-CA6
26	P	306	CDL	OB7-CB5-OB6-CB4
18	C	305	PGV	C30-C31-C32-C33
19	O	304	TGL	C17-C18-C19-C33
25	G	101	PEK	C34-C35-C36-C37
26	G	102	CDL	C63-C64-C65-C66
19	L	101	TGL	CA9-C20-C21-C22
18	P	301	PGV	C5-C6-C7-C8
18	P	301	PGV	C25-C26-C27-C28
19	I	101	TGL	CC3-CC4-CC5-CC6
19	Y	101	TGL	C21-C22-C23-C24
25	G	103	PEK	C16-C17-C18-C19
26	G	102	CDL	C52-C53-C54-C55
18	A	606	PGV	O12-C04-C05-O05
18	A	607	PGV	O12-C04-C05-O05
18	C	301	PGV	C13-C14-C15-C16
19	O	304	TGL	C11-C12-C13-C14
19	L	101	TGL	CC3-CC4-CC5-CC6
25	C	308	PEK	C1-C2-C3-C4
18	P	304	PGV	C20-C19-O03-C01
25	P	303	PEK	C26-C27-C28-C29
26	C	306	CDL	C16-C17-C18-C19
26	C	306	CDL	C54-C55-C56-C57
24	T	101	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	C2-C3-C4-C5
18	P	305	PGV	C22-C23-C24-C25
22	B	302	PSC	C21-C22-C23-C24
19	O	304	TGL	CA5-CA6-CA7-CA8
19	O	304	TGL	CC5-CC6-CC7-CC8
19	L	101	TGL	C22-C23-C24-C25
19	A	608	TGL	OA1-CA1-OG1-CG1
26	P	306	CDL	C35-C36-C37-C38
26	P	306	CDL	C43-C44-C45-C46
26	C	306	CDL	C18-C19-C20-C21
26	C	306	CDL	C38-C39-C40-C41
25	G	103	PEK	C26-C27-C28-C29
19	O	304	TGL	C21-C22-C23-C24
19	L	101	TGL	C17-C18-C19-C33
19	L	101	TGL	C23-C24-C25-C26
25	C	304	PEK	C21-C22-C23-C24
18	C	305	PGV	C1-C2-C3-C4
18	P	301	PGV	C7-C8-C9-C10
19	I	101	TGL	CA5-CA6-CA7-CA8
19	I	101	TGL	CB6-CB7-CB8-CB9
19	I	101	TGL	CC2-CC3-CC4-CC5
26	P	306	CDL	C34-C35-C36-C37
26	P	306	CDL	C74-C75-C76-C77
19	Y	101	TGL	CC7-CC8-CC9-C15
18	A	607	PGV	C20-C21-C22-C23
19	A	608	TGL	C17-C18-C19-C33
19	L	101	TGL	CB7-CB8-CB9-C10
24	C	302	DMU	C19-C22-C25-C28
26	P	306	CDL	C13-C14-C15-C16
25	G	103	PEK	O02-C1-O01-C02
19	I	101	TGL	C19-C33-C34-C35
26	T	103	CDL	C21-C22-C23-C24
19	A	608	TGL	C15-C16-C17-C18
25	C	308	PEK	C25-C26-C27-C28
25	C	308	PEK	C27-C28-C29-C30
18	P	304	PGV	C30-C31-C32-C33
22	B	302	PSC	C13-C14-C15-C16
19	Y	101	TGL	CA1-CA2-CA3-CA4
19	I	101	TGL	C13-C14-C29-C30
19	I	101	TGL	C23-C24-C25-C26
26	P	306	CDL	C71-C72-C73-C74
26	P	306	CDL	C81-C82-C83-C84

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	C13-C14-C29-C30
26	C	306	CDL	C41-C42-C43-C44
18	C	305	PGV	C22-C23-C24-C25
18	P	305	PGV	C26-C27-C28-C29
19	O	304	TGL	C12-C13-C14-C29
25	G	101	PEK	C16-C17-C18-C19
26	G	102	CDL	C23-C24-C25-C26
19	A	608	TGL	CA9-C20-C21-C22
19	V	101	TGL	CC2-CC3-CC4-CC5
22	O	303	PSC	C04-C05-N-C06
19	I	101	TGL	CC4-CC5-CC6-CC7
26	P	306	CDL	C59-C60-C61-C62
18	A	607	PGV	C30-C31-C32-C33
19	O	304	TGL	CB9-C10-C11-C12
26	G	102	CDL	C31-C32-C33-C34
19	A	608	TGL	CA6-CA7-CA8-CA9
19	A	608	TGL	CC2-CC3-CC4-CC5
25	T	102	PEK	C34-C35-C36-C37
26	C	306	CDL	C62-C63-C64-C65
18	C	301	PGV	C5-C6-C7-C8
19	A	608	TGL	CB5-CB6-CB7-CB8
19	V	101	TGL	CB5-CB6-CB7-CB8
19	I	101	TGL	CB5-CB6-CB7-CB8
18	N	606	PGV	C22-C23-C24-C25
26	C	306	CDL	C53-C54-C55-C56
26	C	306	CDL	C75-C76-C77-C78
18	A	606	PGV	C27-C28-C29-C30
19	O	304	TGL	C22-C23-C24-C25
18	P	304	PGV	C13-C14-C15-C16
22	O	303	PSC	C29-C30-C31-C32
26	C	306	CDL	C82-C83-C84-C85
18	A	607	PGV	C26-C27-C28-C29
18	C	301	PGV	C21-C22-C23-C24
25	C	308	PEK	C33-C34-C35-C36
25	C	308	PEK	C34-C35-C36-C37
26	P	306	CDL	C73-C74-C75-C76
19	O	304	TGL	CB6-CB7-CB8-CB9
19	O	304	TGL	CC4-CC5-CC6-CC7
18	P	304	PGV	C20-C21-C22-C23
25	P	303	PEK	O03-C01-C02-C03
26	G	102	CDL	C21-C22-C23-C24
19	A	608	TGL	C19-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	L	101	TGL	C12-C13-C14-C29
24	C	302	DMU	C25-C28-C31-C34
18	C	301	PGV	C23-C24-C25-C26
25	G	101	PEK	C2-C1-O01-C02
19	I	101	TGL	CA9-C20-C21-C22
24	C	302	DMU	O16-C18-C19-C22
26	C	306	CDL	C52-C53-C54-C55
18	A	606	PGV	C30-C31-C32-C33
25	G	103	PEK	C30-C31-C32-C33
19	O	304	TGL	CA7-CA8-CA9-C20
19	V	101	TGL	C16-C17-C18-C19
18	A	607	PGV	C11-C10-C9-C8
18	P	305	PGV	C12-C13-C14-C15
19	L	101	TGL	C21-C22-C23-C24
25	G	101	PEK	C30-C31-C32-C33
18	P	304	PGV	C22-C23-C24-C25
18	A	607	PGV	O12-C04-C05-C06
26	P	306	CDL	C79-C80-C81-C82
22	O	303	PSC	C27-C28-C29-C30
25	G	101	PEK	O02-C1-O01-C02
19	Y	101	TGL	CB7-CB8-CB9-C10
19	A	608	TGL	CC7-CC8-CC9-C15
18	P	304	PGV	O04-C19-O03-C01
19	Y	101	TGL	CC5-CC6-CC7-CC8
26	T	103	CDL	C39-C40-C41-C42
26	G	102	CDL	C72-C73-C74-C75
19	V	101	TGL	CA5-CA6-CA7-CA8
22	O	303	PSC	C5-C6-C7-C8
24	M	101	DMU	C22-C25-C28-C31
19	O	304	TGL	CA2-CA1-OG1-CG1
26	C	306	CDL	C11-C12-C13-C14
18	A	607	PGV	C3-C4-C5-C6
22	O	303	PSC	C3-C4-C5-C6
18	C	305	PGV	C19-C20-C21-C22
19	A	608	TGL	CB9-C10-C11-C12
26	T	103	CDL	C80-C81-C82-C83
19	O	304	TGL	C15-C16-C17-C18
19	O	304	TGL	OA1-CA1-OG1-CG1
18	A	606	PGV	C13-C14-C15-C16
19	A	608	TGL	C21-C20-CA9-CA8
18	A	607	PGV	C12-C13-C14-C15
22	O	303	PSC	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	OB7-CB5-OB6-CB4
19	A	608	TGL	OB1-CB1-OG2-CG2
25	P	303	PEK	C22-C21-O03-C01
18	C	305	PGV	C20-C19-O03-C01
19	Y	101	TGL	CA9-C20-C21-C22
26	C	306	CDL	C36-C37-C38-C39
26	T	103	CDL	C20-C21-C22-C23
18	C	301	PGV	C4-C5-C6-C7
18	C	305	PGV	C28-C29-C30-C31
19	O	304	TGL	CC6-CC7-CC8-CC9
26	G	102	CDL	C55-C56-C57-C58
18	A	606	PGV	C24-C25-C26-C27
18	C	305	PGV	C25-C26-C27-C28
25	G	101	PEK	C26-C27-C28-C29
25	C	304	PEK	C27-C28-C29-C30
19	Y	101	TGL	CB4-CB5-CB6-CB7
26	G	102	CDL	C13-C14-C15-C16
19	L	101	TGL	CC7-CC8-CC9-C15
26	P	306	CDL	C20-C21-C22-C23
19	Y	101	TGL	C18-C19-C33-C34
26	T	103	CDL	C51-CB5-OB6-CB4
19	A	608	TGL	CB2-CB1-OG2-CG2
25	C	308	PEK	C2-C1-O01-C02
18	P	305	PGV	O01-C02-C03-O11
19	I	101	TGL	C18-C19-C33-C34
26	C	306	CDL	C20-C21-C22-C23
19	A	608	TGL	C12-C13-C14-C29
19	O	304	TGL	CC9-C15-C16-C17
25	C	308	PEK	C30-C31-C32-C33
26	G	102	CDL	OB7-CB5-OB6-CB4
25	C	308	PEK	O02-C1-O01-C02
18	N	606	PGV	C14-C15-C16-C17
19	V	101	TGL	CC3-CC4-CC5-CC6
19	Y	101	TGL	CC3-CC4-CC5-CC6
19	V	101	TGL	C17-C18-C19-C33
18	C	301	PGV	C7-C8-C9-C10
19	V	101	TGL	C11-C12-C13-C14
19	V	101	TGL	C16-C15-CC9-CC8
18	P	305	PGV	C11-C10-C9-C8
25	G	101	PEK	C15-C16-C17-C18
18	N	606	PGV	C4-C5-C6-C7
19	L	101	TGL	CC6-CC7-CC8-CC9

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	C59-C60-C61-C62
18	A	607	PGV	C27-C28-C29-C30
26	P	306	CDL	CB5-C51-C52-C53
26	T	103	CDL	C23-C24-C25-C26
18	C	301	PGV	C29-C30-C31-C32
19	A	608	TGL	C13-C14-C29-C30
26	G	102	CDL	C51-CB5-OB6-CB4
19	I	101	TGL	C11-C10-CB9-CB8
26	T	103	CDL	C82-C83-C84-C85
18	A	607	PGV	C6-C7-C8-C9
18	C	305	PGV	C20-C21-C22-C23
19	A	608	TGL	CB3-CB4-CB5-CB6
18	N	606	PGV	C02-C03-O11-P
18	A	607	PGV	C05-C04-O12-P
18	A	606	PGV	C01-C02-C03-O11
26	T	103	CDL	OA5-CA3-CA4-CA6
18	N	606	PGV	C2-C3-C4-C5
18	P	305	PGV	C4-C5-C6-C7
19	L	101	TGL	C16-C15-CC9-CC8
24	M	101	DMU	C25-C28-C31-C34
19	I	101	TGL	C22-C23-C24-C25
19	O	304	TGL	CA2-CA3-CA4-CA5
22	O	303	PSC	C23-C24-C25-C26
24	M	101	DMU	O16-C18-C19-C22
18	A	606	PGV	O12-C04-C05-C06
26	C	306	CDL	C79-C80-C81-C82
26	G	102	CDL	C61-C62-C63-C64
19	Y	101	TGL	C17-C18-C19-C33
26	C	306	CDL	C76-C77-C78-C79
19	L	101	TGL	C11-C12-C13-C14
25	T	102	PEK	C21-C22-C23-C24
18	C	305	PGV	O04-C19-O03-C01
18	N	606	PGV	O03-C01-C02-C03
26	P	306	CDL	C14-C15-C16-C17
26	C	306	CDL	CA3-CA4-CA6-OA8
26	T	103	CDL	CA3-CA4-CA6-OA8
26	T	103	CDL	CB3-CB4-CB6-OB8
18	C	301	PGV	C6-C7-C8-C9
18	C	301	PGV	C25-C26-C27-C28
22	B	302	PSC	O03-C01-C02-C03
19	A	608	TGL	CG1-CG2-CG3-OG3
26	C	306	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
18	A	607	PGV	C15-C16-C17-C18
25	P	303	PEK	O04-C21-O03-C01
18	P	301	PGV	C31-C32-C33-C34
19	V	101	TGL	C21-C22-C23-C24
23	B	303	CHD	C20-C22-C23-C24
19	I	101	TGL	C21-C20-CA9-CA8
18	N	606	PGV	C25-C26-C27-C28
19	A	608	TGL	CC6-CC7-CC8-CC9
19	V	101	TGL	C25-C26-C27-C28
26	C	306	CDL	C15-C16-C17-C18
26	C	306	CDL	C61-C62-C63-C64
26	T	103	CDL	C64-C65-C66-C67
19	I	101	TGL	C24-C25-C26-C27
18	A	606	PGV	C14-C15-C16-C17
18	C	305	PGV	O05-C05-C06-O06
25	C	308	PEK	C31-C32-C33-C34
18	A	606	PGV	C11-C10-C9-C8
18	C	305	PGV	C12-C13-C14-C15
18	P	301	PGV	C2-C3-C4-C5
26	P	306	CDL	C36-C37-C38-C39
22	O	303	PSC	C2-C1-O01-C02
25	P	303	PEK	C25-C26-C27-C28
26	G	102	CDL	C20-C21-C22-C23
18	P	305	PGV	C28-C29-C30-C31
19	A	608	TGL	CB1-CB2-CB3-CB4
19	L	101	TGL	CC2-CC1-OG3-CG3
26	P	306	CDL	C42-C43-C44-C45
19	I	101	TGL	CB2-CB3-CB4-CB5
26	P	306	CDL	C19-C20-C21-C22
18	N	606	PGV	C03-C02-O01-C1
22	O	303	PSC	C01-C02-O01-C1
25	P	303	PEK	C32-C33-C34-C35
26	P	306	CDL	C84-C85-C86-C87
19	O	304	TGL	CA4-CA5-CA6-CA7
25	C	304	PEK	C31-C32-C33-C34
18	A	607	PGV	C22-C23-C24-C25
18	C	305	PGV	C21-C22-C23-C24
18	A	607	PGV	C20-C19-O03-C01
18	A	607	PGV	O01-C02-C03-O11
24	M	101	DMU	C1-C6-O16-C18
19	O	304	TGL	OG2-CG2-CG3-OG3
18	N	606	PGV	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	C	307	CHD	C20-C22-C23-C24
26	P	306	CDL	C23-C24-C25-C26
25	C	304	PEK	C28-C29-C30-C31
26	P	306	CDL	C11-C12-C13-C14
25	G	101	PEK	C23-C24-C25-C26
25	T	102	PEK	C25-C26-C27-C28
19	I	101	TGL	CA2-CA1-OG1-CG1
19	V	101	TGL	CC2-CC1-OG3-CG3
25	C	304	PEK	C30-C31-C32-C33
18	A	607	PGV	C24-C25-C26-C27
25	T	102	PEK	C28-C29-C30-C31
25	T	102	PEK	C35-C36-C37-C38
26	G	102	CDL	C44-C45-C46-C47
26	C	306	CDL	CA2-C1-CB2-OB2
22	O	303	PSC	O02-C1-O01-C02
18	P	301	PGV	C2-C1-O01-C02
25	G	101	PEK	C28-C29-C30-C31
22	O	303	PSC	C15-C16-C17-C18
26	P	306	CDL	C51-C52-C53-C54
19	Y	101	TGL	CB3-CB4-CB5-CB6
18	C	301	PGV	C15-C16-C17-C18
26	T	103	CDL	C31-C32-C33-C34
22	O	303	PSC	C22-C23-C24-C25
25	C	304	PEK	C01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-CB6
18	P	305	PGV	C01-C02-C03-O11
26	G	102	CDL	C62-C63-C64-C65
26	P	306	CDL	C77-C78-C79-C80
26	C	306	CDL	C17-C18-C19-C20
26	T	103	CDL	O1-C1-CB2-OB2
18	A	607	PGV	O04-C19-O03-C01
25	P	303	PEK	C33-C34-C35-C36
19	L	101	TGL	CC5-CC6-CC7-CC8
19	L	101	TGL	C29-C30-C31-C32
25	C	304	PEK	C35-C36-C37-C38
24	Q	201	DMU	C25-C28-C31-C34
19	V	101	TGL	CA2-CA3-CA4-CA5
25	G	101	PEK	C21-C22-C23-C24
18	A	606	PGV	C05-C04-O12-P
22	B	302	PSC	C02-C03-O11-P
24	M	101	DMU	C3-C4-C57-O61
26	C	306	CDL	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
18	P	305	PGV	C20-C21-C22-C23
26	T	103	CDL	C77-C78-C79-C80
22	O	303	PSC	C21-C22-C23-C24
26	G	102	CDL	C80-C81-C82-C83
26	P	306	CDL	CA3-CA4-CA6-OA8
26	P	306	CDL	CB3-CB4-CB6-OB8
26	C	306	CDL	CB3-CB4-CB6-OB8
18	A	606	PGV	O03-C01-C02-C03
19	O	304	TGL	CG1-CG2-CG3-OG3
25	G	101	PEK	O03-C01-C02-C03
26	G	102	CDL	CA3-CA4-CA6-OA8
19	V	101	TGL	OG1-CG1-CG2-CG3
19	I	101	TGL	CA3-CA4-CA5-CA6
18	N	606	PGV	C21-C22-C23-C24
26	C	306	CDL	C74-C75-C76-C77
22	B	302	PSC	C31-C32-C33-C34
19	A	608	TGL	C33-C34-C35-C36
19	V	101	TGL	CB3-CB4-CB5-CB6
26	P	306	CDL	C61-C62-C63-C64
26	C	306	CDL	C21-C22-C23-C24
18	P	305	PGV	C31-C32-C33-C34
18	C	305	PGV	C24-C25-C26-C27
26	G	102	CDL	C75-C76-C77-C78
25	C	304	PEK	C11-C12-C13-C14
25	C	304	PEK	C12-C13-C14-C15
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
18	P	305	PGV	C03-O11-P-O12
25	C	308	PEK	C6-C7-C8-C9
19	I	101	TGL	OA1-CA1-OG1-CG1
19	L	101	TGL	OC1-CC1-OG3-CG3
19	V	101	TGL	OC1-CC1-OG3-CG3
18	A	606	PGV	C21-C22-C23-C24
18	A	607	PGV	C29-C30-C31-C32
26	G	102	CDL	C77-C78-C79-C80
18	N	606	PGV	O01-C02-C03-O11
19	L	101	TGL	CB5-CB6-CB7-CB8
18	C	305	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C12-C11-CA5-OA6
26	T	103	CDL	C44-C45-C46-C47
18	N	606	PGV	O03-C01-C02-O01
22	B	302	PSC	O03-C01-C02-O01
25	G	101	PEK	O03-C01-C02-O01
26	G	102	CDL	OA6-CA4-CA6-OA8
19	A	608	TGL	OG2-CG2-CG3-OG3
19	A	608	TGL	C23-C24-C25-C26
24	Q	201	DMU	C19-C22-C25-C28
18	C	301	PGV	C2-C3-C4-C5
26	G	102	CDL	C16-C17-C18-C19
22	O	303	PSC	C31-C32-C33-C34
26	T	103	CDL	CB2-C1-CA2-OA2
18	P	301	PGV	O02-C1-O01-C02
26	T	103	CDL	C56-C57-C58-C59
26	T	103	CDL	C63-C64-C65-C66
26	T	103	CDL	C71-C72-C73-C74
19	V	101	TGL	CA9-C20-C21-C22
26	C	306	CDL	C1-CA2-OA2-PA1
18	P	305	PGV	C02-C03-O11-P
25	P	303	PEK	C29-C30-C31-C32
26	P	306	CDL	C64-C65-C66-C67
18	A	607	PGV	C2-C3-C4-C5
22	B	302	PSC	C27-C28-C29-C30
26	G	102	CDL	OB5-CB3-CB4-CB6
19	Y	101	TGL	CC9-C15-C16-C17
19	Y	101	TGL	C23-C24-C25-C26
25	G	103	PEK	C34-C35-C36-C37
24	M	101	DMU	C19-C22-C25-C28
25	T	102	PEK	C15-C16-C17-C18
25	C	308	PEK	C16-C17-C18-C19
22	O	303	PSC	C14-C15-C16-C17
19	V	101	TGL	C20-C21-C22-C23
26	C	306	CDL	C31-CA7-OA8-CA6
19	L	101	TGL	C24-C25-C26-C27
25	C	304	PEK	C23-C24-C25-C26
26	P	306	CDL	C83-C84-C85-C86
24	M	101	DMU	C34-C37-C40-C43
18	A	606	PGV	C03-C02-O01-C1
22	B	302	PSC	C01-C02-O01-C1
18	A	606	PGV	C4-C5-C6-C7
22	B	302	PSC	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	Y	101	TGL	C22-C23-C24-C25
18	P	301	PGV	O03-C01-C02-C03
18	N	606	PGV	C05-C04-O12-P
19	A	608	TGL	OG1-CG1-CG2-CG3
22	O	303	PSC	O03-C01-C02-C03
25	C	304	PEK	O01-C02-C03-O11
18	N	606	PGV	C30-C31-C32-C33
19	Y	101	TGL	CC4-CC5-CC6-CC7
26	T	103	CDL	CA2-C1-CB2-OB2
26	T	103	CDL	C51-C52-C53-C54
18	P	301	PGV	O03-C01-C02-O01
26	P	306	CDL	OA6-CA4-CA6-OA8
26	P	306	CDL	OB6-CB4-CB6-OB8
26	C	306	CDL	OB6-CB4-CB6-OB8
26	T	103	CDL	OA6-CA4-CA6-OA8
25	C	304	PEK	C24-C25-C26-C27
19	I	101	TGL	C21-C22-C23-C24
18	C	305	PGV	C23-C24-C25-C26
22	O	303	PSC	C04-C05-N-C08
19	A	608	TGL	CB2-CB3-CB4-CB5
19	L	101	TGL	CA6-CA7-CA8-CA9
25	G	101	PEK	C2-C3-C4-C5
25	C	304	PEK	O04-C21-O03-C01
18	C	305	PGV	O02-C1-O01-C02
26	T	103	CDL	C74-C75-C76-C77
18	P	305	PGV	C24-C25-C26-C27
18	C	301	PGV	C31-C32-C33-C34
26	P	306	CDL	C75-C76-C77-C78
18	C	305	PGV	C04-O12-P-O11
18	P	305	PGV	C04-O12-P-O11
26	G	102	CDL	CB2-OB2-PB2-OB5
26	P	306	CDL	C40-C41-C42-C43
18	P	305	PGV	C19-C20-C21-C22
26	P	306	CDL	CA4-CA3-OA5-PA1
18	P	304	PGV	C02-C03-O11-P
26	G	102	CDL	C11-C12-C13-C14
26	C	306	CDL	OA9-CA7-OA8-CA6
26	P	306	CDL	CA2-OA2-PA1-OA4
25	T	102	PEK	C03-O11-P-O14
25	T	102	PEK	C04-O12-P-O13
26	C	306	CDL	CA2-OA2-PA1-OA4
26	C	306	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	C	306	CDL	CB3-OB5-PB2-OB4
18	A	606	PGV	C03-O11-P-O14
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	C	304	PEK	C22-C21-O03-C01
18	N	606	PGV	C01-C02-C03-O11
18	A	607	PGV	C01-C02-C03-O11
18	C	305	PGV	C31-C32-C33-C34
18	C	305	PGV	C2-C1-O01-C02
18	P	305	PGV	C5-C6-C7-C8
22	B	302	PSC	C05-C04-O12-P
19	V	101	TGL	C15-C16-C17-C18
24	Q	201	DMU	C34-C37-C40-C43
18	A	606	PGV	O01-C02-C03-O11
26	T	103	CDL	OA5-CA3-CA4-OA6
26	T	103	CDL	OB5-CB3-CB4-OB6
26	G	102	CDL	OB5-CB3-CB4-OB6
26	C	306	CDL	C81-C82-C83-C84
26	T	103	CDL	C52-C53-C54-C55
25	T	102	PEK	C29-C30-C31-C32
25	C	308	PEK	C29-C30-C31-C32
19	I	101	TGL	C16-C17-C18-C19
26	C	306	CDL	C78-C79-C80-C81
18	C	305	PGV	O03-C01-C02-C03
25	P	303	PEK	O03-C01-C02-O01
26	C	306	CDL	OA6-CA4-CA6-OA8
18	A	606	PGV	O03-C01-C02-O01
22	O	303	PSC	O03-C01-C02-O01
18	P	301	PGV	O03-C19-C20-C21
18	C	305	PGV	C02-C03-O11-P
26	C	306	CDL	C84-C85-C86-C87
19	V	101	TGL	CA4-CA5-CA6-CA7
26	P	306	CDL	C52-C53-C54-C55
19	V	101	TGL	CB7-CB8-CB9-C10
19	O	304	TGL	C18-C19-C33-C34
18	A	606	PGV	O05-C05-C06-O06
19	L	101	TGL	CB2-CB3-CB4-CB5
26	T	103	CDL	C60-C61-C62-C63
25	G	103	PEK	C35-C36-C37-C38
19	I	101	TGL	CC7-CC8-CC9-C15
25	T	102	PEK	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
18	P	305	PGV	C15-C16-C17-C18
26	G	102	CDL	C41-C42-C43-C44
19	Y	101	TGL	C29-C30-C31-C32
19	L	101	TGL	CB6-CB7-CB8-CB9
19	A	608	TGL	CG1-CG2-OG2-CB1
19	V	101	TGL	CG3-CG2-OG2-CB1
19	O	304	TGL	OB1-CB1-OG2-CG2
17	A	604	HEA	C11-C12-C13-C14
26	G	102	CDL	CB4-CB3-OB5-PB2
19	I	101	TGL	C15-C16-C17-C18
26	T	103	CDL	C17-C18-C19-C20
26	C	306	CDL	C63-C64-C65-C66
18	C	301	PGV	C9-C10-C11-C12
19	O	304	TGL	C19-C33-C34-C35
26	C	306	CDL	CA3-OA5-PA1-OA2
18	A	607	PGV	C04-O12-P-O11
25	G	103	PEK	C03-O11-P-O12
25	G	103	PEK	C04-O12-P-O11
25	C	308	PEK	C04-O12-P-O11
24	M	101	DMU	O5-C4-C57-O61
18	N	606	PGV	C3-C4-C5-C6
18	N	606	PGV	C13-C14-C15-C16
19	I	101	TGL	CB1-CB2-CB3-CB4
19	I	101	TGL	C29-C30-C31-C32
26	C	306	CDL	C13-C14-C15-C16
19	V	101	TGL	CA3-CA4-CA5-CA6
18	C	301	PGV	C30-C31-C32-C33
19	A	608	TGL	C18-C19-C33-C34
18	P	304	PGV	C19-C20-C21-C22
25	T	102	PEK	C33-C34-C35-C36
19	O	304	TGL	CA9-C20-C21-C22
26	T	103	CDL	C1-CA2-OA2-PA1
18	A	607	PGV	C02-C03-O11-P
18	C	305	PGV	C05-C04-O12-P
19	Y	101	TGL	CC1-CC2-CC3-CC4
19	I	101	TGL	C11-C12-C13-C14
26	C	306	CDL	C23-C24-C25-C26
26	C	306	CDL	C56-C57-C58-C59
23	B	303	CHD	C13-C17-C20-C22
26	G	102	CDL	C39-C40-C41-C42
26	P	306	CDL	C63-C64-C65-C66
25	P	303	PEK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C39-C40-C41-C42
26	G	102	CDL	C24-C25-C26-C27
26	C	306	CDL	C80-C81-C82-C83
19	O	304	TGL	CC1-CC2-CC3-CC4
26	P	306	CDL	C44-C45-C46-C47
26	T	103	CDL	C36-C37-C38-C39
26	C	306	CDL	C14-C15-C16-C17
19	V	101	TGL	CC5-CC6-CC7-CC8
26	C	306	CDL	C43-C44-C45-C46
23	B	303	CHD	C16-C17-C20-C22
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	P	304	PGV	C15-C16-C17-C18
19	Y	101	TGL	CB5-CB6-CB7-CB8
18	C	305	PGV	C6-C7-C8-C9
26	C	306	CDL	O1-C1-CB2-OB2
19	V	101	TGL	CA6-CA7-CA8-CA9
26	P	306	CDL	CA3-CA4-OA6-CA5
19	O	304	TGL	CG1-CG2-OG2-CB1
18	P	305	PGV	O04-C19-O03-C01
19	I	101	TGL	CC6-CC7-CC8-CC9
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
18	P	301	PGV	C22-C23-C24-C25
24	T	101	DMU	C31-C34-C37-C40
25	G	103	PEK	C32-C33-C34-C35
22	B	302	PSC	O01-C02-C03-O11
26	T	103	CDL	C16-C17-C18-C19
26	P	306	CDL	OA5-CA3-CA4-CA6
25	C	304	PEK	C16-C17-C18-C19
25	C	304	PEK	C29-C30-C31-C32
18	P	305	PGV	C20-C19-O03-C01
25	G	103	PEK	C31-C32-C33-C34
18	C	301	PGV	C26-C27-C28-C29
25	C	304	PEK	C3-C4-C5-C6
25	C	304	PEK	C32-C33-C34-C35
26	T	103	CDL	C72-C73-C74-C75
19	I	101	TGL	CA4-CA5-CA6-CA7
26	P	306	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
25	G	101	PEK	C27-C28-C29-C30
25	G	103	PEK	C28-C29-C30-C31
25	C	308	PEK	C3-C4-C5-C6
26	P	306	CDL	C52-C51-CB5-OB6
19	V	101	TGL	CG2-CG3-OG3-CC1
26	P	306	CDL	C53-C54-C55-C56
19	A	608	TGL	C16-C17-C18-C19
24	C	302	DMU	C18-C19-C22-C25
19	O	304	TGL	C24-C25-C26-C27
23	B	303	CHD	C13-C17-C20-C21
25	C	308	PEK	C32-C33-C34-C35
19	Y	101	TGL	C21-C20-CA9-CA8
18	P	305	PGV	C3-C4-C5-C6
25	C	308	PEK	C22-C23-C24-C25
18	A	606	PGV	C11-C12-C13-C14
22	B	302	PSC	C7-C8-C9-C10
24	T	101	DMU	C22-C25-C28-C31
17	N	605	HEA	C26-C15-C16-C17
25	P	303	PEK	C22-C23-C24-C25
26	P	306	CDL	C1-CA2-OA2-PA1
26	T	103	CDL	C52-C51-CB5-OB6
19	O	304	TGL	OG3-CC1-CC2-CC3
19	A	608	TGL	OG1-CA1-CA2-CA3
24	C	302	DMU	C5-C10-O7-C3
19	V	101	TGL	C21-C20-CA9-CA8
25	G	103	PEK	O01-C1-C2-C3
25	P	303	PEK	C23-C24-C25-C26
25	G	101	PEK	O01-C1-C2-C3
18	P	301	PGV	C9-C10-C11-C12
25	T	102	PEK	C3-C4-C5-C6
18	C	301	PGV	C11-C12-C13-C14
26	P	306	CDL	C37-C38-C39-C40
26	P	306	CDL	CA6-CA4-OA6-CA5
26	C	306	CDL	C12-C13-C14-C15
19	V	101	TGL	CB6-CB7-CB8-CB9
19	I	101	TGL	OG1-CA1-CA2-CA3
26	G	102	CDL	C32-C31-CA7-OA8
18	P	305	PGV	O01-C1-C2-C3
18	C	301	PGV	C22-C23-C24-C25
18	P	304	PGV	C11-C12-C13-C14
22	O	303	PSC	C7-C8-C9-C10
18	P	301	PGV	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
18	P	301	PGV	C02-C03-O11-P
19	A	608	TGL	C25-C26-C27-C28
22	B	302	PSC	C4-C5-C6-C7
25	T	102	PEK	O01-C1-C2-C3
18	N	606	PGV	C11-C12-C13-C14
25	G	103	PEK	C14-C15-C16-C17
19	O	304	TGL	OG1-CA1-CA2-CA3
19	O	304	TGL	CB2-CB1-OG2-CG2
17	N	605	HEA	C12-C13-C14-C15
19	I	101	TGL	C20-C21-C22-C23
19	O	304	TGL	CB3-CB4-CB5-CB6
26	G	102	CDL	C82-C83-C84-C85
18	A	606	PGV	O01-C1-C2-C3
26	G	102	CDL	C43-C44-C45-C46
18	P	301	PGV	C11-C12-C13-C14
22	B	302	PSC	C12-C13-C14-C15
19	O	304	TGL	CA6-CA7-CA8-CA9
25	G	103	PEK	O03-C21-C22-C23
19	V	101	TGL	OG3-CC1-CC2-CC3
19	L	101	TGL	CA5-CA6-CA7-CA8
17	N	605	HEA	C14-C15-C16-C17
25	G	103	PEK	C3-C4-C5-C6
18	P	304	PGV	C9-C10-C11-C12
26	G	102	CDL	C32-C31-CA7-OA9
19	L	101	TGL	C25-C26-C27-C28
18	P	305	PGV	O02-C1-C2-C3
19	I	101	TGL	OA1-CA1-CA2-CA3
26	P	306	CDL	C54-C55-C56-C57
18	N	606	PGV	O01-C1-C2-C3
19	L	101	TGL	C21-C20-CA9-CA8
18	P	301	PGV	C19-C20-C21-C22
26	C	306	CDL	C83-C84-C85-C86
19	L	101	TGL	OG3-CC1-CC2-CC3
17	N	605	HEA	O11-C11-C12-C13
26	T	103	CDL	C52-C51-CB5-OB7
25	C	304	PEK	C03-O11-P-O12
26	C	306	CDL	C39-C40-C41-C42
26	T	103	CDL	C15-C16-C17-C18
19	I	101	TGL	CB7-CB8-CB9-C10
19	V	101	TGL	OB1-CB1-OG2-CG2
19	Y	101	TGL	CA3-CA4-CA5-CA6
25	G	103	PEK	O02-C1-C2-C3

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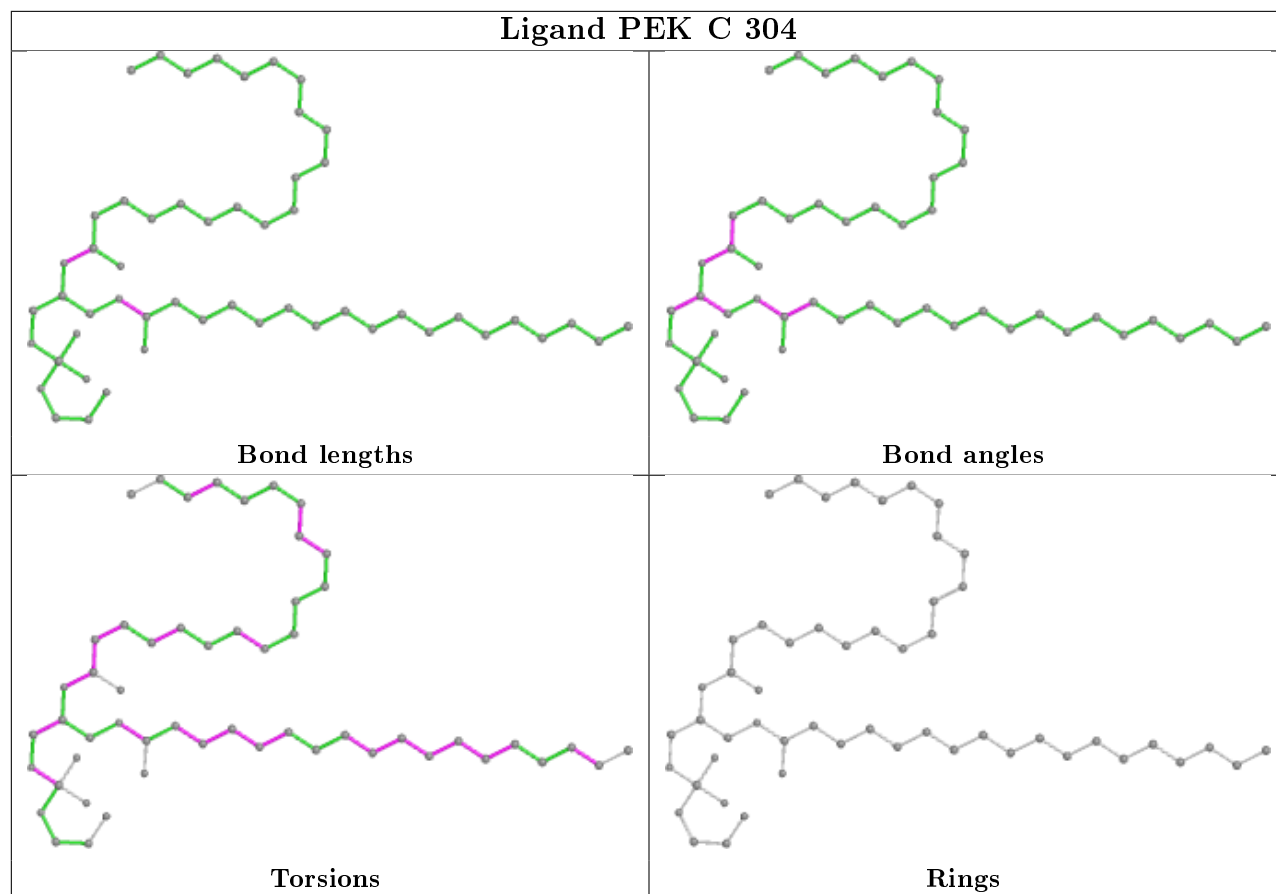
Mol	Chain	Res	Type	Atoms
19	O	304	TGL	OC1-CC1-CC2-CC3
24	Q	201	DMU	C18-C19-C22-C25
25	C	304	PEK	C03-O11-P-O14
26	T	103	CDL	CA2-OA2-PA1-OA3
18	C	305	PGV	C04-O12-P-O14
18	P	305	PGV	C04-O12-P-O14
26	G	102	CDL	CA3-OA5-PA1-OA3
26	G	102	CDL	CA3-OA5-PA1-OA4
19	O	304	TGL	OA1-CA1-CA2-CA3
25	G	101	PEK	O02-C1-C2-C3
26	T	103	CDL	C75-C76-C77-C78
22	B	302	PSC	C2-C3-C4-C5
25	P	303	PEK	O12-C04-C05-N
25	T	102	PEK	O02-C1-C2-C3
25	C	304	PEK	C22-C23-C24-C25
26	T	103	CDL	C38-C39-C40-C41
19	L	101	TGL	CC4-CC5-CC6-CC7
19	V	101	TGL	OC1-CC1-CC2-CC3
26	T	103	CDL	C57-C58-C59-C60
18	C	301	PGV	C27-C28-C29-C30
26	P	306	CDL	C32-C33-C34-C35
26	P	306	CDL	C80-C81-C82-C83
25	P	303	PEK	C05-C04-O12-P
25	G	103	PEK	C05-C04-O12-P
25	G	101	PEK	C05-C04-O12-P
19	I	101	TGL	OG2-CB1-CB2-CB3
19	Y	101	TGL	OG1-CA1-CA2-CA3
26	G	102	CDL	C81-C82-C83-C84
18	P	305	PGV	C2-C3-C4-C5
25	G	103	PEK	O04-C21-C22-C23
19	L	101	TGL	OC1-CC1-CC2-CC3
22	O	303	PSC	O03-C19-C20-C21
24	Q	201	DMU	C19-C18-O16-C6
25	C	308	PEK	O03-C21-C22-C23
26	P	306	CDL	C60-C61-C62-C63
19	Y	101	TGL	OA1-CA1-CA2-CA3
18	A	606	PGV	O02-C1-C2-C3
19	I	101	TGL	CC5-CC6-CC7-CC8
25	C	304	PEK	O01-C1-C2-C3
26	G	102	CDL	C52-C51-CB5-OB6

There are no ring outliers.

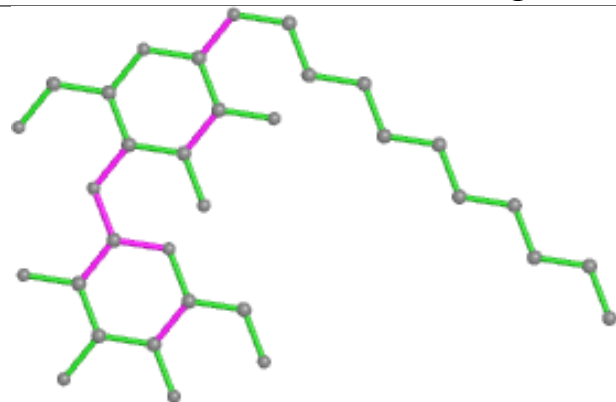
26 monomers are involved in 47 short contacts:

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

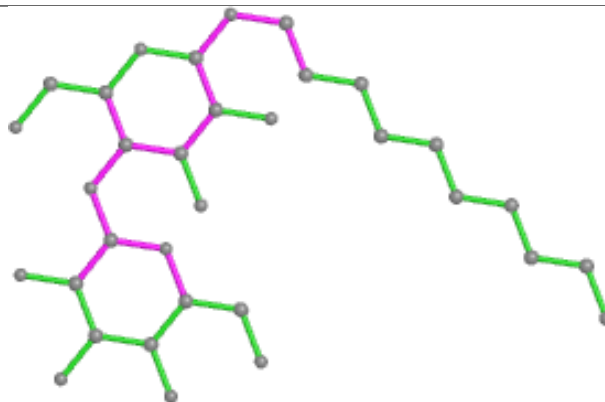
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



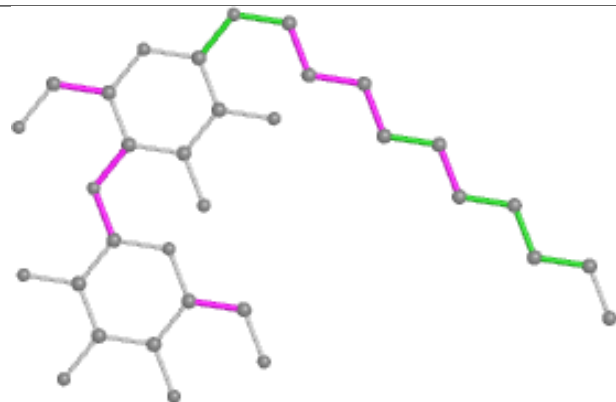
Ligand DMU C 302



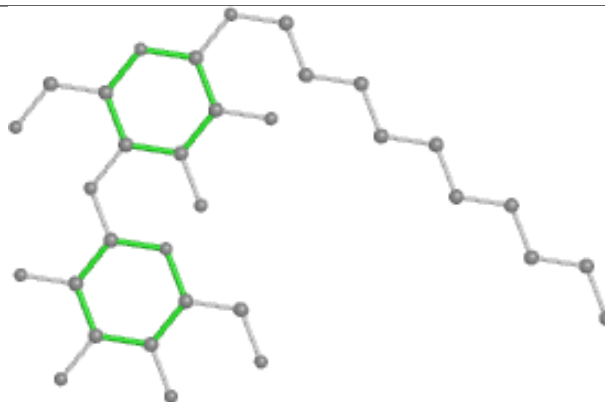
Bond lengths



Bond angles

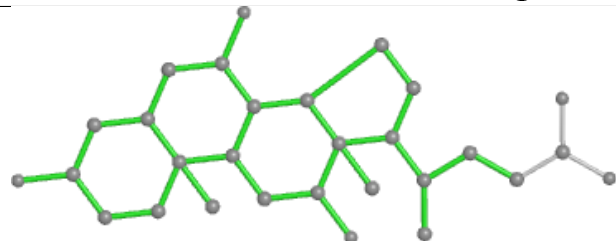


Torsions

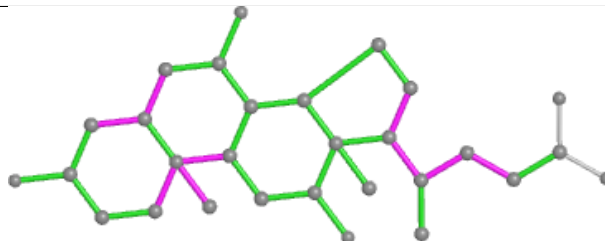


Rings

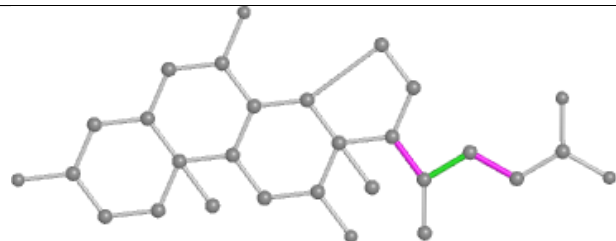
Ligand CHD B 303



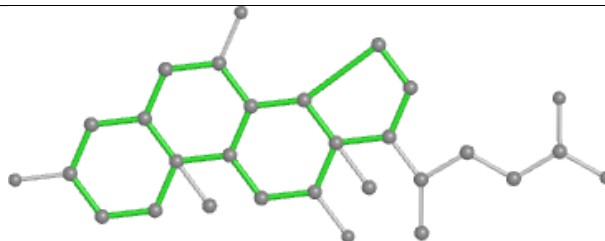
Bond lengths



Bond angles

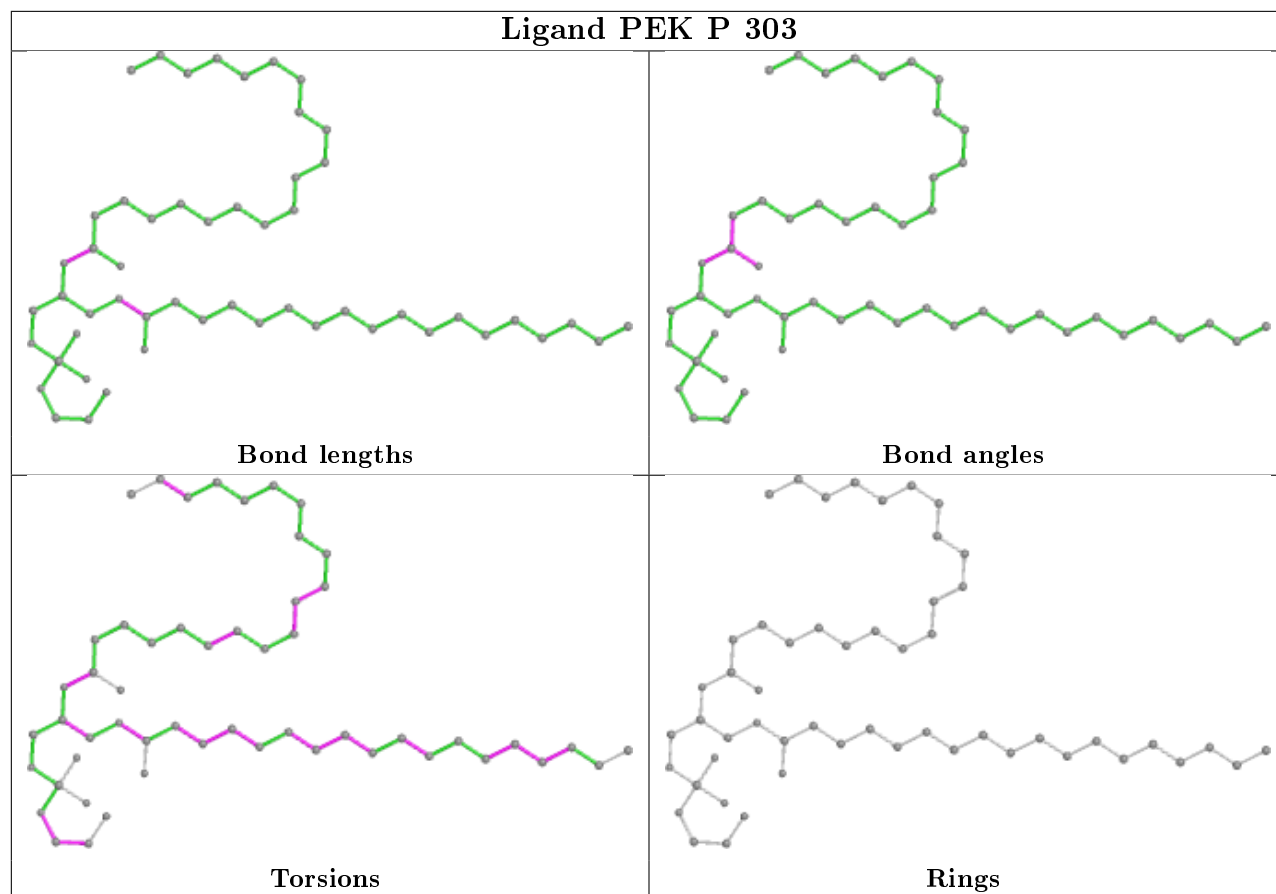


Torsions

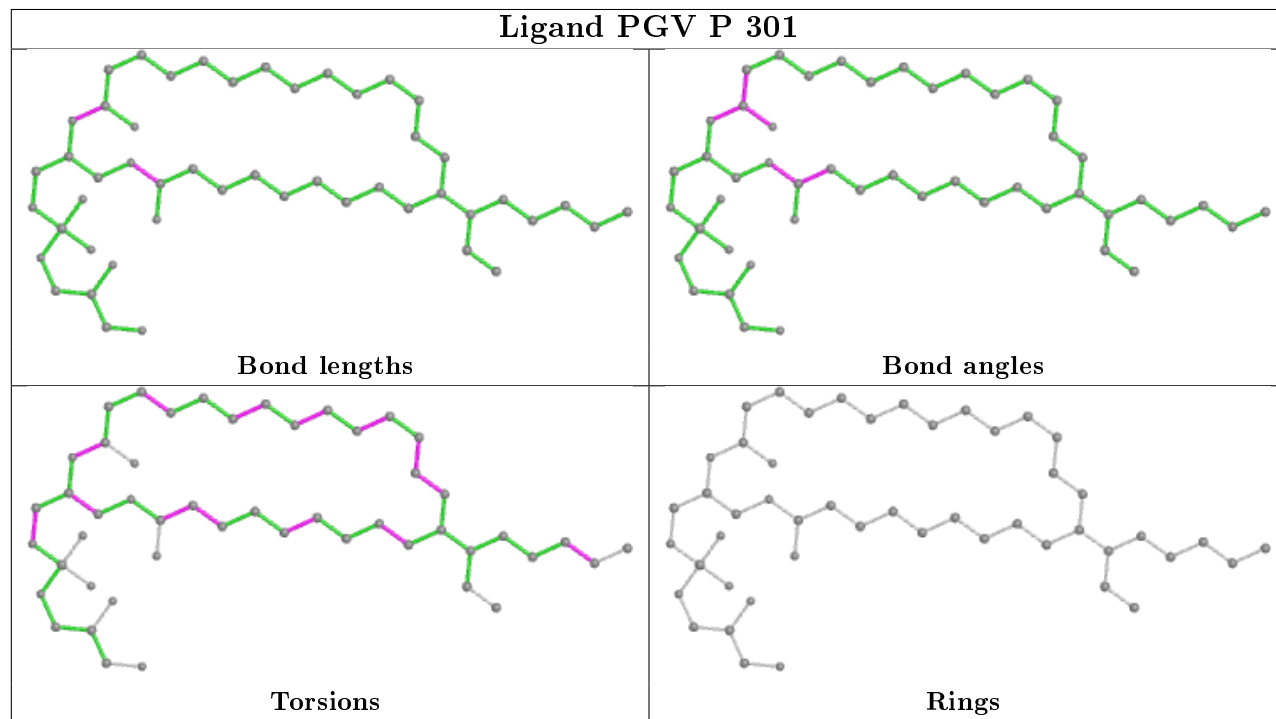


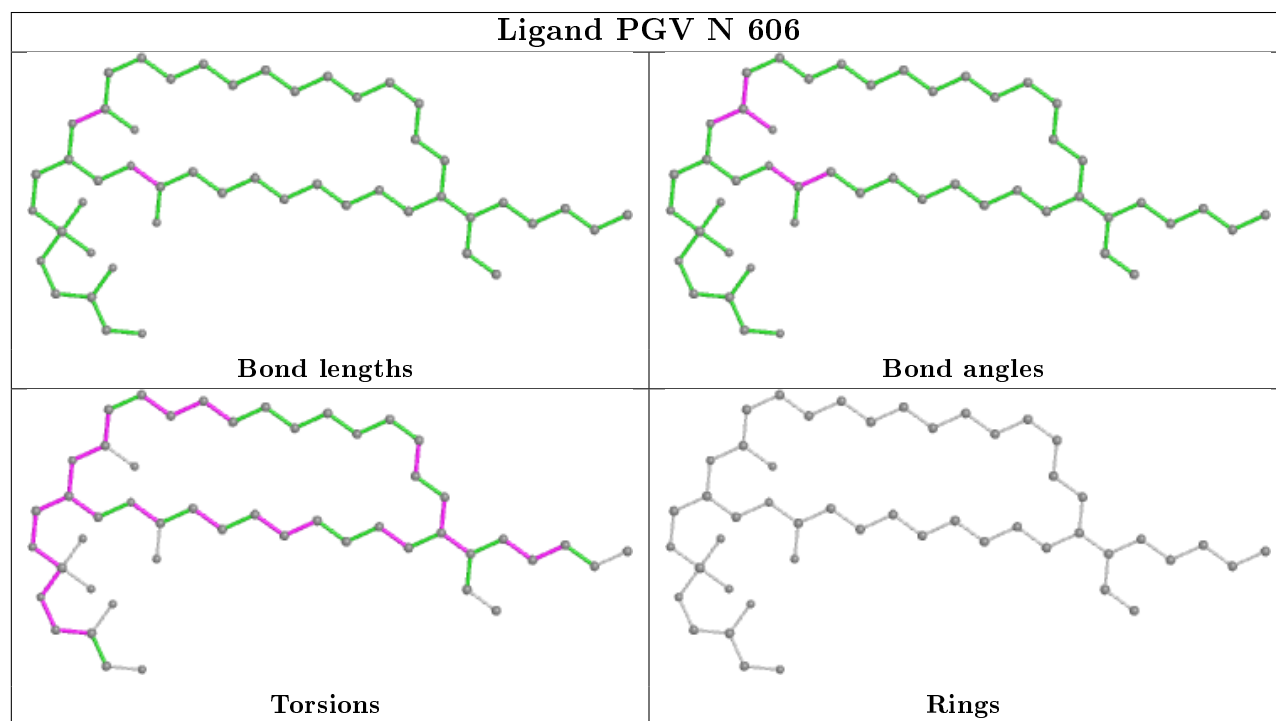
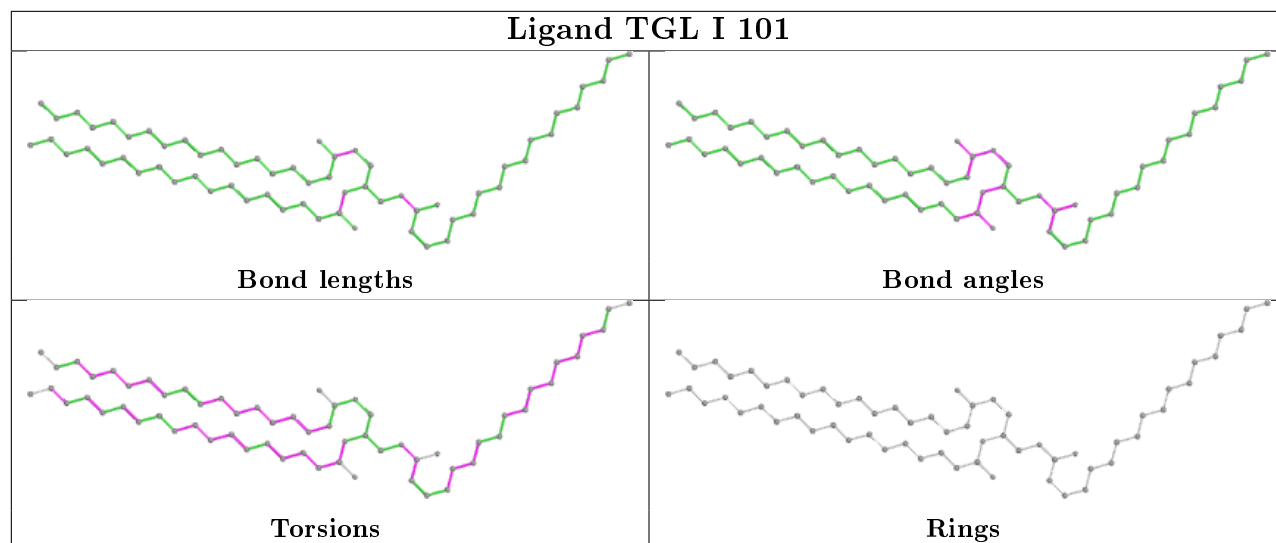
Rings

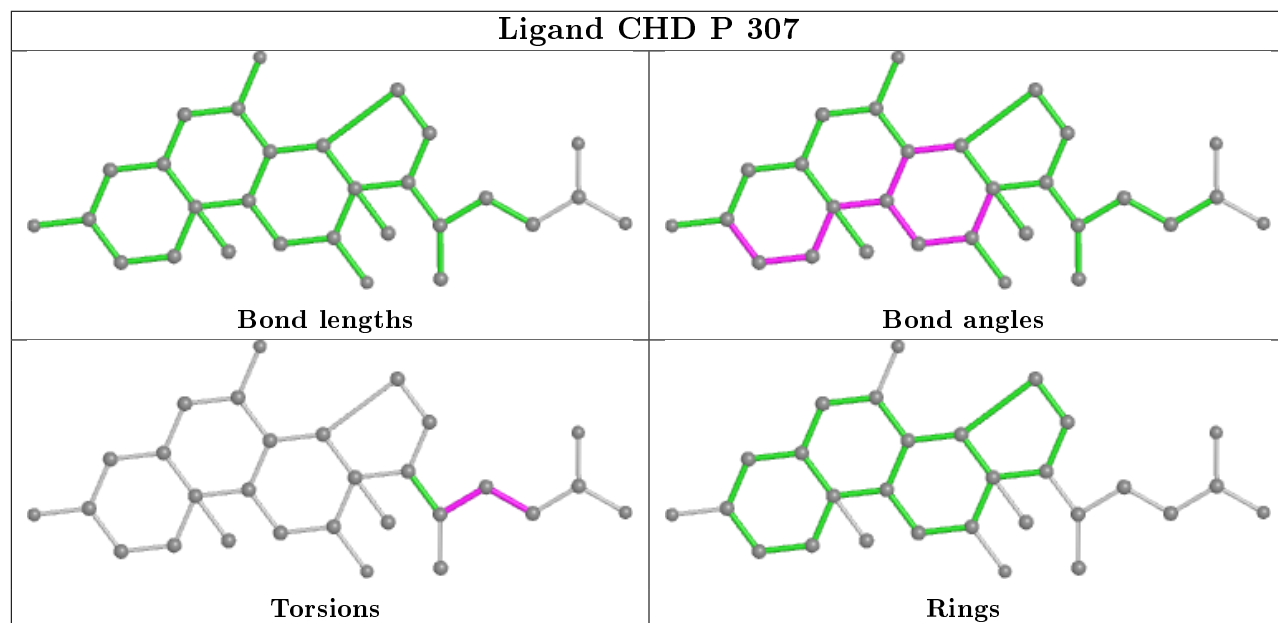
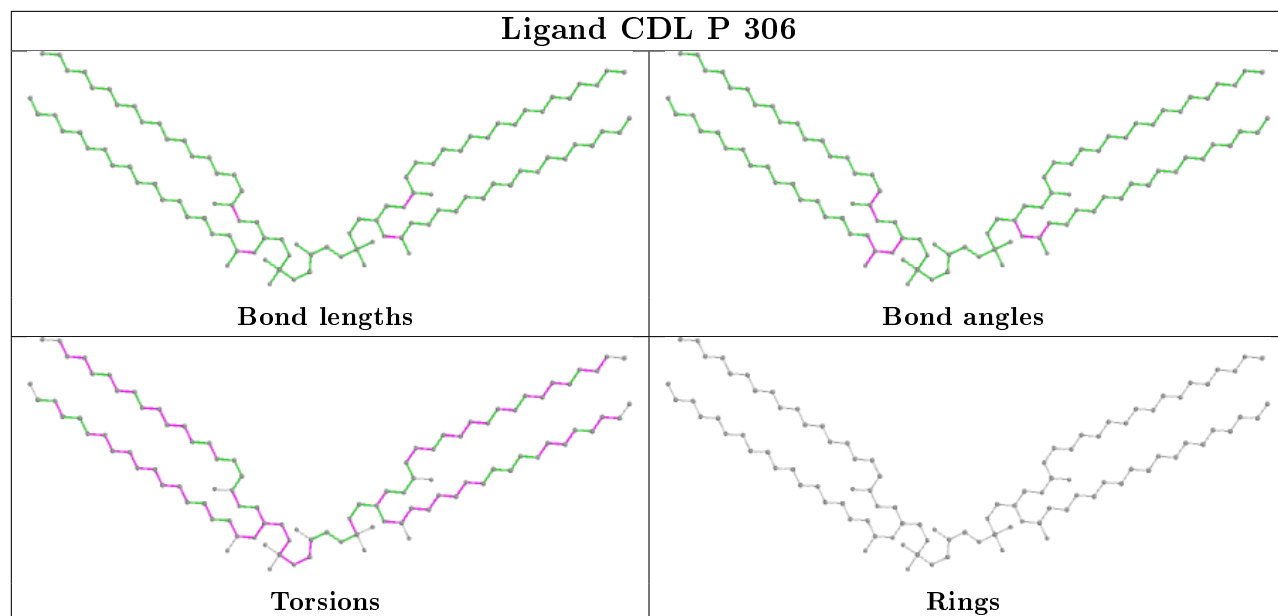
Ligand PEK P 303

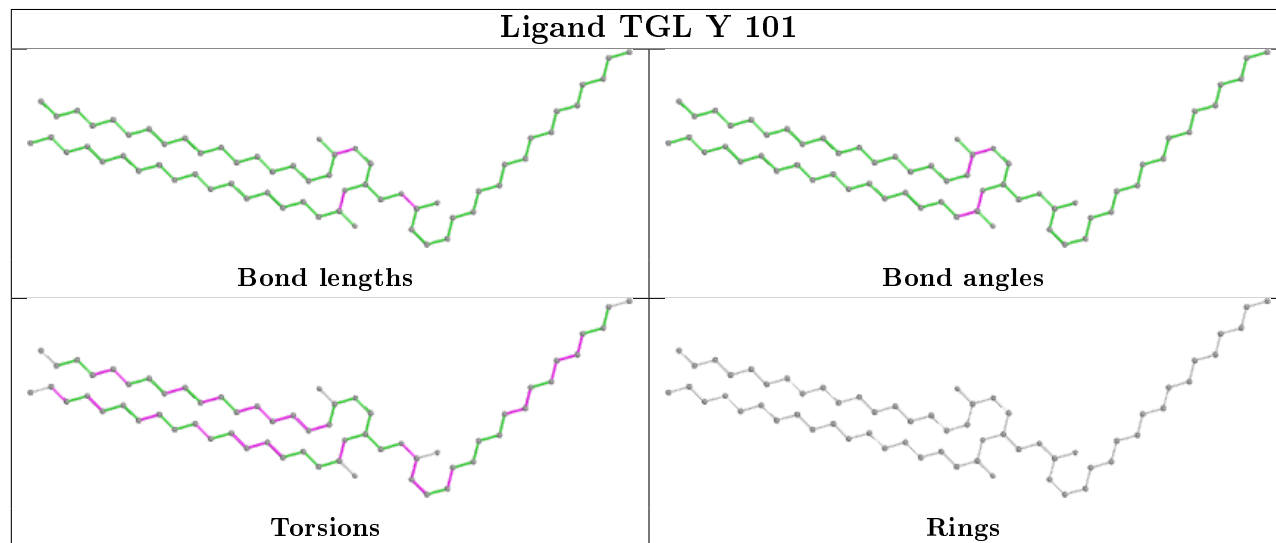
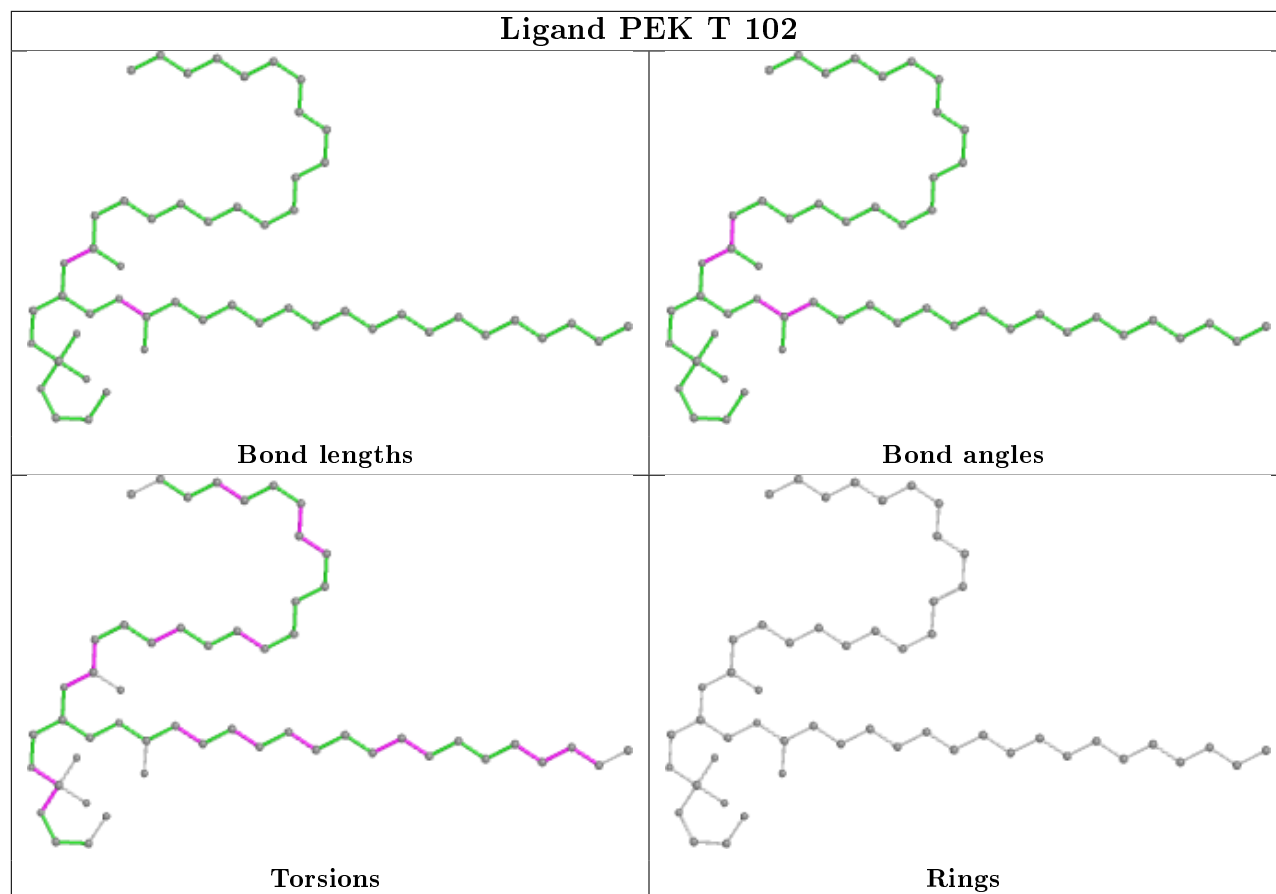


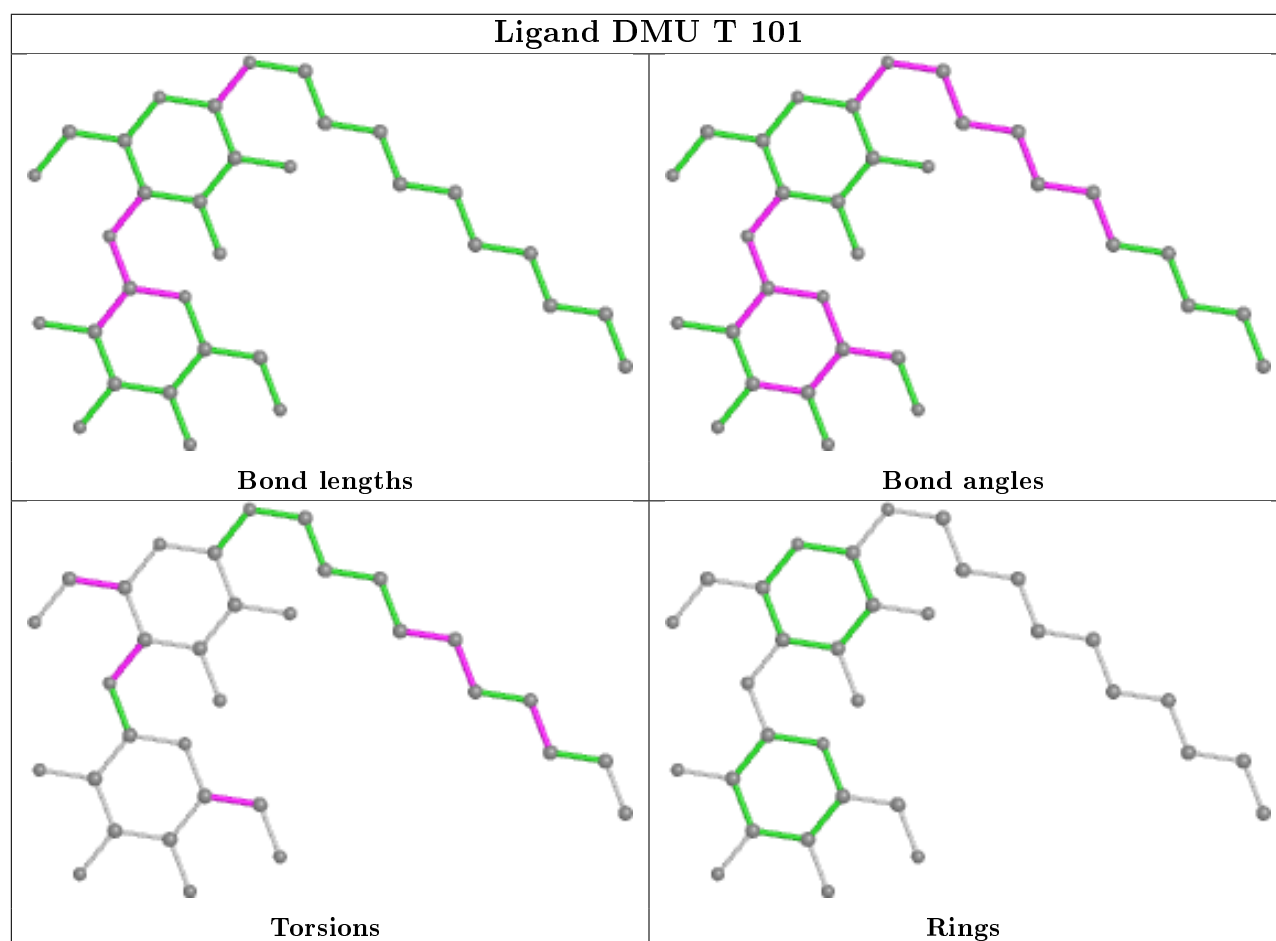
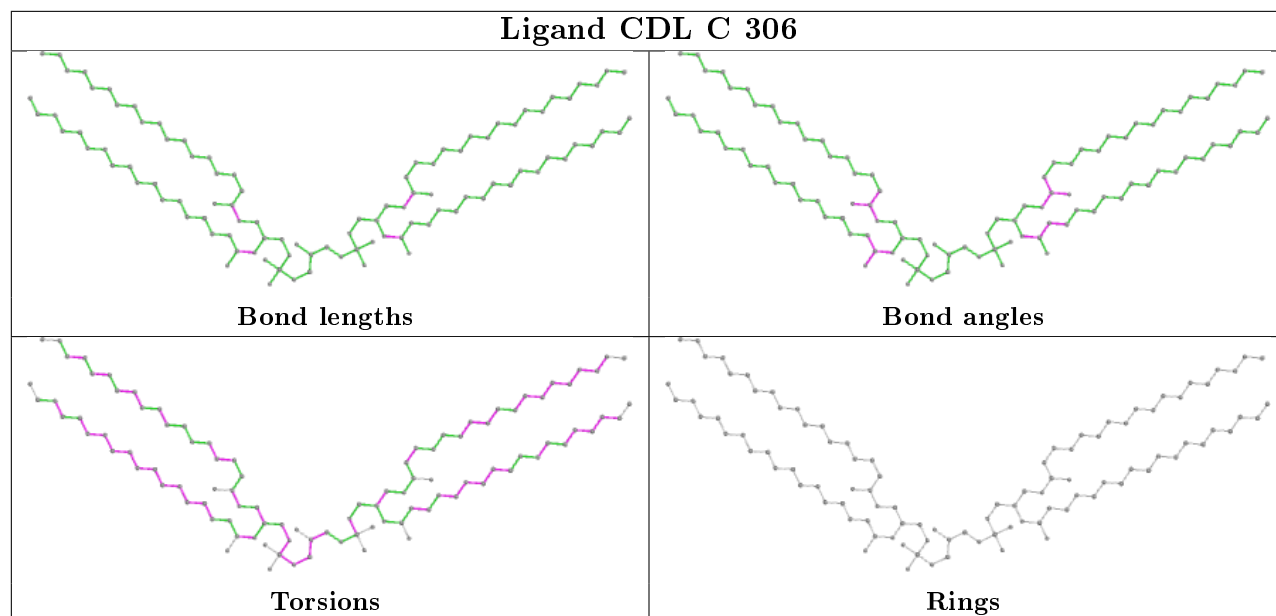
Ligand PGV P 301

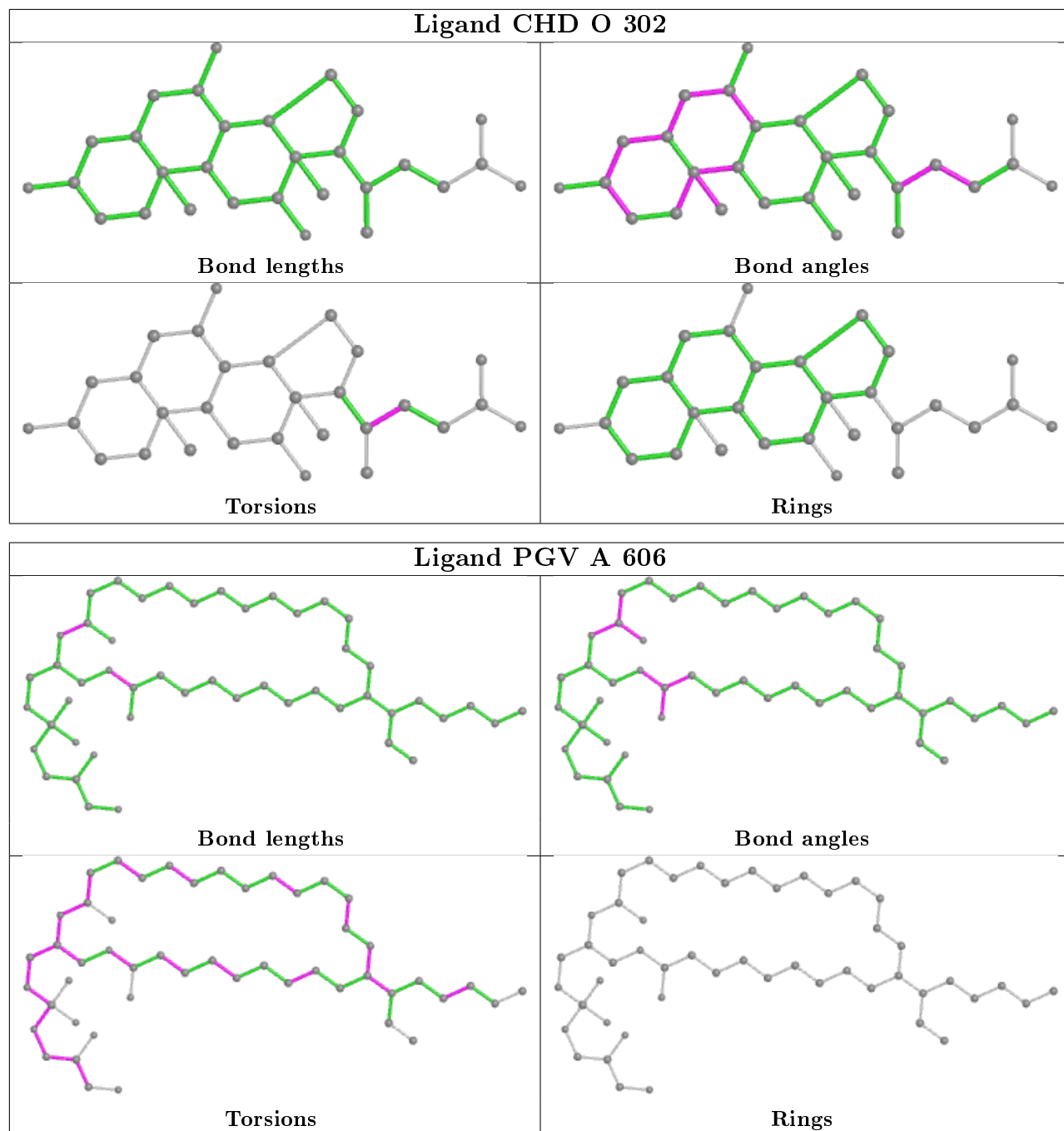


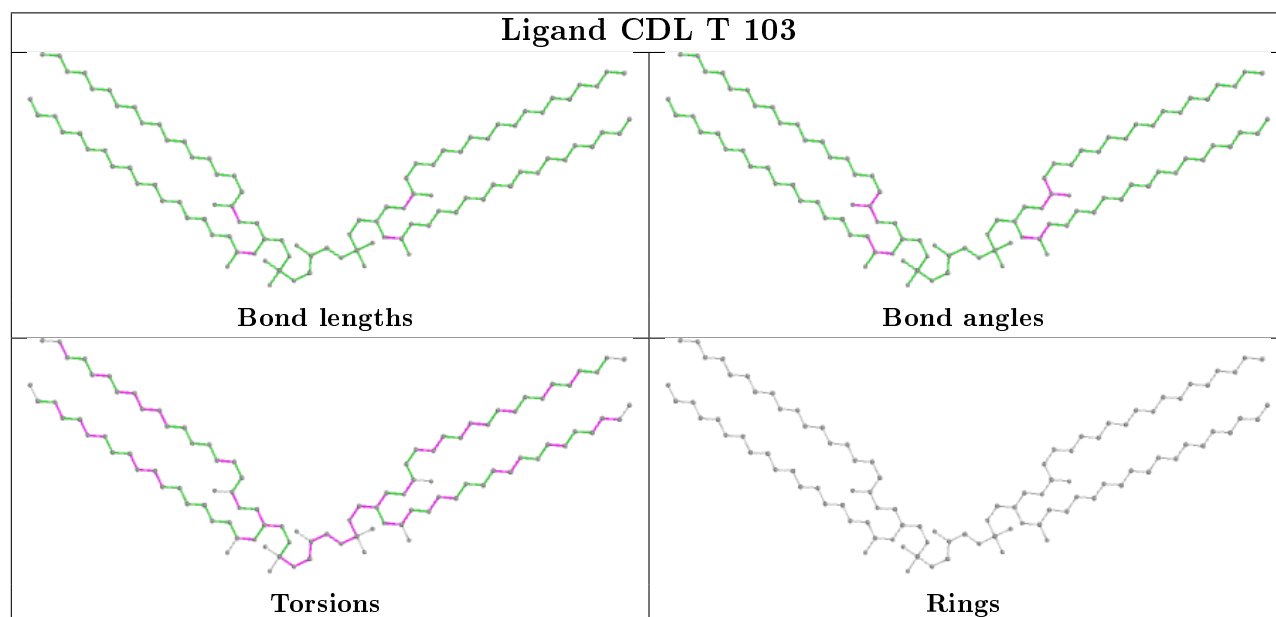
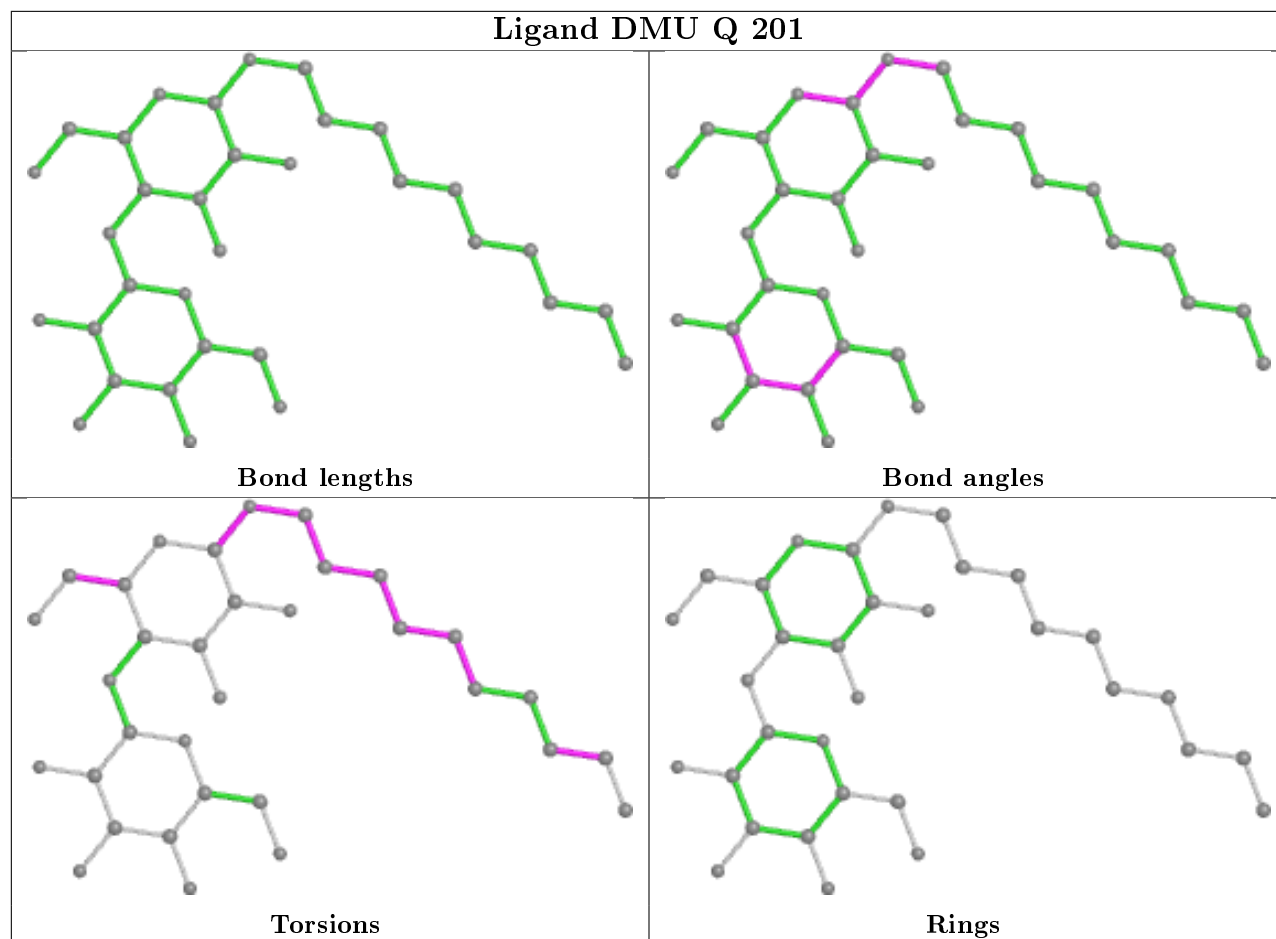


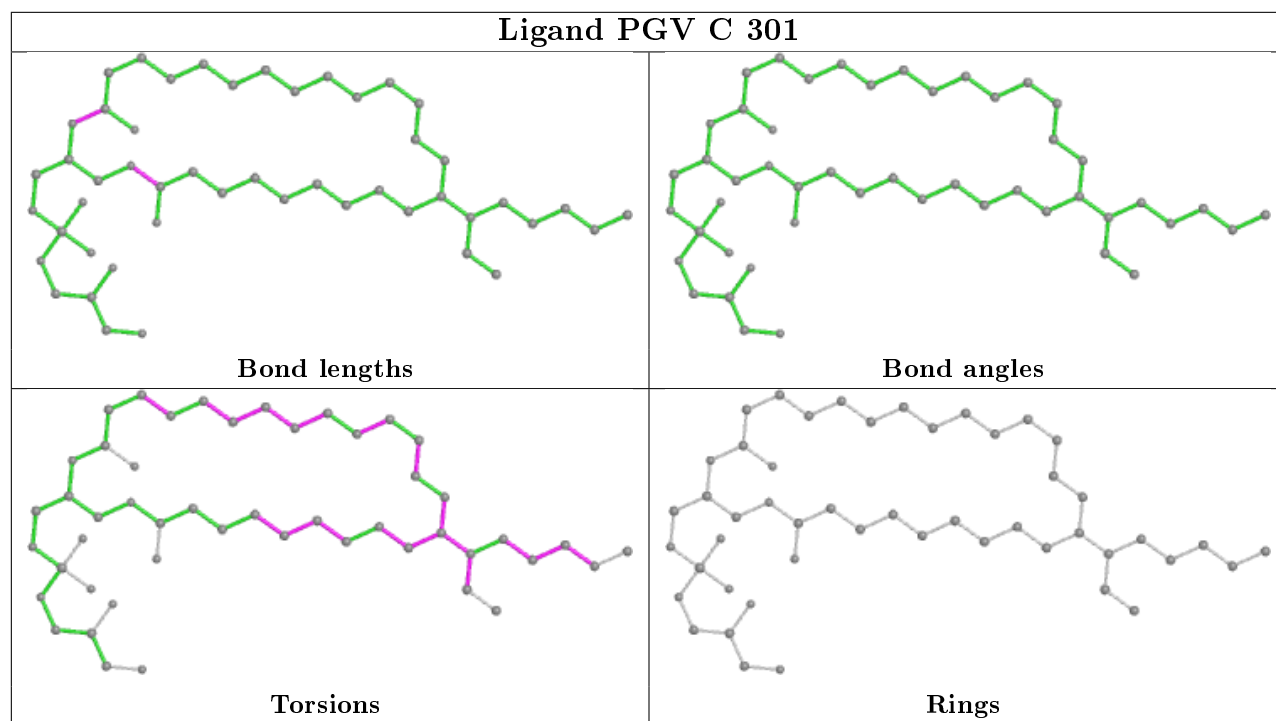
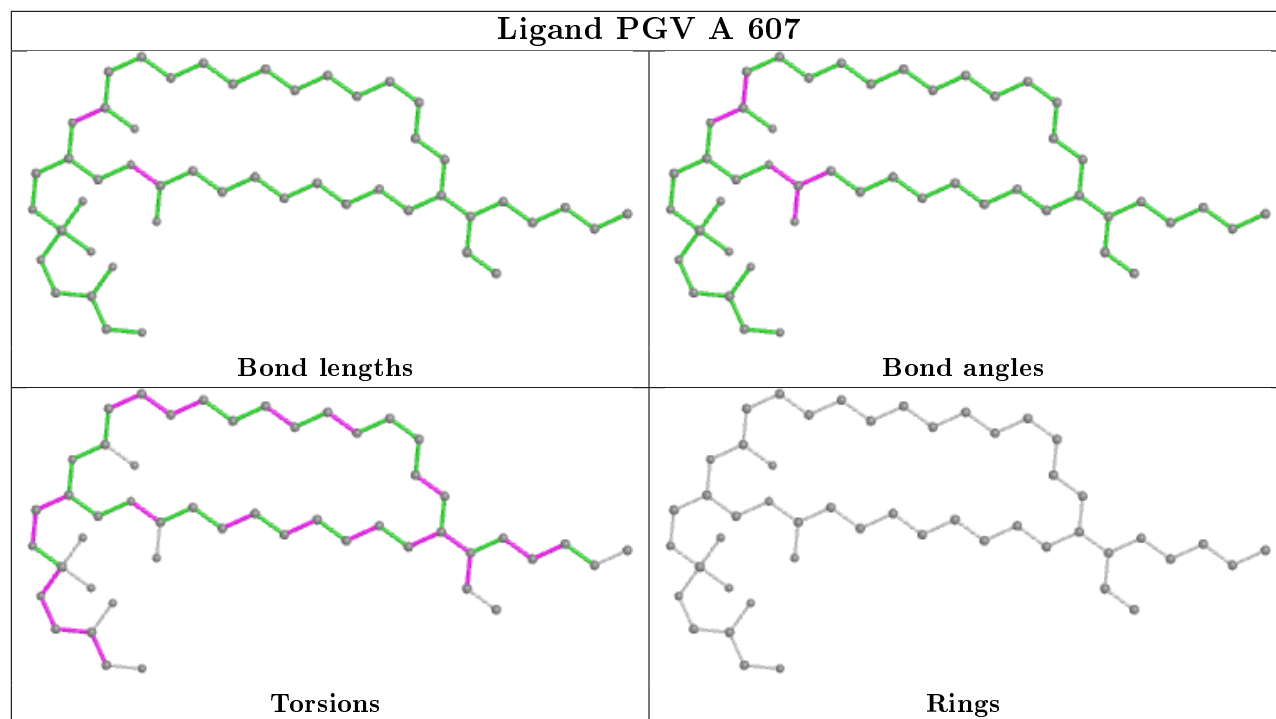




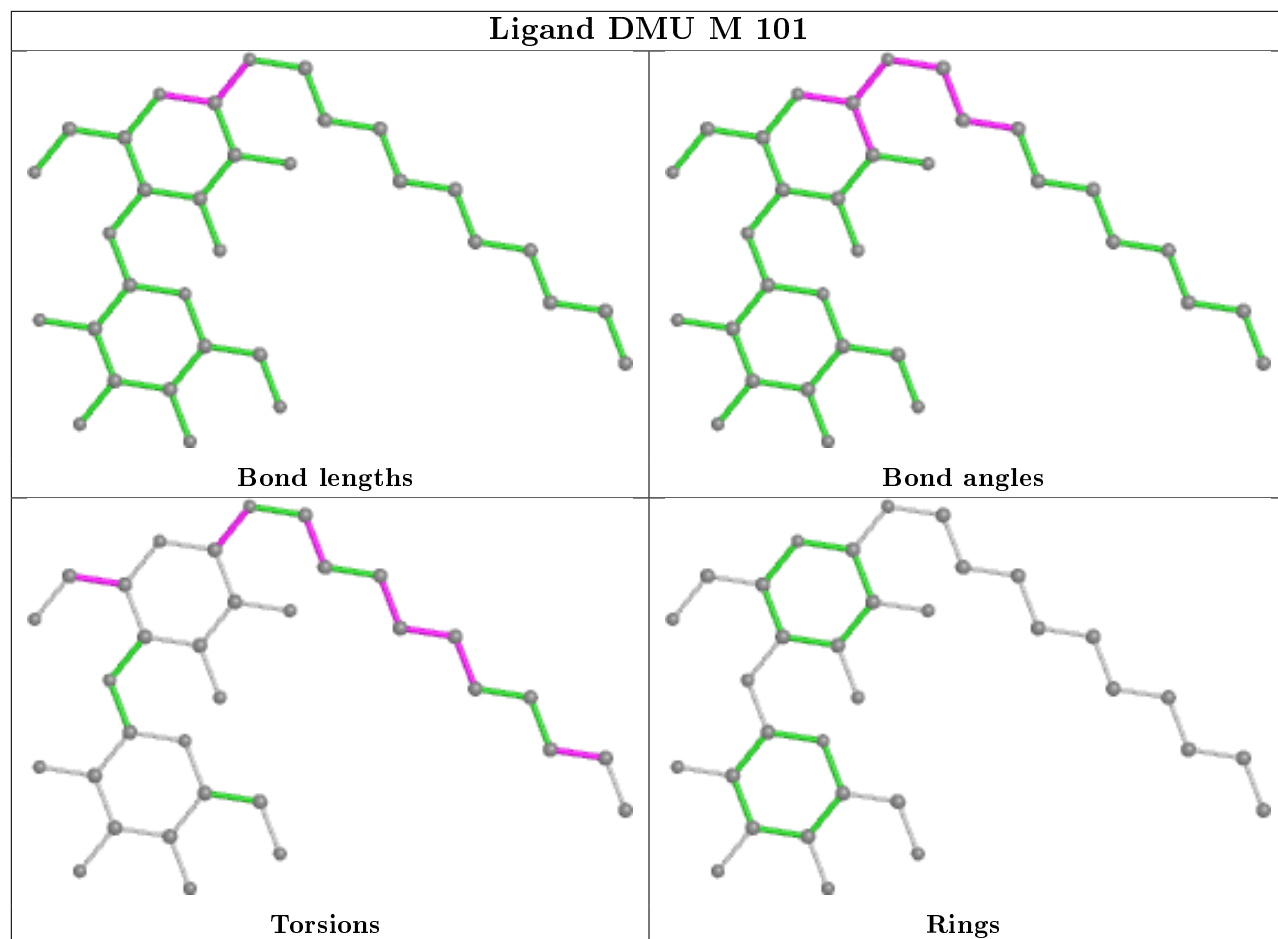




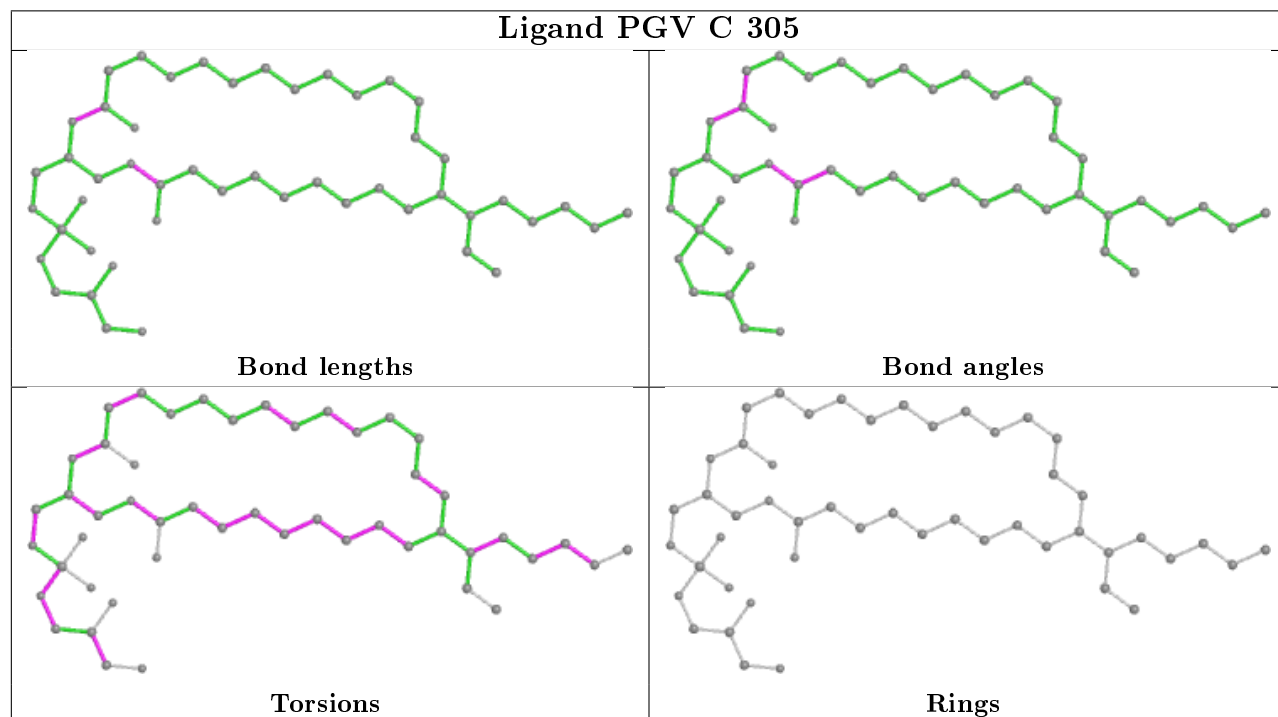


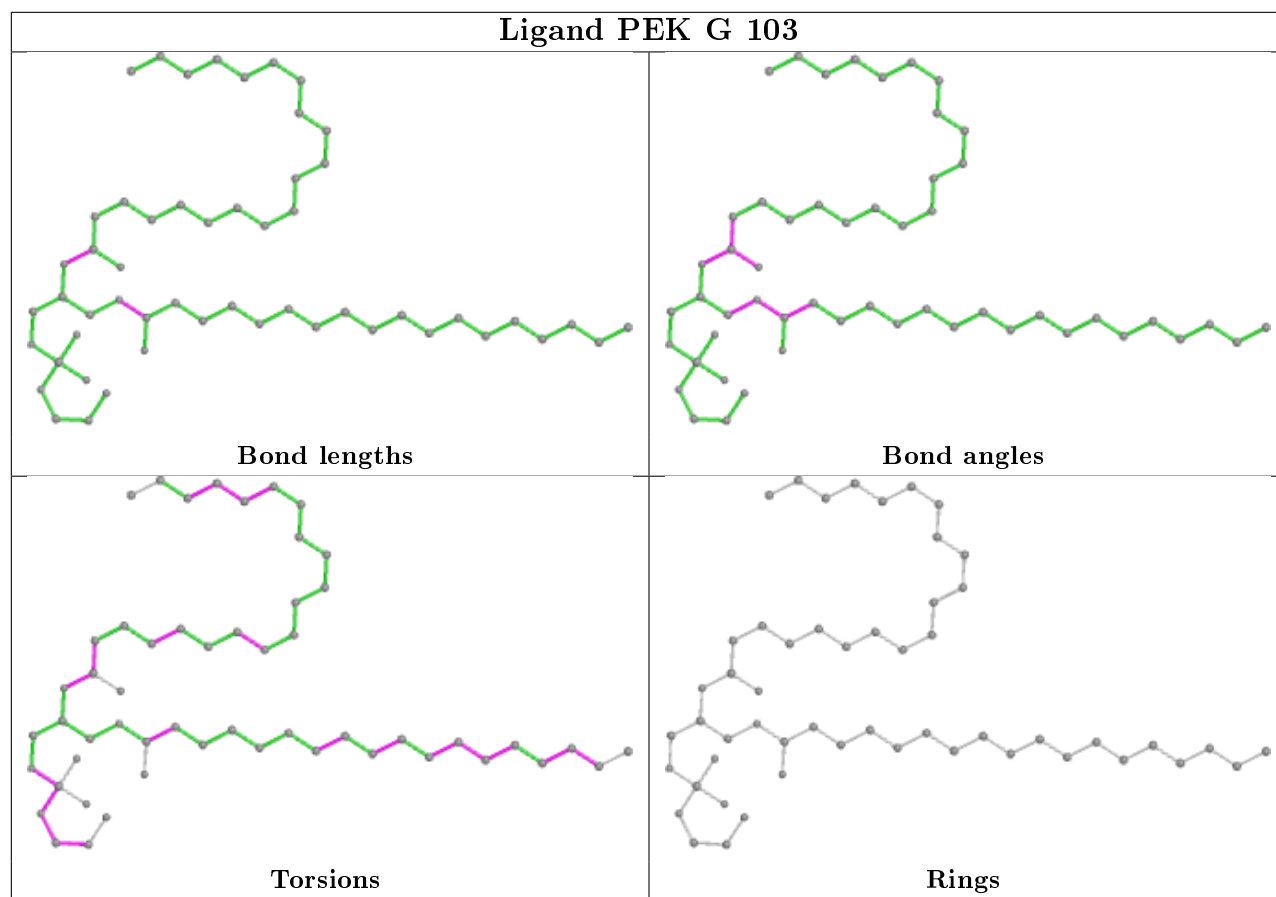
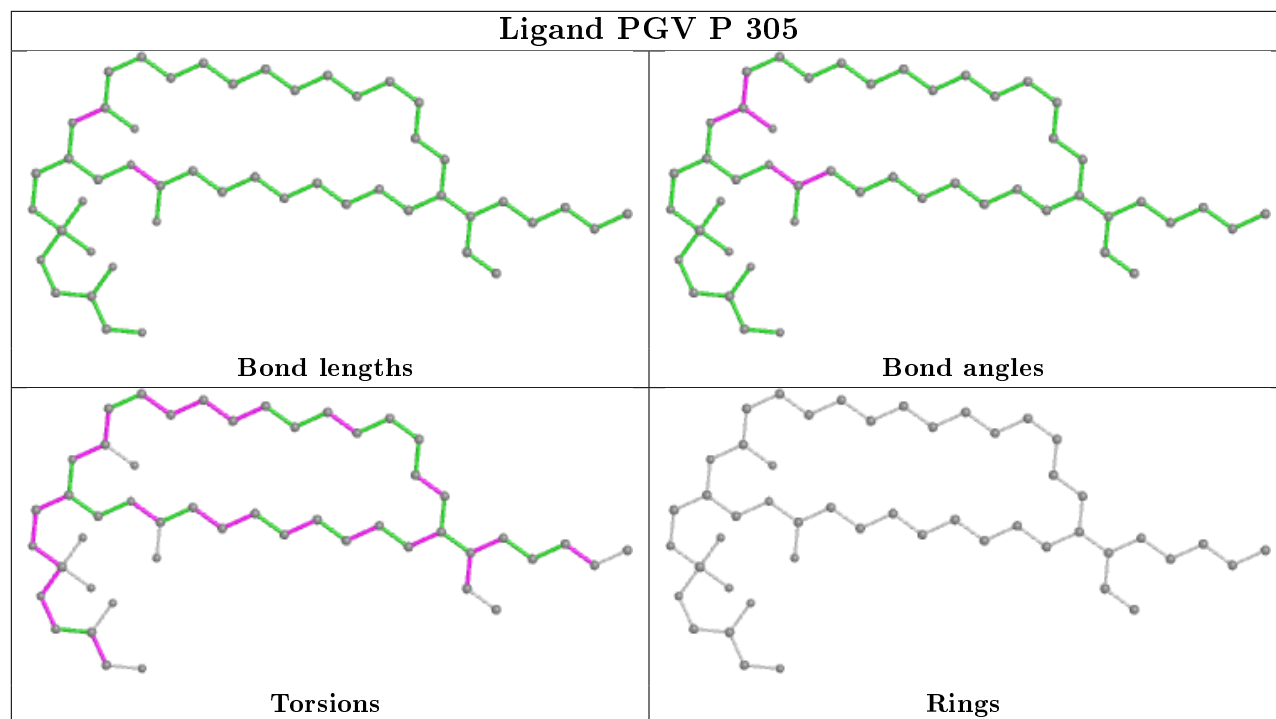


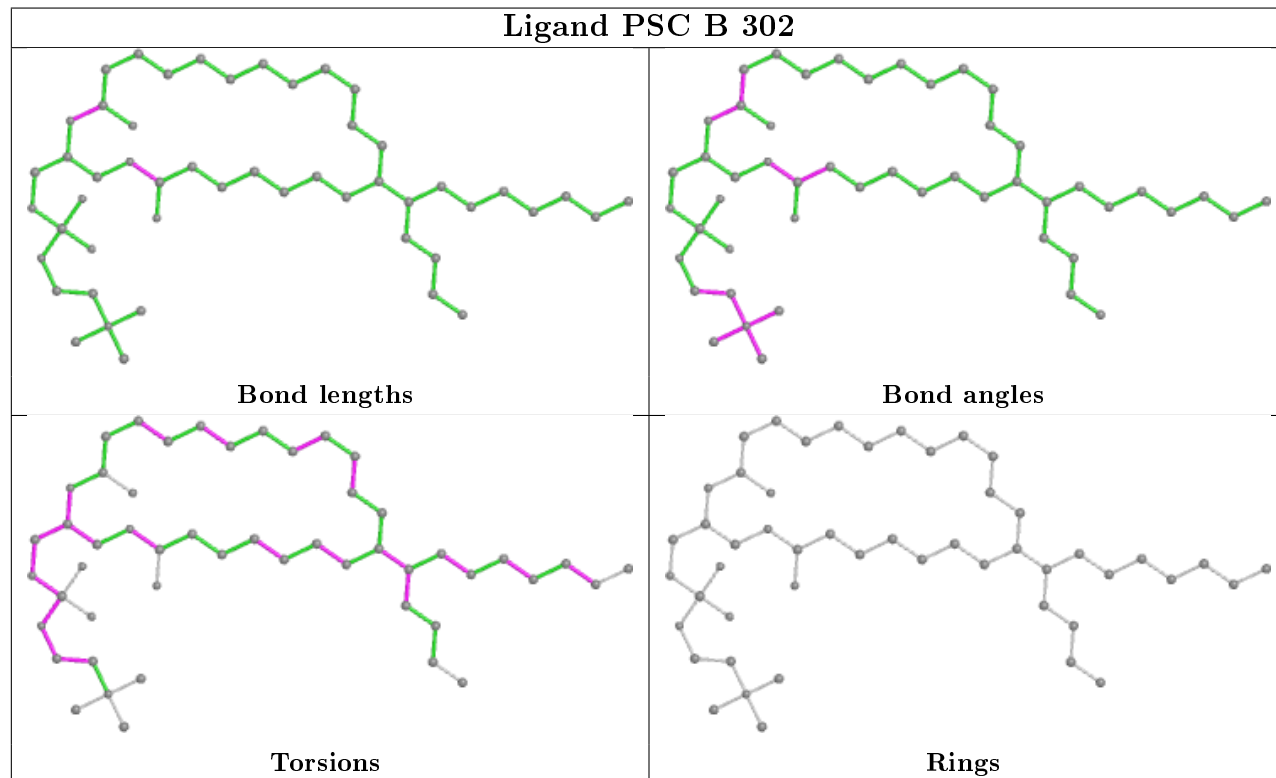
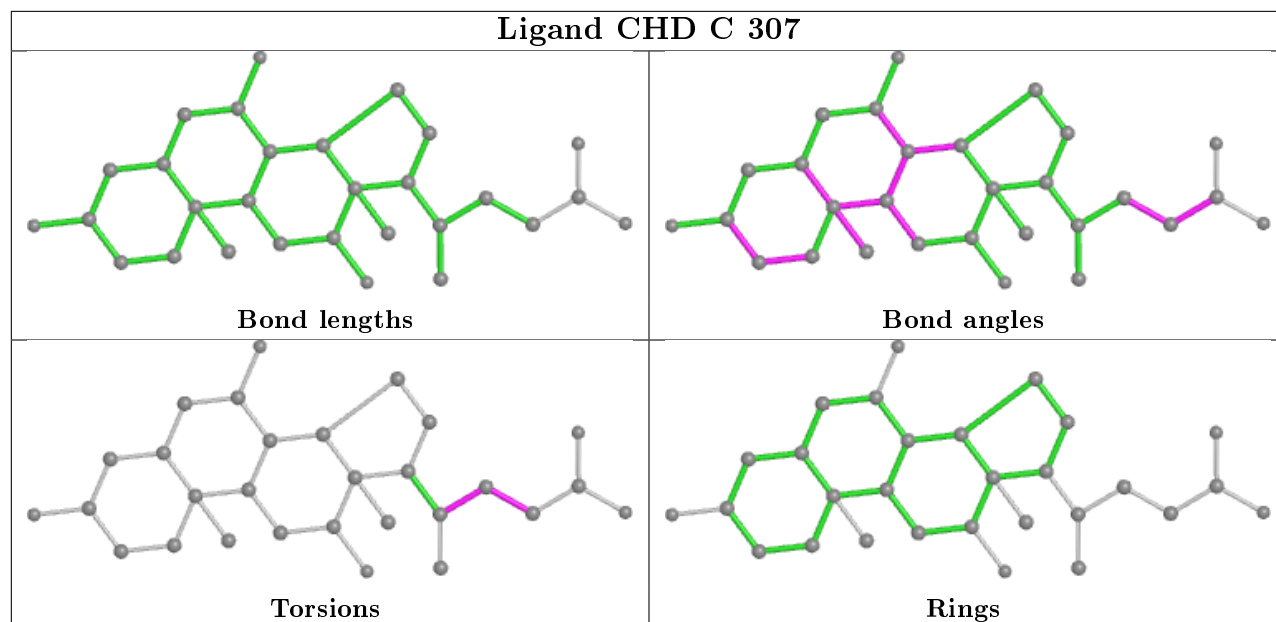
Ligand DMU M 101

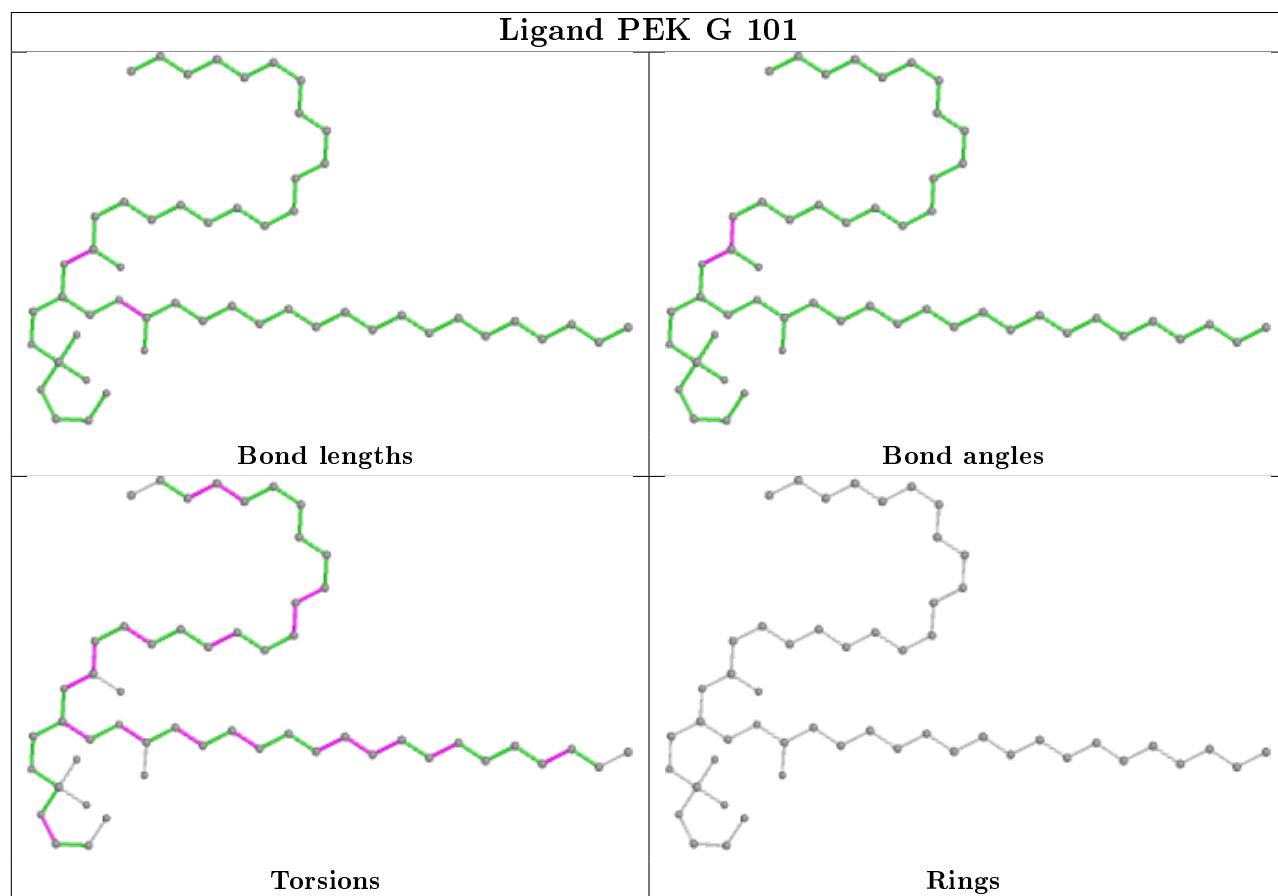
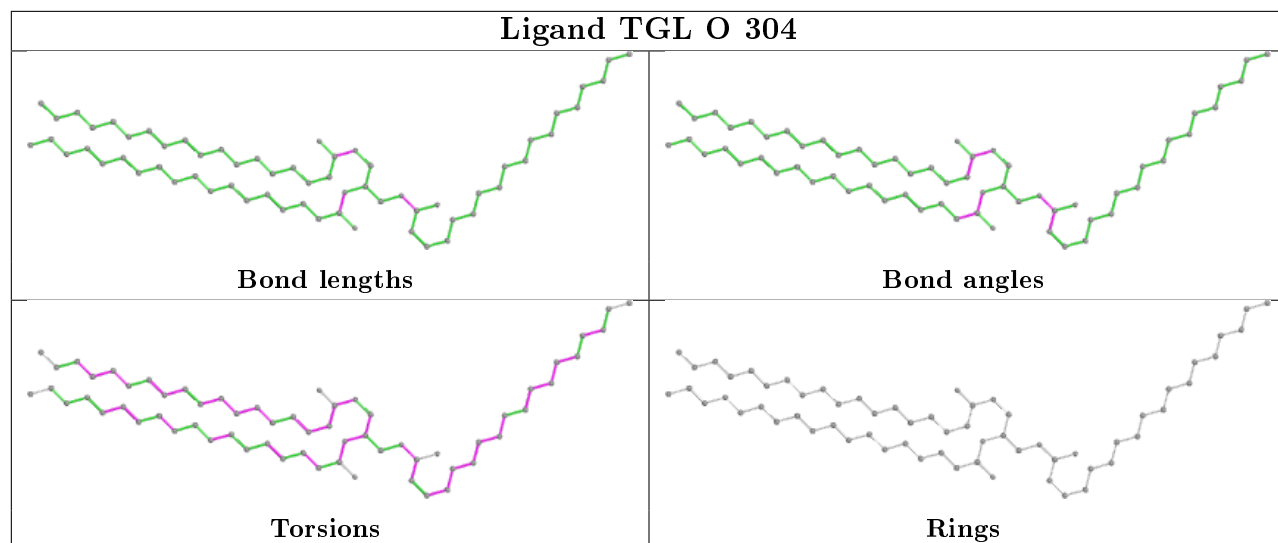


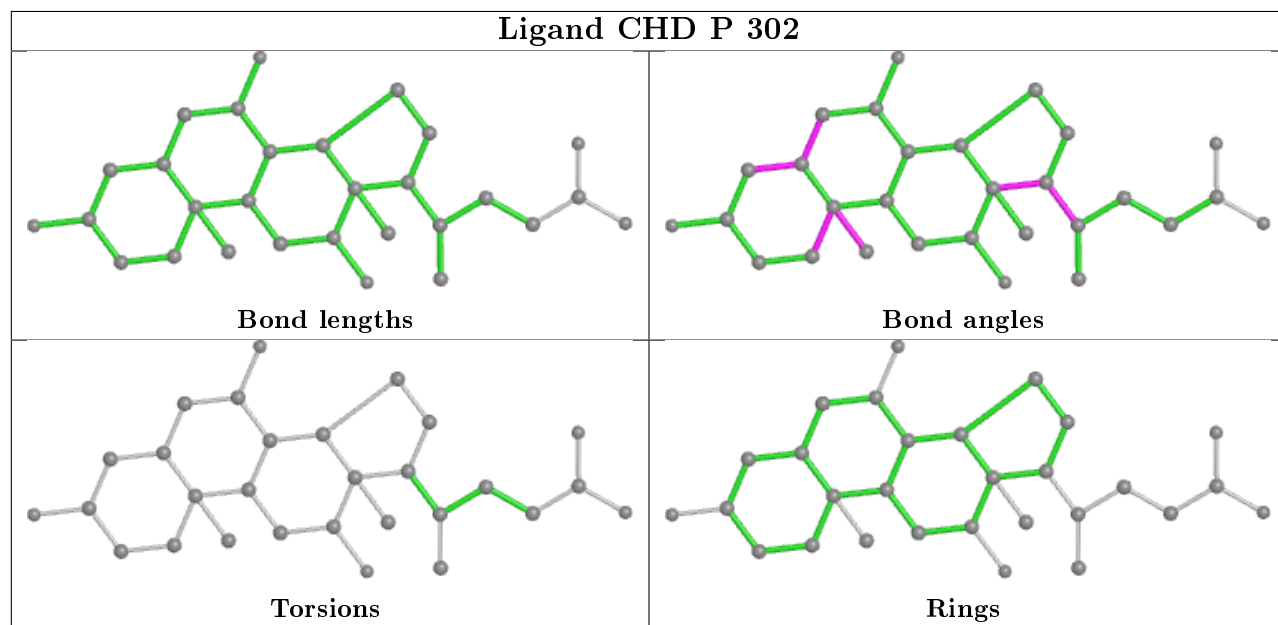
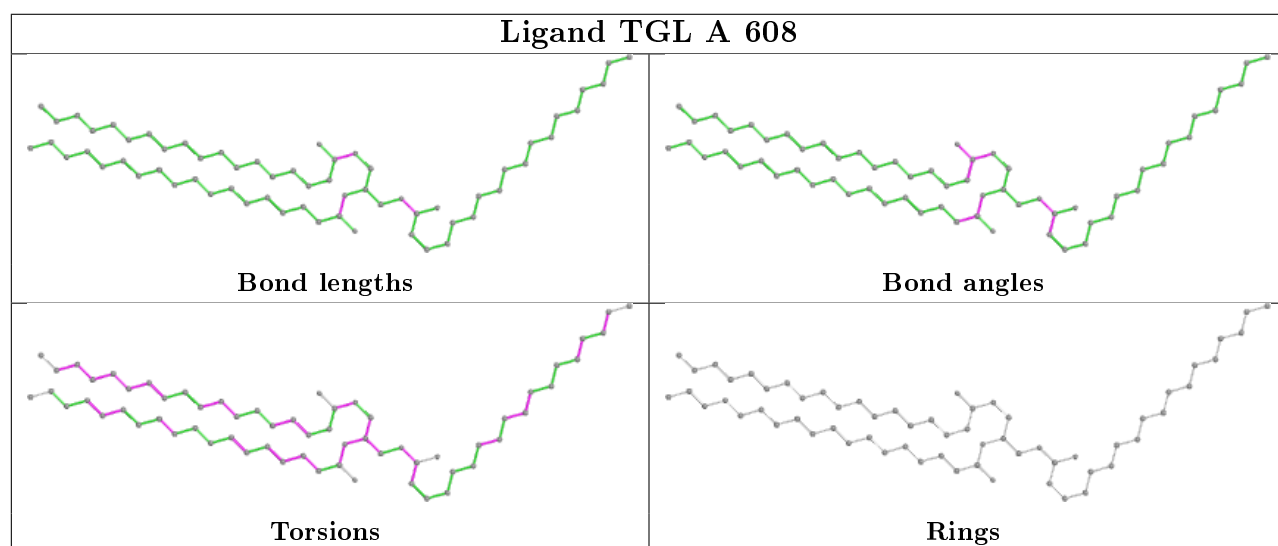
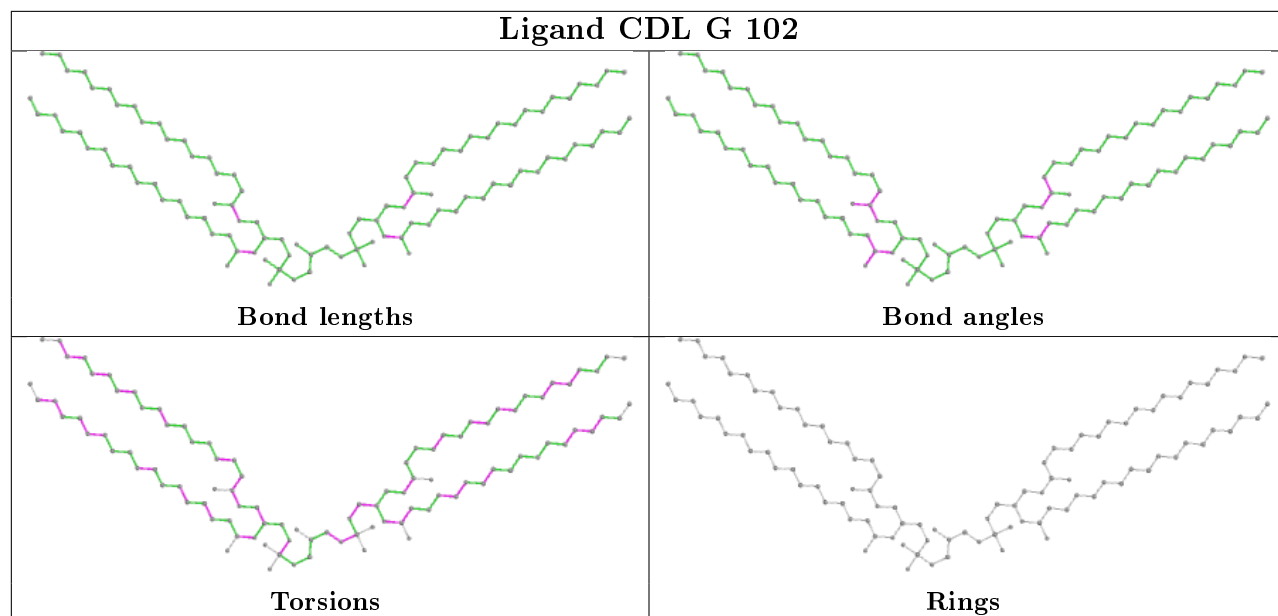
Ligand PGV C 305

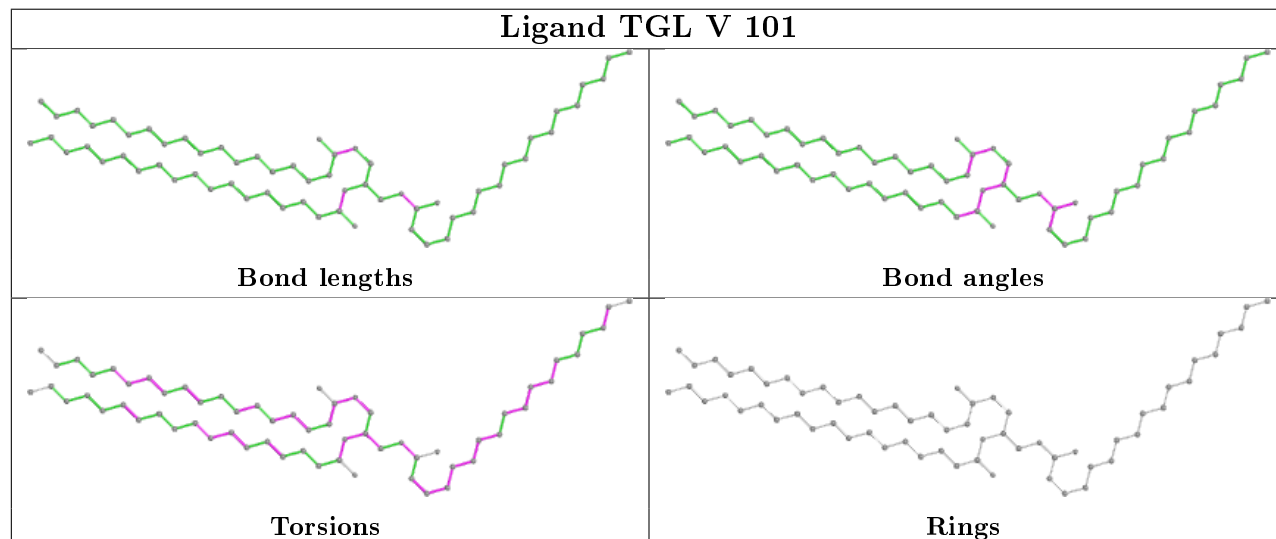
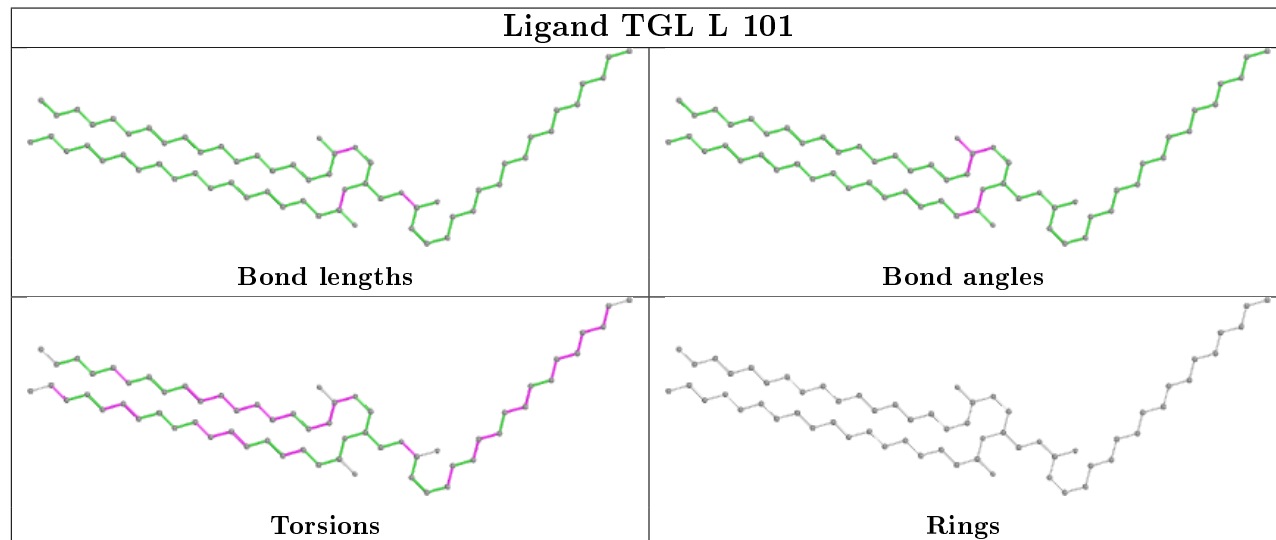
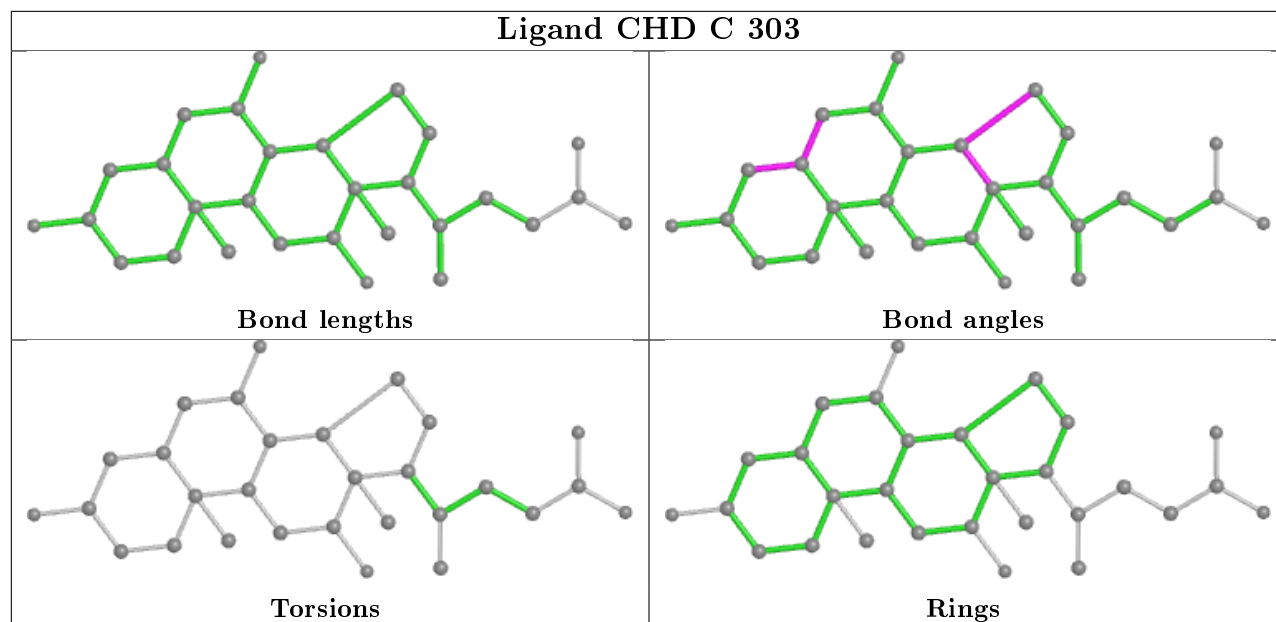


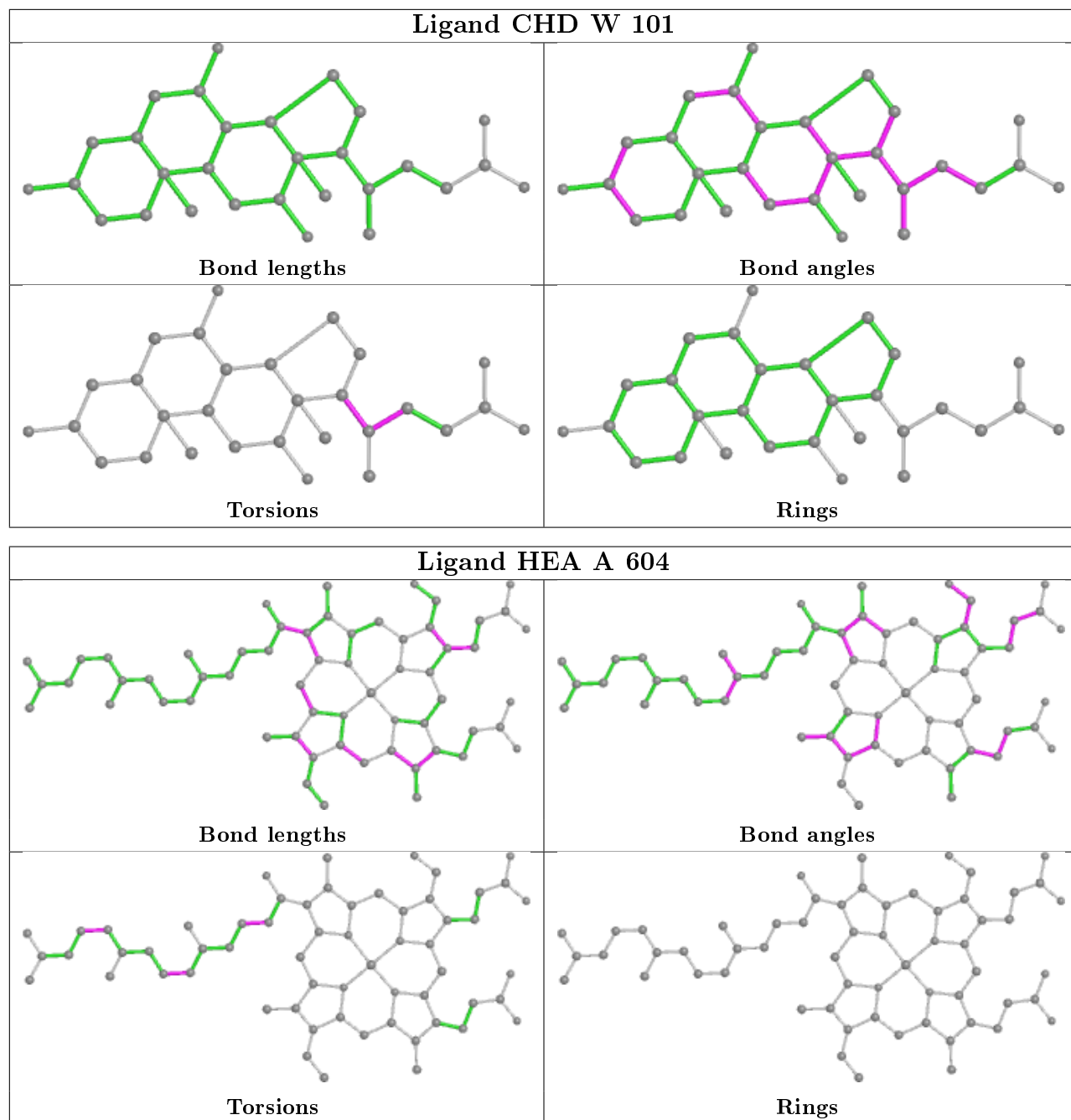


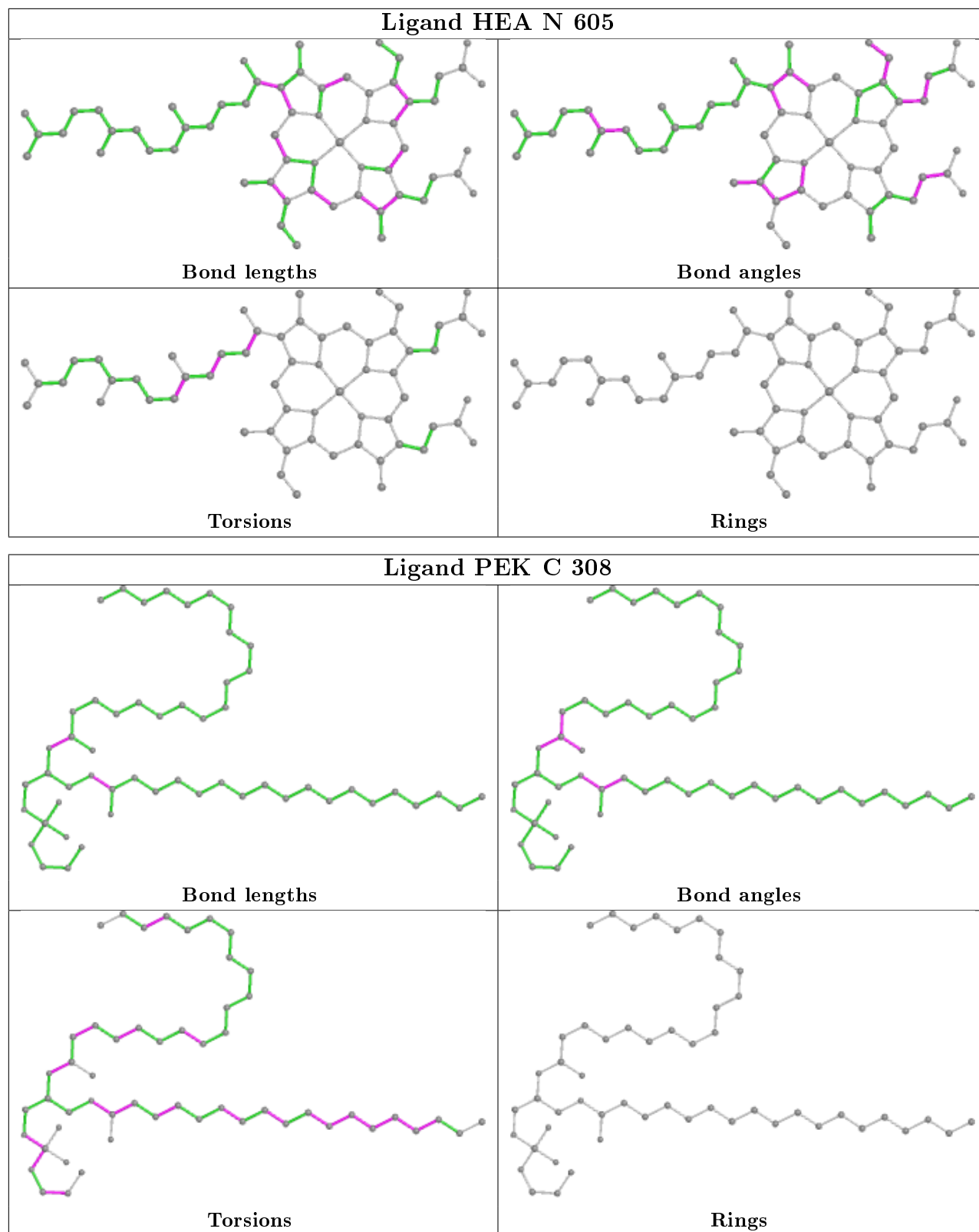


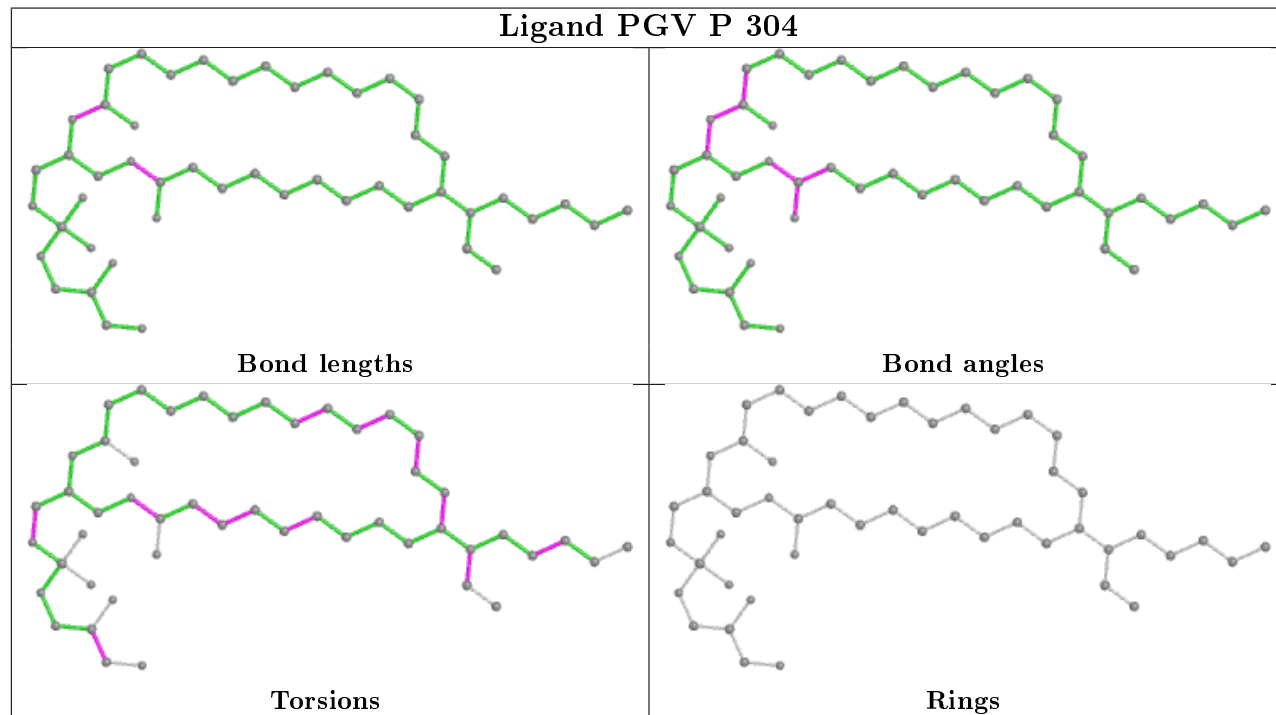
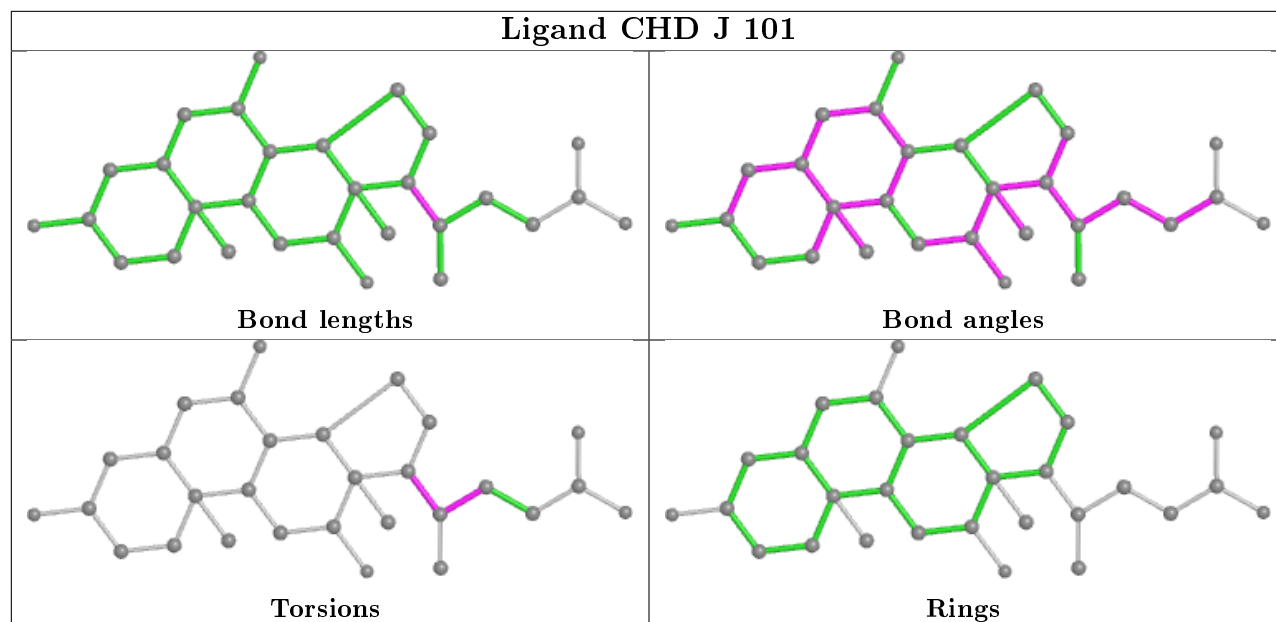


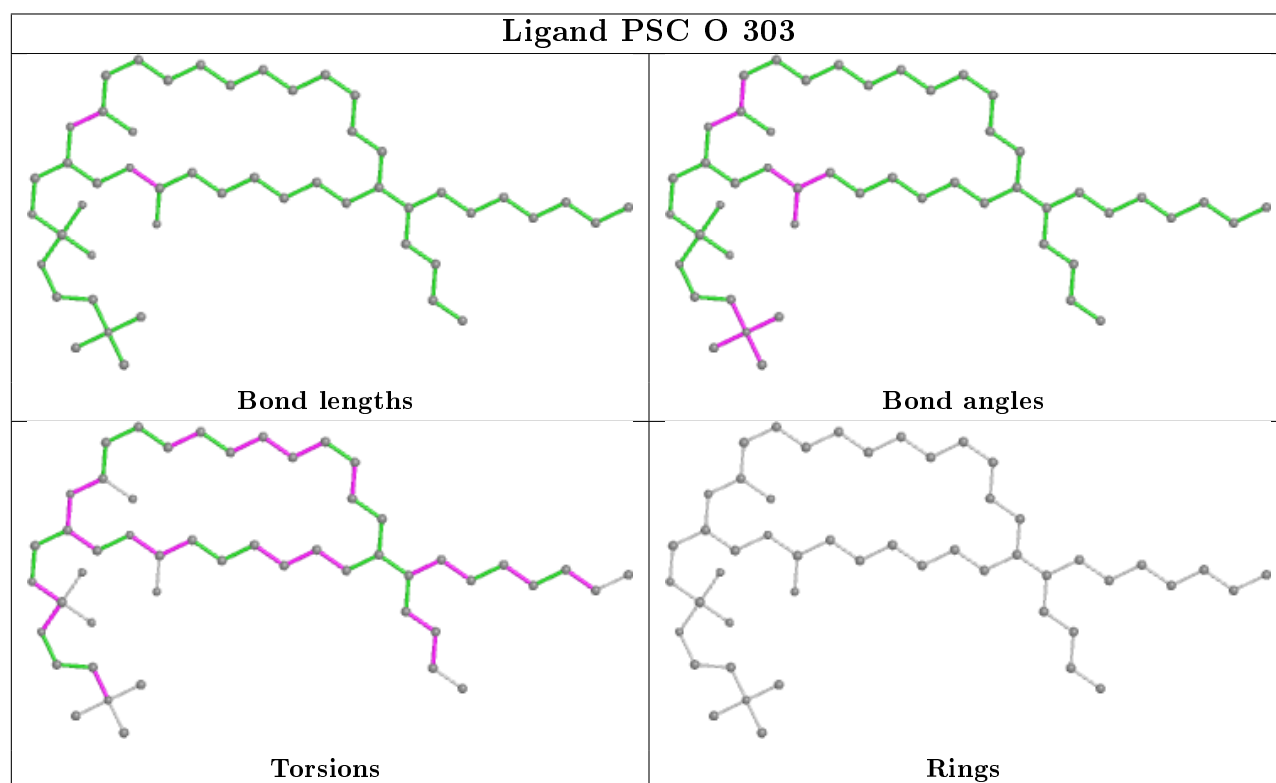
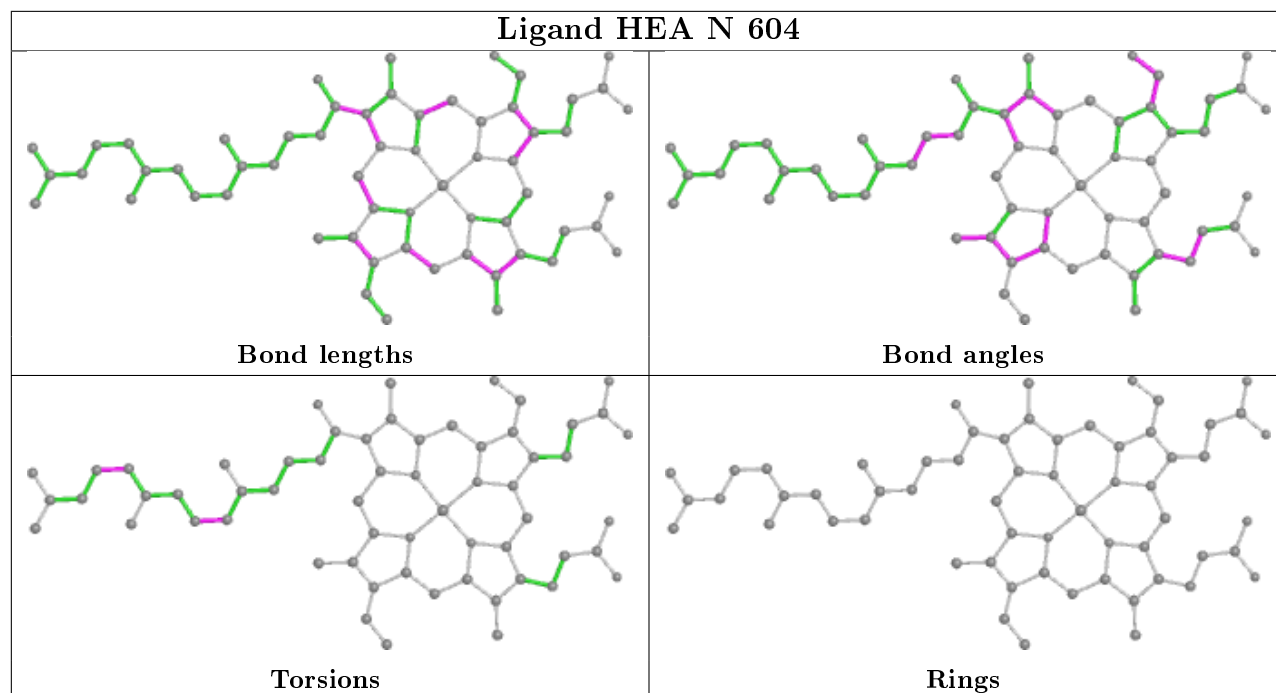


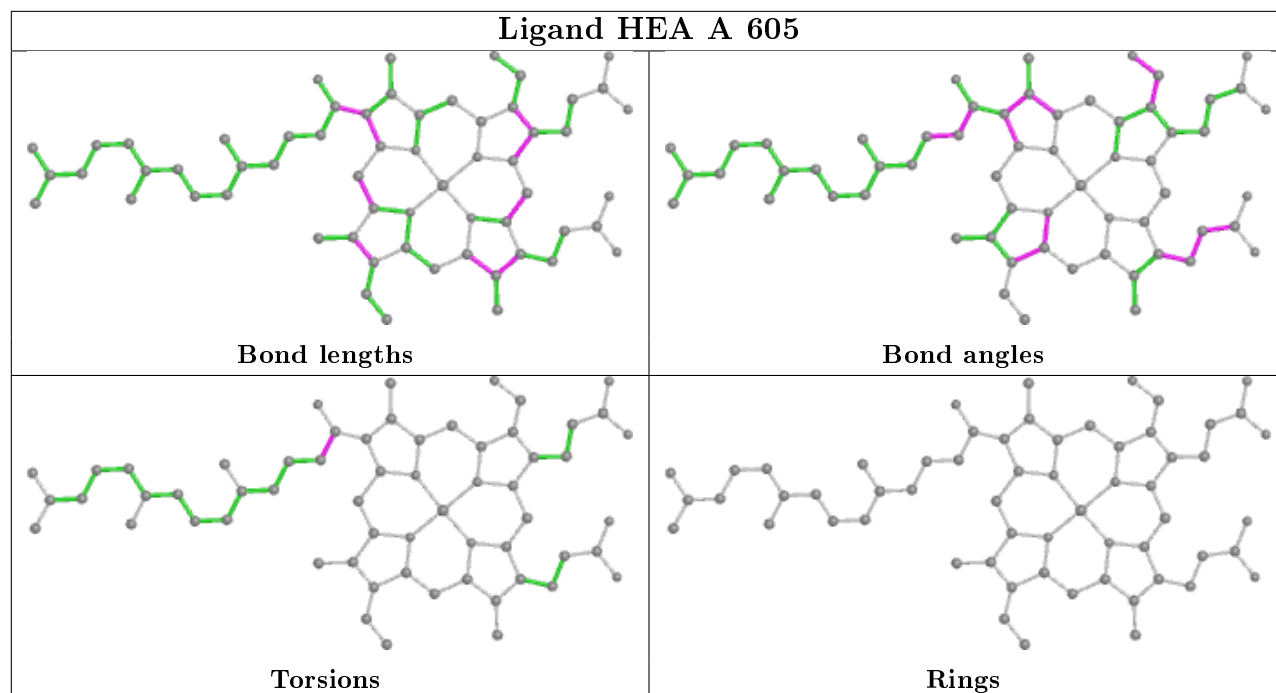












5.7 Other polymers [i](#)

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%)	-1.01	0 100 100	31, 41, 54, 91	0
1	N	513/514 (99%)	-0.91	0 100 100	36, 55, 75, 108	0
2	B	226/227 (99%)	-0.74	2 (0%) 84 84	33, 50, 83, 128	0
2	O	226/227 (99%)	-0.51	5 (2%) 62 59	49, 68, 104, 155	0
3	C	259/261 (99%)	-0.83	0 100 100	34, 46, 65, 98	0
3	P	259/261 (99%)	-0.75	1 (0%) 92 93	42, 57, 80, 124	0
4	D	144/147 (97%)	-0.53	2 (1%) 75 75	39, 53, 80, 110	0
4	Q	144/147 (97%)	0.07	8 (5%) 24 20	56, 83, 120, 202	0
5	E	105/109 (96%)	-0.55	2 (1%) 66 65	39, 53, 84, 140	0
5	R	105/109 (96%)	-0.36	2 (1%) 66 65	52, 69, 90, 134	0
6	F	98/98 (100%)	-0.05	9 (9%) 9 6	38, 56, 130, 154	0
6	S	98/98 (100%)	0.15	9 (9%) 9 6	47, 68, 152, 176	0
7	G	83/85 (97%)	0.12	10 (12%) 4 3	40, 59, 144, 161	0
7	T	83/85 (97%)	0.14	13 (15%) 2 1	43, 72, 144, 163	0
8	H	79/85 (92%)	-0.27	2 (2%) 57 55	43, 60, 119, 135	0
8	U	79/85 (92%)	-0.03	7 (8%) 9 7	54, 75, 129, 157	0
9	I	72/73 (98%)	-0.36	1 (1%) 75 75	46, 63, 93, 114	0
9	V	72/73 (98%)	0.00	5 (6%) 16 13	49, 79, 112, 127	0
10	J	58/59 (98%)	-0.23	2 (3%) 45 40	44, 60, 104, 138	0
10	W	58/59 (98%)	0.10	5 (8%) 10 8	61, 79, 130, 151	0
11	K	49/56 (87%)	-0.29	1 (2%) 65 63	47, 60, 81, 96	0
11	X	49/56 (87%)	0.15	2 (4%) 37 32	59, 80, 104, 123	0
12	L	46/47 (97%)	-0.68	1 (2%) 62 59	40, 49, 75, 124	0
12	Y	46/47 (97%)	-0.31	2 (4%) 35 31	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%)	-0.34	2 (4%)	31 28	40, 48, 95, 139	0
13	Z	43/46 (93%)	0.17	3 (6%)	16 12	62, 74, 131, 153	0
All	All	3550/3614 (98%)	-0.54	96 (2%)	54 50	31, 56, 101, 202	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	10.1
7	G	40	GLY	9.9
7	G	39	SER	7.7
6	S	1	ALA	7.7
6	F	98	HIS	7.6
6	S	98	HIS	7.6
4	Q	7	LYS	6.7
13	Z	43	SER	6.6
7	T	40	GLY	6.5
7	G	3	ALA	6.3
4	Q	8	SER	6.3
6	S	2	SER	6.2
6	F	94	HIS	6.2
6	F	1	ALA	6.2
13	M	43	SER	6.1
6	S	95	GLN	6.0
7	G	41	HIS	5.5
7	T	39	SER	5.4
10	W	57	HIS	5.4
7	T	41	HIS	5.2
6	S	94	HIS	5.2
7	T	3	ALA	5.1
6	F	2	SER	4.8
2	O	59	GLN	4.6
13	Z	42	LYS	4.6
10	J	58	LYS	4.4
7	T	84	LYS	4.1
13	M	42	LYS	4.1
5	E	5	HIS	4.0
2	O	90	ILE	4.0
10	J	57	HIS	3.9
8	H	45	ALA	3.8
4	Q	5	VAL	3.8
8	U	8	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
5	R	5	HIS	3.7
9	V	2	THR	3.6
8	U	10	ASN	3.5
8	U	45	ALA	3.5
7	G	42	ARG	3.4
10	W	58	LYS	3.3
4	D	4	SER	3.3
2	O	227	LEU	3.2
12	Y	2	HIS	3.1
7	T	42	ARG	3.1
7	T	43	GLU	3.1
10	W	52	TRP	3.1
4	Q	6	VAL	3.1
6	F	95	GLN	3.1
7	G	2	SER	3.0
6	S	3	GLY	3.0
13	Z	39	ASN	3.0
7	G	84	LYS	3.0
9	V	37	PHE	2.9
7	T	1	ALA	2.9
4	Q	32	ASN	2.9
4	Q	147	LYS	2.9
7	T	36	TRP	2.8
10	W	56	PRO	2.8
9	V	53	ASN	2.7
4	Q	9	GLU	2.7
7	G	43	GLU	2.6
3	P	3	HIS	2.6
7	T	8	HIS	2.6
9	V	3	ALA	2.6
8	H	8	ILE	2.6
6	F	97	ALA	2.6
10	W	48	TYR	2.5
6	S	96	LEU	2.4
7	T	10	GLY	2.4
9	I	25	PHE	2.4
12	Y	47	LYS	2.4
11	X	7	PRO	2.4
6	S	97	ALA	2.4
8	U	77	ALA	2.4
7	G	8	HIS	2.3
2	B	90	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
12	L	47	LYS	2.3
7	T	9	GLY	2.3
5	E	9	GLU	2.3
2	B	59	GLN	2.3
6	F	27	GLY	2.2
8	U	7	LYS	2.2
6	F	3	GLY	2.2
7	G	9	GLY	2.2
6	F	28	GLN	2.2
8	U	51	SER	2.2
11	X	35	GLN	2.2
9	V	55	ASP	2.2
7	T	2	SER	2.2
11	K	6	ALA	2.1
2	O	58	ALA	2.1
6	S	4	GLY	2.1
2	O	57	ASP	2.1
5	R	108	LYS	2.1
4	D	141	ASP	2.0
8	U	49	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.65	0.65	144,155,160,162	0
9	SAC	I	1	9/10	0.66	0.58	122,141,150,151	0
7	TPO	T	11	11/12	0.72	0.49	139,153,169,174	0
7	TPO	G	11	11/12	0.76	0.48	112,136,147,154	0
1	FME	N	1	10/11	0.92	0.39	86,103,121,132	0
1	FME	A	1	10/11	0.94	0.39	80,84,135,138	0
2	FME	O	1	10/11	0.96	0.14	60,73,78,88	0
2	FME	B	1	10/11	0.98	0.10	46,49,54,64	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

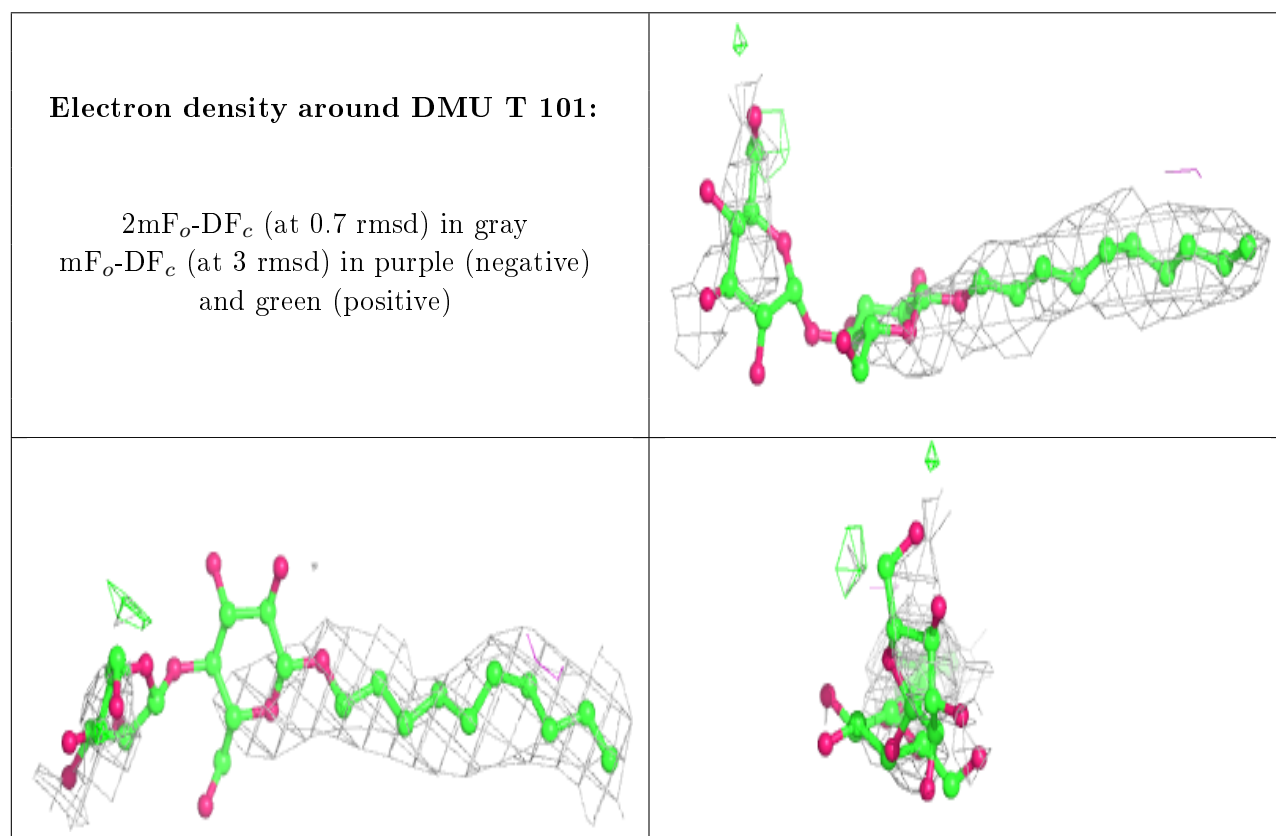
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	DMU	T	101	33/33	0.40	0.49	116,164,194,199	0
25	PEK	G	103	53/53	0.52	0.44	79,133,192,210	0
18	PGV	N	606	51/51	0.61	0.37	59,100,150,166	0
25	PEK	T	102	53/53	0.62	0.31	73,108,155,162	0
24	DMU	C	302	33/33	0.66	0.39	112,136,174,194	0
22	PSC	O	303	52/52	0.68	0.35	79,119,224,231	0
26	CDL	T	103	100/100	0.69	0.32	76,113,183,211	0
19	TGL	Y	101	63/63	0.70	0.31	76,102,153,164	0
25	PEK	C	304	53/53	0.70	0.29	75,104,180,197	0
18	PGV	A	606	51/51	0.70	0.31	57,108,156,190	0
26	CDL	G	102	100/100	0.71	0.33	78,128,168,200	0
23	CHD	W	101	29/29	0.73	0.36	105,123,144,151	0
25	PEK	C	308	53/53	0.73	0.34	71,111,178,196	0
18	PGV	P	305	51/51	0.73	0.32	77,111,129,133	0
24	DMU	Q	201	33/33	0.75	0.35	86,103,119,123	0
22	PSC	B	302	52/52	0.75	0.31	69,119,211,230	0
26	CDL	C	306	100/100	0.76	0.29	60,109,150,157	0
19	TGL	I	101	63/63	0.76	0.26	44,91,123,136	0
26	CDL	P	306	100/100	0.76	0.28	66,112,142,143	0
19	TGL	L	101	63/63	0.77	0.29	58,93,123,133	0
19	TGL	V	101	63/63	0.77	0.25	50,93,138,147	0
19	TGL	O	304	63/63	0.77	0.28	89,112,126,138	0
18	PGV	A	607	51/51	0.77	0.29	76,107,130,136	0
19	TGL	A	608	63/63	0.77	0.25	57,92,112,120	0
23	CHD	J	101	29/29	0.83	0.31	82,94,112,120	0
24	DMU	M	101	33/33	0.86	0.23	50,57,74,75	0
23	CHD	P	307	29/29	0.91	0.24	85,103,118,128	0
16	NA	N	603	1/1	0.92	0.17	64,64,64,64	0
25	PEK	P	303	53/53	0.93	0.21	56,83,135,148	0
15	MG	N	602	1/1	0.93	0.11	46,46,46,46	0
18	PGV	P	304	51/51	0.95	0.18	45,54,149,162	0
25	PEK	G	101	53/53	0.95	0.18	37,67,111,123	0
23	CHD	C	307	29/29	0.95	0.20	77,85,92,93	0
16	NA	A	603	1/1	0.95	0.08	39,39,39,39	0
18	PGV	C	305	51/51	0.96	0.15	37,51,97,105	0
23	CHD	P	302	29/29	0.96	0.12	45,49,60,63	0
18	PGV	P	301	51/51	0.96	0.16	37,65,89,93	0

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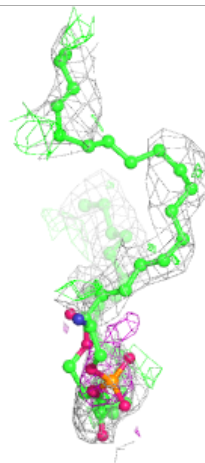
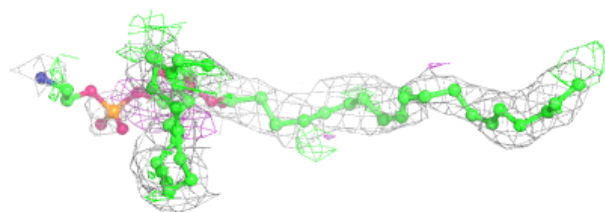
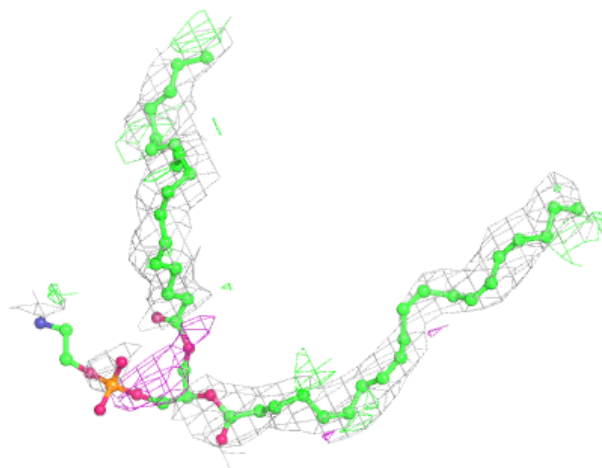
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
18	PGV	C	301	51/51	0.97	0.17	35,61,86,95	0
23	CHD	O	302	29/29	0.97	0.11	41,46,52,54	0
15	MG	A	602	1/1	0.97	0.09	38,38,38,38	0
23	CHD	B	303	29/29	0.97	0.12	41,44,57,69	0
17	HEA	N	604	60/60	0.97	0.13	45,52,71,75	0
17	HEA	A	604	60/60	0.97	0.12	33,39,78,81	0
27	ZN	S	101	1/1	0.97	0.03	65,65,65,65	0
27	ZN	F	101	1/1	0.98	0.02	54,54,54,54	0
21	CUA	O	301	2/2	0.98	0.05	62,62,62,62	0
23	CHD	C	303	29/29	0.98	0.07	36,41,44,48	0
17	HEA	A	605	60/60	0.98	0.12	28,34,47,55	0
17	HEA	N	605	60/60	0.98	0.11	39,43,47,52	0
21	CUA	B	301	2/2	0.98	0.05	42,42,42,43	0
14	CU	A	601	1/1	0.99	0.07	44,44,44,44	0
20	PER	N	607	2/2	0.99	0.07	50,50,50,53	0
14	CU	N	601	1/1	0.99	0.06	58,58,58,58	0
20	PER	A	609	2/2	1.00	0.05	38,38,38,38	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.



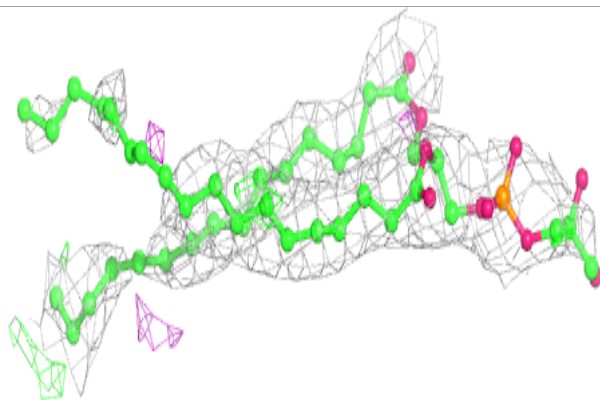
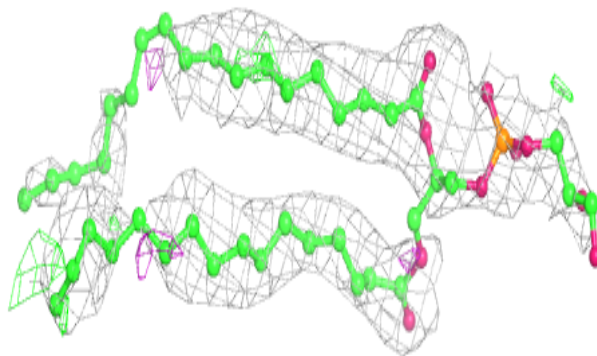
Electron density around PEK G 103:

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



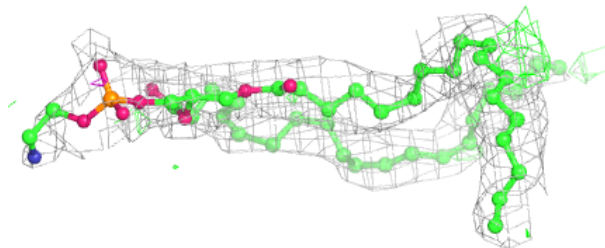
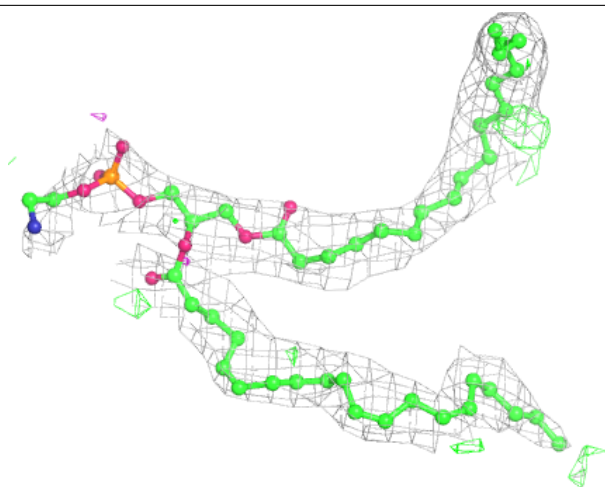
Electron density around PGV N 606:

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



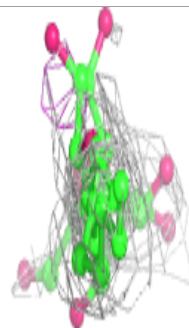
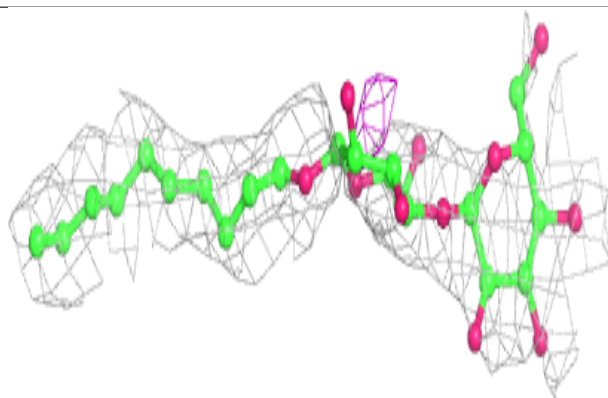
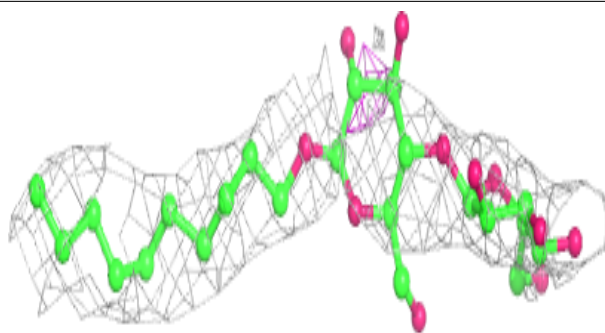
Electron density around PEK T 102:

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

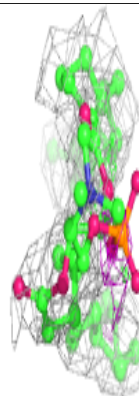
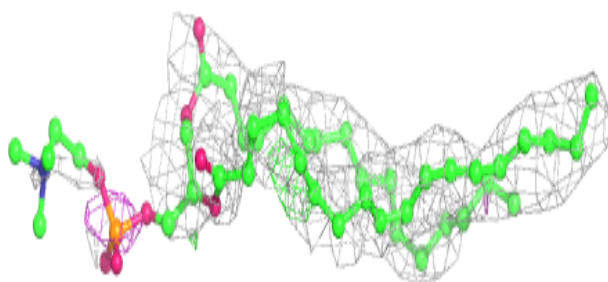
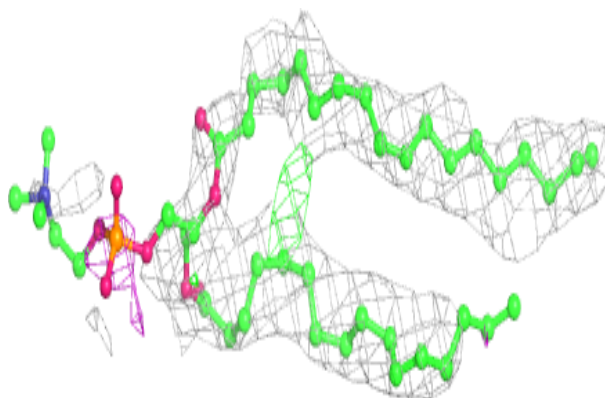


Electron density around DMU C 302:

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

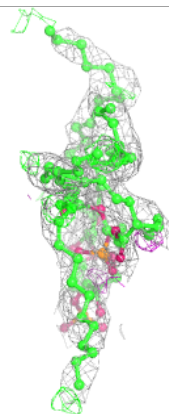
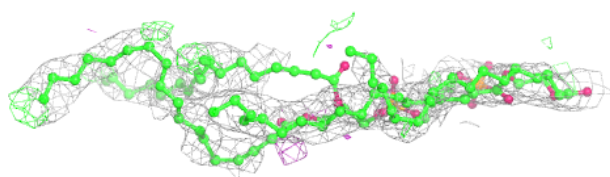
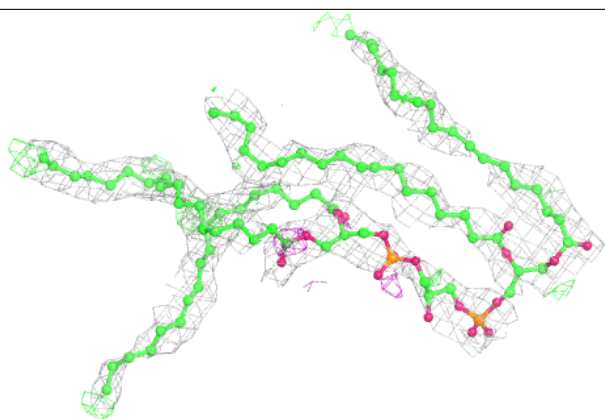
**Electron density around PSC O 303:**

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

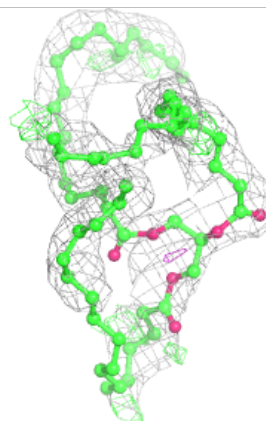
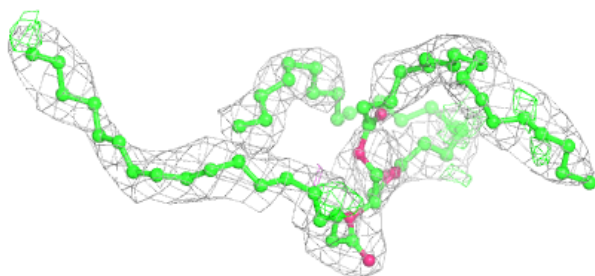
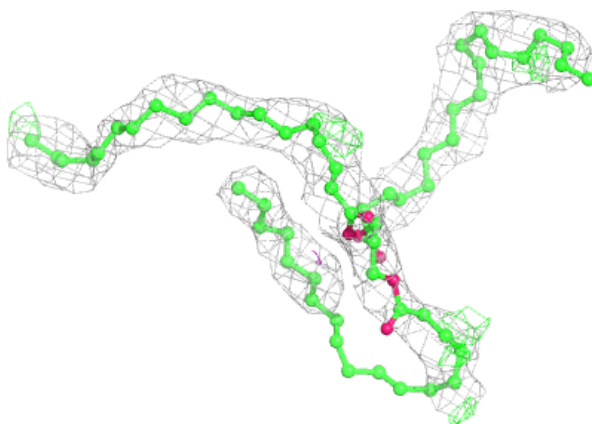


Electron density around CDL T 103:

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

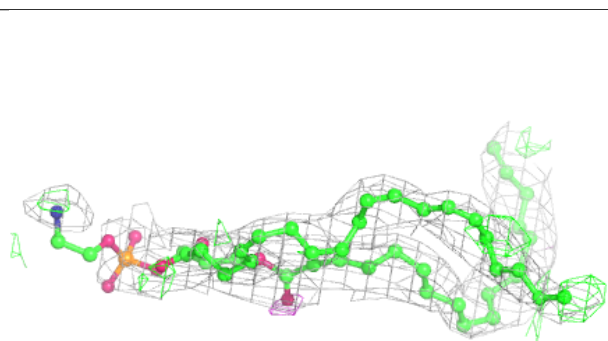
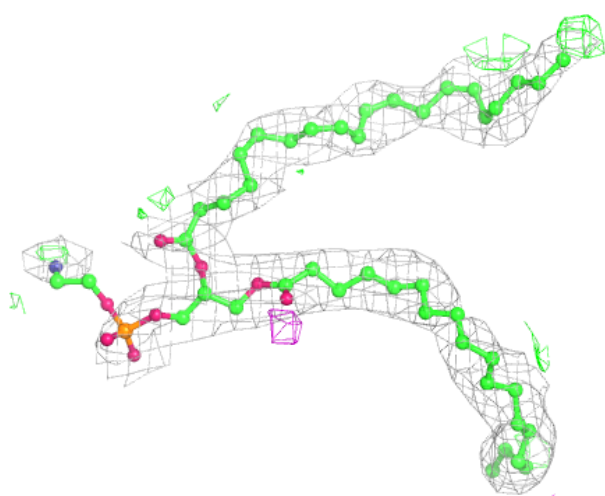
**Electron density around TGL Y 101:**

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



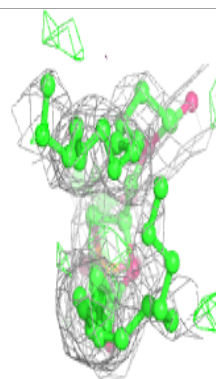
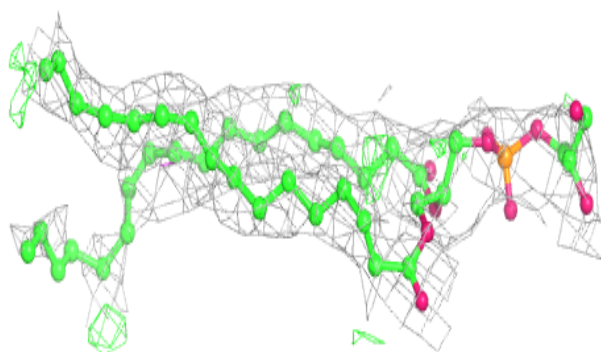
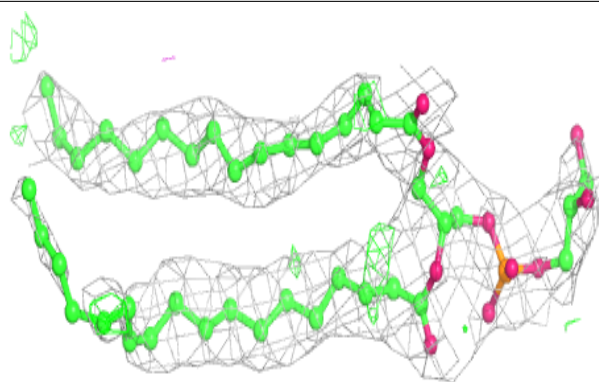
Electron density around PEK C 304:

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

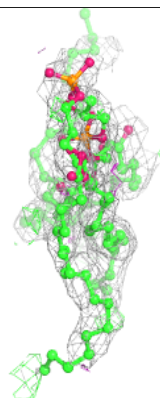
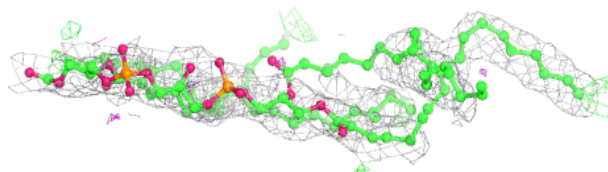
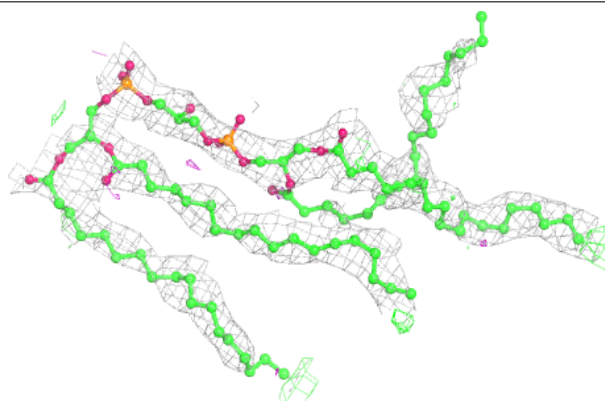


Electron density around PGV A 606:

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

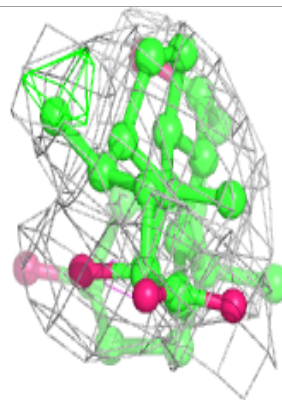
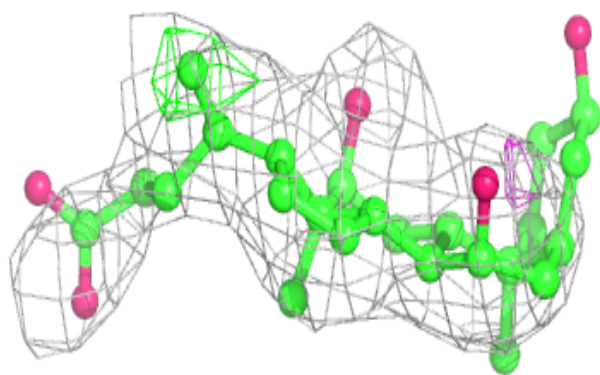
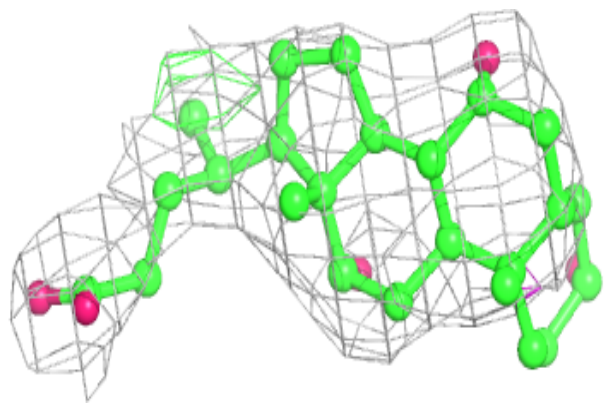
**Electron density around CDL G 102:**

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



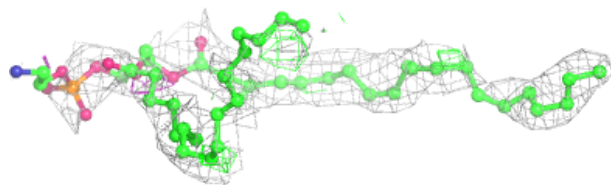
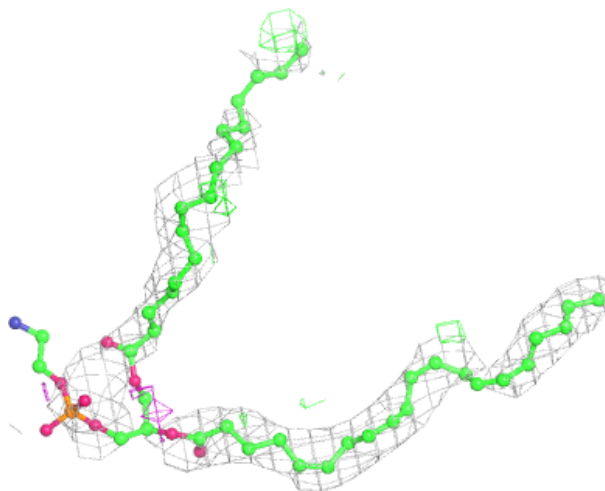
Electron density around CHD W 101:

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



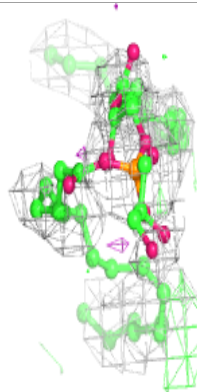
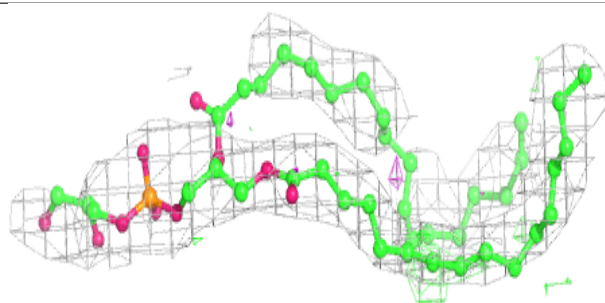
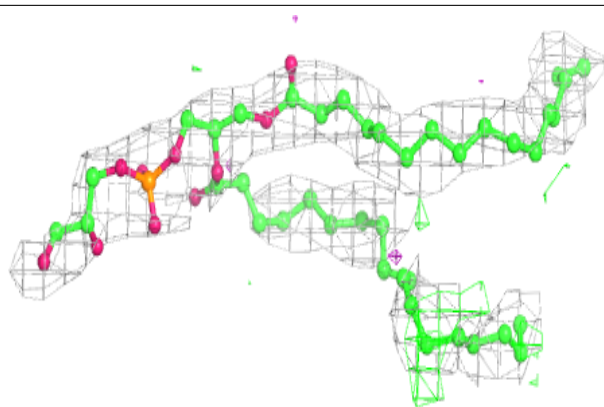
Electron density around PEK C 308:

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and green (positive)

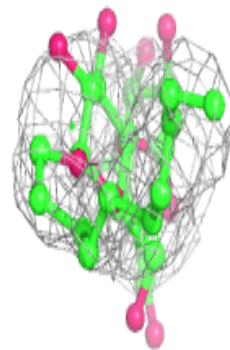
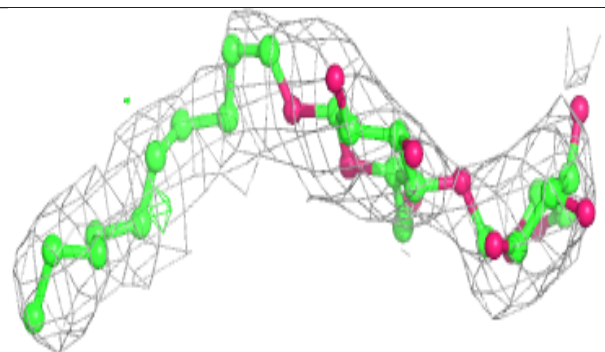
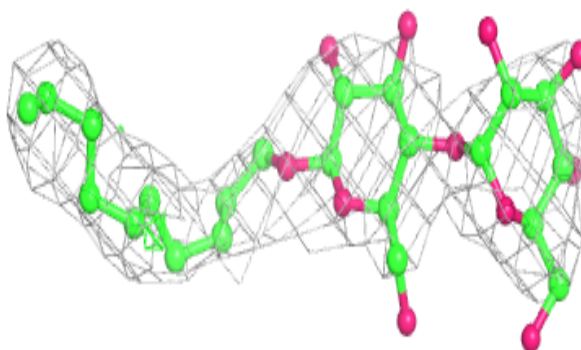


Electron density around PGV P 305:

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

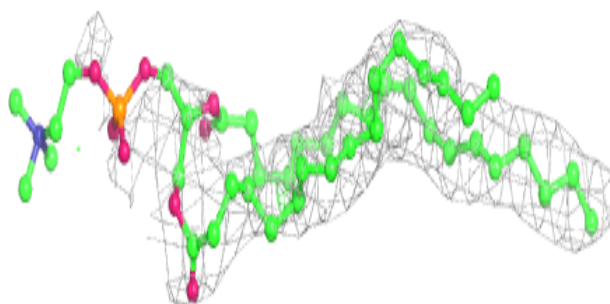
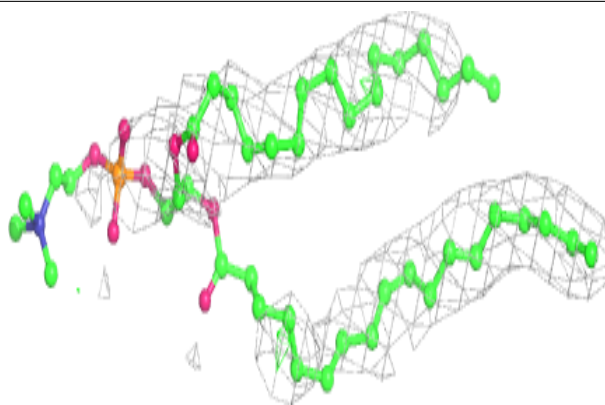
**Electron density around DMU Q 201:**

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

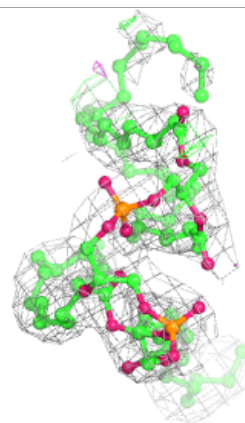
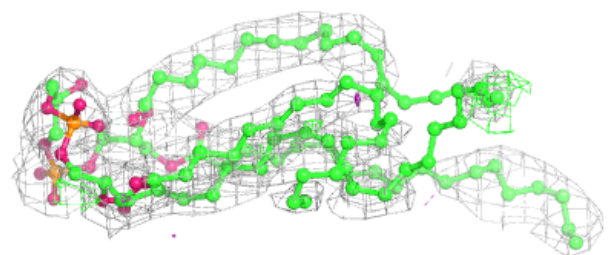
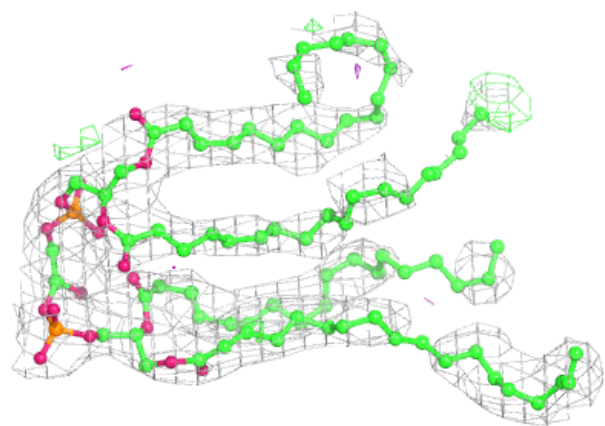


Electron density around PSC B 302:

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

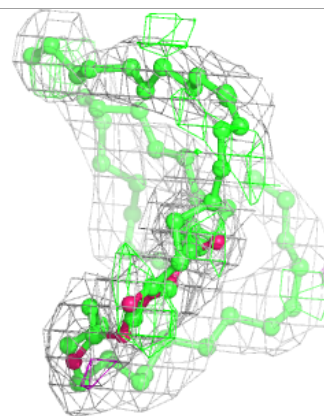
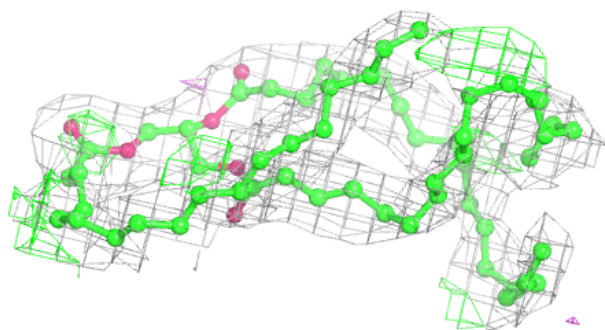
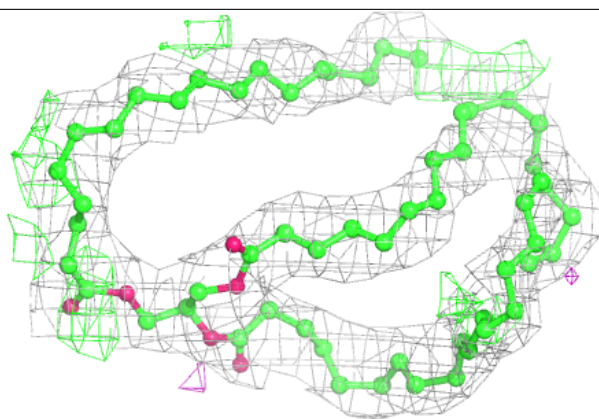
**Electron density around CDL C 306:**

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



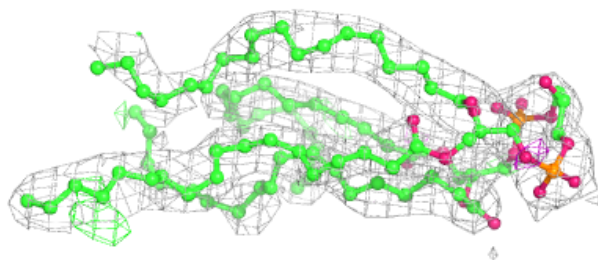
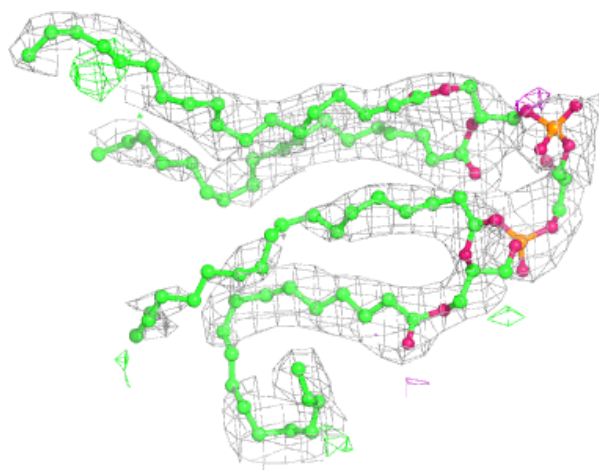
Electron density around TGL I 101:

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



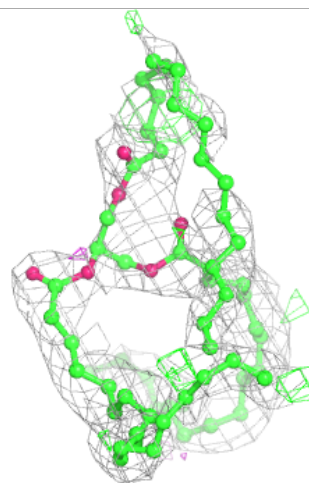
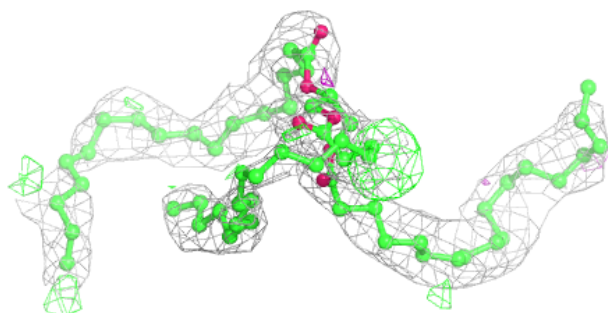
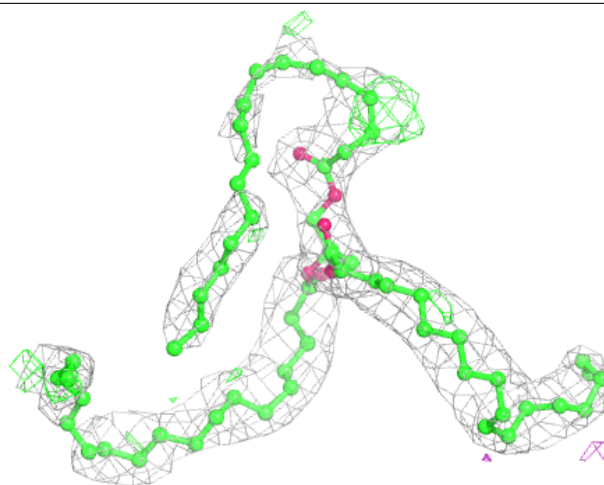
Electron density around CDL P 306:

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



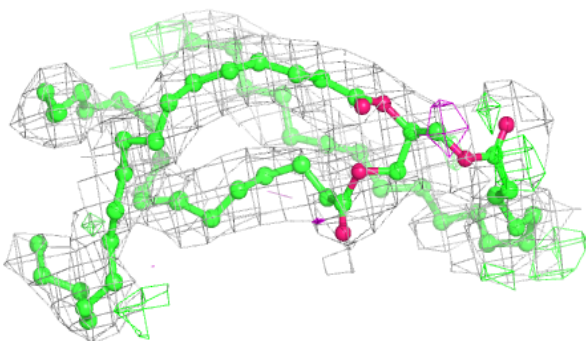
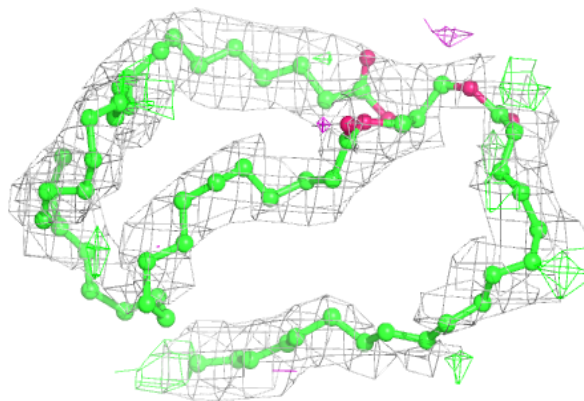
Electron density around TGL L 101:

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

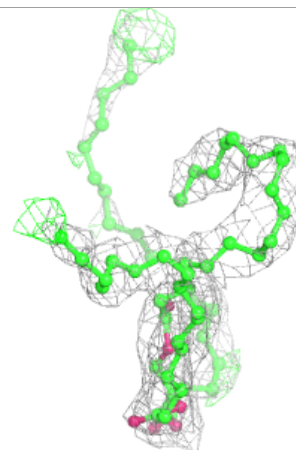
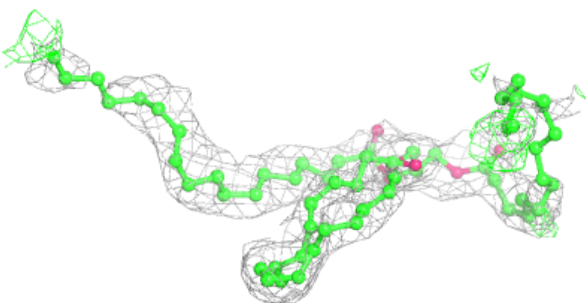
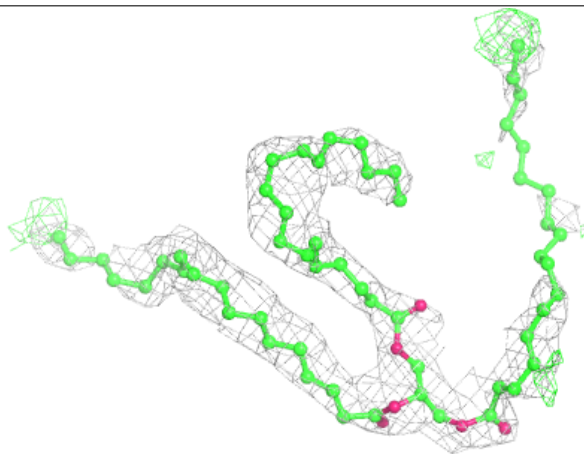


Electron density around TGL V 101:

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

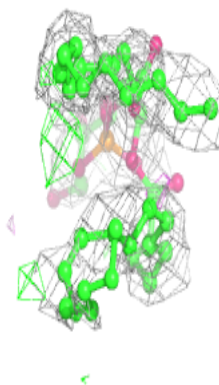
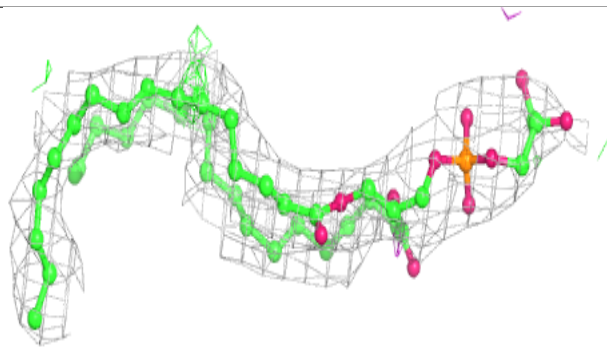
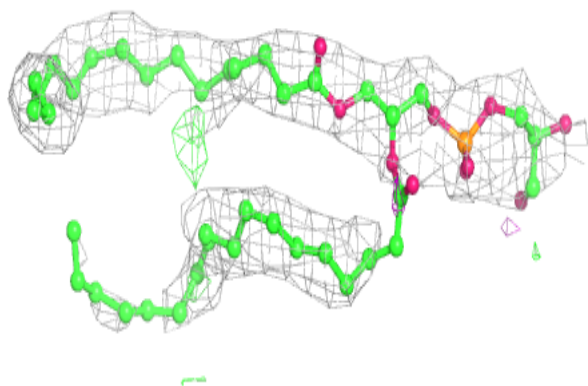
**Electron density around TGL O 304:**

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



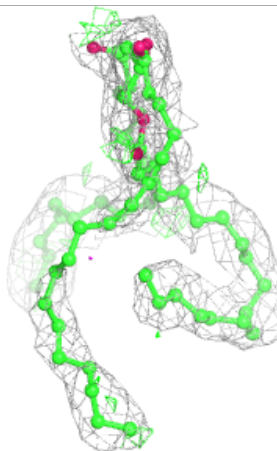
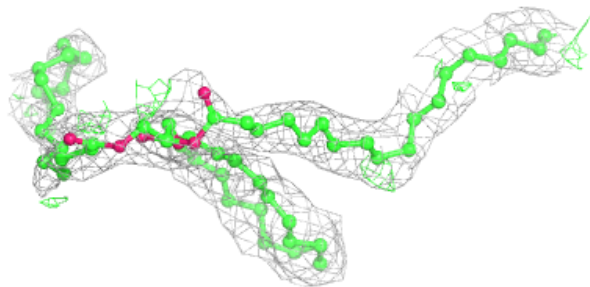
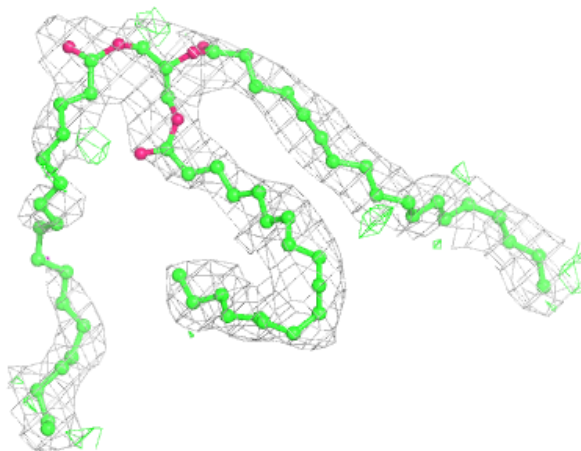
Electron density around PGV A 607:

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



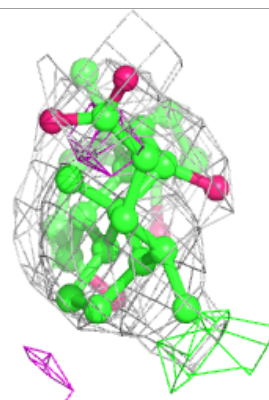
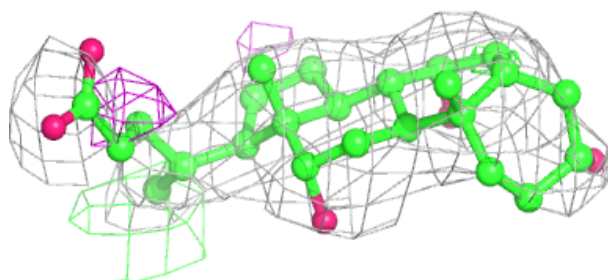
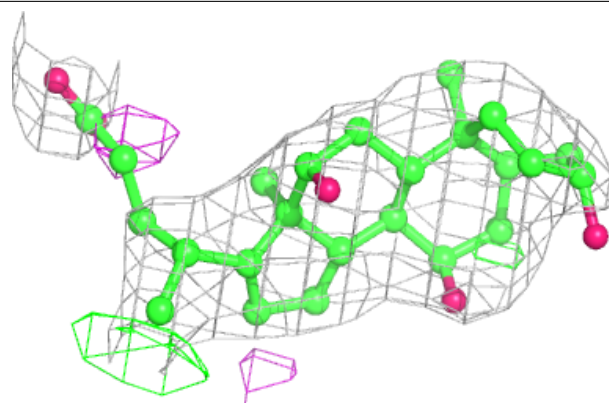
Electron density around TGL A 608:

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

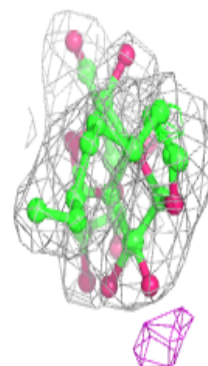
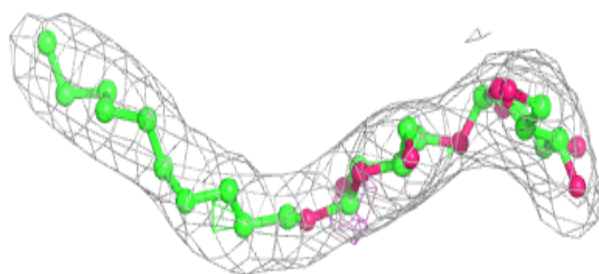
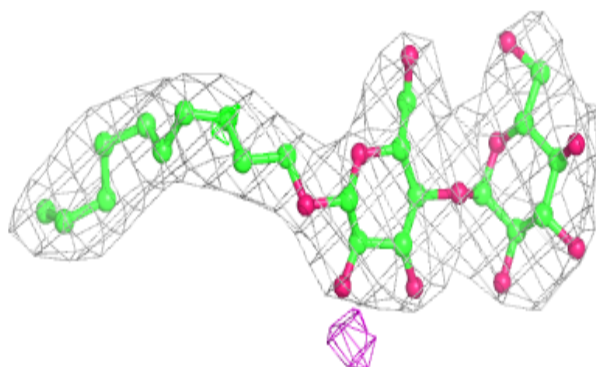


Electron density around CHD J 101:

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

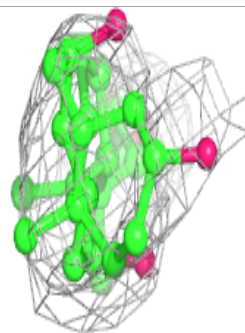
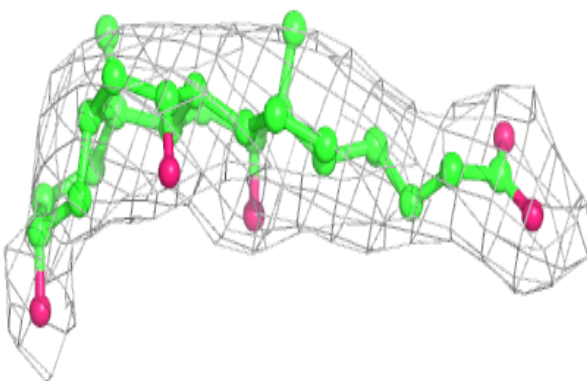
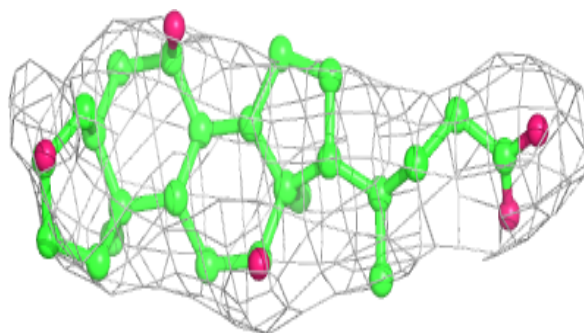
**Electron density around DMU M 101:**

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

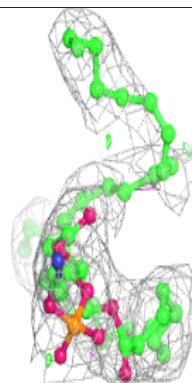
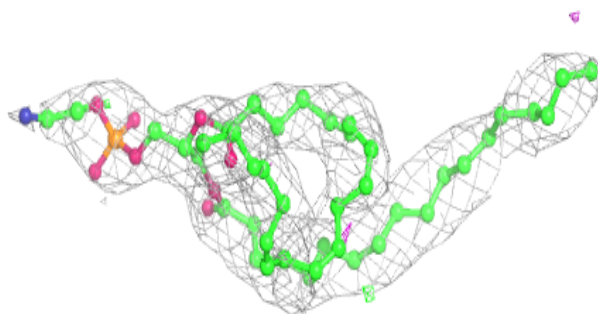
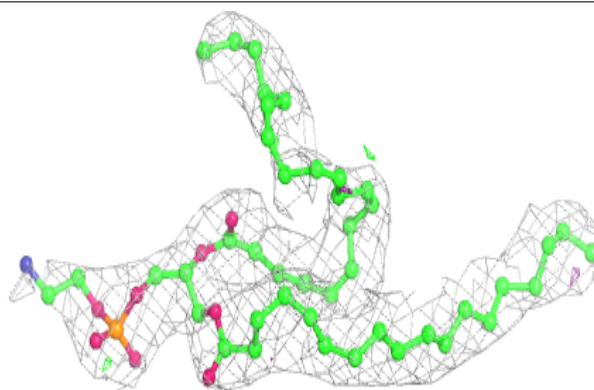


Electron density around CHD P 307:

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

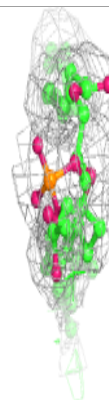
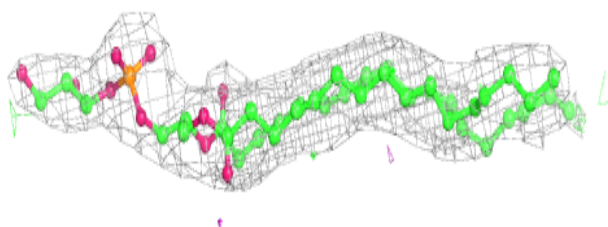
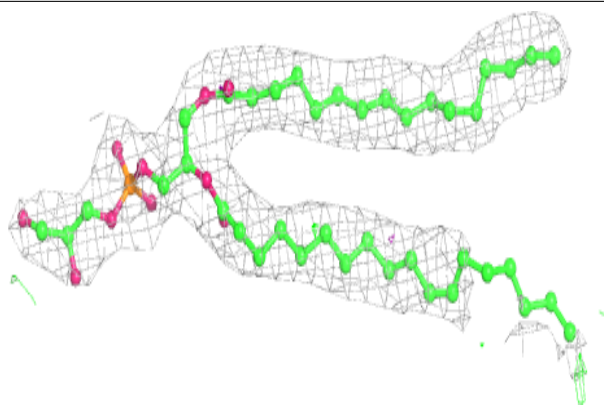
**Electron density around PEK P 303:**

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

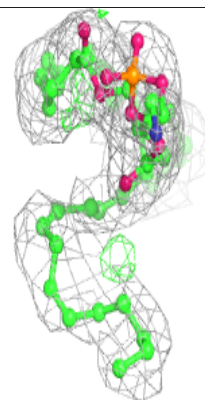
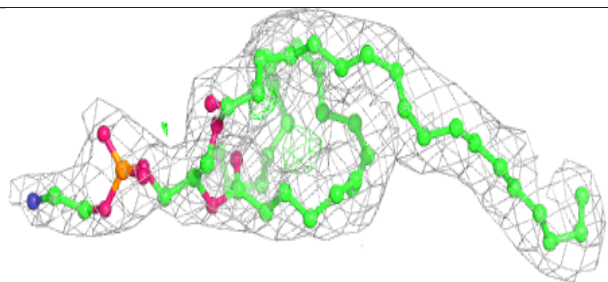
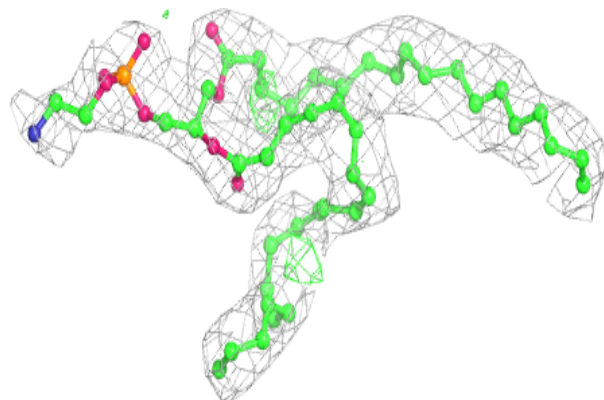


Electron density around PGV P 304:

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

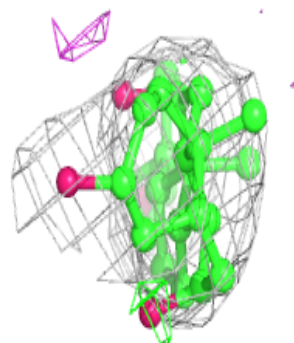
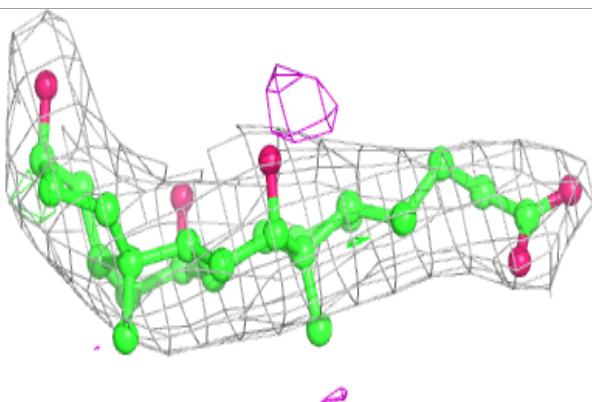
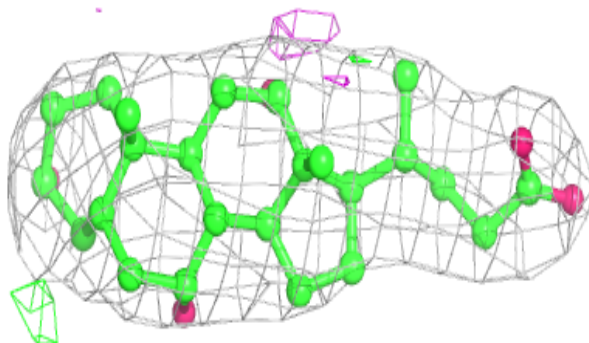
**Electron density around PEK G 101:**

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

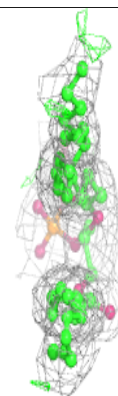
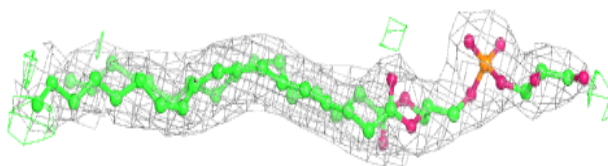
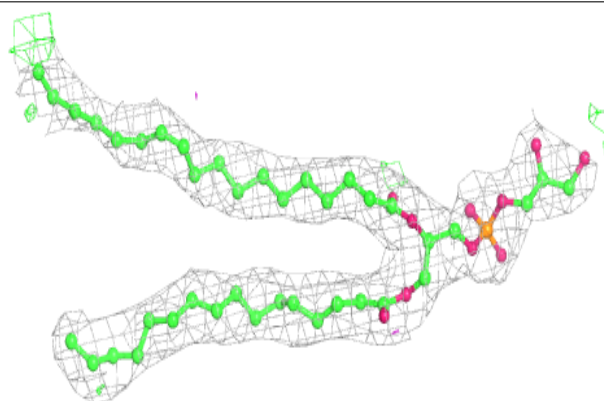


Electron density around CHD C 307:

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

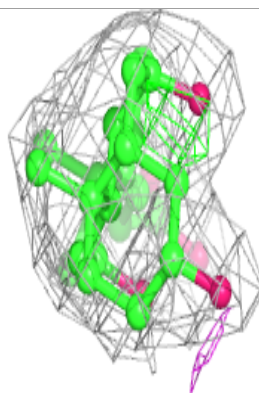
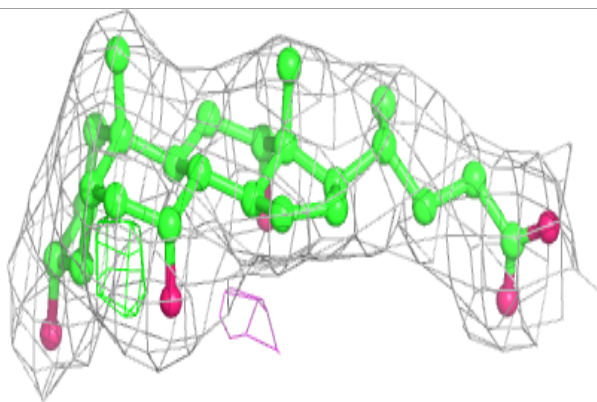
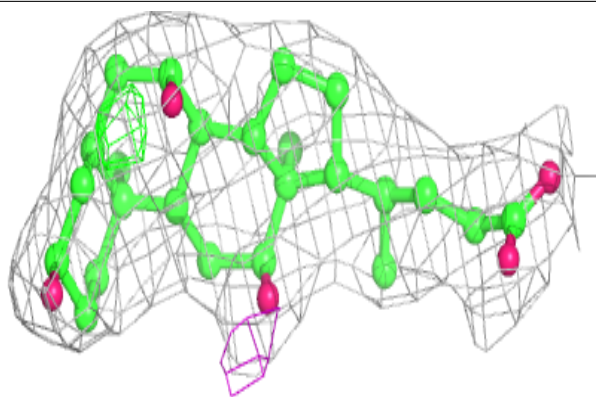
**Electron density around PGV C 305:**

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

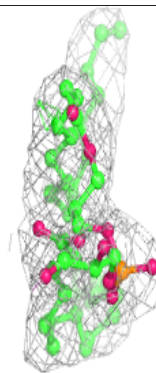
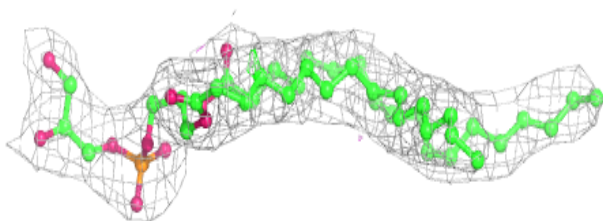
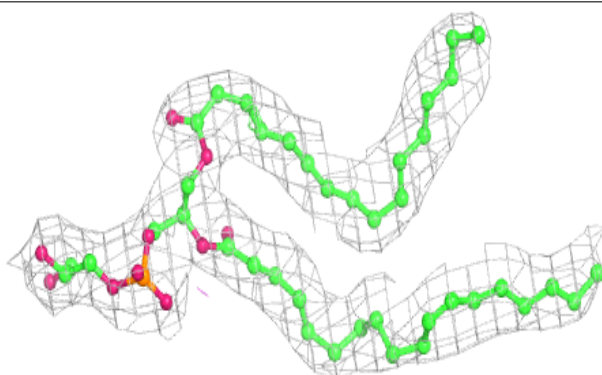


Electron density around CHD P 302:

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

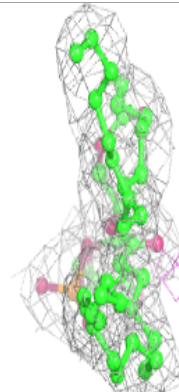
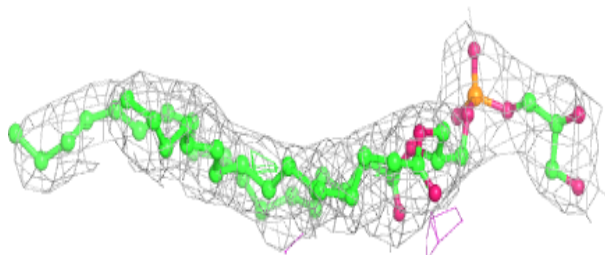
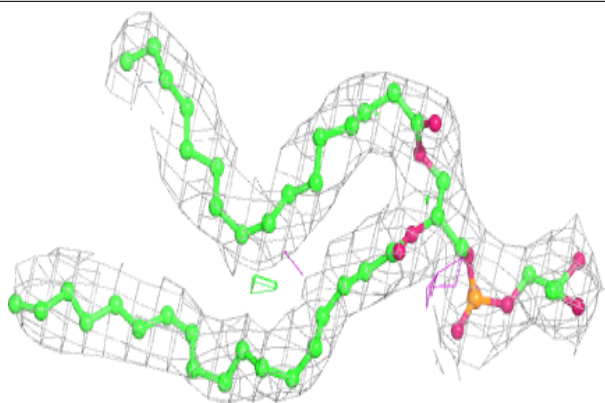
**Electron density around PGV P 301:**

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

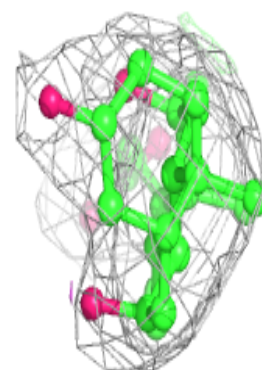
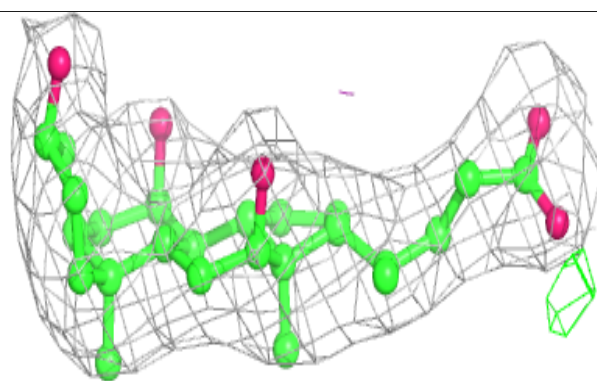
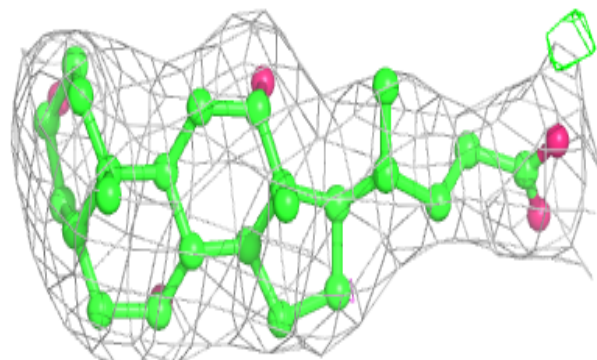


Electron density around PGV C 301:

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

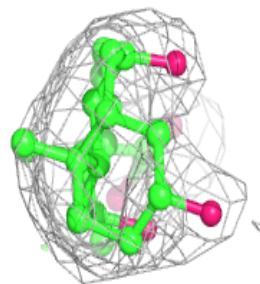
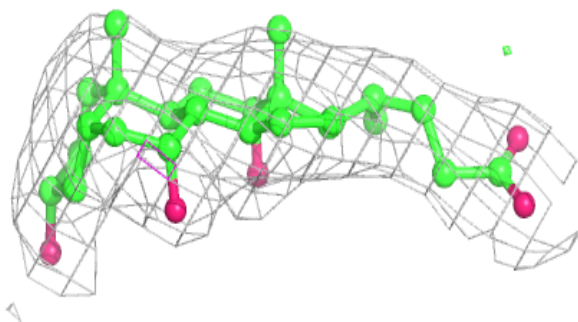
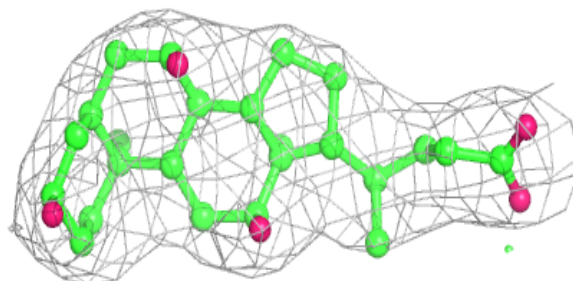
**Electron density around CHD O 302:**

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

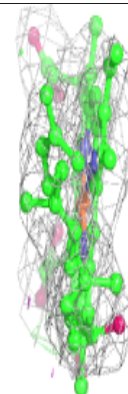
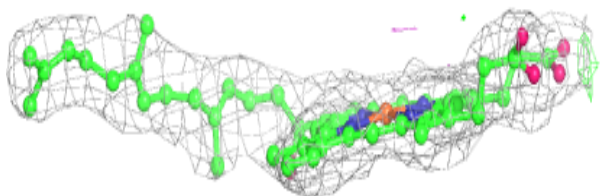
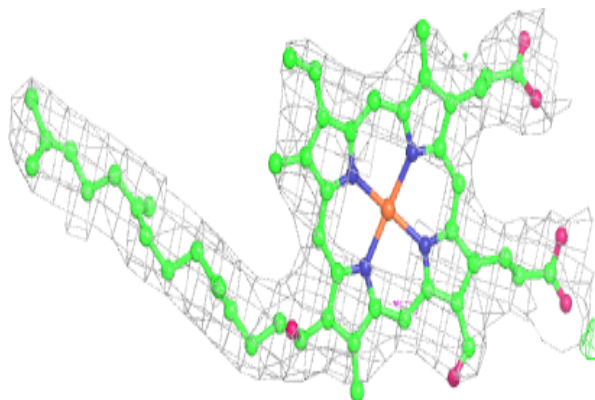


Electron density around CHD B 303:

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

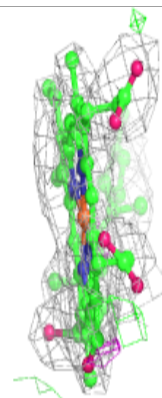
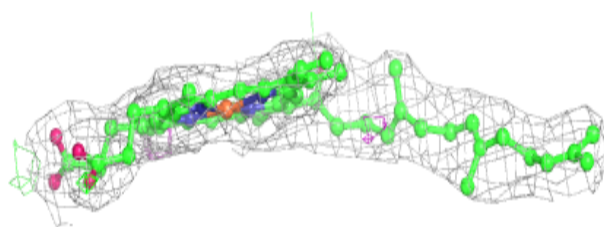
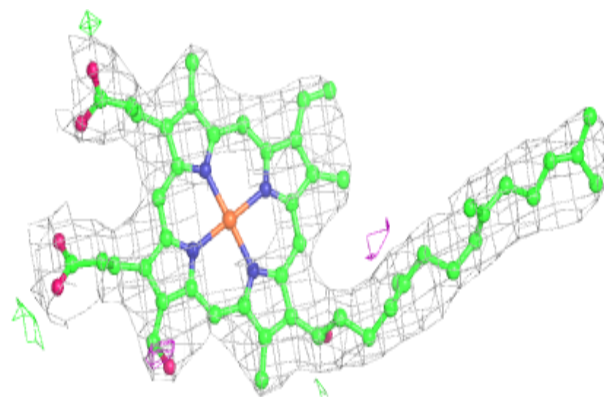
**Electron density around HEA N 604:**

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

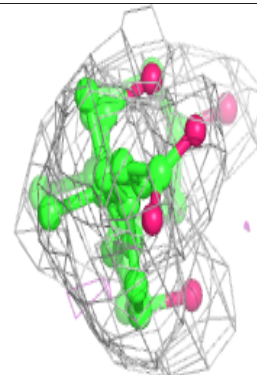
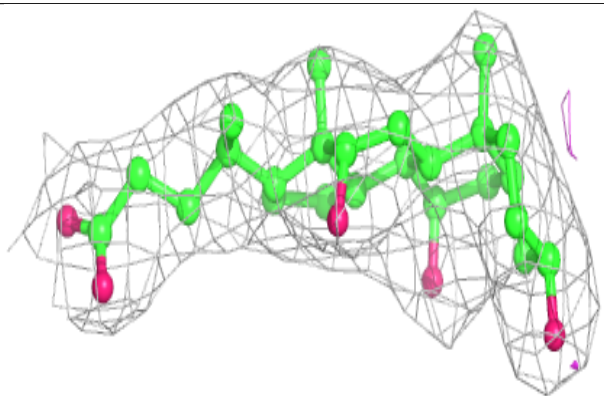
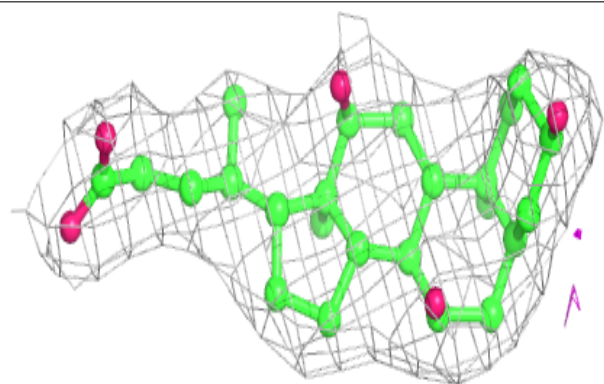


Electron density around HEA A 604:

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

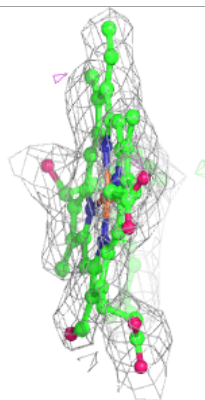
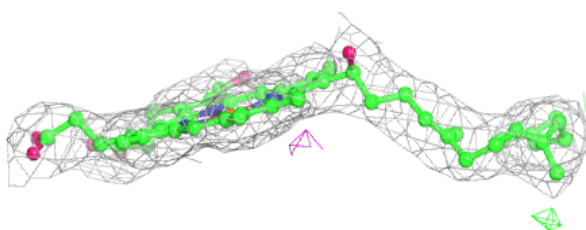
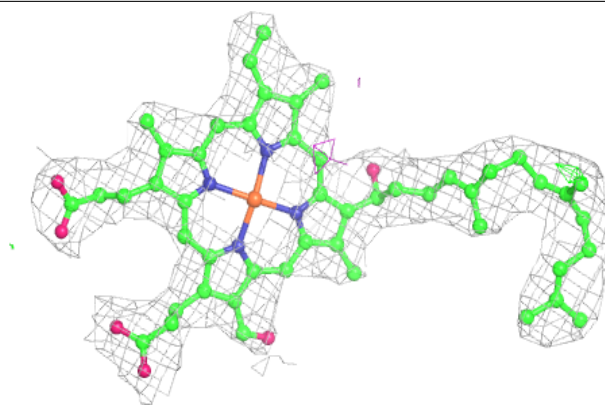
**Electron density around CHD C 303:**

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

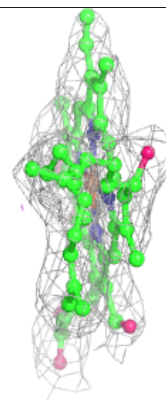
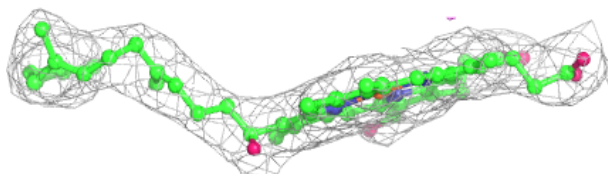
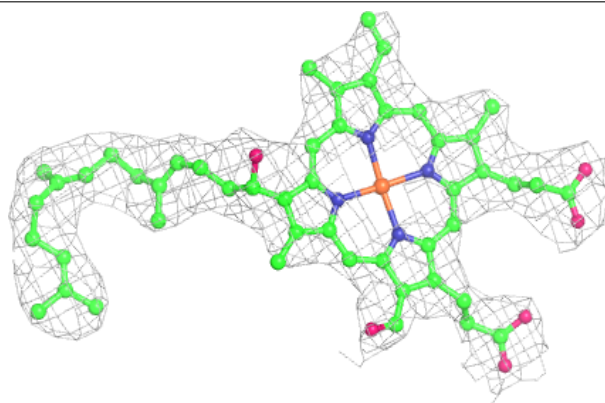


Electron density around HEA A 605:

$2mF_o-DF_c$ (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.