



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 09:10 pm BST

PDB ID : 5XDQ  
Title : Bovine heart cytochrome c oxidase in the fully oxidized state with pH 7.3 at 1.77 angstrom resolution  
Authors : Luo, F.J.; Shimada, A.; Hagimoto, N.; Shimada, S.; Shinzawa-Itoh, K.; Yamashita, E.; Yoshikawa, S.; Tsukihara, T.  
Deposited on : 2017-03-29  
Resolution : 1.77 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](mailto: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.

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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

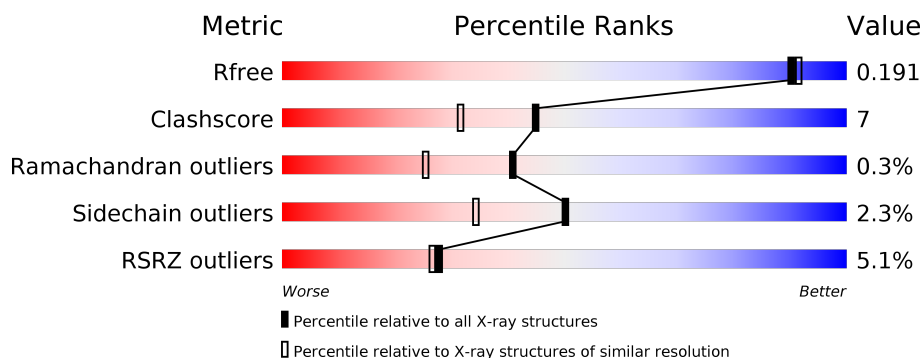
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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  $\geq 3$ , 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>85%</div> <div>15%</div> <div>.</div> </div>
1	N	514	<div> <div>89%</div> <div>11%</div> </div>
2	B	227	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
2	O	227	<div> <div>4%</div> <div>87%</div> <div>13%</div> </div>
3	C	261	<div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	P	261	<div> <div>86%</div> <div>13%</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	94	
6	S	94	
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
14	HEA	A	602	X	-	-	-
14	HEA	N	602	X	-	-	-
20	EDO	A	619	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	EDO	T	105	-	-	-	X
20	EDO	W	102	-	-	-	X
27	DMU	C	313	-	-	-	X
27	DMU	W	104	-	-	-	X



## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 34218 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	33	0
			4118	2757	626	690	45			
1	N	514	Total	C	N	O	S	0	30	0
			4109	2744	627	689	49			

- 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	11	0
			1859	1207	285	345	22			
2	O	227	Total	C	N	O	S	0	10	0
			1851	1200	284	345	22			

- 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	13	0
			2143	1434	336	357	16			
3	P	259	Total	C	N	O	S	0	12	0
			2140	1430	337	357	16			

- 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	1	0
			1200	780	198	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	2	0
			858	549	144	162	3			
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	94	Total	C	N	O	S	0	1	0
			719	446	127	140	6			
6	S	94	Total	C	N	O	S	0	2	0
			722	449	127	140	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
7	G	84	Total 674	C 431	N 129	O 112	P 1	S 1	0	0	0
7	T	84	Total 674	C 431	N 129	O 112	P 1	S 1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	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	2	0
			466	301	78	83	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	1	0
			462	299	78	81	4			

- 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	1	0
			388	254	65	66	3			
11	X	49	Total	C	N	O	S	0	0	0
			383	250	65	66	2			

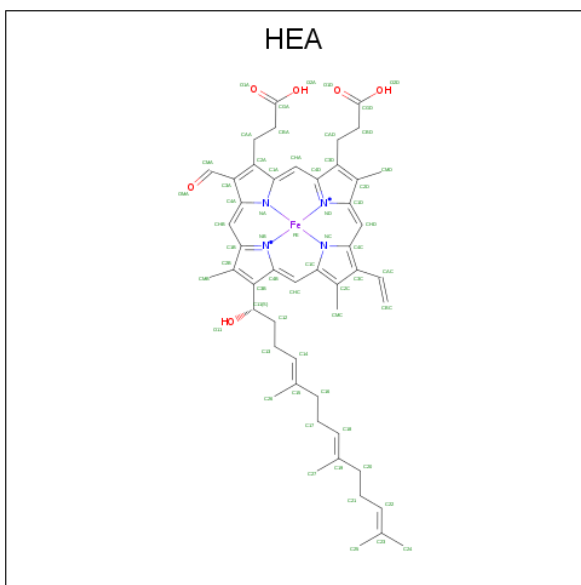
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	4	0
			399	266	66	64	3			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	60	3			

- 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	1	0
			339	228	53	58			
13	Z	43	Total	C	N	O	0	0	0
			334	223	53	58			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
14	N	1	Total 69	C 58	Fe 1	N 4	O 6	0	1
14	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

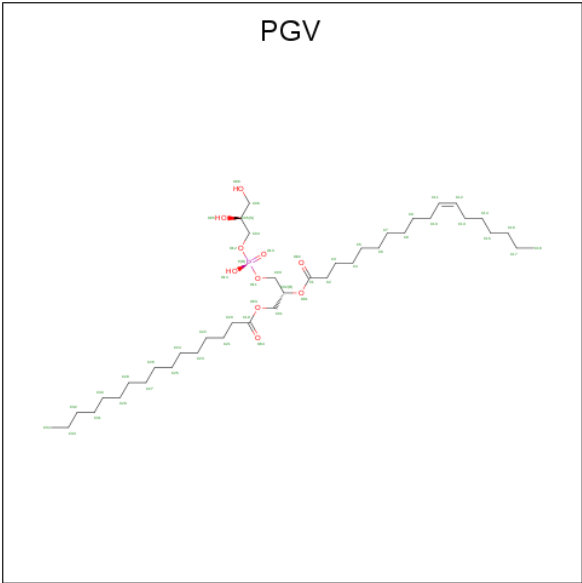
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- 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: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



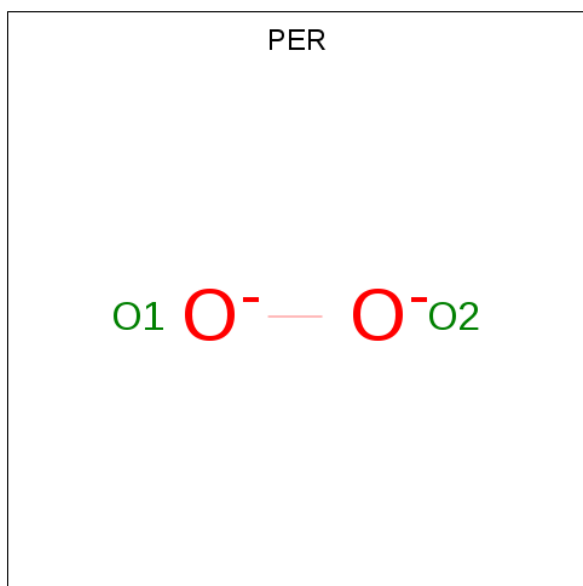
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	1	Total C O P 51 40 10 1	0	0
18	A	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	C	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	N	1	Total C O P 51 40 10 1	0	0
18	P	1	Total C O P 51 40 10 1	0	0

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

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	1
			4	4		
19	N	1	Total	O	0	1
			4	4		

- Molecule 20 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

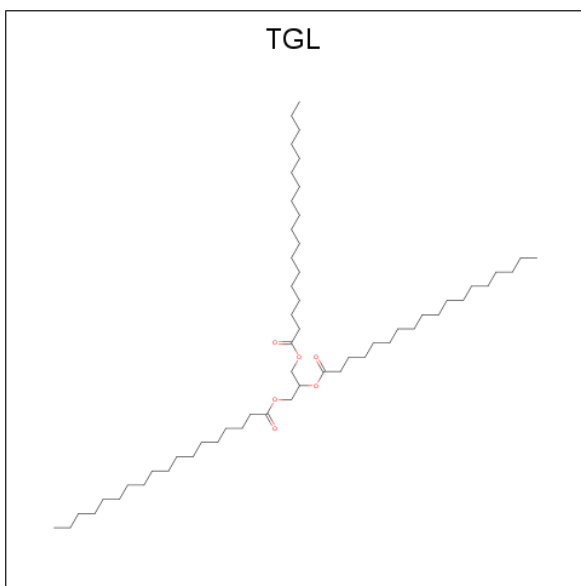
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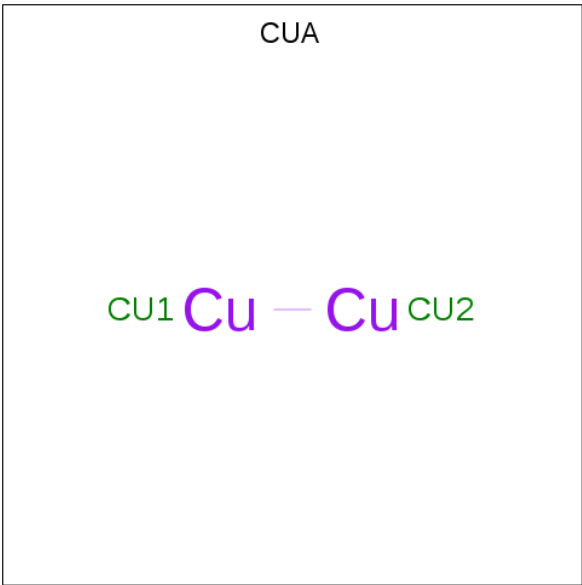
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	N	1	Total 4	C 2	O 2	0	0
20	O	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	P	1	Total 4	C 2	O 2	0	0
20	Q	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	R	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	S	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	T	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	W	1	Total 4	C 2	O 2	0	0
20	Y	1	Total 4	C 2	O 2	0	0

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula:  $C_{57}H_{110}O_6$ ).



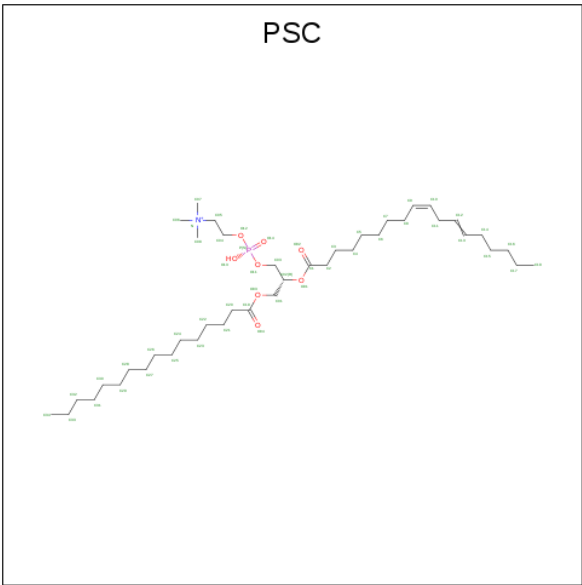
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	O	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula:  $Cu_2$ ).



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

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



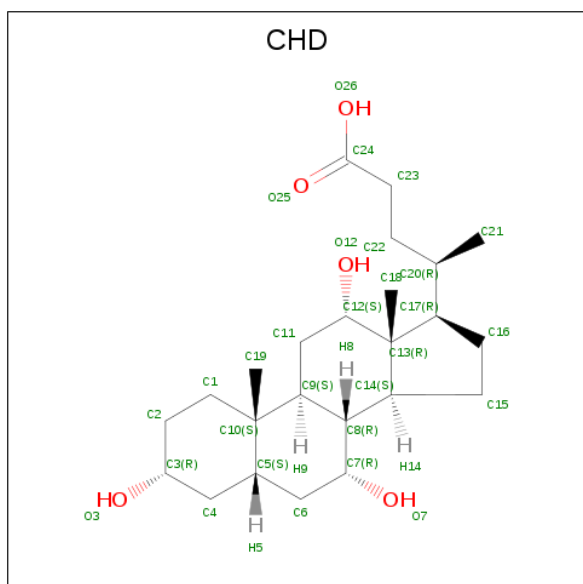
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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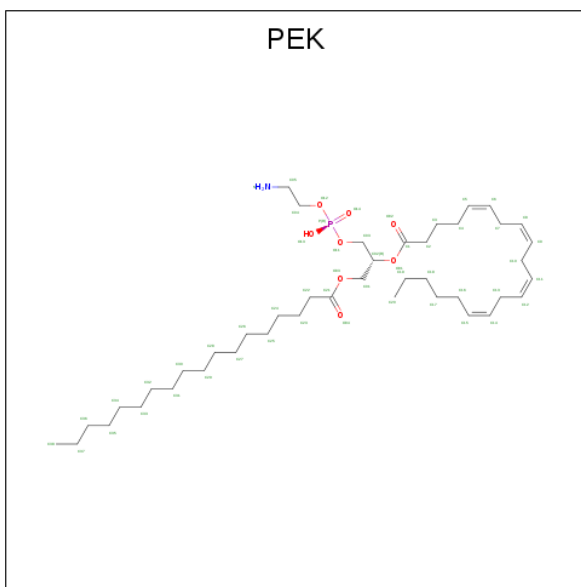
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



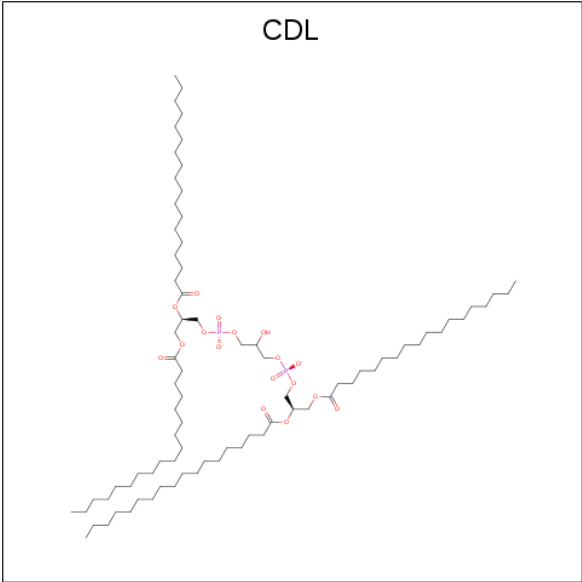
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	B	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	C	1	Total	C	O	0	0
			29	24	5		
24	G	1	Total	C	O	0	0
			29	24	5		
24	J	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	P	1	Total	C	O	0	0
			29	24	5		
24	W	1	Total	C	O	0	0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

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula:  $C_{43}H_{78}NO_8P$ ).



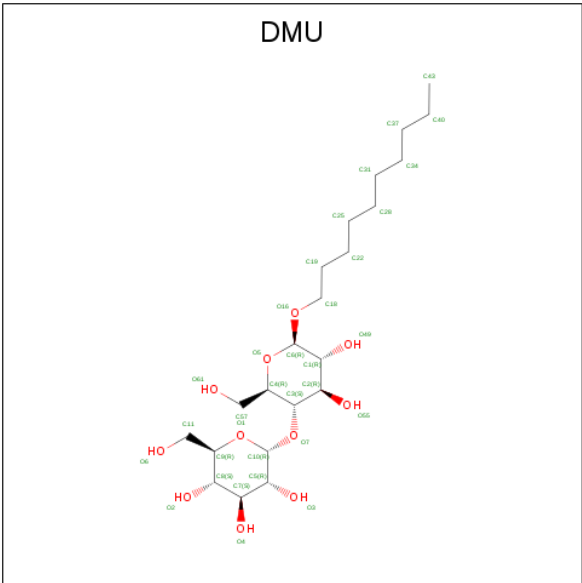
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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 DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	257	Total O 257 257	0	0
29	B	229	Total O 230 230	0	1
29	C	164	Total O 164 164	0	0
29	D	214	Total O 214 214	0	0
29	E	154	Total O 154 154	0	0
29	F	162	Total O 162 162	0	0
29	G	95	Total O 95 95	0	0
29	H	84	Total O 84 84	0	0
29	I	78	Total O 78 78	0	0
29	J	44	Total O 44 44	0	0

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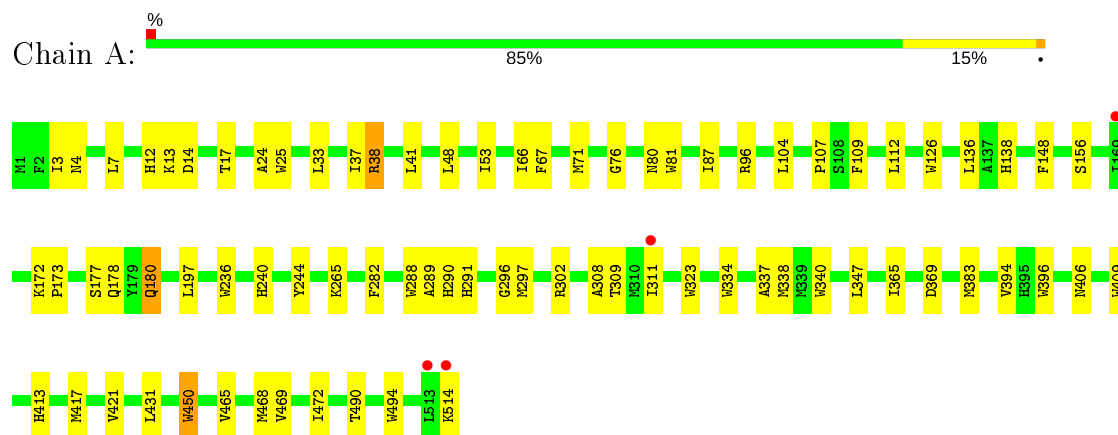
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	K	42	Total 42	O 42	0	0
29	L	57	Total 57	O 57	0	0
29	M	29	Total 29	O 29	0	0
29	N	267	Total 267	O 267	0	0
29	O	186	Total 186	O 186	0	0
29	P	151	Total 151	O 151	0	0
29	Q	98	Total 98	O 98	0	0
29	R	115	Total 115	O 115	0	0
29	S	126	Total 126	O 126	0	0
29	T	87	Total 87	O 87	0	0
29	U	74	Total 74	O 74	0	0
29	V	57	Total 57	O 57	0	0
29	W	32	Total 32	O 32	0	0
29	X	22	Total 22	O 22	0	0
29	Y	37	Total 37	O 37	0	0
29	Z	21	Total 21	O 21	0	0



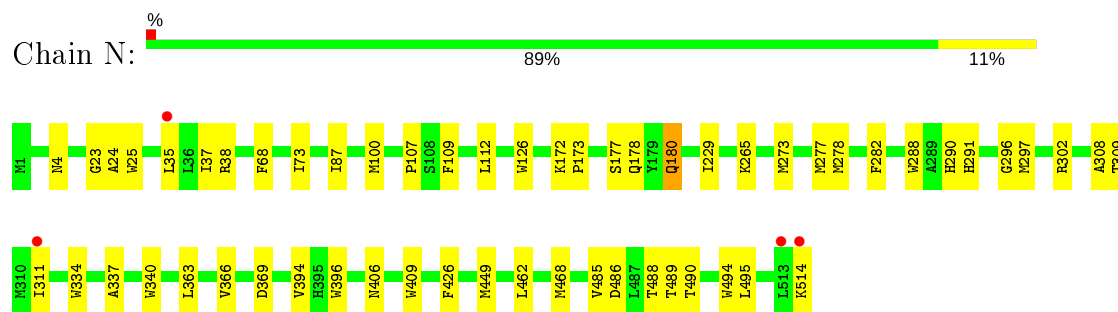
### 3 Residue-property plots [i](#)

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.

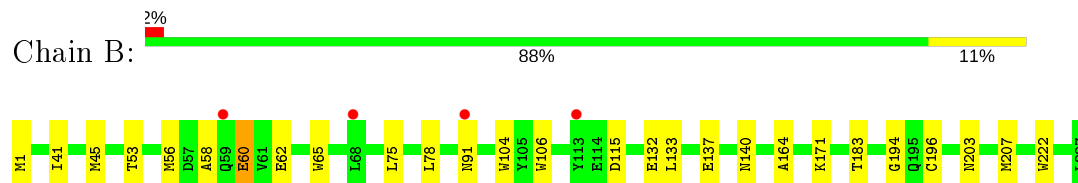
#### • Molecule 1: Cytochrome c oxidase subunit 1



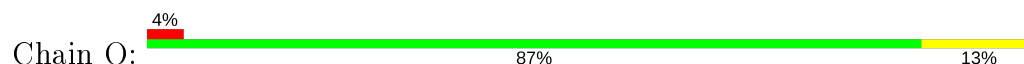
#### • Molecule 1: Cytochrome c oxidase subunit 1

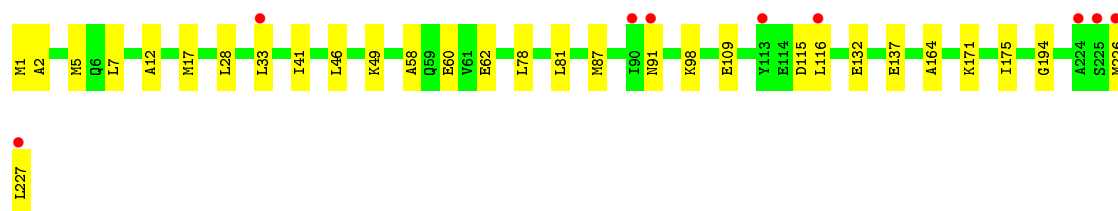


#### • Molecule 2: Cytochrome c oxidase subunit 2

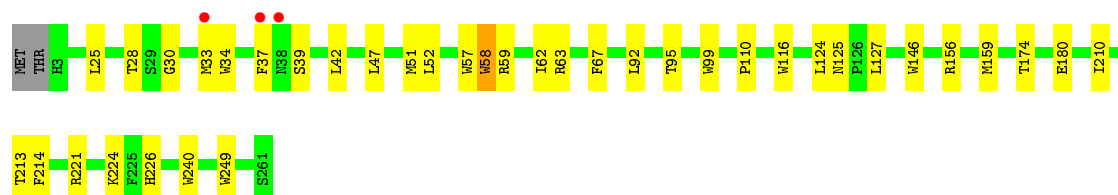
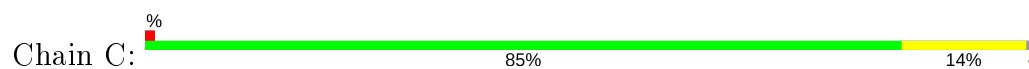


#### • Molecule 2: Cytochrome c oxidase subunit 2

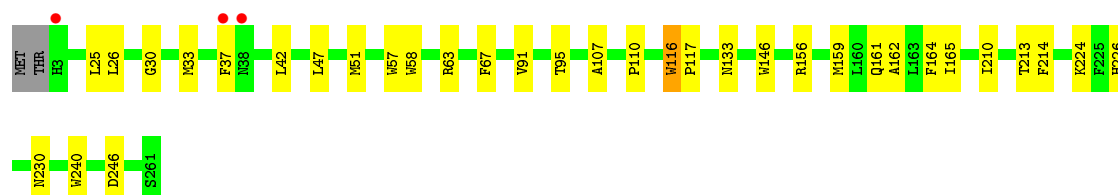
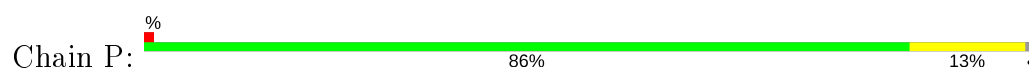




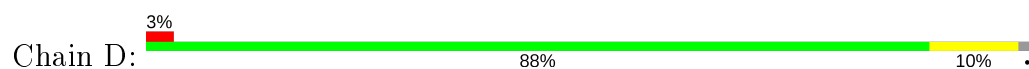
• Molecule 3: Cytochrome c oxidase subunit 3



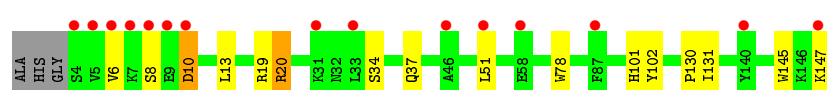
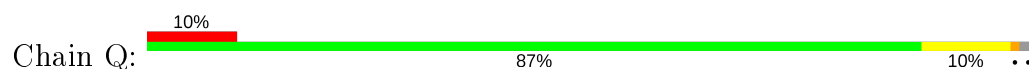
• Molecule 3: Cytochrome c oxidase subunit 3



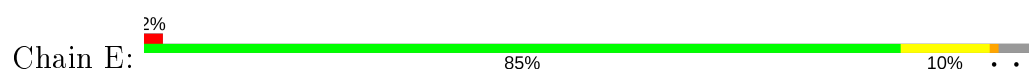
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



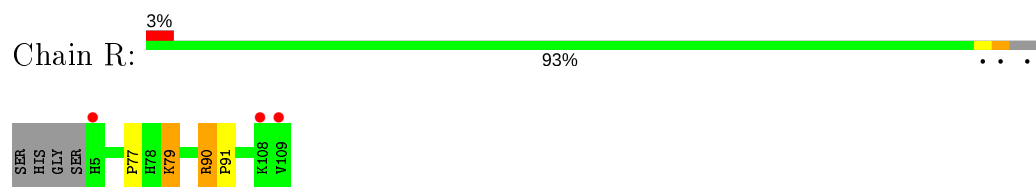
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



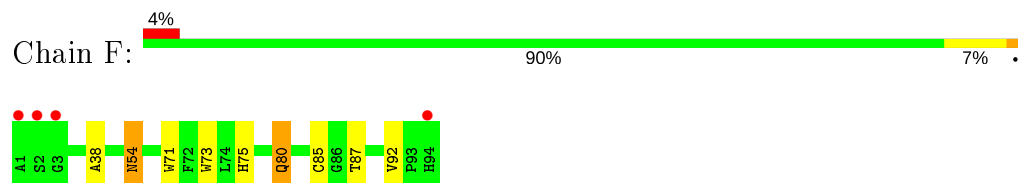
• Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



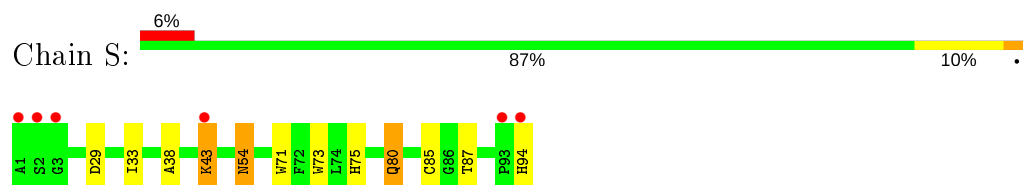
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



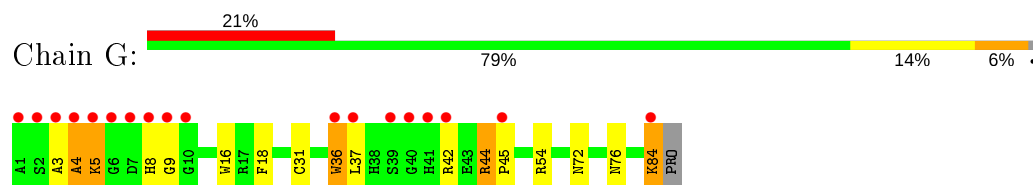
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



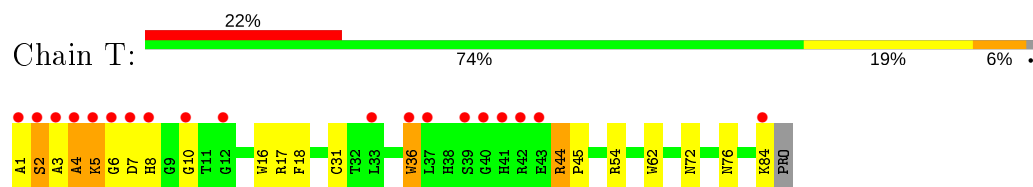
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



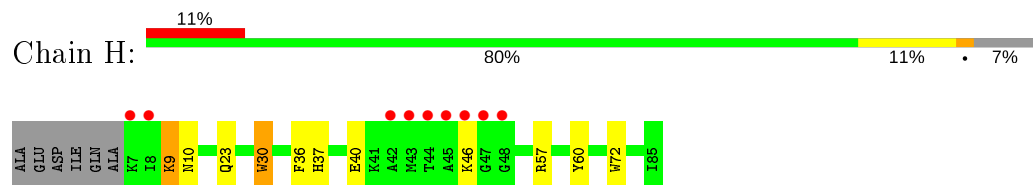
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



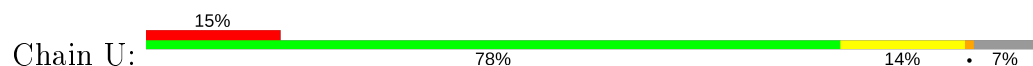
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

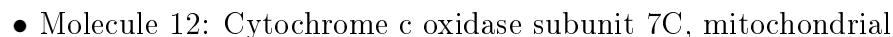


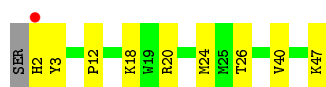
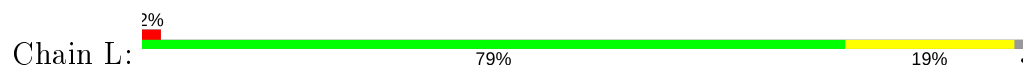
- Molecule 8: Cytochrome c oxidase subunit 6B1



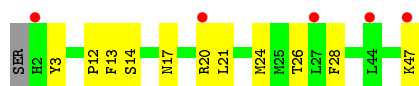
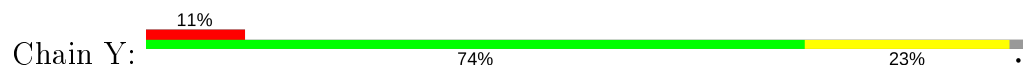
- Molecule 8: Cytochrome c oxidase subunit 6B1



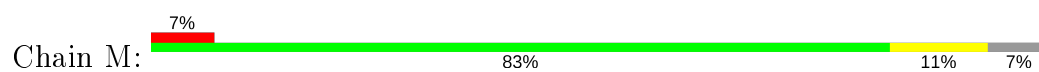




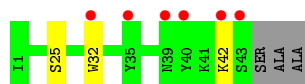
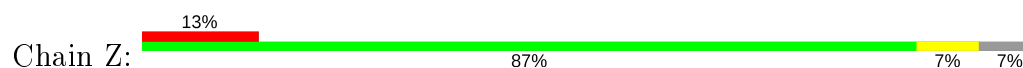
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.31Å 205.90Å 177.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.45 – 1.77 134.45 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.6 (134.45-1.77) 99.7 (134.45-1.77)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.164 , 0.190 0.166 , 0.191	Depositor DCC
$R_{free}$ test set	32362 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 85.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, EDO, 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	0.65	10/4405 (0.2%)	0.58	1/6009 (0.0%)
1	N	0.62	7/4385 (0.2%)	0.57	0/5979
2	B	0.55	3/1946 (0.2%)	0.64	0/2648
2	O	0.51	0/1938	0.57	0/2637
3	C	0.70	7/2298 (0.3%)	0.52	0/3139
3	P	0.69	4/2292 (0.2%)	0.53	0/3131
4	D	0.62	4/1229 (0.3%)	0.53	0/1658
4	Q	0.58	2/1240 (0.2%)	0.51	0/1673
5	E	0.52	0/886	0.53	0/1202
5	R	0.49	0/871	0.53	0/1182
6	F	0.55	2/740 (0.3%)	0.58	0/1003
6	S	0.52	1/748 (0.1%)	0.54	0/1014
7	G	0.68	2/689 (0.3%)	0.60	0/936
7	T	0.67	3/689 (0.4%)	0.59	0/936
8	H	0.62	2/682 (0.3%)	0.54	0/921
8	U	0.62	2/682 (0.3%)	0.52	0/921
9	I	0.40	0/605	0.49	0/802
9	V	0.37	0/605	0.48	0/802
10	J	0.51	0/487	0.49	0/657
10	W	0.51	0/478	0.48	0/645
11	K	0.67	1/405 (0.2%)	0.51	0/555
11	X	0.66	0/397	0.49	0/545
12	L	0.59	0/430	0.51	0/575
12	Y	0.54	0/401	0.49	0/536
13	M	0.54	0/352	0.50	0/480
13	Z	0.52	1/344 (0.3%)	0.47	0/469
All	All	0.60	51/30224 (0.2%)	0.55	1/41055 (0.0%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	57	TRP	CD2-CE2	5.75	1.48	1.41
3	C	57	TRP	CD2-CE2	5.73	1.48	1.41
1	A	288	TRP	CD2-CE2	5.54	1.48	1.41
1	A	340	TRP	CD2-CE2	5.49	1.48	1.41
7	G	16	TRP	CD2-CE2	5.46	1.48	1.41
1	A	409	TRP	CD2-CE2	5.44	1.47	1.41
3	C	58	TRP	CD2-CE2	5.43	1.47	1.41
11	K	29	TRP	CD2-CE2	5.40	1.47	1.41
3	P	240	TRP	CD2-CE2	5.38	1.47	1.41
3	P	58	TRP	CD2-CE2	5.37	1.47	1.41
1	A	126	TRP	CD2-CE2	5.35	1.47	1.41
1	N	340	TRP	CD2-CE2	5.32	1.47	1.41
1	A	323	TRP	CD2-CE2	5.31	1.47	1.41
3	P	116	TRP	CD2-CE2	5.31	1.47	1.41
2	B	65	TRP	CD2-CE2	5.29	1.47	1.41
4	D	48	TRP	CD2-CE2	5.29	1.47	1.41
1	A	236	TRP	CD2-CE2	5.28	1.47	1.41
8	H	72	TRP	CD2-CE2	5.28	1.47	1.41
1	N	494	TRP	CD2-CE2	5.25	1.47	1.41
7	T	36	TRP	CD2-CE2	5.24	1.47	1.41
2	B	222	TRP	CD2-CE2	5.23	1.47	1.41
3	C	116	TRP	CD2-CE2	5.23	1.47	1.41
8	U	72	TRP	CD2-CE2	5.22	1.47	1.41
3	C	249	TRP	CD2-CE2	5.22	1.47	1.41
1	A	396	TRP	CD2-CE2	5.21	1.47	1.41
1	N	396	TRP	CD2-CE2	5.21	1.47	1.41
7	T	16	TRP	CD2-CE2	5.20	1.47	1.41
1	N	288	TRP	CD2-CE2	5.20	1.47	1.41
8	H	30	TRP	CD2-CE2	5.17	1.47	1.41
7	G	36	TRP	CD2-CE2	5.17	1.47	1.41
1	N	126	TRP	CD2-CE2	5.15	1.47	1.41
3	C	99	TRP	CD2-CE2	5.14	1.47	1.41
4	D	98	TRP	CD2-CE2	5.14	1.47	1.41
4	Q	78	TRP	CD2-CE2	5.14	1.47	1.41
3	C	34	TRP	CD2-CE2	5.12	1.47	1.41
6	S	73	TRP	CD2-CE2	5.12	1.47	1.41
2	B	106	TRP	CD2-CE2	5.11	1.47	1.41
1	A	450	TRP	CD2-CE2	5.09	1.47	1.41
4	D	115	TRP	CD2-CE2	5.09	1.47	1.41
1	N	409	TRP	CD2-CE2	5.08	1.47	1.41
1	N	25	TRP	CD2-CE2	5.08	1.47	1.41
1	A	25	TRP	CD2-CE2	5.06	1.47	1.41
6	F	73	TRP	CD2-CE2	5.06	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	145	TRP	CD2-CE2	5.06	1.47	1.41
7	T	62	TRP	CD2-CE2	5.04	1.47	1.41
6	F	71	TRP	CD2-CE2	5.04	1.47	1.41
13	Z	32	TRP	CD2-CE2	5.04	1.47	1.41
8	U	55	TRP	CD2-CE2	5.02	1.47	1.41
1	A	334	TRP	CD2-CE2	5.02	1.47	1.41
3	C	146	TRP	CD2-CE2	5.01	1.47	1.41
4	D	138	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4118	0	4147	75	0
1	N	4109	0	4118	57	0
2	B	1859	0	1889	17	0
2	O	1851	0	1866	23	0
3	C	2143	0	2072	40	0
3	P	2140	0	2058	33	0
4	D	1195	0	1183	15	0
4	Q	1200	0	1186	7	0
5	E	858	0	855	21	0
5	R	852	0	845	2	0
6	F	719	0	702	6	0
6	S	722	0	709	10	0
7	G	674	0	644	14	0
7	T	674	0	644	15	0
8	H	662	0	623	7	0
8	U	662	0	623	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	601	0	613	5	0
9	V	601	0	613	7	0
10	J	466	0	466	7	0
10	W	462	0	464	8	0
11	K	388	0	375	1	0
11	X	383	0	366	0	0
12	L	399	0	395	9	0
12	Y	382	0	381	10	0
13	M	339	0	363	6	0
13	Z	334	0	352	2	0
14	A	129	0	88	8	0
14	N	129	0	88	17	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	102	0	152	8	0
18	C	102	0	152	7	0
18	N	102	0	152	3	0
18	P	51	0	76	1	0
18	U	51	0	76	2	0
19	A	4	0	0	0	0
19	N	4	0	0	0	0
20	A	44	0	66	8	0
20	B	20	0	30	2	0
20	C	12	0	18	0	0
20	E	4	0	6	0	0
20	F	8	0	12	0	0
20	G	4	0	6	0	0
20	H	4	0	6	1	0
20	J	4	0	6	2	0
20	L	16	0	24	2	0
20	M	8	0	12	0	0
20	N	20	0	30	1	0
20	O	4	0	6	0	0
20	P	24	0	36	0	0
20	Q	4	0	6	0	0
20	R	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	S	12	0	18	0	0
20	T	8	0	12	0	0
20	W	8	0	12	0	0
20	Y	4	0	6	0	0
21	B	63	0	110	3	0
21	D	63	0	110	6	0
21	L	63	0	110	4	0
21	N	63	0	110	4	0
21	O	63	0	110	4	0
21	Q	63	0	110	2	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	52	0	80	6	0
23	O	52	0	80	5	0
24	B	29	0	39	1	0
24	C	58	0	78	2	0
24	G	29	0	39	0	0
24	J	29	0	39	2	0
24	P	58	0	78	5	0
24	W	29	0	39	2	0
25	C	106	0	154	6	0
25	G	53	0	77	1	0
25	P	53	0	77	2	0
25	T	106	0	154	7	0
26	C	100	0	156	16	0
26	G	100	0	156	12	0
26	P	100	0	156	9	0
26	T	100	0	156	7	0
27	C	66	0	84	10	0
27	M	33	0	42	0	0
27	P	33	0	42	0	0
27	W	33	0	42	11	0
27	Z	33	0	42	1	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	A	257	0	0	3	0
29	B	230	0	0	4	0
29	C	164	0	0	1	0
29	D	214	0	0	6	0
29	E	154	0	0	3	0
29	F	162	0	0	0	0
29	G	95	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	H	84	0	0	1	0
29	I	78	0	0	1	0
29	J	44	0	0	0	0
29	K	42	0	0	1	0
29	L	57	0	0	4	0
29	M	29	0	0	0	0
29	N	267	0	0	3	0
29	O	186	0	0	0	0
29	P	151	0	0	2	0
29	Q	98	0	0	0	0
29	R	115	0	0	0	0
29	S	126	0	0	1	0
29	T	87	0	0	1	0
29	U	74	0	0	0	0
29	V	57	0	0	2	0
29	W	32	0	0	1	0
29	X	22	0	0	0	0
29	Y	37	0	0	0	0
29	Z	21	0	0	0	0
All	All	34218	0	32142	413	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 7.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33[A]:MET:SD	27:C:313:DMU:H11	1.64	1.36
27:C:313:DMU:H8	10:J:53:ALA:HB2	1.25	1.18
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C23	1.77	1.13
3:P:33[A]:MET:SD	27:W:104:DMU:H11	1.88	1.13
1:A:468[B]:MET:HE1	14:A:601[B]:HEA:H212	1.35	1.09
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C24	1.82	1.09
1:N:468[B]:MET:CE	14:N:601[B]:HEA:C23	2.34	1.04
5:E:37:VAL:HG11	5:E:70[B]:VAL:HG11	1.39	1.03
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:H243	1.35	1.03
27:C:313:DMU:C19	10:J:53:ALA:HB2	1.95	0.96
2:O:41:ILE:HD13	23:O:303:PSC:H342	1.47	0.96
1:A:468[B]:MET:CE	14:A:601[B]:HEA:H212	1.98	0.92
3:C:67:PHE:HE2	26:C:307:CDL:H1	1.36	0.90
10:W:53:ALA:HB2	27:W:104:DMU:C19	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136[A]:LEU:HD23	20:B:306:EDO:H21	1.55	0.88
7:G:84:LYS:HD2	7:G:84:LYS:H	1.36	0.87
3:P:33[A]:MET:HG3	3:P:42[A]:LEU:HD12	1.55	0.86
6:S:43:LYS:H	6:S:43:LYS:HD2	1.40	0.85
6:S:43:LYS:CD	6:S:43:LYS:H	1.90	0.84
25:C:303:PEK:HN2	7:G:76:ASN:HD21	1.25	0.83
14:A:602:HEA:HBC1	14:A:602:HEA:HMC1	1.60	0.83
3:C:92:LEU:O	3:C:95[B]:THR:HG22	1.79	0.83
3:P:63:ARG:HE	26:P:305:CDL:HA22	1.40	0.83
6:F:75:HIS:H	6:F:80:GLN:HE22	1.28	0.81
6:S:75:HIS:H	6:S:80:GLN:HE22	1.24	0.81
3:C:224:LYS:HD3	26:C:307:CDL:HB31	1.62	0.81
3:C:33[A]:MET:SD	27:C:313:DMU:C22	2.59	0.81
6:F:85:CYS:SG	6:F:87:THR:HG23	2.20	0.81
3:C:63:ARG:HE	26:C:307:CDL:HA22	1.46	0.81
5:E:67:ILE:O	5:E:70[A]:VAL:HG22	1.81	0.81
1:N:366[B]:VAL:HG11	2:O:17[B]:MET:CE	2.11	0.81
12:Y:14:SER:O	12:Y:20:ARG:NH2	2.14	0.81
7:G:72:ASN:H	7:G:76:ASN:HD22	1.29	0.80
7:T:72:ASN:H	7:T:76:ASN:HD22	1.29	0.80
9:V:8:GLN:HG2	29:V:101:HOH:O	1.82	0.79
1:N:297[B]:MET:HG3	1:N:302:ARG:HG3	1.65	0.79
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C22	2.12	0.79
1:A:468[B]:MET:HE1	14:A:601[B]:HEA:C21	2.13	0.79
1:N:273:MET:O	1:N:277[B]:MET:HG2	1.82	0.79
14:N:602:HEA:HBC1	14:N:602:HEA:HMC1	1.65	0.78
10:W:53:ALA:HB2	27:W:104:DMU:H9	1.64	0.78
9:V:6:LYS:HE2	29:V:113:HOH:O	1.84	0.75
1:N:468[B]:MET:HE2	14:N:601[B]:HEA:C23	2.15	0.75
1:N:468[B]:MET:CE	14:N:601[B]:HEA:C22	2.64	0.75
21:D:201:TGL:HG32	29:D:312:HOH:O	1.85	0.75
29:D:301:HOH:O	5:E:70[B]:VAL:HG13	1.85	0.74
27:C:313:DMU:H9	10:J:49:CYS:O	1.87	0.74
1:N:366[B]:VAL:HG11	2:O:17[B]:MET:HE1	1.68	0.74
3:C:224:LYS:CD	26:C:307:CDL:HB31	2.18	0.73
10:W:53:ALA:HB2	27:W:104:DMU:H8	1.70	0.73
3:C:62[B]:ILE:HD11	18:C:305:PGV:H21	1.71	0.72
1:N:468[B]:MET:CE	14:N:601[B]:HEA:C24	2.65	0.72
5:E:83:PRO:HB2	29:E:301:HOH:O	1.91	0.71
20:L:103:EDO:H12	29:L:232:HOH:O	1.89	0.71
25:P:303:PEK:HN2	7:T:76:ASN:HD21	1.36	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:303:PSC:H202	23:O:303:PSC:H02	1.73	0.70
5:E:37:VAL:HG11	5:E:70[B]:VAL:CG1	2.20	0.70
3:C:58:TRP:O	3:C:62[B]:ILE:HG12	1.92	0.69
1:A:104:LEU:HB2	1:A:156[B]:SER:OG	1.92	0.69
12:Y:17:ASN:H	12:Y:20:ARG:HH12	1.39	0.69
1:N:297[B]:MET:CG	1:N:302:ARG:HG3	2.23	0.68
2:O:116:LEU:HD13	2:O:226:MET:HG2	1.74	0.68
1:N:297[B]:MET:HG2	29:N:788:HOH:O	1.95	0.67
7:T:5:LYS:HG3	25:T:101:PEK:H351	1.77	0.67
27:C:313:DMU:H10	10:J:49:CYS:HB3	1.76	0.67
4:D:34:SER:H	4:D:37:GLN:HE21	1.42	0.67
2:O:41:ILE:CD1	23:O:303:PSC:H342	2.24	0.67
4:D:23:PRO:HB3	5:E:70[A]:VAL:CG1	2.26	0.66
1:A:178[B]:GLN:HG2	7:T:7:ASP:HB2	1.76	0.66
6:F:54:ASN:HD22	6:F:54:ASN:H	1.44	0.66
3:P:91:VAL:O	3:P:95[B]:THR:HG23	1.95	0.66
26:G:101:CDL:H541	26:G:101:CDL:H242	1.78	0.65
3:P:224:LYS:HD3	26:P:305:CDL:HB31	1.78	0.65
1:A:468[B]:MET:CE	14:A:601[B]:HEA:C21	2.72	0.65
3:P:224:LYS:CD	26:P:305:CDL:HB31	2.27	0.65
1:N:468[B]:MET:CE	14:N:601[B]:HEA:H243	2.21	0.64
1:N:265:LYS:HE3	29:N:940:HOH:O	1.98	0.64
5:E:37:VAL:CG1	5:E:70[B]:VAL:HG11	2.22	0.64
26:G:101:CDL:H432	1:N:311[B]:ILE:HG13	1.80	0.63
29:N:891:HOH:O	25:P:303:PEK:H383	1.98	0.63
21:O:301:TGL:HA72	21:O:301:TGL:H102	1.78	0.63
26:G:101:CDL:H351	2:O:78:LEU:HD12	1.80	0.63
7:G:84:LYS:N	7:G:84:LYS:HD2	2.12	0.63
12:L:24[A]:MET:HG3	29:L:201:HOH:O	1.98	0.62
1:A:468[B]:MET:HE1	20:A:619:EDO:H21	1.80	0.62
1:A:4[B]:ASN:ND2	29:A:701:HOH:O	2.32	0.62
26:T:103:CDL:H171	26:T:103:CDL:HB32	1.81	0.62
1:A:37[B]:ILE:HG13	1:A:38:ARG:N	2.15	0.62
5:E:86:ILE:O	5:E:90:ARG:HG2	2.00	0.62
5:E:12:ASP:HB3	5:E:46:LYS:HE3	1.82	0.61
1:N:308:ALA:O	1:N:311[A]:ILE:HG22	2.01	0.60
2:B:53:THR:HG21	29:D:307:HOH:O	2.00	0.60
2:B:60:GLU:CD	2:B:60:GLU:H	2.04	0.60
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.82	0.60
7:T:5:LYS:NZ	29:T:201:HOH:O	2.25	0.60
18:A:606:PGV:H061	13:M:5:PRO:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:301:TGL:H121	21:B:301:TGL:HA82	1.83	0.60
1:A:14:ASP:HA	1:A:17[B]:THR:HG22	1.84	0.60
1:A:337:ALA:HB2	1:A:394[A]:VAL:HG23	1.83	0.60
27:W:104:DMU:H36	27:W:104:DMU:H29	1.83	0.60
3:P:213:THR:HG23	26:P:305:CDL:H761	1.85	0.59
11:K:29:TRP:HA	11:K:32[B]:MET:HG2	1.84	0.59
5:E:67:ILE:O	5:E:70[A]:VAL:CG2	2.50	0.59
8:H:9:LYS:HG3	8:H:10:ASN:H	1.68	0.59
1:A:66:ILE:O	1:A:71[B]:MET:HG2	2.03	0.59
1:N:172:LYS:NZ	1:N:178[A]:GLN:HE22	2.01	0.59
1:A:297[B]:MET:SD	1:A:302:ARG:HG2	2.43	0.59
3:C:224:LYS:HD3	26:C:307:CDL:CB3	2.33	0.58
3:P:67:PHE:HE2	26:P:305:CDL:H1	1.69	0.58
2:B:183:THR:HG23	29:B:586:HOH:O	2.04	0.57
1:N:35[B]:LEU:HD11	1:N:462:LEU:HB2	1.85	0.57
4:D:78:TRP:N	21:D:201:TGL:HB22	2.20	0.57
1:A:468[B]:MET:CE	20:A:619:EDO:H21	2.34	0.57
12:L:26:THR:HG23	13:M:25:SER:CB	2.34	0.57
10:J:27:THR:HG22	20:J:102:EDO:H22	1.86	0.57
6:S:43:LYS:N	6:S:43:LYS:HD2	2.17	0.57
18:A:608:PGV:H281	18:C:305:PGV:H301	1.86	0.56
3:C:124:LEU:HD13	3:C:180[B]:GLU:OE2	2.05	0.56
27:C:313:DMU:H7	10:J:52:TRP:CE3	2.40	0.56
21:N:606:TGL:HC31	12:Y:13:PHE:HA	1.88	0.56
7:T:31:CYS:SG	26:T:103:CDL:H552	2.46	0.56
25:C:304:PEK:H383	26:G:101:CDL:H273	1.87	0.56
1:A:468[B]:MET:SD	20:A:619:EDO:H12	2.46	0.56
29:E:301:HOH:O	9:I:4:LEU:HD13	2.05	0.56
1:A:347:LEU:HD13	1:A:383[B]:MET:CE	2.35	0.56
18:A:608:PGV:H183	25:C:303:PEK:H322	1.88	0.56
8:U:9:LYS:HG3	8:U:10:ASN:H	1.72	0.56
1:A:33:LEU:O	1:A:37[B]:ILE:HG23	2.06	0.55
3:C:67:PHE:CE2	26:C:307:CDL:H1	2.28	0.55
1:A:37[B]:ILE:HG13	1:A:38:ARG:HG2	1.88	0.55
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.41	0.55
3:C:33[A]:MET:HG3	3:C:42[A]:LEU:HD12	1.88	0.55
26:C:307:CDL:H212	26:C:307:CDL:H772	1.89	0.55
1:A:347:LEU:HD13	1:A:383[B]:MET:HE2	1.88	0.55
6:S:85:CYS:SG	6:S:87:THR:HG23	2.47	0.55
7:G:3:ALA:O	7:G:4:ALA:CB	2.54	0.55
12:L:20:ARG:NH2	29:L:201:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:307:CDL:HB21	26:C:307:CDL:OB6	2.07	0.55
1:N:87:ILE:O	1:N:173:PRO:HD3	2.07	0.54
12:L:18:LYS:HG2	20:L:103:EDO:H21	1.89	0.54
1:A:468[B]:MET:HG2	1:A:469:VAL:N	2.23	0.54
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.38	0.54
18:A:606:PGV:H231	13:M:12:PRO:HG3	1.89	0.54
1:N:449[A]:MET:SD	2:O:5:MET:HG2	2.47	0.54
2:B:1:FME:SD	2:B:133[B]:LEU:HD21	2.48	0.54
3:P:226:HIS:CE1	26:P:305:CDL:HB32	2.42	0.54
3:C:226:HIS:CE1	26:C:307:CDL:HB32	2.43	0.54
10:W:27:THR:HG22	29:W:221:HOH:O	2.08	0.53
7:T:3:ALA:O	7:T:4:ALA:CB	2.57	0.53
2:O:7:LEU:HD11	21:O:301:TGL:H152	1.90	0.53
5:E:67:ILE:HA	5:E:70[A]:VAL:HG22	1.90	0.53
12:L:26:THR:HG23	13:M:25:SER:HB3	1.88	0.53
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.08	0.53
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.91	0.53
1:N:468[B]:MET:HE2	14:N:601[B]:HEA:C25	2.39	0.53
18:A:606:PGV:H302	18:A:606:PGV:H132	1.91	0.53
21:Q:201:TGL:OB1	21:Q:201:TGL:HG32	2.08	0.53
20:A:615:EDO:H21	4:D:11:TYR:HB3	1.91	0.53
1:N:468[B]:MET:HE2	14:N:601[B]:HEA:H252	1.91	0.53
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.39	0.53
25:C:304:PEK:C38	26:G:101:CDL:H273	2.39	0.52
3:C:47:LEU:O	3:C:51[A]:MET:HG2	2.09	0.52
3:C:156:ARG:HE	24:C:308:CHD:C24	2.22	0.52
4:D:23:PRO:CB	5:E:70[A]:VAL:HG11	2.40	0.52
6:S:29:ASP:OD1	6:S:33[B]:ILE:HG12	2.09	0.52
4:D:23:PRO:HB3	5:E:70[A]:VAL:HG11	1.92	0.52
8:H:37:HIS:HA	8:H:40:GLU:HG2	1.90	0.52
3:C:47:LEU:O	3:C:51[B]:MET:HG3	2.10	0.51
23:O:303:PSC:H071	9:V:10:ARG:HH21	1.76	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
1:A:308:ALA:O	1:A:311[B]:ILE:HG22	2.10	0.51
1:A:365[B]:ILE:HD11	29:A:707:HOH:O	2.09	0.51
3:C:33[B]:MET:SD	29:C:404:HOH:O	2.59	0.51
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.51
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.40	0.51
4:D:78:TRP:CA	21:D:201:TGL:HB22	2.40	0.51
1:N:172:LYS:HZ2	1:N:178[A]:GLN:HE22	1.59	0.51
26:P:305:CDL:H342	26:P:305:CDL:H391	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:ALA:O	2:B:194:GLY:HA3	2.10	0.51
3:C:33[A]:MET:SD	27:C:313:DMU:H6	2.51	0.51
4:Q:10:ASP:HB3	4:Q:13:LEU:HD12	1.92	0.51
10:W:58:LYS:H	10:W:58:LYS:HD2	1.74	0.51
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.10	0.51
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.93	0.51
1:A:71[B]:MET:HG3	29:A:787:HOH:O	2.10	0.51
24:P:301:CHD:H152	18:U:101:PGV:H11	1.93	0.51
2:O:58:ALA:O	2:O:62:GLU:HG3	2.10	0.50
4:D:19:ARG:NH1	29:D:302:HOH:O	2.44	0.50
6:F:92:VAL:O	6:F:92:VAL:HG23	2.11	0.50
3:C:174:THR:HG21	26:C:307:CDL:H861	1.93	0.50
3:C:213:THR:HG23	26:C:307:CDL:H781	1.94	0.50
21:L:101:TGL:HC32	29:L:201:HOH:O	2.11	0.50
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.10	0.50
27:W:104:DMU:H36	27:W:104:DMU:C57	2.41	0.50
4:D:23:PRO:HB3	5:E:70[B]:VAL:CG2	2.41	0.50
3:C:62[B]:ILE:CD1	18:C:305:PGV:H21	2.41	0.50
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.12	0.50
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.77	0.50
1:A:3:ILE:HG23	1:A:7[B]:LEU:HD12	1.94	0.50
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.92	0.50
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.94	0.49
1:A:13[B]:LYS:HG2	1:A:81:TRP:CZ3	2.48	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.59	0.49
4:D:23:PRO:HB3	5:E:70[B]:VAL:HG22	1.94	0.49
5:E:66:ARG:O	5:E:70[B]:VAL:HG23	2.13	0.49
3:P:161:GLN:HE22	25:T:102:PEK:H22	1.78	0.49
3:C:125:ASN:HB2	7:G:42:ARG:NH2	2.27	0.49
26:T:103:CDL:H782	26:T:103:CDL:H571	1.95	0.49
2:B:41:ILE:HG21	23:B:303:PSC:H332	1.93	0.49
3:P:30:GLY:HA2	3:P:42[B]:LEU:HB3	1.95	0.49
3:C:62[B]:ILE:HD12	3:C:221:ARG:CZ	2.43	0.48
3:C:30:GLY:HA2	3:C:42[B]:LEU:HB3	1.95	0.48
1:A:177:SER:H	1:A:180:GLN:HE21	1.61	0.48
1:A:197:LEU:HD21	7:T:2:SER:HB2	1.95	0.48
2:B:60:GLU:CD	2:B:60:GLU:N	2.64	0.48
25:C:303:PEK:H131	25:C:303:PEK:H242	1.95	0.48
26:G:101:CDL:H751	1:N:282:PHE:HZ	1.78	0.48
21:N:606:TGL:HA22	12:Y:13:PHE:HB3	1.95	0.48
18:N:607:PGV:H011	18:N:607:PGV:H22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297[B]:MET:SD	1:A:302:ARG:CG	3.01	0.48
1:A:494:TRP:O	20:A:612:EDO:H21	2.14	0.48
1:A:13[B]:LYS:HG2	1:A:81:TRP:CE3	2.48	0.48
1:A:48:LEU:HD23	13:M:37[B]:LEU:HD21	1.96	0.48
10:W:36[B]:MET:HG2	24:W:101:CHD:H221	1.94	0.48
18:A:606:PGV:H311	13:M:19:LEU:HD23	1.95	0.48
1:N:406:ASN:HD21	18:N:607:PGV:H21	1.78	0.48
8:H:46:LYS:HD3	8:U:7:LYS:HG2	1.95	0.48
21:D:201:TGL:CG3	29:D:312:HOH:O	2.53	0.48
12:L:12:PRO:HG2	21:L:101:TGL:HG11	1.94	0.48
27:W:104:DMU:C10	27:W:104:DMU:H29	2.44	0.48
26:G:101:CDL:H873	25:G:103:PEK:H371	1.95	0.47
3:P:224:LYS:HD3	26:P:305:CDL:CB3	2.43	0.47
24:C:308:CHD:H162	24:C:308:CHD:H231	1.96	0.47
3:C:125:ASN:HB2	7:G:42:ARG:HH22	1.80	0.47
3:P:156:ARG:HE	24:P:306:CHD:C24	2.27	0.47
1:N:309:THR:HG22	14:N:602:HEA:HMB2	1.96	0.47
2:B:41:ILE:HD13	23:B:303:PSC:H342	1.96	0.47
7:T:17:ARG:HH22	25:T:102:PEK:H041	1.80	0.47
3:C:63:ARG:HE	26:C:307:CDL:CA2	2.21	0.47
3:P:33[A]:MET:SD	27:W:104:DMU:H6	2.55	0.47
1:A:309:THR:HG22	14:A:602:HEA:HMB2	1.97	0.47
1:A:76:GLY:O	1:A:80:ASN:HB2	2.15	0.47
23:B:303:PSC:H042	23:B:303:PSC:H062	1.75	0.47
9:I:2:THR:HG23	29:I:110:HOH:O	2.14	0.47
3:C:226:HIS:HE1	26:C:307:CDL:HB32	1.80	0.46
7:G:5:LYS:HB3	1:N:278[A]:MET:CE	2.45	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.62	0.46
1:A:178[A]:GLN:HG2	7:T:7:ASP:HB2	1.97	0.46
26:C:307:CDL:HA61	20:J:102:EDO:H12	1.97	0.46
7:G:3:ALA:O	7:G:4:ALA:HB2	2.15	0.46
6:S:43:LYS:HG3	29:S:286:HOH:O	2.15	0.46
1:N:488:THR:HB	1:N:495:LEU:HD13	1.98	0.46
1:A:383[B]:MET:HE3	1:A:421:VAL:HG23	1.97	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.15	0.46
3:P:156:ARG:HH21	24:P:306:CHD:C24	2.29	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.98	0.45
23:O:303:PSC:C20	23:O:303:PSC:H02	2.45	0.45
3:P:107:ALA:HB2	18:U:101:PGV:H031	1.98	0.45
21:B:301:TGL:OG1	21:B:301:TGL:CB1	2.65	0.45
2:B:41:ILE:O	2:B:45:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:77:PRO:HA	5:R:79:LYS:HE3	1.98	0.45
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.99	0.45
2:B:41:ILE:HD13	23:B:303:PSC:C34	2.46	0.45
25:C:304:PEK:H361	26:G:101:CDL:H273	1.97	0.45
1:N:24:ALA:HA	14:N:601[A]:HEA:H22	1.98	0.45
2:O:12:ALA:HA	2:O:17[B]:MET:HG3	1.99	0.45
1:A:178[B]:GLN:CD	1:A:178[B]:GLN:H	2.19	0.45
21:D:201:TGL:H341	9:I:16:ARG:HH21	1.81	0.45
27:C:313:DMU:H9	10:J:53:ALA:HB2	1.94	0.45
4:D:19:ARG:HB3	4:D:21:ASP:OD1	2.17	0.45
8:U:57:ARG:O	8:U:61:LYS:HB2	2.17	0.45
21:N:606:TGL:HG11	12:Y:12:PRO:HG2	1.99	0.44
7:G:9:GLY:HA3	1:N:178[A]:GLN:HE21	1.81	0.44
10:W:49:CYS:HB3	27:W:104:DMU:H10	1.98	0.44
1:A:172:LYS:HZ2	1:A:178[A]:GLN:HE22	1.65	0.44
1:N:468[B]:MET:HE1	14:N:601[B]:HEA:C21	2.48	0.44
9:I:35:TYR:C	9:I:35:TYR:CD1	2.91	0.44
3:P:246:ASP:HB2	29:P:513:HOH:O	2.16	0.44
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.15	0.44
1:A:177:SER:H	1:A:180:GLN:NE2	2.15	0.44
1:A:67:PHE:HA	1:A:71[B]:MET:SD	2.58	0.44
20:B:306:EDO:H22	29:B:544:HOH:O	2.18	0.44
3:C:62[B]:ILE:HD11	18:C:305:PGV:C2	2.43	0.44
7:G:72:ASN:H	7:G:76:ASN:ND2	2.06	0.44
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.44
1:A:14:ASP:O	1:A:17[B]:THR:HG22	2.18	0.44
1:N:468[B]:MET:HE2	14:N:601[B]:HEA:C22	2.43	0.44
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.00	0.44
3:C:37:PHE:HB3	27:C:313:DMU:H29	2.00	0.44
3:P:37:PHE:CE2	27:W:104:DMU:H13	2.53	0.44
9:V:1:SAC:H2A1	9:V:1:SAC:HA	1.79	0.44
2:O:28:LEU:HD21	21:O:301:TGL:HG12	1.99	0.43
18:A:606:PGV:H011	29:K:116:HOH:O	2.18	0.43
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.01	0.43
1:A:37[B]:ILE:CD1	1:A:41:LEU:HD12	2.48	0.43
3:C:240:TRP:HB3	25:T:101:PEK:H5	2.00	0.43
5:E:67:ILE:C	5:E:70[A]:VAL:HG22	2.37	0.43
7:G:5:LYS:HD3	1:N:278[A]:MET:HB3	2.00	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.54	0.43
25:T:102:PEK:H332	25:T:102:PEK:H362	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468[B]:MET:HE2	14:A:601[B]:HEA:C21	2.48	0.43
2:B:56:MET:HB3	23:B:303:PSC:H211	2.01	0.43
3:C:59:ARG:HA	26:C:307:CDL:H512	2.00	0.43
1:A:472:ILE:HG21	21:L:101:TGL:HA82	2.01	0.43
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.53	0.43
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.06	0.43
26:G:101:CDL:H342	2:O:81:LEU:HB2	2.00	0.43
3:C:33[B]:MET:HG2	3:C:39:SER:HB3	2.00	0.43
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.54	0.43
7:G:31:CYS:SG	26:G:101:CDL:H532	2.58	0.43
2:B:183:THR:HG22	29:B:440:HOH:O	2.19	0.42
18:N:607:PGV:H011	18:N:607:PGV:C2	2.48	0.42
12:Y:21:LEU:HA	12:Y:24[A]:MET:HE2	2.00	0.42
1:A:347:LEU:HD22	1:A:383[B]:MET:HE1	2.01	0.42
3:P:165:ILE:HD11	25:T:102:PEK:H72	2.01	0.42
25:T:101:PEK:H361	26:T:103:CDL:H851	2.01	0.42
7:T:44:ARG:HA	7:T:45:PRO:HD3	1.90	0.42
1:A:514:LYS:HG3	6:F:38:ALA:CB	2.50	0.42
3:C:210:ILE:HG12	18:C:305:PGV:H132	2.02	0.42
3:C:62[B]:ILE:HD12	3:C:221:ARG:NE	2.34	0.42
26:G:101:CDL:H341	26:G:101:CDL:OA7	2.20	0.42
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.37	0.42
6:S:54:ASN:HD22	6:S:54:ASN:C	2.23	0.42
3:P:133[A]:ASN:ND2	29:P:402:HOH:O	2.52	0.42
3:P:210:ILE:HD13	18:P:304:PGV:H301	2.01	0.42
26:T:103:CDL:H341	26:T:103:CDL:OA7	2.19	0.42
10:W:33:ARG:HG2	24:W:101:CHD:H151	2.01	0.42
20:H:101:EDO:H22	29:H:208:HOH:O	2.19	0.42
12:L:2[A]:HIS:CG	12:L:3:TYR:H	2.37	0.42
1:N:4[B]:ASN:ND2	12:Y:3:TYR:OH	2.51	0.42
24:P:306:CHD:H112	24:P:306:CHD:H12A	1.90	0.42
4:Q:130:PRO:HD2	4:Q:131:ILE:HD12	2.02	0.42
2:B:196:CYS:HB2	2:B:207:MET:HG3	2.00	0.42
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.02	0.42
3:P:224:LYS:HD2	26:P:305:CDL:HB31	2.02	0.42
1:A:112:LEU:C	1:A:112:LEU:HD23	2.39	0.42
1:A:413:HIS:NE2	20:A:619:EDO:H11	2.35	0.42
1:A:514:LYS:HA	6:F:38:ALA:HB3	2.00	0.42
1:A:406:ASN:HD21	18:A:606:PGV:H22	1.84	0.42
1:A:311[A]:ILE:HG13	26:T:103:CDL:H441	2.02	0.42
1:A:12:HIS:CE1	1:A:13[B]:LYS:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.01	0.42
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.02	0.42
1:A:53:ILE:HD11	12:L:40:VAL:HG13	2.01	0.42
24:B:304:CHD:H12	24:B:304:CHD:H212	2.02	0.41
3:P:33[A]:MET:SD	27:W:104:DMU:C22	2.82	0.41
24:J:101:CHD:H183	24:J:101:CHD:H222	2.02	0.41
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.35	0.41
26:G:101:CDL:H541	26:G:101:CDL:H221	2.02	0.41
12:L:12:PRO:HB2	21:L:101:TGL:HG2	2.02	0.41
4:D:109:HIS:HD2	29:D:410:HOH:O	2.03	0.41
1:N:426:PHE:HZ	21:O:301:TGL:HA51	1.85	0.41
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.96	0.41
8:H:9:LYS:HA	8:H:9:LYS:HD3	1.83	0.41
21:N:606:TGL:H331	12:Y:28:PHE:HA	2.03	0.41
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.41
4:D:78:TRP:HA	21:D:201:TGL:HB22	2.02	0.41
1:A:465:VAL:HA	20:A:619:EDO:H12	2.01	0.41
23:B:303:PSC:H072	5:E:11:PHE:HB2	2.03	0.41
4:D:23:PRO:HB3	5:E:70[A]:VAL:HG12	2.02	0.41
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.21	0.41
1:N:172:LYS:NZ	1:N:178[A]:GLN:NE2	2.68	0.41
1:N:486:ASP:OD2	4:Q:19:ARG:NE	2.54	0.41
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.03	0.41
1:A:240:HIS:CE1	1:A:244:TYR:OH	2.72	0.41
1:A:347:LEU:HD13	1:A:383[B]:MET:HE1	2.03	0.41
1:A:37[B]:ILE:HD12	1:A:41:LEU:HD12	2.03	0.41
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.56	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.21	0.41
14:N:602:HEA:HMC1	14:N:602:HEA:CBC	2.45	0.41
2:O:33:LEU:HD13	9:V:31:PHE:HD1	1.85	0.41
26:T:103:CDL:H542	26:T:103:CDL:H241	2.02	0.41
7:T:84:LYS:H	7:T:84:LYS:CE	2.34	0.41
3:C:210:ILE:HG21	18:C:305:PGV:H282	2.03	0.41
3:C:52:LEU:HD23	26:C:307:CDL:H362	2.03	0.41
2:B:58:ALA:O	2:B:62:GLU:HG3	2.20	0.40
5:E:84:TYR:N	29:E:301:HOH:O	2.54	0.40
1:N:297[B]:MET:CG	1:N:302:ARG:CG	2.96	0.40
3:P:116:TRP:HA	3:P:117:PRO:C	2.41	0.40
18:C:306:PGV:H332	7:T:1:ALA:HB2	2.04	0.40
1:A:24:ALA:HA	14:A:601[A]:HEA:H22	2.02	0.40
2:B:140:ASN:HB3	29:B:551:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.57	0.40
2:O:1:FME:HE2	2:O:2:ALA:O	2.21	0.40
1:A:148:PHE:HB3	3:C:28:THR:HB	2.04	0.40
9:I:57:MET:O	9:I:61:GLU:HG2	2.21	0.40
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.87	0.40
1:N:177:SER:H	1:N:180:GLN:NE2	2.19	0.40
3:P:164:PHE:CD1	24:P:306:CHD:H192	2.56	0.40
21:B:301:TGL:H301	21:B:301:TGL:HA91	2.02	0.40
5:E:82:TYR:HB3	5:E:83:PRO:HD3	2.02	0.40
1:N:180:GLN:HB2	1:N:180:GLN:HE21	1.72	0.40
1:A:289:ALA:HB1	1:A:297[B]:MET:CE	2.51	0.40
24:J:101:CHD:C18	24:J:101:CHD:H222	2.52	0.40
1:N:337:ALA:HB2	1:N:394[A]:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	545/514 (106%)	532 (98%)	13 (2%)	0	100	100
1	N	542/514 (105%)	528 (97%)	14 (3%)	0	100	100
2	B	236/227 (104%)	230 (98%)	6 (2%)	0	100	100
2	O	235/227 (104%)	231 (98%)	4 (2%)	0	100	100
3	C	270/261 (103%)	266 (98%)	4 (2%)	0	100	100
3	P	269/261 (103%)	265 (98%)	4 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	143/147 (97%)	136 (95%)	5 (4%)	2 (1%)	11	2
5	E	105/109 (96%)	105 (100%)	0	0	100	100
5	R	103/109 (94%)	103 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	93/94 (99%)	91 (98%)	2 (2%)	0	100	100
6	S	94/94 (100%)	93 (99%)	1 (1%)	0	100	100
7	G	81/85 (95%)	71 (88%)	8 (10%)	2 (2%)	5	1
7	T	81/85 (95%)	72 (89%)	4 (5%)	5 (6%)	1	0
8	H	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
8	U	77/85 (91%)	75 (97%)	1 (1%)	1 (1%)	12	3
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	71 (100%)	0	0	100	100
10	J	58/59 (98%)	57 (98%)	1 (2%)	0	100	100
10	W	57/59 (97%)	57 (100%)	0	0	100	100
11	K	48/56 (86%)	47 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	47/47 (100%)	44 (94%)	3 (6%)	0	100	100
12	Y	45/47 (96%)	43 (96%)	2 (4%)	0	100	100
13	M	42/46 (91%)	42 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3620/3606 (100%)	3528 (98%)	82 (2%)	10 (0%)	41	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	T	4	ALA
7	T	5	LYS
7	G	5	LYS
4	Q	8	SER
7	T	8	HIS
4	Q	6	VAL
7	T	10	GLY
8	U	8	ILE
7	T	6	GLY

### 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	459/426 (108%)	453 (99%)	6 (1%)	69	59
1	N	456/426 (107%)	450 (99%)	6 (1%)	69	59
2	B	221/210 (105%)	214 (97%)	7 (3%)	39	22
2	O	220/210 (105%)	214 (97%)	6 (3%)	44	28
3	C	237/226 (105%)	234 (99%)	3 (1%)	69	59
3	P	236/226 (104%)	233 (99%)	3 (1%)	69	59
4	D	128/129 (99%)	127 (99%)	1 (1%)	81	76
4	Q	129/129 (100%)	125 (97%)	4 (3%)	40	22
5	E	94/95 (99%)	93 (99%)	1 (1%)	73	65
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	36
6	F	79/78 (101%)	77 (98%)	2 (2%)	47	31
6	S	80/78 (103%)	76 (95%)	4 (5%)	24	9
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	1
7	T	67/68 (98%)	62 (92%)	5 (8%)	13	3
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	27
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	7
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	45
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	19
10	J	51/50 (102%)	51 (100%)	0	100	100
10	W	50/50 (100%)	48 (96%)	2 (4%)	31	14
11	K	40/46 (87%)	40 (100%)	0	100	100
11	X	39/46 (85%)	39 (100%)	0	100	100
12	L	43/40 (108%)	42 (98%)	1 (2%)	50	34
12	Y	40/40 (100%)	39 (98%)	1 (2%)	47	31
13	M	38/38 (100%)	38 (100%)	0	100	100
13	Z	37/38 (97%)	36 (97%)	1 (3%)	44	28
All	All	3159/3076 (103%)	3088 (98%)	71 (2%)	50	36

All (71) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	338	MET
1	A	369	ASP
2	B	60	GLU
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115[A]	ASP
2	B	115[B]	ASP
2	B	171	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
4	D	31	LYS
5	E	90	ARG
6	F	54	ASN
6	F	80	GLN
7	G	8	HIS
7	G	18	PHE
7	G	36	TRP
7	G	37	LEU
7	G	44	ARG
7	G	54	ARG
7	G	84	LYS
8	H	9	LYS
8	H	60	TYR
9	I	2	THR
12	L	47	LYS
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	363	LEU
1	N	369	ASP
1	N	485	VAL
2	O	60	GLU
2	O	91	ASN
2	O	115[A]	ASP
2	O	115[B]	ASP
2	O	171	LYS
2	O	227	LEU

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Mol	Chain	Res	Type
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	10	ASP
4	Q	20	ARG
4	Q	51	LEU
4	Q	147	LYS
5	R	79	LYS
5	R	90	ARG
6	S	43	LYS
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	2	SER
7	T	18	PHE
7	T	36	TRP
7	T	44	ARG
7	T	54	ARG
8	U	7	LYS
8	U	29	CYS
8	U	50	VAL
8	U	60	TYR
9	V	36	LYS
9	V	70	GLN
10	W	50	LEU
10	W	58	LYS
12	Y	47	LYS
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
2	B	10	GLN
2	B	52	HIS
2	B	59	GLN
2	B	181	GLN
2	B	195	GLN
3	C	68	GLN
3	C	161	GLN
4	D	29	HIS
4	D	32	ASN

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Mol	Chain	Res	Type
4	D	37	GLN
4	D	101	HIS
4	D	143	ASN
5	E	5	HIS
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
1	N	180	GLN
2	O	10	GLN
2	O	52	HIS
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
3	P	161	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	5	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
7	T	76	ASN
9	V	8	GLN
10	W	29	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	$\# Z  > 2$
2	FME	B	1	2	8,9,10	0.78	0	7,9,11	3.14	2 (28%)
2	FME	O	1	2	8,9,10	0.60	0	7,9,11	1.17	0
1	FME	A	1	1	8,9,10	0.56	0	7,9,11	1.59	2 (28%)
7	TPO	G	11	7	8,10,11	1.34	1 (12%)	10,14,16	0.78	0
9	SAC	I	1	9	7,8,9	2.04	2 (28%)	8,9,11	1.08	0
9	SAC	V	1	9	7,8,9	2.04	2 (28%)	8,9,11	1.37	1 (12%)
1	FME	N	1	1	8,9,10	0.57	0	7,9,11	1.29	0
7	TPO	T	11	7	8,10,11	1.30	1 (12%)	10,14,16	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	B	1	2	-	1/7/9/11	-
2	FME	O	1	2	-	0/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
9	SAC	I	1	9	-	2/7/8/10	-
9	SAC	V	1	9	-	5/7/8/10	-
1	FME	N	1	1	-	2/7/9/11	-
7	TPO	T	11	7	-	2/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	4.66	1.33	1.23
9	V	1	SAC	OAC-C1A	4.49	1.33	1.23
7	G	11	TPO	P-O1P	2.81	1.59	1.50
9	V	1	SAC	CA-N	2.80	1.50	1.46
7	T	11	TPO	P-O1P	2.80	1.59	1.50
9	I	1	SAC	CA-N	2.49	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-6.99	112.07	122.82
1	A	1	FME	C-CA-N	3.05	115.23	109.73
2	B	1	FME	C-CA-N	2.94	115.03	109.73
9	V	1	SAC	CB-CA-N	-2.46	105.03	110.55
1	A	1	FME	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C-CA-CB-OG
9	V	1	SAC	O-C-CA-CB
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	O-C-CA-CB
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	N-CA-CB-OG
1	A	1	FME	CB-CG-SD-CE
9	V	1	SAC	C-CA-CB-OG
9	V	1	SAC	N-CA-CB-OG
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	FME	1	0
2	O	1	FME	1	0
9	V	1	SAC	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 118 ligands modelled in this entry, 10 are monoatomic - leaving 108 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	$\# Z  > 2$
20	EDO	A	615	-	3,3,3	0.37	0	2,2,2	0.51	0
20	EDO	P	309	-	3,3,3	0.46	0	2,2,2	0.29	0
20	EDO	B	305	-	3,3,3	0.49	0	2,2,2	0.21	0
18	PGV	N	607	-	50,50,50	0.95	2 (4%)	53,56,56	0.97	5 (9%)
27	DMU	M	101	-	34,34,34	0.44	0	45,45,45	0.88	1 (2%)
20	EDO	B	309	-	3,3,3	0.56	0	2,2,2	0.22	0
19	PER	N	608[A]	15,14	0,1,1	0.00	-	-		
20	EDO	Y	101	-	3,3,3	0.46	0	2,2,2	0.33	0
22	CUA	B	302	2	0,1,1	0.00	-	-		
20	EDO	B	306	-	3,3,3	0.34	0	2,2,2	0.29	0
20	EDO	B	308	-	3,3,3	0.42	0	2,2,2	0.41	0
14	HEA	A	602	1,19	44,67,67	0.87	1 (2%)	37,103,103	1.46	7 (18%)
20	EDO	L	102	-	3,3,3	0.41	0	2,2,2	0.45	0
20	EDO	L	105	-	3,3,3	0.43	0	2,2,2	0.33	0
18	PGV	U	101	-	50,50,50	0.96	2 (4%)	53,56,56	1.02	3 (5%)
20	EDO	O	304	-	3,3,3	0.46	0	2,2,2	0.36	0
20	EDO	A	614	-	3,3,3	0.39	0	2,2,2	0.41	0
20	EDO	R	202	-	3,3,3	0.41	0	2,2,2	0.41	0
25	PEK	C	304	-	52,52,52	0.94	2 (3%)	55,57,57	0.98	2 (3%)
20	EDO	T	105	-	3,3,3	0.45	0	2,2,2	0.35	0
20	EDO	H	101	-	3,3,3	0.41	0	2,2,2	0.41	0
20	EDO	F	102	-	3,3,3	0.50	0	2,2,2	0.20	0
20	EDO	N	613	-	3,3,3	0.44	0	2,2,2	0.17	0
20	EDO	J	102	-	3,3,3	0.42	0	2,2,2	0.46	0
27	DMU	C	312	-	34,34,34	0.49	0	45,45,45	0.87	2 (4%)
20	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.19	0
24	CHD	P	306	-	29,32,32	0.49	0	48,51,51	1.45	7 (14%)
20	EDO	A	619	-	3,3,3	0.44	0	2,2,2	0.25	0
20	EDO	S	104	-	3,3,3	0.40	0	2,2,2	0.48	0
20	EDO	M	103	-	3,3,3	0.45	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	EDO	N	611	-	3,3,3	0.48	0	2,2,2	0.36	0
18	PGV	C	306	-	50,50,50	0.99	2 (4%)	53,56,56	0.99	3 (5%)
24	CHD	C	301	-	29,32,32	0.60	0	48,51,51	1.07	3 (6%)
20	EDO	P	308	-	3,3,3	0.43	0	2,2,2	0.39	0
20	EDO	A	613	-	3,3,3	0.58	0	2,2,2	0.50	0
25	PEK	C	303	-	52,52,52	0.87	2 (3%)	55,57,57	0.80	2 (3%)
25	PEK	G	103	-	52,52,52	0.91	2 (3%)	55,57,57	0.97	4 (7%)
20	EDO	P	311	-	3,3,3	0.54	0	2,2,2	0.20	0
20	EDO	A	616	-	3,3,3	0.41	0	2,2,2	0.43	0
14	HEA	A	601[B]	-	44,67,67	0.93	2 (4%)	37,103,103	1.64	10 (27%)
18	PGV	C	305	-	50,50,50	0.88	2 (4%)	53,56,56	0.81	1 (1%)
24	CHD	P	301	-	29,32,32	0.54	0	48,51,51	1.05	3 (6%)
20	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.44	0
20	EDO	N	614	-	3,3,3	0.50	0	2,2,2	0.33	0
20	EDO	N	610	-	3,3,3	0.48	0	2,2,2	0.28	0
21	TGL	N	606	-	62,62,62	1.26	6 (9%)	65,65,65	1.10	3 (4%)
21	TGL	O	301	-	62,62,62	1.25	6 (9%)	65,65,65	1.08	3 (4%)
19	PER	A	607[B]	15,14	0,1,1	0.00	-	-	-	-
20	EDO	W	103	-	3,3,3	0.42	0	2,2,2	0.42	0
19	PER	A	607[A]	15,14	0,1,1	0.00	-	-	-	-
14	HEA	N	601[A]	-	44,67,67	0.87	0	37,103,103	1.62	9 (24%)
20	EDO	C	310	-	3,3,3	0.53	0	2,2,2	0.24	0
20	EDO	P	310	-	3,3,3	0.43	0	2,2,2	0.35	0
23	PSC	B	303	-	51,51,51	1.12	3 (5%)	57,59,59	0.96	2 (3%)
27	DMU	W	104	-	34,34,34	0.55	1 (2%)	45,45,45	0.75	1 (2%)
20	EDO	R	204	-	3,3,3	0.49	0	2,2,2	0.30	0
20	EDO	A	618	-	3,3,3	0.47	0	2,2,2	0.28	0
19	PER	N	608[B]	15,14	0,1,1	0.00	-	-	-	-
14	HEA	N	602	1,19	44,67,67	0.91	1 (2%)	37,103,103	1.53	6 (16%)
20	EDO	S	103	-	3,3,3	0.50	0	2,2,2	0.28	0
20	EDO	C	309	-	3,3,3	0.39	0	2,2,2	0.58	0
27	DMU	Z	101	-	34,34,34	0.45	0	45,45,45	0.78	0
20	EDO	T	104	-	3,3,3	0.43	0	2,2,2	0.37	0
27	DMU	P	313	-	34,34,34	0.54	0	45,45,45	1.17	5 (11%)
20	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.36	0
26	CDL	T	103	-	99,99,99	1.32	12 (12%)	105,111,111	1.09	5 (4%)
20	EDO	E	201	-	3,3,3	0.44	0	2,2,2	0.40	0
20	EDO	A	610	-	3,3,3	0.49	0	2,2,2	0.33	0
20	EDO	N	612	-	3,3,3	0.45	0	2,2,2	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	DMU	C	313	-	34,34,34	0.53	1 (2%)	45,45,45	0.90	2 (4%)
21	TGL	B	301	-	62,62,62	1.21	6 (9%)	65,65,65	1.10	4 (6%)
24	CHD	B	304	-	29,32,32	0.57	0	48,51,51	1.02	2 (4%)
18	PGV	N	609	-	50,50,50	0.87	2 (4%)	53,56,56	0.91	2 (3%)
26	CDL	P	305	-	99,99,99	1.33	12 (12%)	105,111,111	1.07	5 (4%)
20	EDO	R	203	-	3,3,3	0.42	0	2,2,2	0.37	0
20	EDO	Q	202	-	3,3,3	0.46	0	2,2,2	0.24	0
20	EDO	L	103	-	3,3,3	0.47	0	2,2,2	0.26	0
18	PGV	P	304	-	50,50,50	0.88	2 (4%)	53,56,56	0.78	1 (1%)
22	CUA	O	302	2	0,1,1	0.00	-	-		
20	EDO	A	612	-	3,3,3	0.39	0	2,2,2	0.24	0
23	PSC	O	303	-	51,51,51	1.10	3 (5%)	57,59,59	1.07	3 (5%)
24	CHD	G	102	-	29,32,32	0.59	0	48,51,51	1.08	3 (6%)
20	EDO	M	102	-	3,3,3	0.42	0	2,2,2	0.37	0
24	CHD	J	101	-	29,32,32	0.49	0	48,51,51	1.43	8 (16%)
24	CHD	W	101	-	29,32,32	0.48	0	48,51,51	1.46	7 (14%)
25	PEK	P	303	-	52,52,52	0.90	2 (3%)	55,57,57	0.89	2 (3%)
20	EDO	L	104	-	3,3,3	0.44	0	2,2,2	0.35	0
21	TGL	Q	201	-	62,62,62	1.27	6 (9%)	65,65,65	1.08	4 (6%)
26	CDL	C	307	-	99,99,99	1.33	12 (12%)	105,111,111	1.07	4 (3%)
14	HEA	N	601[B]	-	44,67,67	0.86	0	37,103,103	1.57	8 (21%)
20	EDO	B	307	-	3,3,3	0.50	0	2,2,2	0.28	0
18	PGV	A	606	-	50,50,50	0.97	2 (4%)	53,56,56	1.01	3 (5%)
20	EDO	W	102	-	3,3,3	0.46	0	2,2,2	0.33	0
14	HEA	A	601[A]	-	44,67,67	0.94	2 (4%)	37,103,103	1.69	11 (29%)
20	EDO	S	102	-	3,3,3	0.47	0	2,2,2	0.16	0
20	EDO	P	312	-	3,3,3	0.49	0	2,2,2	0.28	0
24	CHD	C	308	-	29,32,32	0.61	0	48,51,51	1.84	10 (20%)
20	EDO	F	103	-	3,3,3	0.43	0	2,2,2	0.33	0
21	TGL	D	201	-	62,62,62	1.25	6 (9%)	65,65,65	0.99	4 (6%)
20	EDO	R	201	-	3,3,3	0.47	0	2,2,2	0.34	0
21	TGL	L	101	-	62,62,62	1.28	6 (9%)	65,65,65	1.12	3 (4%)
20	EDO	C	311	-	3,3,3	0.52	0	2,2,2	0.25	0
20	EDO	P	307	-	3,3,3	0.43	0	2,2,2	0.43	0
25	PEK	T	101	-	52,52,52	0.95	2 (3%)	55,57,57	0.96	3 (5%)
18	PGV	A	608	-	50,50,50	0.95	2 (4%)	53,56,56	0.85	3 (5%)
25	PEK	T	102	-	52,52,52	0.96	2 (3%)	55,57,57	0.88	3 (5%)
20	EDO	G	104	-	3,3,3	0.48	0	2,2,2	0.23	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
26	CDL	G	101	-	99,99,99	1.31	12 (12%)	105,111,111	1.10	6 (5%)

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
20	EDO	A	615	-	-	1/1/1/1	-
20	EDO	P	309	-	-	1/1/1/1	-
20	EDO	B	305	-	-	0/1/1/1	-
18	PGV	N	607	-	-	29/55/55/55	-
27	DMU	M	101	-	-	8/19/59/59	0/2/2/2
20	EDO	B	309	-	-	0/1/1/1	-
20	EDO	B	307	-	-	0/1/1/1	-
20	EDO	Y	101	-	-	0/1/1/1	-
20	EDO	B	306	-	-	1/1/1/1	-
20	EDO	B	308	-	-	1/1/1/1	-
14	HEA	A	602	1,19	3/3/7/16	0/24/76/76	-
20	EDO	L	102	-	-	0/1/1/1	-
20	EDO	L	105	-	-	1/1/1/1	-
18	PGV	U	101	-	-	29/55/55/55	-
20	EDO	O	304	-	-	0/1/1/1	-
20	EDO	A	614	-	-	0/1/1/1	-
20	EDO	R	202	-	-	0/1/1/1	-
25	PEK	C	304	-	-	26/56/56/56	-
20	EDO	T	105	-	-	1/1/1/1	-
20	EDO	H	101	-	-	1/1/1/1	-
20	EDO	F	102	-	-	0/1/1/1	-
20	EDO	N	613	-	-	1/1/1/1	-
20	EDO	J	102	-	-	0/1/1/1	-
27	DMU	C	312	-	-	10/19/59/59	0/2/2/2
20	EDO	A	617	-	-	1/1/1/1	-
24	CHD	P	306	-	-	7/7/74/74	0/4/4/4
20	EDO	A	619	-	-	1/1/1/1	-
20	EDO	S	104	-	-	1/1/1/1	-
20	EDO	M	103	-	-	1/1/1/1	-
20	EDO	N	611	-	-	0/1/1/1	-
18	PGV	C	306	-	-	26/55/55/55	-
24	CHD	C	301	-	-	0/7/74/74	0/4/4/4
20	EDO	P	308	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	A	613	-	-	0/1/1/1	-
25	PEK	C	303	-	-	17/56/56/56	-
25	PEK	G	103	-	-	31/56/56/56	-
20	EDO	P	311	-	-	0/1/1/1	-
20	EDO	A	616	-	-	0/1/1/1	-
14	HEA	A	601[B]	-	-	3/24/76/76	-
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
20	EDO	A	609	-	-	1/1/1/1	-
20	EDO	N	614	-	-	0/1/1/1	-
20	EDO	N	610	-	-	0/1/1/1	-
21	TGL	N	606	-	-	33/65/65/65	-
21	TGL	O	301	-	-	34/65/65/65	-
20	EDO	W	103	-	-	1/1/1/1	-
14	HEA	N	601[A]	-	-	2/24/76/76	-
20	EDO	C	310	-	-	0/1/1/1	-
20	EDO	P	310	-	-	1/1/1/1	-
23	PSC	B	303	-	-	29/55/55/55	-
27	DMU	W	104	-	-	9/19/59/59	0/2/2/2
20	EDO	R	204	-	-	0/1/1/1	-
20	EDO	A	618	-	-	0/1/1/1	-
14	HEA	N	602	1,19	3/3/7/16	0/24/76/76	-
20	EDO	S	103	-	-	0/1/1/1	-
20	EDO	C	309	-	-	0/1/1/1	-
27	DMU	Z	101	-	-	7/19/59/59	0/2/2/2
20	EDO	T	104	-	-	0/1/1/1	-
27	DMU	P	313	-	-	8/19/59/59	0/2/2/2
20	EDO	A	611	-	-	0/1/1/1	-
26	CDL	T	103	-	-	61/110/110/110	-
20	EDO	E	201	-	-	0/1/1/1	-
20	EDO	A	610	-	-	0/1/1/1	-
20	EDO	N	612	-	-	0/1/1/1	-
27	DMU	C	313	-	-	10/19/59/59	0/2/2/2
21	TGL	B	301	-	-	43/65/65/65	-
24	CHD	B	304	-	-	0/7/74/74	0/4/4/4
18	PGV	N	609	-	-	12/55/55/55	-
26	CDL	P	305	-	-	69/110/110/110	-
20	EDO	R	203	-	-	0/1/1/1	-
20	EDO	Q	202	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	EDO	L	103	-	-	0/1/1/1	-
18	PGV	P	304	-	-	18/55/55/55	-
20	EDO	A	612	-	-	0/1/1/1	-
23	PSC	O	303	-	-	31/55/55/55	-
24	CHD	G	102	-	-	0/7/74/74	0/4/4/4
20	EDO	M	102	-	-	0/1/1/1	-
24	CHD	J	101	-	-	3/7/74/74	0/4/4/4
24	CHD	W	101	-	-	4/7/74/74	1/4/4/4
25	PEK	P	303	-	-	16/56/56/56	-
20	EDO	L	104	-	-	0/1/1/1	-
21	TGL	Q	201	-	-	34/65/65/65	-
26	CDL	C	307	-	-	66/110/110/110	-
14	HEA	N	601[B]	-	-	4/24/76/76	-
18	PGV	C	305	-	-	19/55/55/55	-
18	PGV	A	606	-	-	25/55/55/55	-
20	EDO	W	102	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	3/24/76/76	-
20	EDO	S	102	-	-	0/1/1/1	-
20	EDO	P	312	-	-	0/1/1/1	-
24	CHD	C	308	-	-	6/7/74/74	0/4/4/4
20	EDO	F	103	-	-	0/1/1/1	-
21	TGL	D	201	-	-	38/65/65/65	-
20	EDO	R	201	-	-	0/1/1/1	-
21	TGL	L	101	-	-	33/65/65/65	-
20	EDO	C	311	-	-	0/1/1/1	-
20	EDO	P	307	-	-	1/1/1/1	-
25	PEK	T	101	-	-	26/56/56/56	-
18	PGV	A	608	-	-	11/55/55/55	-
25	PEK	T	102	-	-	31/56/56/56	-
20	EDO	G	104	-	-	0/1/1/1	-
26	CDL	G	101	-	-	64/110/110/110	-

All (126) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG2-CB1	4.71	1.47	1.34
26	C	307	CDL	OA8-CA7	4.65	1.46	1.33
21	N	606	TGL	OG2-CB1	4.59	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	305	CDL	OB8-CB7	4.57	1.46	1.33
26	P	305	CDL	OA8-CA7	4.57	1.46	1.33
23	B	303	PSC	O01-C1	4.56	1.47	1.34
21	Q	201	TGL	OG2-CB1	4.55	1.47	1.34
21	D	201	TGL	OG1-CA1	4.55	1.46	1.33
21	Q	201	TGL	OG3-CC1	4.54	1.46	1.33
21	L	101	TGL	OG3-CC1	4.53	1.46	1.33
26	T	103	CDL	OB8-CB7	4.52	1.46	1.33
18	C	306	PGV	O03-C19	4.52	1.46	1.33
21	Q	201	TGL	OG1-CA1	4.52	1.46	1.33
21	O	301	TGL	OG2-CB1	4.52	1.47	1.34
26	C	307	CDL	OA6-CA5	4.50	1.47	1.34
21	O	301	TGL	OG1-CA1	4.50	1.46	1.33
26	G	101	CDL	OB8-CB7	4.49	1.46	1.33
26	C	307	CDL	OB8-CB7	4.49	1.46	1.33
25	T	102	PEK	O03-C21	4.47	1.46	1.33
21	N	606	TGL	OG3-CC1	4.47	1.46	1.33
25	T	101	PEK	O03-C21	4.46	1.46	1.33
26	T	103	CDL	OB6-CB5	4.45	1.46	1.34
21	O	301	TGL	OG3-CC1	4.45	1.46	1.33
18	C	306	PGV	O01-C1	4.43	1.46	1.34
21	L	101	TGL	OG1-CA1	4.42	1.46	1.33
21	B	301	TGL	OG3-CC1	4.40	1.46	1.33
18	A	606	PGV	O03-C19	4.40	1.46	1.33
25	C	304	PEK	O03-C21	4.40	1.46	1.33
23	B	303	PSC	O03-C19	4.39	1.46	1.33
21	D	201	TGL	OG3-CC1	4.39	1.46	1.33
21	N	606	TGL	OG1-CA1	4.39	1.46	1.33
18	A	606	PGV	O01-C1	4.38	1.46	1.34
26	P	305	CDL	OA6-CA5	4.38	1.46	1.34
25	T	102	PEK	O01-C1	4.38	1.46	1.34
25	T	101	PEK	O01-C1	4.37	1.46	1.34
18	A	608	PGV	O03-C19	4.37	1.46	1.33
23	O	303	PSC	O03-C19	4.36	1.46	1.33
18	U	101	PGV	O01-C1	4.36	1.46	1.34
18	U	101	PGV	O03-C19	4.35	1.46	1.33
18	N	607	PGV	O01-C1	4.35	1.46	1.34
25	C	304	PEK	O01-C1	4.34	1.46	1.34
18	N	607	PGV	O03-C19	4.33	1.46	1.33
23	O	303	PSC	O01-C1	4.32	1.46	1.34
25	G	103	PEK	O03-C21	4.32	1.46	1.33
26	T	103	CDL	OA8-CA7	4.30	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	103	CDL	OA6-CA5	4.28	1.46	1.34
26	G	101	CDL	OB6-CB5	4.27	1.46	1.34
25	P	303	PEK	O03-C21	4.27	1.45	1.33
26	G	101	CDL	OA8-CA7	4.25	1.45	1.33
26	G	101	CDL	OA6-CA5	4.25	1.46	1.34
21	D	201	TGL	OG2-CB1	4.24	1.46	1.34
18	N	609	PGV	O03-C19	4.11	1.45	1.33
26	P	305	CDL	OB6-CB5	4.07	1.45	1.34
21	B	301	TGL	OG1-CA1	4.05	1.45	1.33
25	G	103	PEK	O01-C1	4.04	1.45	1.34
18	P	304	PGV	O03-C19	4.00	1.45	1.33
25	C	303	PEK	O03-C21	3.97	1.44	1.33
21	B	301	TGL	OG2-CB1	3.96	1.45	1.34
26	C	307	CDL	OB6-CB5	3.96	1.45	1.34
25	C	303	PEK	O01-C1	3.89	1.45	1.34
18	A	608	PGV	O01-C1	3.88	1.45	1.34
18	C	305	PGV	O03-C19	3.88	1.44	1.33
25	P	303	PEK	O01-C1	3.87	1.45	1.34
18	C	305	PGV	O01-C1	3.74	1.44	1.34
23	O	303	PSC	C13-C12	3.69	1.53	1.31
23	B	303	PSC	C13-C12	3.65	1.53	1.31
18	P	304	PGV	O01-C1	3.61	1.44	1.34
21	L	101	TGL	C20-CA9	-3.32	1.32	1.51
26	C	307	CDL	C59-C58	-3.28	1.33	1.51
18	N	609	PGV	O01-C1	3.28	1.43	1.34
26	C	307	CDL	C79-C78	-3.27	1.33	1.51
26	T	103	CDL	C22-C21	-3.26	1.33	1.51
21	B	301	TGL	C10-CB9	-3.26	1.33	1.51
26	G	101	CDL	C59-C58	-3.25	1.33	1.51
26	G	101	CDL	C19-C18	-3.23	1.33	1.51
21	B	301	TGL	C15-CC9	-3.22	1.33	1.51
21	D	201	TGL	C10-CB9	-3.22	1.33	1.51
21	N	606	TGL	C20-CA9	-3.22	1.33	1.51
26	G	101	CDL	C22-C21	-3.22	1.33	1.51
26	T	103	CDL	C19-C18	-3.21	1.33	1.51
26	G	101	CDL	C62-C61	-3.21	1.33	1.51
26	T	103	CDL	C59-C58	-3.21	1.33	1.51
26	C	307	CDL	C19-C18	-3.21	1.33	1.51
26	C	307	CDL	C62-C61	-3.20	1.33	1.51
21	Q	201	TGL	C10-CB9	-3.20	1.33	1.51
21	O	301	TGL	C20-CA9	-3.20	1.33	1.51
21	L	101	TGL	C15-CC9	-3.20	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	305	CDL	C42-C41	-3.19	1.33	1.51
21	B	301	TGL	C20-CA9	-3.19	1.33	1.51
21	Q	201	TGL	C15-CC9	-3.19	1.33	1.51
26	P	305	CDL	C22-C21	-3.19	1.33	1.51
26	P	305	CDL	C59-C58	-3.19	1.33	1.51
26	P	305	CDL	C19-C18	-3.18	1.33	1.51
26	C	307	CDL	C82-C81	-3.18	1.33	1.51
26	G	101	CDL	C39-C38	-3.18	1.33	1.51
26	C	307	CDL	C22-C21	-3.17	1.33	1.51
21	D	201	TGL	C15-CC9	-3.17	1.33	1.51
21	L	101	TGL	C10-CB9	-3.17	1.33	1.51
21	N	606	TGL	C10-CB9	-3.17	1.33	1.51
21	N	606	TGL	C15-CC9	-3.16	1.33	1.51
26	T	103	CDL	C39-C38	-3.16	1.33	1.51
26	C	307	CDL	C42-C41	-3.16	1.33	1.51
26	G	101	CDL	C79-C78	-3.16	1.33	1.51
26	P	305	CDL	C62-C61	-3.15	1.33	1.51
26	T	103	CDL	C42-C41	-3.14	1.34	1.51
26	T	103	CDL	C79-C78	-3.14	1.34	1.51
26	T	103	CDL	C62-C61	-3.14	1.34	1.51
26	G	101	CDL	C42-C41	-3.14	1.34	1.51
21	Q	201	TGL	C20-CA9	-3.13	1.34	1.51
21	O	301	TGL	C15-CC9	-3.13	1.34	1.51
26	G	101	CDL	C82-C81	-3.13	1.34	1.51
26	P	305	CDL	C82-C81	-3.12	1.34	1.51
26	P	305	CDL	C79-C78	-3.12	1.34	1.51
26	P	305	CDL	C39-C38	-3.10	1.34	1.51
21	D	201	TGL	C20-CA9	-3.10	1.34	1.51
26	C	307	CDL	C39-C38	-3.09	1.34	1.51
21	O	301	TGL	C10-CB9	-3.08	1.34	1.51
26	T	103	CDL	C82-C81	-3.06	1.34	1.51
14	N	602	HEA	C3B-C11	-2.93	1.50	1.52
14	A	601[B]	HEA	C3B-C11	-2.80	1.50	1.52
14	A	601[A]	HEA	C3B-C11	-2.80	1.50	1.52
27	W	104	DMU	O16-C6	2.25	1.44	1.40
14	A	602	HEA	C3B-C11	-2.22	1.51	1.52
27	C	313	DMU	O16-C6	2.21	1.44	1.40
14	A	601[B]	HEA	O11-C11	2.16	1.47	1.42
14	A	601[A]	HEA	O11-C11	2.16	1.47	1.42

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	308	CHD	C17-C13-C12	-4.59	113.47	117.67
21	L	101	TGL	OG2-CB1-CB2	4.59	121.39	111.50
26	G	101	CDL	OA6-CA5-C11	4.58	121.37	111.50
23	O	303	PSC	O01-C1-C2	4.43	121.05	111.50
24	C	308	CHD	C16-C17-C20	4.41	118.97	112.15
21	N	606	TGL	OG2-CB1-CB2	4.36	120.90	111.50
26	G	101	CDL	OB6-CB5-C51	4.29	120.74	111.50
25	C	304	PEK	O01-C1-C2	4.25	120.65	111.50
26	T	103	CDL	OB6-CB5-C51	4.23	120.62	111.50
26	C	307	CDL	OA6-CA5-C11	4.21	120.58	111.50
24	C	308	CHD	C22-C23-C24	-4.18	104.60	113.59
18	A	606	PGV	O01-C1-C2	4.15	120.44	111.50
14	A	602	HEA	CAD-CBD-CGD	-4.08	105.83	112.67
21	O	301	TGL	OG2-CB1-CB2	4.07	120.27	111.50
26	P	305	CDL	OA6-CA5-C11	4.06	120.26	111.50
25	T	101	PEK	O01-C1-C2	4.02	120.17	111.50
25	G	103	PEK	O01-C1-C2	4.01	120.14	111.50
26	T	103	CDL	OA6-CA5-C11	4.00	120.12	111.50
24	C	308	CHD	C13-C17-C20	-4.00	114.72	119.50
14	N	602	HEA	CAD-CBD-CGD	-3.95	106.04	112.67
24	C	308	CHD	C23-C22-C20	-3.94	109.41	114.72
18	U	101	PGV	O01-C1-C2	3.91	119.92	111.50
21	B	301	TGL	OG2-CB1-CB2	3.82	119.73	111.50
14	N	601[A]	HEA	CAA-CBA-CGA	-3.81	106.29	112.67
14	N	601[B]	HEA	CAA-CBA-CGA	-3.81	106.29	112.67
18	C	306	PGV	O01-C1-C2	3.77	119.62	111.50
24	J	101	CHD	C16-C17-C20	3.73	117.92	112.15
18	N	607	PGV	O01-C1-C2	3.69	119.45	111.50
23	B	303	PSC	O01-C1-C2	3.67	119.41	111.50
14	A	601[A]	HEA	C27-C19-C20	3.59	121.31	115.27
25	T	102	PEK	O01-C1-C2	3.58	119.22	111.50
18	N	609	PGV	O03-C19-C20	3.54	123.03	111.91
24	W	101	CHD	C16-C17-C20	3.47	117.52	112.15
14	N	602	HEA	OMA-CMA-C3A	-3.45	117.39	124.91
18	U	101	PGV	O03-C19-C20	3.36	122.47	111.91
24	P	306	CHD	C22-C23-C24	-3.34	106.40	113.59
25	P	303	PEK	O01-C1-C2	3.34	118.69	111.50
24	J	101	CHD	C14-C13-C12	3.32	110.50	107.40
14	N	601[A]	HEA	C27-C19-C20	3.32	120.86	115.27
24	P	306	CHD	C23-C22-C20	-3.31	110.26	114.72
24	W	101	CHD	C14-C13-C12	3.28	110.46	107.40
21	Q	201	TGL	OG3-CC1-CC2	3.28	122.20	111.91
24	C	308	CHD	C15-C14-C8	3.27	122.90	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	101	CHD	C22-C20-C17	3.26	117.03	110.28
18	C	306	PGV	O03-C19-C20	3.26	122.13	111.91
18	A	608	PGV	O03-C19-C20	3.25	122.12	111.91
21	B	301	TGL	OG3-CC1-CC2	3.25	122.10	111.91
27	P	313	DMU	C6-C1-C2	3.22	116.69	110.00
26	P	305	CDL	OB6-CB5-C51	3.19	118.38	111.50
21	D	201	TGL	OG1-CA1-CA2	3.15	121.79	111.91
21	L	101	TGL	OG1-CA1-CA2	3.15	121.78	111.91
27	W	104	DMU	O7-C3-C4	3.12	118.00	109.45
14	A	602	HEA	C1B-C2B-C3B	-3.07	104.86	107.00
24	C	308	CHD	C6-C7-C8	3.04	114.73	111.48
26	C	307	CDL	OB6-CB5-C51	3.04	118.04	111.50
14	A	601[B]	HEA	C13-C12-C11	-3.02	109.81	114.35
14	A	601[A]	HEA	C13-C12-C11	-3.02	109.81	114.35
14	A	601[B]	HEA	CMC-C2C-C1C	-2.99	123.86	128.46
14	A	601[A]	HEA	CMC-C2C-C1C	-2.99	123.86	128.46
24	J	101	CHD	C22-C20-C17	2.99	116.47	110.28
14	N	601[A]	HEA	OMA-CMA-C3A	-2.99	118.41	124.91
14	N	601[B]	HEA	OMA-CMA-C3A	-2.99	118.41	124.91
24	J	101	CHD	C17-C13-C14	-2.97	97.10	100.09
18	N	609	PGV	O03-C19-O04	-2.96	116.12	123.59
27	P	313	DMU	O5-C6-C1	2.96	116.60	110.35
21	Q	201	TGL	OG2-CB1-CB2	2.95	117.86	111.50
14	A	601[B]	HEA	CMC-C2C-C3C	2.93	130.16	124.68
14	A	601[A]	HEA	CMC-C2C-C3C	2.93	130.16	124.68
25	P	303	PEK	O03-C21-C22	2.93	121.10	111.91
14	N	602	HEA	CAA-CBA-CGA	-2.92	107.77	112.67
21	N	606	TGL	OG1-CA1-CA2	2.91	121.05	111.91
21	D	201	TGL	OG3-CC1-CC2	2.90	121.00	111.91
25	T	102	PEK	O03-C21-C22	2.90	121.00	111.91
14	A	602	HEA	OMA-CMA-C3A	-2.88	118.64	124.91
24	W	101	CHD	C17-C13-C14	-2.88	97.19	100.09
14	N	602	HEA	C27-C19-C20	2.85	120.07	115.27
26	P	305	CDL	OB8-CB7-C71	2.84	120.81	111.91
14	A	601[B]	HEA	C21-C22-C23	-2.83	118.07	127.75
23	B	303	PSC	O03-C19-C20	2.83	120.79	111.91
18	A	606	PGV	O03-C19-C20	2.83	120.79	111.91
21	Q	201	TGL	OG1-CA1-CA2	2.83	120.78	111.91
24	B	304	CHD	C15-C14-C13	2.78	106.28	103.55
14	N	602	HEA	C1B-C2B-C3B	-2.77	105.07	107.00
24	W	101	CHD	C6-C5-C10	2.76	115.59	112.66
14	A	602	HEA	C27-C19-C20	2.76	119.91	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	303	PEK	O01-C1-C2	2.75	117.43	111.50
26	T	103	CDL	OA8-CA7-C31	2.73	120.47	111.91
21	N	606	TGL	OG3-CC1-CC2	2.71	120.42	111.91
14	A	602	HEA	CAA-CBA-CGA	-2.71	108.13	112.67
23	O	303	PSC	O03-C19-C20	2.69	120.36	111.91
26	G	101	CDL	OA8-CA7-C31	2.69	120.34	111.91
21	L	101	TGL	OG3-CC1-CC2	2.65	120.23	111.91
27	C	312	DMU	C1-C2-C3	2.64	115.72	109.68
24	G	102	CHD	C6-C5-C4	-2.62	108.18	111.19
14	A	601[B]	HEA	OMA-CMA-C3A	-2.62	119.21	124.91
14	A	601[A]	HEA	OMA-CMA-C3A	-2.62	119.21	124.91
25	C	304	PEK	O03-C21-C22	2.62	120.12	111.91
21	O	301	TGL	OG1-CA1-CA2	2.61	120.10	111.91
14	A	601[A]	HEA	C20-C19-C18	-2.59	115.87	121.12
27	C	313	DMU	O16-C6-C1	2.59	112.34	108.30
14	A	601[B]	HEA	CBA-CAA-C2A	2.58	117.23	112.48
14	A	601[A]	HEA	CBA-CAA-C2A	2.58	117.23	112.48
14	N	601[A]	HEA	CBA-CAA-C2A	2.58	117.23	112.48
14	N	601[B]	HEA	CBA-CAA-C2A	2.58	117.23	112.48
24	P	306	CHD	C6-C7-C8	2.57	114.23	111.48
26	G	101	CDL	OB8-CB7-C71	2.57	119.96	111.91
26	T	103	CDL	OB8-CB7-C71	2.56	119.95	111.91
24	J	101	CHD	C1-C10-C5	2.56	111.55	107.77
25	T	101	PEK	O03-C21-C22	2.55	119.92	111.91
27	C	312	DMU	C6-C1-C2	2.54	115.29	110.00
18	N	607	PGV	O03-C19-C20	2.53	119.85	111.91
24	P	301	CHD	C6-C7-C8	2.51	114.16	111.48
14	N	602	HEA	C13-C12-C11	-2.48	110.62	114.35
25	G	103	PEK	C02-O01-C1	-2.48	111.69	117.79
25	G	103	PEK	O03-C21-C22	2.47	119.67	111.91
18	A	608	PGV	O03-C19-O04	-2.47	117.37	123.59
14	A	602	HEA	C13-C12-C11	-2.46	110.66	114.35
18	C	305	PGV	O01-C1-C2	2.43	116.75	111.50
18	A	608	PGV	O01-C1-C2	2.43	116.73	111.50
26	C	307	CDL	OB8-CB7-C71	2.42	119.50	111.91
14	A	601[B]	HEA	C26-C15-C16	2.41	119.33	115.27
14	A	601[A]	HEA	C26-C15-C16	2.41	119.33	115.27
14	N	601[A]	HEA	C20-C19-C18	-2.40	116.25	121.12
21	O	301	TGL	OG3-CC1-CC2	2.40	119.43	111.91
24	C	301	CHD	C15-C14-C13	2.39	105.90	103.55
21	Q	201	TGL	OG3-CC1-OC1	-2.39	117.57	123.59
26	P	305	CDL	OA8-CA7-C31	2.39	119.39	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	306	CHD	C13-C17-C20	-2.38	116.66	119.50
18	U	101	PGV	O03-C19-O04	-2.34	117.67	123.59
14	N	601[B]	HEA	C21-C22-C23	-2.34	119.75	127.75
24	W	101	CHD	C9-C10-C5	2.33	111.85	108.58
26	G	101	CDL	OA6-CA5-OA7	-2.33	118.07	123.70
24	P	306	CHD	C4-C3-C2	-2.33	107.77	110.55
26	C	307	CDL	OA8-CA7-C31	2.33	119.21	111.91
24	P	306	CHD	C15-C14-C13	2.32	105.83	103.55
27	M	101	DMU	C7-C8-C9	2.32	114.37	110.24
14	N	601[A]	HEA	CMB-C2B-C3B	2.31	129.21	124.69
14	N	601[B]	HEA	CMB-C2B-C3B	2.31	129.21	124.69
21	B	301	TGL	OG3-CC1-OC1	-2.31	117.77	123.59
14	A	602	HEA	C20-C19-C18	-2.30	116.45	121.12
23	O	303	PSC	O01-C1-O02	-2.29	118.16	123.70
14	A	601[B]	HEA	C16-C15-C14	-2.28	116.50	121.12
14	A	601[A]	HEA	C16-C15-C14	-2.28	116.50	121.12
24	W	101	CHD	C21-C20-C17	-2.27	109.45	112.92
24	J	101	CHD	C23-C22-C20	-2.26	111.67	114.72
14	N	601[A]	HEA	CMB-C2B-C1B	-2.26	124.99	128.46
14	N	601[B]	HEA	CMB-C2B-C1B	-2.26	124.99	128.46
14	A	601[B]	HEA	C1B-C2B-C3B	-2.26	105.42	107.00
14	A	601[A]	HEA	C1B-C2B-C3B	-2.26	105.42	107.00
14	A	601[B]	HEA	CMB-C2B-C3B	2.25	129.09	124.69
14	A	601[A]	HEA	CMB-C2B-C3B	2.25	129.09	124.69
24	C	308	CHD	C10-C9-C8	2.24	114.22	111.82
24	G	102	CHD	C15-C14-C13	2.23	105.74	103.55
24	P	306	CHD	C15-C14-C8	2.23	121.45	118.33
24	G	102	CHD	C13-C17-C20	-2.21	116.86	119.50
24	P	301	CHD	C19-C10-C1	-2.21	104.70	108.26
27	P	313	DMU	C2-C3-C4	-2.20	105.87	110.93
24	C	308	CHD	O12-C12-C13	-2.20	107.31	111.03
25	T	102	PEK	O03-C21-O04	-2.20	118.04	123.59
25	T	101	PEK	O01-C1-O02	-2.20	118.38	123.70
21	D	201	TGL	OG3-CC1-OC1	-2.19	118.06	123.59
24	J	101	CHD	C6-C5-C4	-2.18	108.68	111.19
24	C	301	CHD	C22-C23-C24	-2.17	108.93	113.59
25	C	303	PEK	O03-C21-C22	2.15	118.67	111.91
24	J	101	CHD	C10-C9-C8	2.14	114.12	111.82
24	C	301	CHD	C11-C9-C8	2.14	114.01	110.88
24	C	308	CHD	C14-C13-C12	2.14	109.39	107.40
27	C	313	DMU	C1-C2-C3	2.13	114.55	109.68
18	N	607	PGV	O03-C19-O04	-2.13	118.22	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	301	TGL	OG1-CA1-CA2	2.13	118.58	111.91
21	D	201	TGL	OG2-CB1-CB2	2.12	116.06	111.50
26	T	103	CDL	OA6-CA5-OA7	-2.11	118.61	123.70
24	P	301	CHD	C15-C14-C13	2.10	105.61	103.55
18	C	306	PGV	O03-C19-O04	-2.10	118.29	123.59
14	N	601[A]	HEA	CMD-C2D-C3D	2.09	128.89	124.94
14	N	601[B]	HEA	CMD-C2D-C3D	2.09	128.89	124.94
25	G	103	PEK	O01-C1-O02	-2.08	118.67	123.70
26	G	101	CDL	OB8-CB7-OB9	-2.05	118.41	123.59
24	B	304	CHD	C6-C5-C4	-2.05	108.83	111.19
27	P	313	DMU	C6-O5-C4	2.05	117.71	113.69
18	N	607	PGV	O01-C1-O02	-2.05	118.75	123.70
18	N	607	PGV	C03-C02-C01	-2.05	106.95	111.79
26	P	305	CDL	OB8-CB7-OB9	-2.04	118.44	123.59
14	N	601[A]	HEA	CMC-C2C-C3C	2.04	128.49	124.68
14	N	601[B]	HEA	CMC-C2C-C3C	2.04	128.49	124.68
18	P	304	PGV	O03-C19-C20	2.04	118.30	111.91
18	A	606	PGV	O03-C01-C02	2.03	114.35	108.43
27	P	313	DMU	O7-C3-C2	2.02	112.65	107.28

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	602	HEA	ND
14	A	602	HEA	NA
14	A	602	HEA	NB
14	N	602	HEA	ND
14	N	602	HEA	NA
14	N	602	HEA	NB

All (953) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	N	607	PGV	O02-C1-O01-C02
18	N	607	PGV	C2-C1-O01-C02
18	U	101	PGV	C03-O11-P-O13
18	U	101	PGV	C04-C05-C06-O06
25	C	304	PEK	C04-O12-P-O14
25	C	304	PEK	C7-C8-C9-C10
25	C	304	PEK	C10-C11-C12-C13
25	C	304	PEK	C13-C14-C15-C16
27	C	312	DMU	C19-C18-O16-C6

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Mol	Chain	Res	Type	Atoms
24	P	306	CHD	C20-C22-C23-C24
18	C	306	PGV	C03-O11-P-O12
18	C	306	PGV	C03-O11-P-O13
18	C	306	PGV	C03-O11-P-O14
25	C	303	PEK	C10-C11-C12-C13
25	G	103	PEK	O12-C04-C05-N
25	G	103	PEK	C2-C1-O01-C02
25	G	103	PEK	C9-C10-C11-C12
23	B	303	PSC	C03-O11-P-O14
23	B	303	PSC	O12-C04-C05-N
27	W	104	DMU	O5-C6-O16-C18
27	Z	101	DMU	C19-C18-O16-C6
27	P	313	DMU	C1-C6-O16-C18
26	T	103	CDL	OA5-CA3-CA4-OA6
26	T	103	CDL	C11-CA5-OA6-CA4
21	B	301	TGL	OB1-CB1-OG2-CG2
26	P	305	CDL	CA2-OA2-PA1-OA4
26	P	305	CDL	C11-CA5-OA6-CA4
26	P	305	CDL	OB7-CB5-OB6-CB4
26	P	305	CDL	C51-CB5-OB6-CB4
23	O	303	PSC	C03-O11-P-O13
23	O	303	PSC	C04-O12-P-O13
23	O	303	PSC	O12-C04-C05-N
23	O	303	PSC	C2-C1-O01-C02
25	P	303	PEK	C7-C8-C9-C10
25	P	303	PEK	C11-C10-C9-C8
25	P	303	PEK	C10-C11-C12-C13
21	Q	201	TGL	CC2-CC1-OG3-CG3
21	Q	201	TGL	OC1-CC1-OG3-CG3
26	C	307	CDL	O1-C1-CB2-OB2
26	C	307	CDL	CA2-C1-CB2-OB2
26	C	307	CDL	CA2-OA2-PA1-OA4
26	C	307	CDL	C11-CA5-OA6-CA4
26	C	307	CDL	OB7-CB5-OB6-CB4
26	C	307	CDL	C51-CB5-OB6-CB4
18	C	305	PGV	C10-C11-C12-C13
18	A	606	PGV	C04-O12-P-O14
18	A	606	PGV	C02-C03-O11-P
21	D	201	TGL	CB2-CB1-OG2-CG2
21	D	201	TGL	OG1-CG1-CG2-OG2
25	T	101	PEK	C03-O11-P-O13
25	T	101	PEK	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	T	101	PEK	C2-C1-O01-C02
25	T	101	PEK	C7-C8-C9-C10
26	G	101	CDL	O1-C1-CA2-OA2
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	C11-CA5-OA6-CA4
27	W	104	DMU	C4-C3-O7-C10
23	O	303	PSC	O04-C19-O03-C01
21	D	201	TGL	OC1-CC1-OG3-CG3
21	B	301	TGL	CG2-CG3-OG3-CC1
27	P	313	DMU	O1-C10-O7-C3
23	O	303	PSC	C20-C19-O03-C01
21	D	201	TGL	CC2-CC1-OG3-CG3
21	N	606	TGL	OA1-CA1-OG1-CG1
23	B	303	PSC	O04-C19-O03-C01
18	A	606	PGV	O04-C19-O03-C01
24	C	308	CHD	C13-C17-C20-C21
25	G	103	PEK	O02-C1-O01-C02
21	O	301	TGL	OB1-CB1-OG2-CG2
26	T	103	CDL	OA7-CA5-OA6-CA4
26	P	305	CDL	OA7-CA5-OA6-CA4
23	O	303	PSC	O02-C1-O01-C02
26	C	307	CDL	OA7-CA5-OA6-CA4
18	A	606	PGV	O02-C1-O01-C02
21	D	201	TGL	OB1-CB1-OG2-CG2
26	G	101	CDL	OA7-CA5-OA6-CA4
21	N	606	TGL	CA2-CA1-OG1-CG1
23	B	303	PSC	C20-C19-O03-C01
21	O	301	TGL	CB2-CB1-OG2-CG2
21	B	301	TGL	CB2-CB1-OG2-CG2
24	C	308	CHD	C16-C17-C20-C21
24	C	308	CHD	C16-C17-C20-C22
24	C	308	CHD	C13-C17-C20-C22
18	N	607	PGV	C20-C19-O03-C01
21	B	301	TGL	CA2-CA1-OG1-CG1
21	B	301	TGL	CC2-CC1-OG3-CG3
18	A	606	PGV	C20-C19-O03-C01
26	G	101	CDL	C31-CA7-OA8-CA6
27	C	313	DMU	O6-C11-C9-O1
18	U	101	PGV	C10-C11-C12-C13
25	C	303	PEK	C13-C14-C15-C16
23	B	303	PSC	C11-C12-C13-C14
25	P	303	PEK	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
18	N	607	PGV	O04-C19-O03-C01
26	T	103	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	OA9-CA7-OA8-CA6
23	B	303	PSC	C04-C05-N-C06
21	O	301	TGL	CC2-CC1-OG3-CG3
26	T	103	CDL	C31-CA7-OA8-CA6
21	B	301	TGL	OA1-CA1-OG1-CG1
18	A	606	PGV	C2-C1-O01-C02
27	C	312	DMU	O5-C4-C57-O61
27	W	104	DMU	O6-C11-C9-O1
27	P	313	DMU	O6-C11-C9-C8
25	T	102	PEK	C33-C34-C35-C36
27	C	313	DMU	O6-C11-C9-C8
27	C	313	DMU	O5-C4-C57-O61
21	B	301	TGL	OC1-CC1-OG3-CG3
24	C	308	CHD	C21-C20-C22-C23
27	P	313	DMU	O6-C11-C9-O1
21	O	301	TGL	OC1-CC1-OG3-CG3
14	A	601[B]	HEA	C19-C20-C21-C22
14	N	601[A]	HEA	C19-C20-C21-C22
14	N	601[B]	HEA	C15-C16-C17-C18
14	N	601[B]	HEA	C19-C20-C21-C22
26	P	305	CDL	C31-CA7-OA8-CA6
24	P	306	CHD	C17-C20-C22-C23
18	N	607	PGV	C10-C11-C12-C13
26	T	103	CDL	CA2-C1-CB2-OB2
26	C	307	CDL	CB2-C1-CA2-OA2
26	G	101	CDL	CB2-C1-CA2-OA2
26	P	305	CDL	OA9-CA7-OA8-CA6
26	T	103	CDL	C71-CB7-OB8-CB6
26	P	305	CDL	C71-CB7-OB8-CB6
21	L	101	TGL	CA2-CA1-OG1-CG1
25	T	101	PEK	C22-C21-O03-C01
26	G	101	CDL	C71-CB7-OB8-CB6
23	O	303	PSC	C1-C2-C3-C4
21	Q	201	TGL	CC1-CC2-CC3-CC4
24	C	308	CHD	C17-C20-C22-C23
27	C	312	DMU	C3-C4-C57-O61
25	G	103	PEK	O01-C02-C03-O11
26	C	307	CDL	O1-C1-CA2-OA2
23	B	303	PSC	C1-C2-C3-C4
26	P	305	CDL	CA5-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	P	305	CDL	OB9-CB7-OB8-CB6
24	J	101	CHD	C13-C17-C20-C22
26	T	103	CDL	OB9-CB7-OB8-CB6
21	L	101	TGL	OA1-CA1-OG1-CG1
26	G	101	CDL	OB9-CB7-OB8-CB6
24	P	306	CHD	C21-C20-C22-C23
26	T	103	CDL	C79-C80-C81-C82
21	Q	201	TGL	CB1-CB2-CB3-CB4
25	G	103	PEK	C4-C5-C6-C7
25	G	103	PEK	C7-C8-C9-C10
18	N	609	PGV	C10-C11-C12-C13
18	P	304	PGV	C10-C11-C12-C13
25	P	303	PEK	C4-C5-C6-C7
24	W	101	CHD	C13-C17-C20-C22
18	U	101	PGV	C19-C20-C21-C22
26	P	305	CDL	CB5-C51-C52-C53
26	C	307	CDL	CB5-C51-C52-C53
26	G	101	CDL	CB5-C51-C52-C53
27	M	101	DMU	O6-C11-C9-O1
23	B	303	PSC	C04-C05-N-C08
25	G	103	PEK	C1-C2-C3-C4
24	J	101	CHD	C13-C17-C20-C21
24	W	101	CHD	C13-C17-C20-C21
27	C	313	DMU	C3-C4-C57-O61
27	C	312	DMU	O16-C18-C19-C22
25	T	101	PEK	O04-C21-O03-C01
27	C	312	DMU	O5-C6-O16-C18
27	P	313	DMU	O5-C6-O16-C18
14	A	601[B]	HEA	C15-C16-C17-C18
14	A	601[A]	HEA	C19-C20-C21-C22
27	Z	101	DMU	O16-C18-C19-C22
27	Z	101	DMU	O6-C11-C9-O1
24	J	101	CHD	C16-C17-C20-C21
18	A	606	PGV	C10-C11-C12-C13
25	T	102	PEK	C4-C5-C6-C7
25	T	102	PEK	C7-C8-C9-C10
25	C	304	PEK	C2-C1-O01-C02
21	N	606	TGL	CB2-CB1-OG2-CG2
25	G	103	PEK	C04-O12-P-O11
23	B	303	PSC	C04-O12-P-O11
26	P	305	CDL	CA2-OA2-PA1-OA5
26	P	305	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
23	O	303	PSC	C03-O11-P-O12
23	O	303	PSC	C04-O12-P-O11
26	C	307	CDL	CA2-OA2-PA1-OA5
26	C	307	CDL	CA3-OA5-PA1-OA2
26	C	307	CDL	CB2-OB2-PB2-OB5
18	A	606	PGV	C03-O11-P-O12
18	A	606	PGV	C04-O12-P-O11
25	T	101	PEK	C03-O11-P-O12
26	C	307	CDL	C31-CA7-OA8-CA6
24	W	101	CHD	C16-C17-C20-C21
25	C	304	PEK	O02-C1-O01-C02
21	N	606	TGL	OB1-CB1-OG2-CG2
25	T	102	PEK	C22-C21-O03-C01
21	L	101	TGL	CA9-C20-C21-C22
18	A	606	PGV	C19-C20-C21-C22
18	U	101	PGV	C6-C7-C8-C9
21	N	606	TGL	CA2-CA3-CA4-CA5
23	B	303	PSC	C5-C6-C7-C8
23	B	303	PSC	C30-C31-C32-C33
26	G	101	CDL	C54-C55-C56-C57
23	B	303	PSC	C2-C1-O01-C02
18	N	607	PGV	C22-C23-C24-C25
18	U	101	PGV	C4-C5-C6-C7
27	C	312	DMU	C19-C22-C25-C28
18	C	306	PGV	C20-C21-C22-C23
21	N	606	TGL	CB5-CB6-CB7-CB8
21	O	301	TGL	C11-C10-CB9-CB8
26	T	103	CDL	C34-C35-C36-C37
26	T	103	CDL	C52-C53-C54-C55
21	B	301	TGL	CB3-CB4-CB5-CB6
21	B	301	TGL	CC5-CC6-CC7-CC8
21	B	301	TGL	C23-C24-C25-C26
26	P	305	CDL	C35-C36-C37-C38
26	C	307	CDL	C57-C58-C59-C60
26	C	307	CDL	C77-C78-C79-C80
21	D	201	TGL	C14-C29-C30-C31
21	L	101	TGL	CA3-CA4-CA5-CA6
21	L	101	TGL	C19-C33-C34-C35
25	T	101	PEK	C26-C27-C28-C29
26	G	101	CDL	C38-C39-C40-C41
18	U	101	PGV	C13-C14-C15-C16
18	U	101	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
21	N	606	TGL	C21-C20-CA9-CA8
21	N	606	TGL	CB6-CB7-CB8-CB9
23	B	303	PSC	C23-C24-C25-C26
27	Z	101	DMU	C19-C22-C25-C28
26	T	103	CDL	C53-C54-C55-C56
26	P	305	CDL	C39-C40-C41-C42
26	P	305	CDL	C78-C79-C80-C81
18	P	304	PGV	C30-C31-C32-C33
26	C	307	CDL	C36-C37-C38-C39
26	C	307	CDL	C58-C59-C60-C61
21	D	201	TGL	CC2-CC3-CC4-CC5
21	L	101	TGL	CC7-CC8-CC9-C15
25	T	102	PEK	C28-C29-C30-C31
21	B	301	TGL	CG1-CG2-OG2-CB1
23	B	303	PSC	O02-C1-O01-C02
18	U	101	PGV	C20-C21-C22-C23
25	G	103	PEK	C26-C27-C28-C29
26	P	305	CDL	C53-C54-C55-C56
21	Q	201	TGL	C11-C10-CB9-CB8
26	C	307	CDL	C73-C74-C75-C76
25	G	103	PEK	C13-C14-C15-C16
25	T	101	PEK	C10-C11-C12-C13
26	T	103	CDL	C19-C20-C21-C22
21	B	301	TGL	CC7-CC8-CC9-C15
26	P	305	CDL	C51-C52-C53-C54
26	C	307	CDL	C35-C36-C37-C38
26	T	103	CDL	O1-C1-CB2-OB2
18	U	101	PGV	C14-C15-C16-C17
18	C	306	PGV	C14-C15-C16-C17
21	O	301	TGL	CB3-CB4-CB5-CB6
27	W	104	DMU	C19-C22-C25-C28
26	T	103	CDL	C41-C42-C43-C44
27	C	313	DMU	C28-C31-C34-C37
21	B	301	TGL	C21-C22-C23-C24
21	B	301	TGL	C22-C23-C24-C25
26	P	305	CDL	C20-C21-C22-C23
21	D	201	TGL	C11-C12-C13-C14
21	L	101	TGL	CA6-CA7-CA8-CA9
21	L	101	TGL	CB5-CB6-CB7-CB8
21	L	101	TGL	C16-C15-CC9-CC8
26	T	103	CDL	CB7-C71-C72-C73
18	P	304	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
27	C	312	DMU	C1-C6-O16-C18
18	N	607	PGV	C4-C5-C6-C7
18	N	607	PGV	C28-C29-C30-C31
18	C	306	PGV	C4-C5-C6-C7
21	N	606	TGL	CC3-CC4-CC5-CC6
21	N	606	TGL	CC5-CC6-CC7-CC8
27	C	313	DMU	C19-C22-C25-C28
21	B	301	TGL	CA5-CA6-CA7-CA8
26	P	305	CDL	C57-C58-C59-C60
18	P	304	PGV	C22-C23-C24-C25
23	O	303	PSC	C22-C23-C24-C25
23	O	303	PSC	C24-C25-C26-C27
21	D	201	TGL	CC5-CC6-CC7-CC8
26	G	101	CDL	C23-C24-C25-C26
18	N	607	PGV	C24-C25-C26-C27
21	O	301	TGL	CC5-CC6-CC7-CC8
26	P	305	CDL	C12-C13-C14-C15
18	C	305	PGV	C28-C29-C30-C31
21	L	101	TGL	C18-C19-C33-C34
21	D	201	TGL	CB1-CB2-CB3-CB4
18	C	306	PGV	C23-C24-C25-C26
21	B	301	TGL	CA2-CA3-CA4-CA5
18	N	609	PGV	C23-C24-C25-C26
23	O	303	PSC	C29-C30-C31-C32
21	Q	201	TGL	C23-C24-C25-C26
26	C	307	CDL	C18-C19-C20-C21
18	C	305	PGV	C27-C28-C29-C30
21	D	201	TGL	CA6-CA7-CA8-CA9
26	G	101	CDL	C15-C16-C17-C18
26	G	101	CDL	C32-C33-C34-C35
26	G	101	CDL	C43-C44-C45-C46
25	G	103	PEK	C30-C31-C32-C33
21	N	606	TGL	C24-C25-C26-C27
26	C	307	CDL	C34-C35-C36-C37
21	D	201	TGL	C16-C17-C18-C19
26	G	101	CDL	C42-C43-C44-C45
18	N	607	PGV	C04-C05-C06-O06
18	U	101	PGV	C28-C29-C30-C31
18	C	306	PGV	C21-C22-C23-C24
25	C	303	PEK	C34-C35-C36-C37
21	N	606	TGL	C10-C11-C12-C13
21	N	606	TGL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
27	W	104	DMU	C28-C31-C34-C37
21	B	301	TGL	C12-C13-C14-C29
26	P	305	CDL	C61-C62-C63-C64
21	Q	201	TGL	C17-C18-C19-C33
18	N	609	PGV	C11-C10-C9-C8
25	C	304	PEK	C32-C33-C34-C35
18	C	306	PGV	C2-C3-C4-C5
21	O	301	TGL	C16-C17-C18-C19
26	T	103	CDL	C21-C22-C23-C24
26	T	103	CDL	C37-C38-C39-C40
26	T	103	CDL	C59-C60-C61-C62
26	T	103	CDL	C63-C64-C65-C66
26	P	305	CDL	C77-C78-C79-C80
26	C	307	CDL	C72-C73-C74-C75
18	C	305	PGV	C13-C14-C15-C16
18	A	606	PGV	C13-C14-C15-C16
21	D	201	TGL	C13-C14-C29-C30
25	T	102	PEK	C32-C33-C34-C35
23	B	303	PSC	C04-C05-N-C07
18	N	607	PGV	C2-C3-C4-C5
18	C	306	PGV	C28-C29-C30-C31
26	T	103	CDL	C23-C24-C25-C26
26	T	103	CDL	C62-C63-C64-C65
26	C	307	CDL	C53-C54-C55-C56
21	L	101	TGL	CB2-CB3-CB4-CB5
25	T	101	PEK	C23-C24-C25-C26
26	G	101	CDL	C41-C42-C43-C44
26	G	101	CDL	C63-C64-C65-C66
25	C	304	PEK	O12-C04-C05-N
27	M	101	DMU	C22-C25-C28-C31
18	C	306	PGV	C29-C30-C31-C32
21	N	606	TGL	CA3-CA4-CA5-CA6
21	O	301	TGL	CA5-CA6-CA7-CA8
23	B	303	PSC	C3-C4-C5-C6
26	T	103	CDL	C75-C76-C77-C78
26	C	307	CDL	C54-C55-C56-C57
26	C	307	CDL	C74-C75-C76-C77
21	L	101	TGL	C12-C13-C14-C29
21	L	101	TGL	C21-C22-C23-C24
26	G	101	CDL	C57-C58-C59-C60
26	C	307	CDL	CA5-C11-C12-C13
18	N	607	PGV	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	C	303	PEK	C16-C17-C18-C19
21	O	301	TGL	CB7-CB8-CB9-C10
21	B	301	TGL	CA7-CA8-CA9-C20
21	Q	201	TGL	CA6-CA7-CA8-CA9
21	Q	201	TGL	CC5-CC6-CC7-CC8
26	C	307	CDL	C56-C57-C58-C59
18	A	608	PGV	C30-C31-C32-C33
26	C	307	CDL	C71-CB7-OB8-CB6
25	C	304	PEK	C26-C27-C28-C29
27	C	312	DMU	C31-C34-C37-C40
23	B	303	PSC	C29-C30-C31-C32
26	P	305	CDL	C75-C76-C77-C78
26	P	305	CDL	C81-C82-C83-C84
25	P	303	PEK	C26-C27-C28-C29
26	C	307	CDL	C14-C15-C16-C17
21	D	201	TGL	CB7-CB8-CB9-C10
21	L	101	TGL	CC4-CC5-CC6-CC7
21	O	301	TGL	C20-C21-C22-C23
26	C	307	CDL	C51-C52-C53-C54
21	D	201	TGL	C18-C19-C33-C34
21	L	101	TGL	C17-C18-C19-C33
26	G	101	CDL	C71-C72-C73-C74
26	C	307	CDL	OA9-CA7-OA8-CA6
25	G	103	PEK	C34-C35-C36-C37
21	N	606	TGL	C12-C13-C14-C29
21	O	301	TGL	CA2-CA3-CA4-CA5
21	B	301	TGL	CC6-CC7-CC8-CC9
26	P	305	CDL	C15-C16-C17-C18
26	P	305	CDL	C43-C44-C45-C46
18	A	606	PGV	C27-C28-C29-C30
21	D	201	TGL	CC9-C15-C16-C17
21	L	101	TGL	C11-C12-C13-C14
25	T	102	PEK	C27-C28-C29-C30
25	T	102	PEK	C13-C14-C15-C16
26	C	307	CDL	C63-C64-C65-C66
21	D	201	TGL	CB9-C10-C11-C12
21	N	606	TGL	CC9-C15-C16-C17
21	O	301	TGL	CB9-C10-C11-C12
26	T	103	CDL	C81-C82-C83-C84
21	L	101	TGL	C11-C10-CB9-CB8
27	W	104	DMU	O6-C11-C9-C8
25	C	303	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	G	103	PEK	C23-C24-C25-C26
21	O	301	TGL	CA4-CA5-CA6-CA7
26	C	307	CDL	C17-C18-C19-C20
18	C	305	PGV	C24-C25-C26-C27
26	G	101	CDL	C21-C22-C23-C24
18	P	304	PGV	C12-C13-C14-C15
25	P	303	PEK	C15-C16-C17-C18
18	N	609	PGV	C26-C27-C28-C29
26	G	101	CDL	C35-C36-C37-C38
27	C	312	DMU	C28-C31-C34-C37
26	G	101	CDL	C62-C63-C64-C65
25	T	102	PEK	O04-C21-O03-C01
25	T	101	PEK	C21-C22-C23-C24
26	T	103	CDL	C58-C59-C60-C61
26	P	305	CDL	C36-C37-C38-C39
21	Q	201	TGL	C19-C33-C34-C35
26	G	101	CDL	C56-C57-C58-C59
21	B	301	TGL	CB7-CB8-CB9-C10
21	B	301	TGL	C14-C29-C30-C31
21	Q	201	TGL	C21-C20-CA9-CA8
26	C	307	CDL	C22-C23-C24-C25
26	C	307	CDL	C38-C39-C40-C41
26	C	307	CDL	OB9-CB7-OB8-CB6
21	O	301	TGL	CC4-CC5-CC6-CC7
18	P	304	PGV	C24-C25-C26-C27
26	C	307	CDL	C40-C41-C42-C43
26	C	307	CDL	C83-C84-C85-C86
25	T	102	PEK	C30-C31-C32-C33
20	A	615	EDO	O1-C1-C2-O2
20	P	309	EDO	O1-C1-C2-O2
20	L	105	EDO	O1-C1-C2-O2
20	H	101	EDO	O1-C1-C2-O2
20	M	103	EDO	O1-C1-C2-O2
20	A	609	EDO	O1-C1-C2-O2
20	W	103	EDO	O1-C1-C2-O2
25	G	103	PEK	C31-C32-C33-C34
26	T	103	CDL	C51-CB5-OB6-CB4
25	C	303	PEK	C28-C29-C30-C31
26	T	103	CDL	C31-C32-C33-C34
25	C	304	PEK	C1-C2-C3-C4
26	T	103	CDL	CA5-C11-C12-C13
27	M	101	DMU	C25-C28-C31-C34

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Mol	Chain	Res	Type	Atoms
21	O	301	TGL	C13-C14-C29-C30
18	A	606	PGV	C26-C27-C28-C29
27	W	104	DMU	C18-C19-C22-C25
23	O	303	PSC	C11-C12-C13-C14
25	T	101	PEK	C4-C5-C6-C7
23	B	303	PSC	C6-C7-C8-C9
26	G	101	CDL	CA5-C11-C12-C13
21	N	606	TGL	CB2-CB3-CB4-CB5
21	Q	201	TGL	CA5-CA6-CA7-CA8
21	B	301	TGL	C19-C33-C34-C35
21	O	301	TGL	CA1-CA2-CA3-CA4
25	G	103	PEK	C33-C34-C35-C36
21	O	301	TGL	C17-C18-C19-C33
18	C	305	PGV	C7-C8-C9-C10
21	D	201	TGL	C21-C22-C23-C24
27	C	312	DMU	C18-C19-C22-C25
27	C	313	DMU	C18-C19-C22-C25
21	B	301	TGL	C11-C10-CB9-CB8
21	B	301	TGL	C13-C14-C29-C30
26	C	307	CDL	C21-C22-C23-C24
25	G	103	PEK	C21-C22-C23-C24
18	P	304	PGV	C1-C2-C3-C4
18	C	305	PGV	C1-C2-C3-C4
21	Q	201	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	CB2-CB1-OG2-CG2
25	G	103	PEK	C29-C30-C31-C32
26	T	103	CDL	C17-C18-C19-C20
21	B	301	TGL	CC4-CC5-CC6-CC7
26	C	307	CDL	C23-C24-C25-C26
18	A	608	PGV	C27-C28-C29-C30
18	N	607	PGV	C26-C27-C28-C29
26	T	103	CDL	C14-C15-C16-C17
21	L	101	TGL	OB1-CB1-OG2-CG2
21	D	201	TGL	CA9-C20-C21-C22
21	B	301	TGL	C16-C17-C18-C19
26	P	305	CDL	C54-C55-C56-C57
26	P	305	CDL	C56-C57-C58-C59
21	D	201	TGL	C11-C10-CB9-CB8
25	C	304	PEK	C2-C3-C4-C5
25	T	102	PEK	C2-C3-C4-C5
25	G	103	PEK	C22-C23-C24-C25
21	O	301	TGL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	P	305	CDL	C23-C24-C25-C26
21	Q	201	TGL	C21-C22-C23-C24
18	N	607	PGV	C25-C26-C27-C28
21	N	606	TGL	CC4-CC5-CC6-CC7
25	C	303	PEK	C7-C8-C9-C10
18	U	101	PGV	C2-C3-C4-C5
21	D	201	TGL	C10-C11-C12-C13
18	C	306	PGV	C3-C4-C5-C6
21	O	301	TGL	CA7-CA8-CA9-C20
21	L	101	TGL	CC3-CC4-CC5-CC6
27	P	313	DMU	C18-C19-C22-C25
26	T	103	CDL	OB7-CB5-OB6-CB4
21	Q	201	TGL	OB1-CB1-OG2-CG2
23	O	303	PSC	C2-C3-C4-C5
21	L	101	TGL	C24-C25-C26-C27
26	T	103	CDL	C61-C62-C63-C64
26	T	103	CDL	C74-C75-C76-C77
26	G	101	CDL	C1-CA2-OA2-PA1
26	T	103	CDL	C73-C74-C75-C76
26	T	103	CDL	OA5-CA3-CA4-CA6
26	C	307	CDL	OA5-CA3-CA4-CA6
21	L	101	TGL	C10-C11-C12-C13
26	G	101	CDL	CB7-C71-C72-C73
27	C	313	DMU	C22-C25-C28-C31
21	B	301	TGL	CA3-CA4-CA5-CA6
25	T	102	PEK	C25-C26-C27-C28
25	C	304	PEK	C15-C16-C17-C18
25	C	303	PEK	C25-C26-C27-C28
18	P	304	PGV	C7-C8-C9-C10
21	Q	201	TGL	CC6-CC7-CC8-CC9
27	W	104	DMU	C22-C25-C28-C31
26	G	101	CDL	CA3-CA4-CA6-OA8
26	G	101	CDL	C37-C38-C39-C40
26	P	305	CDL	C84-C85-C86-C87
26	C	307	CDL	C44-C45-C46-C47
26	C	307	CDL	C64-C65-C66-C67
23	O	303	PSC	C31-C32-C33-C34
18	C	306	PGV	C5-C6-C7-C8
26	T	103	CDL	C72-C73-C74-C75
21	Q	201	TGL	C13-C14-C29-C30
25	C	304	PEK	C35-C36-C37-C38
21	O	301	TGL	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	C	307	CDL	C84-C85-C86-C87
21	D	201	TGL	CC4-CC5-CC6-CC7
18	N	607	PGV	C15-C16-C17-C18
26	P	305	CDL	C41-C42-C43-C44
25	T	102	PEK	C35-C36-C37-C38
18	N	607	PGV	C31-C32-C33-C34
21	N	606	TGL	C16-C17-C18-C19
21	N	606	TGL	C29-C30-C31-C32
26	P	305	CDL	C24-C25-C26-C27
21	Q	201	TGL	C29-C30-C31-C32
26	G	101	CDL	C77-C78-C79-C80
18	N	609	PGV	C12-C13-C14-C15
25	C	303	PEK	C22-C23-C24-C25
25	C	303	PEK	C30-C31-C32-C33
18	P	304	PGV	C13-C14-C15-C16
18	C	305	PGV	C15-C16-C17-C18
26	P	305	CDL	CB7-C71-C72-C73
21	N	606	TGL	CC2-CC1-OG3-CG3
21	L	101	TGL	C29-C30-C31-C32
27	M	101	DMU	C34-C37-C40-C43
21	O	301	TGL	C15-C16-C17-C18
26	C	307	CDL	C31-C32-C33-C34
21	O	301	TGL	CG1-CG2-OG2-CB1
21	D	201	TGL	C33-C34-C35-C36
26	G	101	CDL	C40-C41-C42-C43
26	G	101	CDL	C64-C65-C66-C67
21	Q	201	TGL	CC2-CC3-CC4-CC5
25	T	101	PEK	C27-C28-C29-C30
18	C	306	PGV	C13-C14-C15-C16
21	B	301	TGL	C10-C11-C12-C13
18	N	607	PGV	O01-C02-C03-O11
25	C	303	PEK	C4-C5-C6-C7
21	D	201	TGL	OG1-CA1-CA2-CA3
23	O	303	PSC	C13-C14-C15-C16
26	P	305	CDL	C71-C72-C73-C74
26	P	305	CDL	OB6-CB4-CB6-OB8
21	L	101	TGL	OG1-CG1-CG2-OG2
18	C	306	PGV	C24-C25-C26-C27
18	P	304	PGV	C29-C30-C31-C32
26	P	305	CDL	C19-C20-C21-C22
21	D	201	TGL	C15-C16-C17-C18
26	G	101	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
26	C	307	CDL	C20-C21-C22-C23
26	C	307	CDL	C41-C42-C43-C44
25	T	102	PEK	C23-C24-C25-C26
26	P	305	CDL	C79-C80-C81-C82
26	P	305	CDL	C82-C83-C84-C85
18	P	304	PGV	C15-C16-C17-C18
25	P	303	PEK	C17-C18-C19-C20
21	N	606	TGL	C20-C21-C22-C23
21	O	301	TGL	CC7-CC8-CC9-C15
18	A	608	PGV	C31-C32-C33-C34
24	P	306	CHD	C16-C17-C20-C21
18	N	607	PGV	C20-C21-C22-C23
18	C	306	PGV	O12-C04-C05-C06
21	O	301	TGL	C14-C29-C30-C31
26	P	305	CDL	C14-C15-C16-C17
26	P	305	CDL	C44-C45-C46-C47
18	A	608	PGV	C10-C11-C12-C13
21	N	606	TGL	CA1-CA2-CA3-CA4
21	D	201	TGL	CC7-CC8-CC9-C15
18	N	607	PGV	C01-C02-C03-O11
25	C	304	PEK	C01-C02-C03-O11
21	N	606	TGL	CC6-CC7-CC8-CC9
21	N	606	TGL	C18-C19-C33-C34
27	P	313	DMU	O16-C18-C19-C22
21	D	201	TGL	CC1-CC2-CC3-CC4
26	T	103	CDL	C12-C13-C14-C15
26	P	305	CDL	C42-C43-C44-C45
21	N	606	TGL	C21-C22-C23-C24
21	O	301	TGL	C21-C22-C23-C24
26	P	305	CDL	C52-C53-C54-C55
26	C	307	CDL	C15-C16-C17-C18
18	C	305	PGV	C29-C30-C31-C32
26	G	101	CDL	C12-C13-C14-C15
18	U	101	PGV	C20-C19-O03-C01
25	C	304	PEK	C22-C21-O03-C01
23	O	303	PSC	C15-C16-C17-C18
24	P	306	CHD	C16-C17-C20-C22
18	N	609	PGV	C13-C14-C15-C16
26	P	305	CDL	CB3-CB4-CB6-OB8
21	Q	201	TGL	CG1-CG2-CG3-OG3
26	C	307	CDL	CB3-CB4-CB6-OB8
21	D	201	TGL	OG1-CG1-CG2-CG3

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Mol	Chain	Res	Type	Atoms
21	O	301	TGL	C23-C24-C25-C26
21	Q	201	TGL	CB2-CB3-CB4-CB5
21	D	201	TGL	C29-C30-C31-C32
26	G	101	CDL	C13-C14-C15-C16
26	G	101	CDL	C18-C19-C20-C21
18	N	609	PGV	C31-C32-C33-C34
25	C	304	PEK	C25-C26-C27-C28
18	A	606	PGV	C15-C16-C17-C18
21	N	606	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	CA9-C20-C21-C22
21	D	201	TGL	CA5-CA6-CA7-CA8
25	P	303	PEK	C34-C35-C36-C37
21	Q	201	TGL	C24-C25-C26-C27
25	C	304	PEK	C11-C10-C9-C8
25	G	103	PEK	C6-C7-C8-C9
25	G	103	PEK	C12-C13-C14-C15
26	T	103	CDL	CA2-OA2-PA1-OA5
23	O	303	PSC	C9-C10-C11-C12
23	O	303	PSC	C10-C11-C12-C13
25	P	303	PEK	C9-C10-C11-C12
25	T	101	PEK	C5-C6-C7-C8
25	T	101	PEK	C6-C7-C8-C9
25	T	101	PEK	C11-C10-C9-C8
25	T	101	PEK	C12-C13-C14-C15
25	T	102	PEK	C11-C10-C9-C8
25	T	102	PEK	C9-C10-C11-C12
25	T	102	PEK	C12-C13-C14-C15
26	C	307	CDL	CA7-C31-C32-C33
23	O	303	PSC	O01-C02-C03-O11
25	T	101	PEK	O01-C02-C03-O11
21	B	301	TGL	CB5-CB6-CB7-CB8
18	C	306	PGV	C31-C32-C33-C34
26	G	101	CDL	C36-C37-C38-C39
26	T	103	CDL	C32-C33-C34-C35
18	U	101	PGV	O03-C01-C02-O01
18	C	306	PGV	O03-C01-C02-O01
21	B	301	TGL	OG2-CG2-CG3-OG3
26	C	307	CDL	OB6-CB4-CB6-OB8
18	U	101	PGV	C31-C32-C33-C34
21	B	301	TGL	C20-C21-C22-C23
24	P	306	CHD	C13-C17-C20-C22
25	C	304	PEK	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
21	O	301	TGL	C21-C20-CA9-CA8
25	T	102	PEK	C22-C23-C24-C25
25	T	102	PEK	C24-C25-C26-C27
25	C	303	PEK	C24-C25-C26-C27
21	Q	201	TGL	CC9-C15-C16-C17
18	N	607	PGV	C6-C7-C8-C9
26	G	101	CDL	C14-C15-C16-C17
26	C	307	CDL	C13-C14-C15-C16
18	C	306	PGV	C02-C03-O11-P
26	T	103	CDL	CA4-CA3-OA5-PA1
26	T	103	CDL	C1-CB2-OB2-PB2
18	P	304	PGV	C02-C03-O11-P
18	C	305	PGV	C02-C03-O11-P
26	G	101	CDL	CA4-CA3-OA5-PA1
18	C	306	PGV	C6-C7-C8-C9
25	T	101	PEK	C32-C33-C34-C35
18	P	304	PGV	C11-C12-C13-C14
20	B	306	EDO	O1-C1-C2-O2
20	P	308	EDO	O1-C1-C2-O2
21	D	201	TGL	C23-C24-C25-C26
21	Q	201	TGL	CB5-CB6-CB7-CB8
18	N	607	PGV	C23-C24-C25-C26
25	G	103	PEK	C24-C25-C26-C27
23	O	303	PSC	C3-C4-C5-C6
18	A	606	PGV	C31-C32-C33-C34
25	G	103	PEK	C01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-CB6
26	G	101	CDL	OA5-CA3-CA4-CA6
26	T	103	CDL	C54-C55-C56-C57
18	A	606	PGV	C25-C26-C27-C28
21	B	301	TGL	C25-C26-C27-C28
18	P	304	PGV	C21-C22-C23-C24
26	G	101	CDL	C24-C25-C26-C27
21	O	301	TGL	CA6-CA7-CA8-CA9
25	P	303	PEK	C28-C29-C30-C31
23	B	303	PSC	C2-C3-C4-C5
21	L	101	TGL	C21-C20-CA9-CA8
26	G	101	CDL	C34-C35-C36-C37
25	T	102	PEK	C16-C17-C18-C19
21	Q	201	TGL	CA2-CA1-OG1-CG1
26	G	101	CDL	C58-C59-C60-C61
26	T	103	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
26	P	305	CDL	C16-C17-C18-C19
21	Q	201	TGL	CG3-CG2-OG2-CB1
26	T	103	CDL	C56-C57-C58-C59
21	Q	201	TGL	CC4-CC5-CC6-CC7
18	A	608	PGV	C14-C15-C16-C17
27	Z	101	DMU	C28-C31-C34-C37
18	A	606	PGV	C05-C04-O12-P
21	B	301	TGL	CC2-CC3-CC4-CC5
25	C	304	PEK	O01-C02-C03-O11
26	C	307	CDL	OA5-CA3-CA4-OA6
24	P	306	CHD	C13-C17-C20-C21
18	C	305	PGV	C22-C23-C24-C25
26	P	305	CDL	O1-C1-CA2-OA2
25	C	304	PEK	O04-C21-O03-C01
26	P	305	CDL	C60-C61-C62-C63
18	A	606	PGV	O03-C01-C02-O01
21	L	101	TGL	OG2-CG2-CG3-OG3
25	T	101	PEK	O03-C01-C02-O01
21	B	301	TGL	C21-C20-CA9-CA8
18	U	101	PGV	O04-C19-O03-C01
21	Q	201	TGL	OA1-CA1-OG1-CG1
26	T	103	CDL	C20-C21-C22-C23
21	Q	201	TGL	CA4-CA5-CA6-CA7
26	C	307	CDL	C12-C13-C14-C15
21	B	301	TGL	CB9-C10-C11-C12
21	B	301	TGL	CC3-CC4-CC5-CC6
18	U	101	PGV	C11-C10-C9-C8
25	C	303	PEK	C15-C16-C17-C18
18	P	304	PGV	C11-C10-C9-C8
21	N	606	TGL	CB3-CB4-CB5-CB6
18	C	305	PGV	C14-C15-C16-C17
25	T	102	PEK	C34-C35-C36-C37
25	T	102	PEK	O02-C1-O01-C02
21	B	301	TGL	CA4-CA5-CA6-CA7
23	O	303	PSC	C5-C6-C7-C8
27	Z	101	DMU	C18-C19-C22-C25
18	N	607	PGV	C21-C22-C23-C24
18	N	607	PGV	C03-O11-P-O12
18	C	306	PGV	C04-O12-P-O11
23	B	303	PSC	C03-O11-P-O12
18	C	306	PGV	O12-C04-C05-O05
26	T	103	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	U	101	PGV	C02-C03-O11-P
18	U	101	PGV	C05-C04-O12-P
25	G	103	PEK	C02-C03-O11-P
26	P	305	CDL	CA4-CA3-OA5-PA1
26	C	307	CDL	CA4-CA3-OA5-PA1
26	G	101	CDL	C83-C84-C85-C86
25	G	103	PEK	C04-O12-P-O14
23	B	303	PSC	C04-O12-P-O14
26	P	305	CDL	CA3-OA5-PA1-OA3
26	C	307	CDL	CA3-OA5-PA1-OA3
26	C	307	CDL	CB2-OB2-PB2-OB3
18	A	606	PGV	C03-O11-P-O13
18	A	606	PGV	C04-O12-P-O13
26	G	101	CDL	CA2-OA2-PA1-OA4
26	P	305	CDL	OA5-CA3-CA4-CA6
25	T	101	PEK	C01-C02-C03-O11
25	T	102	PEK	C01-C02-C03-O11
20	T	105	EDO	O1-C1-C2-O2
21	L	101	TGL	OG1-CA1-CA2-CA3
21	D	201	TGL	C19-C33-C34-C35
21	N	606	TGL	C16-C15-CC9-CC8
18	A	606	PGV	C29-C30-C31-C32
25	T	102	PEK	C10-C11-C12-C13
25	T	102	PEK	C2-C1-O01-C02
25	G	103	PEK	C05-C04-O12-P
23	O	303	PSC	C05-C04-O12-P
18	U	101	PGV	C1-C2-C3-C4
21	O	301	TGL	C22-C23-C24-C25
21	O	301	TGL	C16-C15-CC9-CC8
18	C	306	PGV	C20-C19-O03-C01
26	P	305	CDL	CB2-C1-CA2-OA2
18	A	608	PGV	C23-C24-C25-C26
23	B	303	PSC	O01-C02-C03-O11
26	T	103	CDL	OB5-CB3-CB4-OB6
26	P	305	CDL	OA5-CA3-CA4-OA6
25	G	103	PEK	C35-C36-C37-C38
26	C	307	CDL	C61-C62-C63-C64
21	D	201	TGL	C21-C20-CA9-CA8
26	C	307	CDL	C33-C34-C35-C36
23	B	303	PSC	C19-C20-C21-C22
26	T	103	CDL	C13-C14-C15-C16
26	P	305	CDL	C64-C65-C66-C67

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Mol	Chain	Res	Type	Atoms
18	A	606	PGV	O03-C01-C02-C03
18	A	606	PGV	C21-C22-C23-C24
21	L	101	TGL	OG1-CG1-CG2-CG3
21	L	101	TGL	CG1-CG2-CG3-OG3
25	T	101	PEK	O03-C01-C02-C03
26	T	103	CDL	OA6-CA4-CA6-OA8
26	P	305	CDL	C58-C59-C60-C61
18	C	305	PGV	C31-C32-C33-C34
21	Q	201	TGL	C11-C12-C13-C14
21	L	101	TGL	CC5-CC6-CC7-CC8
26	G	101	CDL	C20-C21-C22-C23
26	P	305	CDL	C21-C22-C23-C24
25	G	103	PEK	C28-C29-C30-C31
21	D	201	TGL	CC3-CC4-CC5-CC6
25	P	303	PEK	C25-C26-C27-C28
23	O	303	PSC	C02-C01-O03-C19
26	T	103	CDL	C40-C41-C42-C43
18	A	606	PGV	C14-C15-C16-C17
26	P	305	CDL	C31-C32-C33-C34
18	C	306	PGV	O04-C19-O03-C01
18	U	101	PGV	O05-C05-C06-O06
26	G	101	CDL	C79-C80-C81-C82
23	O	303	PSC	C23-C24-C25-C26
25	P	303	PEK	C23-C24-C25-C26
21	Q	201	TGL	C10-C11-C12-C13
26	C	307	CDL	C19-C20-C21-C22
23	B	303	PSC	C03-C02-O01-C1
23	O	303	PSC	C01-C02-C03-O11
18	N	607	PGV	C14-C15-C16-C17
26	P	305	CDL	C34-C35-C36-C37
18	P	304	PGV	C23-C24-C25-C26
26	C	307	CDL	C82-C83-C84-C85
21	D	201	TGL	OG2-CB1-CB2-CB3
20	N	613	EDO	O1-C1-C2-O2
20	P	310	EDO	O1-C1-C2-O2
26	G	101	CDL	C11-C12-C13-C14
27	C	313	DMU	O5-C6-O16-C18
21	Q	201	TGL	OG2-CG2-CG3-OG3
26	G	101	CDL	OA6-CA4-CA6-OA8
18	U	101	PGV	C03-O11-P-O12
18	U	101	PGV	C04-O12-P-O11
25	C	304	PEK	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
25	T	101	PEK	C04-O12-P-O11
25	T	102	PEK	C04-O12-P-O11
26	G	101	CDL	CB3-OB5-PB2-OB2
23	B	303	PSC	C21-C22-C23-C24
26	C	307	CDL	C16-C17-C18-C19
18	C	306	PGV	O03-C01-C02-C03
21	B	301	TGL	CG1-CG2-CG3-OG3
26	G	101	CDL	C72-C73-C74-C75
26	T	103	CDL	C82-C83-C84-C85
23	O	303	PSC	C02-C03-O11-P
21	O	301	TGL	C12-C13-C14-C29
18	N	607	PGV	O05-C05-C06-O06
21	L	101	TGL	OG2-CB1-CB2-CB3
21	Q	201	TGL	CB9-C10-C11-C12
18	A	608	PGV	C11-C10-C9-C8
18	N	607	PGV	C19-C20-C21-C22
26	G	101	CDL	C81-C82-C83-C84
18	N	609	PGV	C27-C28-C29-C30
25	G	103	PEK	C25-C26-C27-C28
18	N	607	PGV	C13-C14-C15-C16
14	A	601[A]	HEA	C27-C19-C20-C21
18	A	606	PGV	C11-C10-C9-C8
21	L	101	TGL	C33-C34-C35-C36
21	D	201	TGL	CA2-CA3-CA4-CA5
18	C	305	PGV	C11-C10-C9-C8
20	A	617	EDO	O1-C1-C2-O2
27	P	313	DMU	C28-C31-C34-C37
18	N	607	PGV	O12-C04-C05-C06
18	U	101	PGV	O03-C01-C02-C03
21	D	201	TGL	OA1-CA1-CA2-CA3
18	U	101	PGV	C7-C8-C9-C10
27	C	313	DMU	C34-C37-C40-C43
21	B	301	TGL	C33-C34-C35-C36
26	C	307	CDL	C32-C33-C34-C35
18	U	101	PGV	C29-C30-C31-C32
25	C	303	PEK	C29-C30-C31-C32
25	G	103	PEK	C3-C4-C5-C6
25	C	304	PEK	C12-C13-C14-C15
25	G	103	PEK	C11-C10-C9-C8
23	B	303	PSC	C9-C10-C11-C12
25	T	101	PEK	C9-C10-C11-C12
18	C	305	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	T	103	CDL	C22-C23-C24-C25
26	P	305	CDL	C11-C12-C13-C14
26	P	305	CDL	C17-C18-C19-C20
27	M	101	DMU	O6-C11-C9-C8
21	O	301	TGL	C18-C19-C33-C34
18	N	609	PGV	C24-C25-C26-C27
26	T	103	CDL	C76-C77-C78-C79
25	C	304	PEK	C30-C31-C32-C33
18	A	608	PGV	C28-C29-C30-C31
18	C	305	PGV	C05-C04-O12-P
18	N	609	PGV	O03-C19-C20-C21
23	O	303	PSC	C30-C31-C32-C33
23	B	303	PSC	C7-C8-C9-C10
25	T	102	PEK	C14-C15-C16-C17
26	T	103	CDL	CA3-CA4-CA6-OA8
20	A	619	EDO	O1-C1-C2-O2
20	S	104	EDO	O1-C1-C2-O2
20	Q	202	EDO	O1-C1-C2-O2
26	G	101	CDL	C31-C32-C33-C34
18	A	608	PGV	O03-C19-C20-C21
27	M	101	DMU	C28-C31-C34-C37
18	U	101	PGV	C11-C12-C13-C14
25	T	102	PEK	C3-C4-C5-C6
25	T	102	PEK	O01-C02-C03-O11
26	G	101	CDL	OA5-CA3-CA4-OA6
18	C	306	PGV	C15-C16-C17-C18
23	B	303	PSC	C01-C02-C03-O11
21	D	201	TGL	CC6-CC7-CC8-CC9
25	C	304	PEK	C14-C15-C16-C17
18	C	305	PGV	C12-C13-C14-C15
18	N	607	PGV	C30-C31-C32-C33
18	P	304	PGV	C25-C26-C27-C28
14	N	601[A]	HEA	C12-C13-C14-C15
14	N	601[B]	HEA	C12-C13-C14-C15
18	C	305	PGV	C9-C10-C11-C12
14	A	601[A]	HEA	C18-C19-C20-C21
25	C	303	PEK	C17-C18-C19-C20
27	Z	101	DMU	O6-C11-C9-C8
25	P	303	PEK	C14-C15-C16-C17
21	N	606	TGL	C11-C10-CB9-CB8
21	L	101	TGL	C23-C24-C25-C26
26	G	101	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
18	A	608	PGV	C12-C13-C14-C15
18	P	304	PGV	C05-C04-O12-P
23	B	303	PSC	C11-C10-C9-C8
25	C	303	PEK	O03-C21-C22-C23
25	C	304	PEK	C23-C24-C25-C26
25	T	101	PEK	C22-C23-C24-C25
27	M	101	DMU	C19-C22-C25-C28
26	P	305	CDL	C22-C23-C24-C25
20	B	308	EDO	O1-C1-C2-O2
20	P	307	EDO	O1-C1-C2-O2
25	P	303	PEK	C22-C21-O03-C01
26	G	101	CDL	OB6-CB4-CB6-OB8
26	P	305	CDL	C13-C14-C15-C16
26	P	305	CDL	C62-C63-C64-C65
21	B	301	TGL	CA6-CA7-CA8-CA9
26	P	305	CDL	C18-C19-C20-C21
18	U	101	PGV	C12-C13-C14-C15
21	B	301	TGL	CC9-C15-C16-C17
18	N	609	PGV	C11-C12-C13-C14
18	C	305	PGV	C11-C12-C13-C14
26	T	103	CDL	C32-C31-CA7-OA8
26	G	101	CDL	C32-C31-CA7-OA8
18	N	609	PGV	C15-C16-C17-C18
26	G	101	CDL	C78-C79-C80-C81
27	M	101	DMU	O16-C18-C19-C22
23	O	303	PSC	C4-C5-C6-C7
25	C	303	PEK	O04-C21-C22-C23
14	N	601[B]	HEA	C16-C17-C18-C19
26	T	103	CDL	C32-C31-CA7-OA9
25	C	304	PEK	C29-C30-C31-C32
25	P	303	PEK	C22-C23-C24-C25
21	N	606	TGL	OG3-CC1-CC2-CC3
21	B	301	TGL	OG3-CC1-CC2-CC3
26	C	307	CDL	C79-C80-C81-C82
21	O	301	TGL	CA9-C20-C21-C22
18	U	101	PGV	C03-O11-P-O14
26	T	103	CDL	CA2-OA2-PA1-OA4
26	T	103	CDL	CA3-OA5-PA1-OA3
26	P	305	CDL	CA2-OA2-PA1-OA3
26	G	101	CDL	CB3-OB5-PB2-OB3
26	G	101	CDL	C32-C31-CA7-OA9
26	G	101	CDL	C12-C11-CA5-OA7

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Mol	Chain	Res	Type	Atoms
26	P	305	CDL	C52-C51-CB5-OB6
27	W	104	DMU	C34-C37-C40-C43
26	G	101	CDL	C55-C56-C57-C58
26	P	305	CDL	C33-C34-C35-C36
14	A	601[B]	HEA	C16-C17-C18-C19
25	T	101	PEK	C34-C35-C36-C37
23	O	303	PSC	C19-C20-C21-C22
25	T	102	PEK	O01-C1-C2-C3
26	P	305	CDL	CA2-C1-CB2-OB2
26	T	103	CDL	C1-CA2-OA2-PA1
26	G	101	CDL	C73-C74-C75-C76
21	N	606	TGL	C25-C26-C27-C28
26	C	307	CDL	C37-C38-C39-C40
21	N	606	TGL	OC1-CC1-CC2-CC3
26	P	305	CDL	C52-C51-CB5-OB7
26	T	103	CDL	C52-C51-CB5-OB6
25	T	102	PEK	O02-C1-C2-C3
24	W	101	CHD	C21-C20-C22-C23
21	B	301	TGL	C15-C16-C17-C18
18	A	608	PGV	C26-C27-C28-C29

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	W	101	CHD	C1-C10-C2-C3-C4-C5

48 monomers are involved in 181 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	615	EDO	1	0
18	N	607	PGV	3	0
20	B	306	EDO	2	0
14	A	602	HEA	2	0
18	U	101	PGV	2	0
25	C	304	PEK	3	0
20	H	101	EDO	1	0
20	N	613	EDO	1	0
20	J	102	EDO	2	0
24	P	306	CHD	4	0
20	A	619	EDO	6	0
18	C	306	PGV	1	0
25	C	303	PEK	3	0

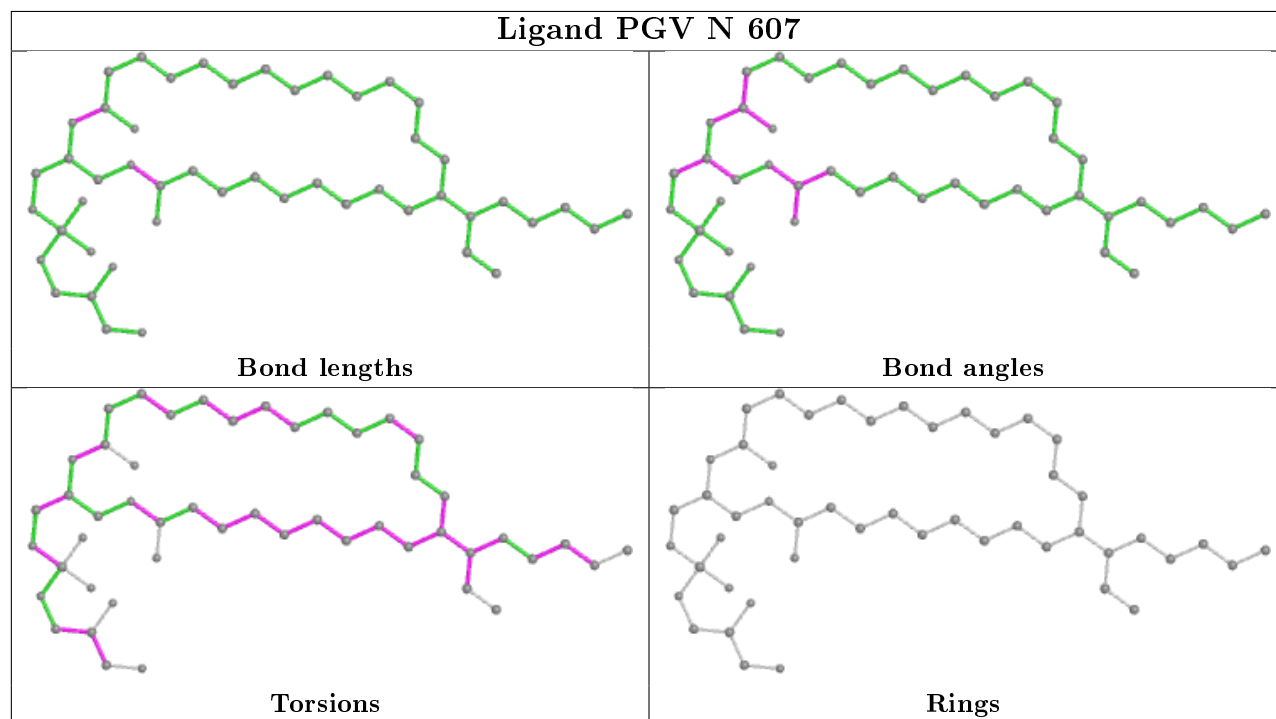
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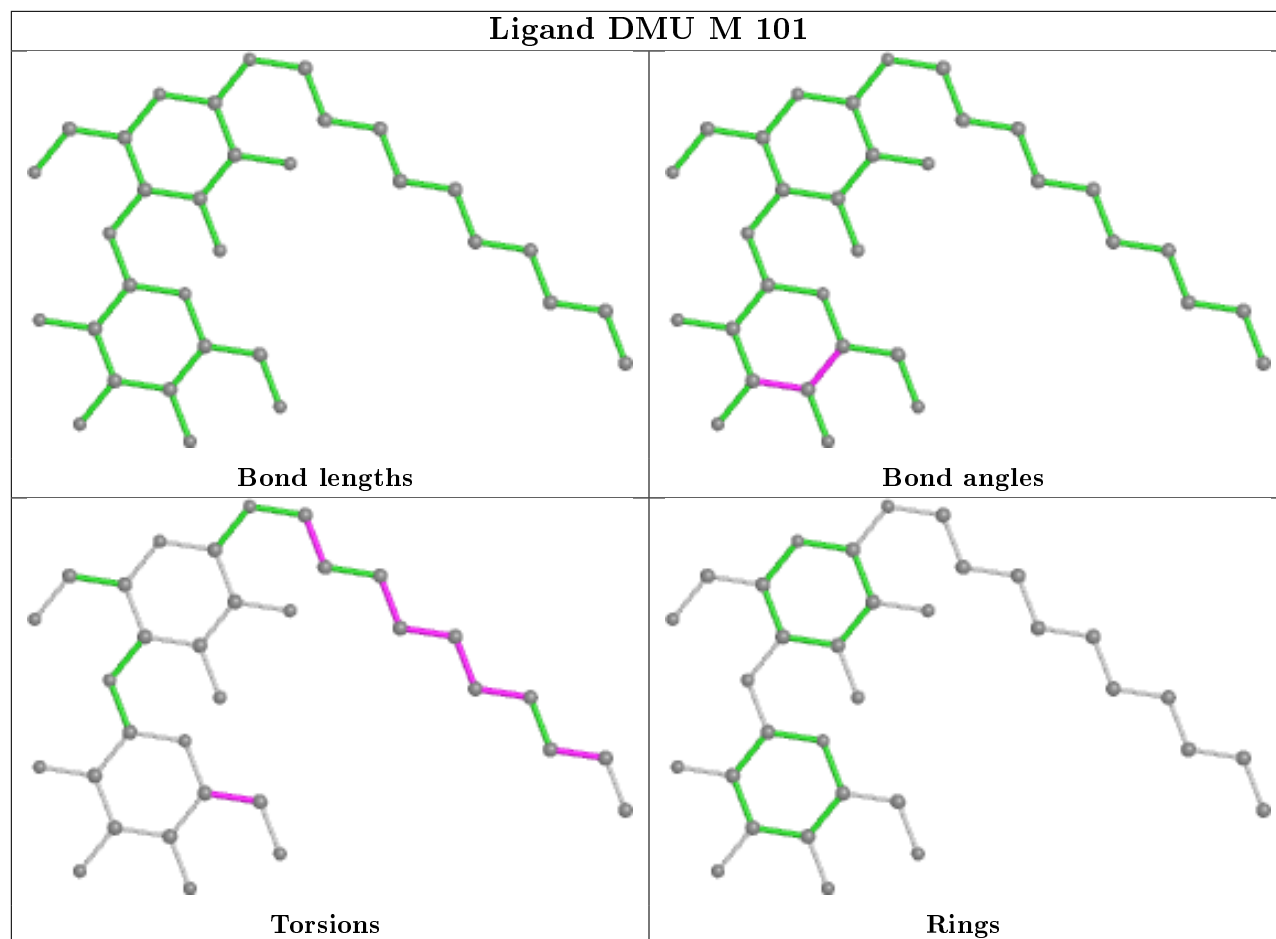
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	G	103	PEK	1	0
14	A	601[B]	HEA	5	0
18	C	305	PGV	6	0
24	P	301	CHD	1	0
21	N	606	TGL	4	0
21	O	301	TGL	4	0
14	N	601[A]	HEA	1	0
23	B	303	PSC	6	0
27	W	104	DMU	11	0
14	N	602	HEA	3	0
27	Z	101	DMU	1	0
26	T	103	CDL	7	0
27	C	313	DMU	10	0
21	B	301	TGL	3	0
24	B	304	CHD	1	0
26	P	305	CDL	9	0
20	L	103	EDO	2	0
18	P	304	PGV	1	0
20	A	612	EDO	1	0
23	O	303	PSC	5	0
24	J	101	CHD	2	0
24	W	101	CHD	2	0
25	P	303	PEK	2	0
21	Q	201	TGL	2	0
26	C	307	CDL	16	0
14	N	601[B]	HEA	13	0
18	A	606	PGV	6	0
14	A	601[A]	HEA	1	0
24	C	308	CHD	2	0
21	D	201	TGL	6	0
21	L	101	TGL	4	0
25	T	101	PEK	3	0
18	A	608	PGV	2	0
25	T	102	PEK	4	0
26	G	101	CDL	12	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

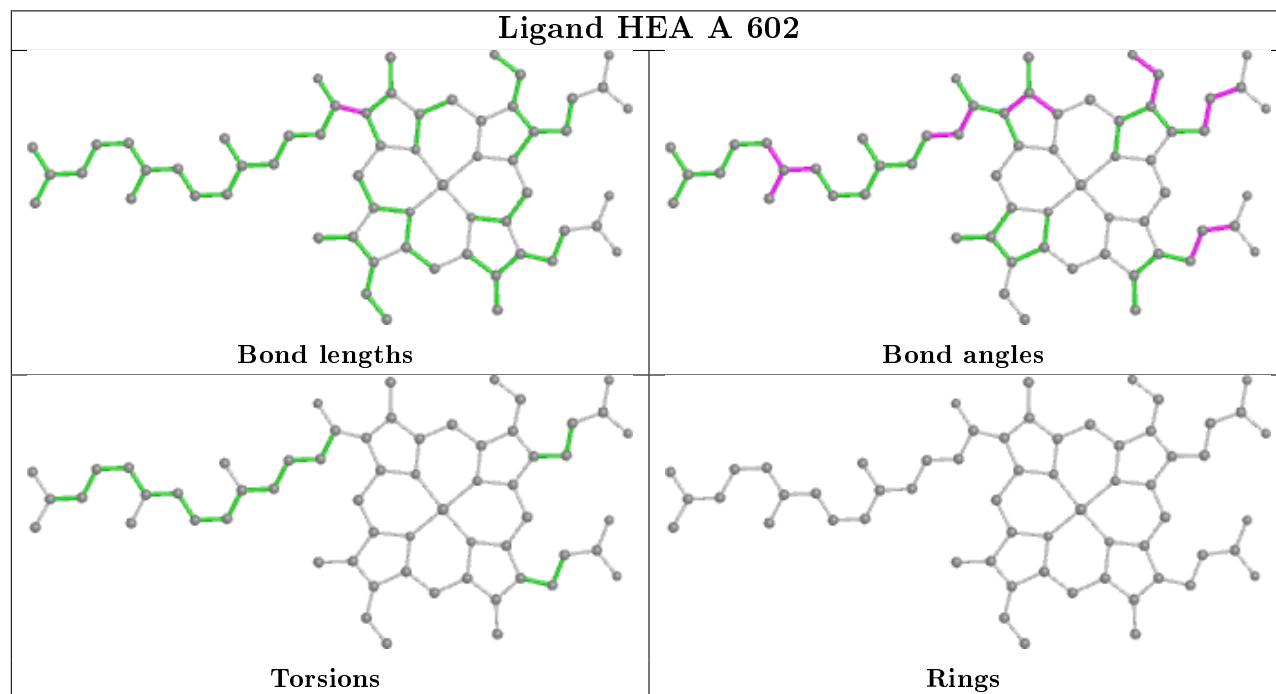
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

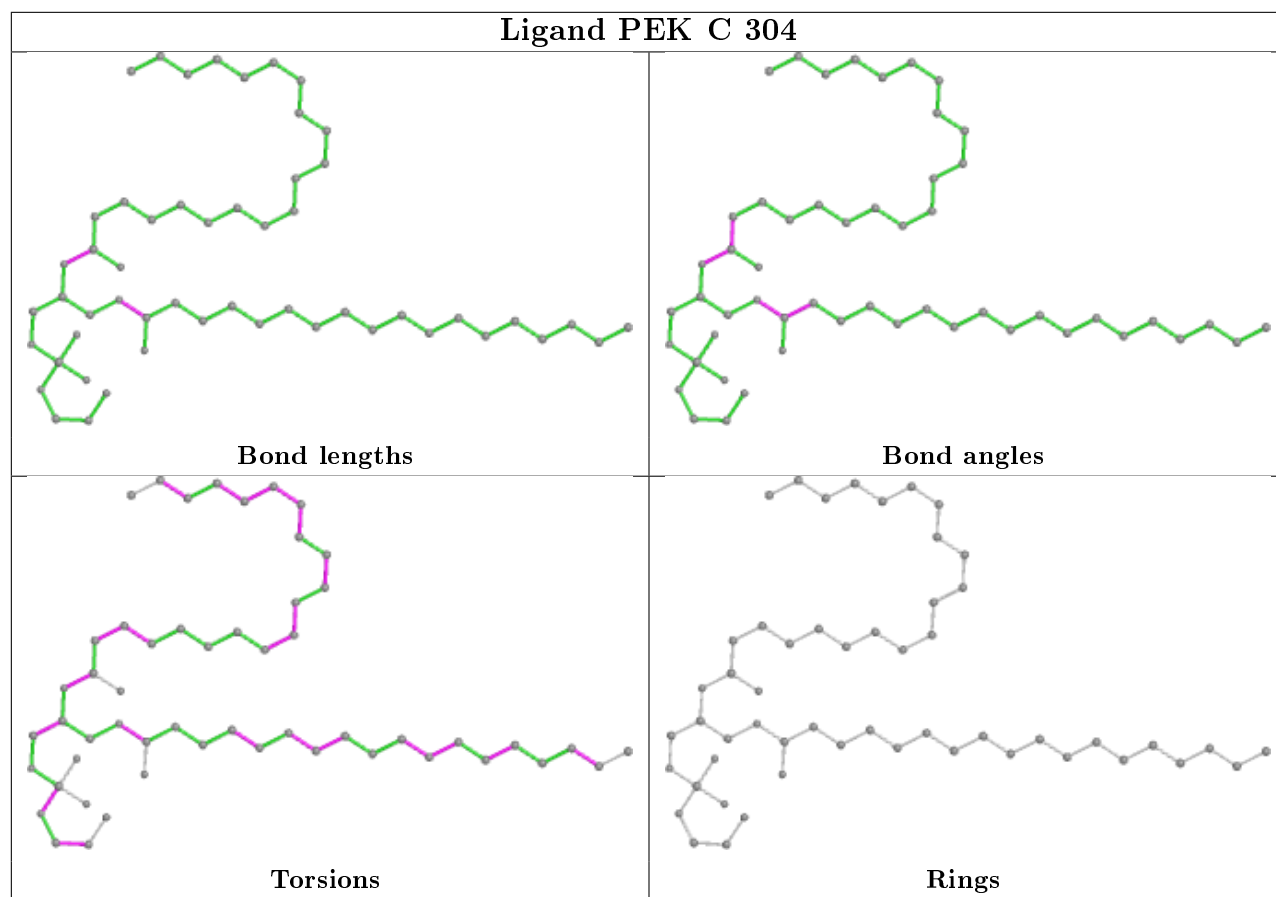
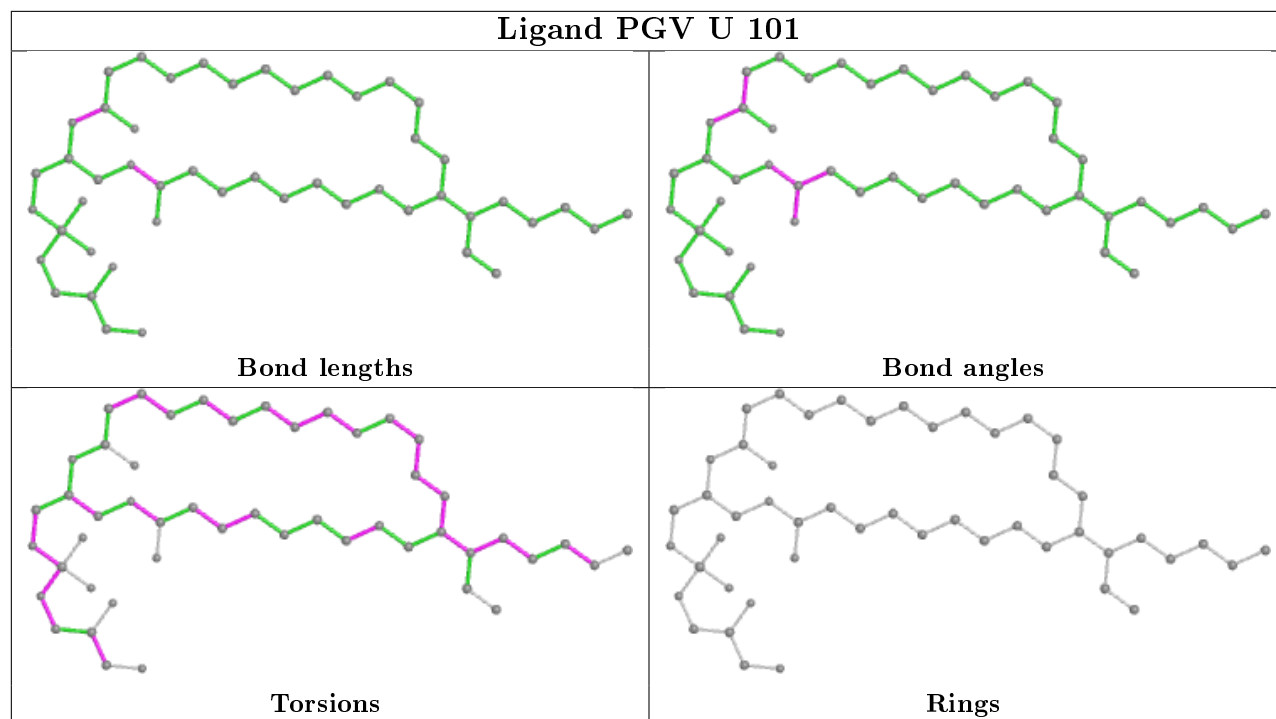


## Ligand DMU M 101

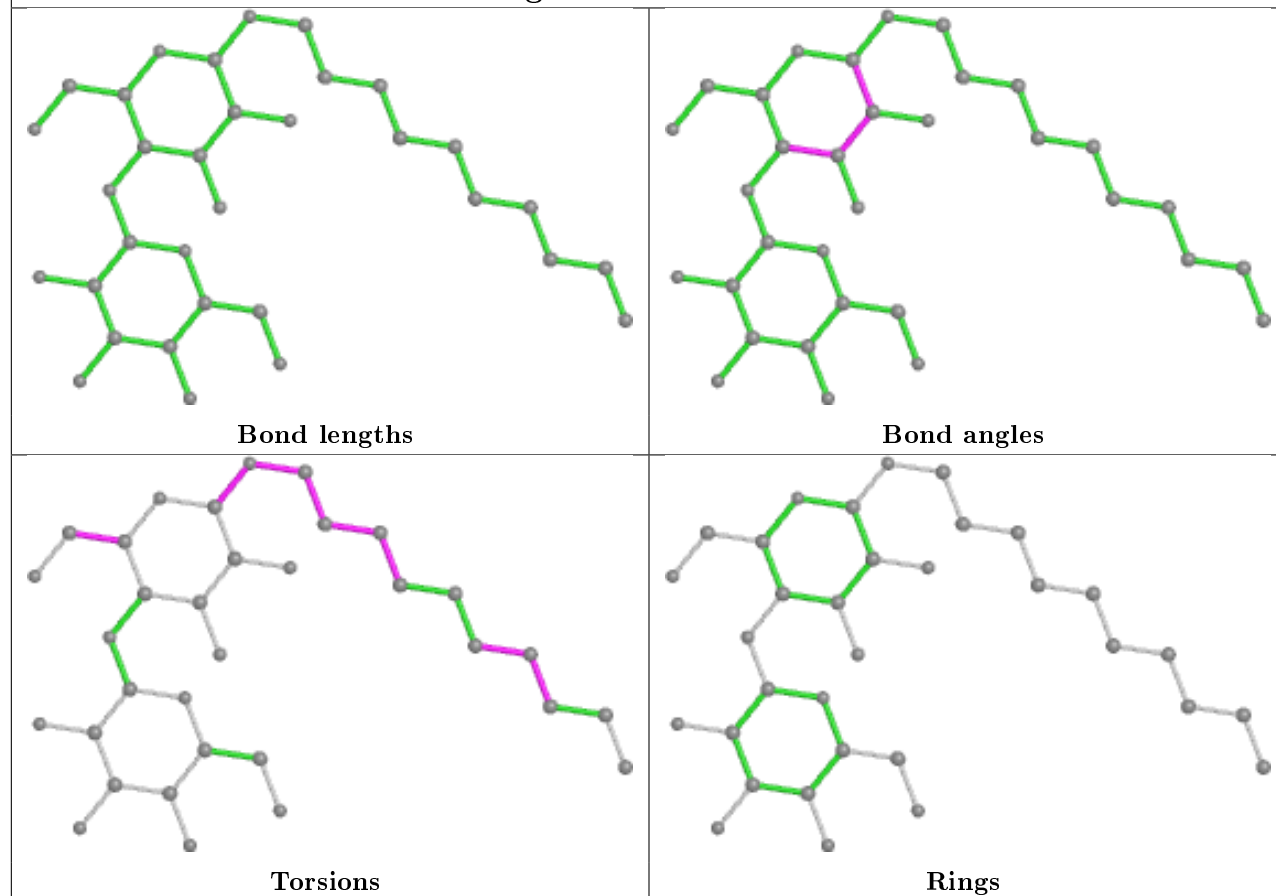


## Ligand HEA A 602

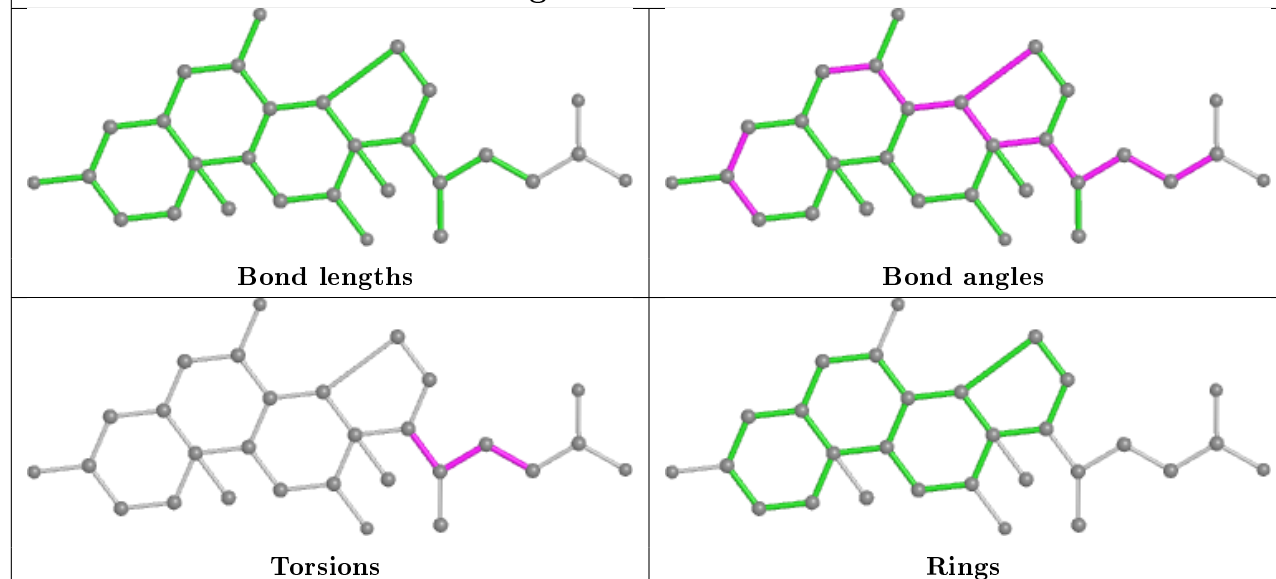


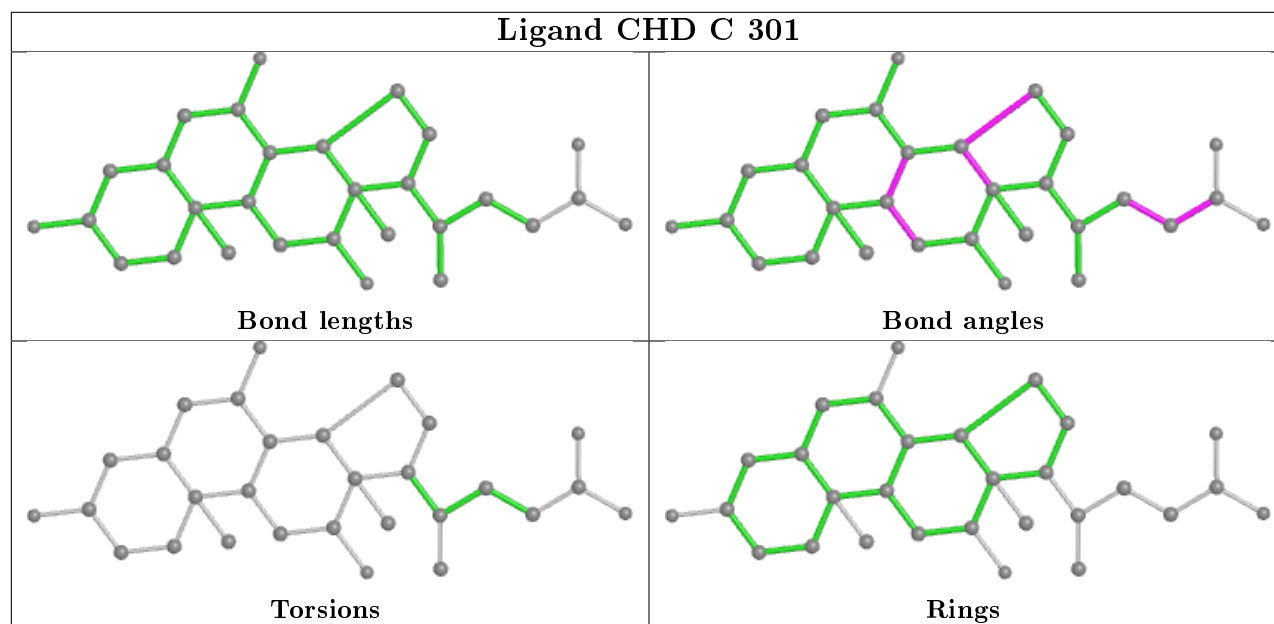
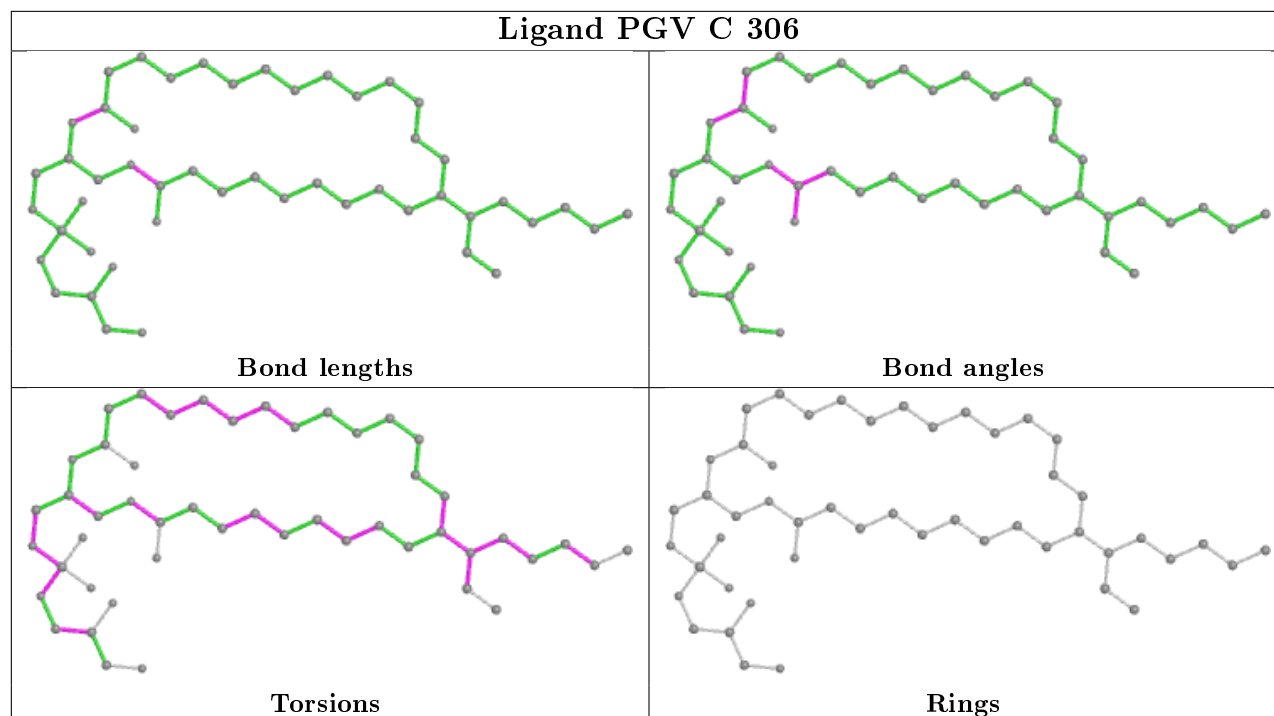


## Ligand DMU C 312



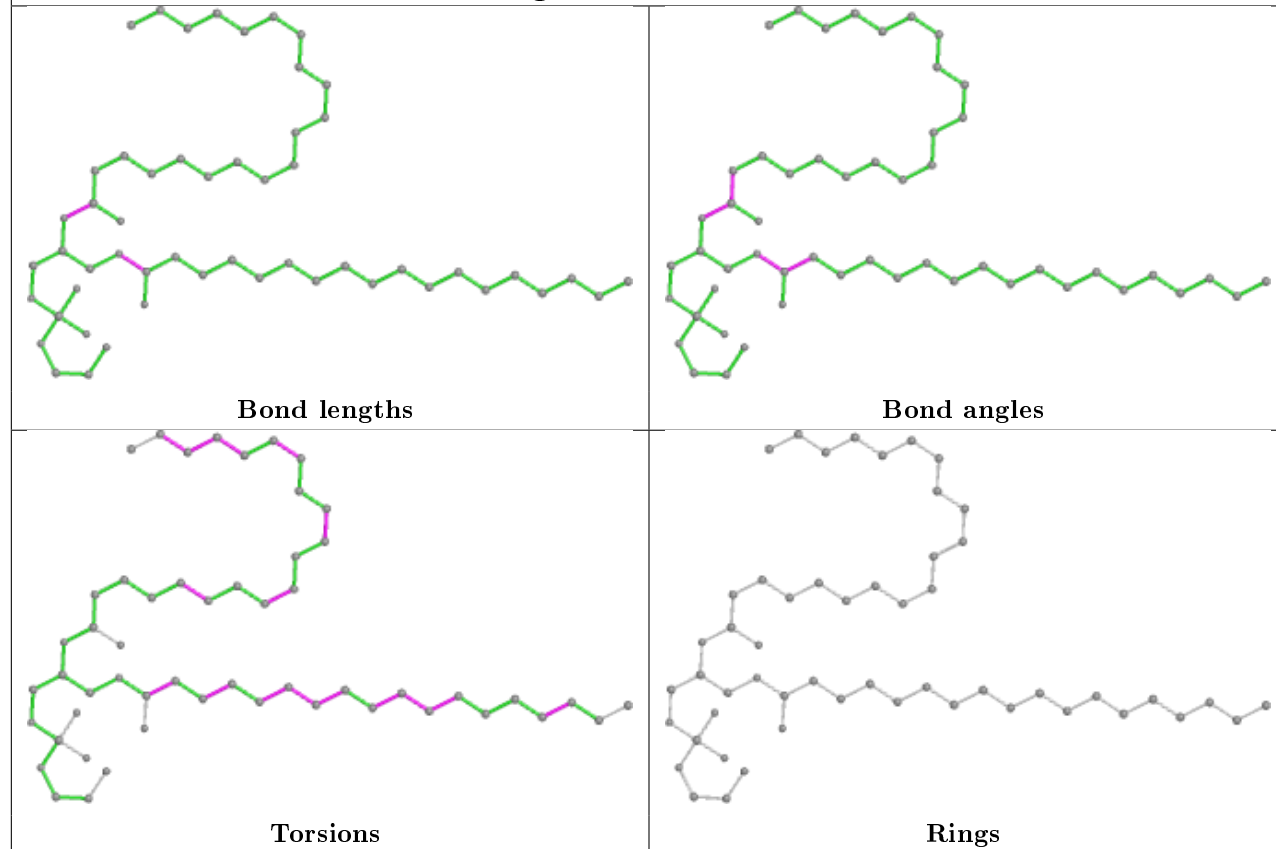
## Ligand CHD P 306



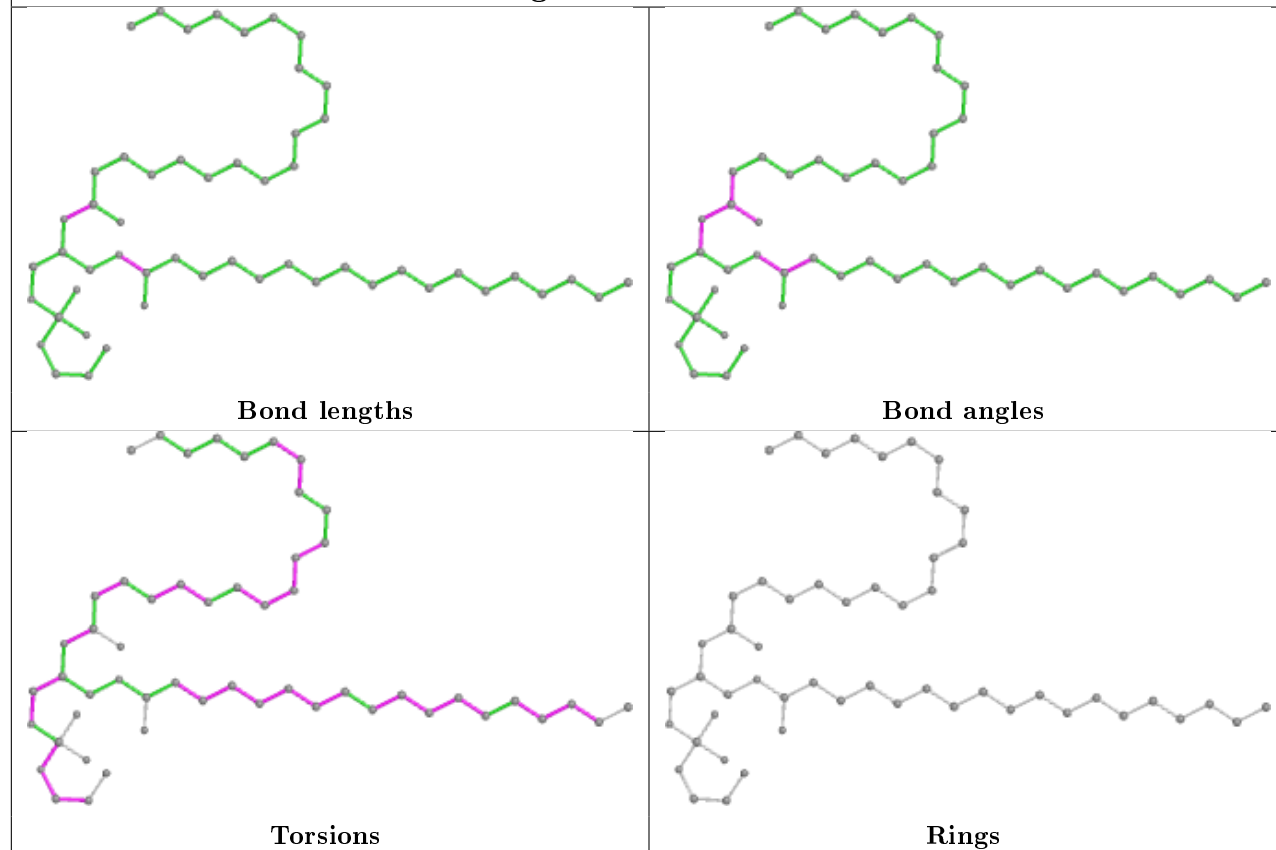


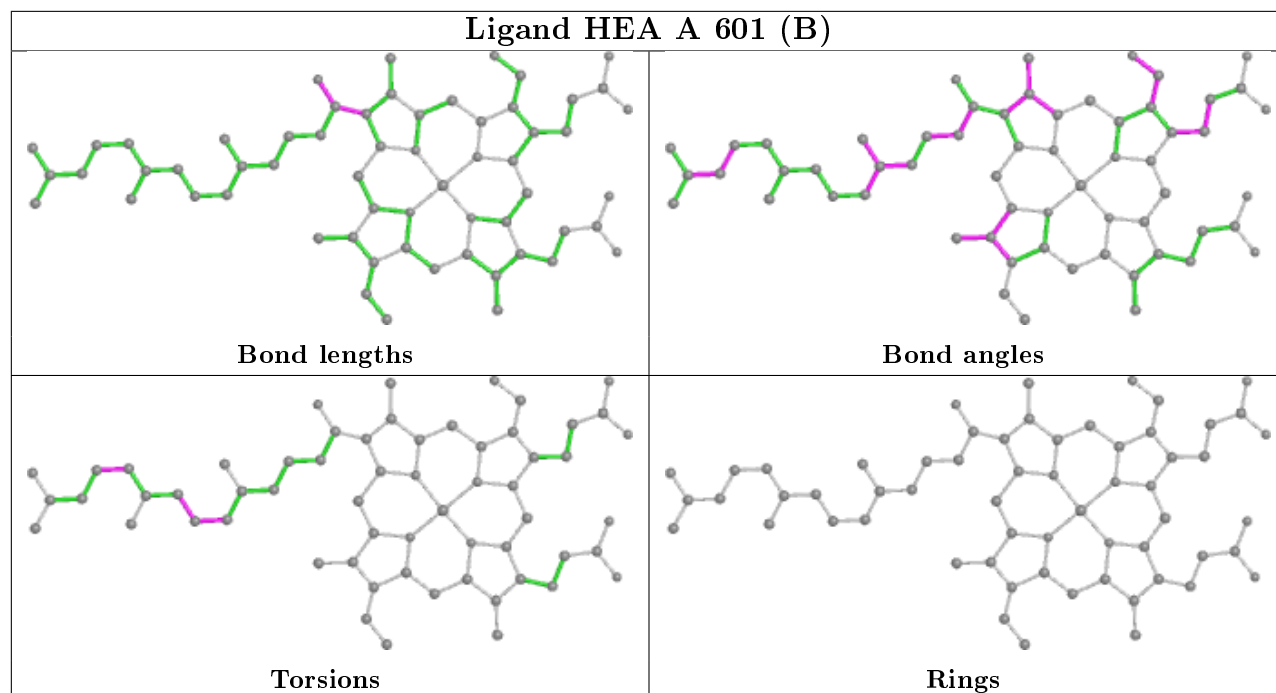
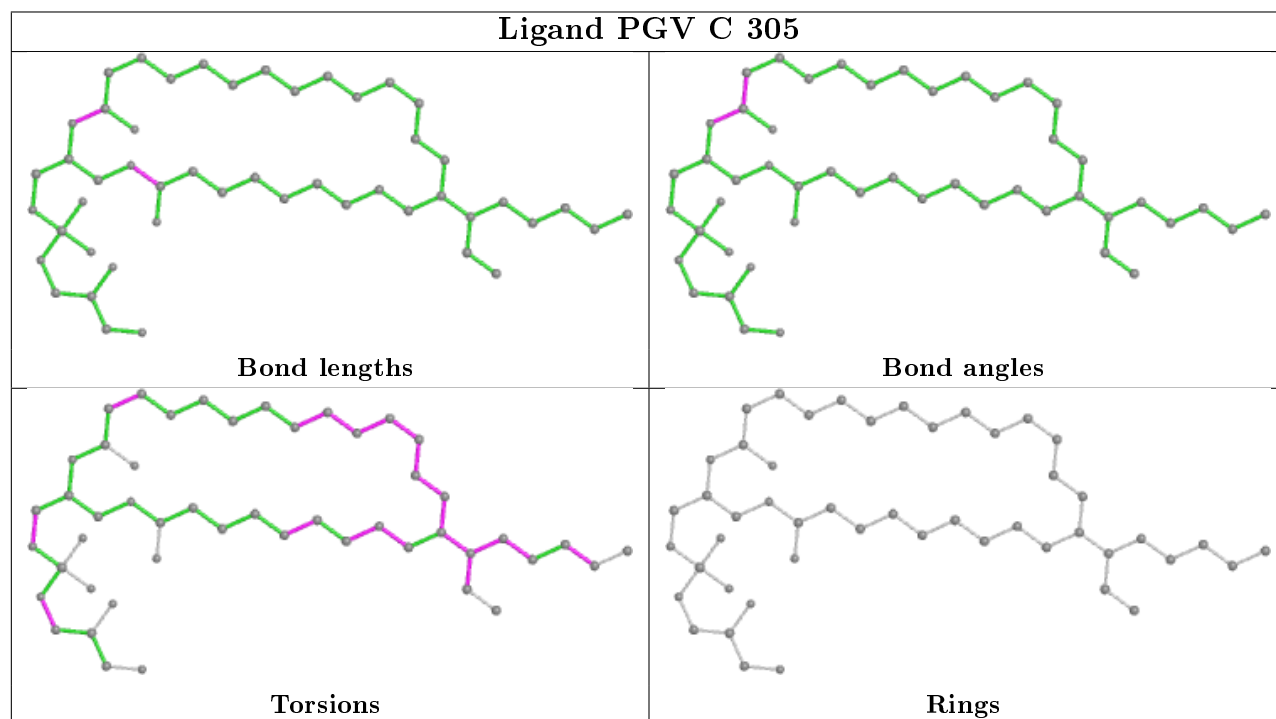


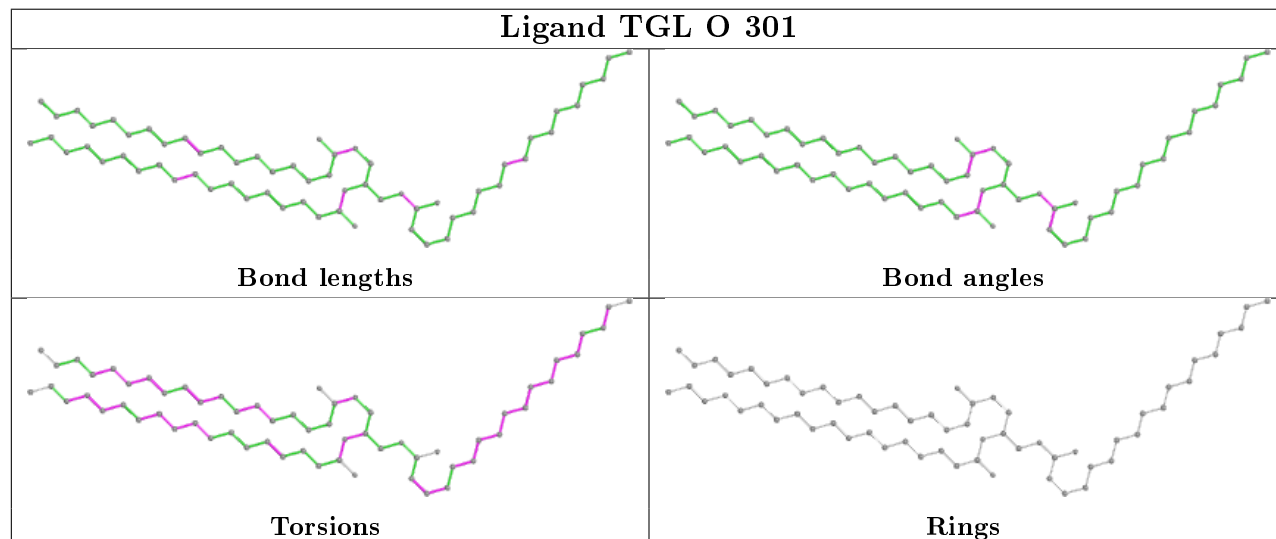
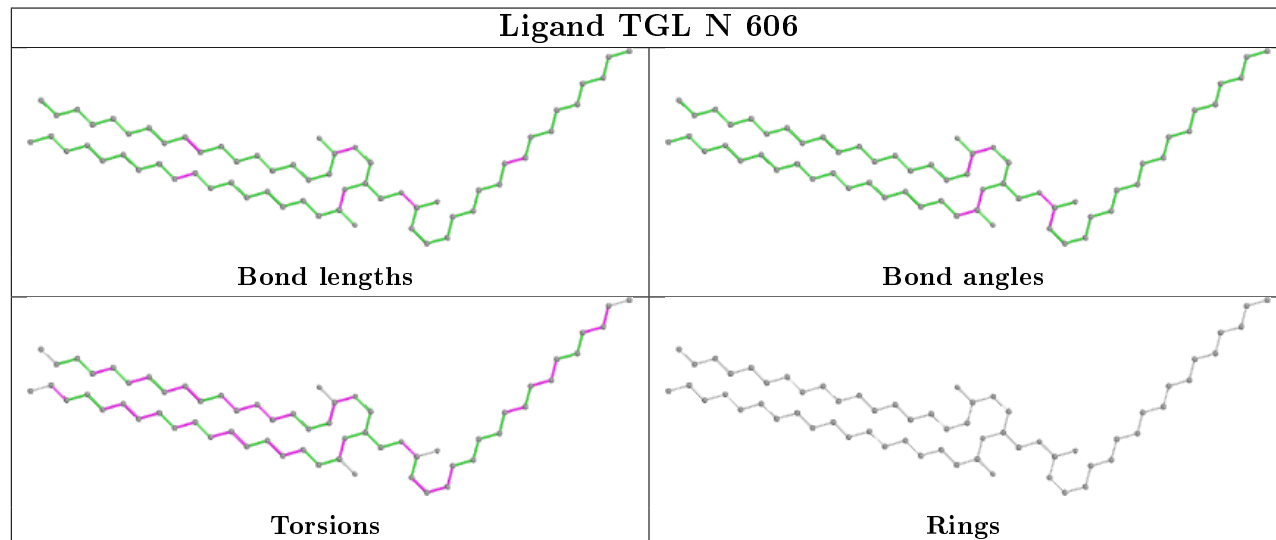
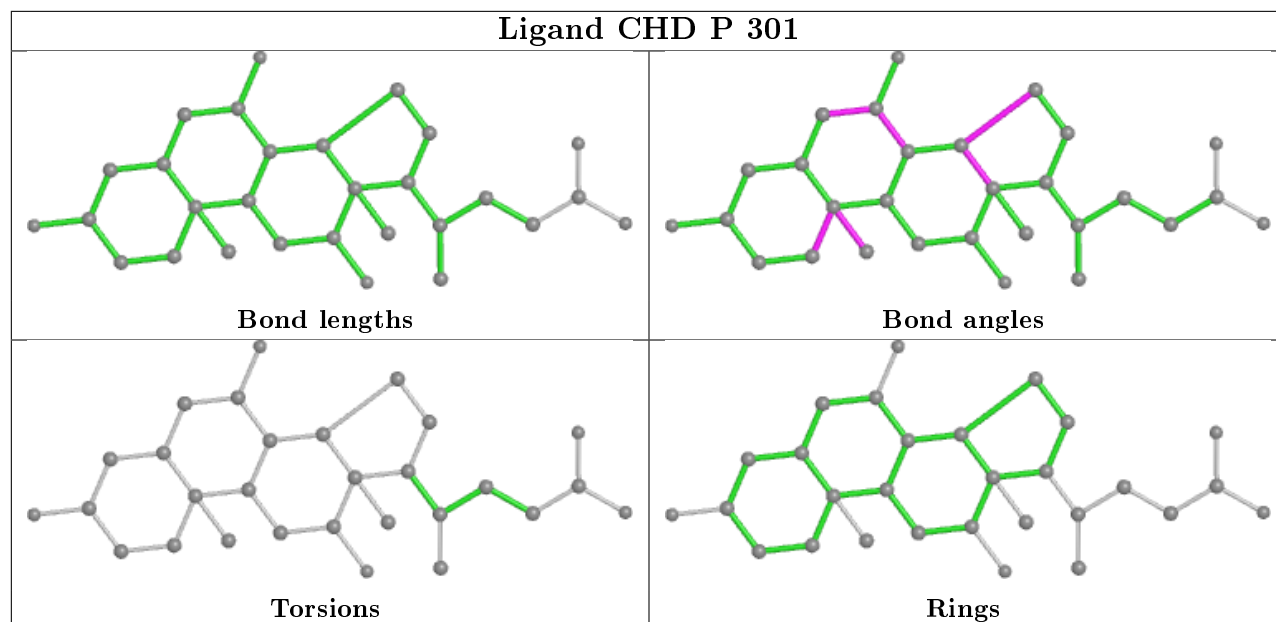
## Ligand PEK C 303

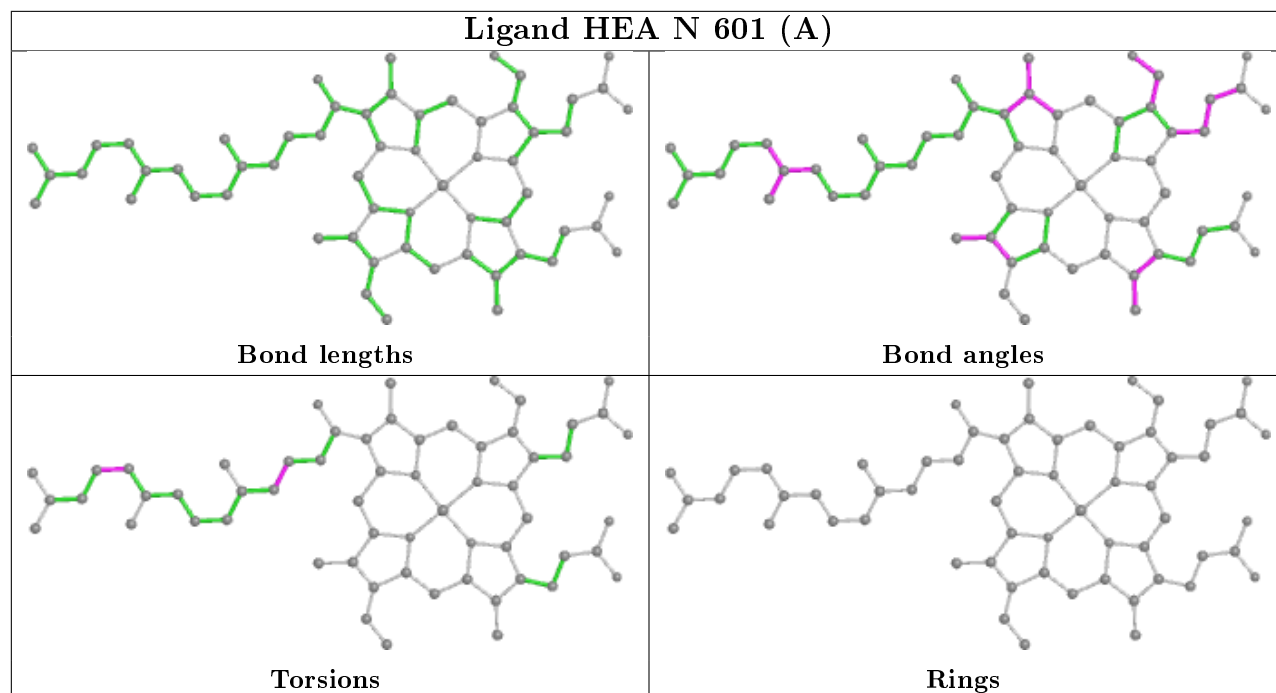
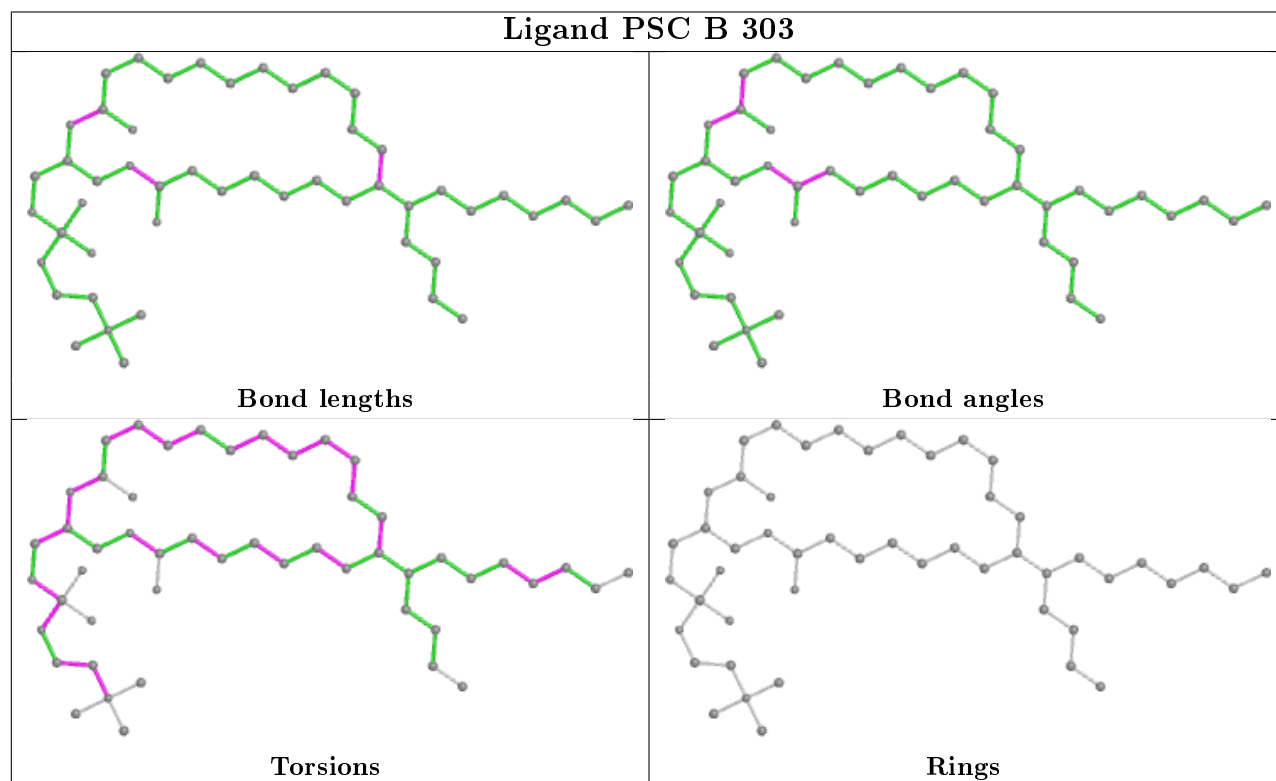


## Ligand PEK G 103

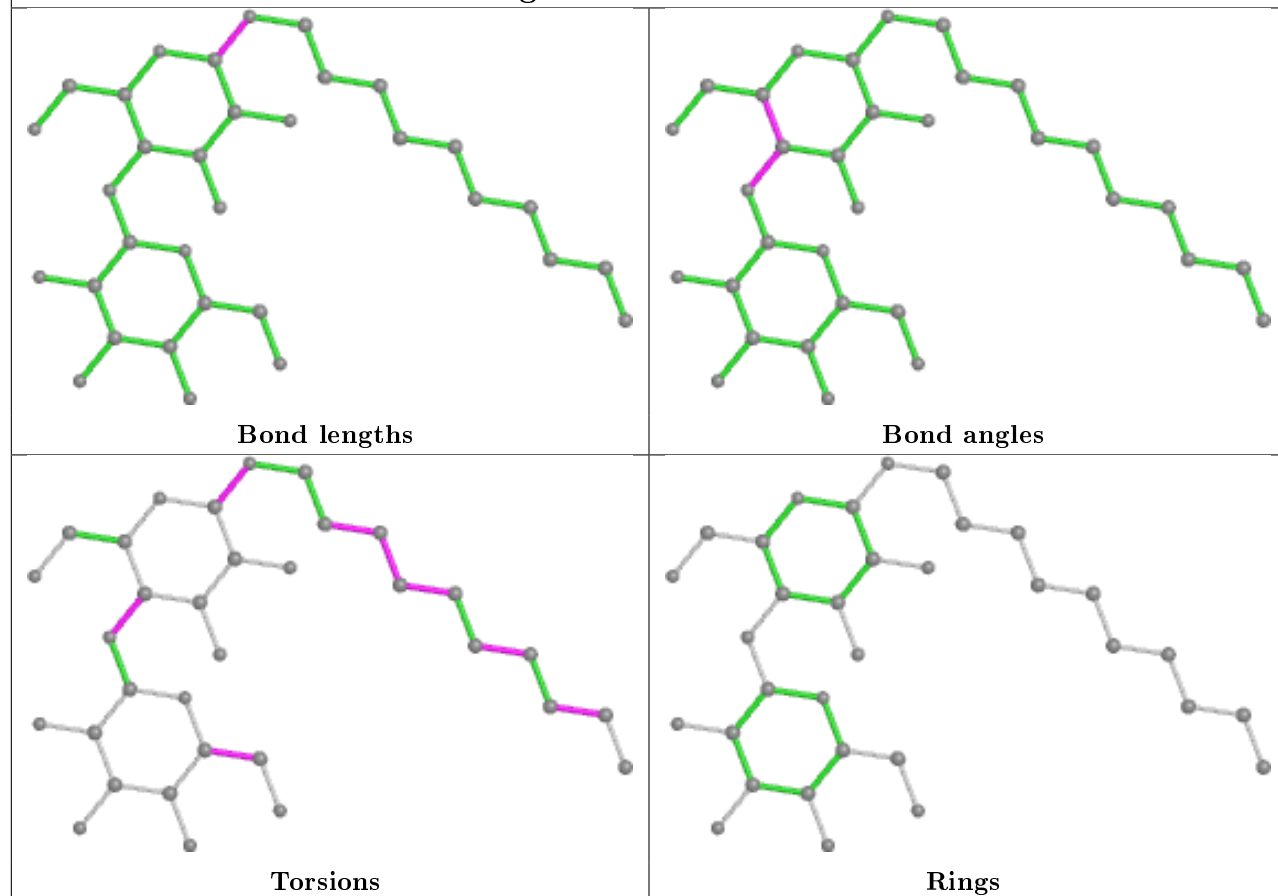


**Ligand HEA A 601 (B)****Ligand PGV C 305**

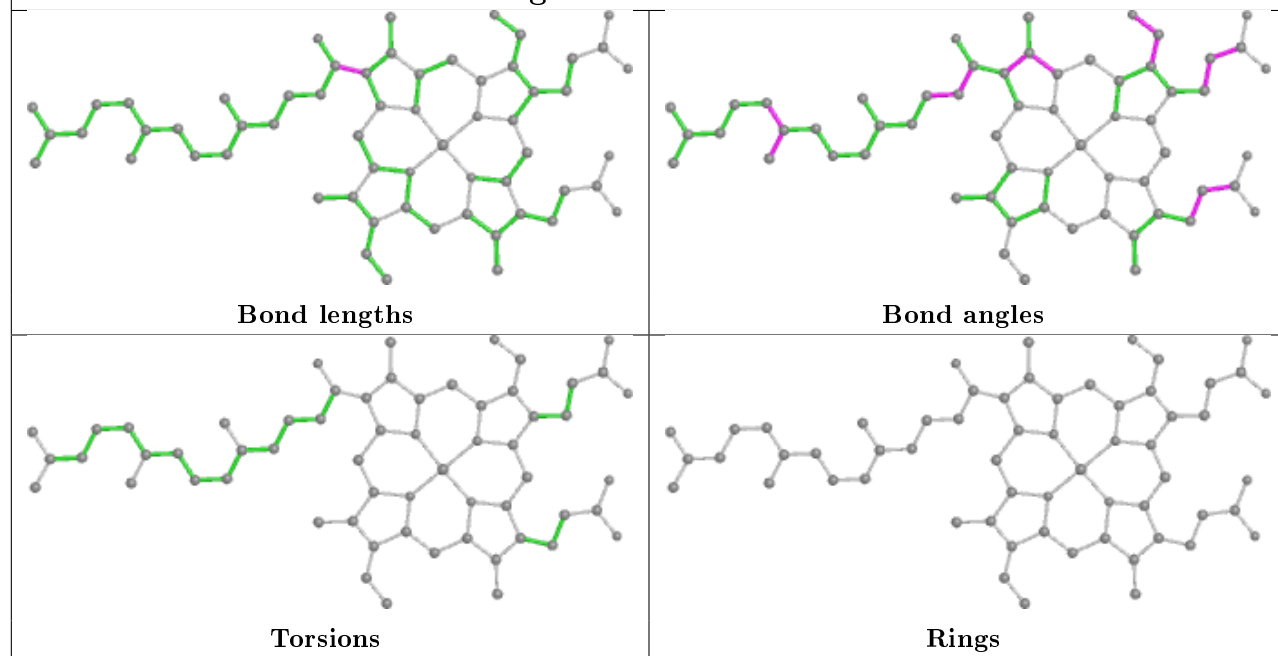


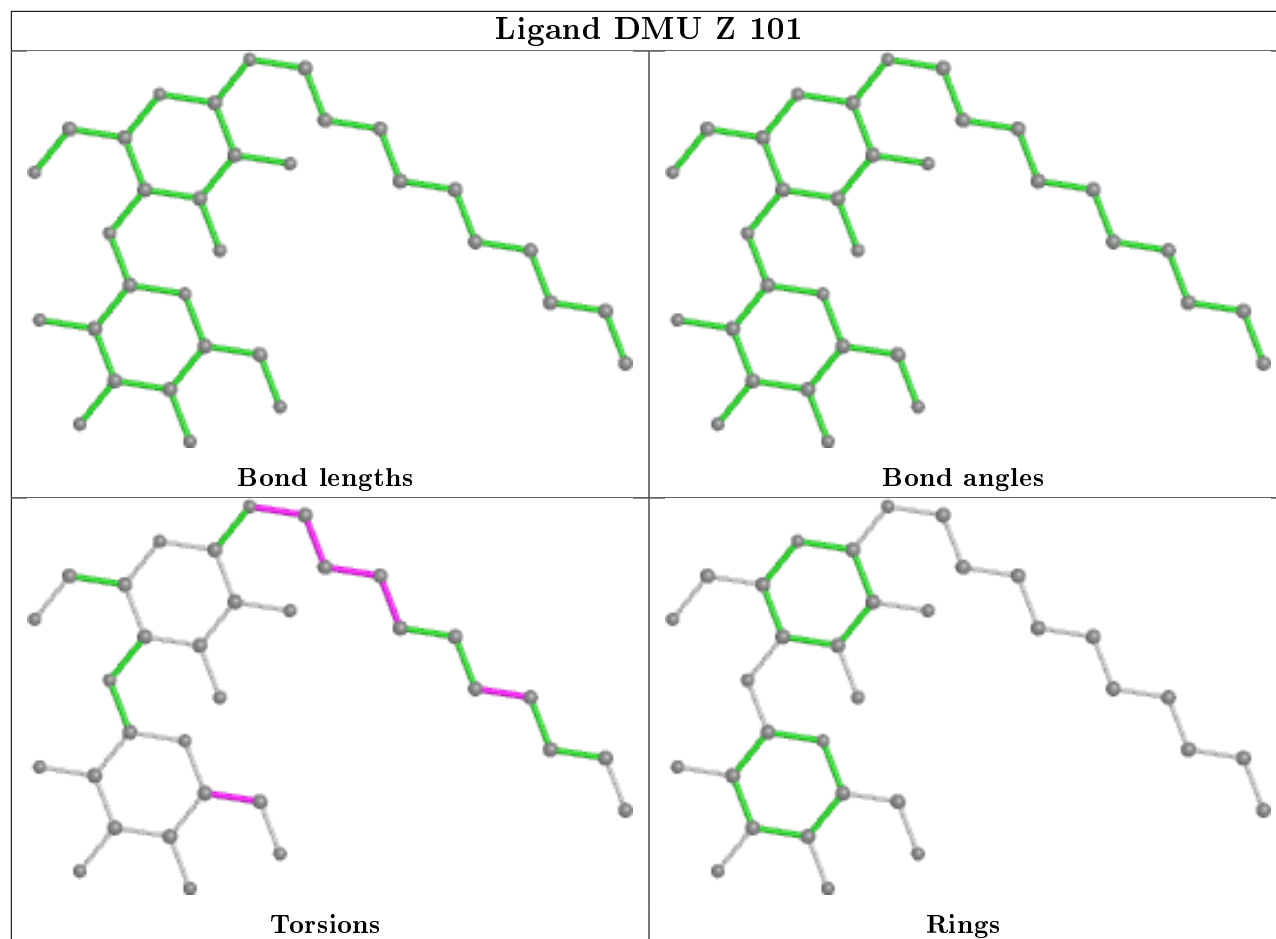
**Ligand HEA N 601 (A)****Ligand PSC B 303**

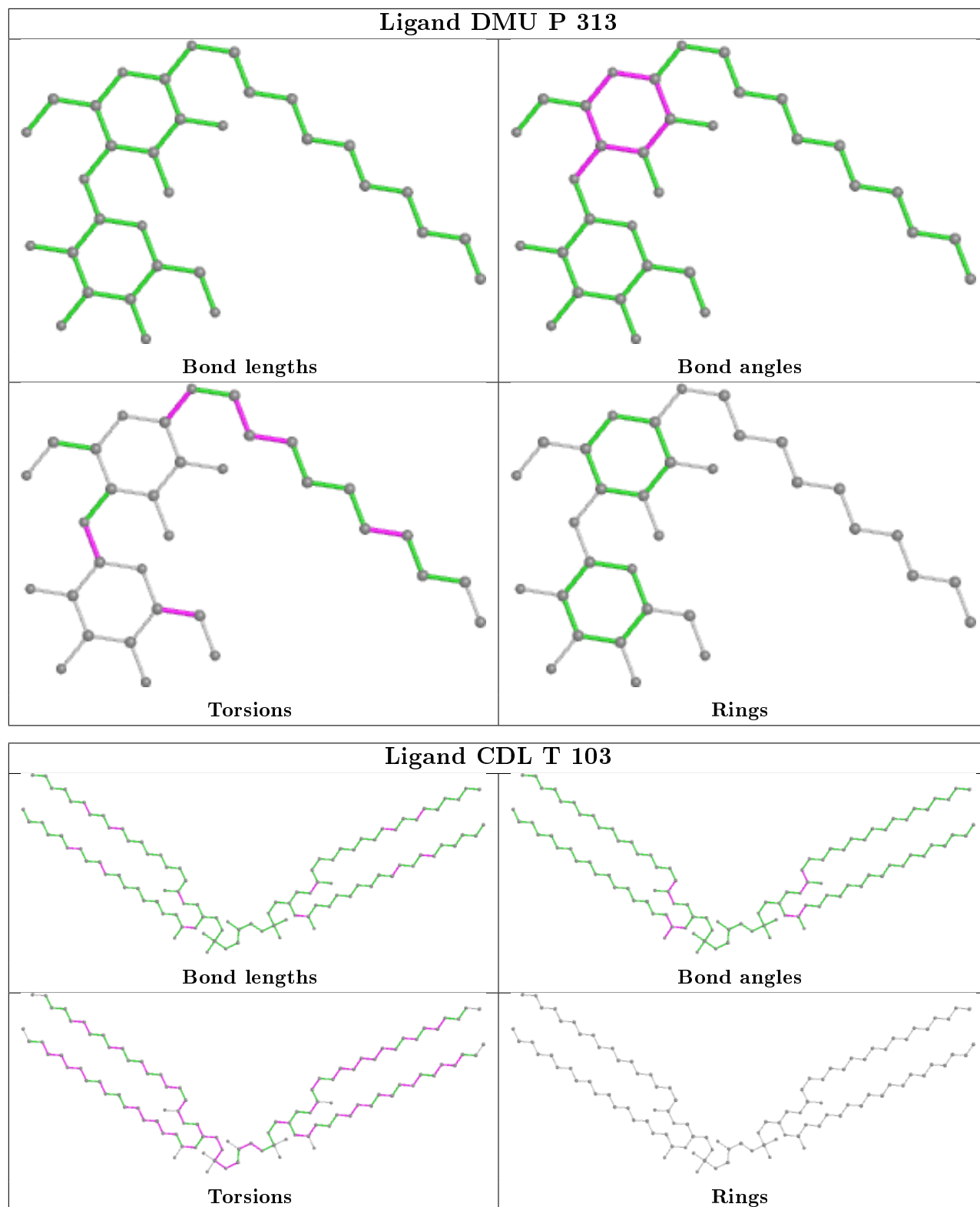
## Ligand DMU W 104



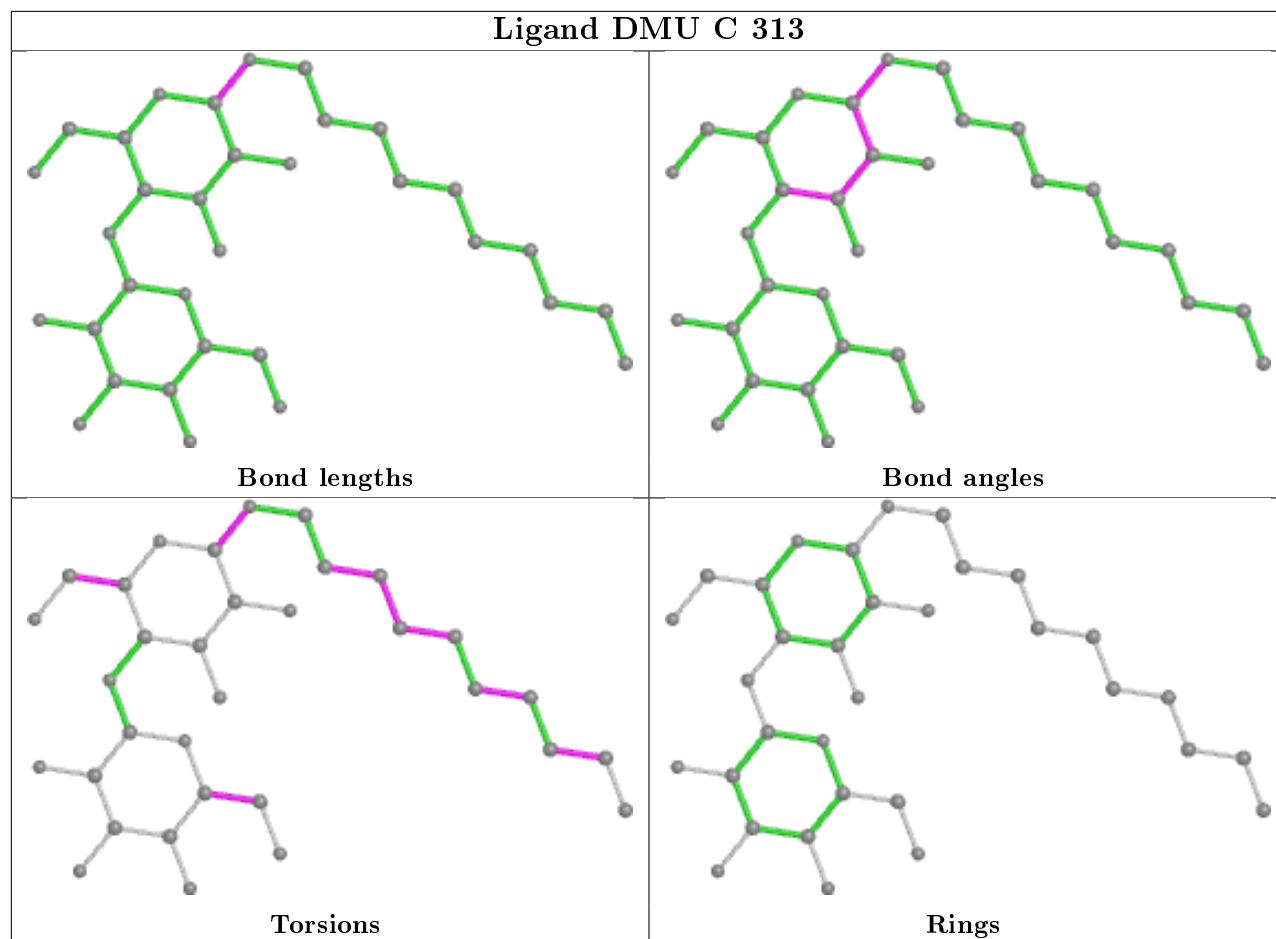
## Ligand HEA N 602



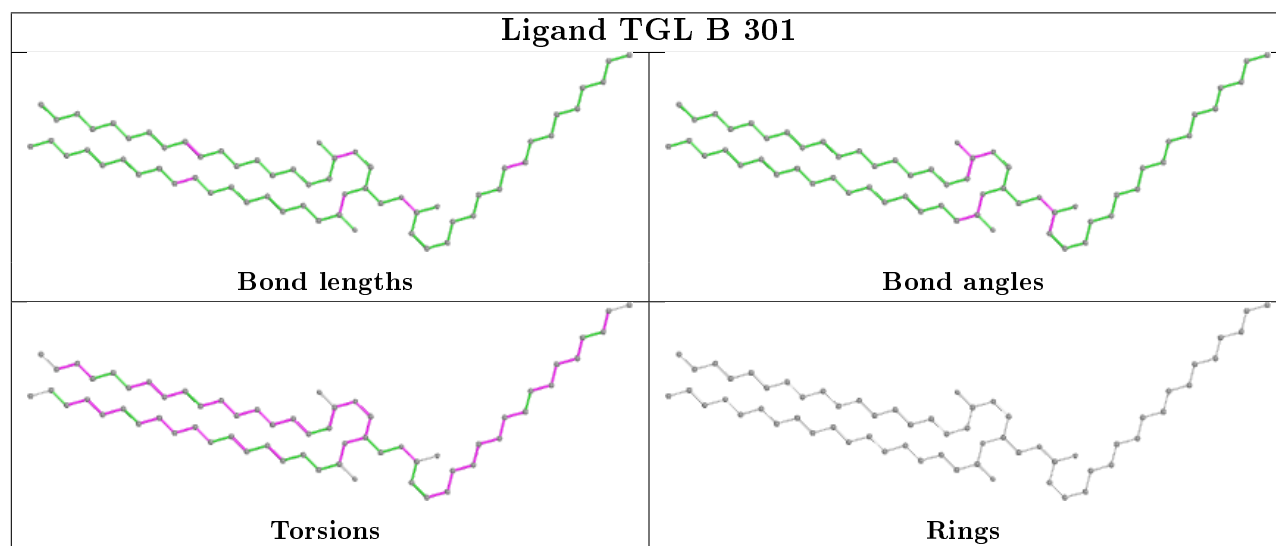




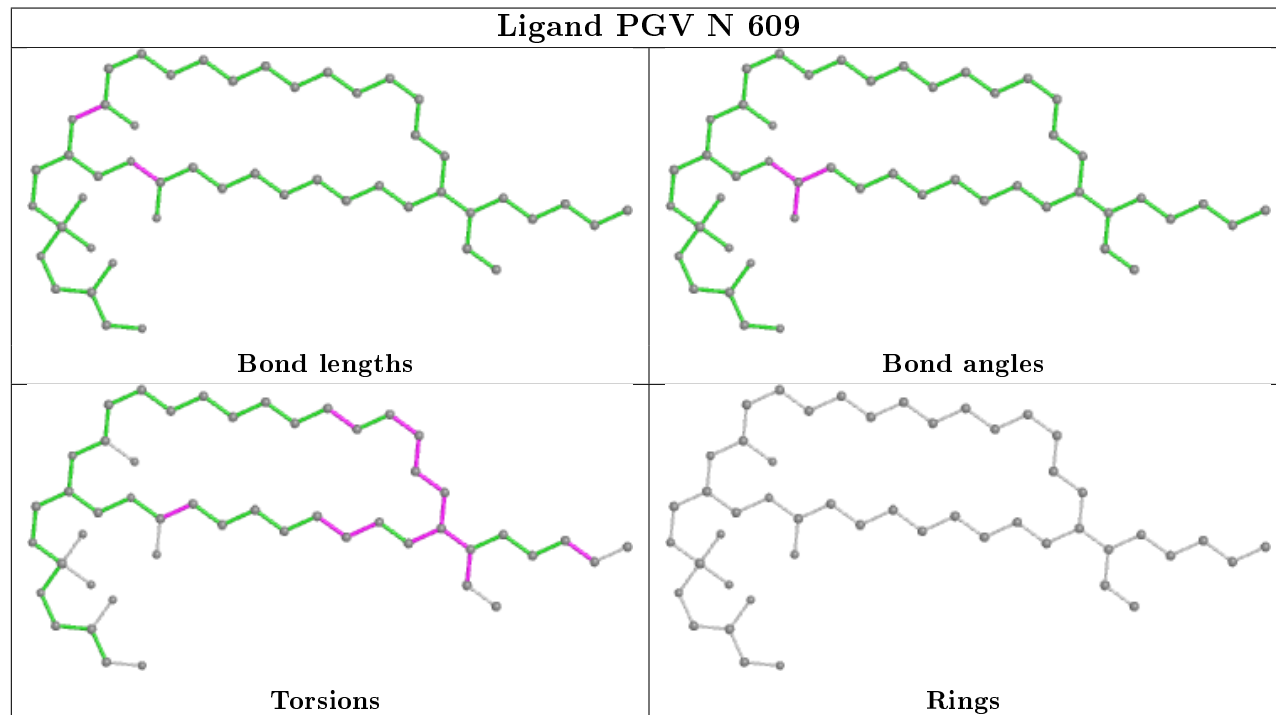
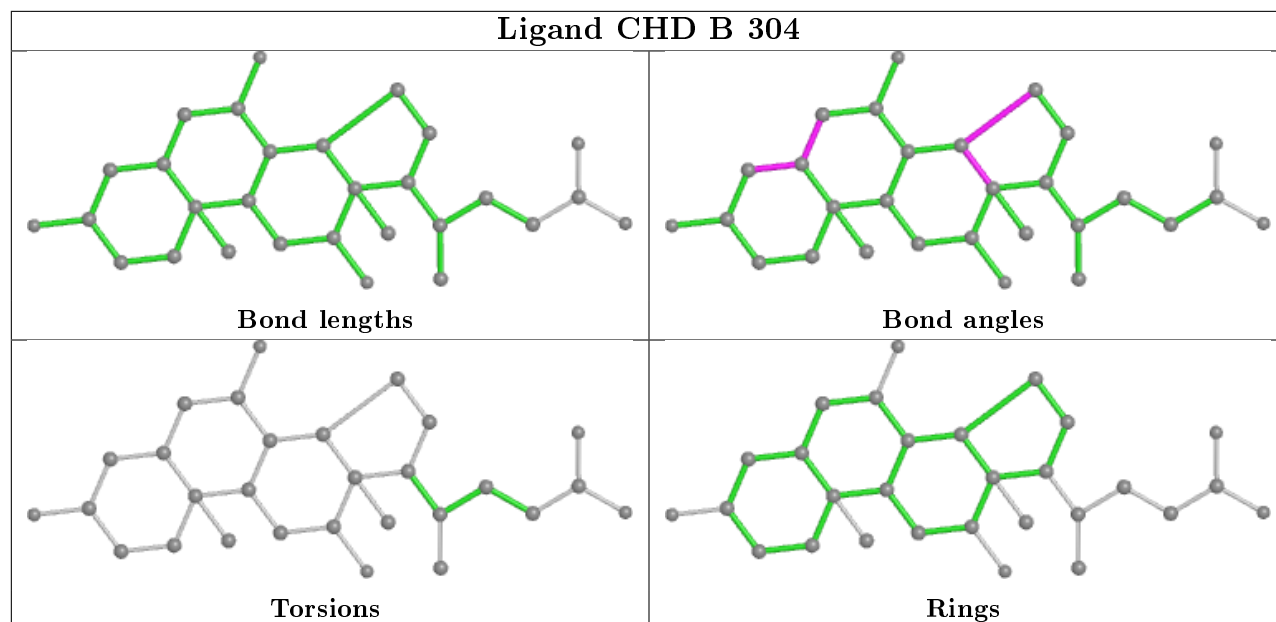
## Ligand DMU C 313

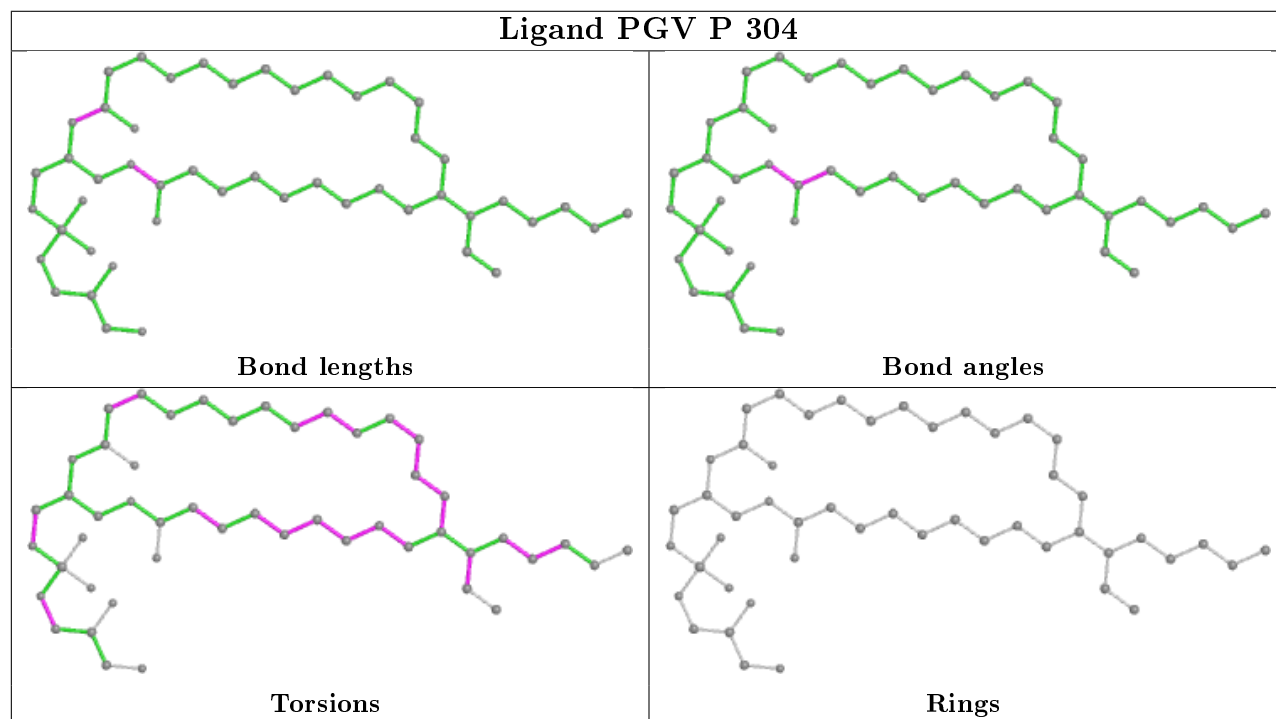
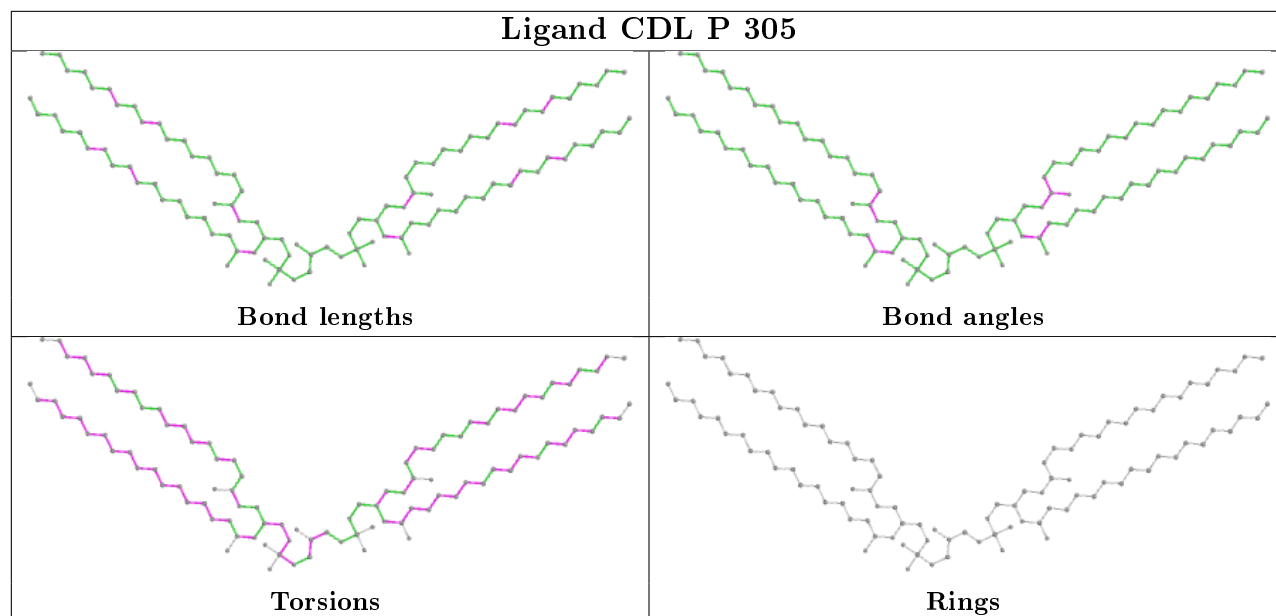


## Ligand TGL B 301

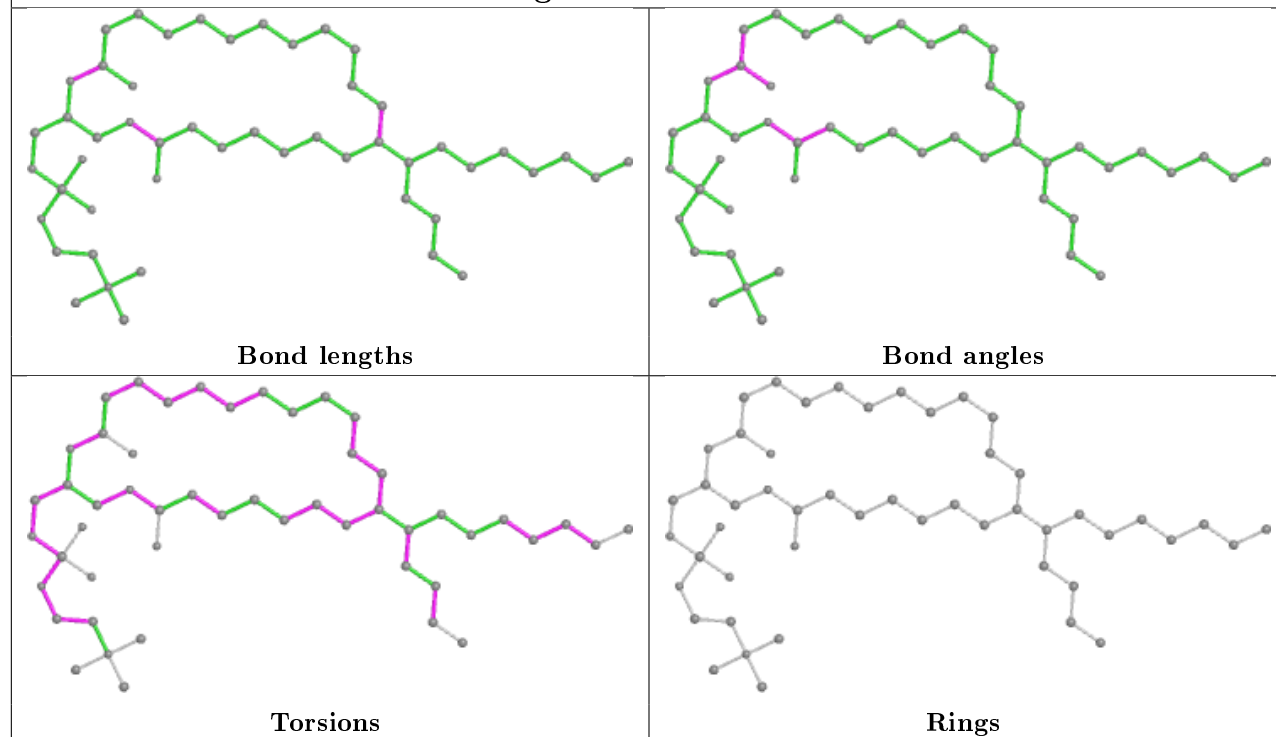




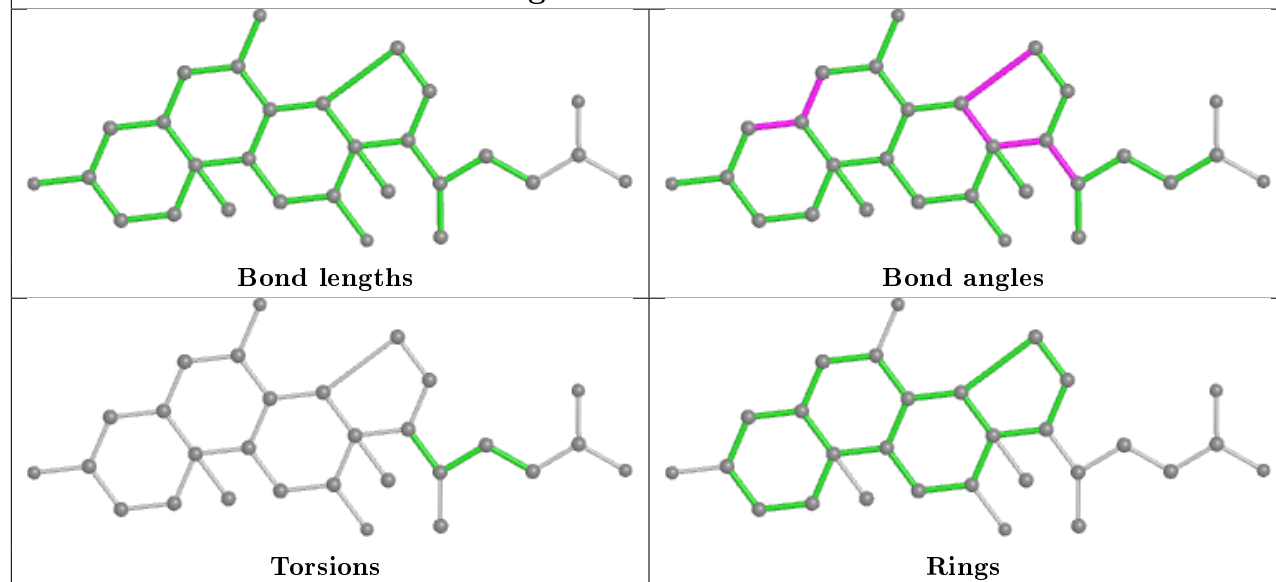




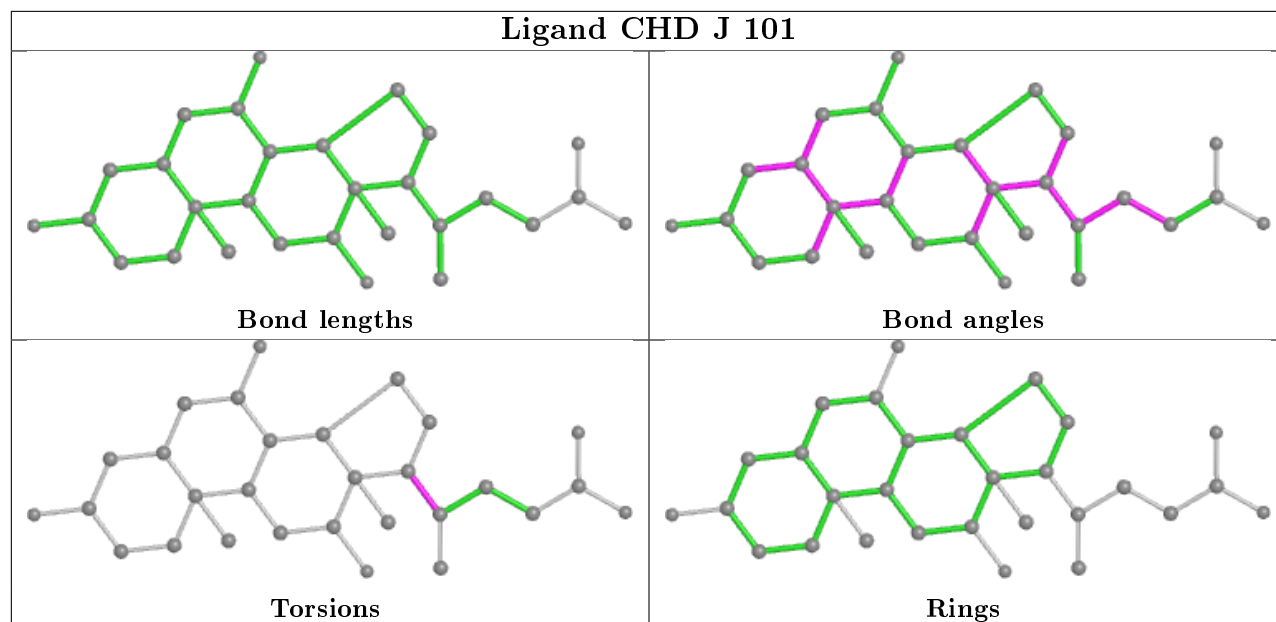
## Ligand PSC O 303



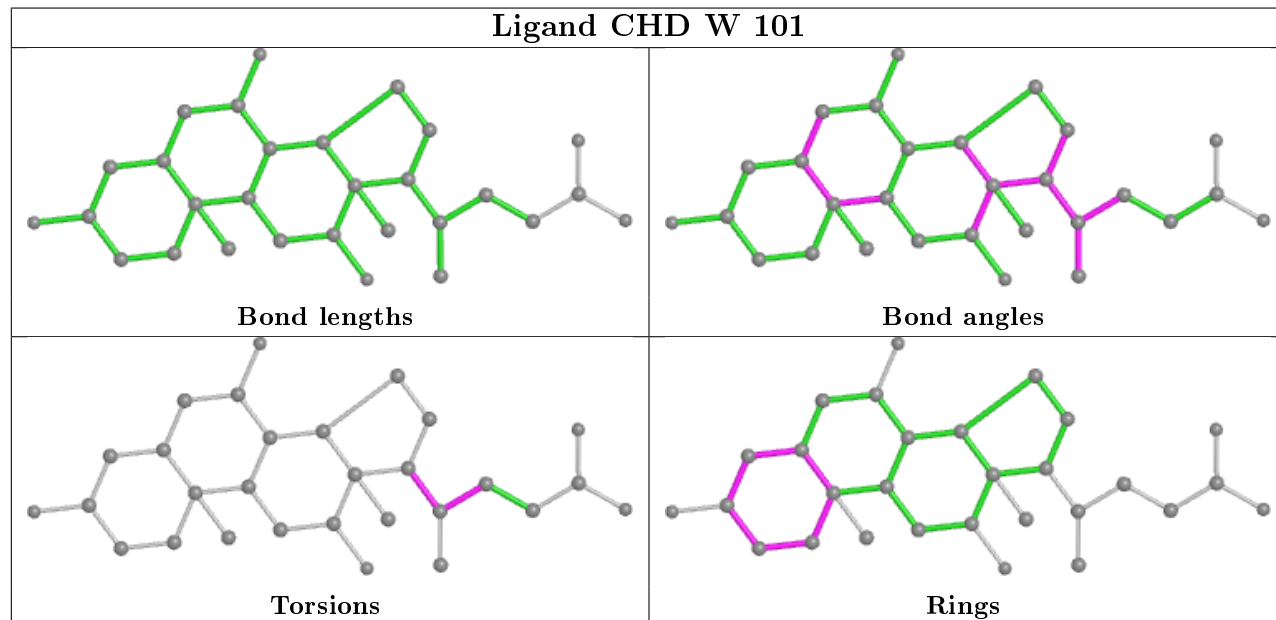
## Ligand CHD G 102



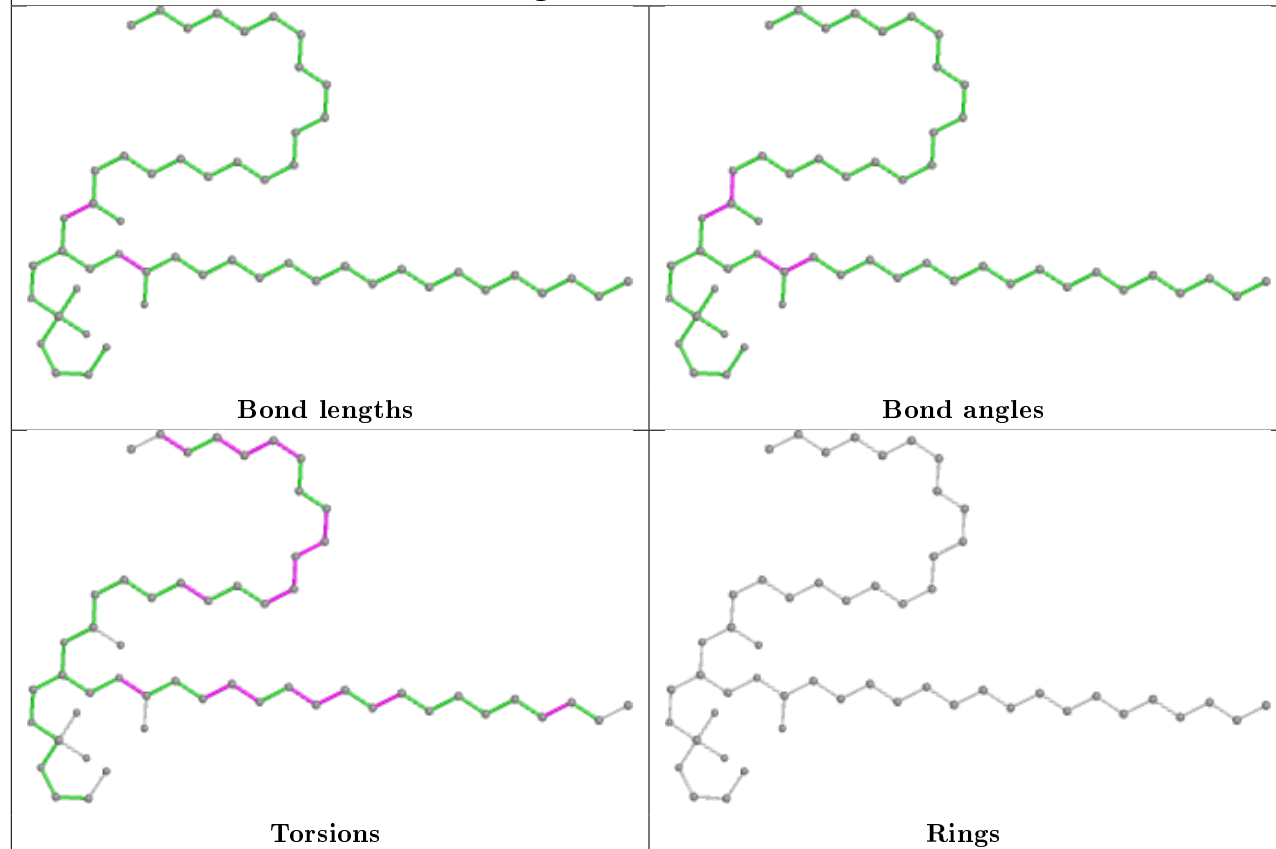
## Ligand CHD J 101



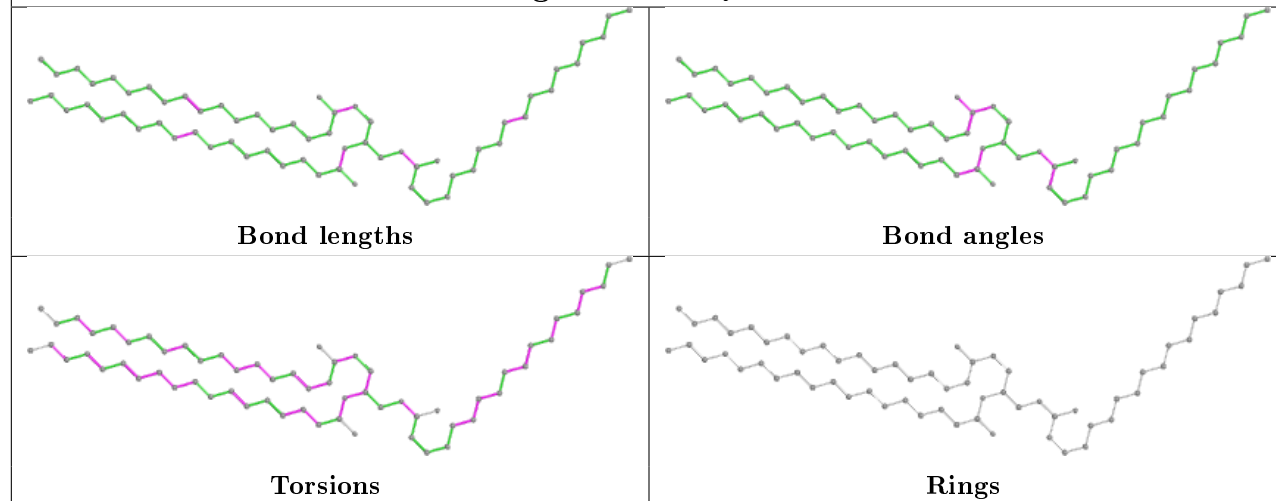
## Ligand CHD W 101

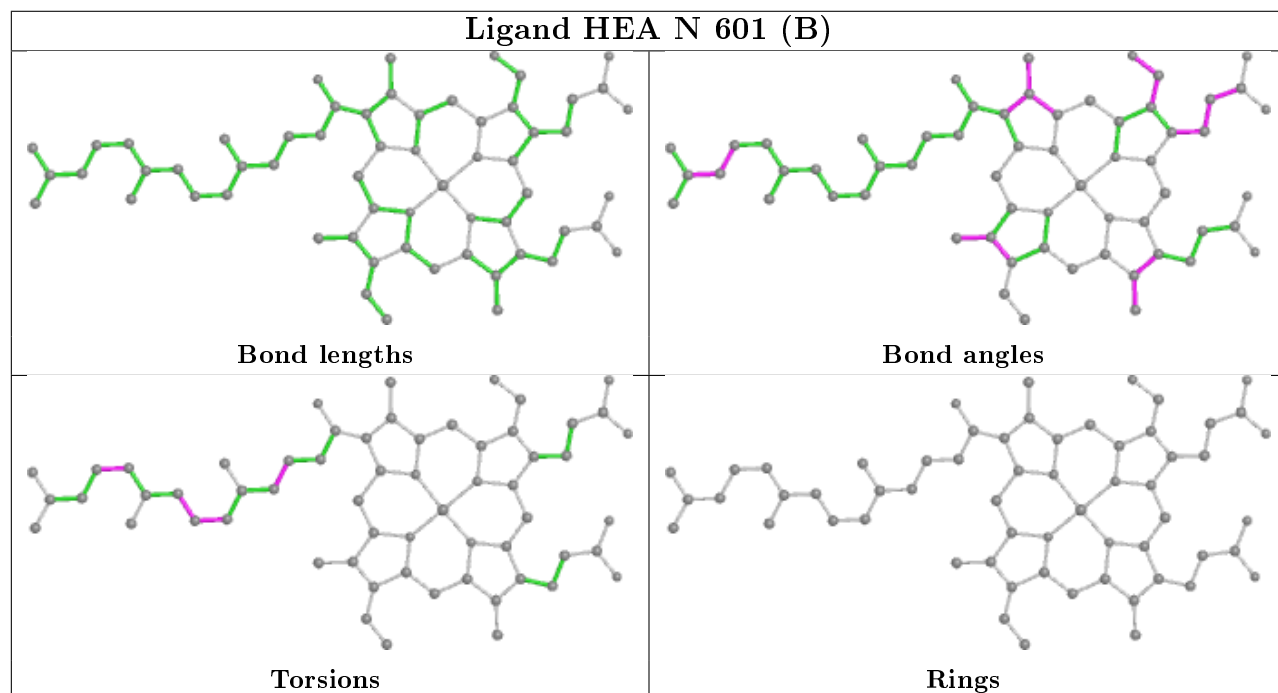
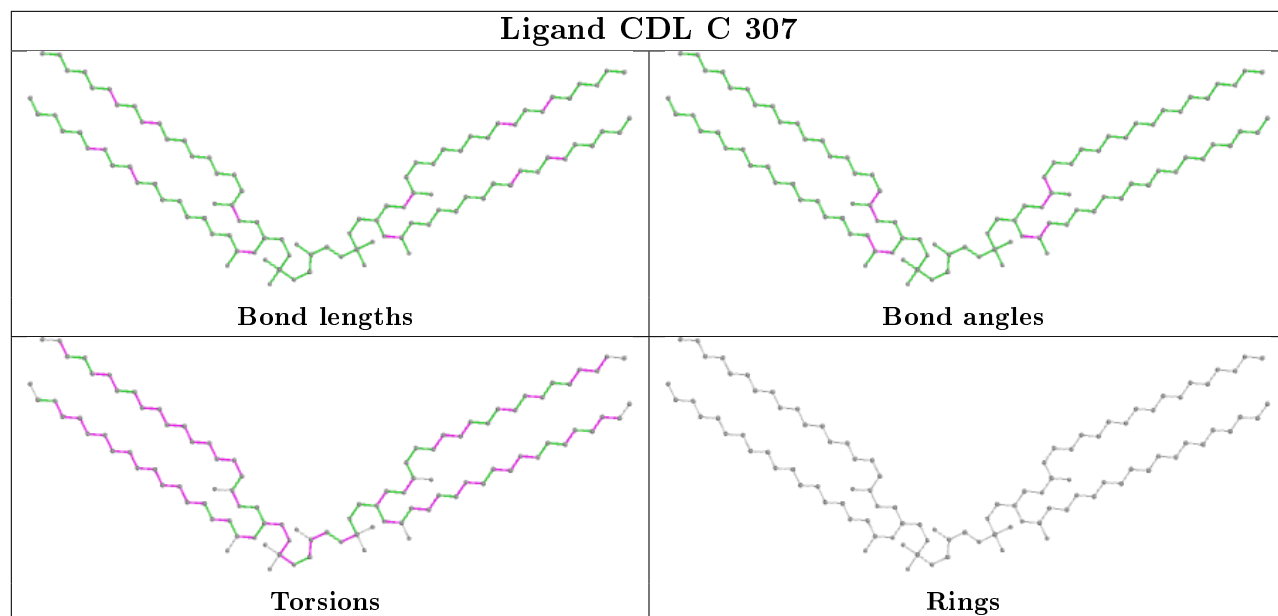


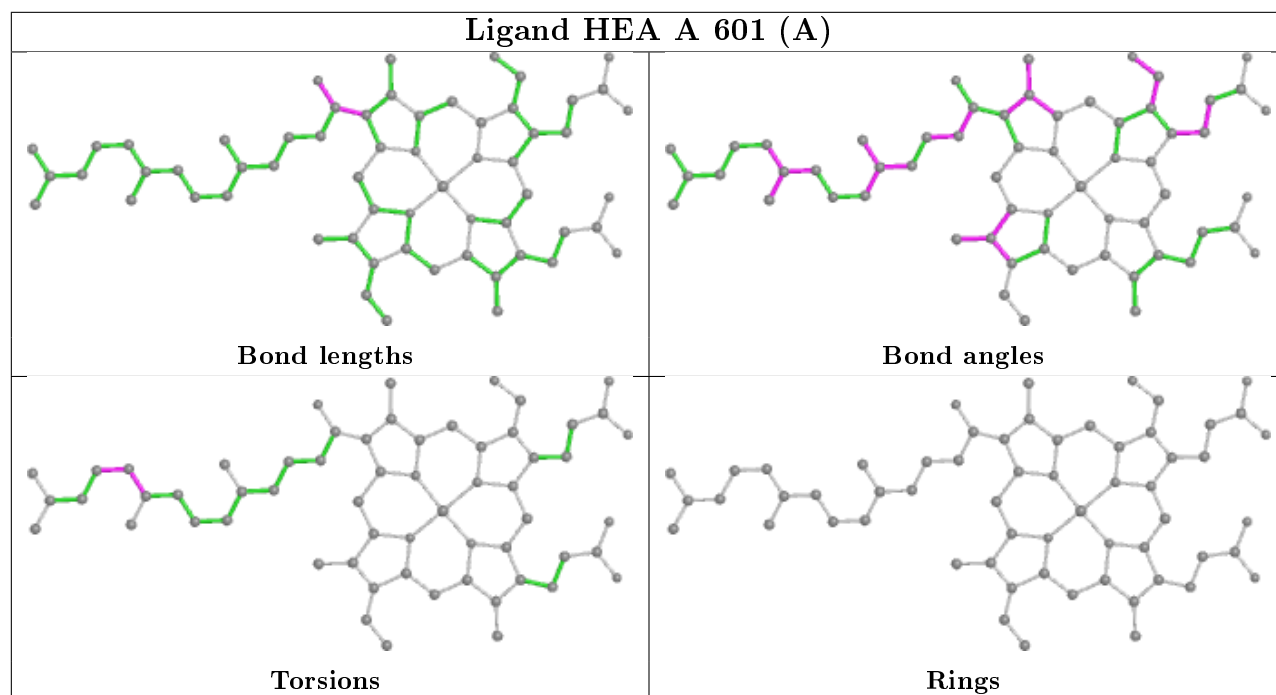
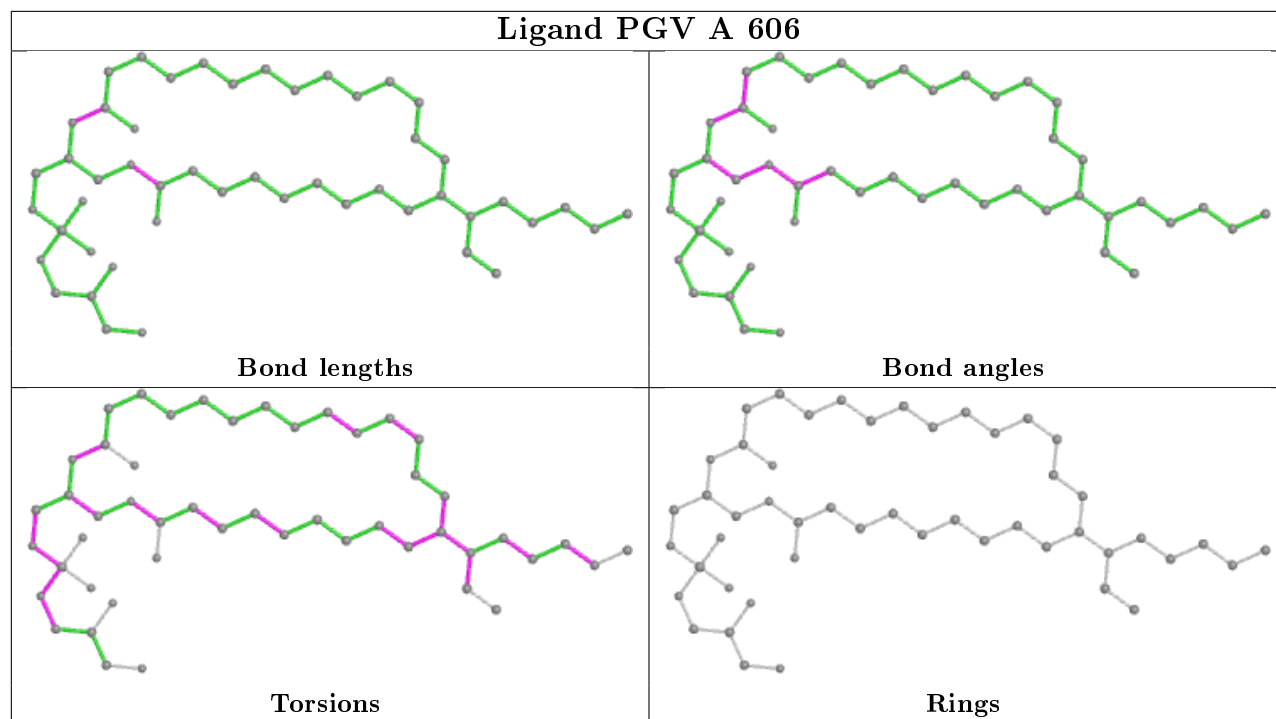
## Ligand PEK P 303

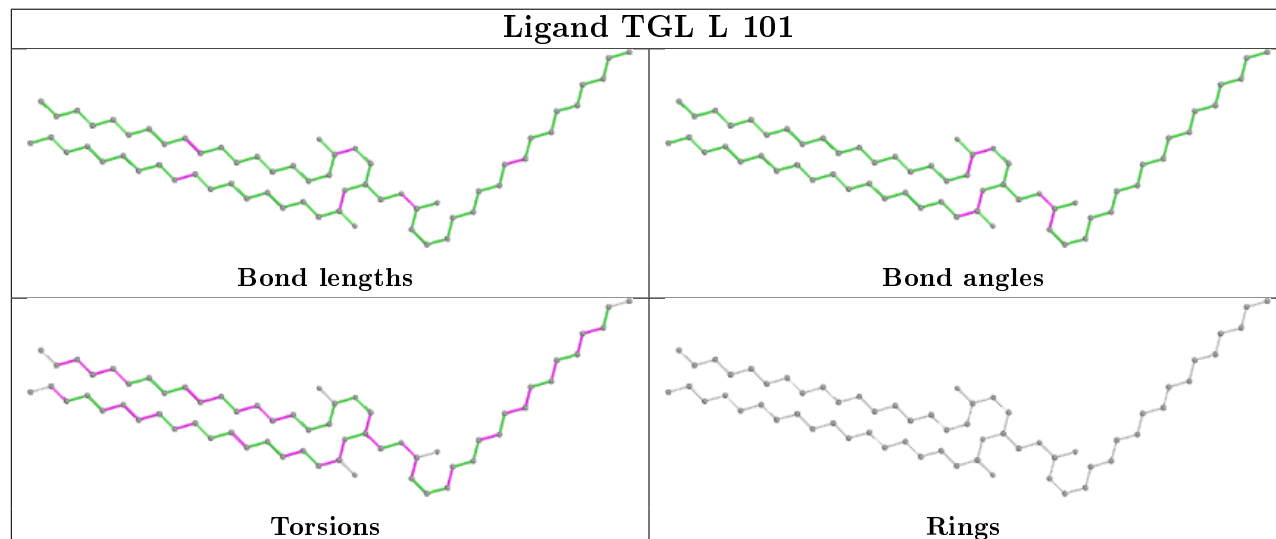
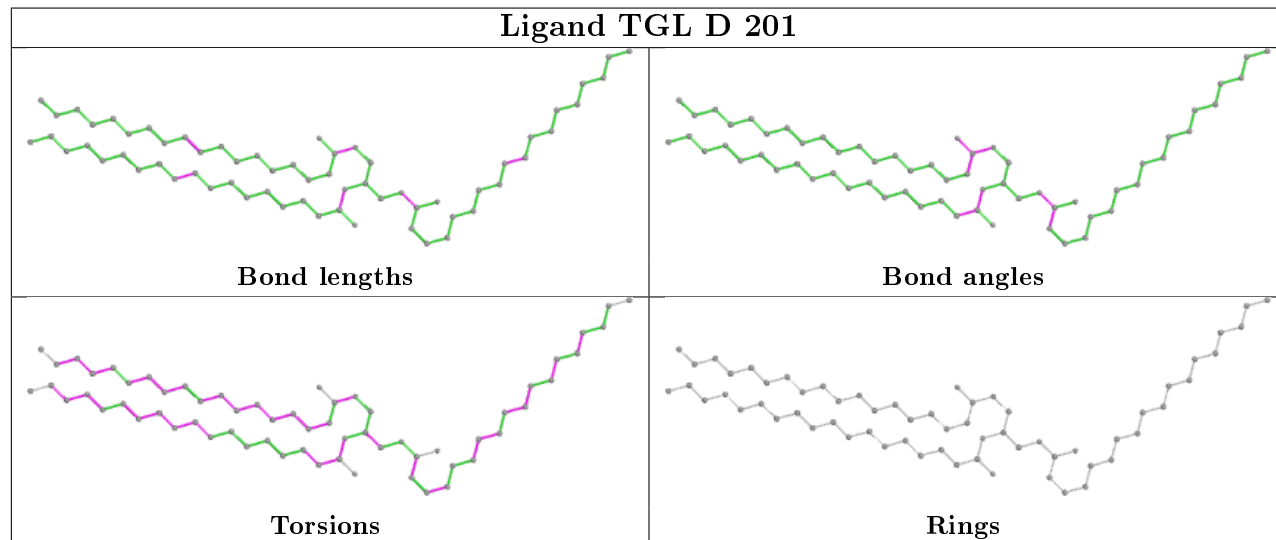
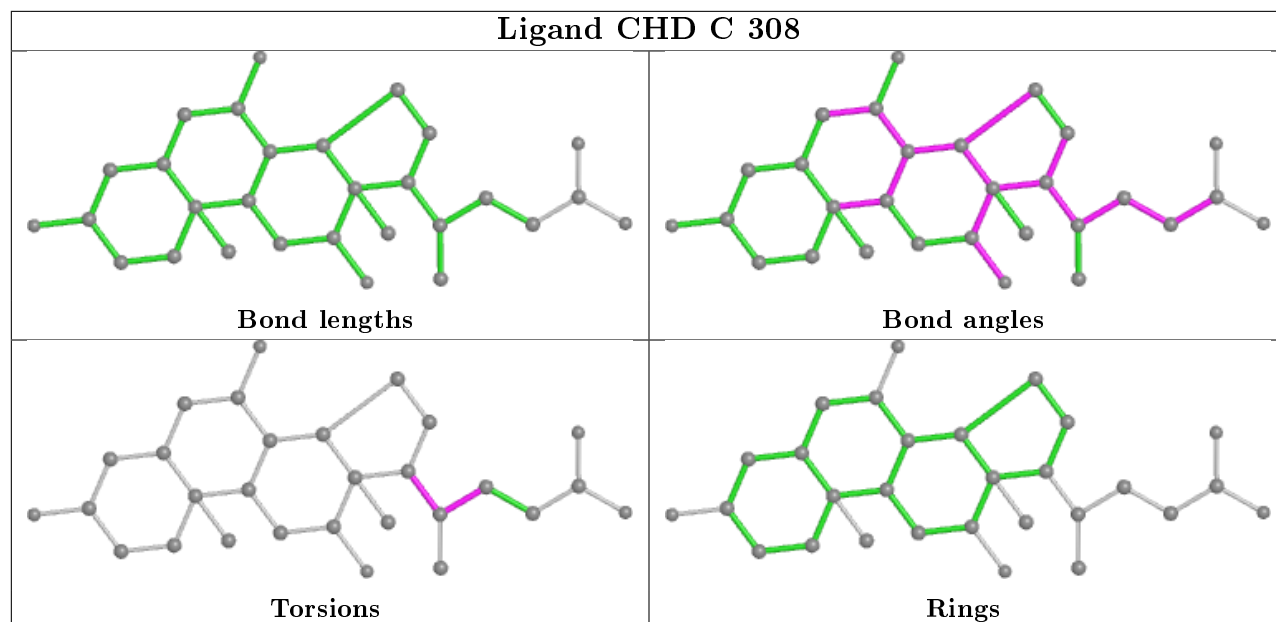


## Ligand TGL Q 201



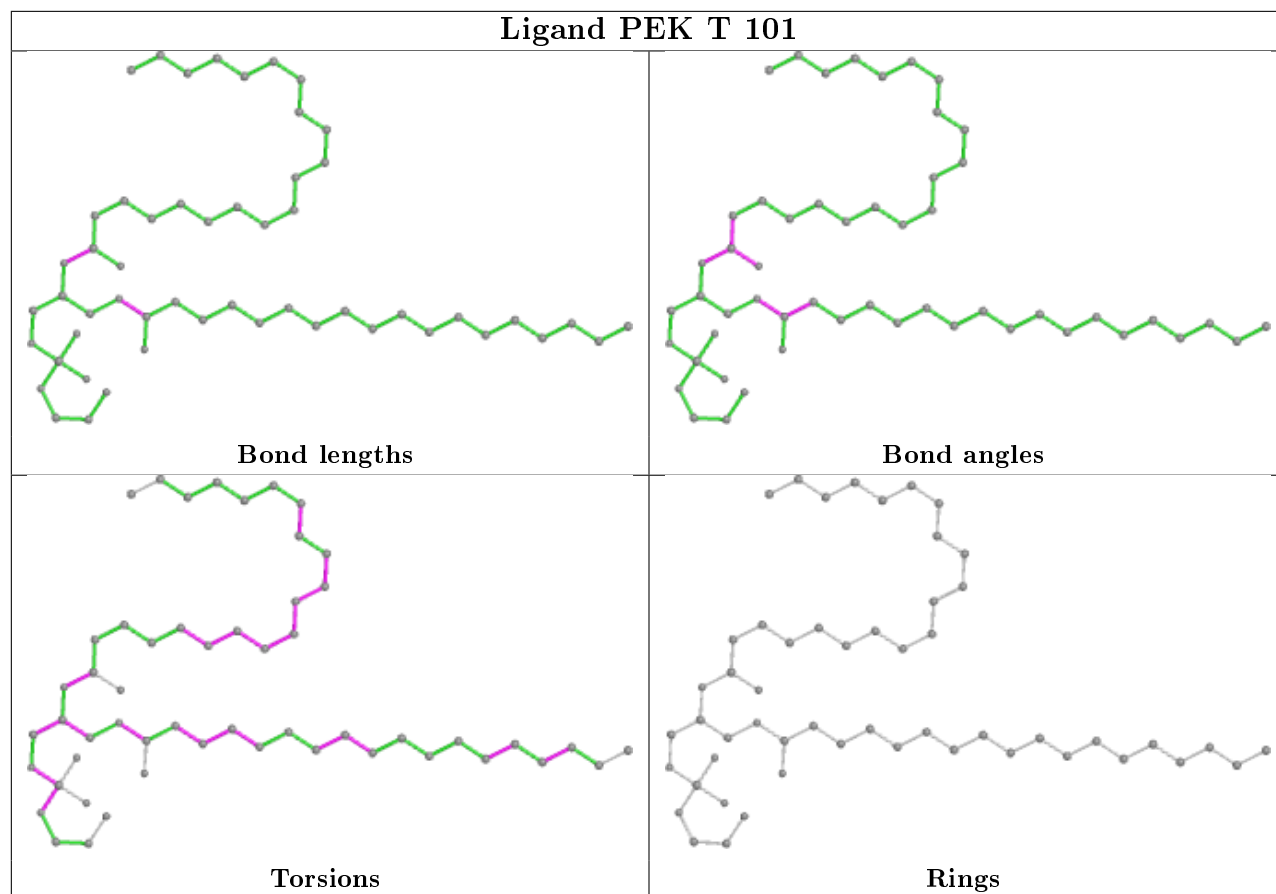




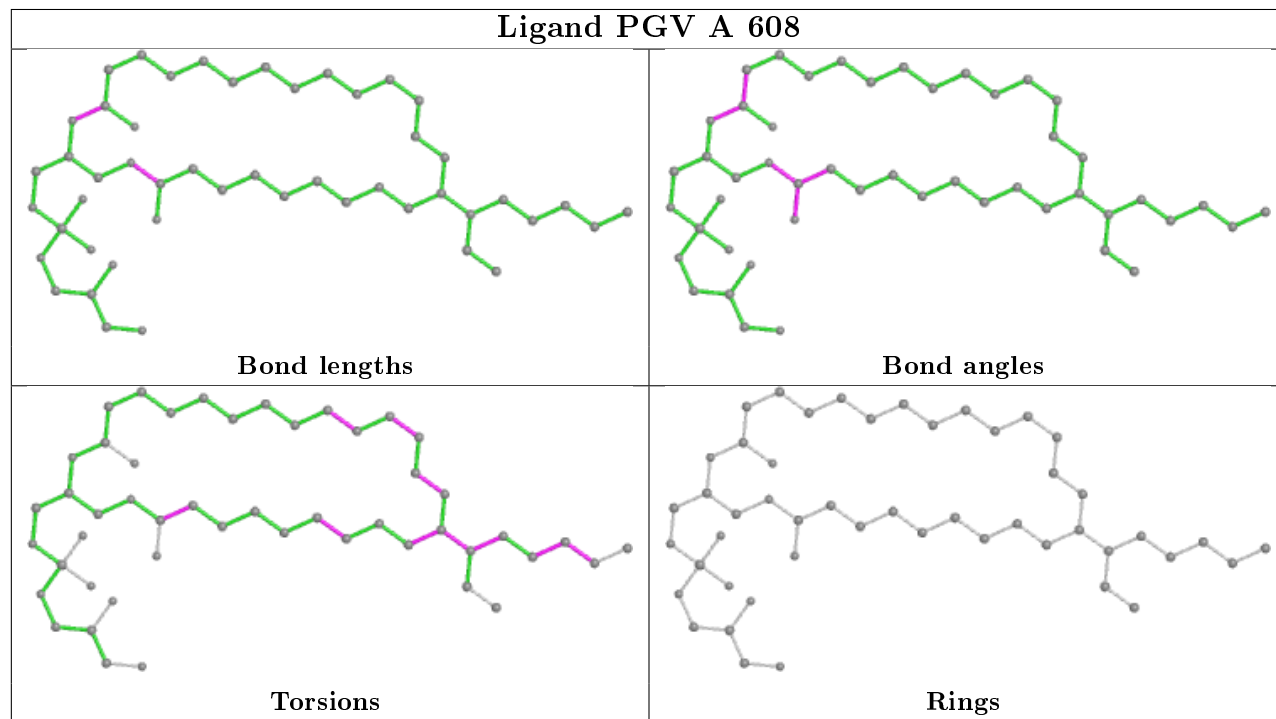


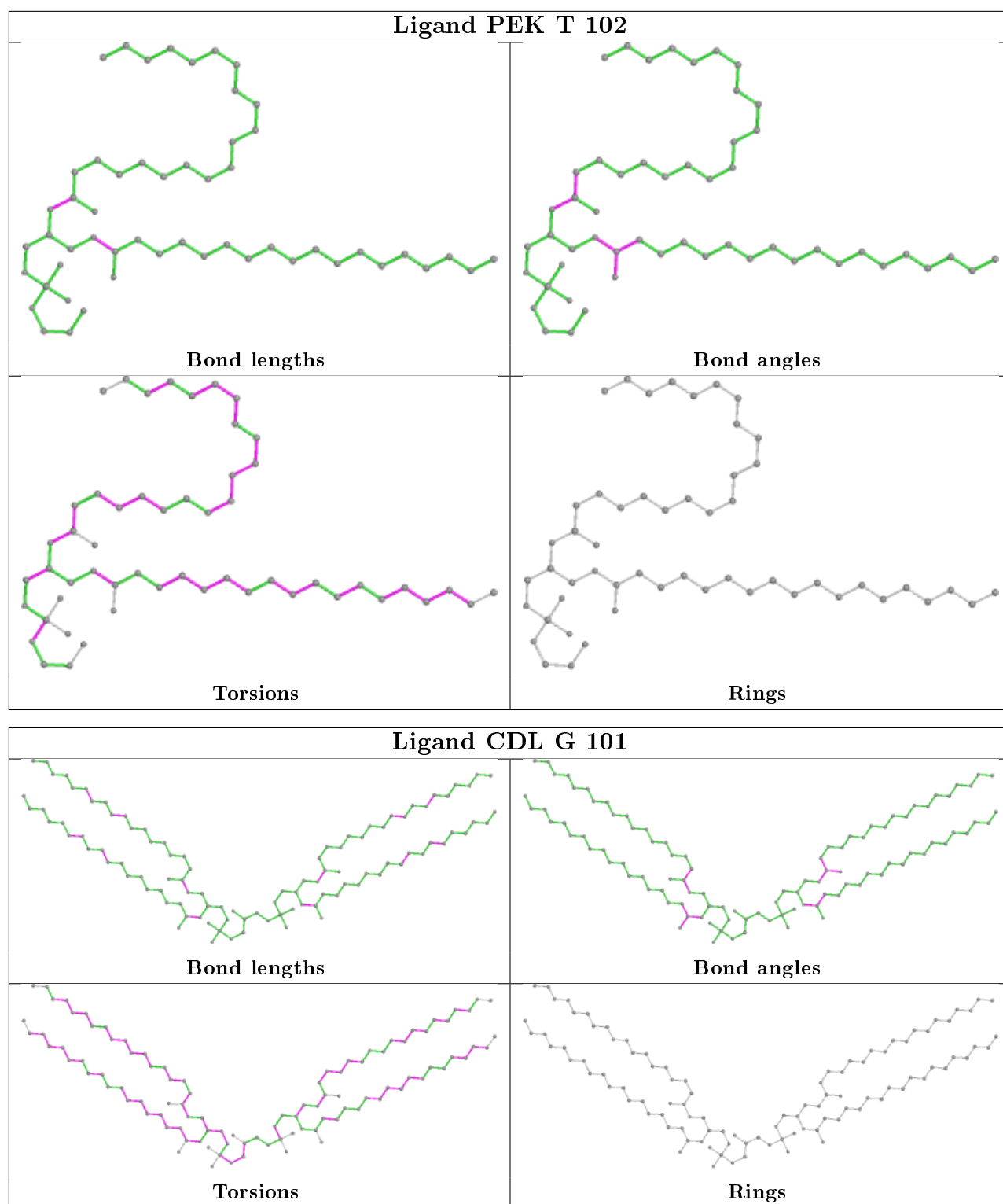


## Ligand PEK T 101



## Ligand PGV A 608





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.24	4 (0%) 86 86	23, 28, 35, 78	0
1	N	513/514 (99%)	0.19	4 (0%) 86 86	26, 33, 44, 76	0
2	B	226/227 (99%)	0.17	4 (1%) 68 68	27, 34, 49, 70	0
2	O	226/227 (99%)	0.40	9 (3%) 38 36	31, 44, 67, 98	0
3	C	259/261 (99%)	0.18	3 (1%) 79 79	26, 31, 42, 77	0
3	P	259/261 (99%)	0.20	3 (1%) 79 79	27, 34, 45, 70	0
4	D	144/147 (97%)	0.08	4 (2%) 53 51	29, 37, 55, 75	0
4	Q	144/147 (97%)	0.96	15 (10%) 6 6	36, 54, 80, 139	0
5	E	105/109 (96%)	0.14	2 (1%) 66 67	29, 35, 56, 108	0
5	R	105/109 (96%)	0.35	3 (2%) 51 50	34, 43, 60, 131	0
6	F	94/94 (100%)	0.42	4 (4%) 35 33	28, 39, 59, 116	0
6	S	94/94 (100%)	0.45	6 (6%) 19 18	29, 40, 71, 116	0
7	G	83/85 (97%)	1.12	18 (21%) 0 0	30, 39, 106, 139	0
7	T	83/85 (97%)	1.44	19 (22%) 0 0	30, 43, 98, 139	0
8	H	79/85 (92%)	0.64	9 (11%) 5 4	32, 42, 87, 103	0
8	U	79/85 (92%)	0.89	13 (16%) 1 1	39, 49, 95, 120	0
9	I	72/73 (98%)	1.15	15 (20%) 1 0	32, 44, 78, 97	0
9	V	72/73 (98%)	1.41	17 (23%) 0 0	33, 59, 86, 93	0
10	J	58/59 (98%)	0.49	4 (6%) 16 16	31, 41, 64, 106	0
10	W	58/59 (98%)	0.67	4 (6%) 16 16	37, 48, 72, 120	0
11	K	49/56 (87%)	0.06	1 (2%) 65 65	35, 42, 55, 61	0
11	X	49/56 (87%)	0.65	5 (10%) 6 6	47, 57, 74, 79	0
12	L	46/47 (97%)	0.27	1 (2%) 62 61	29, 34, 50, 94	0
12	Y	46/47 (97%)	0.55	5 (10%) 5 5	37, 46, 64, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.45	3 (6%) 16 16	31, 35, 72, 105	0
13	Z	43/46 (93%)	0.59	6 (13%) 2 2	42, 49, 81, 124	0
All	All	3542/3606 (98%)	0.40	181 (5%) 28 26	23, 36, 67, 139	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	22.9
4	Q	6	VAL	20.3
2	O	227	LEU	13.1
7	T	10	GLY	12.7
4	Q	4	SER	12.6
6	F	1	ALA	12.6
8	U	8	ILE	12.4
9	I	25	PHE	11.9
9	I	29	LEU	11.7
7	T	3	ALA	11.4
8	H	8	ILE	11.2
7	T	36	TRP	10.2
8	H	45	ALA	9.8
6	F	2	SER	9.3
7	G	3	ALA	9.1
9	V	25	PHE	8.6
6	S	1	ALA	8.5
5	R	5	HIS	8.3
9	V	34	PHE	8.1
5	R	109	VAL	7.9
9	V	29	LEU	7.8
10	J	58	LYS	7.1
7	T	8	HIS	6.9
8	U	7	LYS	6.8
7	T	2	SER	6.7
4	Q	7	LYS	6.7
9	I	33	THR	6.5
6	S	2	SER	6.4
7	T	37	LEU	6.3
7	G	40	GLY	6.2
10	W	58	LYS	6.2
2	O	113	TYR	6.2
7	G	2	SER	6.1
3	P	3	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
9	I	30	GLY	6.0
9	V	31	PHE	6.0
7	T	42	ARG	5.9
7	G	42	ARG	5.9
7	G	6	GLY	5.8
8	U	50	VAL	5.7
9	I	26	MET	5.7
9	V	37	PHE	5.6
6	F	94	HIS	5.6
5	E	5	HIS	5.4
7	T	39	SER	5.4
7	G	36	TRP	5.2
4	Q	8	SER	5.2
9	V	30	GLY	5.2
7	G	8	HIS	5.2
7	T	41	HIS	5.1
8	H	46	LYS	5.0
4	D	4	SER	4.9
8	U	10	ASN	4.9
6	S	93	PRO	4.8
8	U	45	ALA	4.8
7	T	7	ASP	4.8
13	M	43	SER	4.8
9	I	31	PHE	4.8
7	G	5	LYS	4.7
12	L	2[A]	HIS	4.5
7	T	1	ALA	4.4
9	I	34	PHE	4.3
13	M	42	LYS	4.3
10	W	57	HIS	4.2
2	O	224	ALA	4.2
12	Y	47	LYS	4.2
8	U	9	LYS	4.2
7	T	40	GLY	4.1
7	G	84	LYS	4.1
9	V	33	THR	4.0
10	W	52	TRP	4.0
9	V	2	THR	4.0
7	T	33	LEU	4.0
7	T	5	LYS	4.0
3	P	37	PHE	3.9
9	I	37	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
4	Q	10	ASP	3.9
7	G	4	ALA	3.9
2	B	113	TYR	3.8
6	S	94	HIS	3.8
2	O	91	ASN	3.8
9	V	26	MET	3.7
13	Z	42	LYS	3.7
9	V	32	ALA	3.7
6	F	3	GLY	3.6
7	T	6	GLY	3.6
7	G	41	HIS	3.6
4	Q	51	LEU	3.6
8	U	48	GLY	3.6
2	B	59	GLN	3.5
7	G	1	ALA	3.5
1	N	311[A]	ILE	3.5
7	T	43	GLU	3.4
1	A	513	LEU	3.4
2	O	116	LEU	3.4
11	X	13	TYR	3.4
10	J	52	TRP	3.4
7	G	37	LEU	3.3
10	J	1	PHE	3.3
7	T	84	LYS	3.3
13	Z	43	SER	3.3
4	Q	31	LYS	3.3
9	I	19	PHE	3.2
4	Q	46	ALA	3.2
9	V	39	VAL	3.2
5	E	70[A]	VAL	3.2
13	M	40	TYR	3.2
9	I	28	SER	3.2
2	B	68[A]	LEU	3.1
3	P	38	ASN	3.1
4	Q	147	LYS	3.0
2	O	90	ILE	3.0
9	I	15	ARG	3.0
12	Y	20	ARG	3.0
11	X	52	GLU	3.0
13	Z	32	TRP	3.0
11	X	23	THR	2.9
8	U	44	THR	2.9

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Mol	Chain	Res	Type	RSRZ
9	I	27	VAL	2.9
9	I	22	VAL	2.8
8	U	47	GLY	2.8
9	V	27	VAL	2.8
13	Z	35	TYR	2.7
2	O	226	MET	2.7
8	H	47	GLY	2.7
8	H	48	GLY	2.7
13	Z	39	ASN	2.7
9	I	32	ALA	2.6
9	V	73	LYS	2.6
7	T	4	ALA	2.6
6	S	3	GLY	2.6
7	G	7	ASP	2.6
2	B	91	ASN	2.6
4	Q	87	PHE	2.5
4	Q	9	GLU	2.5
8	U	11	TYR	2.5
13	Z	40	TYR	2.5
7	G	9	GLY	2.5
10	W	56	PRO	2.5
1	A	514	LYS	2.5
9	V	21	ILE	2.5
7	G	10	GLY	2.4
8	U	52	VAL	2.4
5	R	108	LYS	2.4
3	C	37	PHE	2.4
10	J	57	HIS	2.4
1	A	311[A]	ILE	2.3
2	O	33	LEU	2.3
9	I	36	LYS	2.3
12	Y	27	LEU	2.3
1	A	169[A]	ILE	2.3
9	V	18	ARG	2.3
7	G	39	SER	2.3
8	H	7	LYS	2.3
4	D	87	PHE	2.3
8	H	43	MET	2.3
4	D	5	VAL	2.3
8	U	55	TRP	2.3
9	V	38	ALA	2.3
1	N	514	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
6	S	43	LYS	2.2
3	C	38	ASN	2.2
4	Q	33	LEU	2.2
4	D	19	ARG	2.2
11	K	47	ARG	2.2
1	N	35[A]	LEU	2.2
4	Q	58	GLU	2.2
2	O	225	SER	2.1
3	C	33[A]	MET	2.1
8	U	46	LYS	2.1
8	H	42	ALA	2.1
7	G	45	PRO	2.1
9	V	65	LYS	2.1
12	Y	2	HIS	2.1
1	N	513	LEU	2.1
11	X	6	ALA	2.1
11	X	27	ALA	2.1
7	T	12	GLY	2.0
4	Q	140	TYR	2.0
12	Y	44	LEU	2.0
8	H	44	THR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.51	0.38	109,117,122,124	0
7	TPO	T	11	11/12	0.51	0.35	107,125,143,144	0
7	TPO	G	11	11/12	0.55	0.28	74,90,145,146	0
9	SAC	I	1	9/10	0.84	0.18	62,71,77,78	0
2	FME	B	1	10/11	0.94	0.14	32,35,51,58	0
1	FME	A	1	10/11	0.94	0.14	40,47,73,88	0
1	FME	N	1	10/11	0.96	0.12	47,55,88,93	0
2	FME	O	1	10/11	0.97	0.10	43,46,57,65	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
27	DMU	P	313	33/33	0.28	0.32	84,143,147,148	0
20	EDO	M	103	4/4	0.48	0.24	113,116,116,117	0
27	DMU	C	313	33/33	0.55	0.52	76,136,146,147	0
25	PEK	C	304	53/53	0.57	0.24	45,80,138,146	0
27	DMU	W	104	33/33	0.60	0.43	78,131,146,146	0
26	CDL	T	103	100/100	0.65	0.28	56,83,115,139	0
27	DMU	C	312	33/33	0.66	0.23	83,116,143,145	0
20	EDO	L	102	4/4	0.66	0.30	86,90,91,91	0
20	EDO	T	105	4/4	0.66	0.88	144,145,145,145	4
20	EDO	W	102	4/4	0.67	0.42	103,107,108,109	0
21	TGL	Q	201	63/63	0.69	0.21	56,76,92,95	0
26	CDL	G	101	100/100	0.69	0.32	58,89,138,147	0
25	PEK	T	102	53/53	0.70	0.23	39,77,126,137	0
25	PEK	T	101	53/53	0.71	0.27	51,87,142,148	0
23	PSC	B	303	52/52	0.72	0.33	45,83,142,149	0
20	EDO	L	104	4/4	0.73	0.24	97,97,98,99	0
20	EDO	Y	101	4/4	0.73	0.28	96,97,99,100	0
21	TGL	N	606	63/63	0.74	0.26	49,73,104,120	0
25	PEK	G	103	53/53	0.74	0.24	52,87,125,139	0
26	CDL	P	305	100/100	0.74	0.28	45,82,111,117	0
17	NA	C	302	1/1	0.75	0.27	53,53,53,53	0
26	CDL	C	307	100/100	0.75	0.29	41,74,102,117	0
18	PGV	U	101	51/51	0.75	0.24	48,83,126,143	0
24	CHD	W	101	29/29	0.76	0.31	62,72,98,102	0
20	EDO	H	101	4/4	0.78	0.21	75,75,77,78	0
24	CHD	J	101	29/29	0.78	0.24	53,65,103,108	0
20	EDO	C	311	4/4	0.79	0.24	48,56,58,61	0
20	EDO	P	307	4/4	0.79	0.38	89,96,96,98	0
20	EDO	A	619	4/4	0.79	0.63	81,83,87,89	4
18	PGV	N	607	51/51	0.79	0.31	49,81,128,140	0
21	TGL	D	201	63/63	0.79	0.17	46,68,87,89	0
20	EDO	W	103	4/4	0.80	0.17	72,78,78,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
21	TGL	L	101	63/63	0.80	0.23	37,59,92,99	0
20	EDO	N	613	4/4	0.80	0.36	85,92,94,99	0
20	EDO	L	105	4/4	0.80	0.22	85,86,87,87	0
20	EDO	P	309	4/4	0.80	0.22	88,91,92,95	0
20	EDO	L	103	4/4	0.80	0.28	45,61,62,66	0
20	EDO	P	312	4/4	0.80	0.15	57,65,67,67	0
20	EDO	B	309	4/4	0.81	0.17	42,52,53,55	0
18	PGV	C	306	51/51	0.81	0.20	45,73,111,133	0
23	PSC	O	303	52/52	0.82	0.24	40,76,138,147	0
20	EDO	A	611	4/4	0.82	0.22	70,77,78,81	0
20	EDO	A	618	4/4	0.83	0.18	55,58,59,61	0
17	NA	P	302	1/1	0.83	0.19	49,49,49,49	0
18	PGV	A	606	51/51	0.84	0.23	35,74,106,132	0
21	TGL	B	301	63/63	0.84	0.21	36,69,89,100	0
21	TGL	O	301	63/63	0.85	0.21	50,76,98,105	0
20	EDO	R	204	4/4	0.85	0.30	55,63,67,67	0
27	DMU	Z	101	33/33	0.86	0.20	55,66,92,94	0
20	EDO	P	310	4/4	0.87	0.24	86,90,94,97	0
20	EDO	A	609	4/4	0.87	0.23	45,51,52,53	0
20	EDO	R	202	4/4	0.88	0.25	88,90,90,94	0
20	EDO	R	203	4/4	0.88	0.36	90,92,93,95	0
20	EDO	B	308	4/4	0.88	0.22	88,89,93,97	0
20	EDO	B	306	4/4	0.88	0.20	47,52,54,55	0
20	EDO	M	102	4/4	0.88	0.17	83,84,85,85	0
20	EDO	A	615	4/4	0.89	0.35	64,67,70,72	0
20	EDO	S	104	4/4	0.89	0.26	74,75,77,80	0
20	EDO	P	308	4/4	0.89	0.23	97,100,100,102	0
20	EDO	N	614	4/4	0.90	0.16	52,53,56,57	0
20	EDO	T	104	4/4	0.90	0.23	98,101,103,104	0
24	CHD	P	306	29/29	0.90	0.16	45,55,61,76	0
20	EDO	A	616	4/4	0.90	0.17	85,86,89,93	0
27	DMU	M	101	33/33	0.90	0.12	44,51,71,86	0
20	EDO	Q	202	4/4	0.90	0.22	43,54,59,68	0
20	EDO	B	307	4/4	0.92	0.15	50,54,56,58	0
20	EDO	A	610	4/4	0.92	0.16	36,39,39,40	0
20	EDO	A	617	4/4	0.93	0.15	38,44,48,49	0
16	MG	N	604	1/1	0.93	0.19	39,39,39,39	0
24	CHD	C	308	29/29	0.93	0.15	48,54,65,67	0
20	EDO	C	309	4/4	0.93	0.18	41,47,51,54	0
20	EDO	P	311	4/4	0.93	0.17	48,49,51,52	0
20	EDO	N	612	4/4	0.94	0.15	58,62,66,66	0
20	EDO	A	614	4/4	0.95	0.22	73,73,76,77	0

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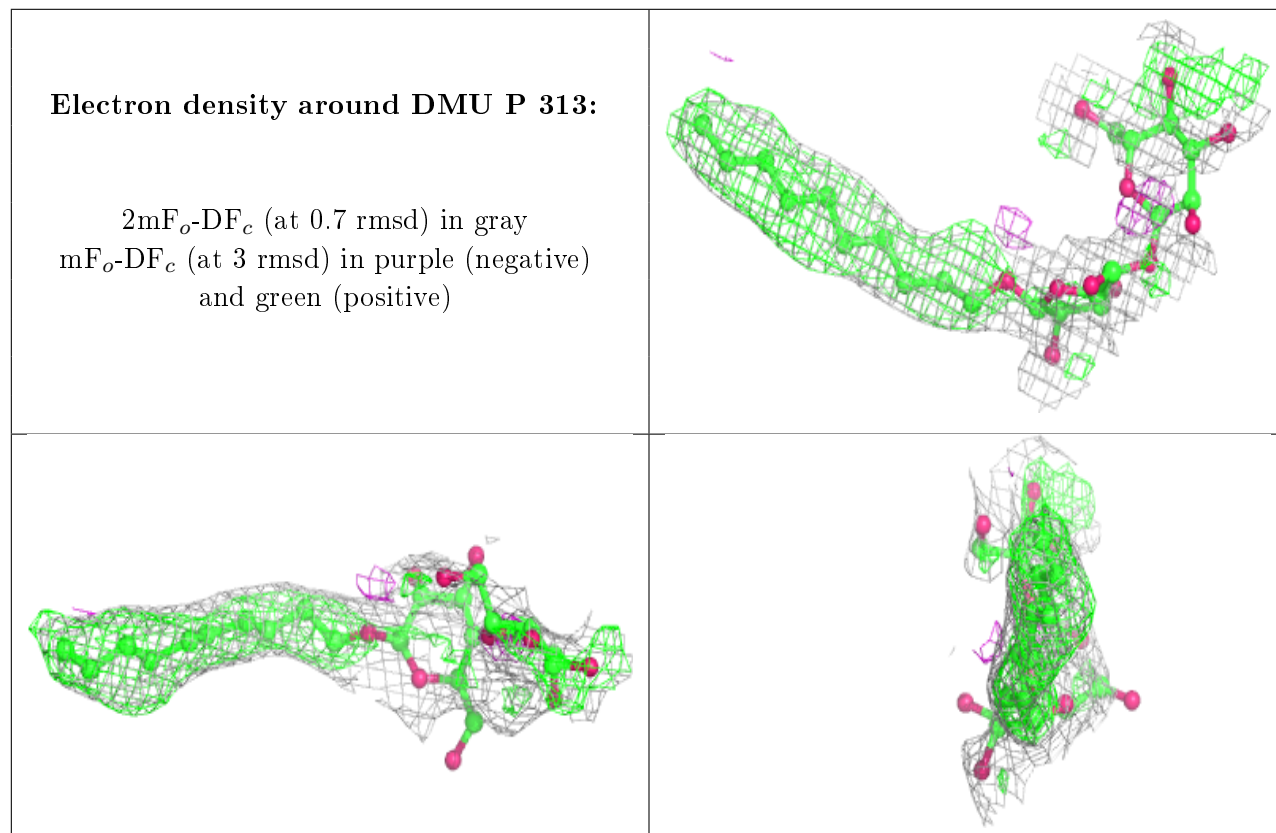
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
20	EDO	A	612	4/4	0.95	0.32	54,63,64,64	0
20	EDO	S	102	4/4	0.95	0.12	31,33,33,34	0
20	EDO	S	103	4/4	0.95	0.11	44,44,46,46	0
20	EDO	J	102	4/4	0.95	0.21	55,65,65,67	0
20	EDO	N	611	4/4	0.95	0.13	34,35,38,39	0
24	CHD	B	304	29/29	0.96	0.11	29,32,35,41	0
20	EDO	R	201	4/4	0.96	0.19	49,49,49,52	0
20	EDO	F	102	4/4	0.96	0.14	29,30,30,32	0
20	EDO	A	613	4/4	0.96	0.13	28,28,32,32	0
24	CHD	C	301	29/29	0.96	0.09	28,31,35,36	0
20	EDO	C	310	4/4	0.96	0.09	39,43,43,43	0
20	EDO	N	610	4/4	0.96	0.12	40,40,42,42	0
20	EDO	F	103	4/4	0.96	0.14	43,45,45,46	0
20	EDO	O	304	4/4	0.97	0.12	44,46,48,48	0
24	CHD	P	301	29/29	0.97	0.10	30,33,36,39	0
25	PEK	P	303	53/53	0.97	0.15	30,49,94,97	0
25	PEK	C	303	53/53	0.97	0.15	30,47,86,95	0
20	EDO	G	104	4/4	0.97	0.11	37,39,40,40	0
20	EDO	E	201	4/4	0.97	0.10	48,49,51,51	0
14	HEA	N	602	60/60	0.98	0.11	25,29,34,37	0
14	HEA	A	601[B]	60/60	0.98	0.12	22,26,33,38	9
14	HEA	N	601[A]	60/60	0.98	0.12	28,34,43,49	9
20	EDO	B	305	4/4	0.98	0.12	34,36,36,37	0
18	PGV	P	304	51/51	0.98	0.13	31,40,70,78	0
22	CUA	O	302	2/2	0.98	0.14	39,39,39,39	0
14	HEA	N	601[B]	60/60	0.98	0.12	28,33,39,41	9
18	PGV	C	305	51/51	0.98	0.13	29,34,81,94	0
18	PGV	N	609	51/51	0.98	0.13	30,43,65,70	0
18	PGV	A	608	51/51	0.98	0.13	27,38,61,65	0
24	CHD	G	102	29/29	0.98	0.11	29,32,34,42	0
14	HEA	A	601[A]	60/60	0.98	0.12	22,26,38,41	9
16	MG	A	604	1/1	0.98	0.17	30,30,30,30	0
17	NA	N	605	1/1	0.99	0.07	41,41,41,41	0
22	CUA	B	302	2/2	0.99	0.16	29,29,29,30	0
14	HEA	A	602	60/60	0.99	0.10	21,25,30,34	0
19	PER	N	608[A]	2/2	1.00	0.17	28,28,28,31	0
15	CU	A	603	1/1	1.00	0.17	27,27,27,27	0
19	PER	A	607[A]	2/2	1.00	0.17	24,24,24,25	0
28	ZN	S	101	1/1	1.00	0.13	37,37,37,37	0
28	ZN	F	101	1/1	1.00	0.15	35,35,35,35	0
19	PER	N	608[B]	2/2	1.00	0.17	15,15,15,16	2
15	CU	N	603	1/1	1.00	0.18	31,31,31,31	0

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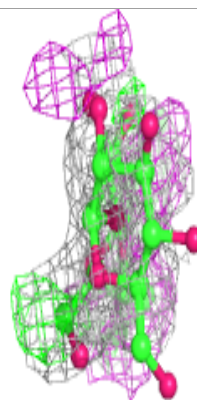
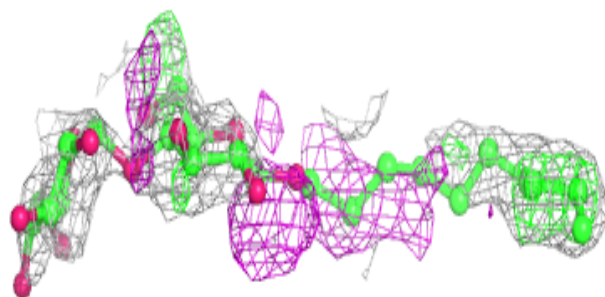
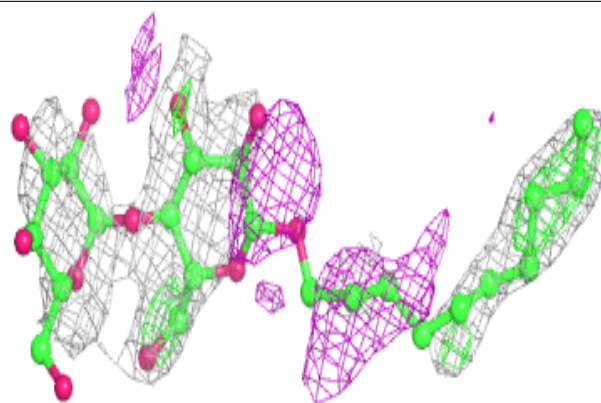
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
17	NA	A	605	1/1	1.00	0.09	30,30,30,30	0
19	PER	A	607[B]	2/2	1.00	0.17	6,6,6,6	2

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.



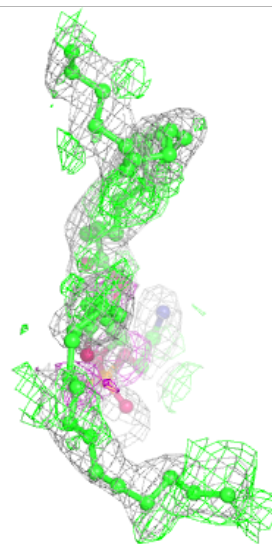
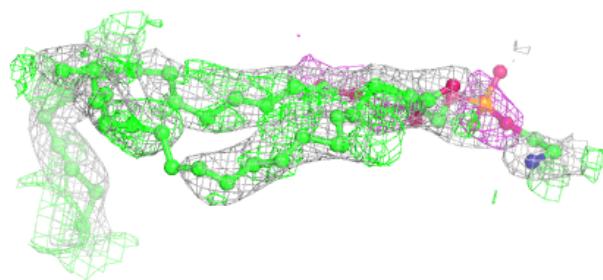
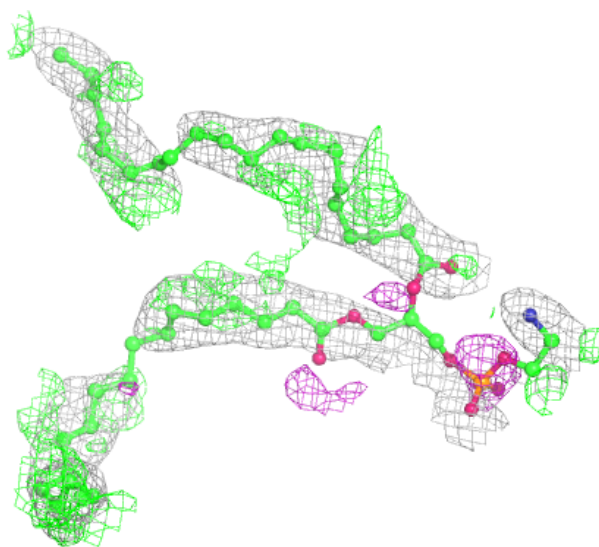
**Electron density around DMU C 313:**

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



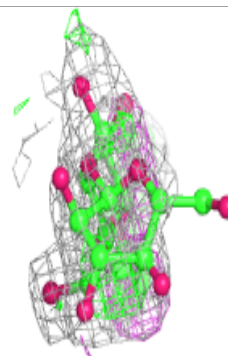
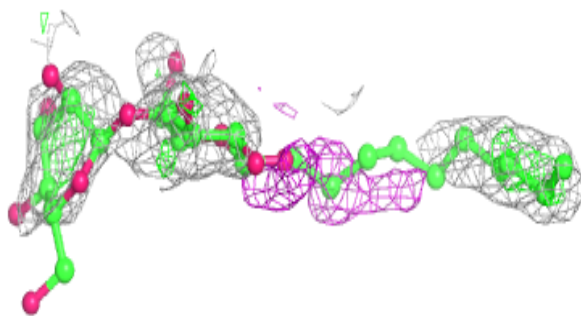
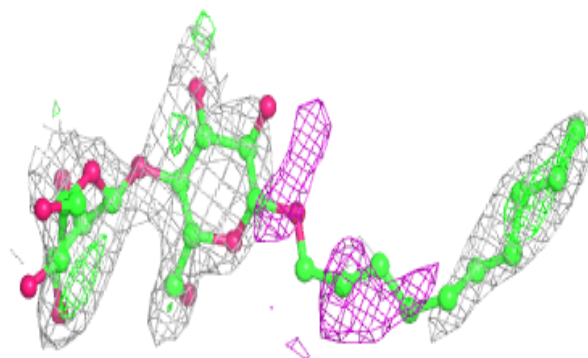
**Electron density around PEK C 304:**

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and green (positive)

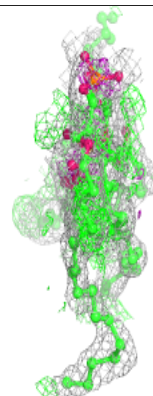
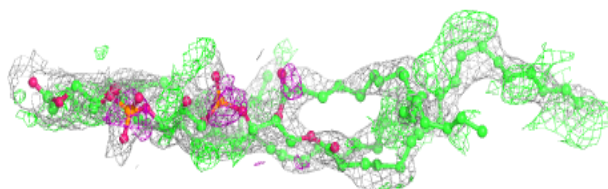
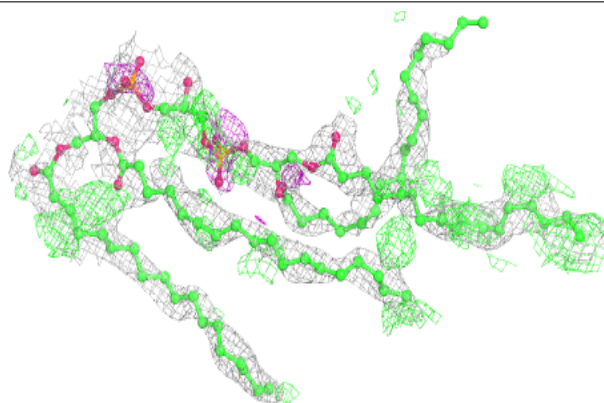


**Electron density around DMU W 104:**

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

**Electron density around CDL T 103:**

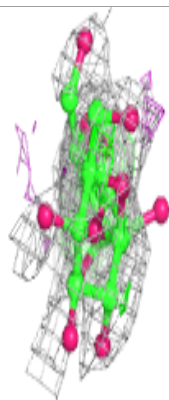
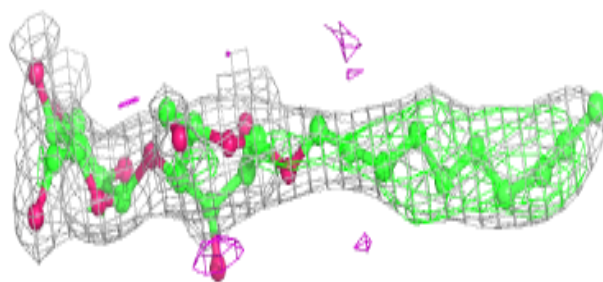
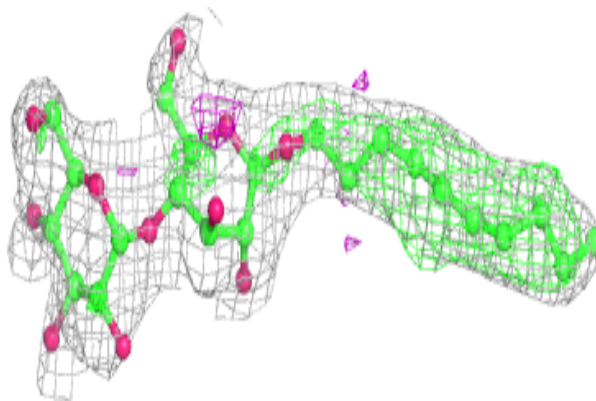
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



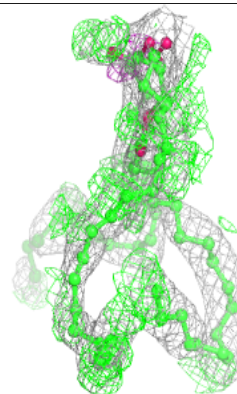
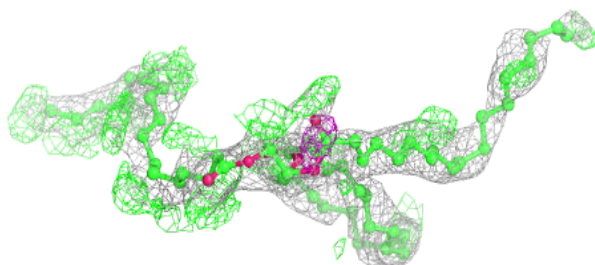
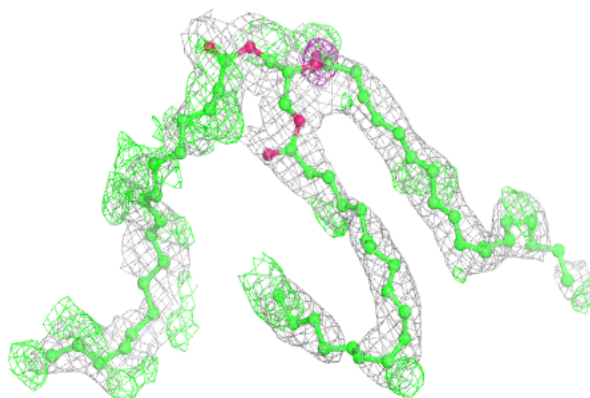


**Electron density around DMU C 312:**

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

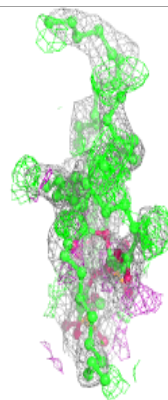
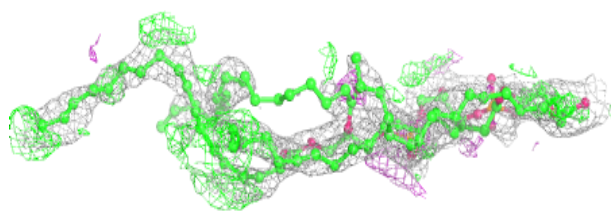
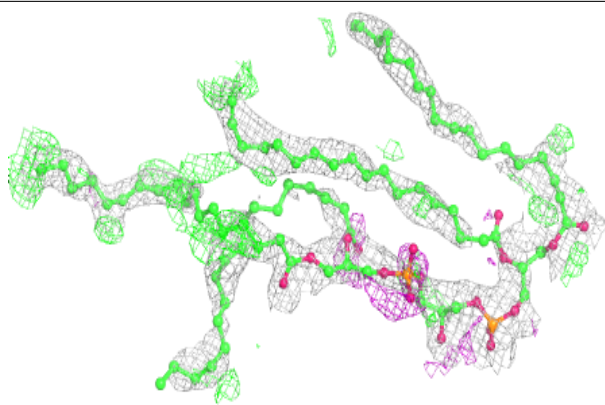
**Electron density around TGL Q 201:**

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



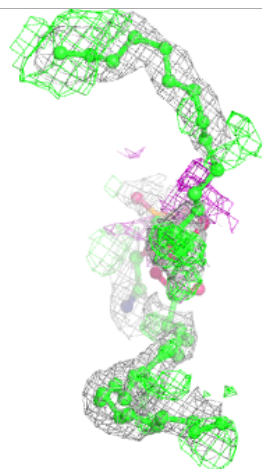
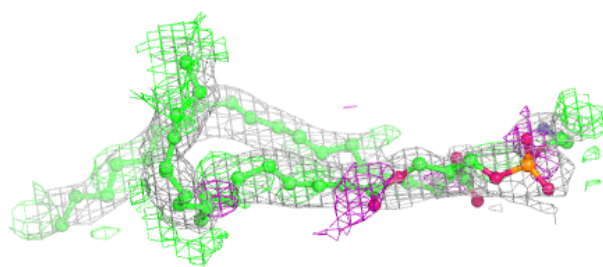
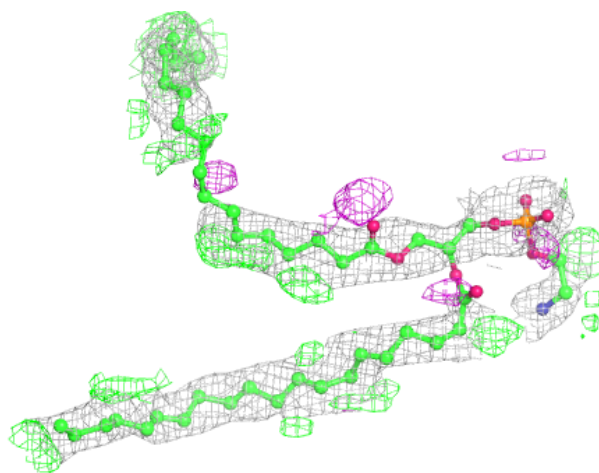
**Electron density around CDL G 101:**

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



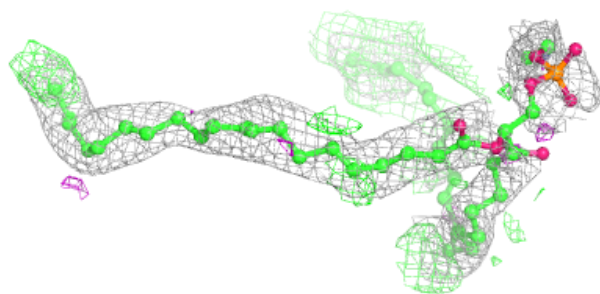
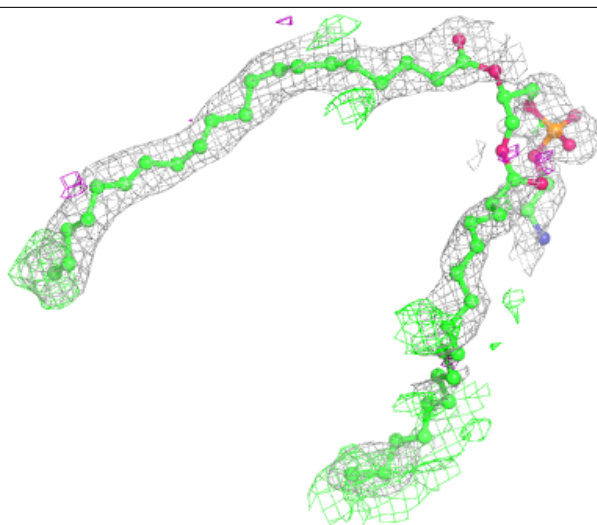
**Electron density around PEK T 102:**

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



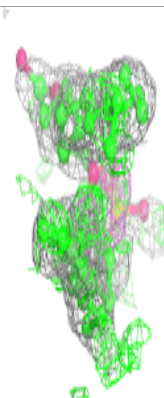
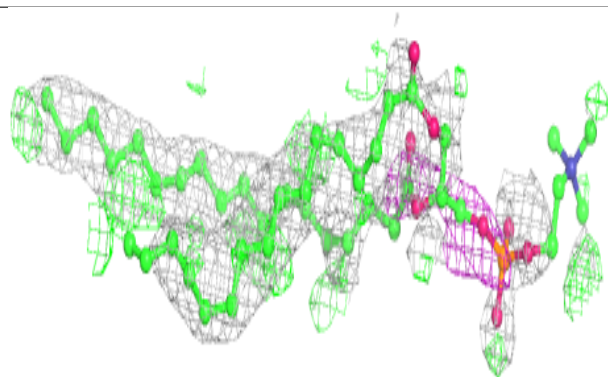
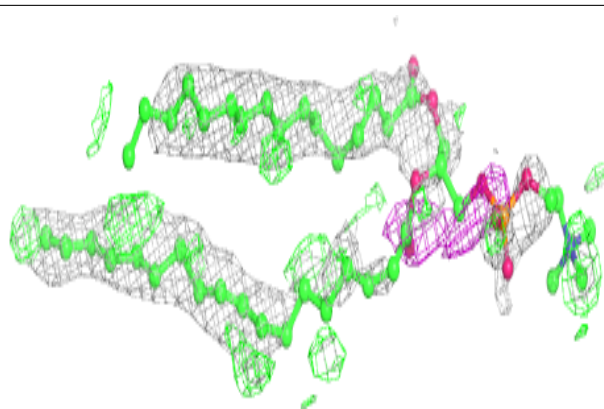
**Electron density around PEK T 101:**

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



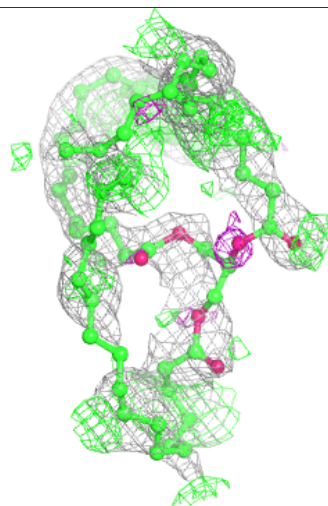
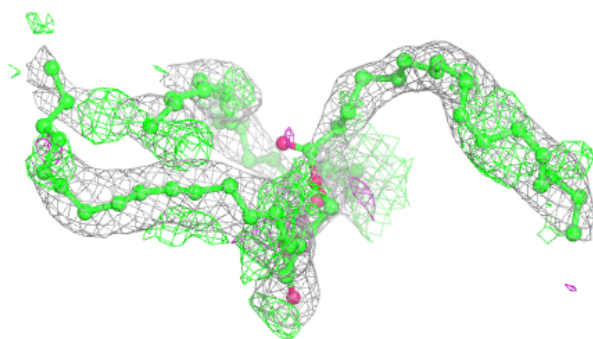
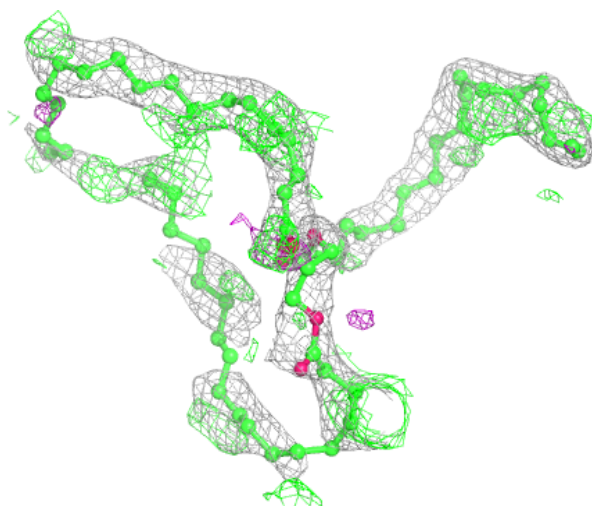
**Electron density around PSC B 303:**

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



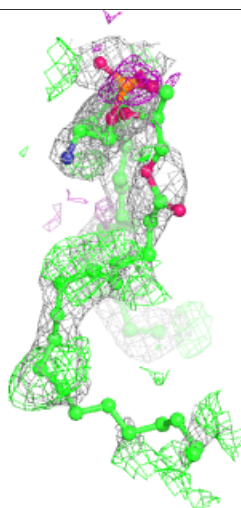
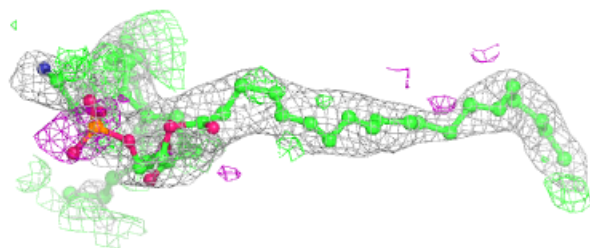
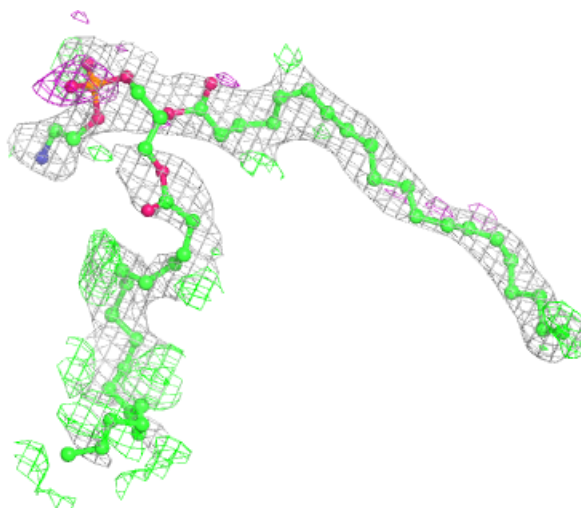
**Electron density around TGL N 606:**

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



**Electron density around PEK G 103:**

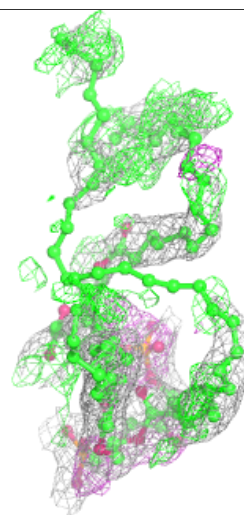
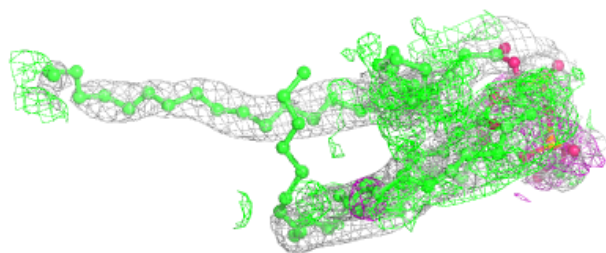
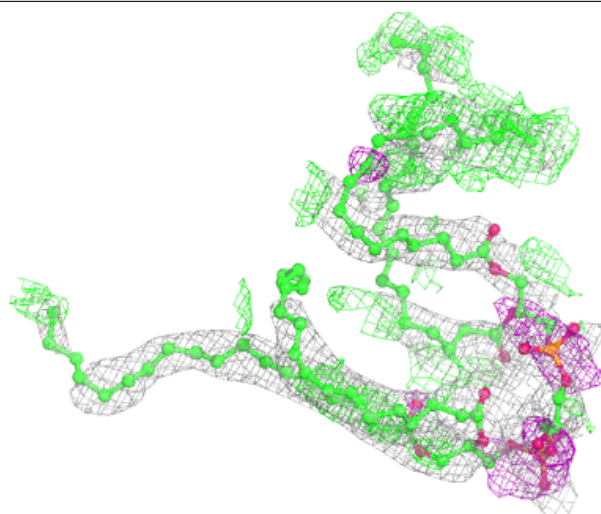
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around CDL P 305:**

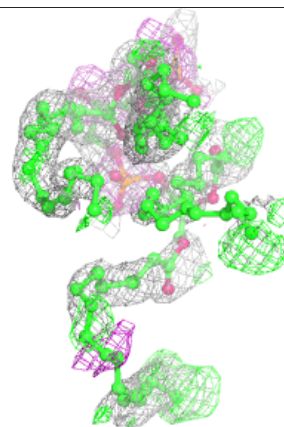
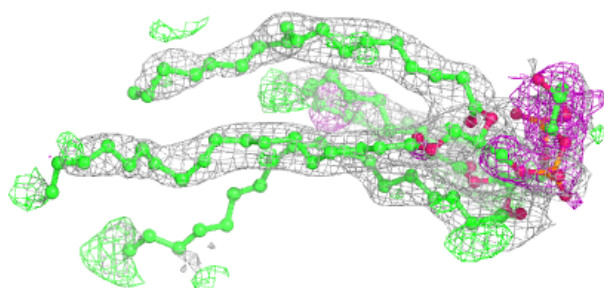
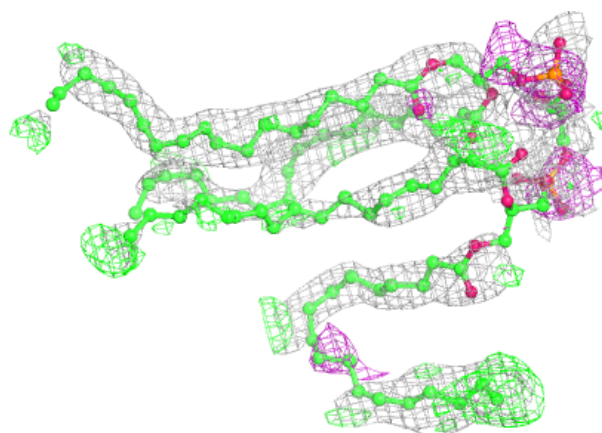
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



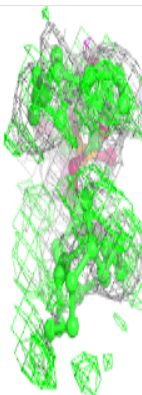
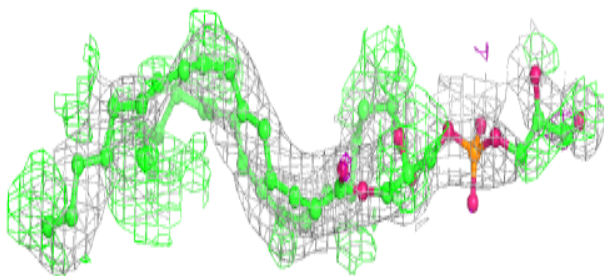
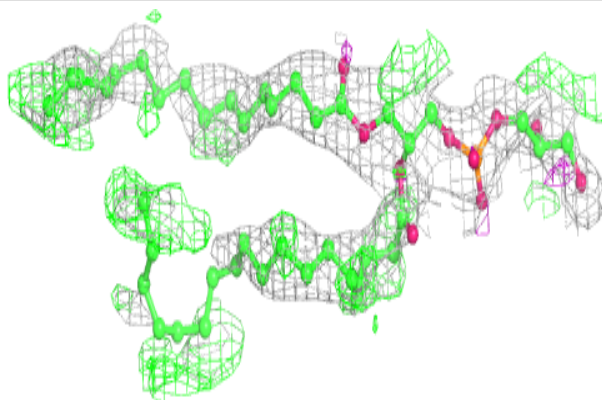


**Electron density around CDL C 307:**

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

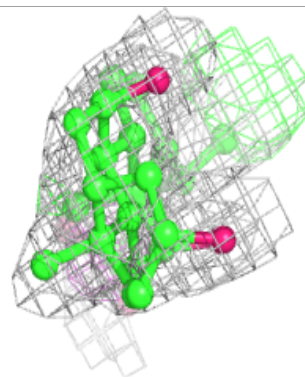
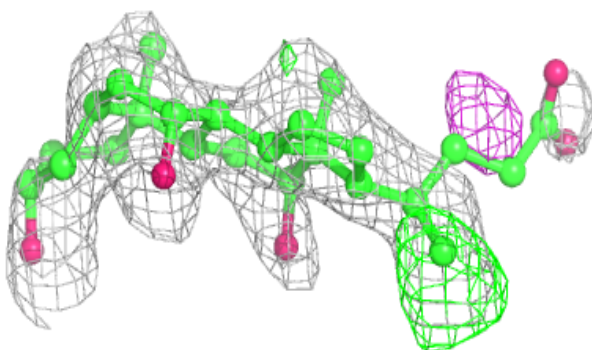
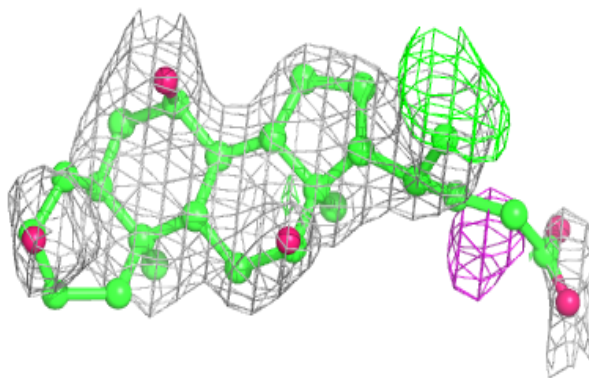
**Electron density around PGV U 101:**

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

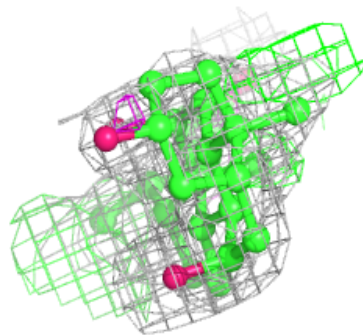
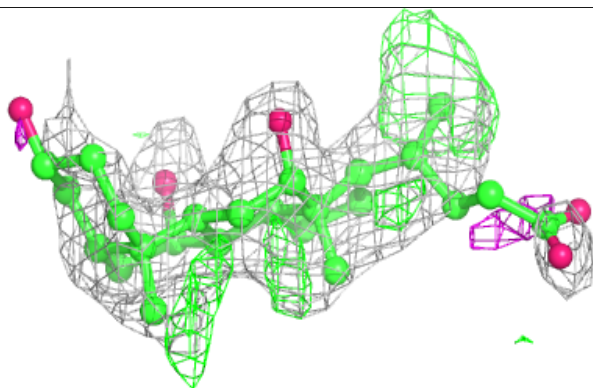
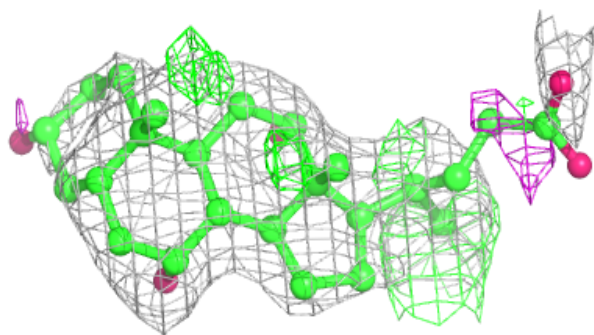


**Electron density around CHD W 101:**

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

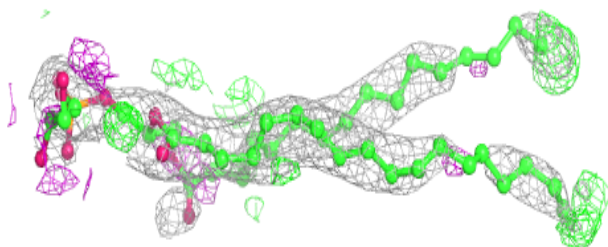
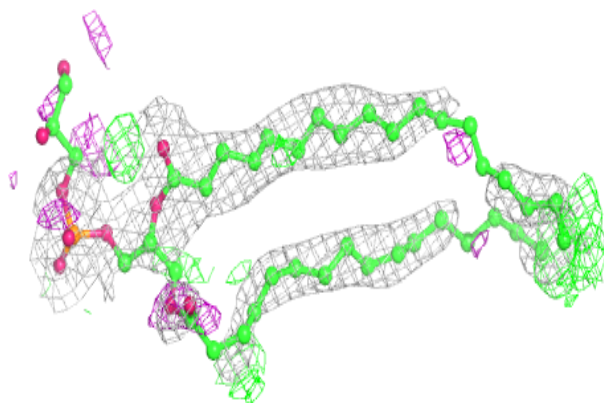
**Electron density around CHD J 101:**

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

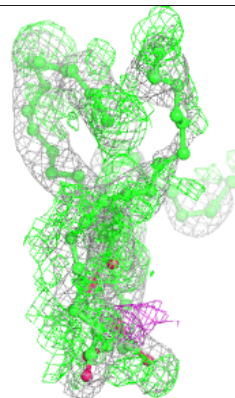
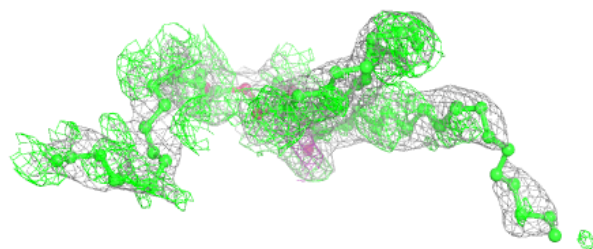
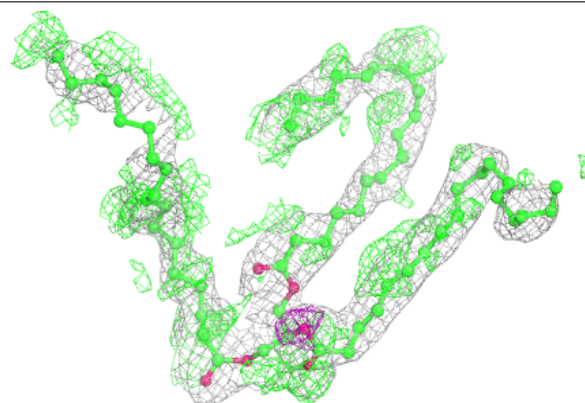


**Electron density around PGV N 607:**

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

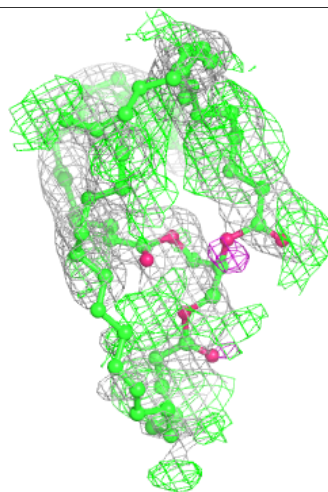
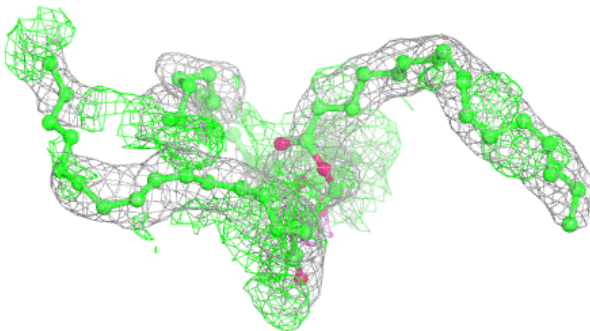
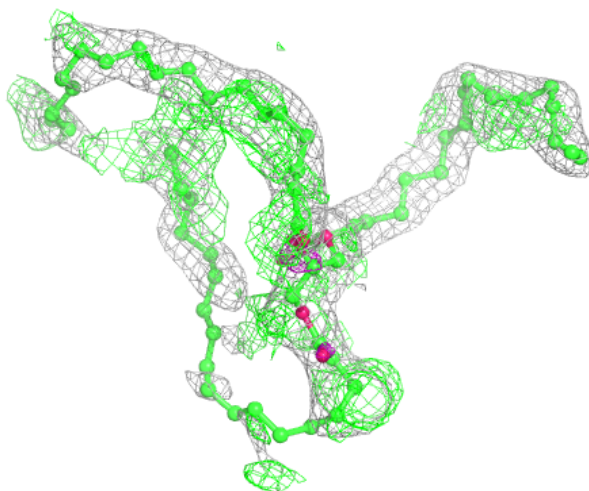
**Electron density around TGL D 201:**

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



**Electron density around TGL L 101:**

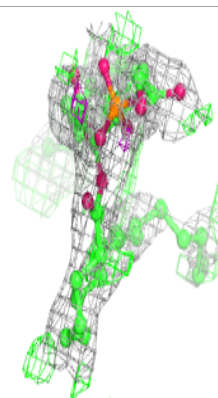
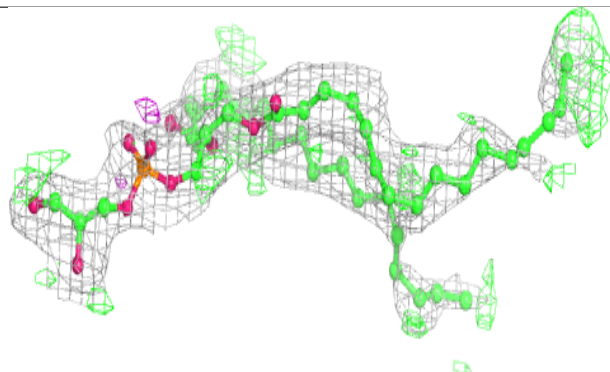
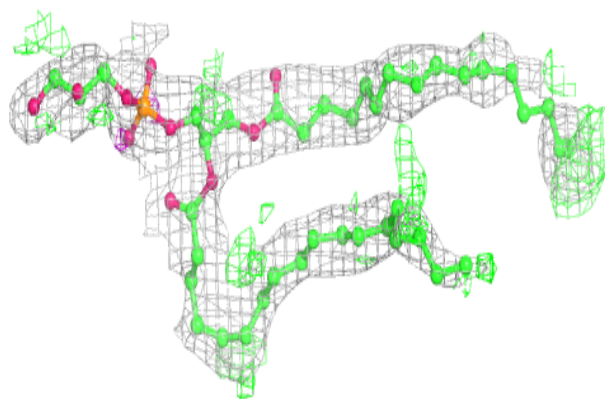
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



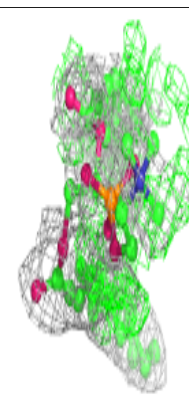
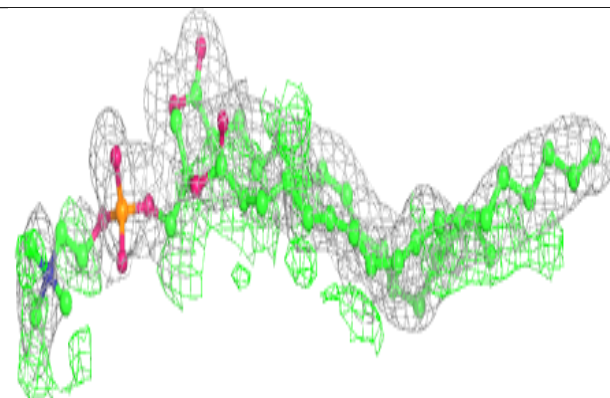
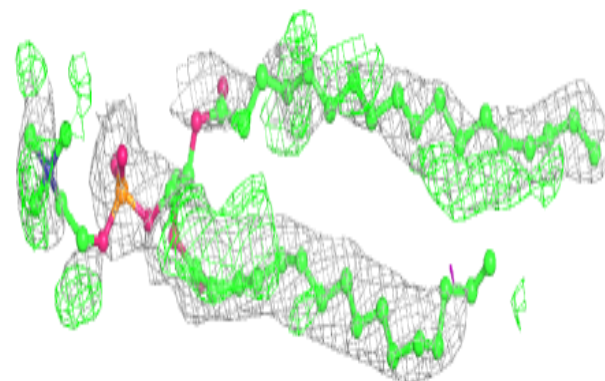


**Electron density around PGV C 306:**

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

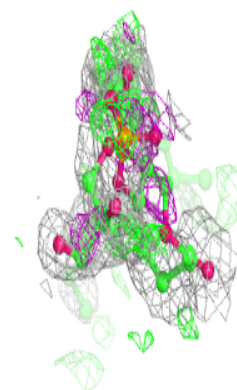
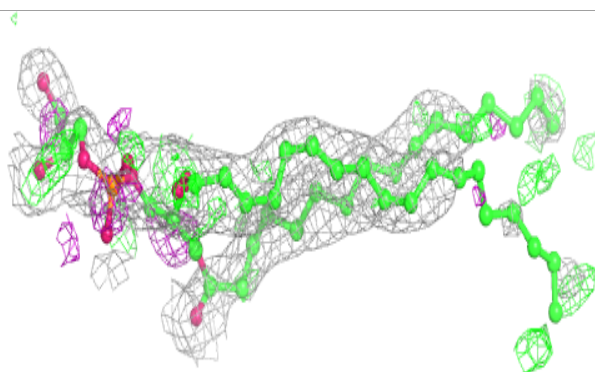
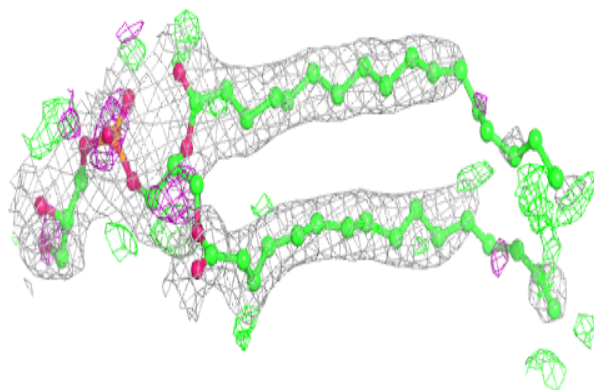
**Electron density around PSC O 303:**

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

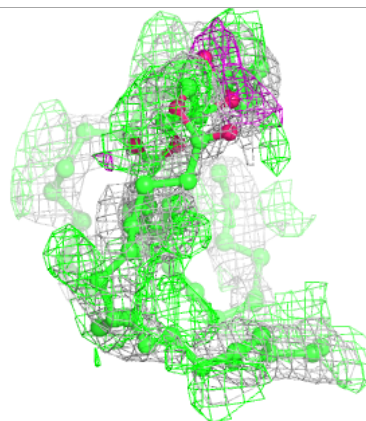
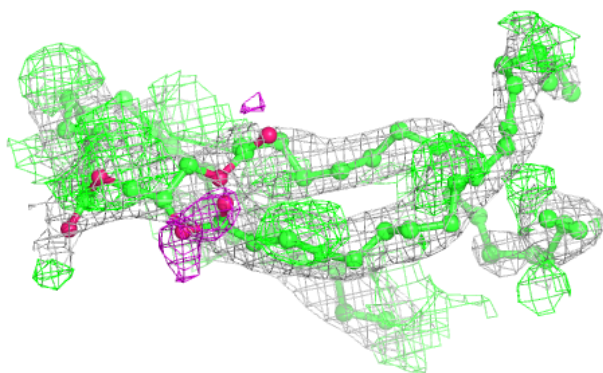
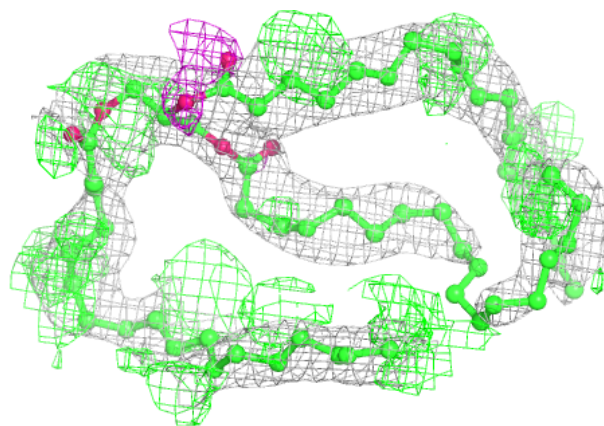


**Electron density around PGV A 606:**

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

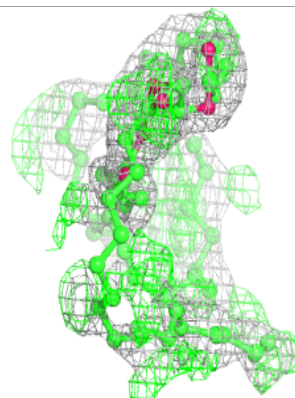
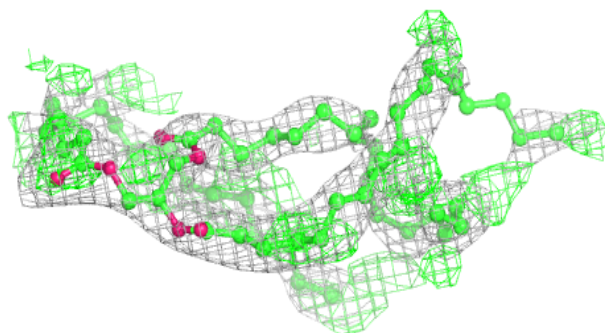
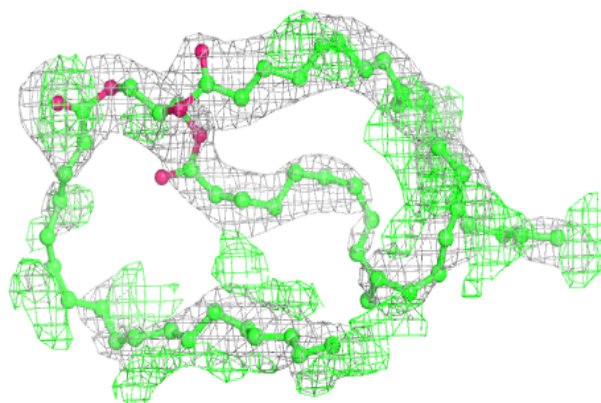
**Electron density around TGL B 301:**

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

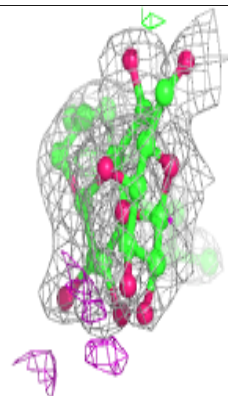
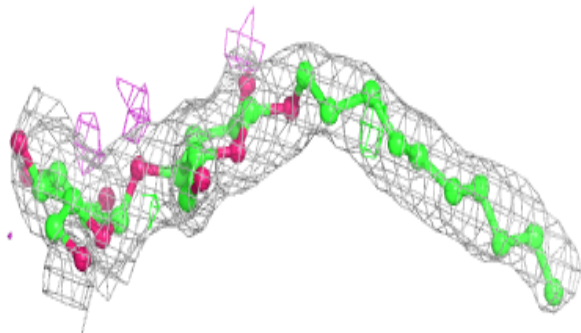
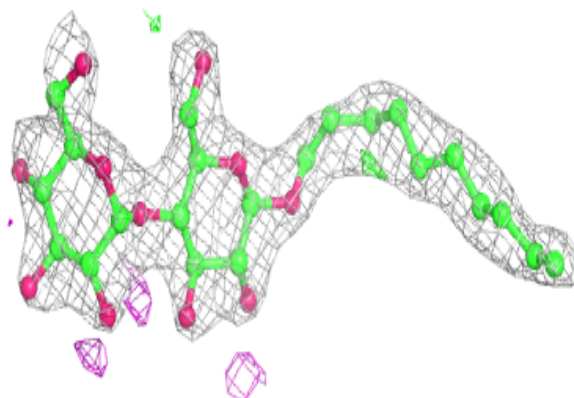


**Electron density around TGL O 301:**

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

**Electron density around DMU Z 101:**

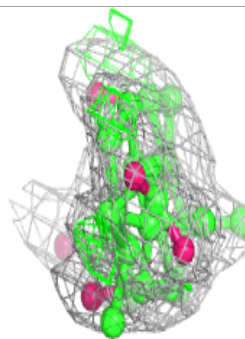
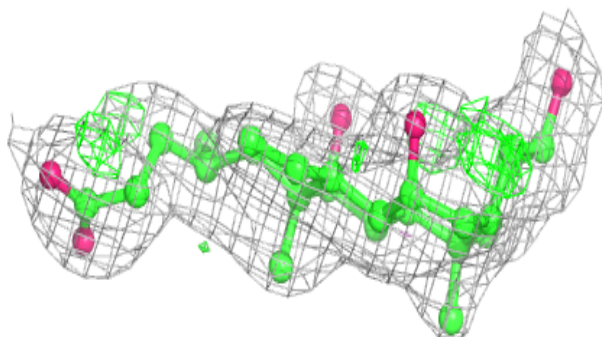
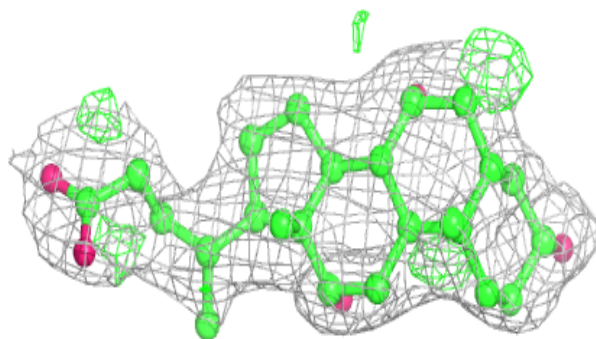
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



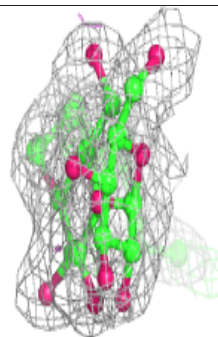
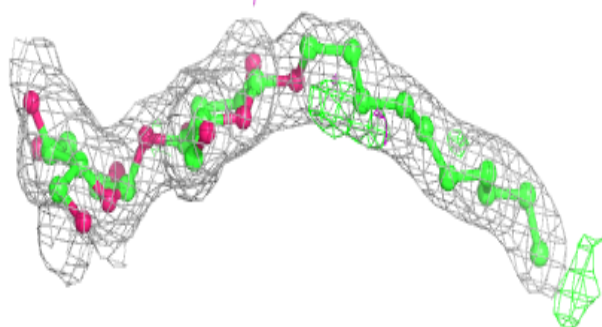
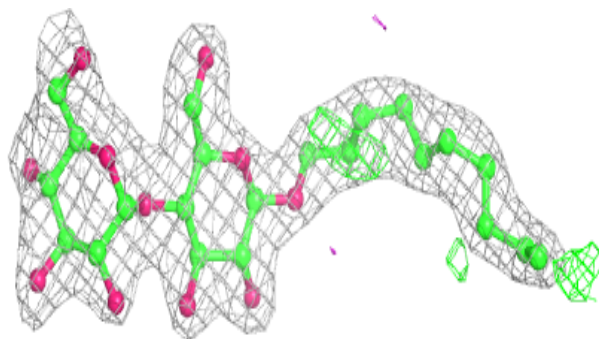


**Electron density around CHD P 306:**

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

**Electron density around DMU M 101:**

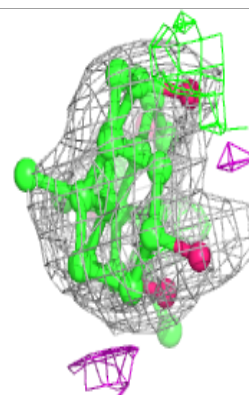
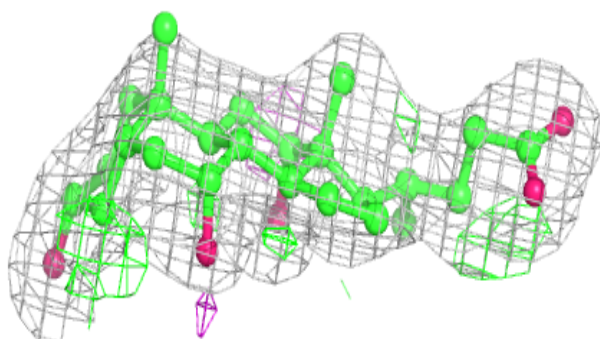
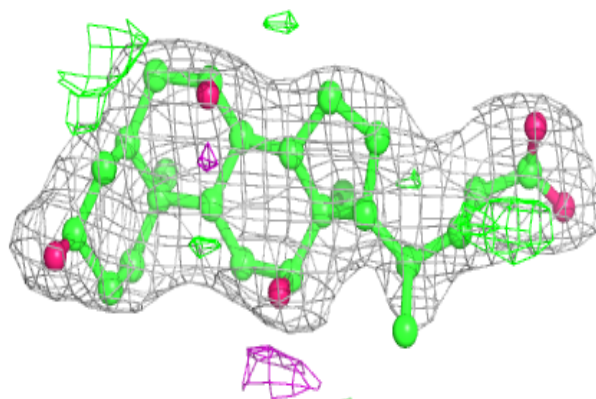
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



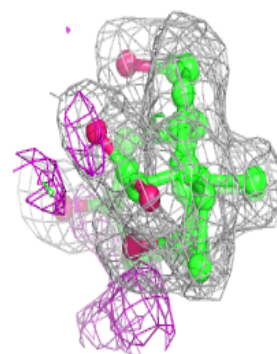
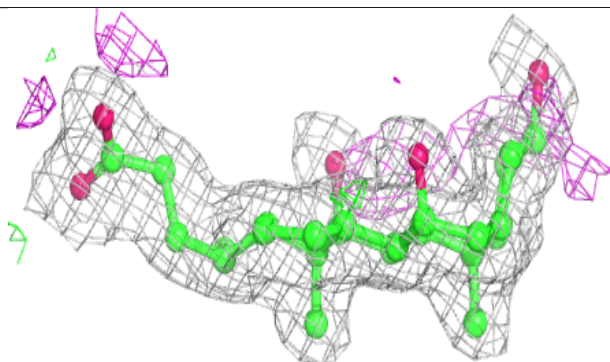
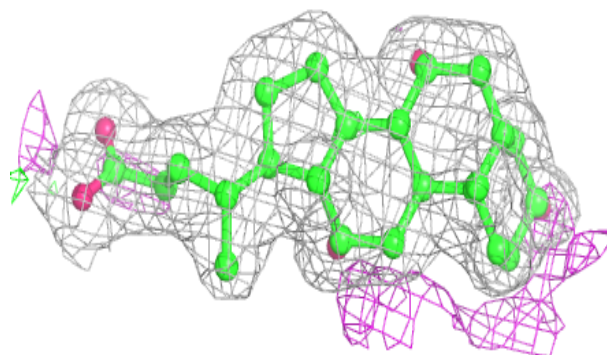


**Electron density around CHD C 308:**

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

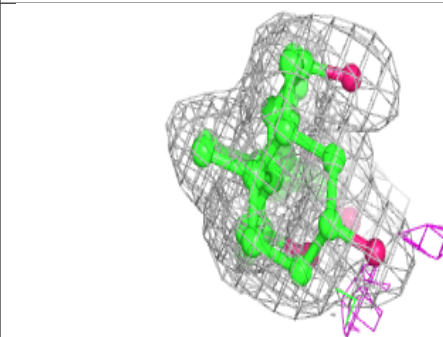
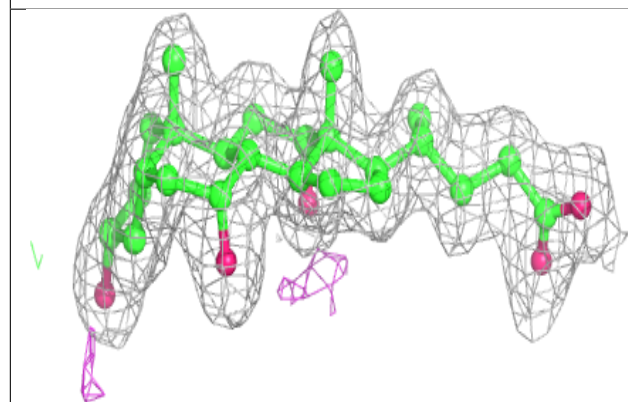
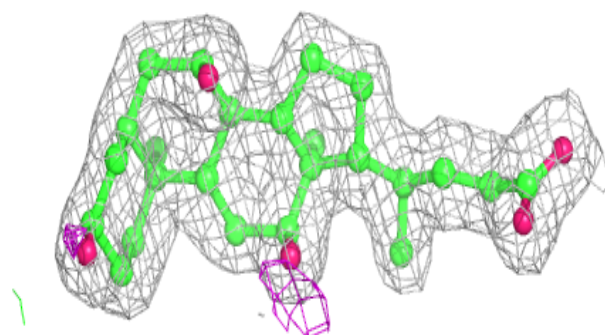
**Electron density around CHD B 304:**

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

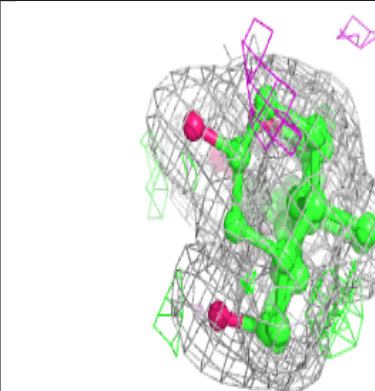
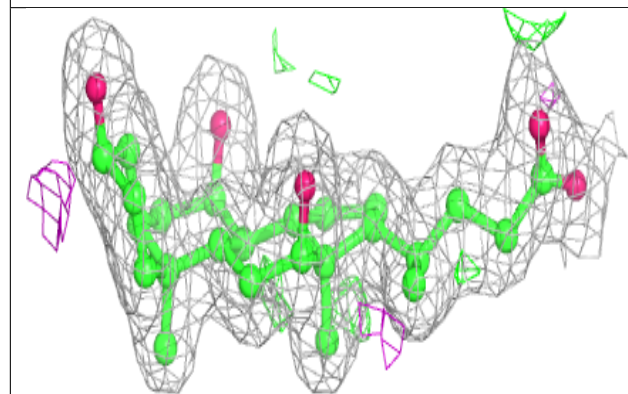
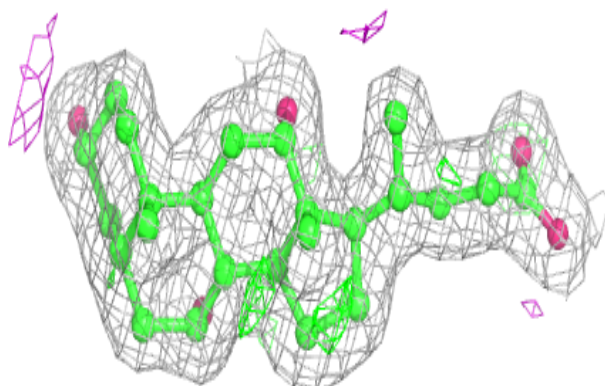


**Electron density around CHD C 301:**

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

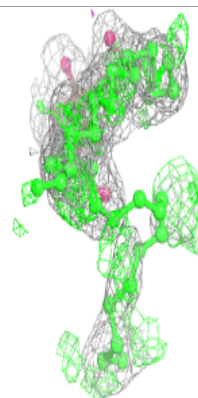
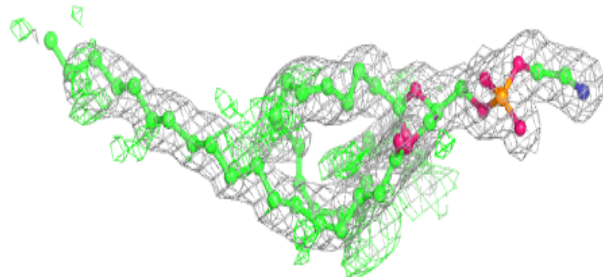
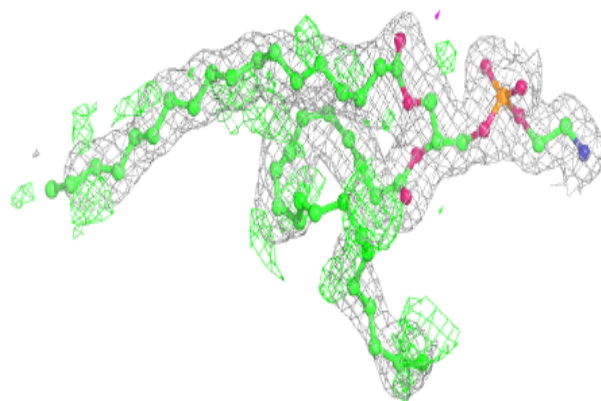
**Electron density around CHD P 301:**

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

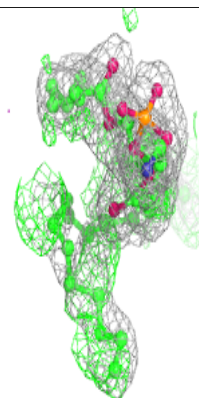
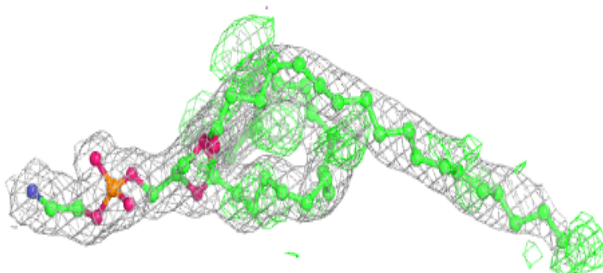
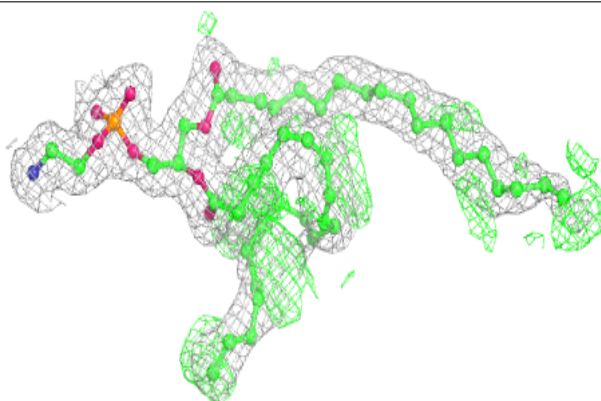


**Electron density around PEK P 303:**

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

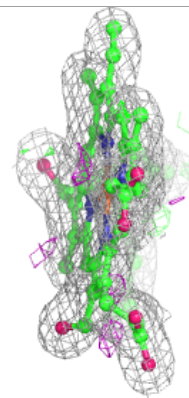
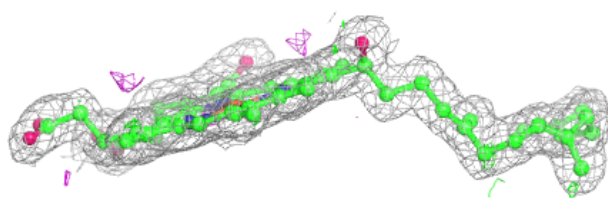
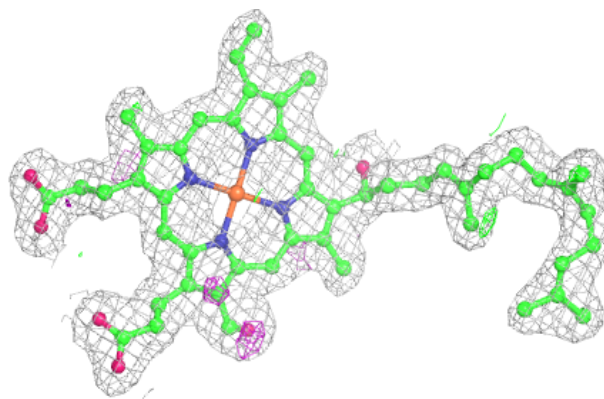
**Electron density around PEK C 303:**

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

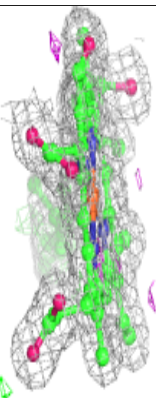
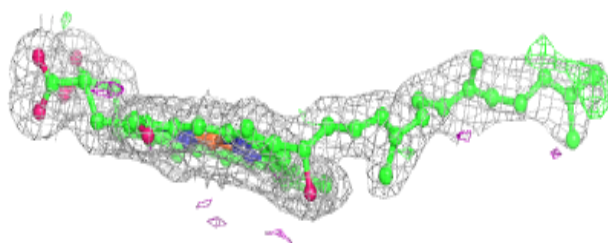
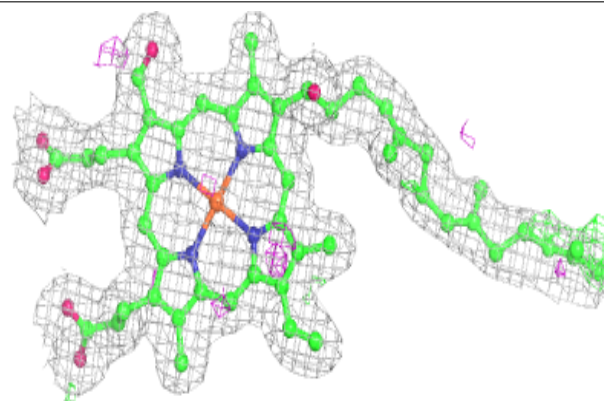


**Electron density around HEA N 602:**

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

**Electron density around HEA A 601 (B):**

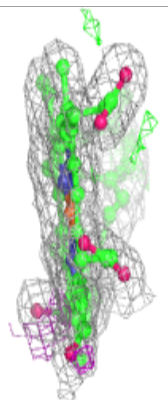
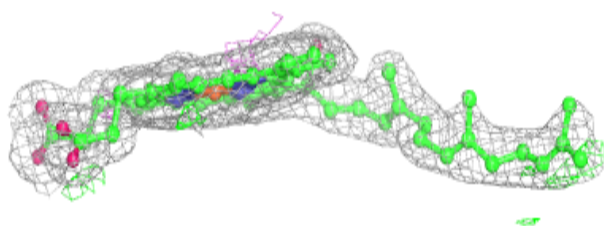
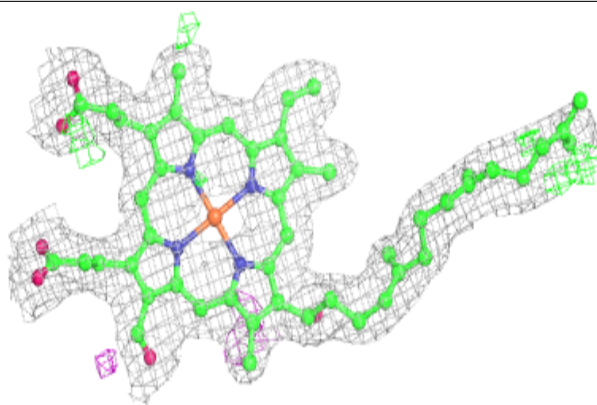
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



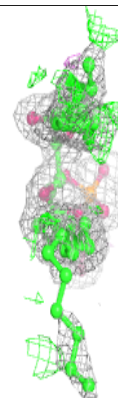
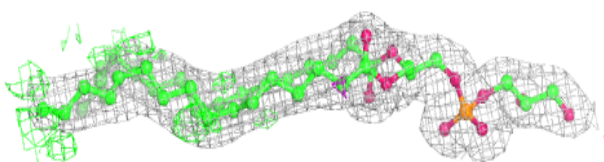
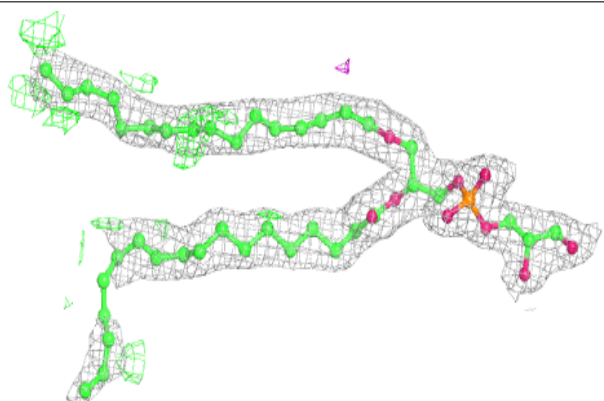


**Electron density around HEA N 601 (A):**

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

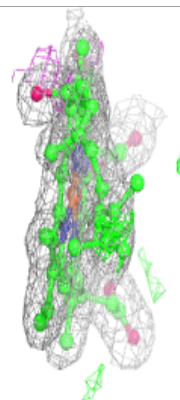
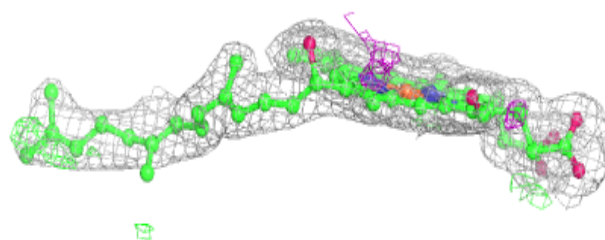
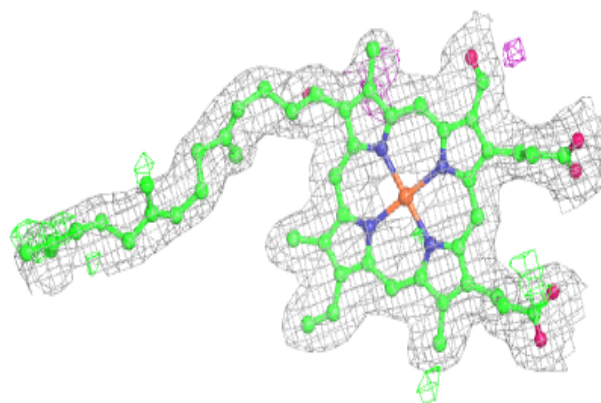
**Electron density around PGV P 304:**

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

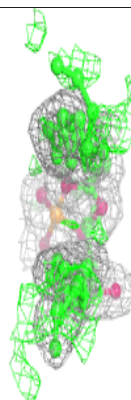
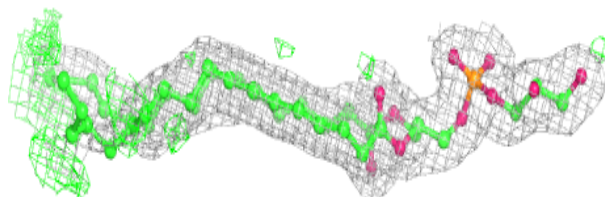
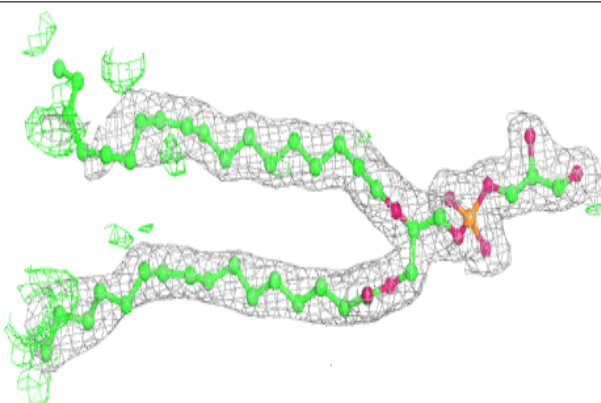


**Electron density around HEA N 601 (B):**

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

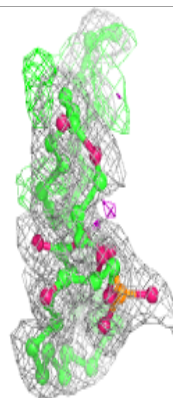
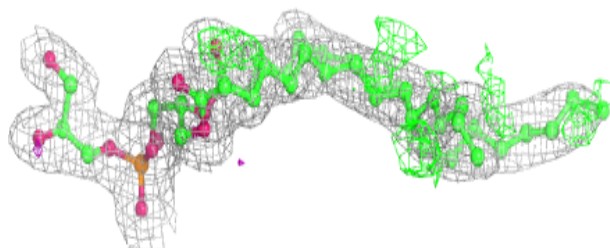
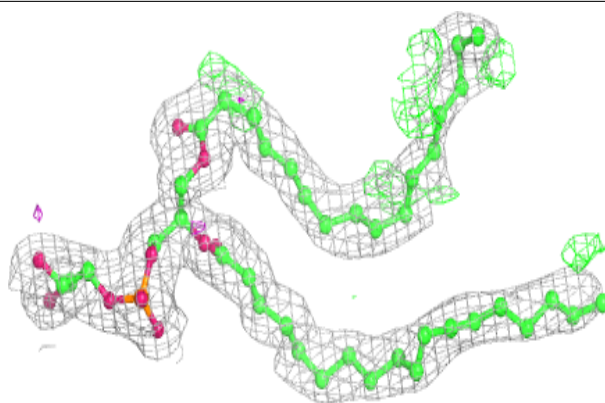
**Electron density around PGV C 305:**

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

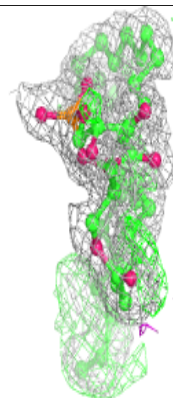
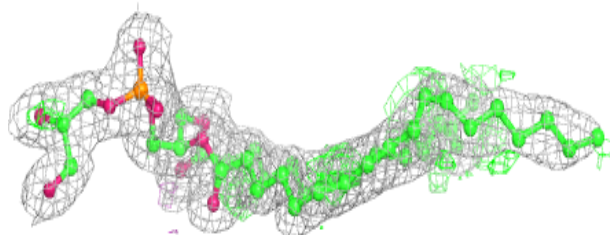
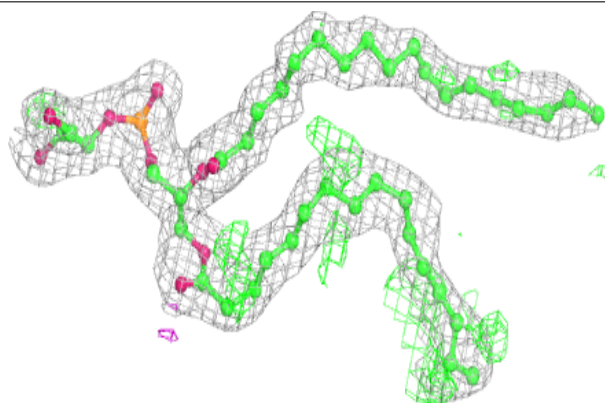


**Electron density around PGV N 609:**

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

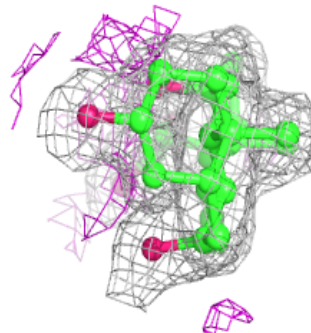
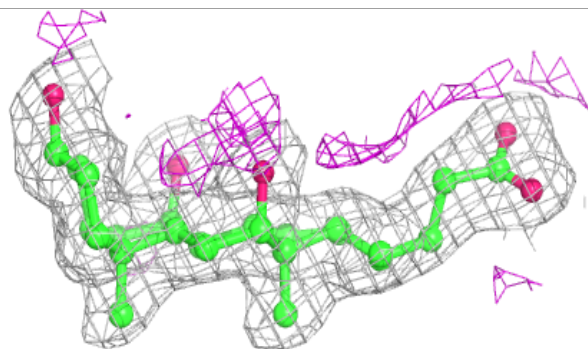
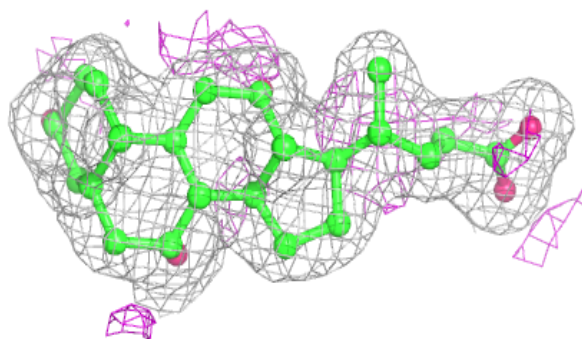
**Electron density around PGV A 608:**

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

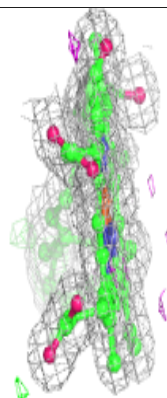
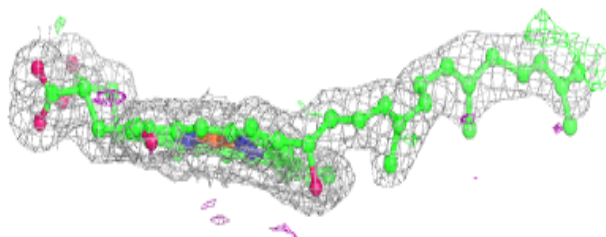
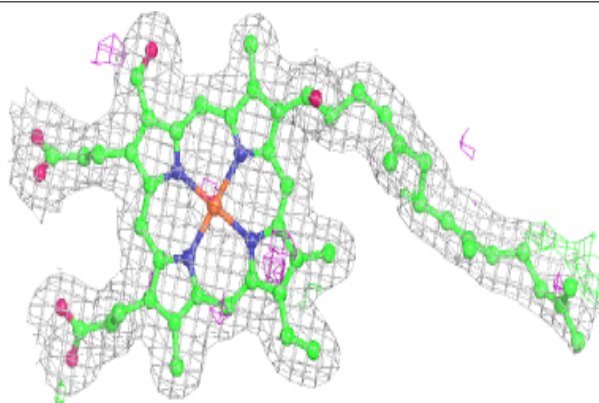


**Electron density around CHD G 102:**

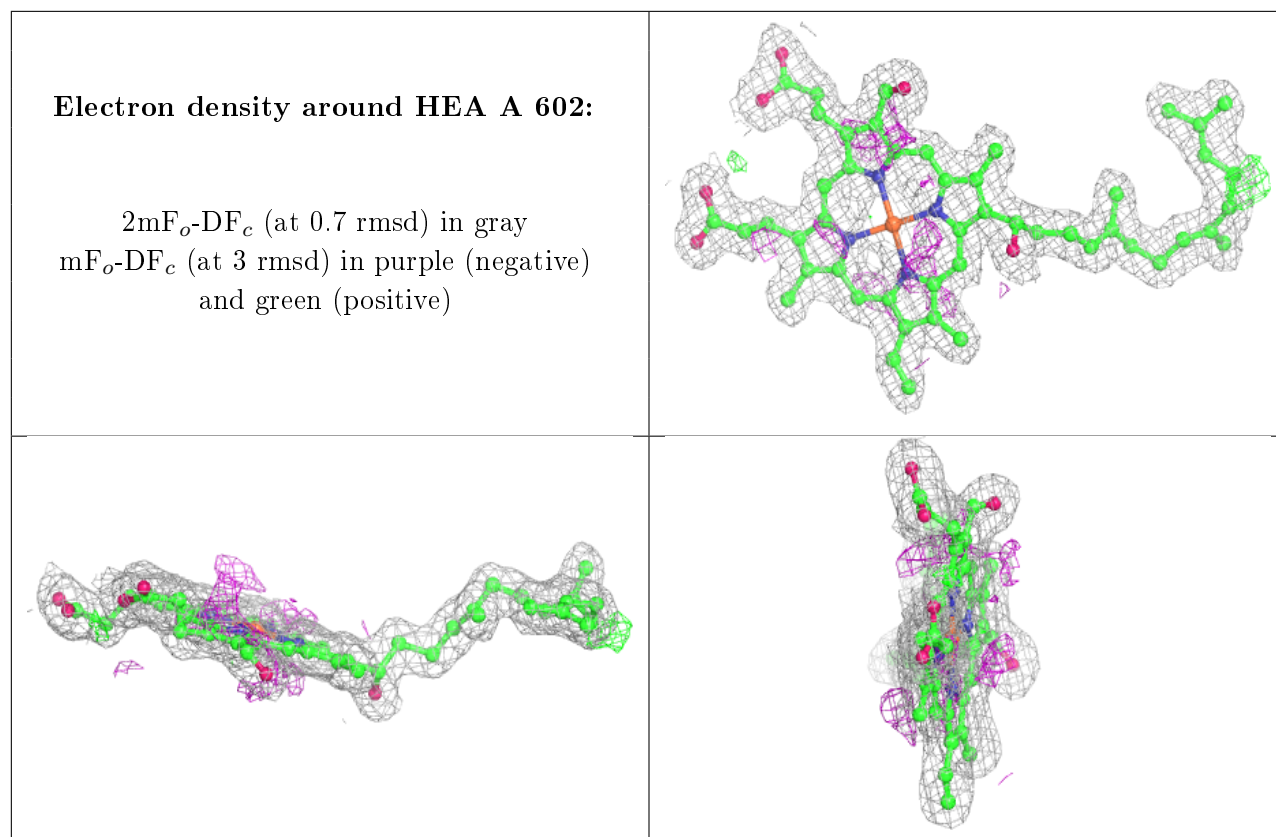
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HEA A 601 (A):**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.