



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 03:17 PM JST

PDB ID : 7W3E
Title : Bovine cytochrome c oxidase in CN-bound fully reduced state at 50 K
Authors : Tsukihara, T.; Shimada, A.
Deposited on : 2021-11-25
Resolution : 1.45 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

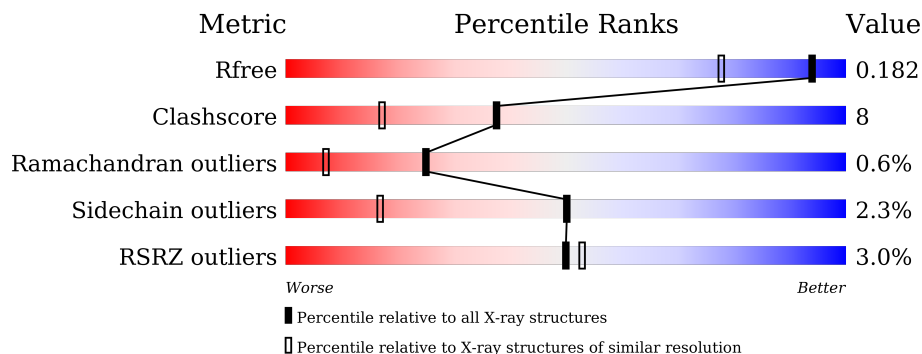
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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.



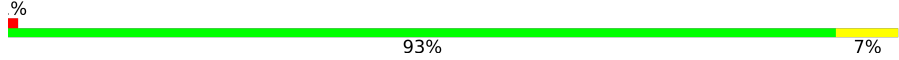

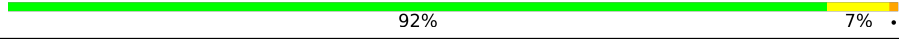
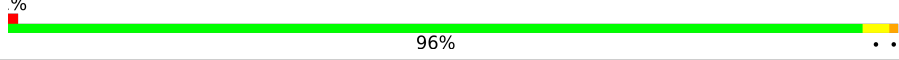
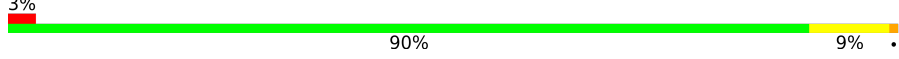








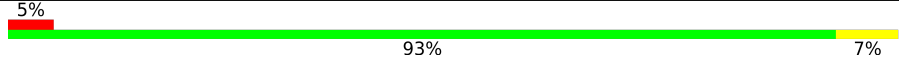

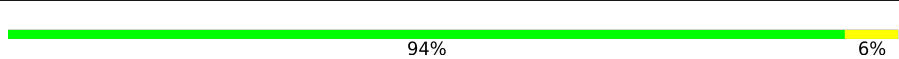
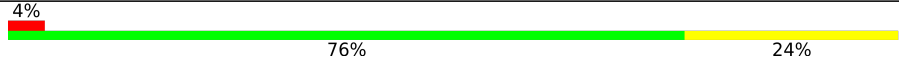
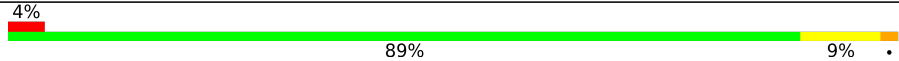
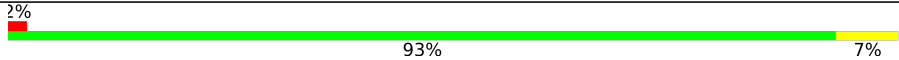
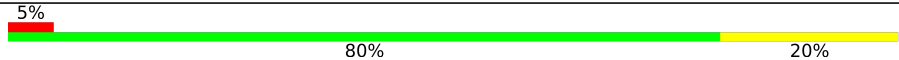
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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

Mol	Chain	Length	Quality of chain
1	A	514	86% (Green), 13% (Yellow), 1% (Orange), 0% (Red)
1	N	514	89% (Green), 11% (Yellow), 0% (Orange), 0% (Red)
2	B	227	3% (Red), 79% (Green), 19% (Yellow), 0% (Orange)
2	O	227	3% (Red), 79% (Green), 19% (Yellow), 0% (Orange)
3	C	259	87% (Green), 13% (Yellow), 0% (Orange), 0% (Red)
3	P	259	92% (Green), 8% (Yellow), 0% (Orange), 0% (Red)

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Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	104	
5	R	104	
6	F	93	
6	S	93	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	57	
10	W	57	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	41	
13	Z	41	

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
21	EDO	B	305	-	-	X	-
9	SAC	V	1	-	-	-	X

2 Entry composition [i](#)

There are 30 unique types of molecules in this entry. The entry contains 35109 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
			Total	C	N	O	S			
1	A	514	4162	2778	639	699	46	0	34	0
1	N	514	4160	2776	639	698	47	1	33	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	227	2000	1306	302	372	20	0	26	0
2	O	227	1999	1305	303	369	22	0	26	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	259	2125	1419	337	355	14	0	7	0
3	P	259	2121	1417	339	351	14	0	6	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	144	1201	783	196	218	4	0	1	0
4	Q	144	1209	783	202	220	4	0	3	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	3	0
			720	445	128	142	5			
6	S	93	Total	C	N	O	S	0	4	0
			721	447	127	141	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	S	0	0	0
			642	413	122	106	1			
7	T	84	Total	C	N	O	S	0	2	0
			663	423	126	113	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	2	0
			389	253	65	68	3			
11	X	49	Total	C	N	O	S	0	0	0
			385	250	65	68	2			

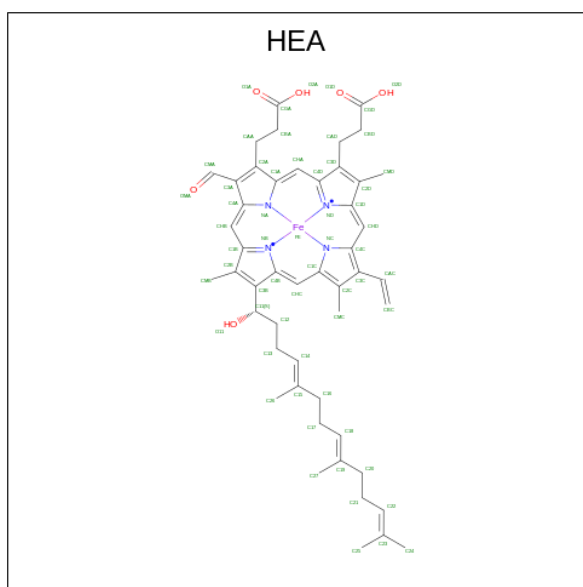
- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	1	0
			382	255	64	61	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	41	Total	C	N	O	0	1	0
			322	216	50	56			
13	Z	41	Total	C	N	O	0	0	0
			320	214	50	56			

- Molecule 14 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
14	A	1	Total	C	Fe	N	O	0	1
			79	67	1	4	7		
14	A	1	Total	C	Fe	N	O	0	1
			111	89	2	8	12		
14	N	1	Total	C	Fe	N	O	0	1
			79	67	1	4	7		
14	N	1	Total	C	Fe	N	O	0	1
			111	89	2	8	12		

- 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		

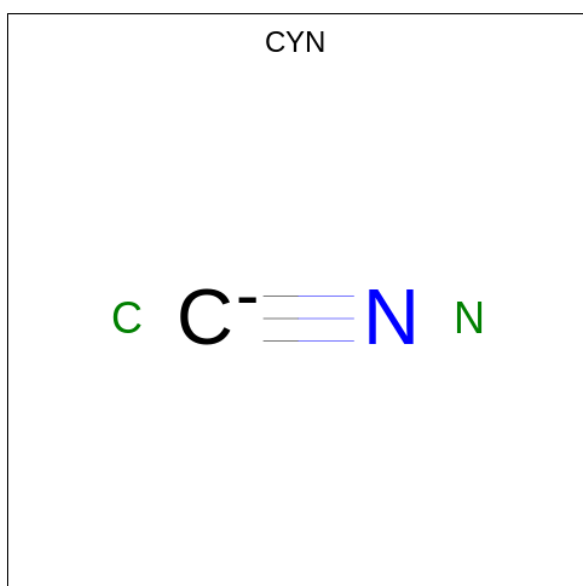
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

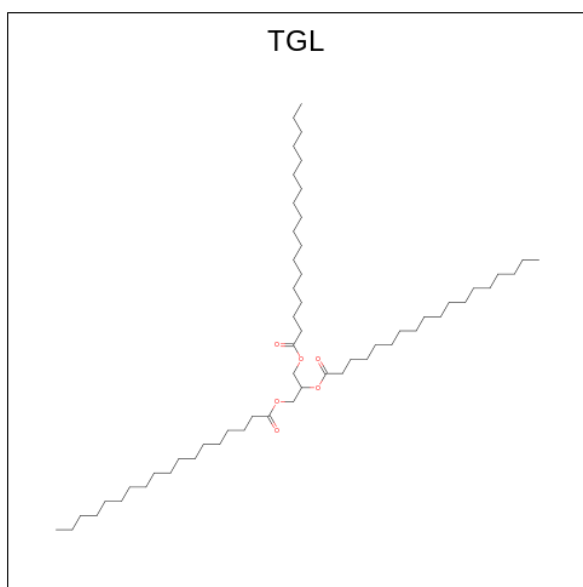
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Na	0	0
			1	1		
17	C	1	Total	Na	0	0
			1	1		
17	N	1	Total	Na	0	0
			1	1		
17	P	1	Total	Na	0	0
			1	1		

- Molecule 18 is CYANIDE ION (three-letter code: CYN) (formula: CN).



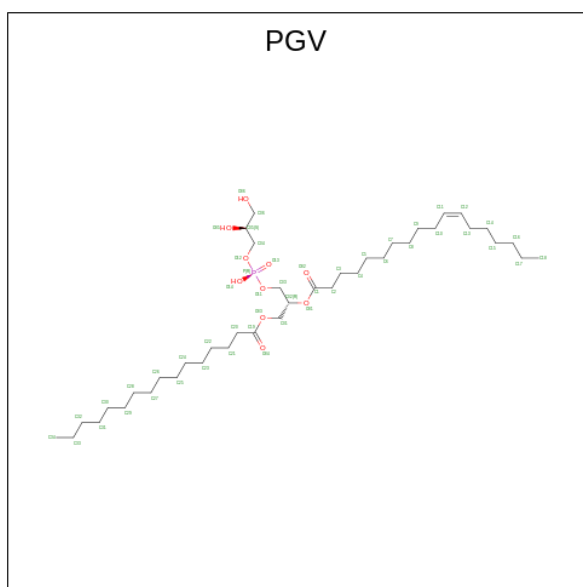
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	N	0	1
			4	2	2		
18	N	1	Total	C	N	0	1
			4	2	2		

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



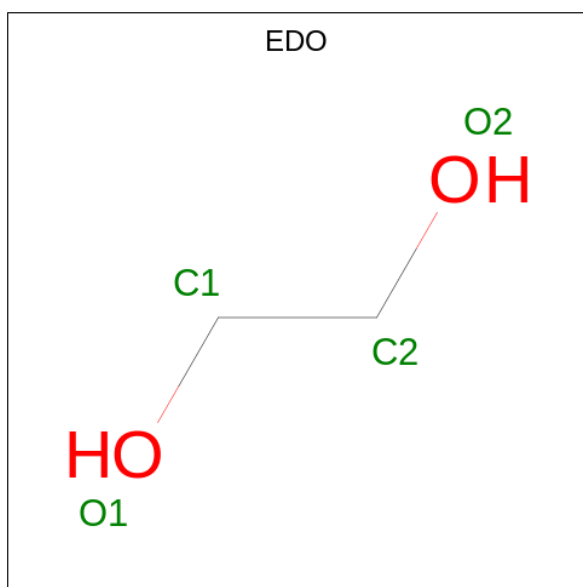
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
19	A	1	63	57	6	0	0
19	B	1	62	56	6	0	0
19	D	1	48	42	6	0	0
19	O	1	63	57	6	0	0
19	O	1	63	57	6	0	0

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
20	A	1	46	37	8	1	0	0
20	C	1	51	40	10	1	0	0
20	C	1	51	40	10	1	0	0
20	C	1	47	36	10	1	0	0
20	N	1	51	40	10	1	0	0
20	P	1	45	34	10	1	0	0
20	P	1	51	40	10	1	0	0
20	Q	1	51	40	10	1	0	0

- Molecule 21 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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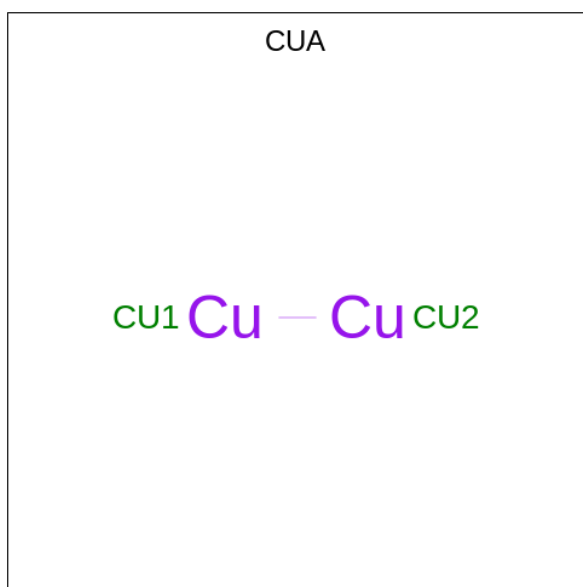
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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21	D	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	E	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	F	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	G	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	N	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0
21	O	1	Total 4	C 2	O 2	0	0

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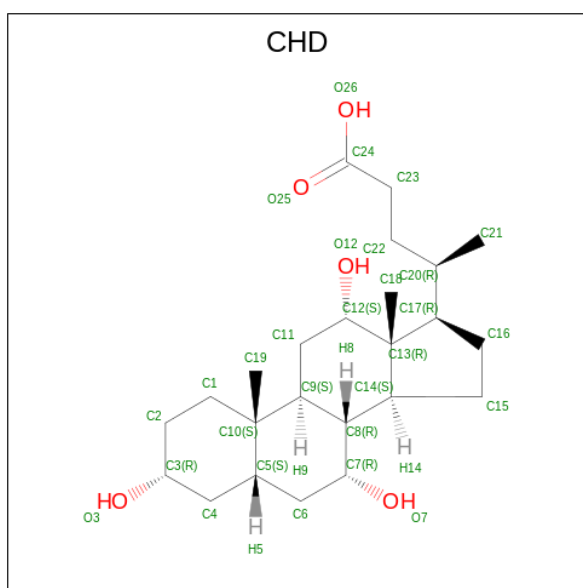
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	P	1	Total 4	C 2	O 2	0	0
21	P	1	Total 4	C 2	O 2	0	0
21	Q	1	Total 4	C 2	O 2	0	0
21	R	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	S	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	T	1	Total 4	C 2	O 2	0	0
21	U	1	Total 4	C 2	O 2	0	0
21	Y	1	Total 4	C 2	O 2	0	0

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

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



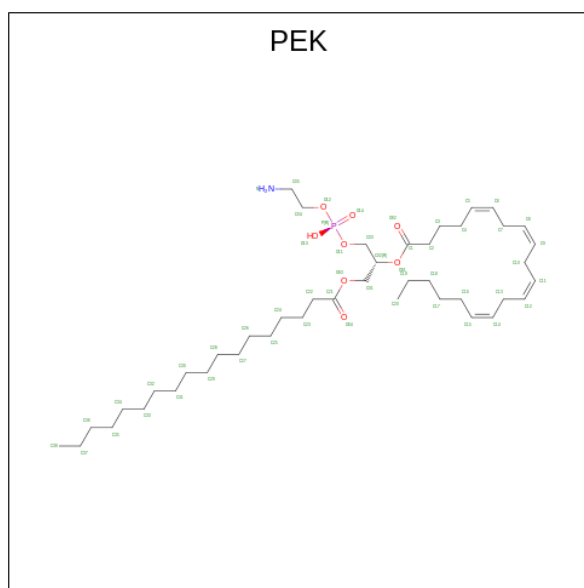
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 29 24 5	0	0
23	C	1	Total C O 29 24 5	0	0

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

- Molecule 24 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C₄₃H₇₈NO₈P).



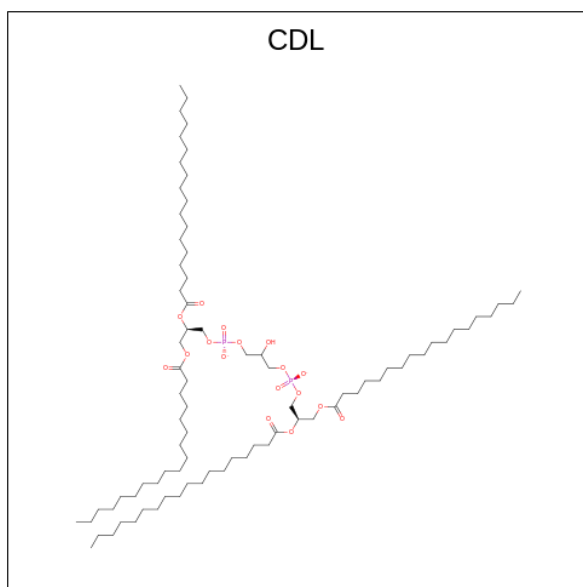
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			51	41	1	8	1		
24	C	1	Total	C	O			0	0
			44	40	4				
24	P	1	Total	C	O			0	0
			22	20	2				
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

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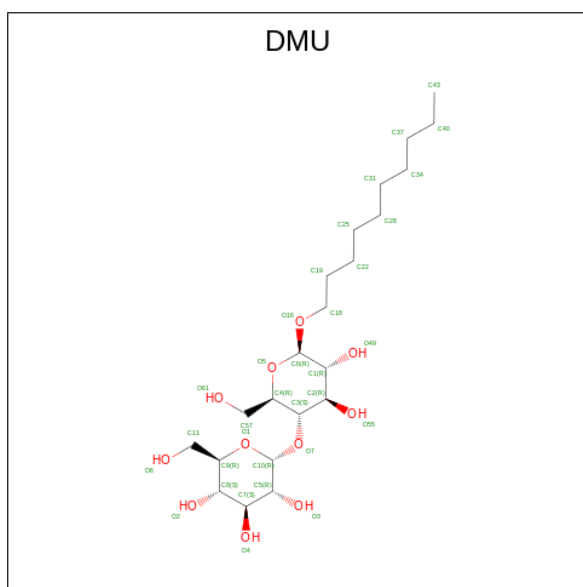
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	P	1	Total	C	O				
			46	41	5		0	0	
24	T	1	Total	C	N	O	P		
			49	39	1	8	1	0	

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	C	1	Total	C	O	P		
			86	68	16	2	0	0
25	G	1	Total	C	O	P		
			89	71	16	2	0	0
25	P	1	Total	C	O	P		
			76	64	11	1	0	0
25	T	1	Total	C	O	P		
			80	63	15	2	0	0
25	Y	1	Total	C	O	P		
			87	68	17	2	0	0

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



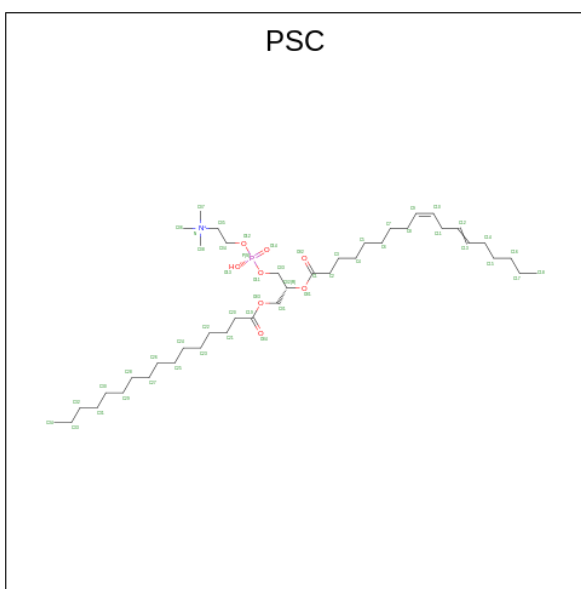
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	C	1	Total	C	O	0	0
			33	22	11		
26	G	1	Total	C	O	0	0
			21	16	5		
26	J	1	Total	C	O	0	0
			33	22	11		
26	K	1	Total	C	O	0	0
			22	16	6		
26	K	1	Total	C	O	0	0
			22	16	6		
26	K	1	Total	C	O	0	0
			17	15	2		
26	L	1	Total	C	O	0	0
			18	12	6		
26	M	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			33	22	11		
26	P	1	Total	C	O	0	0
			22	16	6		
26	X	1	Total	C	O	0	0
			22	16	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	X	1	Total	C	O	0	0
			22	16	6		
26	X	1	Total	C	O	0	0
			22	16	6		
26	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 27 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: C₄₂H₈₁NO₈P).

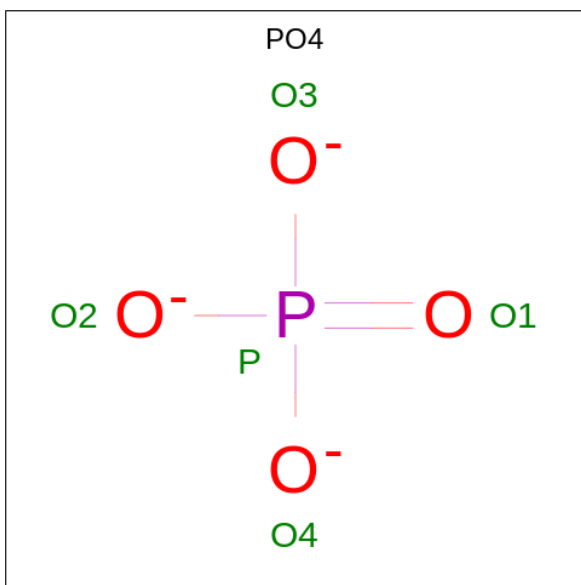


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
27	O	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

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

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

- Molecule 29 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	U	1	Total	O	P	0	0
			5	4	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	286	Total	O	0	3
			286	286		
30	B	245	Total	O	0	0
			245	245		
30	C	196	Total	O	0	0
			196	196		
30	D	250	Total	O	0	0
			250	250		
30	E	178	Total	O	0	0
			178	178		
30	F	177	Total	O	0	2
			177	177		
30	G	97	Total	O	0	0
			97	97		
30	H	111	Total	O	0	0
			111	111		
30	I	81	Total	O	0	0
			81	81		
30	J	63	Total	O	0	0
			63	63		
30	K	63	Total	O	0	0
			63	63		

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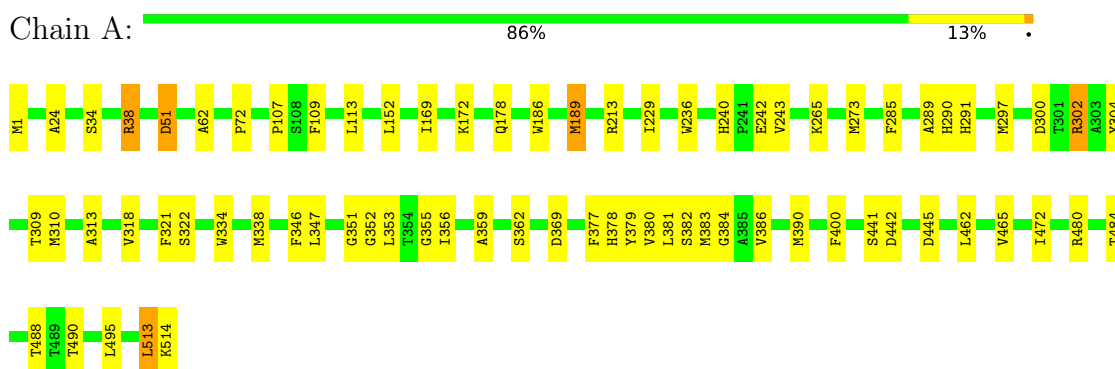
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	L	57	Total 57	O 57	0	0
30	M	46	Total 46	O 46	0	0
30	N	263	Total 263	O 263	0	1
30	O	204	Total 204	O 204	0	0
30	P	179	Total 179	O 179	0	0
30	Q	128	Total 128	O 128	0	0
30	R	131	Total 131	O 131	0	0
30	S	126	Total 126	O 126	0	0
30	T	78	Total 78	O 78	0	0
30	U	121	Total 121	O 121	0	0
30	V	68	Total 68	O 68	0	0
30	W	51	Total 51	O 51	0	0
30	X	50	Total 50	O 50	0	0
30	Y	48	Total 48	O 48	0	0
30	Z	30	Total 30	O 30	0	0

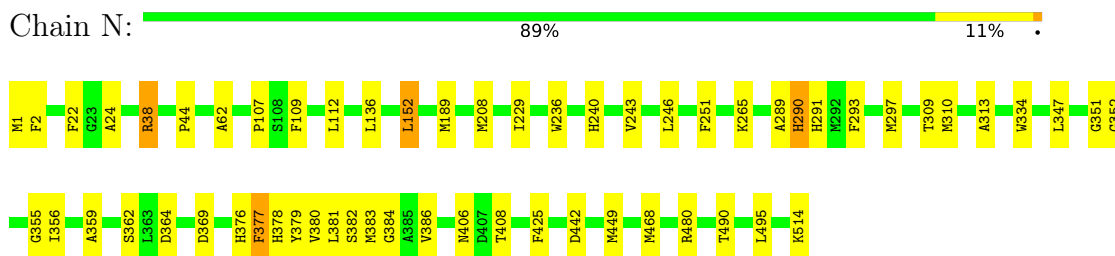
3 Residue-property plots [i](#)

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

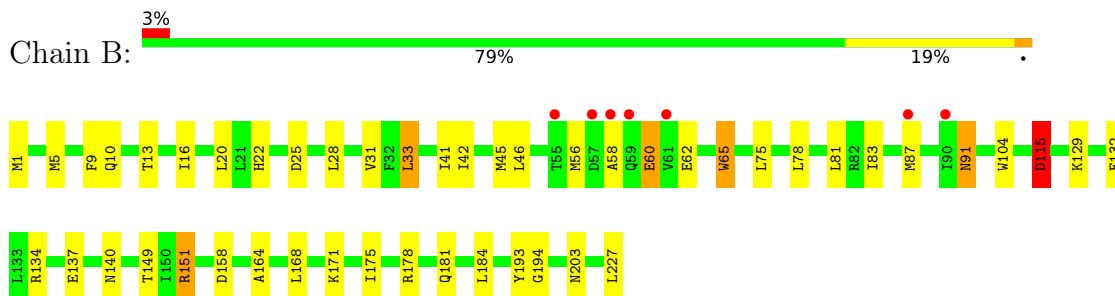
- Molecule 1: Cytochrome c oxidase subunit 1



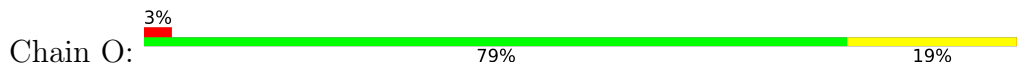
- Molecule 1: Cytochrome c oxidase subunit 1

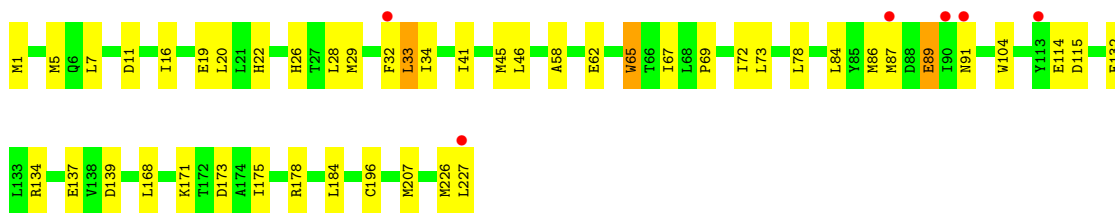


- Molecule 2: Cytochrome c oxidase subunit 2



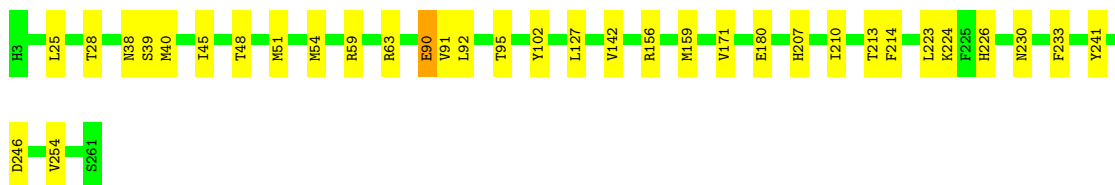
- Molecule 2: Cytochrome c oxidase subunit 2





- Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 87% 13%



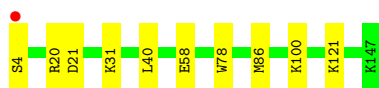
- Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 92% 8%



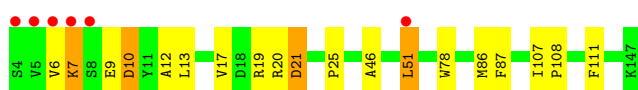
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial

Chain D: 93% 7%



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

Chain Q: 4% 87% 10%



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

Chain E: 92% 7%

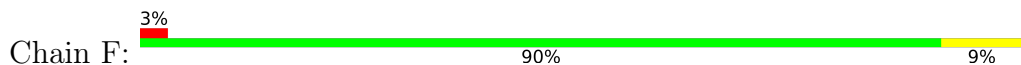


- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial

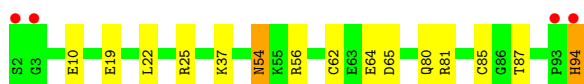
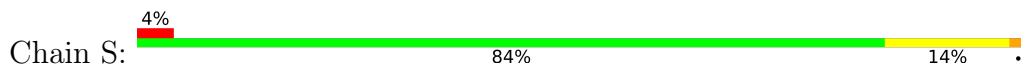
Chain R: 96%



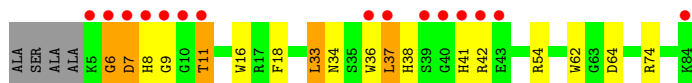
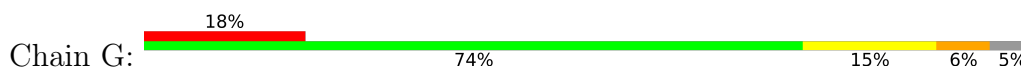
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



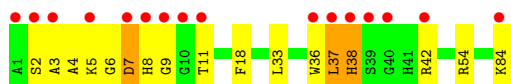
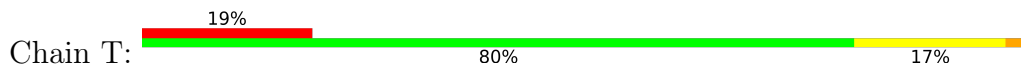
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



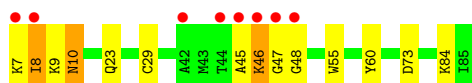
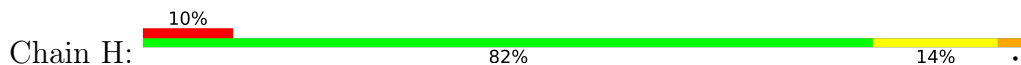
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



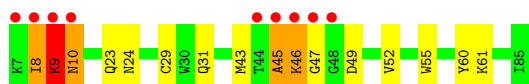
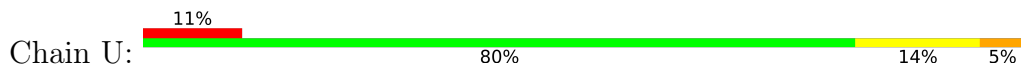
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial



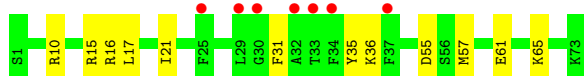
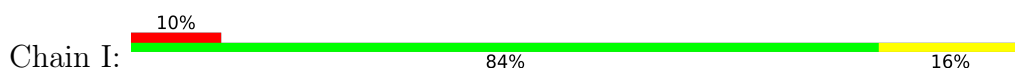
- Molecule 8: Cytochrome c oxidase subunit 6B1



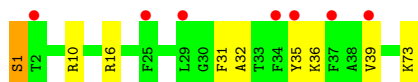
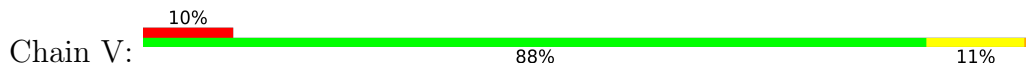
- Molecule 8: Cytochrome c oxidase subunit 6B1



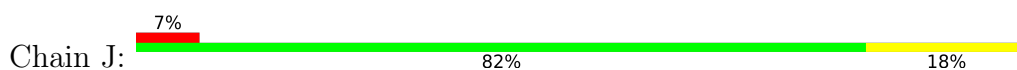
- Molecule 9: Cytochrome c oxidase subunit 6C



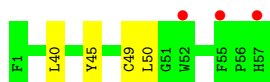
- Molecule 9: Cytochrome c oxidase subunit 6C



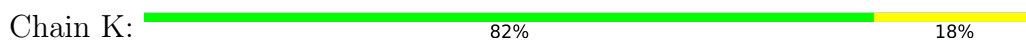
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



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



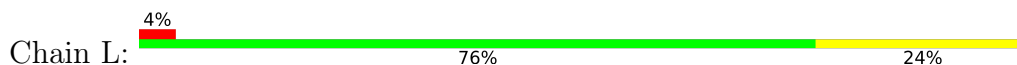
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



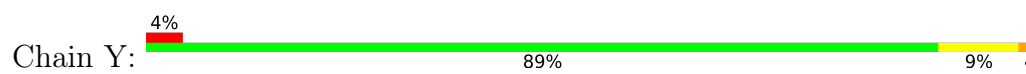
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



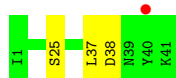
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



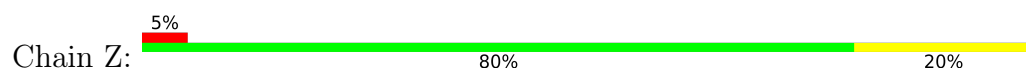
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	181.67Å 203.75Å 177.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.76 – 1.45 135.60 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.76-1.45) 99.9 (135.60-1.45)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 1.45Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.162 , 0.182 0.162 , 0.182	Depositor DCC
R_{free} test set	57695 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	22.7	Xtrriage
Anisotropy	0.652	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35109	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CU, PO4, PGV, CDL, PSC, CUA, NA, EDO, FME, SAC, HEA, DMU, TGL, PEK, CHD, CYN, MG, ZN

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	0.95	3/4449 (0.1%)	1.07	18/6067 (0.3%)
1	N	0.90	2/4447 (0.0%)	0.95	10/6066 (0.2%)
2	B	0.85	1/2067 (0.0%)	1.00	7/2815 (0.2%)
2	O	0.80	0/2065	0.94	6/2811 (0.2%)
3	C	0.89	4/2252 (0.2%)	0.89	2/3077 (0.1%)
3	P	0.88	0/2246	0.89	3/3068 (0.1%)
4	D	0.84	0/1241	0.91	2/1674 (0.1%)
4	Q	0.65	0/1259	0.81	3/1697 (0.2%)
5	E	0.92	1/860 (0.1%)	0.99	4/1167 (0.3%)
5	R	0.76	0/860	0.84	1/1167 (0.1%)
6	F	0.96	1/751 (0.1%)	1.04	0/1019
6	S	0.85	1/758 (0.1%)	0.97	2/1029 (0.2%)
7	G	0.87	1/668 (0.1%)	0.97	2/909 (0.2%)
7	T	0.74	0/699	0.88	0/950
8	H	0.85	0/682	0.96	1/921 (0.1%)
8	U	0.81	0/682	0.85	0/921
9	I	0.71	0/605	0.87	2/802 (0.2%)
9	V	0.71	0/605	0.76	0/802
10	J	0.64	0/462	0.81	2/625 (0.3%)
10	W	0.60	0/462	0.76	0/625
11	K	0.84	1/414 (0.2%)	0.94	1/566 (0.2%)
11	X	0.67	0/399	0.76	0/546
12	L	0.99	1/393 (0.3%)	0.89	0/526
12	Y	0.77	0/400	0.75	0/536
13	M	0.95	0/338	0.94	0/462
13	Z	0.81	1/330 (0.3%)	0.77	0/451
All	All	0.85	17/30394 (0.1%)	0.94	66/41299 (0.2%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
6	F	0	1
All	All	0	5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	16	GLU	CG-CD	6.54	1.61	1.51
7	G	36	TRP	CB-CG	6.34	1.61	1.50
3	C	102	TYR	CG-CD2	-6.28	1.30	1.39
1	N	514	LYS	CE-NZ	6.24	1.64	1.49
6	F	85	CYS	CB-SG	-6.11	1.71	1.82
11	K	39	GLU	CB-CG	6.10	1.63	1.52
5	E	70	VAL	CB-CG1	-5.73	1.40	1.52
6	S	62	CYS	CB-SG	-5.54	1.72	1.81
1	N	377	PHE	CE2-CZ	5.24	1.47	1.37
13	Z	35	TYR	CD2-CE2	5.20	1.47	1.39
1	A	346	PHE	CB-CG	5.17	1.60	1.51
3	C	102	TYR	CD2-CE2	5.12	1.47	1.39
2	B	193	TYR	CD2-CE2	5.09	1.47	1.39
3	C	90[A]	GLU	CB-CG	5.07	1.61	1.52
3	C	90[B]	GLU	CB-CG	5.07	1.61	1.52
1	A	242	GLU	CD-OE1	5.04	1.31	1.25
1	A	34	SER	CB-OG	5.02	1.48	1.42

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189[A]	MET	CG-SD-CE	-13.95	77.88	100.20
1	A	189[B]	MET	CG-SD-CE	-13.95	77.88	100.20
5	E	60	ASP	CB-CG-OD2	-10.69	108.68	118.30
11	K	47	ARG	NE-CZ-NH1	8.55	124.58	120.30
2	O	134	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	N	38	ARG	NE-CZ-NH1	8.16	124.38	120.30
9	I	16	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	38	ARG	NE-CZ-NH1	7.59	124.09	120.30
5	E	40	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	442	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	51[A]	ASP	CB-CG-OD2	-7.13	111.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51[B]	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	400	PHE	CB-CG-CD2	-7.12	115.82	120.80
1	A	38	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	513	LEU	CA-CB-CG	-6.98	99.25	115.30
1	N	251	PHE	CB-CG-CD2	-6.63	116.16	120.80
1	N	208[A]	MET	CB-CG-SD	6.59	132.18	112.40
1	N	208[B]	MET	CB-CG-SD	6.59	132.18	112.40
3	C	223	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	A	442	ASP	CB-CG-OD2	-6.50	112.45	118.30
8	H	73	ASP	CB-CG-OD2	-6.48	112.47	118.30
4	D	20	ARG	NE-CZ-NH2	6.44	123.52	120.30
3	P	155	ASP	CB-CG-OD1	6.34	124.01	118.30
9	I	55	ASP	CB-CG-OD1	6.26	123.94	118.30
2	O	139	ASP	CB-CG-OD1	6.11	123.80	118.30
2	B	184	LEU	CA-CB-CG	6.07	129.25	115.30
1	A	445	ASP	CB-CG-OD1	5.98	123.69	118.30
10	J	28	ASP	CB-CG-OD2	-5.96	112.93	118.30
4	D	21	ASP	CB-CG-OD1	5.95	123.66	118.30
1	N	377	PHE	CB-CG-CD2	5.93	124.95	120.80
7	G	64	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	213	ARG	NE-CZ-NH2	-5.89	117.36	120.30
5	E	73	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	302[A]	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	A	302[B]	ARG	NE-CZ-NH1	-5.74	117.43	120.30
2	O	173	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	310[A]	MET	CG-SD-CE	-5.66	91.15	100.20
1	A	310[B]	MET	CG-SD-CE	-5.66	91.15	100.20
1	N	442	ASP	CB-CG-OD2	-5.57	113.29	118.30
6	S	56	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	B	151	ARG	NE-CZ-NH1	5.53	123.06	120.30
2	B	158	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	300	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	N	38	ARG	NE-CZ-NH2	-5.49	117.56	120.30
3	P	233	PHE	CB-CG-CD1	-5.48	116.96	120.80
4	Q	21[A]	ASP	CB-CG-OD2	5.46	123.21	118.30
4	Q	21[B]	ASP	CB-CG-OD2	5.46	123.21	118.30
3	C	233	PHE	CB-CG-CD1	-5.44	116.99	120.80
10	J	36	MET	CG-SD-CE	-5.38	91.58	100.20
2	O	11	ASP	CB-CG-OD1	5.37	123.13	118.30
4	Q	51	LEU	CA-CB-CG	5.35	127.61	115.30
3	P	90	GLU	OE1-CD-OE2	5.33	129.69	123.30
5	R	36	LEU	CB-CG-CD2	-5.30	101.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	189[A]	MET	CG-SD-CE	-5.27	91.77	100.20
1	N	189[B]	MET	CG-SD-CE	-5.27	91.77	100.20
2	O	139	ASP	CB-CG-OD2	-5.25	113.57	118.30
2	O	65	TRP	CB-CA-C	-5.25	99.91	110.40
2	B	25	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	B	134	ARG	NE-CZ-NH2	-5.19	117.70	120.30
2	B	115[A]	ASP	CB-CA-C	5.19	120.77	110.40
2	B	115[B]	ASP	CB-CA-C	5.19	120.77	110.40
1	A	480	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	S	81	ARG	NE-CZ-NH1	-5.09	117.75	120.30
5	E	66	ARG	NE-CZ-NH2	-5.04	117.78	120.30
7	G	6	GLY	N-CA-C	5.04	125.70	113.10
1	N	480	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	379	TYR	Mainchain
6	F	93	PRO	Peptide
1	N	240	HIS	Sidechain
1	N	379	TYR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4162	0	4144	83	0
1	N	4160	0	4135	66	0
2	B	2000	0	2024	41	0
2	O	1999	0	2031	35	0
3	C	2125	0	2033	32	0
3	P	2121	0	2029	18	0
4	D	1201	0	1188	8	0
4	Q	1209	0	1197	16	0
5	E	842	0	838	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	R	842	0	838	4	0
6	F	720	0	698	7	0
6	S	721	0	702	12	0
7	G	642	0	606	7	0
7	T	663	0	626	14	0
8	H	662	0	623	12	0
8	U	662	0	623	18	0
9	I	601	0	613	8	0
9	V	601	0	613	9	0
10	J	451	0	446	8	0
10	W	451	0	446	3	0
11	K	389	0	372	7	0
11	X	385	0	366	3	0
12	L	380	0	380	9	0
12	Y	382	0	383	5	0
13	M	322	0	337	2	0
13	Z	320	0	334	5	0
14	A	190	0	138	28	0
14	N	190	0	138	23	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	4	0	0	0	0
18	N	4	0	0	0	0
19	A	63	0	110	10	0
19	B	62	0	105	6	0
19	D	48	0	77	7	0
19	O	126	0	220	14	0
20	A	46	0	69	7	0
20	C	149	0	217	8	0
20	N	51	0	76	4	0
20	P	96	0	138	1	0
20	Q	51	0	76	6	0
21	A	36	0	54	2	0
21	B	20	0	30	5	0
21	C	4	0	6	0	0
21	D	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	8	0	12	0	0
21	F	12	0	18	0	0
21	G	8	0	12	0	0
21	N	32	0	48	0	0
21	O	16	0	24	1	0
21	P	8	0	12	0	0
21	Q	4	0	6	0	0
21	R	4	0	6	0	0
21	S	28	0	42	3	0
21	T	8	0	12	0	0
21	U	4	0	6	3	0
21	Y	4	0	6	0	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	29	0	39	0	0
23	C	58	0	78	5	0
23	G	29	0	39	1	0
23	J	29	0	39	4	0
23	P	58	0	78	3	0
23	W	29	0	38	1	0
24	C	95	0	138	4	0
24	P	121	0	179	9	0
24	T	49	0	66	0	0
25	C	86	0	122	14	0
25	G	89	0	133	8	0
25	P	76	0	113	6	0
25	T	80	0	120	15	0
25	Y	87	0	127	4	0
26	C	33	0	42	5	0
26	G	21	0	30	2	0
26	J	33	0	42	3	0
26	K	61	0	84	2	0
26	L	18	0	20	3	0
26	M	33	0	42	0	0
26	P	154	0	199	7	0
26	X	66	0	93	5	0
26	Z	33	0	42	1	0
27	E	52	0	80	8	0
27	O	51	0	75	9	0
28	F	1	0	0	0	0
28	S	1	0	0	0	0
29	U	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	286	0	0	13	0
30	B	245	0	0	5	0
30	C	196	0	0	6	0
30	D	250	0	0	3	0
30	E	178	0	0	2	0
30	F	177	0	0	3	0
30	G	97	0	0	0	0
30	H	111	0	0	0	0
30	I	81	0	0	4	0
30	J	63	0	0	3	0
30	K	63	0	0	0	0
30	L	57	0	0	3	0
30	M	46	0	0	0	0
30	N	263	0	0	7	0
30	O	204	0	0	6	0
30	P	179	0	0	4	0
30	Q	128	0	0	3	0
30	R	131	0	0	3	0
30	S	126	0	0	4	0
30	T	78	0	0	1	0
30	U	121	0	0	5	0
30	V	68	0	0	1	0
30	W	51	0	0	0	0
30	X	50	0	0	0	0
30	Y	48	0	0	1	0
30	Z	30	0	0	1	0
All	All	35109	0	32347	493	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 8.

All (493) 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)
6:S:94:HIS:HE1	21:S:108:EDO:H22	1.28	0.96
8:U:24:ASN:HD21	21:U:101:EDO:H21	1.31	0.93
10:J:50:LEU:HB2	26:J:101:DMU:H20	1.51	0.93
1:N:356:ILE:HD13	14:N:602[C]:HEA:HMB1	1.51	0.91
1:A:347:LEU:HD22	1:A:383[A]:MET:SD	2.10	0.91
1:A:347:LEU:HD13	1:A:383[A]:MET:HB3	1.57	0.86
1:A:356:ILE:HD13	14:A:602[C]:HEA:HMB1	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:201:PGV:H22	20:Q:201:PGV:H011	1.64	0.79
7:G:11:THR:HG23	7:G:16:TRP:HE1	1.48	0.79
4:D:78:TRP:HB3	19:D:201:TGL:HB22	1.62	0.79
2:B:10:GLN:H	21:B:305:EDO:C1	1.98	0.77
12:Y:2:HIS:N	30:Y:201:HOH:O	2.17	0.77
1:N:359:ALA:HA	14:N:602[C]:HEA:OMA	1.86	0.75
10:J:55:PHE:HE1	26:L:101:DMU:H29	1.52	0.75
19:A:607:TGL:HC32	12:L:20:ARG:HH12	1.51	0.73
2:B:10:GLN:H	21:B:305:EDO:H12	1.53	0.73
2:O:26:HIS:HA	2:O:29[C]:MET:HE3	1.69	0.73
19:A:607:TGL:HC41	30:A:933:HOH:O	1.88	0.72
4:D:100:LYS:HE3	30:D:344:HOH:O	1.89	0.71
1:A:347:LEU:HB3	1:A:383[A]:MET:HB3	1.71	0.71
1:N:347:LEU:HD13	1:N:383[A]:MET:HB3	1.72	0.71
1:A:347:LEU:CB	1:A:383[A]:MET:HB3	2.22	0.69
27:E:201:PSC:H42	27:E:201:PSC:H262	1.73	0.69
1:N:309:THR:HG22	14:N:602[C]:HEA:HMB2	1.75	0.68
23:P:309:CHD:H231	30:P:547:HOH:O	1.94	0.68
6:S:94:HIS:CE1	21:S:108:EDO:H22	2.20	0.68
1:A:347:LEU:CD1	1:A:383[A]:MET:HB3	2.23	0.68
10:J:55:PHE:CE1	26:L:101:DMU:H29	2.28	0.68
1:A:386:VAL:HG21	14:A:601[A]:HEA:H261	1.76	0.68
19:A:607:TGL:HC22	19:A:607:TGL:HC82	1.77	0.67
1:N:356:ILE:HA	14:N:602[C]:HEA:HMB3	1.77	0.66
2:B:33[C]:LEU:HD22	30:B:624:HOH:O	1.96	0.65
1:N:24:ALA:HB2	14:N:601[A]:HEA:H253	1.79	0.65
1:N:352:GLY:O	14:N:602[C]:HEA:H121	1.98	0.64
8:U:23:GLN:NE2	30:U:201:HOH:O	2.30	0.64
1:N:309:THR:O	30:N:702:HOH:O	2.15	0.64
1:N:356:ILE:HD13	14:N:602[C]:HEA:CMB	2.26	0.64
1:N:386:VAL:HG21	14:N:601[A]:HEA:H261	1.80	0.63
24:P:305:PEK:C38	25:T:102:CDL:H273	2.29	0.63
1:A:352:GLY:O	14:A:602[C]:HEA:H121	1.99	0.63
2:B:42[A]:ILE:HG21	19:D:201:TGL:H232	1.79	0.63
3:C:63:ARG:HE	25:C:308:CDL:CA2	2.12	0.63
19:A:607:TGL:HC51	19:A:607:TGL:CC1	2.30	0.62
4:D:78:TRP:CB	19:D:201:TGL:HB22	2.29	0.62
1:A:347:LEU:HD13	1:A:383[A]:MET:CB	2.28	0.62
1:A:390[B]:MET:HE1	14:A:601[B]:HEA:H211	1.81	0.62
20:N:607:PGV:H343	24:P:304:PEK:H381	1.81	0.62
1:N:362:SER:HA	2:O:87[A]:MET:HE1	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:84:LEU:HA	2:O:87[A]:MET:HE2	1.83	0.61
19:O:302:TGL:HG32	30:O:577:HOH:O	1.99	0.61
8:U:23:GLN:NE2	30:U:202:HOH:O	2.31	0.60
1:N:334:TRP:CH2	2:O:46[A]:LEU:HD13	2.36	0.60
1:A:359:ALA:HA	14:A:602[C]:HEA:OMA	2.02	0.60
19:O:302:TGL:H181	30:O:567:HOH:O	2.00	0.60
3:C:213:THR:HG23	25:C:308:CDL:H771	1.83	0.60
19:B:301:TGL:HC61	30:I:170:HOH:O	2.01	0.60
1:N:136[B]:LEU:HD11	30:T:267:HOH:O	2.03	0.59
2:O:22:HIS:HB3	30:V:160:HOH:O	2.01	0.59
19:O:302:TGL:HG31	30:Q:352:HOH:O	2.00	0.59
1:A:514:LYS:HE2	30:F:223:HOH:O	2.00	0.59
30:A:809:HOH:O	27:E:201:PSC:H31	2.02	0.59
1:N:356:ILE:CD1	14:N:602[C]:HEA:HMB1	2.29	0.59
1:A:390[B]:MET:HE1	14:A:601[B]:HEA:H242	1.85	0.59
1:A:334:TRP:CH2	2:B:46[A]:LEU:HD13	2.37	0.59
2:B:10:GLN:HG3	21:B:305:EDO:H11	1.84	0.59
1:A:356:ILE:HD13	14:A:602[C]:HEA:CMB	2.32	0.58
1:A:390[B]:MET:CE	14:A:601[B]:HEA:H242	2.33	0.58
1:A:229[B]:ILE:HD12	2:B:178:ARG:NH1	2.19	0.58
2:O:33[C]:LEU:HD21	9:V:32:ALA:HB2	1.85	0.58
8:U:24:ASN:HD21	21:U:101:EDO:C2	2.13	0.58
20:N:607:PGV:H183	24:P:304:PEK:H342	1.85	0.58
25:T:102:CDL:HA62	25:T:102:CDL:H352	1.86	0.58
1:A:347:LEU:HB3	1:A:383[A]:MET:CB	2.34	0.57
12:L:26:THR:OG1	30:L:201:HOH:O	2.16	0.57
30:A:927:HOH:O	8:H:23:GLN:HG2	2.03	0.57
6:S:94:HIS:NE2	30:S:201:HOH:O	2.11	0.57
2:B:22:HIS:HB3	30:I:166:HOH:O	2.04	0.57
14:N:602[C]:HEA:HBD1	14:N:602[C]:HEA:HMD1	1.87	0.57
3:C:91:VAL:O	3:C:95[B]:THR:HG23	2.04	0.57
2:B:83:ILE:O	2:B:87:MET:HG3	2.05	0.57
3:P:63:ARG:HE	25:P:308:CDL:CA2	2.16	0.57
8:U:43:MET:HE3	8:U:49:ASP:N	2.20	0.57
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.87	0.57
1:A:313:ALA:HB2	1:A:356:ILE:HD11	1.87	0.57
6:S:80[B]:GLN:NE2	30:S:203:HOH:O	2.38	0.56
7:G:62:TRP:HB2	26:G:105:DMU:H5	1.86	0.56
8:U:45:ALA:O	8:U:47:GLY:N	2.39	0.56
11:X:40:TRP:CD1	26:X:103:DMU:H9	2.40	0.56
2:B:129:LYS:HE3	30:B:569:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51[A]:ASP:OD2	1:A:441:SER:OG	2.21	0.56
1:N:290[A]:HIS:HD1	1:N:309:THR:HG1	1.53	0.56
1:A:353:LEU:HB3	2:B:31[A]:VAL:HG13	1.88	0.56
25:P:308:CDL:H521	25:P:308:CDL:HB62	1.88	0.56
3:C:40:MET:SD	26:G:105:DMU:H11	2.46	0.56
1:A:290[A]:HIS:CD2	1:A:291:HIS:CD2	2.95	0.55
20:A:608:PGV:H212	30:A:981:HOH:O	2.05	0.55
26:P:310:DMU:H10	26:P:311:DMU:H12	1.89	0.55
1:A:24:ALA:HB2	14:A:601[A]:HEA:H253	1.87	0.55
1:A:356:ILE:HA	14:A:602[C]:HEA:HMB3	1.87	0.55
1:N:112:LEU:HG	30:N:904:HOH:O	2.05	0.55
1:N:468:MET:HG3	30:N:930:HOH:O	2.06	0.55
2:O:104:TRP:HB2	21:O:307:EDO:H22	1.88	0.55
3:C:39:SER:OG	26:C:311:DMU:H29	2.05	0.55
11:X:24:PHE:O	11:X:28:VAL:HG23	2.07	0.55
1:N:377:PHE:CD1	14:N:602[C]:HEA:HBD2	2.41	0.55
12:L:42:HIS:HB2	26:L:101:DMU:H6	1.89	0.55
1:A:513:LEU:O	30:A:702:HOH:O	2.18	0.55
2:O:67:ILE:HD11	30:O:588:HOH:O	2.06	0.55
1:A:273:MET:SD	1:A:322[B]:SER:OG	2.63	0.55
1:A:514:LYS:HD2	30:F:212:HOH:O	2.07	0.55
8:U:43:MET:HE3	8:U:49:ASP:H	1.71	0.55
1:A:236:TRP:CH2	14:A:602[A]:HEA:HBD1	2.42	0.54
30:A:703:HOH:O	2:B:203:ASN:ND2	2.41	0.54
3:C:171:VAL:HG22	25:C:308:CDL:H852	1.89	0.54
8:H:55:TRP:H	8:U:46:LYS:HZ3	1.56	0.54
3:C:90[B]:GLU:OE2	20:C:305:PGV:H321	2.07	0.54
1:N:347:LEU:CD1	1:N:383[A]:MET:HB3	2.36	0.54
1:N:449[A]:MET:SD	2:O:5:MET:HG2	2.48	0.54
6:S:22:LEU:HD12	30:S:298:HOH:O	2.07	0.54
19:B:301:TGL:H111	19:B:301:TGL:HA72	1.90	0.53
19:O:301:TGL:HA22	19:O:301:TGL:H162	1.90	0.53
1:A:322[B]:SER:HB2	30:A:718:HOH:O	2.08	0.53
1:A:484[A]:THR:HG22	30:A:921:HOH:O	2.08	0.53
2:B:56:MET:HA	27:E:201:PSC:H211	1.90	0.53
10:J:52:TRP:O	10:J:57:HIS:HE1	1.92	0.53
2:O:58:ALA:O	2:O:62:GLU:HG3	2.08	0.53
14:A:602[C]:HEA:HMD1	14:A:602[C]:HEA:HBD1	1.91	0.53
2:O:65:TRP:HE1	27:O:304:PSC:H12	1.74	0.52
2:B:78:LEU:HD23	25:T:102:CDL:H342	1.92	0.52
24:C:303:PEK:H322	20:C:305:PGV:C18	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:MET:HG3	30:L:227:HOH:O	2.09	0.52
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.92	0.52
3:C:224:LYS:HD3	25:C:308:CDL:HB31	1.90	0.52
7:T:38:HIS:HD1	7:T:38:HIS:N	2.06	0.52
1:N:243:VAL:HG11	14:N:602[C]:HEA:HMD2	1.90	0.52
26:P:312:DMU:H11	10:W:49:CYS:HB3	1.92	0.52
27:O:304:PSC:H061	5:R:8:ASP:OD1	2.09	0.52
8:U:31:GLN:NE2	30:U:203:HOH:O	2.36	0.52
2:B:227:LEU:HD21	30:B:535:HOH:O	2.08	0.52
19:A:607:TGL:HG31	30:A:926:HOH:O	2.10	0.52
8:U:8:ILE:HG13	8:U:8:ILE:O	2.10	0.51
5:R:90:ARG:NH2	30:R:301:HOH:O	2.28	0.51
2:B:81:LEU:HD12	25:T:102:CDL:H371	1.92	0.51
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.93	0.51
14:A:602[A]:HEA:HMB1	30:A:708:HOH:O	2.10	0.51
1:A:169[B]:ILE:HD11	1:A:189[B]:MET:CE	2.41	0.51
1:A:356:ILE:CD1	14:A:602[C]:HEA:HMB1	2.38	0.51
7:G:33:LEU:O	7:G:37:LEU:HB2	2.11	0.51
25:G:101:CDL:H131	25:G:101:CDL:OB4	2.11	0.51
7:T:38:HIS:NE2	25:T:102:CDL:H112	2.25	0.50
1:A:334:TRP:HH2	2:B:46[A]:LEU:HD13	1.76	0.50
1:A:488:THR:HB	1:A:495[B]:LEU:HG	1.93	0.50
14:A:602[C]:HEA:HMD1	14:A:602[C]:HEA:CBD	2.42	0.50
1:A:377:PHE:HA	1:A:380[B]:VAL:HG12	1.93	0.50
2:B:10:GLN:CG	21:B:305:EDO:H11	2.42	0.50
3:C:226:HIS:CE1	25:C:308:CDL:HB32	2.46	0.50
10:J:49:CYS:HB3	26:J:101:DMU:H11	1.94	0.50
30:N:919:HOH:O	20:Q:201:PGV:H032	2.10	0.50
8:H:8:ILE:HG12	8:H:8:ILE:O	2.10	0.50
3:P:62:ILE:HD12	25:P:308:CDL:H522	1.93	0.50
1:A:113:LEU:HB2	19:A:607:TGL:H323	1.93	0.49
19:O:302:TGL:HB21	4:Q:78:TRP:CA	2.42	0.49
1:N:229[B]:ILE:HD12	2:O:178:ARG:NH1	2.27	0.49
27:E:201:PSC:H12	27:E:201:PSC:C34	2.43	0.49
6:S:64:GLU:O	6:S:65:ASP:HB2	2.13	0.49
1:A:362:SER:HB3	2:B:20:LEU:HD21	1.94	0.49
7:T:38:HIS:N	7:T:38:HIS:ND1	2.60	0.49
3:C:254:VAL:CG2	25:G:101:CDL:H652	2.42	0.49
1:A:334:TRP:CZ2	2:B:46[A]:LEU:HB3	2.47	0.49
6:F:85:CYS:SG	6:F:87[A]:THR:HG23	2.53	0.49
1:A:355:GLY:C	14:A:602[C]:HEA:HMB3	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:HA	1:A:380[A]:VAL:HG22	1.93	0.49
7:G:38:HIS:HE1	25:G:101:CDL:H122	1.77	0.49
1:N:112:LEU:HD23	1:N:112:LEU:C	2.32	0.49
19:O:302:TGL:H312	4:Q:86:MET:HG2	1.94	0.49
10:J:7:GLU:HG3	30:J:239:HOH:O	2.12	0.49
19:O:302:TGL:H342	9:V:16:ARG:HE	1.78	0.49
11:K:40:TRP:CD1	26:K:103:DMU:H12	2.48	0.49
1:N:290[A]:HIS:CD2	1:N:291:HIS:CD2	3.01	0.49
30:A:776:HOH:O	12:L:7:PRO:HG3	2.12	0.48
3:C:207:HIS:HD2	3:C:241:TYR:OH	1.96	0.48
19:D:201:TGL:HG32	30:D:440:HOH:O	2.13	0.48
1:A:462:LEU:O	1:A:465[B]:VAL:HG12	2.13	0.48
2:B:13:THR:HB	2:B:168:LEU:HD23	1.95	0.48
3:C:226:HIS:HE1	25:C:308:CDL:HB32	1.76	0.48
4:D:31:LYS:HE2	30:D:384:HOH:O	2.12	0.48
25:G:101:CDL:H421	1:N:310[B]:MET:HG3	1.95	0.48
1:N:334:TRP:CE3	19:O:302:TGL:HA31	2.48	0.48
8:U:47:GLY:HA2	30:U:268:HOH:O	2.13	0.48
1:N:310[B]:MET:HB2	2:O:73:LEU:HD22	1.95	0.48
4:Q:87:PHE:CD2	20:Q:201:PGV:H141	2.47	0.48
1:A:178[B]:GLN:HE21	7:T:7:ASP:HB2	1.78	0.48
14:A:602[A]:HEA:CMB	30:A:708:HOH:O	2.62	0.48
7:T:37:LEU:HD23	25:T:102:CDL:H381	1.95	0.48
26:X:101:DMU:H11	26:X:102:DMU:H12	1.96	0.48
1:N:376:HIS:CE1	1:N:380[C]:VAL:HG11	2.48	0.48
1:N:378:HIS:HA	1:N:382[C]:SER:HB2	1.96	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.48
1:N:236:TRP:CH2	14:N:602[A]:HEA:HBD1	2.48	0.48
1:N:377:PHE:HA	1:N:380[A]:VAL:HG22	1.94	0.48
1:A:304:TYR:HD1	25:T:102:CDL:HB32	1.79	0.48
20:A:608:PGV:C3	20:A:608:PGV:H011	2.44	0.48
5:E:46:LYS:NZ	30:E:301:HOH:O	2.23	0.48
6:F:87[A]:THR:HG21	30:F:315:HOH:O	2.14	0.48
6:F:41:GLY:HA3	6:F:87[B]:THR:HG22	1.96	0.48
2:O:28[C]:LEU:HG	2:O:32[C]:PHE:CE2	2.49	0.48
20:P:307:PGV:H241	20:P:307:PGV:H272	1.63	0.48
1:A:169[B]:ILE:HD12	7:T:9:GLY:H	1.79	0.47
8:H:45:ALA:C	8:H:47:GLY:H	2.18	0.47
10:W:40:LEU:HD12	23:W:101:CHD:H183	1.95	0.47
27:E:201:PSC:H12	27:E:201:PSC:H343	1.96	0.47
30:N:902:HOH:O	24:P:304:PEK:H382	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:48:THR:HG23	25:P:308:CDL:H392	1.96	0.47
25:Y:101:CDL:HB61	25:Y:101:CDL:H111	1.96	0.47
2:B:41[A]:ILE:O	2:B:45[A]:MET:HG2	2.14	0.47
3:C:48:THR:HG23	25:C:308:CDL:H412	1.96	0.47
1:N:334:TRP:CZ2	2:O:46[A]:LEU:HB3	2.50	0.47
19:O:302:TGL:H192	9:V:16:ARG:HH21	1.78	0.47
1:A:377:PHE:O	1:A:381[B]:LEU:HB3	2.15	0.47
23:J:102:CHD:H111	23:J:102:CHD:H193	1.45	0.47
1:A:273:MET:HE2	30:A:718:HOH:O	2.14	0.47
1:A:309:THR:HG22	14:A:602[C]:HEA:HMB2	1.96	0.47
20:A:608:PGV:H321	20:A:608:PGV:H141	1.95	0.47
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.96	0.47
27:O:304:PSC:H071	9:V:10:ARG:HH21	1.79	0.47
3:C:210:ILE:HD13	20:C:306:PGV:H302	1.96	0.47
23:J:102:CHD:H211	23:J:102:CHD:H231	1.66	0.47
1:N:229[B]:ILE:HD11	2:O:175:ILE:HD13	1.96	0.47
1:N:347:LEU:CB	1:N:383[A]:MET:HB3	2.45	0.47
1:N:406:ASN:HD21	20:Q:201:PGV:H21	1.80	0.47
1:N:408:THR:HB	20:Q:201:PGV:H51	1.96	0.47
8:U:24:ASN:ND2	21:U:101:EDO:H21	2.14	0.47
11:X:40:TRP:CD1	26:X:103:DMU:H14	2.49	0.47
1:A:355:GLY:O	14:A:602[C]:HEA:HMB3	2.15	0.47
19:B:301:TGL:H111	19:B:301:TGL:H142	1.63	0.47
3:C:39:SER:HB2	26:C:311:DMU:O61	2.15	0.47
8:H:7:LYS:HD2	8:U:46:LYS:HG2	1.97	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.47
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.47
23:C:309:CHD:H161	30:C:589:HOH:O	2.14	0.47
4:D:86:MET:CE	11:K:22:ALA:HB2	2.45	0.47
1:N:313:ALA:HB2	1:N:356:ILE:HD11	1.95	0.47
1:N:377:PHE:HA	1:N:380[B]:VAL:HG12	1.96	0.47
5:R:90:ARG:NH1	30:R:303:HOH:O	2.48	0.47
6:S:94:HIS:HE1	21:S:108:EDO:C2	2.14	0.47
1:A:172:LYS:NZ	1:A:178[A]:GLN:HE22	2.13	0.46
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.97	0.46
14:A:601[A]:HEA:H122	14:A:601[A]:HEA:H262	1.98	0.46
2:B:31[A]:VAL:CG1	19:B:301:TGL:HB72	2.44	0.46
2:B:140:ASN:HB3	30:B:517:HOH:O	2.15	0.46
2:O:114:GLU:HG3	2:O:227:LEU:HD21	1.97	0.46
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.67	0.46
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:309:CHD:H162	23:C:309:CHD:H231	1.97	0.46
5:E:86:ILE:O	5:E:90:ARG:HG2	2.15	0.46
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.98	0.46
3:C:54[A]:MET:HE1	20:C:306:PGV:H152	1.97	0.46
1:N:310[A]:MET:HB3	2:O:73:LEU:HD22	1.98	0.46
2:O:168:LEU:HD13	2:O:184:LEU:HG	1.97	0.46
25:T:102:CDL:H402	25:T:102:CDL:H161	1.97	0.46
19:O:302:TGL:H362	30:R:394:HOH:O	2.14	0.46
24:P:304:PEK:H161	24:P:304:PEK:H132	1.72	0.46
7:T:37:LEU:CD2	25:T:102:CDL:H381	2.45	0.46
1:A:229[A]:ILE:HD11	2:B:175:ILE:HD13	1.97	0.46
1:N:289:ALA:HB1	1:N:297[B]:MET:HE1	1.96	0.46
4:Q:19[A]:ARG:HD2	4:Q:21[A]:ASP:OD1	2.15	0.46
1:A:321:PHE:CD2	2:B:65:TRP:HB2	2.51	0.46
3:C:142:VAL:HG21	25:G:101:CDL:H822	1.97	0.46
6:F:64:GLU:O	6:F:65:ASP:HB2	2.16	0.46
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.15	0.46
27:E:201:PSC:H252	27:E:201:PSC:H221	1.27	0.46
6:F:41:GLY:HA3	6:F:87[B]:THR:CG2	2.45	0.46
7:T:38:HIS:NE2	25:T:102:CDL:C11	2.79	0.46
1:A:243:VAL:HG11	14:A:602[C]:HEA:HMD2	1.98	0.46
19:A:607:TGL:HC42	30:L:238:HOH:O	2.16	0.46
3:C:156:ARG:HE	23:C:309:CHD:C24	2.28	0.46
2:B:28[C]:LEU:HD12	2:B:28[C]:LEU:HA	1.80	0.45
1:N:243:VAL:CG1	14:N:602[C]:HEA:HMD2	2.47	0.45
25:G:101:CDL:H151	25:G:101:CDL:H182	1.54	0.45
27:O:304:PSC:C07	9:V:10:ARG:HH21	2.30	0.45
3:P:38:ASN:O	26:P:310:DMU:H32	2.17	0.45
6:S:19:GLU:HG2	30:S:308:HOH:O	2.16	0.45
1:A:289:ALA:HB1	1:A:297[B]:MET:CE	2.47	0.45
2:B:115[B]:ASP:OD1	30:B:401:HOH:O	2.21	0.45
1:N:347:LEU:HB3	1:N:383[A]:MET:HB3	1.98	0.45
27:O:304:PSC:H31	30:O:550:HOH:O	2.16	0.45
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.16	0.45
9:I:35:TYR:C	9:I:35:TYR:CD2	2.90	0.45
23:J:102:CHD:H213	30:J:237:HOH:O	2.16	0.45
2:O:41[A]:ILE:O	2:O:45[A]:MET:HG2	2.16	0.45
27:O:304:PSC:C01	27:O:304:PSC:H212	2.46	0.45
1:N:152[B]:LEU:HD11	3:P:28:THR:HG21	1.99	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.97	0.45
26:P:315:DMU:H13	26:P:315:DMU:H18	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178[B]:GLN:NE2	7:T:8:HIS:O	2.50	0.45
3:C:51[A]:MET:CE	20:C:306:PGV:H161	2.47	0.45
1:A:186:TRP:HH2	7:T:7:ASP:HB3	1.80	0.45
1:A:285:PHE:CD2	7:T:3:ALA:O	2.69	0.45
7:G:34:ASN:HD22	25:G:101:CDL:H142	1.82	0.45
3:C:38:ASN:HA	30:C:410:HOH:O	2.17	0.45
25:C:308:CDL:H561	25:C:308:CDL:H532	1.75	0.45
7:G:41:HIS:HB3	7:G:74:ARG:NH1	2.32	0.45
1:N:290[C]:HIS:HB2	1:N:293:PHE:CE2	2.52	0.45
3:P:29:SER:HB2	26:P:312:DMU:H21	1.99	0.45
26:P:310:DMU:H7	26:P:311:DMU:H8	1.98	0.45
20:Q:201:PGV:H311	13:Z:16:ALA:HA	1.98	0.45
26:X:103:DMU:H11	26:X:103:DMU:O49	2.17	0.45
1:A:347:LEU:CG	1:A:383[A]:MET:HB3	2.47	0.45
19:D:201:TGL:HA41	19:D:201:TGL:HB51	1.99	0.45
1:N:2:PHE:CZ	25:Y:101:CDL:H721	2.51	0.45
19:O:301:TGL:HC32	30:O:569:HOH:O	2.16	0.45
27:O:304:PSC:C07	9:V:10:ARG:HE	2.30	0.45
3:P:51[A]:MET:HE1	30:P:557:HOH:O	2.15	0.44
25:T:102:CDL:H451	25:T:102:CDL:H422	1.68	0.44
26:X:103:DMU:H9	26:X:103:DMU:H14	1.58	0.44
1:A:169[B]:ILE:CD1	1:A:189[B]:MET:HE1	2.48	0.44
3:C:246:ASP:HB2	30:C:491:HOH:O	2.17	0.44
12:L:26:THR:HG23	13:M:25:SER:CB	2.47	0.44
2:B:60:GLU:H	2:B:60:GLU:HG3	1.48	0.44
4:D:121:LYS:NZ	21:D:202:EDO:O2	2.51	0.44
8:H:46:LYS:HZ3	8:U:55:TRP:H	1.64	0.44
1:N:22:PHE:HA	25:Y:101:CDL:H791	1.98	0.44
1:A:236:TRP:HH2	14:A:602[A]:HEA:HBD1	1.80	0.44
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.77	0.44
14:N:602[A]:HEA:HBC1	14:N:602[A]:HEA:HMC1	2.00	0.44
12:Y:47:LYS:HE3	12:Y:47:LYS:HB3	1.71	0.44
1:A:113:LEU:HB2	19:A:607:TGL:H302	2.00	0.44
4:D:78:TRP:CA	19:D:201:TGL:HB22	2.48	0.44
12:Y:2:HIS:CG	12:Y:3:TYR:H	2.35	0.44
27:E:201:PSC:H51	9:I:17:LEU:HD23	2.00	0.44
2:O:19:GLU:HG3	2:O:86[A]:MET:HE1	1.99	0.44
3:P:246:ASP:HB2	30:P:510:HOH:O	2.18	0.44
1:A:321:PHE:CD1	27:E:201:PSC:H341	2.53	0.44
1:A:378:HIS:HA	1:A:382[C]:SER:HB2	2.00	0.44
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B:301:TGL:H221	19:B:301:TGL:H252	1.56	0.44
9:I:31:PHE:CD1	9:I:31:PHE:C	2.90	0.44
30:N:719:HOH:O	19:O:302:TGL:HB31	2.18	0.44
3:C:180:GLU:HG3	30:C:401:HOH:O	2.18	0.44
4:Q:46:ALA:HB3	30:Q:353:HOH:O	2.16	0.44
1:N:229[A]:ILE:HD11	2:O:175:ILE:HD13	1.99	0.43
20:A:608:PGV:H011	20:A:608:PGV:H31	2.00	0.43
8:H:7:LYS:HG2	8:H:8:ILE:H	1.83	0.43
2:O:41[C]:ILE:O	2:O:45[C]:MET:HG2	2.17	0.43
4:Q:9:GLU:HG2	4:Q:12:ALA:HB3	2.00	0.43
1:A:318:VAL:O	1:A:322[B]:SER:OG	2.36	0.43
24:C:303:PEK:H322	20:C:305:PGV:H183	1.99	0.43
8:H:9:LYS:O	8:H:10:ASN:ND2	2.52	0.43
1:N:152[B]:LEU:CD1	3:P:28:THR:HG21	2.48	0.43
24:P:305:PEK:H381	25:T:102:CDL:H273	2.00	0.43
1:A:169[B]:ILE:HD11	1:A:189[B]:MET:HE1	2.00	0.43
7:G:38:HIS:CE1	25:G:101:CDL:H122	2.52	0.43
2:O:34[C]:ILE:HD11	2:O:72:ILE:HG21	2.01	0.43
2:O:89:GLU:O	2:O:91:ASN:ND2	2.52	0.43
3:P:156:ARG:HE	23:P:309:CHD:C24	2.31	0.43
12:Y:26[B]:THR:HG21	13:Z:21:VAL:HG12	2.00	0.43
20:C:307:PGV:H241	20:C:307:PGV:H272	1.50	0.43
9:V:1:SAC:HA	9:V:1:SAC:H2A1	1.73	0.43
2:B:58:ALA:O	2:B:62:GLU:HG3	2.18	0.43
8:H:46:LYS:HD3	8:U:52:VAL:HA	2.00	0.43
9:I:65:LYS:NZ	30:I:102:HOH:O	2.51	0.43
2:O:86[A]:MET:HE2	2:O:86[A]:MET:HB2	1.71	0.43
27:O:304:PSC:H212	27:O:304:PSC:H22	2.00	0.43
25:T:102:CDL:H382	25:T:102:CDL:H141	2.01	0.43
2:B:42[A]:ILE:HG22	19:D:201:TGL:H251	1.99	0.43
23:C:309:CHD:H183	23:C:309:CHD:H20	1.88	0.43
11:K:24:PHE:O	11:K:28[B]:VAL:HG23	2.18	0.43
1:N:364:ASP:OD1	14:N:602[A]:HEA:O1A	2.37	0.43
1:A:351:GLY:HA3	1:A:380[C]:VAL:HB	2.01	0.43
1:A:472:ILE:HG21	19:A:607:TGL:HA91	2.00	0.43
24:C:303:PEK:H203	24:C:303:PEK:H171	1.89	0.43
26:C:311:DMU:H2	26:J:101:DMU:O3	2.19	0.43
23:J:102:CHD:H191	23:J:102:CHD:H8	1.88	0.43
3:P:246:ASP:HB2	30:P:497:HOH:O	2.19	0.43
25:T:102:CDL:H832	25:T:102:CDL:H801	1.83	0.43
1:A:513:LEU:O	1:A:514:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:7:LYS:HB3	4:Q:10:ASP:OD1	2.19	0.43
2:B:91:ASN:HB3	2:B:149:THR:HG21	2.00	0.42
9:I:15:ARG:HD3	30:I:160:HOH:O	2.19	0.42
7:T:36:TRP:CG	7:T:36:TRP:O	2.71	0.42
1:A:152[B]:LEU:CD1	3:C:28:THR:HG21	2.49	0.42
14:A:602[A]:HEA:HHA	14:A:602[A]:HEA:HAD2	1.77	0.42
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.48	0.42
14:N:602[A]:HEA:HMB1	30:N:702:HOH:O	2.19	0.42
20:N:607:PGV:H343	24:P:304:PEK:C38	2.47	0.42
3:C:224:LYS:CD	25:C:308:CDL:HB31	2.49	0.42
8:H:45:ALA:O	8:H:47:GLY:N	2.53	0.42
25:P:308:CDL:H521	25:P:308:CDL:OB9	2.19	0.42
1:N:309:THR:CG2	14:N:602[C]:HEA:HMB2	2.46	0.42
6:S:10:GLU:OE2	6:S:25:ARG:NH2	2.46	0.42
24:C:303:PEK:H201	30:C:563:HOH:O	2.19	0.42
11:K:54:ARG:HE	11:K:54:ARG:HB3	1.64	0.42
25:T:102:CDL:HA62	25:T:102:CDL:H311	1.70	0.42
21:A:615:EDO:H12	2:B:58:ALA:HB3	2.02	0.42
2:B:16:ILE:HD12	2:B:87:MET:HG2	2.01	0.42
3:P:156:ARG:HE	23:P:309:CHD:C23	2.32	0.42
26:C:311:DMU:H26	10:J:38:LEU:HD23	2.00	0.42
12:L:45:LEU:HD23	12:L:45:LEU:HA	1.89	0.42
1:N:362:SER:OG	2:O:87[A]:MET:HE2	2.20	0.42
24:P:304:PEK:H31	24:P:304:PEK:H71	2.01	0.42
3:C:92:LEU:O	3:C:95[B]:THR:OG1	2.28	0.42
9:I:57:MET:O	9:I:61:GLU:HG2	2.19	0.42
1:N:378:HIS:O	1:N:383[C]:MET:HG2	2.20	0.42
1:A:321:PHE:HB3	2:B:65:TRP:CE3	2.55	0.42
2:B:9:PHE:HA	21:B:305:EDO:H12	2.01	0.42
27:O:304:PSC:H292	27:O:304:PSC:H261	1.51	0.42
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.19	0.42
1:A:243:VAL:CG1	14:A:602[C]:HEA:HMD2	2.49	0.41
20:A:608:PGV:H142	20:A:608:PGV:H301	2.02	0.41
3:C:45:ILE:HD13	26:C:311:DMU:H21	2.02	0.41
3:C:246:ASP:HB2	30:C:521:HOH:O	2.20	0.41
25:C:308:CDL:H162	25:C:308:CDL:H361	2.02	0.41
25:C:308:CDL:H312	25:C:308:CDL:HA61	1.89	0.41
12:L:44:LEU:O	12:L:47:LYS:HD2	2.19	0.41
1:N:347:LEU:HB3	1:N:383[A]:MET:CB	2.50	0.41
14:N:602[C]:HEA:HMB1	14:N:602[C]:HEA:H11	1.84	0.41
5:R:80:GLU:H	5:R:80:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:9:LYS:HA	8:U:9:LYS:HD3	1.49	0.41
19:B:301:TGL:HA92	19:B:301:TGL:HA62	1.82	0.41
1:N:355:GLY:O	14:N:602[C]:HEA:CHB	2.68	0.41
19:O:302:TGL:HB21	4:Q:78:TRP:HB3	2.02	0.41
9:V:35:TYR:CZ	9:V:39:VAL:HG11	2.55	0.41
1:A:377:PHE:CD2	14:A:602[C]:HEA:HBD2	2.55	0.41
6:S:37:LYS:HD2	6:S:37:LYS:HA	1.80	0.41
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.92	0.41
3:P:80[A]:ARG:NH2	3:P:236:GLU:OE1	2.49	0.41
6:S:85:CYS:SG	6:S:87[A]:THR:HG23	2.61	0.41
8:H:9:LYS:HA	8:H:9:LYS:HD2	1.76	0.41
1:N:246:LEU:HB3	1:N:381[C]:LEU:HD11	2.03	0.41
4:Q:20[A]:ARG:HG2	30:Q:360:HOH:O	2.20	0.41
13:Z:28:LEU:HD23	26:Z:101:DMU:H7	2.02	0.41
3:C:51[A]:MET:HE2	20:C:306:PGV:H161	2.02	0.41
1:N:355:GLY:O	14:N:602[C]:HEA:HMB3	2.20	0.41
14:A:602[A]:HEA:HBC1	14:A:602[A]:HEA:HMC1	2.02	0.41
20:A:608:PGV:H51	20:A:608:PGV:H22	1.97	0.41
21:A:617:EDO:H11	12:L:10:ASN:HD22	1.85	0.41
1:N:362:SER:HB3	2:O:20:LEU:HD21	2.03	0.41
4:Q:19[A]:ARG:CD	4:Q:21[A]:ASP:OD1	2.69	0.41
7:T:37:LEU:C	7:T:38:HIS:HD1	2.24	0.41
13:Z:24:LEU:HD23	13:Z:24:LEU:HA	1.91	0.41
10:J:33:ARG:HD3	30:J:232:HOH:O	2.20	0.41
2:O:16:ILE:HD12	2:O:16:ILE:HG23	1.71	0.41
12:Y:22:LEU:O	12:Y:26[B]:THR:HG23	2.20	0.41
1:A:152[B]:LEU:HD11	3:C:28:THR:HG21	2.01	0.41
25:C:308:CDL:HB62	25:C:308:CDL:H522	2.03	0.41
1:N:44:PRO:HG3	4:Q:111:PHE:CZ	2.56	0.41
1:N:351:GLY:HA3	1:N:380[C]:VAL:HB	2.03	0.41
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.50	0.41
7:T:84:LYS:H	7:T:84:LYS:NZ	2.19	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.86	0.41
30:E:351:HOH:O	9:I:10:ARG:HG2	2.21	0.41
25:P:308:CDL:H402	25:P:308:CDL:H431	1.93	0.41
3:C:51[A]:MET:SD	25:C:308:CDL:H621	2.61	0.40
11:K:24:PHE:O	11:K:28[A]:VAL:HG12	2.21	0.40
2:O:7:LEU:HD11	19:O:301:TGL:H161	2.04	0.40
26:P:310:DMU:H17	10:W:45:TYR:CG	2.56	0.40
4:Q:7:LYS:HG2	4:Q:13:LEU:HD12	2.04	0.40
8:U:9:LYS:HA	30:U:264:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:607:PGV:C18	24:P:304:PEK:H322	2.51	0.40
8:U:9:LYS:O	8:U:10:ASN:HB2	2.21	0.40
2:B:5[A]:MET:HE2	11:K:43:SER:HB2	2.03	0.40
6:F:62:CYS:HB3	6:F:85:CYS:HB3	2.03	0.40
23:G:102:CHD:H12	23:G:102:CHD:H212	2.02	0.40
30:O:459:HOH:O	4:Q:21[B]:ASP:HB2	2.20	0.40
6:S:54:ASN:HD22	6:S:54:ASN:C	2.23	0.40
9:V:31:PHE:CD1	9:V:31:PHE:C	2.93	0.40
20:A:608:PGV:H202	20:A:608:PGV:H232	1.74	0.40
23:C:309:CHD:H112	23:C:309:CHD:H12A	1.86	0.40
1:N:383[B]:MET:HE2	1:N:425:PHE:HD2	1.86	0.40
3:P:3:HIS:CD2	3:P:3:HIS:N	2.87	0.40
25:Y:101:CDL:OB9	25:Y:101:CDL:H122	2.21	0.40
1:A:113:LEU:HB2	19:A:607:TGL:C30	2.52	0.40
1:A:377:PHE:CD2	14:A:602[A]:HEA:HAD1	2.57	0.40
3:C:59:ARG:HB2	25:C:308:CDL:H512	2.04	0.40
11:K:26:VAL:HG13	26:K:101:DMU:H11	2.03	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	550/514 (107%)	531 (96%)	17 (3%)	2 (0%)	34	13
1	N	549/514 (107%)	532 (97%)	15 (3%)	2 (0%)	34	13
2	B	251/227 (111%)	246 (98%)	5 (2%)	0	100	100
2	O	251/227 (111%)	245 (98%)	6 (2%)	0	100	100
3	C	264/259 (102%)	260 (98%)	4 (2%)	0	100	100
3	P	263/259 (102%)	257 (98%)	6 (2%)	0	100	100
4	D	143/144 (99%)	140 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Q	145/144 (101%)	141 (97%)	2 (1%)	2 (1%)	11	2
5	E	102/104 (98%)	102 (100%)	0	0	100	100
5	R	102/104 (98%)	102 (100%)	0	0	100	100
6	F	94/93 (101%)	92 (98%)	2 (2%)	0	100	100
6	S	95/93 (102%)	93 (98%)	2 (2%)	0	100	100
7	G	78/84 (93%)	71 (91%)	2 (3%)	5 (6%)	1	0
7	T	84/84 (100%)	73 (87%)	7 (8%)	4 (5%)	2	0
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	3	0
8	U	77/79 (98%)	69 (90%)	4 (5%)	4 (5%)	2	0
9	I	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
9	V	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
10	J	55/57 (96%)	55 (100%)	0	0	100	100
10	W	55/57 (96%)	55 (100%)	0	0	100	100
11	K	49/49 (100%)	48 (98%)	1 (2%)	0	100	100
11	X	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
12	L	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
12	Y	45/46 (98%)	44 (98%)	1 (2%)	0	100	100
13	M	40/41 (98%)	39 (98%)	1 (2%)	0	100	100
13	Z	39/41 (95%)	39 (100%)	0	0	100	100
All	All	3641/3540 (103%)	3533 (97%)	86 (2%)	22 (1%)	25	7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384[A]	GLY
1	A	384[B]	GLY
7	G	7	ASP
7	G	8	HIS
8	H	10	ASN
1	N	384[A]	GLY
1	N	384[B]	GLY
7	T	4	ALA
8	U	45	ALA
7	G	37	LEU
8	H	48	GLY

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Mol	Chain	Res	Type
4	Q	7	LYS
7	T	7	ASP
8	U	9	LYS
8	U	46	LYS
8	H	46	LYS
4	Q	6	VAL
7	T	5	LYS
8	U	10	ASN
7	G	9	GLY
7	T	6	GLY
7	G	6	GLY

5.3.2 Protein sidechains [i](#)

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	463/426 (109%)	459 (99%)	4 (1%)	78	57
1	N	462/426 (108%)	455 (98%)	7 (2%)	65	35
2	B	236/210 (112%)	227 (96%)	9 (4%)	33	5
2	O	236/210 (112%)	229 (97%)	7 (3%)	41	9
3	C	231/224 (103%)	227 (98%)	4 (2%)	60	28
3	P	230/224 (103%)	226 (98%)	4 (2%)	60	28
4	D	129/128 (101%)	128 (99%)	1 (1%)	81	62
4	Q	131/128 (102%)	129 (98%)	2 (2%)	65	35
5	E	91/91 (100%)	90 (99%)	1 (1%)	73	48
5	R	91/91 (100%)	90 (99%)	1 (1%)	73	48
6	F	81/78 (104%)	79 (98%)	2 (2%)	47	14
6	S	82/78 (105%)	80 (98%)	2 (2%)	49	16
7	G	65/68 (96%)	59 (91%)	6 (9%)	9	0
7	T	68/68 (100%)	60 (88%)	8 (12%)	5	0
8	H	71/71 (100%)	67 (94%)	4 (6%)	21	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	U	71/71 (100%)	66 (93%)	5 (7%)	15	1
9	I	57/57 (100%)	56 (98%)	1 (2%)	59	26
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	6
10	J	48/48 (100%)	48 (100%)	0	100	100
10	W	48/48 (100%)	47 (98%)	1 (2%)	53	19
11	K	41/39 (105%)	41 (100%)	0	100	100
11	X	39/39 (100%)	39 (100%)	0	100	100
12	L	39/39 (100%)	38 (97%)	1 (3%)	46	13
12	Y	40/39 (103%)	38 (95%)	2 (5%)	24	2
13	M	36/35 (103%)	35 (97%)	1 (3%)	43	11
13	Z	35/35 (100%)	34 (97%)	1 (3%)	42	10
All	All	3178/3028 (105%)	3102 (98%)	76 (2%)	50	16

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	338	MET
1	A	369	ASP
2	B	33[A]	LEU
2	B	33[C]	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	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
3	C	230	ASN
4	D	4	SER
5	E	90	ARG
6	F	54[A]	ASN
6	F	54[B]	ASN
7	G	7	ASP

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Mol	Chain	Res	Type
7	G	11	THR
7	G	18	PHE
7	G	33	LEU
7	G	42	ARG
7	G	54	ARG
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
8	H	84	LYS
9	I	36	LYS
12	L	2	HIS
13	M	38	ASP
1	N	38	ARG
1	N	109	PHE
1	N	152[A]	LEU
1	N	152[B]	LEU
1	N	290[A]	HIS
1	N	290[C]	HIS
1	N	369	ASP
2	O	33[A]	LEU
2	O	33[C]	LEU
2	O	78	LEU
2	O	89	GLU
2	O	115	ASP
2	O	171	LYS
2	O	226	MET
3	P	3	HIS
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	10	ASP
4	Q	51	LEU
5	R	80	GLU
6	S	54	ASN
6	S	94	HIS
7	T	2	SER
7	T	11	THR
7	T	18	PHE
7	T	33	LEU
7	T	37	LEU
7	T	38	HIS
7	T	42	ARG

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Mol	Chain	Res	Type
7	T	54	ARG
8	U	8	ILE
8	U	9	LYS
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	36	LYS
9	V	73	LYS
10	W	50	LEU
12	Y	26[A]	THR
12	Y	26[B]	THR
13	Z	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	10	GLN
2	B	52	HIS
2	B	181	GLN
2	B	195	GLN
2	B	203	ASN
3	C	50	ASN
3	C	68	GLN
4	D	29	HIS
4	D	101	HIS
5	E	94	ASN
7	G	34	ASN
8	H	23	GLN
8	H	37	HIS
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS
3	P	50	ASN
3	P	68	GLN
3	P	76	GLN
4	Q	109	HIS
5	R	78	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	54	ASN
6	S	94	HIS
7	T	34	ASN
8	U	24	ASN
10	W	29	ASN
11	X	35	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SAC	V	1	9	7,8,9	0.65	0	8,9,11	0.94	1 (12%)
1	FME	N	1	1	8,9,10	0.46	0	7,9,11	1.83	2 (28%)
1	FME	A	1	1	8,9,10	1.09	0	7,9,11	2.41	5 (71%)
2	FME	B	1	2	8,9,10	1.34	1 (12%)	7,9,11	1.12	0
2	FME	O	1	2	8,9,10	0.78	0	7,9,11	1.09	1 (14%)
9	SAC	I	1	9	7,8,9	0.72	0	8,9,11	1.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SAC	V	1	9	-	4/7/8/10	-

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CB-CG	2.48	1.61	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	CE-SD-CG	3.66	112.98	100.40
1	A	1	FME	CE-SD-CG	3.50	112.42	100.40
1	A	1	FME	CA-N-CN	-3.37	117.64	122.82
1	N	1	FME	O-C-CA	-2.44	118.37	124.78
1	A	1	FME	CG-CB-CA	-2.33	106.47	112.95
1	A	1	FME	O-C-CA	-2.30	118.74	124.78
2	O	1	FME	O-C-CA	-2.23	118.93	124.78
9	V	1	SAC	O-C-CA	-2.18	119.06	124.78
1	A	1	FME	O1-CN-N	-2.09	119.75	125.27

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	CB-CA-N-CN
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	O-C-CA-CB
9	I	1	SAC	C-CA-CB-OG
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C-CA-CB-OG
9	I	1	SAC	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	N	1	FME	CB-CG-SD-CE
9	V	1	SAC	N-CA-CB-OG
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	N	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	V	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 128 ligands modelled in this entry, 10 are monoatomic - leaving 118 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$
26	DMU	K	103	-	17,17,34	0.65	0	17,18,45	1.20	1 (5%)
23	CHD	P	309	-	32,32,32	0.78	0	51,51,51	1.87	12 (23%)
19	TGL	O	301	-	62,62,62	1.11	3 (4%)	65,65,65	1.40	7 (10%)
21	EDO	B	307	-	3,3,3	0.49	0	2,2,2	0.42	0
14	HEA	A	602[A]	1	57,67,67	1.50	9 (15%)	61,103,103	2.25	26 (42%)
23	CHD	W	101	-	32,32,32	0.87	0	51,51,51	2.36	18 (35%)
26	DMU	P	311	-	34,34,34	0.80	1 (2%)	45,45,45	1.23	6 (13%)
21	EDO	A	616	-	3,3,3	0.81	0	2,2,2	0.55	0
20	PGV	A	608	-	45,45,50	1.18	4 (8%)	49,50,56	1.44	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	P	306	-	44,44,50	0.82	2 (4%)	47,50,56	1.12	3 (6%)
21	EDO	A	609	-	3,3,3	0.42	0	2,2,2	0.32	0
19	TGL	A	607	-	62,62,62	1.22	3 (4%)	65,65,65	2.02	18 (27%)
26	DMU	K	102	-	22,22,34	1.45	5 (22%)	27,27,45	1.78	6 (22%)
21	EDO	O	305	-	3,3,3	0.79	0	2,2,2	0.75	0
24	PEK	T	101	-	48,48,52	1.20	2 (4%)	51,53,57	1.56	9 (17%)
24	PEK	C	304	-	43,43,52	1.16	2 (4%)	44,44,57	1.41	5 (11%)
20	PGV	P	307	-	50,50,50	1.06	2 (4%)	53,56,56	1.60	7 (13%)
14	HEA	N	602[C]	1	57,67,67	1.49	7 (12%)	61,103,103	2.04	19 (31%)
21	EDO	A	612	-	3,3,3	0.33	0	2,2,2	1.09	0
21	EDO	N	613	-	3,3,3	0.64	0	2,2,2	0.54	0
21	EDO	B	305	-	3,3,3	0.91	0	2,2,2	1.48	1 (50%)
26	DMU	P	316	-	22,22,34	1.20	2 (9%)	27,27,45	2.22	9 (33%)
26	DMU	X	102	-	22,22,34	1.35	3 (13%)	27,27,45	1.39	5 (18%)
21	EDO	A	617	-	3,3,3	0.70	0	2,2,2	0.71	0
25	CDL	Y	101	-	86,86,99	1.35	10 (11%)	92,98,111	1.23	8 (8%)
21	EDO	A	613	-	3,3,3	0.78	0	2,2,2	0.28	0
21	EDO	N	608	-	3,3,3	0.79	0	2,2,2	0.65	0
21	EDO	E	202	-	3,3,3	0.65	0	2,2,2	0.40	0
21	EDO	N	610	-	3,3,3	0.34	0	2,2,2	1.04	0
24	PEK	P	303	-	21,21,52	1.11	1 (4%)	21,21,57	1.26	3 (14%)
26	DMU	L	101	-	18,18,34	1.21	1 (5%)	23,23,45	1.56	3 (13%)
25	CDL	C	308	-	84,84,99	1.41	13 (15%)	91,94,111	1.59	17 (18%)
21	EDO	N	611	-	3,3,3	0.65	0	2,2,2	0.86	0
21	EDO	F	102	-	3,3,3	0.89	0	2,2,2	0.55	0
19	TGL	O	302	-	62,62,62	1.12	4 (6%)	65,65,65	1.10	4 (6%)
21	EDO	S	106	-	3,3,3	0.68	0	2,2,2	0.52	0
19	TGL	B	301	-	61,61,62	1.18	3 (4%)	64,64,65	1.61	9 (14%)
18	CYN	N	606[A]	15	0,1,1	-	-	-	-	-
21	EDO	P	314	-	3,3,3	0.39	0	2,2,2	1.36	0
21	EDO	A	614	-	3,3,3	0.73	0	2,2,2	0.57	0
21	EDO	E	203	-	3,3,3	0.48	0	2,2,2	0.59	0
21	EDO	R	201	-	3,3,3	0.61	0	2,2,2	0.60	0
24	PEK	C	303	-	50,50,52	0.75	2 (4%)	53,55,57	1.05	4 (7%)
23	CHD	J	102	-	32,32,32	0.89	1 (3%)	51,51,51	2.70	22 (43%)
21	EDO	O	308	-	3,3,3	0.56	0	2,2,2	0.56	0
21	EDO	S	108	-	3,3,3	0.68	0	2,2,2	0.57	0
21	EDO	B	306	-	3,3,3	0.79	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	Q	201	-	50,50,50	1.02	2 (4%)	53,56,56	1.53	8 (15%)
21	EDO	O	306	-	3,3,3	0.81	0	2,2,2	0.20	0
26	DMU	M	101	-	34,34,34	0.65	1 (2%)	45,45,45	1.38	9 (20%)
18	CYN	A	606[A]	15	0,1,1	-	-	-	-	-
14	HEA	A	601[B]	-	57,67,67	1.65	13 (22%)	61,103,103	1.88	14 (22%)
23	CHD	C	301	-	32,32,32	1.10	2 (6%)	51,51,51	1.67	10 (19%)
29	PO4	U	102	-	4,4,4	0.58	0	6,6,6	0.70	0
22	CUA	O	303	2	0,1,1	-	-	-	-	-
24	PEK	P	305	-	45,45,52	1.21	2 (4%)	47,47,57	1.57	4 (8%)
25	CDL	G	101	-	87,87,99	1.43	13 (14%)	91,97,111	1.52	10 (10%)
21	EDO	U	101	-	3,3,3	0.65	0	2,2,2	0.38	0
21	EDO	Q	202	-	3,3,3	0.60	0	2,2,2	0.14	0
25	CDL	P	308	-	71,74,99	1.60	10 (14%)	72,78,111	1.63	10 (13%)
21	EDO	N	615	-	3,3,3	0.62	0	2,2,2	0.50	0
23	CHD	B	303	-	32,32,32	0.82	1 (3%)	51,51,51	1.91	17 (33%)
26	DMU	X	101	-	22,22,34	1.56	2 (9%)	27,27,45	1.99	9 (33%)
21	EDO	N	609	-	3,3,3	0.28	0	2,2,2	0.55	0
21	EDO	T	104	-	3,3,3	0.56	0	2,2,2	0.28	0
24	PEK	P	304	-	52,52,52	0.56	0	55,57,57	1.17	3 (5%)
14	HEA	N	601[A]	-	57,67,67	1.53	13 (22%)	61,103,103	1.80	13 (21%)
26	DMU	X	103	-	22,22,34	1.18	1 (4%)	27,27,45	1.69	7 (25%)
26	DMU	Z	101	-	34,34,34	0.51	0	45,45,45	1.18	4 (8%)
26	DMU	K	101	-	22,22,34	1.27	1 (4%)	27,27,45	1.61	7 (25%)
21	EDO	C	310	-	3,3,3	0.90	0	2,2,2	0.25	0
26	DMU	P	310	-	34,34,34	0.53	0	45,45,45	1.31	5 (11%)
21	EDO	S	103	-	3,3,3	0.65	0	2,2,2	0.18	0
26	DMU	C	311	-	34,34,34	0.86	0	45,45,45	1.83	12 (26%)
21	EDO	A	615	-	3,3,3	0.35	0	2,2,2	0.67	0
26	DMU	P	315	-	34,34,34	1.05	3 (8%)	45,45,45	1.92	12 (26%)
23	CHD	P	301	-	32,32,32	0.93	2 (6%)	51,51,51	1.47	8 (15%)
21	EDO	F	103	-	3,3,3	0.88	0	2,2,2	0.28	0
20	PGV	C	306	-	50,50,50	0.85	2 (4%)	53,56,56	0.90	2 (3%)
20	PGV	C	307	-	46,46,50	1.27	2 (4%)	49,52,56	1.83	9 (18%)
21	EDO	S	104	-	3,3,3	0.65	0	2,2,2	0.98	0
14	HEA	N	602[A]	1	57,67,67	1.48	9 (15%)	61,103,103	2.15	21 (34%)
21	EDO	S	107	-	3,3,3	0.66	0	2,2,2	0.68	0
21	EDO	B	308	-	3,3,3	1.24	0	2,2,2	0.73	0
25	CDL	T	102	-	79,79,99	1.36	9 (11%)	84,89,111	1.57	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHD	C	309	-	32,32,32	0.91	0	51,51,51	2.52	13 (25%)
14	HEA	A	602[C]	1	57,67,67	1.42	10 (17%)	61,103,103	2.24	25 (40%)
27	PSC	E	201	-	51,51,51	1.21	3 (5%)	57,59,59	1.83	7 (12%)
21	EDO	A	610	-	3,3,3	1.08	0	2,2,2	1.03	0
21	EDO	B	304	-	3,3,3	0.71	0	2,2,2	0.47	0
22	CUA	B	302	2	0,1,1	-	-	-	-	-
26	DMU	G	105	-	21,21,34	1.24	2 (9%)	24,25,45	2.11	7 (29%)
21	EDO	D	202	-	3,3,3	0.47	0	2,2,2	0.53	0
18	CYN	N	606[C]	15	0,1,1	-	-	-	-	-
20	PGV	C	305	-	50,50,50	0.79	0	53,56,56	0.87	0
26	DMU	P	312	-	34,34,34	0.80	1 (2%)	45,45,45	1.25	4 (8%)
21	EDO	G	104	-	3,3,3	0.63	0	2,2,2	0.60	0
21	EDO	O	307	-	3,3,3	0.58	0	2,2,2	0.51	0
21	EDO	S	105	-	3,3,3	0.98	0	2,2,2	0.88	0
27	PSC	O	304	-	50,50,51	1.24	3 (6%)	56,58,59	1.98	11 (19%)
23	CHD	G	102	-	32,32,32	0.80	1 (3%)	51,51,51	1.51	7 (13%)
21	EDO	N	612	-	3,3,3	0.49	0	2,2,2	0.35	0
14	HEA	A	601[A]	-	57,67,67	1.62	14 (24%)	61,103,103	1.96	16 (26%)
21	EDO	G	103	-	3,3,3	0.72	0	2,2,2	0.56	0
14	HEA	N	601[B]	-	57,67,67	1.56	13 (22%)	61,103,103	1.74	15 (24%)
18	CYN	A	606[C]	15	0,1,1	-	-	-	-	-
21	EDO	A	611	-	3,3,3	0.29	0	2,2,2	0.51	0
21	EDO	T	103	-	3,3,3	0.83	0	2,2,2	0.83	0
21	EDO	F	104	-	3,3,3	0.76	0	2,2,2	0.64	0
19	TGL	D	201	-	47,47,62	1.71	5 (10%)	50,50,65	1.27	8 (16%)
21	EDO	Y	102	-	3,3,3	0.48	0	2,2,2	0.06	0
26	DMU	J	101	-	34,34,34	0.95	1 (2%)	45,45,45	1.47	8 (17%)
21	EDO	N	614	-	3,3,3	0.79	0	2,2,2	0.44	0
21	EDO	S	102	-	3,3,3	0.72	0	2,2,2	0.52	0
20	PGV	N	607	-	50,50,50	1.10	6 (12%)	53,56,56	1.26	5 (9%)
21	EDO	P	313	-	3,3,3	0.84	0	2,2,2	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	DMU	K	103	-	-	4/11/19/59	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHD	P	309	-	-	5/9/74/74	0/4/4/4
19	TGL	O	301	-	-	33/65/65/65	-
21	EDO	B	307	-	-	0/1/1/1	-
14	HEA	A	602[A]	1	-	7/32/76/76	-
23	CHD	W	101	-	-	5/9/74/74	0/4/4/4
26	DMU	P	311	-	-	7/19/59/59	0/2/2/2
21	EDO	A	616	-	-	0/1/1/1	-
20	PGV	A	608	-	-	18/47/47/55	-
20	PGV	P	306	-	-	8/49/49/55	-
21	EDO	A	609	-	-	0/1/1/1	-
19	TGL	A	607	-	-	31/65/65/65	-
26	DMU	K	102	-	-	8/13/33/59	0/1/1/2
21	EDO	O	305	-	-	0/1/1/1	-
24	PEK	T	101	-	-	18/52/52/56	-
24	PEK	C	304	-	-	22/43/43/56	-
20	PGV	P	307	-	-	14/55/55/55	-
14	HEA	N	602[C]	1	-	6/32/76/76	-
21	EDO	A	612	-	-	0/1/1/1	-
21	EDO	N	613	-	-	0/1/1/1	-
21	EDO	B	305	-	-	1/1/1/1	-
26	DMU	P	316	-	-	7/13/33/59	0/1/1/2
26	DMU	X	102	-	-	9/13/33/59	0/1/1/2
21	EDO	A	617	-	-	1/1/1/1	-
25	CDL	Y	101	-	-	39/97/97/110	-
21	EDO	A	613	-	-	0/1/1/1	-
21	EDO	N	608	-	-	0/1/1/1	-
21	EDO	E	202	-	-	0/1/1/1	-
21	EDO	N	610	-	-	0/1/1/1	-
24	PEK	P	303	-	-	7/19/19/56	-
26	DMU	L	101	-	-	2/9/29/59	0/1/1/2
25	CDL	C	308	-	-	35/90/90/110	-
21	EDO	N	611	-	-	0/1/1/1	-
21	EDO	F	102	-	-	0/1/1/1	-
19	TGL	O	302	-	-	26/65/65/65	-
21	EDO	S	106	-	-	1/1/1/1	-
19	TGL	B	301	-	-	33/64/64/65	-
21	EDO	P	314	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	EDO	A	614	-	-	0/1/1/1	-
21	EDO	E	203	-	-	0/1/1/1	-
21	EDO	R	201	-	-	0/1/1/1	-
24	PEK	C	303	-	-	14/54/54/56	-
23	CHD	J	102	-	-	7/9/74/74	0/4/4/4
21	EDO	O	308	-	-	0/1/1/1	-
21	EDO	S	108	-	-	1/1/1/1	-
21	EDO	B	306	-	-	0/1/1/1	-
20	PGV	Q	201	-	-	14/55/55/55	-
21	EDO	O	306	-	-	0/1/1/1	-
26	DMU	M	101	-	-	5/19/59/59	0/2/2/2
14	HEA	A	601[B]	-	-	5/32/76/76	-
23	CHD	C	301	-	-	2/9/74/74	0/4/4/4
24	PEK	P	305	-	-	22/47/47/56	-
25	CDL	G	101	-	-	31/94/94/110	-
21	EDO	U	101	-	-	1/1/1/1	-
21	EDO	Q	202	-	-	1/1/1/1	-
25	CDL	P	308	-	-	23/73/77/110	-
21	EDO	N	615	-	-	0/1/1/1	-
23	CHD	B	303	-	-	2/9/74/74	0/4/4/4
26	DMU	X	101	-	-	5/13/33/59	0/1/1/2
21	EDO	N	609	-	-	0/1/1/1	-
21	EDO	T	104	-	-	0/1/1/1	-
24	PEK	P	304	-	-	8/56/56/56	-
14	HEA	N	601[A]	-	-	4/32/76/76	-
26	DMU	X	103	-	-	7/13/33/59	0/1/1/2
26	DMU	Z	101	-	-	6/19/59/59	0/2/2/2
26	DMU	K	101	-	-	4/13/33/59	0/1/1/2
21	EDO	C	310	-	-	0/1/1/1	-
26	DMU	P	310	-	-	9/19/59/59	0/2/2/2
21	EDO	S	103	-	-	0/1/1/1	-
26	DMU	C	311	-	-	7/19/59/59	0/2/2/2
21	EDO	A	615	-	-	0/1/1/1	-
26	DMU	P	315	-	-	10/19/59/59	0/2/2/2
23	CHD	P	301	-	-	1/9/74/74	0/4/4/4
21	EDO	F	103	-	-	0/1/1/1	-
20	PGV	C	306	-	-	12/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	C	307	-	-	18/51/51/55	-
21	EDO	S	104	-	-	0/1/1/1	-
14	HEA	N	602[A]	1	-	7/32/76/76	-
21	EDO	S	107	-	-	1/1/1/1	-
21	EDO	B	308	-	-	0/1/1/1	-
25	CDL	T	102	-	-	30/87/87/110	-
23	CHD	C	309	-	-	6/9/74/74	0/4/4/4
14	HEA	A	602[C]	1	-	5/32/76/76	-
27	PSC	E	201	-	-	28/55/55/55	-
21	EDO	A	610	-	-	0/1/1/1	-
21	EDO	B	304	-	-	0/1/1/1	-
26	DMU	G	105	-	-	6/13/29/59	0/1/1/2
21	EDO	D	202	-	-	1/1/1/1	-
20	PGV	C	305	-	-	7/55/55/55	-
26	DMU	P	312	-	-	5/19/59/59	0/2/2/2
21	EDO	G	104	-	-	0/1/1/1	-
21	EDO	O	307	-	-	0/1/1/1	-
21	EDO	S	105	-	-	0/1/1/1	-
27	PSC	O	304	-	-	24/54/54/55	-
23	CHD	G	102	-	-	2/9/74/74	0/4/4/4
21	EDO	N	612	-	-	0/1/1/1	-
14	HEA	A	601[A]	-	-	8/32/76/76	-
21	EDO	G	103	-	-	0/1/1/1	-
14	HEA	N	601[B]	-	-	5/32/76/76	-
21	EDO	A	611	-	-	0/1/1/1	-
21	EDO	T	103	-	-	0/1/1/1	-
21	EDO	F	104	-	-	0/1/1/1	-
19	TGL	D	201	-	-	19/50/50/65	-
21	EDO	Y	102	-	-	0/1/1/1	-
26	DMU	J	101	-	-	5/19/59/59	0/2/2/2
21	EDO	N	614	-	-	0/1/1/1	-
21	EDO	S	102	-	-	0/1/1/1	-
20	PGV	N	607	-	-	4/55/55/55	-
21	EDO	P	313	-	-	0/1/1/1	-

All (227) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	201	TGL	OB1-CB1	7.11	1.43	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	607	TGL	OG2-CB1	5.83	1.50	1.34
20	C	307	PGV	O03-C19	5.83	1.50	1.33
25	P	308	CDL	OA8-CA7	5.78	1.50	1.33
19	D	201	TGL	OG2-CB1	5.70	1.50	1.34
27	E	201	PSC	O01-C1	5.42	1.49	1.34
24	T	101	PEK	O03-C21	5.42	1.49	1.33
24	P	305	PEK	O01-C1	5.32	1.49	1.34
20	P	307	PGV	O03-C19	5.32	1.48	1.33
25	G	101	CDL	OA6-CA5	5.23	1.49	1.34
27	O	304	PSC	O01-C1	5.21	1.49	1.34
19	O	301	TGL	OG2-CB1	5.18	1.48	1.34
25	P	308	CDL	OA6-CA5	5.11	1.48	1.34
24	C	304	PEK	O01-C1	5.05	1.48	1.33
19	B	301	TGL	OG2-CB1	5.01	1.48	1.34
20	A	608	PGV	O03-C19	5.00	1.48	1.33
25	P	308	CDL	OB6-CB5	5.00	1.47	1.33
19	A	607	TGL	OG3-CC1	4.96	1.47	1.33
24	P	305	PEK	O03-C21	4.95	1.47	1.33
25	G	101	CDL	OA8-CA7	4.91	1.47	1.33
25	Y	101	CDL	OA6-CA5	4.90	1.48	1.34
24	P	303	PEK	O01-C1	4.89	1.47	1.30
25	P	308	CDL	OB8-CB7	4.88	1.47	1.33
25	T	102	CDL	OB8-CB7	4.83	1.47	1.33
20	C	307	PGV	O01-C1	4.82	1.47	1.34
25	T	102	CDL	OA6-CA5	4.80	1.47	1.34
25	C	308	CDL	OA8-CA7	4.76	1.47	1.33
26	X	101	DMU	O16-C6	4.75	1.48	1.40
19	O	302	TGL	OG1-CA1	4.75	1.47	1.33
24	C	304	PEK	O03-C21	4.73	1.47	1.33
25	G	101	CDL	OB8-CB7	4.72	1.47	1.33
25	Y	101	CDL	OB8-CB7	4.68	1.47	1.33
19	B	301	TGL	OG1-CA1	4.68	1.47	1.33
20	Q	201	PGV	O03-C19	4.63	1.46	1.33
19	D	201	TGL	OG1-CA1	4.56	1.46	1.33
19	O	302	TGL	OG2-CB1	4.54	1.47	1.34
24	T	101	PEK	O01-C1	4.46	1.46	1.34
14	N	602[C]	HEA	CHD-C1D	4.43	1.46	1.35
27	O	304	PSC	O03-C19	4.43	1.46	1.33
19	A	607	TGL	OG1-CA1	4.41	1.46	1.33
25	Y	101	CDL	OB6-CB5	4.38	1.46	1.34
19	B	301	TGL	OG3-CC1	4.35	1.46	1.33
14	N	602[A]	HEA	C4D-C3D	-4.35	1.37	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Q	201	PGV	O01-C1	4.28	1.46	1.34
19	O	301	TGL	OG3-CC1	4.20	1.45	1.33
27	E	201	PSC	O03-C19	4.15	1.45	1.33
14	A	602[C]	HEA	CHD-C1D	4.15	1.45	1.35
19	O	301	TGL	OG1-CA1	4.10	1.45	1.33
25	C	308	CDL	OA6-CA5	4.06	1.45	1.34
19	D	201	TGL	OG3-CC1	4.00	1.45	1.33
14	A	601[A]	HEA	CHD-C1D	3.98	1.45	1.35
14	A	601[B]	HEA	CHD-C1D	3.98	1.45	1.35
19	O	302	TGL	OG3-CC1	3.93	1.44	1.33
14	A	602[A]	HEA	CHD-C1D	3.92	1.45	1.35
14	N	602[C]	HEA	CHC-C4B	3.90	1.45	1.35
14	A	602[A]	HEA	C4D-C3D	-3.90	1.38	1.45
20	P	307	PGV	O01-C1	3.87	1.45	1.34
20	A	608	PGV	O01-C1	3.85	1.45	1.34
25	C	308	CDL	C79-C78	-3.79	1.30	1.51
25	T	102	CDL	OA8-CA7	3.77	1.44	1.33
26	J	101	DMU	O16-C6	3.77	1.46	1.40
14	A	602[A]	HEA	CHC-C4B	3.76	1.44	1.35
26	K	101	DMU	O16-C6	3.74	1.46	1.40
14	N	602[A]	HEA	CHC-C4B	3.74	1.44	1.35
25	C	308	CDL	OB8-CB7	3.74	1.44	1.33
20	N	607	PGV	O01-C02	-3.73	1.37	1.46
14	N	601[A]	HEA	CHC-C4B	3.72	1.44	1.35
14	N	601[B]	HEA	CHC-C4B	3.72	1.44	1.35
14	A	601[A]	HEA	C1D-ND	-3.70	1.33	1.40
14	A	601[B]	HEA	C1D-ND	-3.70	1.33	1.40
27	E	201	PSC	C13-C12	3.67	1.53	1.31
26	X	102	DMU	O16-C6	3.66	1.46	1.40
14	N	602[A]	HEA	CHD-C1D	3.65	1.44	1.35
14	N	601[A]	HEA	C4B-NB	-3.62	1.34	1.40
14	N	601[B]	HEA	C4B-NB	-3.62	1.34	1.40
14	N	602[A]	HEA	O11-C11	3.61	1.50	1.42
26	L	101	DMU	O16-C6	3.60	1.46	1.40
27	O	304	PSC	C13-C12	3.60	1.52	1.31
14	N	602[C]	HEA	C1B-C2B	-3.59	1.37	1.44
25	Y	101	CDL	OA8-CA7	3.59	1.43	1.33
25	C	308	CDL	C82-C81	-3.56	1.31	1.51
14	A	601[A]	HEA	C1D-C2D	-3.55	1.37	1.44
14	A	601[B]	HEA	C1D-C2D	-3.55	1.37	1.44
14	N	601[A]	HEA	C1D-ND	-3.53	1.34	1.40
14	N	601[B]	HEA	C1D-ND	-3.53	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	602[C]	HEA	CHC-C4B	3.51	1.44	1.35
25	C	308	CDL	OB6-CB5	3.45	1.44	1.34
25	C	308	CDL	C59-C58	-3.43	1.32	1.51
25	P	308	CDL	C79-C78	-3.42	1.32	1.51
26	K	102	DMU	O16-C6	3.42	1.46	1.40
25	P	308	CDL	C59-C58	-3.40	1.32	1.51
25	T	102	CDL	C42-C41	-3.34	1.32	1.51
25	P	308	CDL	C82-C81	-3.33	1.32	1.51
25	T	102	CDL	C22-C21	-3.30	1.33	1.51
25	Y	101	CDL	C79-C78	-3.27	1.33	1.51
25	T	102	CDL	C19-C18	-3.26	1.33	1.51
25	G	101	CDL	C62-C61	-3.26	1.33	1.51
14	N	601[B]	HEA	O11-C11	3.24	1.49	1.42
25	Y	101	CDL	C82-C81	-3.23	1.33	1.51
25	T	102	CDL	C82-C81	-3.21	1.33	1.51
25	G	101	CDL	C19-C18	-3.19	1.33	1.51
14	N	602[C]	HEA	C4D-C3D	-3.19	1.39	1.45
25	G	101	CDL	C22-C21	-3.16	1.33	1.51
14	A	602[A]	HEA	C1D-C2D	-3.15	1.38	1.44
25	G	101	CDL	C42-C41	-3.14	1.33	1.51
14	A	602[A]	HEA	C4B-C3B	-3.12	1.39	1.44
14	N	602[C]	HEA	C4B-C3B	-3.12	1.39	1.44
25	C	308	CDL	C62-C61	-3.11	1.34	1.51
25	G	101	CDL	C82-C81	-3.09	1.34	1.51
26	X	103	DMU	O16-C6	3.08	1.45	1.40
25	T	102	CDL	C79-C78	-3.02	1.34	1.51
14	A	601[B]	HEA	O11-C11	3.01	1.49	1.42
25	Y	101	CDL	C62-C61	-3.00	1.34	1.51
25	Y	101	CDL	C59-C58	-2.99	1.34	1.51
25	C	308	CDL	C39-C38	-2.98	1.34	1.51
25	Y	101	CDL	C22-C21	-2.97	1.34	1.51
25	G	101	CDL	C79-C78	-2.97	1.34	1.51
25	T	102	CDL	C39-C38	-2.93	1.35	1.51
25	C	308	CDL	C42-C41	-2.92	1.35	1.51
26	P	312	DMU	O16-C6	2.90	1.45	1.40
25	P	308	CDL	C39-C38	-2.90	1.35	1.51
25	G	101	CDL	C39-C38	-2.89	1.35	1.51
25	P	308	CDL	C42-C41	-2.89	1.35	1.51
26	P	316	DMU	C3-C4	2.87	1.59	1.53
14	N	602[C]	HEA	C1D-ND	-2.86	1.35	1.40
14	A	602[C]	HEA	C4B-C3B	-2.83	1.39	1.44
14	N	601[A]	HEA	C1D-C2D	-2.82	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	601[B]	HEA	C1D-C2D	-2.82	1.39	1.44
14	N	602[C]	HEA	C4B-NB	-2.81	1.35	1.40
25	Y	101	CDL	C19-C18	-2.79	1.35	1.51
24	C	303	PEK	O03-C21	2.77	1.41	1.33
26	P	315	DMU	O16-C6	2.77	1.44	1.40
25	P	308	CDL	CA6-CA4	2.75	1.59	1.50
23	C	301	CHD	O25-C24	2.72	1.31	1.22
26	G	105	DMU	O16-C6	2.70	1.44	1.40
14	N	601[A]	HEA	CHD-C1D	2.70	1.41	1.35
14	N	601[B]	HEA	CHD-C1D	2.70	1.41	1.35
14	A	601[A]	HEA	O11-C11	2.70	1.48	1.42
14	A	602[A]	HEA	C18-C19	2.69	1.39	1.33
14	A	602[C]	HEA	C18-C19	2.69	1.39	1.33
26	K	102	DMU	C2-C1	2.68	1.59	1.52
20	A	608	PGV	O02-C1	2.66	1.30	1.22
25	G	101	CDL	C58-C59	-2.61	1.33	1.51
14	A	601[A]	HEA	CHC-C4B	2.59	1.41	1.35
14	A	601[B]	HEA	CHC-C4B	2.59	1.41	1.35
14	A	602[C]	HEA	C4D-C3D	-2.59	1.40	1.45
20	P	306	PGV	P-O14	-2.58	1.43	1.55
14	A	601[A]	HEA	C1B-NB	-2.58	1.33	1.38
14	A	601[B]	HEA	C1B-NB	-2.58	1.33	1.38
14	A	601[A]	HEA	C3A-C2A	-2.57	1.36	1.40
14	A	601[B]	HEA	C3A-C2A	-2.57	1.36	1.40
14	N	601[A]	HEA	C1C-NC	2.56	1.41	1.36
14	N	601[B]	HEA	C1C-NC	2.56	1.41	1.36
14	A	601[A]	HEA	CBD-CGD	2.55	1.56	1.50
14	A	601[B]	HEA	CBD-CGD	2.55	1.56	1.50
26	P	316	DMU	O16-C6	2.53	1.44	1.40
20	N	607	PGV	O01-C1	2.52	1.41	1.34
14	A	602[A]	HEA	O11-C11	2.51	1.48	1.42
25	C	308	CDL	PB2-OB3	2.49	1.58	1.50
14	N	602[A]	HEA	C1C-CHC	2.48	1.47	1.41
14	N	601[A]	HEA	CMD-C2D	2.47	1.56	1.50
14	N	601[B]	HEA	CMD-C2D	2.47	1.56	1.50
14	A	601[A]	HEA	C2A-C1A	-2.47	1.37	1.42
14	A	601[B]	HEA	C2A-C1A	-2.47	1.37	1.42
14	N	601[A]	HEA	C1B-C2B	-2.47	1.39	1.44
14	N	601[B]	HEA	C1B-C2B	-2.47	1.39	1.44
23	J	102	CHD	C13-C14	-2.46	1.51	1.55
23	P	301	CHD	C23-C24	2.43	1.56	1.50
14	N	601[A]	HEA	C12-C11	-2.43	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	X	102	DMU	C3-C2	2.41	1.58	1.52
20	N	607	PGV	O03-C19	2.41	1.40	1.33
14	A	602[C]	HEA	C1B-C2B	-2.41	1.39	1.44
14	A	602[C]	HEA	C4C-CHD	2.40	1.47	1.41
26	M	101	DMU	O16-C6	2.39	1.44	1.40
14	A	601[A]	HEA	C3C-C2C	-2.36	1.37	1.40
14	A	601[B]	HEA	C3C-C2C	-2.36	1.37	1.40
14	N	602[A]	HEA	C4B-C3B	-2.35	1.40	1.44
14	N	601[A]	HEA	O2D-CGD	-2.34	1.22	1.30
14	N	601[B]	HEA	O2D-CGD	-2.34	1.22	1.30
20	N	607	PGV	C01-C02	2.34	1.57	1.50
14	A	602[C]	HEA	C4B-NB	-2.33	1.36	1.40
14	A	601[A]	HEA	C4D-C3D	-2.32	1.41	1.45
14	A	601[B]	HEA	C4D-C3D	-2.32	1.41	1.45
26	X	101	DMU	C3-C2	2.29	1.58	1.52
14	N	601[A]	HEA	O1D-CGD	2.25	1.29	1.22
14	N	601[B]	HEA	O1D-CGD	2.25	1.29	1.22
20	P	306	PGV	O01-C02	-2.24	1.41	1.46
26	G	105	DMU	C2-C1	2.23	1.55	1.52
20	C	306	PGV	O03-C01	2.23	1.50	1.45
14	A	602[C]	HEA	C1D-C2D	-2.21	1.40	1.44
14	A	601[A]	HEA	C1B-C2B	-2.21	1.40	1.44
14	A	601[B]	HEA	C1B-C2B	-2.21	1.40	1.44
23	B	303	CHD	C11-C9	2.18	1.57	1.53
26	P	315	DMU	C8-C9	2.17	1.57	1.53
14	N	601[A]	HEA	O1A-CGA	2.17	1.29	1.22
14	N	601[B]	HEA	O1A-CGA	2.17	1.29	1.22
24	C	303	PEK	O01-C1	2.16	1.40	1.34
14	N	602[A]	HEA	C4B-NB	-2.15	1.36	1.40
26	K	102	DMU	O55-C2	2.15	1.48	1.43
14	N	601[A]	HEA	CBD-CGD	2.14	1.55	1.50
14	N	601[B]	HEA	CBD-CGD	2.14	1.55	1.50
14	N	602[A]	HEA	C1D-C2D	-2.14	1.40	1.44
25	G	101	CDL	CA6-CA4	2.12	1.57	1.50
19	D	201	TGL	CB2-CB1	2.12	1.56	1.50
26	P	315	DMU	C10-C5	2.10	1.58	1.52
26	X	102	DMU	O5-C6	2.10	1.47	1.41
20	N	607	PGV	P-O12	-2.10	1.50	1.59
14	N	602[A]	HEA	C3B-C2B	2.09	1.39	1.34
26	P	311	DMU	O16-C6	2.09	1.43	1.40
25	C	308	CDL	OB6-CB4	-2.07	1.41	1.46
23	G	102	CHD	C10-C9	-2.06	1.52	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	608	PGV	O01-C02	-2.05	1.41	1.46
14	A	602[A]	HEA	C1B-C2B	-2.04	1.40	1.44
26	K	102	DMU	C3-C2	2.04	1.57	1.52
23	P	301	CHD	O25-C24	2.03	1.28	1.22
14	A	602[A]	HEA	C1D-ND	-2.03	1.36	1.40
25	C	308	CDL	PB2-OB2	2.03	1.62	1.54
14	A	601[A]	HEA	C3C-CAC	-2.03	1.43	1.47
14	A	601[B]	HEA	C3C-CAC	-2.03	1.43	1.47
14	A	601[A]	HEA	C12-C11	-2.02	1.49	1.52
26	K	102	DMU	C3-C4	2.02	1.57	1.53
25	G	101	CDL	CA3-CA4	2.02	1.56	1.50
23	C	301	CHD	C18-C13	-2.02	1.51	1.54
19	O	302	TGL	OB1-CB1	2.01	1.28	1.22
20	C	306	PGV	C03-C02	2.00	1.56	1.50
14	A	602[C]	HEA	O11-C11	2.00	1.47	1.42
20	N	607	PGV	O04-C19	-2.00	1.16	1.22

All (566) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	309	CHD	C23-C22-C20	-10.67	95.03	114.52
27	E	201	PSC	C03-C02-C01	-9.39	89.58	111.79
25	G	101	CDL	OA6-CA5-C11	8.69	130.24	111.50
23	W	101	CHD	C13-C17-C20	8.16	129.24	119.50
19	O	301	TGL	OG2-CB1-CB2	7.52	127.70	111.50
19	B	301	TGL	OG2-CB1-CB2	7.15	126.91	111.50
14	N	601[A]	HEA	C13-C12-C11	-7.03	103.78	114.35
27	O	304	PSC	O01-C1-C2	7.00	126.58	111.50
14	N	602[C]	HEA	CHD-C1D-ND	6.83	132.81	124.38
20	C	307	PGV	O03-C19-C20	6.65	132.79	111.91
27	O	304	PSC	C03-C02-C01	-6.58	96.23	111.79
20	P	307	PGV	O03-C19-C20	6.39	131.95	111.91
23	J	102	CHD	C16-C17-C20	6.34	121.96	112.15
19	A	607	TGL	OG2-CB1-CB2	6.25	124.97	111.50
20	Q	201	PGV	C02-O01-C1	-6.23	102.46	117.79
23	C	309	CHD	C21-C20-C17	6.22	122.44	112.92
23	J	102	CHD	C17-C13-C12	-6.17	112.03	117.67
23	J	102	CHD	C11-C9-C10	-6.15	107.39	113.73
27	E	201	PSC	O01-C1-C2	6.06	124.56	111.50
23	J	102	CHD	C19-C10-C9	-5.97	102.96	111.18
25	T	102	CDL	OA6-CA5-C11	5.83	124.06	111.50
14	A	601[A]	HEA	C13-C12-C11	-5.76	105.70	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	307	PGV	O01-C1-C2	5.73	123.85	111.50
14	A	601[A]	HEA	C2D-C1D-ND	5.62	116.50	109.84
14	A	601[B]	HEA	C2D-C1D-ND	5.62	116.50	109.84
26	G	105	DMU	C6-O5-C4	5.61	119.35	113.13
14	N	602[A]	HEA	CHB-C1B-NB	5.50	130.40	124.43
25	P	308	CDL	OB8-CB7-C71	5.48	129.11	111.91
19	A	607	TGL	CG2-OG2-CB1	5.44	131.18	117.79
26	X	101	DMU	O16-C6-C1	5.40	116.74	108.30
25	C	308	CDL	OB2-PB2-OB5	-5.37	92.43	106.73
14	A	602[C]	HEA	C13-C12-C11	-5.35	106.32	114.35
19	A	607	TGL	OG3-CC1-CC2	5.25	128.37	111.91
24	P	305	PEK	O03-C21-C22	5.22	128.31	111.91
14	A	602[C]	HEA	C17-C18-C19	-5.17	115.21	127.66
14	N	601[A]	HEA	C3C-C4C-NC	5.14	115.85	109.21
14	N	601[B]	HEA	C3C-C4C-NC	5.14	115.85	109.21
26	K	102	DMU	O16-C6-C1	5.06	116.20	108.30
20	A	608	PGV	C3-C2-C1	5.05	131.99	113.62
23	P	309	CHD	C15-C14-C13	5.03	108.48	103.55
23	P	309	CHD	C19-C10-C9	-4.98	104.31	111.18
23	W	101	CHD	C17-C13-C14	-4.88	95.17	100.09
14	A	601[B]	HEA	C17-C18-C19	-4.81	116.07	127.66
24	P	305	PEK	O01-C1-C2	4.72	121.68	111.50
23	C	301	CHD	C18-C13-C12	4.71	113.86	109.07
26	P	315	DMU	O7-C10-C5	4.69	120.27	108.10
24	T	101	PEK	O01-C1-C2	4.69	121.62	111.50
23	J	102	CHD	C13-C17-C20	-4.68	113.91	119.50
14	N	602[A]	HEA	C4D-CHA-C1A	-4.67	116.39	122.56
26	P	316	DMU	O5-C4-C3	4.64	118.13	109.69
23	C	309	CHD	C13-C17-C20	-4.64	113.96	119.50
14	A	601[A]	HEA	C2B-C1B-NB	4.62	115.42	109.88
14	A	601[B]	HEA	C2B-C1B-NB	4.62	115.42	109.88
24	T	101	PEK	O03-C01-C02	4.60	121.83	108.43
26	P	316	DMU	O16-C6-C1	4.59	115.47	108.30
27	O	304	PSC	C21-C20-C19	-4.58	96.97	113.62
14	N	602[A]	HEA	C4A-CHB-C1B	-4.58	116.52	122.56
25	P	308	CDL	OA8-CA6-CA4	4.57	121.74	108.43
26	J	101	DMU	C22-C19-C18	-4.50	93.54	113.49
23	C	309	CHD	C15-C14-C13	4.45	107.92	103.55
14	N	602[C]	HEA	C4D-CHA-C1A	-4.44	116.70	122.56
26	P	315	DMU	C6-C1-C2	4.42	119.21	110.00
26	C	311	DMU	O5-C6-C1	4.39	119.63	110.35
23	W	101	CHD	C1-C2-C3	4.34	116.04	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	602[A]	HEA	CHA-C4D-ND	4.32	129.12	124.43
14	A	602[A]	HEA	C17-C18-C19	4.31	138.04	127.66
23	W	101	CHD	C18-C13-C14	-4.30	104.48	111.21
24	P	305	PEK	C01-O03-C21	4.27	132.95	117.12
23	C	301	CHD	C6-C7-C8	-4.26	106.93	111.48
19	B	301	TGL	CG3-CG2-CG1	-4.26	101.71	111.79
24	C	304	PEK	O03-C21-C22	4.25	125.23	111.91
14	A	602[A]	HEA	C21-C20-C19	4.24	126.94	112.98
14	A	602[C]	HEA	C21-C20-C19	4.24	126.94	112.98
14	A	602[A]	HEA	C13-C14-C15	-4.21	117.51	127.66
23	W	101	CHD	C17-C13-C12	4.21	121.51	117.67
14	N	602[A]	HEA	CHD-C1D-ND	4.21	129.58	124.38
14	N	602[A]	HEA	CHB-C1B-C2B	-4.19	118.43	124.98
23	W	101	CHD	C6-C5-C4	-4.17	106.39	111.19
20	P	307	PGV	O01-C1-C2	4.16	120.47	111.50
23	P	309	CHD	C16-C17-C13	4.16	107.63	103.55
20	N	607	PGV	O01-C1-O02	-4.15	113.67	123.70
26	C	311	DMU	C18-O16-C6	-4.10	107.03	113.84
23	B	303	CHD	C17-C13-C14	4.07	104.20	100.09
14	A	602[A]	HEA	C27-C19-C20	4.06	122.11	115.27
14	A	602[C]	HEA	C27-C19-C20	4.06	122.11	115.27
14	A	601[A]	HEA	C1D-C2D-C3D	-4.06	102.69	106.96
14	A	601[B]	HEA	C1D-C2D-C3D	-4.06	102.69	106.96
24	P	305	PEK	O03-C21-O04	-4.06	113.36	123.59
14	N	601[B]	HEA	C17-C18-C19	-4.04	117.94	127.66
25	G	101	CDL	CB6-OB8-CB7	4.01	131.99	117.12
23	J	102	CHD	C15-C14-C8	4.01	123.94	118.33
25	P	308	CDL	OA8-CA7-C31	4.00	124.46	111.91
14	N	602[C]	HEA	CMD-C2D-C1D	-3.99	118.96	125.04
19	O	302	TGL	OG1-CA1-CA2	3.98	124.38	111.91
24	C	304	PEK	C01-O03-C21	3.97	129.76	116.92
19	A	607	TGL	OG1-CA1-CA2	3.95	124.29	111.91
14	A	602[C]	HEA	OMA-CMA-C3A	-3.93	116.35	124.91
25	Y	101	CDL	OA8-CA7-OA9	-3.91	113.73	123.59
23	G	102	CHD	C17-C13-C14	3.89	104.02	100.09
26	C	311	DMU	C6-C1-C2	3.89	118.09	110.00
26	G	105	DMU	O16-C6-C1	3.88	114.36	108.30
20	C	307	PGV	O03-C19-O04	-3.86	113.85	123.59
25	G	101	CDL	OA6-CA5-OA7	-3.85	114.39	123.70
14	N	601[B]	HEA	C27-C19-C20	3.84	121.73	115.27
26	X	101	DMU	C2-C3-C4	3.84	117.09	110.24
25	C	308	CDL	OA8-CA6-CA4	3.83	119.57	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	304	PEK	O03-C21-O04	-3.83	113.94	123.59
24	T	101	PEK	C03-C02-C01	3.83	120.84	111.79
23	C	309	CHD	C19-C10-C9	-3.82	105.92	111.18
26	K	101	DMU	C18-O16-C6	3.81	120.16	113.84
14	A	602[A]	HEA	CHA-C4D-ND	3.81	128.57	124.43
23	P	301	CHD	C11-C9-C10	-3.79	109.82	113.73
14	A	602[C]	HEA	CHA-C4D-C3D	-3.78	119.28	124.84
26	G	105	DMU	O5-C4-C57	3.77	112.88	106.83
23	B	303	CHD	C5-C4-C3	-3.75	107.25	112.76
23	J	102	CHD	C9-C8-C7	-3.75	107.39	111.88
23	W	101	CHD	C9-C11-C12	-3.74	109.37	114.30
26	P	316	DMU	C6-O5-C4	3.73	121.01	113.69
14	A	602[A]	HEA	CMC-C2C-C1C	-3.73	122.73	128.46
26	K	102	DMU	C2-C3-C4	3.72	116.88	110.24
14	N	602[A]	HEA	CHA-C4D-C3D	-3.72	119.37	124.84
20	C	307	PGV	C21-C20-C19	-3.72	100.11	113.62
23	B	303	CHD	C15-C14-C13	-3.71	99.92	103.55
19	B	301	TGL	OG1-CA1-CA2	3.71	123.54	111.91
27	O	304	PSC	O01-C1-O02	-3.70	114.75	123.70
14	A	602[C]	HEA	CMC-C2C-C3C	3.70	131.59	124.68
23	B	303	CHD	C19-C10-C1	-3.68	102.33	108.26
26	L	101	DMU	C18-O16-C6	3.68	119.94	113.84
26	P	316	DMU	O49-C1-C2	3.65	118.78	110.35
20	Q	201	PGV	O01-C1-C2	3.63	119.33	111.50
26	P	315	DMU	C10-C5-C7	3.63	117.56	110.00
26	X	101	DMU	C3-C2-C1	3.63	117.15	110.82
23	J	102	CHD	C21-C20-C17	-3.61	107.39	112.92
23	J	102	CHD	C22-C20-C17	3.59	117.71	110.28
14	A	602[C]	HEA	CAD-C3D-C2D	3.59	134.57	127.88
20	A	608	PGV	P-O11-C03	3.59	128.19	118.30
26	P	315	DMU	C11-C9-C8	3.59	121.41	113.00
25	C	308	CDL	C52-C51-CB5	-3.59	100.57	113.62
26	X	101	DMU	C18-O16-C6	3.58	119.78	113.84
25	T	102	CDL	CB2-C1-CA2	-3.58	102.26	112.79
14	N	601[A]	HEA	C13-C14-C15	-3.57	119.05	127.66
24	P	303	PEK	O01-C1-C2	3.57	125.51	114.03
23	C	309	CHD	C16-C17-C20	3.57	117.67	112.15
24	T	101	PEK	C02-O01-C1	-3.57	109.01	117.79
19	B	301	TGL	OG2-CG2-CG3	3.55	121.27	108.40
19	D	201	TGL	OG3-CC1-OC1	-3.55	114.63	123.59
23	J	102	CHD	C4-C3-C2	-3.55	106.32	110.55
26	X	103	DMU	C6-O5-C4	3.54	120.64	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	308	CDL	C78-C77-C76	-3.53	96.48	114.42
26	J	101	DMU	C18-O16-C6	3.52	119.67	113.84
20	P	307	PGV	O01-C1-O02	-3.52	115.20	123.70
25	Y	101	CDL	OB8-CB7-C71	3.51	122.93	111.91
20	Q	201	PGV	O03-C19-C20	3.49	122.87	111.91
14	N	601[B]	HEA	C13-C12-C11	-3.48	109.11	114.35
23	W	101	CHD	C18-C13-C17	3.47	116.65	111.21
14	N	602[C]	HEA	CHD-C1D-C2D	-3.47	117.12	126.72
14	N	602[C]	HEA	CMC-C2C-C3C	3.47	131.16	124.68
23	P	309	CHD	C22-C23-C24	-3.45	103.35	112.51
14	A	601[A]	HEA	C3C-C4C-NC	3.45	113.67	109.21
14	A	601[B]	HEA	C3C-C4C-NC	3.45	113.67	109.21
19	O	302	TGL	OG1-CA1-OA1	-3.44	114.92	123.59
25	C	308	CDL	OA8-CA7-C31	3.43	122.67	111.91
14	N	602[C]	HEA	CHA-C4D-C3D	-3.43	119.80	124.84
25	P	308	CDL	OB8-CB7-OB9	-3.41	114.99	123.59
14	N	602[C]	HEA	C13-C12-C11	-3.41	109.23	114.35
23	B	303	CHD	C2-C1-C10	-3.39	106.96	112.78
27	E	201	PSC	C02-O01-C1	3.39	126.14	117.79
20	P	306	PGV	O01-C1-O02	-3.38	115.54	123.70
14	A	602[C]	HEA	C26-C15-C14	-3.37	115.02	123.68
14	A	602[A]	HEA	C3C-C4C-NC	3.37	113.57	109.21
23	P	301	CHD	C22-C20-C17	-3.36	103.35	110.28
19	A	607	TGL	CB9-CB8-CB7	-3.35	97.40	114.42
26	L	101	DMU	O61-C57-C4	3.34	122.75	111.29
23	G	102	CHD	C6-C5-C4	-3.34	107.35	111.19
23	P	309	CHD	O25-C24-C23	-3.32	112.40	123.08
26	P	315	DMU	O5-C6-C1	3.32	117.38	110.35
19	A	607	TGL	OG3-CC1-OC1	-3.32	115.21	123.59
26	P	315	DMU	O2-C8-C9	3.32	117.53	109.30
14	A	602[A]	HEA	C1D-C2D-C3D	-3.31	103.48	106.96
25	P	308	CDL	OA6-CA5-C11	3.31	118.63	111.50
14	N	602[A]	HEA	CMB-C2B-C3B	-3.31	124.04	130.34
23	P	301	CHD	C19-C10-C1	-3.30	102.94	108.26
26	P	316	DMU	C2-C3-C4	3.30	116.12	110.24
23	W	101	CHD	C9-C10-C5	3.29	113.21	108.58
26	G	105	DMU	O5-C6-C1	3.28	117.30	110.35
19	A	607	TGL	CA4-CA3-CA2	-3.28	101.39	113.19
26	P	316	DMU	C3-C2-C1	-3.28	105.09	110.82
14	A	602[A]	HEA	C20-C19-C18	-3.28	114.48	121.12
14	A	602[C]	HEA	C20-C19-C18	-3.28	114.48	121.12
26	P	316	DMU	O55-C2-C1	3.27	117.90	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	102	CHD	C1-C2-C3	3.26	114.65	110.47
23	J	102	CHD	C18-C13-C12	3.26	112.39	109.07
25	T	102	CDL	CB6-CB4-CB3	-3.24	102.92	113.70
14	A	602[A]	HEA	C4A-CHB-C1B	-3.24	118.28	122.56
23	J	102	CHD	O3-C3-C4	3.23	116.28	109.85
14	A	602[C]	HEA	C3B-C4B-NB	3.22	113.66	109.84
26	K	103	DMU	C2-C3-C4	3.21	117.88	110.40
14	A	602[A]	HEA	CMC-C2C-C3C	3.20	130.66	124.68
25	P	308	CDL	CA6-OA8-CA7	3.19	128.94	117.12
26	P	312	DMU	C6-O5-C4	3.19	119.95	113.69
19	O	301	TGL	OG1-CA1-CA2	3.17	121.87	111.91
23	G	102	CHD	C15-C14-C13	-3.15	100.46	103.55
19	A	607	TGL	C12-C11-C10	-3.15	98.42	114.42
25	T	102	CDL	CB6-OB8-CB7	3.14	127.06	116.92
23	P	309	CHD	C18-C13-C12	-3.14	105.87	109.07
26	L	101	DMU	O5-C4-C57	3.13	114.23	106.44
26	P	312	DMU	O55-C2-C1	-3.13	103.11	110.35
25	P	308	CDL	OB6-CB5-C51	3.12	121.70	111.91
25	Y	101	CDL	OB6-CB5-C51	3.12	118.23	111.50
23	C	309	CHD	C6-C5-C4	-3.11	107.61	111.19
14	A	601[A]	HEA	C13-C14-C15	-3.10	120.20	127.66
26	G	105	DMU	C18-O16-C6	-3.09	108.71	113.84
26	P	310	DMU	O3-C5-C7	-3.09	103.20	110.35
26	P	315	DMU	O4-C7-C5	3.09	117.49	110.35
14	N	602[C]	HEA	CHA-C4D-ND	3.09	127.78	124.43
23	B	303	CHD	C6-C5-C4	-3.08	107.64	111.19
14	N	601[A]	HEA	O2A-CGA-CBA	3.07	123.89	114.03
14	N	601[B]	HEA	O2A-CGA-CBA	3.07	123.89	114.03
14	A	602[A]	HEA	CHB-C1B-C2B	-3.07	120.19	124.98
20	P	307	PGV	O03-C19-O04	-3.05	115.89	123.59
27	O	304	PSC	P-O11-C03	3.04	139.49	121.68
27	O	304	PSC	C28-C27-C26	-3.03	99.02	114.42
20	A	608	PGV	O03-C19-C20	3.03	121.41	111.91
20	P	307	PGV	O04-C19-C20	-3.03	111.92	123.73
23	J	102	CHD	C14-C13-C12	3.02	110.22	107.40
26	X	103	DMU	C3-C2-C1	3.02	116.09	110.82
26	P	312	DMU	C22-C19-C18	-3.02	100.12	113.49
14	N	602[C]	HEA	O2A-CGA-CBA	3.01	123.71	114.03
26	G	105	DMU	C3-C2-C1	3.01	115.06	110.69
19	O	301	TGL	CG3-CG2-CG1	-3.00	104.69	111.79
14	A	602[A]	HEA	C2D-C1D-ND	2.99	113.38	109.84
23	B	303	CHD	C4-C5-C10	-2.99	109.48	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	308	CDL	C53-C52-C51	-2.99	102.46	113.19
26	C	311	DMU	O1-C9-C11	2.97	113.82	106.44
25	C	308	CDL	OB4-PB2-OB3	2.96	122.27	110.68
26	Z	101	DMU	O61-C57-C4	-2.95	101.16	111.29
27	O	304	PSC	C02-O01-C1	2.95	125.05	117.79
19	B	301	TGL	CC3-CC2-CC1	-2.95	102.91	113.62
14	A	602[C]	HEA	C16-C15-C14	2.94	127.08	121.12
20	A	608	PGV	C01-O03-C19	2.94	128.02	117.12
14	N	602[C]	HEA	CAD-C3D-C2D	2.94	133.35	127.88
26	X	102	DMU	O5-C4-C57	2.93	113.73	106.44
19	A	607	TGL	C25-C24-C23	-2.93	99.54	114.42
23	J	102	CHD	C16-C17-C13	2.93	106.43	103.55
23	J	102	CHD	C10-C9-C8	-2.93	108.67	111.82
25	C	308	CDL	OA8-CA7-OA9	-2.92	116.21	123.59
26	K	101	DMU	O5-C4-C3	2.92	114.99	109.69
26	J	101	DMU	C6-O5-C4	2.91	119.40	113.69
26	M	101	DMU	O5-C6-O16	-2.91	103.09	109.97
14	N	602[A]	HEA	C3C-C4C-NC	2.90	112.96	109.21
25	C	308	CDL	PB2-OB5-CB3	2.90	126.28	118.30
14	A	602[A]	HEA	O1D-CGD-CBD	-2.89	113.79	123.08
26	C	311	DMU	C6-O5-C4	-2.88	108.03	113.69
23	W	101	CHD	C19-C10-C9	-2.88	107.22	111.18
26	K	101	DMU	C6-O5-C4	2.88	119.33	113.69
23	G	102	CHD	C4-C5-C10	-2.88	109.60	112.66
25	Y	101	CDL	OA8-CA7-C31	2.87	120.92	111.91
14	A	602[C]	HEA	CHD-C1D-ND	2.86	127.92	124.38
25	G	101	CDL	C39-C38-C37	2.86	128.93	114.42
14	A	602[C]	HEA	C3D-C4D-ND	2.85	113.12	110.36
26	X	102	DMU	O16-C6-C1	2.85	112.75	108.30
23	C	301	CHD	C22-C23-C24	-2.83	104.99	112.51
25	Y	101	CDL	OA6-CA4-CA3	2.83	118.66	108.40
14	N	602[A]	HEA	CAD-C3D-C2D	2.83	133.15	127.88
23	J	102	CHD	C14-C8-C9	2.83	113.59	109.71
14	A	602[C]	HEA	CMB-C2B-C3B	-2.82	124.97	130.34
14	A	601[B]	HEA	C26-C15-C16	2.82	120.01	115.27
26	K	102	DMU	C3-C2-C1	2.82	115.74	110.82
23	B	303	CHD	C1-C10-C5	2.82	111.93	107.77
14	N	602[A]	HEA	C13-C12-C11	-2.82	110.12	114.35
14	A	602[A]	HEA	CMD-C2D-C1D	2.81	129.32	125.04
23	C	309	CHD	C11-C9-C10	-2.81	110.83	113.73
26	P	315	DMU	O1-C9-C8	2.81	114.79	109.69
26	C	311	DMU	O7-C10-C5	2.80	115.35	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	O	301	TGL	OG2-CG2-CG3	2.80	118.53	108.40
23	C	309	CHD	C9-C11-C12	-2.79	110.61	114.30
14	N	601[A]	HEA	O1D-CGD-CBD	-2.79	114.11	123.08
14	N	601[B]	HEA	O1D-CGD-CBD	-2.79	114.11	123.08
19	O	302	TGL	CG2-OG2-CB1	-2.79	110.92	117.79
26	X	103	DMU	O5-C6-C1	2.78	116.24	110.35
26	X	103	DMU	C18-O16-C6	-2.78	109.23	113.84
14	N	602[A]	HEA	O2D-CGD-O1D	2.78	130.22	123.30
25	G	101	CDL	OA8-CA6-CA4	2.77	116.51	108.43
26	P	310	DMU	C7-C8-C9	2.77	115.17	110.24
14	A	602[C]	HEA	CHA-C4D-ND	2.77	127.44	124.43
26	P	311	DMU	O3-C5-C10	2.77	116.77	110.05
23	W	101	CHD	C4-C5-C10	2.76	115.59	112.66
26	P	310	DMU	O16-C6-C1	-2.76	103.99	108.30
19	A	607	TGL	OG2-CG2-CG1	2.76	118.39	108.40
23	C	309	CHD	C17-C13-C12	-2.75	115.16	117.67
14	N	602[C]	HEA	C13-C14-C15	-2.75	121.04	127.66
14	A	602[A]	HEA	C4D-CHA-C1A	-2.75	118.93	122.56
23	P	309	CHD	C4-C3-C2	-2.75	107.27	110.55
14	N	602[A]	HEA	CAD-CBD-CGD	-2.74	107.71	113.60
14	A	602[A]	HEA	CHC-C4B-NB	2.73	127.75	124.38
25	C	308	CDL	C81-C80-C79	-2.73	100.59	114.42
24	T	101	PEK	O03-C21-C22	2.71	120.42	111.91
20	P	307	PGV	C21-C20-C19	-2.71	103.76	113.62
23	P	309	CHD	C5-C4-C3	-2.71	108.78	112.76
14	A	602[A]	HEA	CHD-C1D-C2D	-2.71	119.22	126.72
14	N	601[A]	HEA	C3B-C4B-NB	2.70	113.04	109.84
14	N	601[B]	HEA	C3B-C4B-NB	2.70	113.04	109.84
26	K	101	DMU	C2-C3-C4	2.70	115.06	110.24
23	B	303	CHD	O3-C3-C4	-2.70	104.47	109.85
23	W	101	CHD	O12-C12-C11	-2.70	103.63	109.12
14	N	602[A]	HEA	CMB-C2B-C1B	2.69	129.14	125.04
19	B	301	TGL	OG1-CA1-OA1	-2.69	116.80	123.59
14	A	602[A]	HEA	CAD-C3D-C4D	-2.69	119.96	124.66
27	O	304	PSC	C24-C23-C22	-2.69	100.79	114.42
14	A	602[A]	HEA	CHA-C4D-C3D	-2.68	120.90	124.84
20	C	307	PGV	O04-C19-C20	-2.67	113.30	123.73
14	A	601[A]	HEA	CMC-C2C-C1C	-2.67	124.36	128.46
14	A	601[B]	HEA	CMC-C2C-C1C	-2.67	124.36	128.46
24	C	304	PEK	O01-C1-C2	2.67	120.28	111.91
23	C	309	CHD	C4-C5-C10	2.67	115.49	112.66
25	T	102	CDL	OB5-CB3-CB4	2.67	117.88	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	301	CHD	C23-C22-C20	-2.66	109.66	114.52
20	C	307	PGV	O03-C01-C02	2.65	116.16	108.43
19	A	607	TGL	OG2-CB1-OB1	-2.64	117.32	123.70
26	P	315	DMU	O7-C10-O1	-2.64	103.29	110.67
14	N	601[A]	HEA	CAA-CBA-CGA	-2.63	106.38	113.76
14	N	601[B]	HEA	CAA-CBA-CGA	-2.63	106.38	113.76
23	C	301	CHD	C1-C2-C3	-2.63	107.10	110.47
14	A	601[A]	HEA	C21-C22-C23	-2.62	118.78	127.75
14	N	602[A]	HEA	CAD-C3D-C4D	-2.62	120.08	124.66
19	D	201	TGL	CG3-CG2-CG1	-2.62	105.59	111.79
26	K	102	DMU	O5-C4-C3	2.62	114.45	109.69
26	C	311	DMU	O61-C57-C4	-2.62	102.31	111.29
14	N	602[A]	HEA	C26-C15-C16	2.62	119.67	115.27
20	Q	201	PGV	O03-C19-O04	-2.61	117.00	123.59
19	O	301	TGL	OG2-CB1-OB1	-2.60	117.41	123.70
23	C	301	CHD	C17-C13-C12	-2.60	115.30	117.67
26	J	101	DMU	O5-C4-C57	2.59	112.89	106.44
24	P	303	PEK	O01-C1-O02	-2.59	116.84	123.30
20	A	608	PGV	C4-C3-C2	-2.59	103.87	113.19
26	K	102	DMU	O55-C2-C1	2.59	116.33	110.35
23	J	102	CHD	C4-C5-C10	2.59	115.40	112.66
14	N	602[C]	HEA	CMC-C2C-C1C	-2.57	124.51	128.46
23	G	102	CHD	O3-C3-C4	-2.57	104.74	109.85
23	P	309	CHD	C13-C17-C20	-2.56	116.44	119.50
19	A	607	TGL	C26-C25-C24	-2.56	101.44	114.42
25	Y	101	CDL	C78-C77-C76	-2.56	101.44	114.42
23	P	301	CHD	C21-C20-C22	-2.56	106.36	110.36
23	J	102	CHD	C11-C9-C8	2.56	114.62	110.88
24	C	304	PEK	C24-C23-C22	2.55	122.37	113.19
25	T	102	CDL	PB2-OB5-CB3	-2.55	109.02	121.59
23	W	101	CHD	C22-C20-C17	2.55	115.56	110.28
23	B	303	CHD	O12-C12-C13	-2.55	106.73	111.03
19	D	201	TGL	OG3-CC1-CC2	2.54	118.05	111.38
23	C	301	CHD	C13-C17-C20	2.54	122.53	119.50
26	J	101	DMU	O49-C1-C6	2.54	116.22	110.05
27	O	304	PSC	C14-C13-C12	-2.53	105.29	124.73
14	A	602[C]	HEA	CHD-C1D-C2D	-2.53	119.73	126.72
23	P	301	CHD	C22-C23-C24	-2.53	105.80	112.51
26	X	101	DMU	O5-C4-C3	2.52	114.28	109.69
24	C	303	PEK	C14-C13-C12	2.52	124.43	112.02
14	N	601[A]	HEA	O2D-CGD-CBD	2.51	122.08	114.03
14	N	601[B]	HEA	O2D-CGD-CBD	2.51	122.08	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	607	PGV	C9-C10-C11	-2.50	98.09	112.43
25	C	308	CDL	CA4-OA6-CA5	-2.50	111.65	117.79
19	B	301	TGL	OB1-CB1-CB2	-2.49	114.00	123.73
23	B	303	CHD	C19-C10-C5	-2.49	106.14	110.36
26	G	105	DMU	C22-C19-C18	-2.49	102.46	113.49
26	P	311	DMU	O7-C10-C5	2.49	114.55	108.10
27	E	201	PSC	C08-N-C07	-2.48	102.59	108.97
26	M	101	DMU	C22-C19-C18	-2.48	102.51	113.49
19	A	607	TGL	OG3-CG3-CG2	2.47	115.64	108.43
27	E	201	PSC	O01-C1-O02	-2.47	117.73	123.70
26	X	101	DMU	O5-C6-C1	-2.47	105.12	110.35
19	A	607	TGL	CG3-CG2-CG1	-2.46	105.97	111.79
19	D	201	TGL	OG1-CG1-CG2	-2.46	101.27	108.43
19	A	607	TGL	CB6-CB5-CB4	-2.46	101.94	114.42
26	P	310	DMU	O1-C10-C5	2.46	115.55	110.35
23	J	102	CHD	C23-C22-C20	-2.45	110.04	114.52
23	G	102	CHD	C19-C10-C1	-2.45	104.32	108.26
26	X	102	DMU	O7-C3-C2	2.44	116.00	110.35
27	E	201	PSC	C07-N-C06	2.44	115.25	108.97
26	X	102	DMU	C28-C25-C22	-2.44	102.03	114.42
27	O	304	PSC	C25-C24-C23	-2.44	102.04	114.42
25	C	308	CDL	C43-C42-C41	2.44	126.80	114.42
20	P	306	PGV	C03-C02-C01	-2.43	106.03	111.79
26	K	101	DMU	C57-C4-C3	-2.43	107.31	113.00
26	M	101	DMU	C18-O16-C6	-2.43	109.81	113.84
14	N	602[A]	HEA	CMC-C2C-C3C	2.43	129.22	124.68
26	C	311	DMU	O5-C4-C3	2.42	114.86	109.75
14	A	602[A]	HEA	CHB-C1B-NB	2.42	127.06	124.43
20	A	608	PGV	O14-P-O11	2.42	113.17	106.73
23	P	309	CHD	C14-C8-C9	-2.41	106.40	109.71
14	A	602[A]	HEA	CHD-C1D-ND	2.41	127.36	124.38
26	P	311	DMU	O16-C6-C1	2.41	112.06	108.30
14	A	601[A]	HEA	CHA-C4D-ND	2.40	127.04	124.43
14	A	601[B]	HEA	CHA-C4D-ND	2.40	127.04	124.43
25	Y	101	CDL	OA6-CA5-C11	2.40	116.67	111.50
20	N	607	PGV	C22-C21-C20	2.39	121.79	113.19
19	B	301	TGL	CB3-CB2-CB1	-2.39	104.92	113.62
14	A	601[A]	HEA	C1B-C2B-C3B	-2.39	103.94	106.80
14	A	601[B]	HEA	C1B-C2B-C3B	-2.39	103.94	106.80
14	A	602[C]	HEA	O1A-CGA-CBA	-2.38	115.43	123.08
14	A	601[A]	HEA	CHA-C4D-C3D	-2.38	121.34	124.84
14	A	601[B]	HEA	CHA-C4D-C3D	-2.38	121.34	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	602[A]	HEA	O1A-CGA-CBA	-2.38	115.44	123.08
19	D	201	TGL	OG1-CA1-CA2	2.38	119.37	111.91
25	T	102	CDL	OB4-PB2-OB3	2.38	123.99	112.24
23	J	102	CHD	C13-C14-C8	-2.38	111.70	114.74
14	N	602[C]	HEA	CHB-C1B-NB	2.37	127.01	124.43
23	W	101	CHD	C14-C13-C12	-2.37	105.20	107.40
23	C	309	CHD	C1-C2-C3	2.37	113.50	110.47
25	T	102	CDL	C15-C14-C13	-2.36	102.42	114.42
24	C	303	PEK	O11-P-O14	-2.36	99.83	109.07
25	T	102	CDL	C18-C17-C16	-2.36	102.45	114.42
26	X	101	DMU	O5-C4-C57	2.36	112.29	106.44
26	X	102	DMU	C2-C3-C4	2.36	114.44	110.24
25	G	101	CDL	C62-C61-C60	2.35	126.36	114.42
25	C	308	CDL	OA6-CA4-CA3	2.35	116.91	108.40
26	P	315	DMU	O7-C3-C4	-2.35	103.01	109.45
23	J	102	CHD	C5-C4-C3	-2.35	109.31	112.76
14	N	602[A]	HEA	CMD-C2D-C1D	2.34	128.61	125.04
26	M	101	DMU	O5-C6-C1	2.34	115.30	110.35
25	T	102	CDL	C85-C84-C83	2.33	126.27	114.42
26	J	101	DMU	O16-C6-C1	2.33	111.94	108.30
24	T	101	PEK	C3-C4-C5	-2.33	99.09	112.43
26	C	311	DMU	C10-O1-C9	2.32	118.25	113.69
26	K	102	DMU	C6-C1-C2	2.32	114.83	110.00
23	C	309	CHD	O7-C7-C8	2.32	114.61	109.43
23	P	301	CHD	C5-C6-C7	2.32	117.02	114.46
25	C	308	CDL	C76-C75-C74	-2.31	102.69	114.42
24	P	304	PEK	C11-C10-C9	-2.30	100.68	112.02
14	N	602[C]	HEA	CMD-C2D-C3D	2.30	132.37	126.12
14	A	602[C]	HEA	CAD-C3D-C4D	-2.30	120.64	124.66
14	N	602[A]	HEA	CHC-C4B-NB	2.30	127.22	124.38
14	N	601[A]	HEA	O2A-CGA-O1A	-2.30	117.58	123.30
14	N	601[B]	HEA	O2A-CGA-O1A	-2.30	117.58	123.30
14	A	602[A]	HEA	O2A-CGA-CBA	2.29	121.37	114.03
25	P	308	CDL	OA9-CA7-C31	-2.28	114.83	123.73
14	A	601[A]	HEA	C1D-ND-C4D	-2.28	102.72	105.07
14	A	601[B]	HEA	C1D-ND-C4D	-2.28	102.72	105.07
14	N	601[A]	HEA	CMC-C2C-C3C	2.27	128.93	124.68
14	N	601[B]	HEA	CMC-C2C-C3C	2.27	128.93	124.68
20	C	307	PGV	C01-O03-C19	2.27	125.53	117.12
14	A	602[C]	HEA	C12-C13-C14	-2.27	106.24	112.23
19	O	301	TGL	OB1-CB1-CB2	-2.27	114.88	123.73
19	B	301	TGL	CG3-OG3-CC1	2.26	125.49	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	101	DMU	C31-C28-C25	-2.26	102.96	114.42
20	Q	201	PGV	C01-O03-C19	2.26	125.47	117.12
20	Q	201	PGV	C5-C4-C3	-2.26	102.98	114.42
19	A	607	TGL	C20-CA9-CA8	-2.25	102.99	114.42
14	A	601[A]	HEA	O2D-CGD-O1D	2.25	128.91	123.30
14	A	601[B]	HEA	O2D-CGD-O1D	2.25	128.91	123.30
14	A	601[A]	HEA	CHD-C1D-C2D	-2.25	120.50	126.72
14	A	601[B]	HEA	CHD-C1D-C2D	-2.25	120.50	126.72
26	Z	101	DMU	O4-C7-C8	2.25	115.55	110.35
19	O	301	TGL	OG1-CA1-OA1	-2.25	117.92	123.59
14	N	601[A]	HEA	C4B-C3B-C2B	-2.24	103.58	107.41
14	N	601[B]	HEA	C4B-C3B-C2B	-2.24	103.58	107.41
23	W	101	CHD	C1-C10-C5	2.24	111.08	107.77
26	M	101	DMU	C6-C1-C2	-2.24	105.34	110.00
26	J	101	DMU	O1-C9-C11	2.24	112.00	106.44
20	Q	201	PGV	C8-C7-C6	-2.23	103.08	114.42
26	M	101	DMU	C31-C28-C25	-2.23	103.09	114.42
25	T	102	CDL	C17-C16-C15	-2.23	103.09	114.42
23	B	303	CHD	C22-C20-C17	2.23	114.89	110.28
20	N	607	PGV	C01-O03-C19	-2.23	108.86	117.12
14	N	601[A]	HEA	CHA-C4D-ND	2.23	126.85	124.43
14	N	601[B]	HEA	CHA-C4D-ND	2.23	126.85	124.43
23	B	303	CHD	C17-C13-C12	2.22	119.70	117.67
14	A	602[A]	HEA	C2B-C1B-NB	2.22	112.54	109.88
14	A	601[A]	HEA	C17-C18-C19	2.22	133.00	127.66
23	B	303	CHD	O12-C12-C11	2.22	113.64	109.12
26	C	311	DMU	O5-C6-O16	-2.21	104.73	109.97
23	C	301	CHD	C5-C4-C3	-2.21	109.51	112.76
24	T	101	PEK	P-O12-C04	2.21	132.47	121.59
24	C	303	PEK	C16-C15-C14	-2.21	107.78	124.73
23	W	101	CHD	O7-C7-C8	2.21	114.36	109.43
26	P	316	DMU	O49-C1-C6	2.21	115.41	110.05
26	P	315	DMU	C1-C2-C3	2.20	114.71	109.68
26	K	101	DMU	O5-C4-C57	2.20	111.91	106.44
26	X	103	DMU	O16-C6-C1	2.20	111.73	108.30
20	P	306	PGV	C27-C26-C25	-2.20	103.28	114.42
27	E	201	PSC	C25-C24-C23	-2.19	103.31	114.42
23	B	303	CHD	C1-C10-C9	2.18	114.79	111.35
25	G	101	CDL	OA7-CA5-C11	-2.18	115.22	123.73
27	O	304	PSC	C08-N-C06	-2.18	103.36	108.97
26	P	316	DMU	O55-C2-C3	2.18	115.39	110.35
26	M	101	DMU	O2-C8-C9	-2.17	103.90	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	306	PGV	O01-C1-O02	-2.17	118.46	123.70
26	P	315	DMU	O3-C5-C7	-2.16	105.35	110.35
26	X	103	DMU	C2-C3-C4	2.16	114.10	110.24
26	K	101	DMU	O16-C6-C1	2.16	111.68	108.30
14	N	602[A]	HEA	O1A-CGA-CBA	-2.16	116.14	123.08
23	P	309	CHD	C22-C20-C17	-2.16	105.82	110.28
20	N	607	PGV	C30-C29-C28	2.16	125.38	114.42
25	C	308	CDL	OB5-PB2-OB3	2.16	112.52	106.47
19	A	607	TGL	C23-C22-C21	-2.15	103.49	114.42
19	O	302	TGL	OG2-CB1-CB2	2.15	116.14	111.50
14	A	602[C]	HEA	C13-C14-C15	-2.15	122.48	127.66
25	C	308	CDL	OA6-CA5-C11	2.15	116.13	111.50
23	C	301	CHD	C21-C20-C22	-2.14	107.00	110.36
26	P	310	DMU	O3-C5-C10	2.14	115.25	110.05
26	X	101	DMU	C6-O5-C4	2.13	117.88	113.69
24	P	304	PEK	O03-C21-C22	2.13	118.60	111.91
23	P	301	CHD	C9-C11-C12	-2.13	111.49	114.30
14	N	602[C]	HEA	O2A-CGA-O1A	-2.13	117.99	123.30
25	T	102	CDL	OB4-PB2-OB5	-2.13	97.87	107.75
14	N	602[C]	HEA	C3D-C4D-ND	2.13	112.42	110.36
14	A	602[C]	HEA	C2D-C1D-ND	2.12	112.35	109.84
24	C	303	PEK	C24-C23-C22	-2.12	105.57	113.19
14	N	602[C]	HEA	CMB-C2B-C3B	-2.11	126.31	130.34
14	N	601[B]	HEA	C27-C19-C18	-2.11	118.26	123.68
25	G	101	CDL	C61-C60-C59	-2.11	103.71	114.42
24	P	304	PEK	C7-C8-C9	-2.11	105.78	123.57
25	T	102	CDL	OA6-CA4-CA3	2.11	116.03	108.40
26	J	101	DMU	O49-C1-C2	-2.11	105.48	110.35
26	X	101	DMU	O7-C3-C2	2.11	115.22	110.35
14	A	601[A]	HEA	CHB-C1B-C2B	-2.11	121.69	124.98
14	A	601[B]	HEA	CHB-C1B-C2B	-2.11	121.69	124.98
26	X	103	DMU	C34-C31-C28	-2.10	103.78	114.42
20	Q	201	PGV	O01-C02-C03	2.10	116.00	108.40
26	P	311	DMU	C2-C3-C4	-2.09	106.12	110.93
25	P	308	CDL	CA4-OA6-CA5	2.09	122.94	117.79
21	B	305	EDO	O2-C2-C1	2.09	126.94	111.91
14	N	602[C]	HEA	C4D-C3D-C2D	-2.09	103.86	106.90
24	P	303	PEK	C8-C7-C6	-2.08	101.76	112.02
25	C	308	CDL	OB8-CB6-CB4	-2.08	102.37	108.43
19	A	607	TGL	C22-C21-C20	-2.08	103.86	114.42
26	P	311	DMU	C10-O1-C9	-2.08	109.61	113.69
19	D	201	TGL	OG2-CG2-CG3	2.08	115.93	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	303	CHD	C21-C20-C17	-2.08	109.74	112.92
26	P	312	DMU	O16-C18-C19	2.07	116.81	109.56
20	C	307	PGV	C26-C25-C24	-2.07	103.94	114.42
23	G	102	CHD	C13-C17-C20	-2.06	117.04	119.50
25	G	101	CDL	C85-C84-C83	2.05	124.84	114.42
26	M	101	DMU	O1-C9-C8	2.05	113.42	109.69
25	T	102	CDL	OA5-PA1-OA3	2.05	117.08	109.07
14	A	602[A]	HEA	C25-C23-C24	2.05	119.13	114.60
14	A	602[C]	HEA	C25-C23-C24	2.05	119.13	114.60
24	T	101	PEK	O01-C1-O02	-2.05	118.75	123.70
23	P	301	CHD	C6-C7-C8	-2.05	109.30	111.48
14	A	602[C]	HEA	O2A-CGA-CBA	2.05	120.60	114.03
26	M	101	DMU	O3-C5-C10	-2.05	105.08	110.05
25	G	101	CDL	C40-C39-C38	2.04	124.78	114.42
23	B	303	CHD	O7-C7-C6	2.03	114.99	109.94
26	C	311	DMU	O3-C5-C10	2.03	114.99	110.05
25	T	102	CDL	C83-C82-C81	2.03	124.74	114.42
25	Y	101	CDL	C52-C51-CB5	-2.03	106.23	113.62
20	C	306	PGV	O03-C19-O04	-2.03	118.47	123.59
26	P	311	DMU	C18-O16-C6	-2.03	110.48	113.84
23	W	101	CHD	C4-C3-C2	2.03	112.97	110.55
23	W	101	CHD	C15-C14-C13	2.03	105.54	103.55
14	N	601[A]	HEA	CHD-C1D-ND	2.02	126.88	124.38
14	N	601[B]	HEA	CHD-C1D-ND	2.02	126.88	124.38
19	D	201	TGL	CB4-CB3-CB2	-2.02	105.92	113.19
25	T	102	CDL	PB2-OB2-CB2	-2.02	109.82	121.68
23	P	309	CHD	C11-C9-C8	2.02	113.83	110.88
14	A	602[C]	HEA	C4B-NB-C1B	-2.02	102.99	105.07
14	N	602[C]	HEA	OMA-CMA-C3A	-2.02	120.51	124.91
20	P	307	PGV	O03-C01-C02	2.02	114.31	108.43
25	P	308	CDL	OB9-CB7-C71	-2.02	115.87	123.73
14	N	602[A]	HEA	CHD-C1D-C2D	-2.02	121.15	126.72
26	Z	101	DMU	C18-O16-C6	2.01	117.18	113.84
23	C	301	CHD	C16-C17-C20	-2.01	109.04	112.15
24	T	101	PEK	C8-C7-C6	-2.01	102.15	112.02
26	C	311	DMU	C28-C25-C22	-2.00	104.25	114.42
25	T	102	CDL	C40-C39-C38	2.00	124.59	114.42
20	C	307	PGV	O01-C1-O02	-2.00	118.86	123.70
25	T	102	CDL	C19-C18-C17	2.00	124.59	114.42
19	D	201	TGL	OG1-CA1-OA1	-2.00	118.54	123.59

There are no chirality outliers.

All (730) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C12-C11-C3B-C2B
14	A	601[B]	HEA	C14-C15-C16-C17
14	A	601[B]	HEA	C26-C15-C16-C17
14	A	602[C]	HEA	C4D-C3D-CAD-CBD
14	N	601[A]	HEA	C12-C11-C3B-C2B
14	N	601[B]	HEA	C14-C15-C16-C17
14	N	601[B]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C4D-C3D-CAD-CBD
19	A	607	TGL	OB1-CB1-OG2-CG2
19	B	301	TGL	OG1-CG1-CG2-OG2
19	O	301	TGL	OG1-CG1-CG2-OG2
19	O	302	TGL	CB2-CB1-OG2-CG2
20	A	608	PGV	C03-O11-P-O13
20	A	608	PGV	C03-O11-P-O14
20	A	608	PGV	C2-C1-O01-C02
20	A	608	PGV	O04-C19-O03-C01
20	A	608	PGV	C20-C19-O03-C01
20	C	307	PGV	C03-O11-P-O13
20	P	307	PGV	C10-C11-C12-C13
20	Q	201	PGV	C2-C1-O01-C02
20	Q	201	PGV	O04-C19-O03-C01
20	Q	201	PGV	C20-C19-O03-C01
23	J	102	CHD	C13-C17-C20-C21
23	J	102	CHD	C16-C17-C20-C22
23	J	102	CHD	C20-C22-C23-C24
24	C	304	PEK	C4-C5-C6-C7
24	P	305	PEK	C2-C1-O01-C02
24	P	305	PEK	C12-C13-C14-C15
24	P	305	PEK	C13-C14-C15-C16
24	T	101	PEK	C03-O11-P-O12
24	T	101	PEK	C03-O11-P-O13
24	T	101	PEK	C03-O11-P-O14
24	T	101	PEK	C2-C1-O01-C02
25	C	308	CDL	CA3-OA5-PA1-OA3
25	C	308	CDL	OA7-CA5-OA6-CA4
25	C	308	CDL	OA9-CA7-OA8-CA6
25	C	308	CDL	C31-CA7-OA8-CA6
25	C	308	CDL	CB3-OB5-PB2-OB2
25	C	308	CDL	CB3-OB5-PB2-OB3
25	C	308	CDL	CB3-OB5-PB2-OB4
25	G	101	CDL	OA9-CA7-OA8-CA6
25	G	101	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
25	G	101	CDL	C1-CB2-OB2-PB2
25	G	101	CDL	CB3-OB5-PB2-OB2
25	G	101	CDL	CB3-OB5-PB2-OB3
25	G	101	CDL	CB3-OB5-PB2-OB4
25	G	101	CDL	OB6-CB4-CB6-OB8
25	T	102	CDL	CA3-OA5-PA1-OA4
25	T	102	CDL	OA9-CA7-OA8-CA6
25	T	102	CDL	C31-CA7-OA8-CA6
25	Y	101	CDL	CA3-OA5-PA1-OA4
25	Y	101	CDL	CB2-OB2-PB2-OB3
25	Y	101	CDL	CB3-OB5-PB2-OB3
26	C	311	DMU	C1-C6-O16-C18
26	G	105	DMU	C3-C4-C57-O61
26	G	105	DMU	O5-C4-C57-O61
26	G	105	DMU	C19-C18-O16-C6
26	K	101	DMU	C1-C6-O16-C18
26	K	102	DMU	C19-C18-O16-C6
26	P	316	DMU	O5-C6-O16-C18
26	X	102	DMU	C1-C6-O16-C18
26	X	103	DMU	C1-C6-O16-C18
26	X	103	DMU	O5-C6-O16-C18
26	X	103	DMU	C19-C18-O16-C6
27	E	201	PSC	C03-O11-P-O13
27	E	201	PSC	O02-C1-O01-C02
27	E	201	PSC	C2-C1-O01-C02
27	O	304	PSC	C04-O12-P-O14
27	O	304	PSC	O02-C1-O01-C02
27	O	304	PSC	C2-C1-O01-C02
24	C	304	PEK	O04-C21-O03-C01
24	P	305	PEK	O04-C21-O03-C01
24	T	101	PEK	O04-C21-O03-C01
25	C	308	CDL	OB9-CB7-OB8-CB6
25	P	308	CDL	OA9-CA7-OA8-CA6
25	Y	101	CDL	OA9-CA7-OA8-CA6
24	C	304	PEK	C22-C21-O03-C01
24	P	305	PEK	C22-C21-O03-C01
25	C	308	CDL	C71-CB7-OB8-CB6
25	P	308	CDL	C31-CA7-OA8-CA6
25	Y	101	CDL	C31-CA7-OA8-CA6
20	C	307	PGV	O04-C19-O03-C01
20	P	307	PGV	O04-C19-O03-C01
23	J	102	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
19	D	201	TGL	OB1-CB1-OG2-CG2
19	O	302	TGL	OB1-CB1-OG2-CG2
20	A	608	PGV	O02-C1-O01-C02
20	Q	201	PGV	O02-C1-O01-C02
24	P	305	PEK	O02-C1-O01-C02
20	C	307	PGV	C20-C19-O03-C01
20	P	307	PGV	C20-C19-O03-C01
27	O	304	PSC	C20-C19-O03-C01
19	A	607	TGL	CB2-CB1-OG2-CG2
23	J	102	CHD	C13-C17-C20-C22
14	A	602[C]	HEA	C2D-C3D-CAD-CBD
14	N	602[C]	HEA	C2D-C3D-CAD-CBD
19	B	301	TGL	CC2-CC1-OG3-CG3
19	O	301	TGL	CC2-CC1-OG3-CG3
24	T	101	PEK	C22-C21-O03-C01
27	E	201	PSC	C20-C19-O03-C01
20	C	307	PGV	C10-C11-C12-C13
24	T	101	PEK	O02-C1-O01-C02
19	B	301	TGL	OC1-CC1-OG3-CG3
27	O	304	PSC	O04-C19-O03-C01
19	B	301	TGL	C11-C12-C13-C14
19	A	607	TGL	CC2-CC3-CC4-CC5
26	P	311	DMU	O5-C4-C57-O61
26	P	316	DMU	O5-C4-C57-O61
25	C	308	CDL	C11-CA5-OA6-CA4
26	K	102	DMU	O5-C4-C57-O61
26	P	312	DMU	O6-C11-C9-O1
27	E	201	PSC	O04-C19-O03-C01
25	P	308	CDL	C37-C38-C39-C40
19	O	301	TGL	OC1-CC1-OG3-CG3
26	X	102	DMU	O5-C4-C57-O61
26	K	101	DMU	O5-C6-O16-C18
26	K	102	DMU	O5-C6-O16-C18
20	P	306	PGV	C28-C29-C30-C31
26	P	316	DMU	C3-C4-C57-O61
23	P	309	CHD	C17-C20-C22-C23
25	P	308	CDL	OB6-CB4-CB6-OB8
19	D	201	TGL	CB2-CB1-OG2-CG2
26	P	315	DMU	C3-C4-C57-O61
19	O	302	TGL	CA9-C20-C21-C22
27	O	304	PSC	C20-C21-C22-C23
25	T	102	CDL	CA2-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
25	Y	101	CDL	C17-C18-C19-C20
26	P	311	DMU	C3-C4-C57-O61
14	A	602[A]	HEA	C2D-C3D-CAD-CBD
25	T	102	CDL	OA5-CA3-CA4-OA6
23	C	309	CHD	C21-C20-C22-C23
27	E	201	PSC	C1-C2-C3-C4
26	C	311	DMU	O5-C4-C57-O61
26	P	311	DMU	O6-C11-C9-O1
23	P	309	CHD	C21-C20-C22-C23
24	C	304	PEK	C1-C2-C3-C4
24	C	303	PEK	C7-C8-C9-C10
24	C	304	PEK	C7-C8-C9-C10
24	C	304	PEK	C13-C14-C15-C16
26	X	102	DMU	C3-C4-C57-O61
23	W	101	CHD	C13-C17-C20-C22
19	B	301	TGL	CC1-CC2-CC3-CC4
20	C	306	PGV	C19-C20-C21-C22
20	P	307	PGV	C19-C20-C21-C22
24	P	305	PEK	C1-C2-C3-C4
25	P	308	CDL	CB5-C51-C52-C53
20	C	305	PGV	C26-C27-C28-C29
23	C	309	CHD	C17-C20-C22-C23
25	C	308	CDL	C42-C43-C44-C45
25	P	308	CDL	OA7-CA5-OA6-CA4
27	E	201	PSC	C04-C05-N-C06
27	E	201	PSC	C04-C05-N-C07
19	O	301	TGL	CA1-CA2-CA3-CA4
19	O	302	TGL	CC9-C15-C16-C17
26	K	102	DMU	O16-C18-C19-C22
23	P	309	CHD	C20-C22-C23-C24
26	X	103	DMU	O16-C18-C19-C22
26	P	315	DMU	O5-C4-C57-O61
26	K	101	DMU	C3-C4-C57-O61
26	P	310	DMU	O6-C11-C9-C8
26	C	311	DMU	O5-C6-O16-C18
25	T	102	CDL	C11-C12-C13-C14
26	X	101	DMU	O16-C18-C19-C22
20	C	307	PGV	O12-C04-C05-O05
25	G	101	CDL	O1-C1-CA2-OA2
24	C	304	PEK	O02-C1-O01-C02
20	A	608	PGV	C19-C20-C21-C22
26	J	101	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
26	P	312	DMU	O16-C18-C19-C22
24	P	304	PEK	C7-C8-C9-C10
24	P	305	PEK	C10-C11-C12-C13
27	E	201	PSC	C11-C10-C9-C8
25	C	308	CDL	C80-C81-C82-C83
25	P	308	CDL	C11-CA5-OA6-CA4
20	P	307	PGV	C03-O11-P-O12
25	G	101	CDL	CA2-OA2-PA1-OA5
25	G	101	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CA3-OA5-PA1-OA2
25	Y	101	CDL	CA3-OA5-PA1-OA2
27	E	201	PSC	C03-O11-P-O12
27	O	304	PSC	C04-O12-P-O11
19	D	201	TGL	CC2-CC1-OG3-CG3
24	C	304	PEK	C2-C1-O01-C02
23	W	101	CHD	C16-C17-C20-C21
23	W	101	CHD	C13-C17-C20-C21
26	P	311	DMU	O16-C18-C19-C22
25	G	101	CDL	CB2-C1-CA2-OA2
26	X	101	DMU	O5-C4-C57-O61
27	O	304	PSC	C04-C05-N-C06
26	C	311	DMU	O6-C11-C9-O1
25	P	308	CDL	C51-CB5-OB6-CB4
19	A	607	TGL	CA9-C20-C21-C22
19	B	301	TGL	C22-C23-C24-C25
20	A	608	PGV	C20-C21-C22-C23
26	X	103	DMU	O5-C4-C57-O61
25	C	308	CDL	C51-CB5-OB6-CB4
19	A	607	TGL	CC3-CC4-CC5-CC6
19	B	301	TGL	CC4-CC5-CC6-CC7
19	O	301	TGL	C10-C11-C12-C13
20	P	306	PGV	C7-C8-C9-C10
25	C	308	CDL	C82-C83-C84-C85
19	A	607	TGL	C13-C14-C29-C30
19	A	607	TGL	C20-C21-C22-C23
19	O	302	TGL	C21-C22-C23-C24
24	C	303	PEK	C22-C23-C24-C25
24	C	303	PEK	C26-C27-C28-C29
25	C	308	CDL	OB7-CB5-OB6-CB4
25	P	308	CDL	OB7-CB5-OB6-CB4
24	P	304	PEK	C4-C5-C6-C7
24	P	304	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	T	101	PEK	C4-C5-C6-C7
25	G	101	CDL	C15-C16-C17-C18
26	K	102	DMU	C3-C4-C57-O61
25	T	102	CDL	O1-C1-CB2-OB2
25	Y	101	CDL	O1-C1-CB2-OB2
19	A	607	TGL	C21-C22-C23-C24
19	O	301	TGL	CC3-CC4-CC5-CC6
19	O	301	TGL	C20-C21-C22-C23
26	P	315	DMU	C1-C6-O16-C18
19	A	607	TGL	CA3-CA4-CA5-CA6
19	D	201	TGL	CA3-CA4-CA5-CA6
20	C	306	PGV	C20-C21-C22-C23
24	C	303	PEK	C28-C29-C30-C31
19	D	201	TGL	CA7-CA8-CA9-C20
26	K	103	DMU	O16-C18-C19-C22
26	P	310	DMU	C25-C28-C31-C34
19	B	301	TGL	CA5-CA6-CA7-CA8
19	O	302	TGL	CB9-C10-C11-C12
20	C	307	PGV	C2-C3-C4-C5
19	A	607	TGL	C22-C23-C24-C25
19	B	301	TGL	CA4-CA5-CA6-CA7
19	B	301	TGL	CB6-CB7-CB8-CB9
20	C	306	PGV	C7-C8-C9-C10
25	C	308	CDL	C60-C61-C62-C63
25	Y	101	CDL	C20-C21-C22-C23
19	B	301	TGL	C10-C11-C12-C13
19	B	301	TGL	C20-C21-C22-C23
19	O	301	TGL	CA9-C20-C21-C22
19	O	302	TGL	CA6-CA7-CA8-CA9
26	X	102	DMU	C28-C31-C34-C37
27	O	304	PSC	C04-C05-N-C07
26	P	310	DMU	O5-C6-O16-C18
26	P	315	DMU	O5-C6-O16-C18
26	X	102	DMU	O5-C6-O16-C18
19	O	301	TGL	C16-C15-CC9-CC8
19	O	302	TGL	C11-C10-CB9-CB8
19	O	302	TGL	C11-C12-C13-C14
19	O	302	TGL	C16-C15-CC9-CC8
19	O	302	TGL	CC5-CC6-CC7-CC8
26	P	316	DMU	C22-C25-C28-C31
26	C	311	DMU	O6-C11-C9-C8
25	G	101	CDL	C58-C59-C60-C61

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Mol	Chain	Res	Type	Atoms
25	T	102	CDL	C16-C17-C18-C19
24	P	304	PEK	C22-C23-C24-C25
19	O	301	TGL	CC2-CC3-CC4-CC5
26	P	310	DMU	O16-C18-C19-C22
19	D	201	TGL	C23-C24-C25-C26
19	O	301	TGL	C16-C17-C18-C19
24	C	303	PEK	C13-C14-C15-C16
19	A	607	TGL	C10-C11-C12-C13
19	B	301	TGL	C12-C13-C14-C29
19	B	301	TGL	CC5-CC6-CC7-CC8
14	A	602[A]	HEA	C4D-C3D-CAD-CBD
25	T	102	CDL	C34-C35-C36-C37
27	O	304	PSC	C28-C29-C30-C31
19	D	201	TGL	OC1-CC1-OG3-CG3
26	P	315	DMU	C25-C28-C31-C34
26	K	102	DMU	C19-C22-C25-C28
26	X	102	DMU	C18-C19-C22-C25
25	C	308	CDL	C59-C60-C61-C62
26	P	316	DMU	C19-C22-C25-C28
19	D	201	TGL	CB9-C10-C11-C12
25	T	102	CDL	C37-C38-C39-C40
25	Y	101	CDL	C57-C58-C59-C60
20	C	305	PGV	C27-C28-C29-C30
19	A	607	TGL	CC4-CC5-CC6-CC7
27	O	304	PSC	C04-C05-N-C08
21	B	305	EDO	O1-C1-C2-O2
25	P	308	CDL	C43-C44-C45-C46
26	Z	101	DMU	C28-C31-C34-C37
19	O	302	TGL	CC2-CC1-OG3-CG3
19	B	301	TGL	C21-C20-CA9-CA8
19	A	607	TGL	C11-C10-CB9-CB8
19	A	607	TGL	CA2-CA1-OG1-CG1
26	P	315	DMU	C22-C25-C28-C31
19	B	301	TGL	CB9-C10-C11-C12
20	C	305	PGV	C29-C30-C31-C32
26	Z	101	DMU	C22-C25-C28-C31
19	O	301	TGL	CB2-CB1-OG2-CG2
20	C	307	PGV	C2-C1-O01-C02
25	G	101	CDL	C82-C83-C84-C85
19	O	301	TGL	CA3-CA4-CA5-CA6
24	C	304	PEK	C10-C11-C12-C13
27	O	304	PSC	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
26	L	101	DMU	C3-C4-C57-O61
25	G	101	CDL	C60-C61-C62-C63
26	J	101	DMU	C28-C31-C34-C37
20	C	307	PGV	O02-C1-O01-C02
27	O	304	PSC	C5-C6-C7-C8
25	C	308	CDL	C77-C78-C79-C80
20	C	307	PGV	C02-C03-O11-P
20	P	307	PGV	C02-C03-O11-P
25	Y	101	CDL	C51-C52-C53-C54
24	T	101	PEK	C01-C02-C03-O11
25	T	102	CDL	OA5-CA3-CA4-CA6
20	C	307	PGV	O12-C04-C05-C06
25	Y	101	CDL	CA2-C1-CB2-OB2
19	O	301	TGL	OB1-CB1-OG2-CG2
19	A	607	TGL	CC9-C15-C16-C17
20	Q	201	PGV	C20-C21-C22-C23
26	M	101	DMU	C19-C22-C25-C28
19	B	301	TGL	CC6-CC7-CC8-CC9
20	C	307	PGV	C20-C21-C22-C23
27	E	201	PSC	C5-C6-C7-C8
19	A	607	TGL	OA1-CA1-OG1-CG1
19	O	302	TGL	OC1-CC1-OG3-CG3
26	X	102	DMU	C25-C28-C31-C34
24	P	305	PEK	O03-C01-C02-C03
25	Y	101	CDL	C60-C61-C62-C63
19	O	301	TGL	C14-C29-C30-C31
25	G	101	CDL	C37-C38-C39-C40
19	B	301	TGL	C11-C10-CB9-CB8
19	A	607	TGL	CB1-CB2-CB3-CB4
25	Y	101	CDL	C64-C65-C66-C67
26	Z	101	DMU	C25-C28-C31-C34
19	O	301	TGL	CA6-CA7-CA8-CA9
25	T	102	CDL	C20-C21-C22-C23
20	C	307	PGV	O05-C05-C06-O06
20	A	608	PGV	C11-C10-C9-C8
19	O	301	TGL	C13-C14-C29-C30
26	Z	101	DMU	C34-C37-C40-C43
20	A	608	PGV	C15-C16-C17-C18
26	P	312	DMU	O6-C11-C9-C8
19	B	301	TGL	CC3-CC4-CC5-CC6
26	J	101	DMU	C34-C37-C40-C43
26	P	316	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
26	P	315	DMU	O6-C11-C9-O1
20	A	608	PGV	C10-C11-C12-C13
24	C	303	PEK	C4-C5-C6-C7
24	C	303	PEK	C10-C11-C12-C13
24	P	304	PEK	C13-C14-C15-C16
27	E	201	PSC	C04-C05-N-C08
25	T	102	CDL	C77-C78-C79-C80
26	M	101	DMU	C28-C31-C34-C37
14	N	602[A]	HEA	C4D-C3D-CAD-CBD
25	C	308	CDL	C41-C42-C43-C44
25	G	101	CDL	C81-C82-C83-C84
26	P	310	DMU	C1-C6-O16-C18
20	A	608	PGV	O03-C01-C02-O01
19	A	607	TGL	C23-C24-C25-C26
19	A	607	TGL	C14-C29-C30-C31
27	E	201	PSC	C20-C21-C22-C23
27	E	201	PSC	O03-C19-C20-C21
20	P	307	PGV	C1-C2-C3-C4
20	A	608	PGV	C7-C8-C9-C10
25	G	101	CDL	C77-C78-C79-C80
19	D	201	TGL	CA6-CA7-CA8-CA9
25	C	308	CDL	C51-C52-C53-C54
20	C	306	PGV	C27-C28-C29-C30
25	G	101	CDL	C57-C58-C59-C60
26	P	315	DMU	C4-C3-O7-C10
27	E	201	PSC	C19-C20-C21-C22
20	P	307	PGV	C20-C21-C22-C23
25	C	308	CDL	C38-C39-C40-C41
26	X	102	DMU	C19-C22-C25-C28
20	C	305	PGV	C10-C11-C12-C13
20	Q	201	PGV	C10-C11-C12-C13
20	A	608	PGV	C01-C02-C03-O11
20	Q	201	PGV	C01-C02-C03-O11
25	C	308	CDL	OA5-CA3-CA4-CA6
25	G	101	CDL	C80-C81-C82-C83
26	P	316	DMU	C25-C28-C31-C34
19	O	301	TGL	CB1-CB2-CB3-CB4
19	B	301	TGL	CA3-CA4-CA5-CA6
25	Y	101	CDL	CA7-C31-C32-C33
25	C	308	CDL	C40-C41-C42-C43
20	P	307	PGV	O12-C04-C05-O05
19	O	301	TGL	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
27	O	304	PSC	C24-C25-C26-C27
25	G	101	CDL	CA7-C31-C32-C33
26	X	103	DMU	C25-C28-C31-C34
26	K	103	DMU	C19-C18-O16-C6
26	P	310	DMU	C22-C25-C28-C31
24	C	304	PEK	C35-C36-C37-C38
19	B	301	TGL	OG1-CG1-CG2-CG3
19	O	301	TGL	OG1-CG1-CG2-CG3
19	O	302	TGL	C10-C11-C12-C13
20	P	306	PGV	C24-C25-C26-C27
20	N	607	PGV	C10-C11-C12-C13
24	T	101	PEK	C7-C8-C9-C10
26	K	103	DMU	C19-C22-C25-C28
19	O	302	TGL	C17-C18-C19-C33
20	C	307	PGV	C03-O11-P-O12
24	C	303	PEK	C6-C7-C8-C9
24	C	303	PEK	C9-C10-C11-C12
24	C	303	PEK	C11-C12-C13-C14
24	C	304	PEK	C5-C6-C7-C8
24	C	304	PEK	C6-C7-C8-C9
24	C	304	PEK	C11-C10-C9-C8
24	C	304	PEK	C9-C10-C11-C12
24	C	304	PEK	C11-C12-C13-C14
24	C	304	PEK	C12-C13-C14-C15
24	P	303	PEK	C5-C6-C7-C8
24	P	303	PEK	C6-C7-C8-C9
24	P	303	PEK	C11-C10-C9-C8
24	P	303	PEK	C11-C12-C13-C14
24	P	303	PEK	C12-C13-C14-C15
24	P	305	PEK	C5-C6-C7-C8
24	P	305	PEK	C6-C7-C8-C9
24	P	305	PEK	C11-C10-C9-C8
24	P	305	PEK	C9-C10-C11-C12
24	P	305	PEK	C11-C12-C13-C14
24	T	101	PEK	C5-C6-C7-C8
24	T	101	PEK	C11-C10-C9-C8
24	T	101	PEK	C9-C10-C11-C12
24	T	101	PEK	C12-C13-C14-C15
25	Y	101	CDL	CB2-OB2-PB2-OB5
27	E	201	PSC	C9-C10-C11-C12
27	E	201	PSC	C10-C11-C12-C13
27	O	304	PSC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	O	304	PSC	C10-C11-C12-C13
19	B	301	TGL	CB3-CB4-CB5-CB6
20	A	608	PGV	O01-C02-C03-O11
24	T	101	PEK	O01-C02-C03-O11
25	C	308	CDL	C39-C40-C41-C42
25	Y	101	CDL	C76-C77-C78-C79
19	A	607	TGL	C21-C20-CA9-CA8
25	G	101	CDL	C38-C39-C40-C41
25	Y	101	CDL	C77-C78-C79-C80
19	B	301	TGL	CB7-CB8-CB9-C10
19	D	201	TGL	C21-C20-CA9-CA8
20	Q	201	PGV	O03-C01-C02-O01
27	E	201	PSC	C24-C25-C26-C27
19	A	607	TGL	CC6-CC7-CC8-CC9
25	G	101	CDL	CA2-C1-CB2-OB2
26	X	101	DMU	C19-C22-C25-C28
19	B	301	TGL	OB1-CB1-OG2-CG2
25	G	101	CDL	C11-C12-C13-C14
20	P	306	PGV	C02-C03-O11-P
25	C	308	CDL	C36-C37-C38-C39
27	O	304	PSC	C22-C23-C24-C25
21	A	617	EDO	O1-C1-C2-O2
19	A	607	TGL	CB5-CB6-CB7-CB8
19	B	301	TGL	CB5-CB6-CB7-CB8
24	C	303	PEK	C17-C18-C19-C20
26	K	103	DMU	C18-C19-C22-C25
14	N	602[A]	HEA	C2D-C3D-CAD-CBD
26	P	310	DMU	C28-C31-C34-C37
25	P	308	CDL	OA5-CA3-CA4-CA6
24	P	305	PEK	C2-C3-C4-C5
26	J	101	DMU	C18-C19-C22-C25
23	C	309	CHD	C20-C22-C23-C24
20	A	608	PGV	C03-O11-P-O12
25	P	308	CDL	CA7-C31-C32-C33
19	B	301	TGL	CC7-CC8-CC9-C15
25	C	308	CDL	C13-C14-C15-C16
19	A	607	TGL	CG1-CG2-OG2-CB1
19	D	201	TGL	CB4-CB5-CB6-CB7
25	P	308	CDL	C41-C42-C43-C44
19	A	607	TGL	OG1-CG1-CG2-CG3
19	O	302	TGL	CG1-CG2-CG3-OG3
20	C	306	PGV	C02-C03-O11-P

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Mol	Chain	Res	Type	Atoms
25	Y	101	CDL	CA3-CA4-CA6-OA8
25	C	308	CDL	CA7-C31-C32-C33
25	Y	101	CDL	OA7-CA5-OA6-CA4
19	O	301	TGL	C24-C25-C26-C27
26	G	105	DMU	C1-C6-O16-C18
26	P	311	DMU	C1-C6-O16-C18
19	A	607	TGL	OG1-CG1-CG2-OG2
19	B	301	TGL	OG2-CG2-CG3-OG3
19	O	301	TGL	OG2-CG2-CG3-OG3
25	Y	101	CDL	OA6-CA4-CA6-OA8
25	Y	101	CDL	OB6-CB4-CB6-OB8
19	O	301	TGL	CC5-CC6-CC7-CC8
25	P	308	CDL	C82-C83-C84-C85
20	C	306	PGV	C24-C25-C26-C27
24	C	303	PEK	C27-C28-C29-C30
27	E	201	PSC	C23-C24-C25-C26
19	B	301	TGL	CC2-CC3-CC4-CC5
25	P	308	CDL	C58-C59-C60-C61
25	T	102	CDL	CB3-OB5-PB2-OB2
19	A	607	TGL	CA2-CA3-CA4-CA5
24	C	303	PEK	C25-C26-C27-C28
25	C	308	CDL	CA4-CA3-OA5-PA1
19	A	607	TGL	CB6-CB7-CB8-CB9
26	P	315	DMU	C19-C22-C25-C28
20	P	307	PGV	C03-O11-P-O13
25	G	101	CDL	CA2-OA2-PA1-OA3
25	G	101	CDL	CA3-OA5-PA1-OA3
27	E	201	PSC	C03-O11-P-O14
27	O	304	PSC	C04-O12-P-O13
19	D	201	TGL	CA9-C20-C21-C22
27	E	201	PSC	C22-C23-C24-C25
26	P	315	DMU	C2-C3-O7-C10
20	N	607	PGV	C23-C24-C25-C26
26	P	312	DMU	C18-C19-C22-C25
19	B	301	TGL	C16-C15-CC9-CC8
19	D	201	TGL	C11-C10-CB9-CB8
25	Y	101	CDL	C72-C71-CB7-OB8
27	O	304	PSC	O03-C19-C20-C21
19	B	301	TGL	CG1-CG2-CG3-OG3
19	O	301	TGL	CB7-CB8-CB9-C10
19	O	301	TGL	CG1-CG2-CG3-OG3
20	A	608	PGV	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
27	E	201	PSC	O12-C04-C05-N
27	O	304	PSC	O03-C01-C02-C03
27	O	304	PSC	O12-C04-C05-N
19	O	302	TGL	OG2-CG2-CG3-OG3
24	P	305	PEK	O03-C01-C02-O01
27	O	304	PSC	O03-C01-C02-O01
24	P	305	PEK	C4-C5-C6-C7
19	D	201	TGL	CB7-CB8-CB9-C10
20	C	306	PGV	C13-C14-C15-C16
26	P	310	DMU	O6-C11-C9-O1
26	K	102	DMU	C22-C25-C28-C31
25	T	102	CDL	C80-C81-C82-C83
25	Y	101	CDL	C59-C60-C61-C62
20	Q	201	PGV	C01-C02-O01-C1
26	X	103	DMU	C3-C4-C57-O61
25	C	308	CDL	OA5-CA3-CA4-OA6
14	A	601[A]	HEA	C27-C19-C20-C21
19	O	301	TGL	CC6-CC7-CC8-CC9
21	P	314	EDO	O1-C1-C2-O2
21	S	107	EDO	O1-C1-C2-O2
20	C	307	PGV	C4-C5-C6-C7
19	B	301	TGL	CB2-CB1-OG2-CG2
25	Y	101	CDL	C11-CA5-OA6-CA4
26	P	311	DMU	O5-C6-O16-C18
25	Y	101	CDL	C18-C19-C20-C21
27	E	201	PSC	C7-C8-C9-C10
25	C	308	CDL	CA3-OA5-PA1-OA2
25	T	102	CDL	CB2-OB2-PB2-OB5
25	Y	101	CDL	CA2-OA2-PA1-OA5
25	Y	101	CDL	CB3-OB5-PB2-OB2
27	E	201	PSC	C04-O12-P-O11
26	Z	101	DMU	O6-C11-C9-C8
25	Y	101	CDL	CB3-CB4-CB6-OB8
24	P	305	PEK	C14-C15-C16-C17
19	D	201	TGL	CB3-CB4-CB5-CB6
25	P	308	CDL	C55-C56-C57-C58
25	P	308	CDL	CA5-C11-C12-C13
20	C	305	PGV	C11-C12-C13-C14
20	N	607	PGV	C11-C12-C13-C14
24	P	305	PEK	C3-C4-C5-C6
19	B	301	TGL	CA6-CA7-CA8-CA9
26	C	311	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	CAD-CBD-CGD-O1D
14	A	601[B]	HEA	CAD-CBD-CGD-O1D
14	N	602[C]	HEA	CAA-CBA-CGA-O2A
19	A	607	TGL	OG1-CA1-CA2-CA3
25	T	102	CDL	C14-C15-C16-C17
25	T	102	CDL	C81-C82-C83-C84
23	C	309	CHD	C22-C23-C24-O26
14	A	601[A]	HEA	C16-C17-C18-C19
25	Y	101	CDL	C22-C23-C24-C25
25	T	102	CDL	OB5-CB3-CB4-CB6
20	C	307	PGV	C9-C10-C11-C12
25	T	102	CDL	C42-C43-C44-C45
23	W	101	CHD	C22-C23-C24-O25
19	D	201	TGL	CB5-CB6-CB7-CB8
19	O	301	TGL	C12-C13-C14-C29
25	T	102	CDL	CB3-CB4-CB6-OB8
26	L	101	DMU	C1-C6-O16-C18
23	B	303	CHD	C22-C23-C24-O25
23	G	102	CHD	C22-C23-C24-O25
25	T	102	CDL	C1-CB2-OB2-PB2
27	E	201	PSC	O04-C19-C20-C21
19	O	301	TGL	CA7-CA8-CA9-C20
25	P	308	CDL	C34-C35-C36-C37
23	J	102	CHD	C22-C23-C24-O26
20	Q	201	PGV	C12-C13-C14-C15
21	S	108	EDO	O1-C1-C2-O2
26	K	101	DMU	O5-C4-C57-O61
20	C	306	PGV	C15-C16-C17-C18
26	G	105	DMU	C28-C31-C34-C37
23	B	303	CHD	C22-C23-C24-O26
14	N	602[A]	HEA	CAD-CBD-CGD-O1D
19	A	607	TGL	C11-C12-C13-C14
26	K	102	DMU	C28-C31-C34-C37
25	C	308	CDL	C58-C59-C60-C61
23	J	102	CHD	C22-C23-C24-O25
19	A	607	TGL	CC5-CC6-CC7-CC8
14	N	601[A]	HEA	CAD-CBD-CGD-O1D
14	N	601[B]	HEA	CAD-CBD-CGD-O1D
19	O	302	TGL	CB5-CB6-CB7-CB8
24	P	303	PEK	C9-C10-C11-C12
24	P	304	PEK	C11-C12-C13-C14
24	T	101	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	T	101	PEK	C11-C12-C13-C14
19	O	302	TGL	CB4-CB5-CB6-CB7
14	N	602[C]	HEA	CAA-CBA-CGA-O1A
23	G	102	CHD	C22-C23-C24-O26
23	W	101	CHD	C22-C23-C24-O26
20	C	306	PGV	C10-C11-C12-C13
20	P	306	PGV	C20-C21-C22-C23
26	J	101	DMU	C31-C34-C37-C40
19	O	302	TGL	CA5-CA6-CA7-CA8
25	Y	101	CDL	C53-C54-C55-C56
14	A	602[C]	HEA	CAA-CBA-CGA-O2A
24	P	305	PEK	C7-C8-C9-C10
14	N	602[A]	HEA	CAD-CBD-CGD-O2D
14	A	602[A]	HEA	CAD-CBD-CGD-O1D
25	Y	101	CDL	C12-C11-CA5-OA6
19	O	302	TGL	C20-C21-C22-C23
19	O	301	TGL	CC7-CC8-CC9-C15
25	P	308	CDL	C73-C74-C75-C76
20	Q	201	PGV	C2-C3-C4-C5
25	Y	101	CDL	C71-C72-C73-C74
26	X	102	DMU	C34-C37-C40-C43
20	P	306	PGV	C9-C10-C11-C12
24	P	304	PEK	C14-C15-C16-C17
27	E	201	PSC	C12-C13-C14-C15
14	A	602[A]	HEA	CAD-CBD-CGD-O2D
14	N	602[A]	HEA	CAA-CBA-CGA-O1A
23	P	309	CHD	C22-C23-C24-O26
21	Q	202	EDO	O1-C1-C2-O2
21	S	106	EDO	O1-C1-C2-O2
25	T	102	CDL	C12-C13-C14-C15
14	A	602[C]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C26-C15-C16-C17
14	A	602[C]	HEA	CAA-CBA-CGA-O1A
25	T	102	CDL	C32-C33-C34-C35
20	P	307	PGV	C6-C7-C8-C9
27	E	201	PSC	C21-C22-C23-C24
14	A	602[A]	HEA	CAA-CBA-CGA-O1A
19	O	301	TGL	C17-C18-C19-C33
26	M	101	DMU	C22-C25-C28-C31
26	C	311	DMU	C22-C25-C28-C31
25	C	308	CDL	C52-C51-CB5-OB6
14	A	602[A]	HEA	C26-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
14	A	601[A]	HEA	C18-C19-C20-C21
25	G	101	CDL	C12-C11-CA5-OA6
24	C	304	PEK	C14-C15-C16-C17
24	P	303	PEK	C3-C4-C5-C6
14	N	601[A]	HEA	CAD-CBD-CGD-O2D
14	N	601[B]	HEA	CAD-CBD-CGD-O2D
20	Q	201	PGV	C03-C02-O01-C1
25	C	308	CDL	C37-C38-C39-C40
14	A	601[A]	HEA	CAD-CBD-CGD-O2D
14	A	601[B]	HEA	CAD-CBD-CGD-O2D
14	N	602[A]	HEA	C26-C15-C16-C17
14	N	602[C]	HEA	C14-C15-C16-C17
20	C	307	PGV	C13-C14-C15-C16
26	X	101	DMU	C22-C25-C28-C31
20	C	306	PGV	C05-C04-O12-P
20	Q	201	PGV	O03-C01-C02-C03
20	C	307	PGV	C7-C8-C9-C10
19	B	301	TGL	C21-C22-C23-C24
19	O	301	TGL	CB6-CB7-CB8-CB9
14	N	602[A]	HEA	CAA-CBA-CGA-O2A
23	C	309	CHD	C22-C23-C24-O25
19	D	201	TGL	CA2-CA3-CA4-CA5
26	P	311	DMU	C34-C37-C40-C43
19	D	201	TGL	OG2-CB1-CB2-CB3
23	P	301	CHD	C22-C23-C24-O25
23	P	309	CHD	C22-C23-C24-O25
25	T	102	CDL	C13-C14-C15-C16
24	C	304	PEK	O01-C1-C2-C3
25	C	308	CDL	C81-C82-C83-C84
20	C	305	PGV	C11-C10-C9-C8
25	T	102	CDL	C40-C41-C42-C43
26	Z	101	DMU	O16-C18-C19-C22
25	Y	101	CDL	C32-C31-CA7-OA8
19	O	302	TGL	CC1-CC2-CC3-CC4
24	T	101	PEK	C26-C27-C28-C29
23	C	301	CHD	C22-C23-C24-O25
20	Q	201	PGV	C11-C12-C13-C14
25	Y	101	CDL	C31-C32-C33-C34
25	P	308	CDL	C81-C82-C83-C84
23	C	309	CHD	C16-C17-C20-C22
26	M	101	DMU	C34-C37-C40-C43
26	G	105	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
19	O	302	TGL	CA7-CA8-CA9-C20
20	C	306	PGV	C11-C12-C13-C14
14	A	602[A]	HEA	CAA-CBA-CGA-O2A
19	O	301	TGL	C15-C16-C17-C18
26	M	101	DMU	O6-C11-C9-C8
20	A	608	PGV	C23-C24-C25-C26
20	P	306	PGV	C30-C31-C32-C33
26	P	310	DMU	C19-C22-C25-C28
27	O	304	PSC	C12-C13-C14-C15
24	C	304	PEK	C2-C3-C4-C5
20	P	307	PGV	C2-C3-C4-C5
20	C	307	PGV	C24-C25-C26-C27
25	P	308	CDL	C36-C37-C38-C39
24	P	305	PEK	C32-C33-C34-C35
25	G	101	CDL	C12-C11-CA5-OA7
19	A	607	TGL	C16-C15-CC9-CC8
24	C	304	PEK	C31-C32-C33-C34
24	C	304	PEK	O02-C1-C2-C3
24	P	304	PEK	C27-C28-C29-C30
25	Y	101	CDL	C74-C75-C76-C77
25	C	308	CDL	C52-C51-CB5-OB7
26	P	312	DMU	C25-C28-C31-C34
14	A	601[A]	HEA	CAA-CBA-CGA-O2A
14	A	601[B]	HEA	CAA-CBA-CGA-O2A
20	P	307	PGV	C9-C10-C11-C12
25	Y	101	CDL	C32-C31-CA7-OA9
19	O	302	TGL	OG2-CB1-CB2-CB3
14	N	601[A]	HEA	CAA-CBA-CGA-O2A
14	N	601[B]	HEA	CAA-CBA-CGA-O2A
25	G	101	CDL	C20-C21-C22-C23
21	D	202	EDO	O1-C1-C2-O2
21	U	101	EDO	O1-C1-C2-O2
20	P	307	PGV	C12-C13-C14-C15
19	O	302	TGL	C16-C17-C18-C19
24	C	304	PEK	C3-C4-C5-C6
25	P	308	CDL	CA3-CA4-OA6-CA5
27	E	201	PSC	C03-C02-O01-C1
25	G	101	CDL	OB9-CB7-OB8-CB6
25	T	102	CDL	C17-C18-C19-C20
23	C	301	CHD	C22-C23-C24-O26
24	P	305	PEK	C21-C22-C23-C24
26	X	101	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
20	C	306	PGV	C9-C10-C11-C12
27	O	304	PSC	C7-C8-C9-C10
24	C	303	PEK	C16-C17-C18-C19
25	Y	101	CDL	C58-C59-C60-C61
25	T	102	CDL	C32-C31-CA7-OA8
20	P	306	PGV	C1-C2-C3-C4
14	A	601[A]	HEA	O11-C11-C3B-C2B
19	O	301	TGL	C22-C23-C24-C25
20	N	607	PGV	C28-C29-C30-C31
19	O	302	TGL	OG3-CC1-CC2-CC3
25	Y	101	CDL	C52-C51-CB5-OB6
19	D	201	TGL	OG3-CC1-CC2-CC3
25	T	102	CDL	C32-C31-CA7-OA9
20	C	305	PGV	O03-C19-C20-C21
25	P	308	CDL	C80-C81-C82-C83
25	G	101	CDL	C63-C64-C65-C66

There are no ring outliers.

55 monomers are involved in 239 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	K	103	DMU	1	0
23	P	309	CHD	3	0
19	O	301	TGL	3	0
14	A	602[A]	HEA	7	0
23	W	101	CHD	1	0
26	P	311	DMU	2	0
20	A	608	PGV	7	0
19	A	607	TGL	10	0
20	P	307	PGV	1	0
14	N	602[C]	HEA	15	0
21	B	305	EDO	5	0
26	X	102	DMU	1	0
21	A	617	EDO	1	0
25	Y	101	CDL	4	0
26	L	101	DMU	3	0
25	C	308	CDL	14	0
19	O	302	TGL	11	0
19	B	301	TGL	6	0
24	C	303	PEK	4	0
23	J	102	CHD	4	0
21	S	108	EDO	3	0

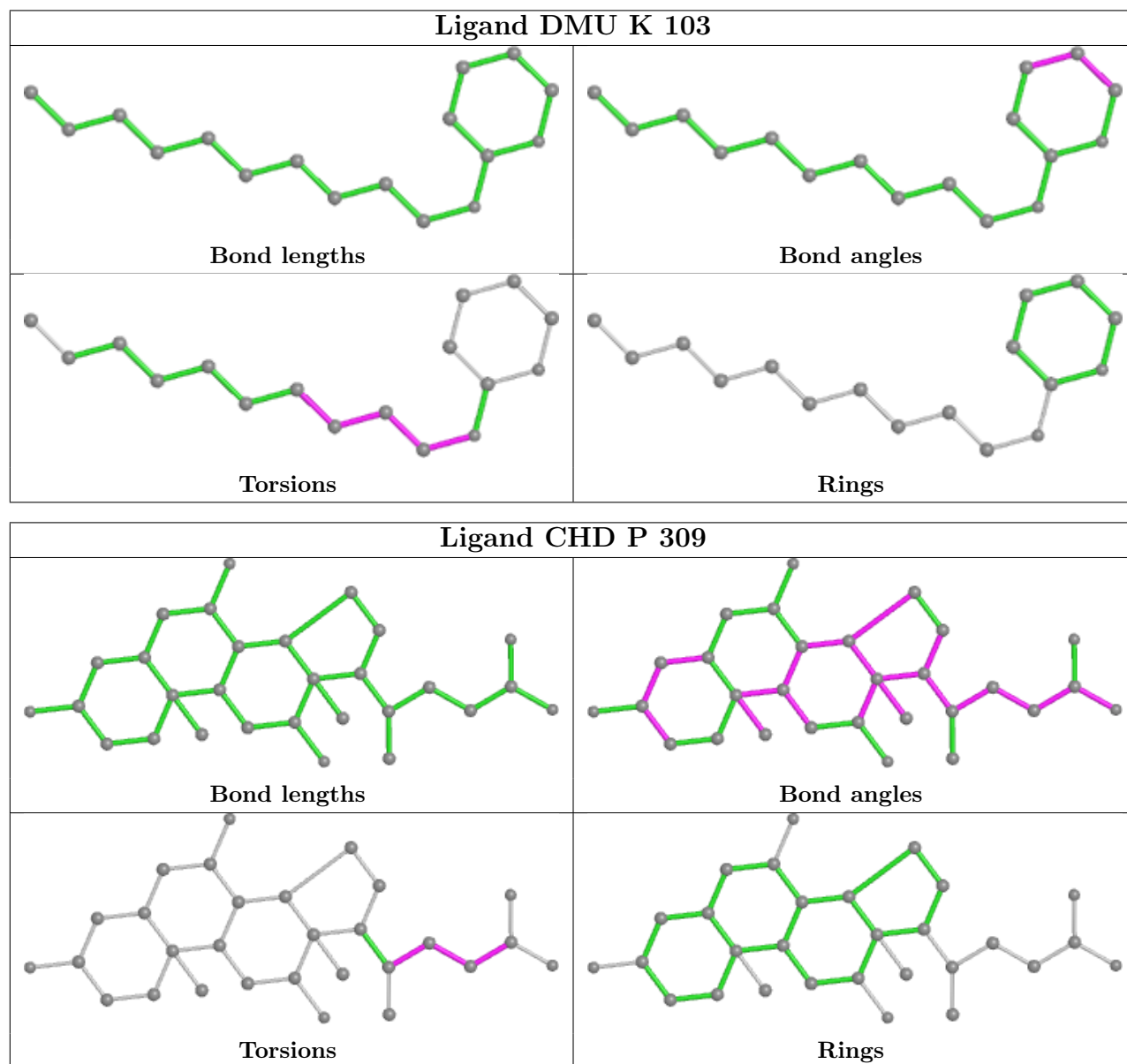
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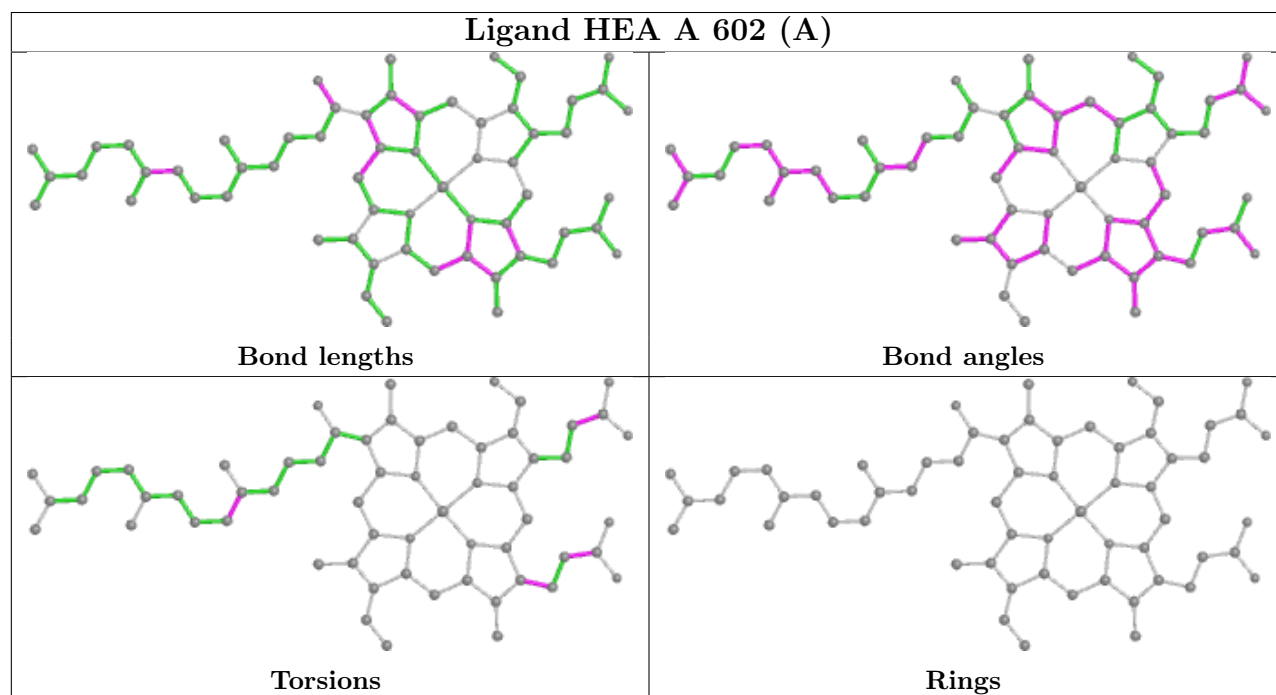
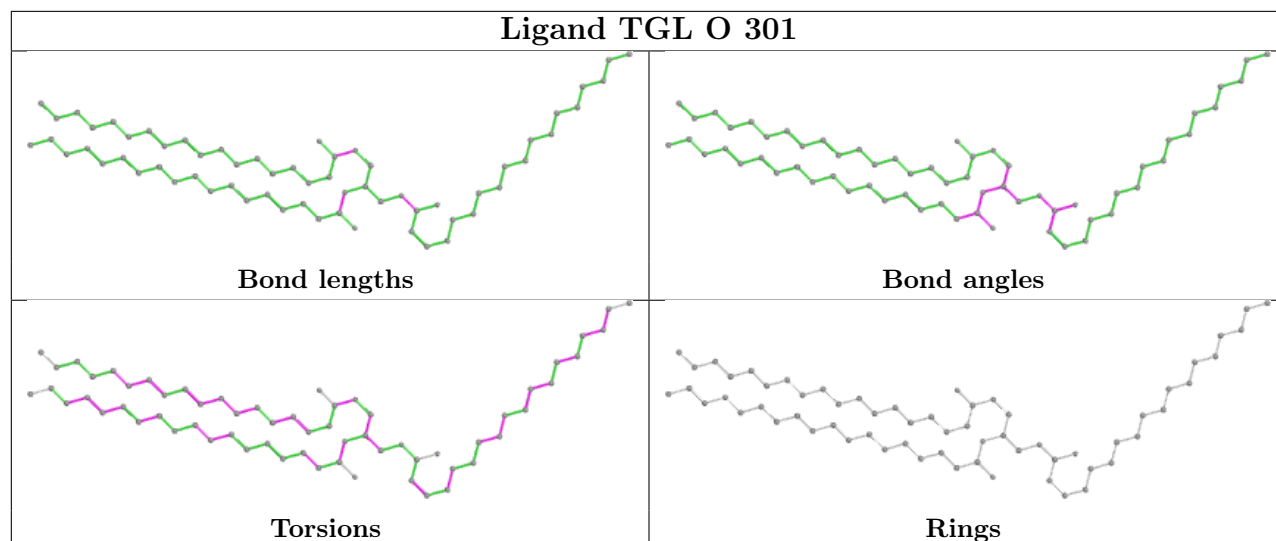
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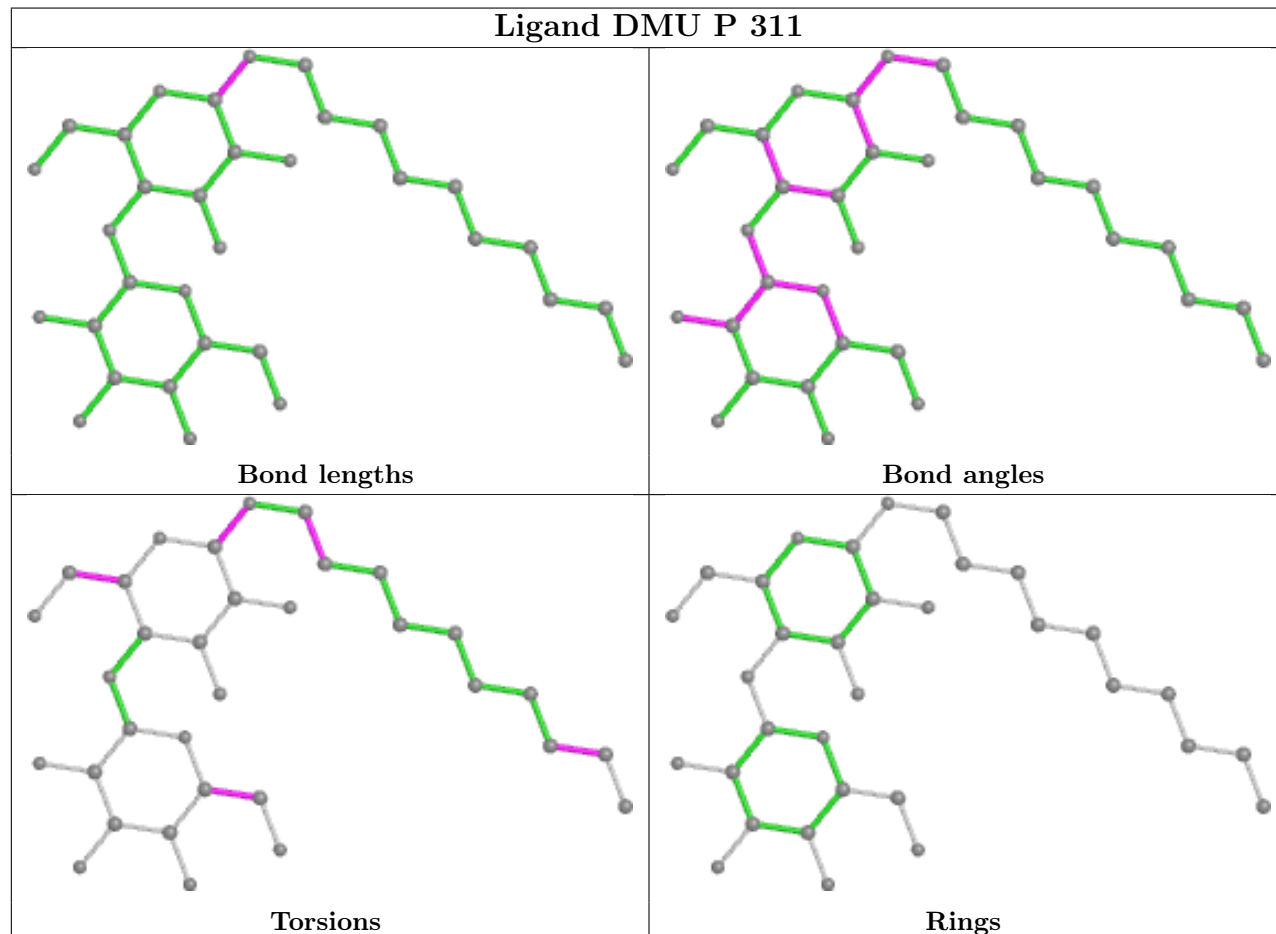
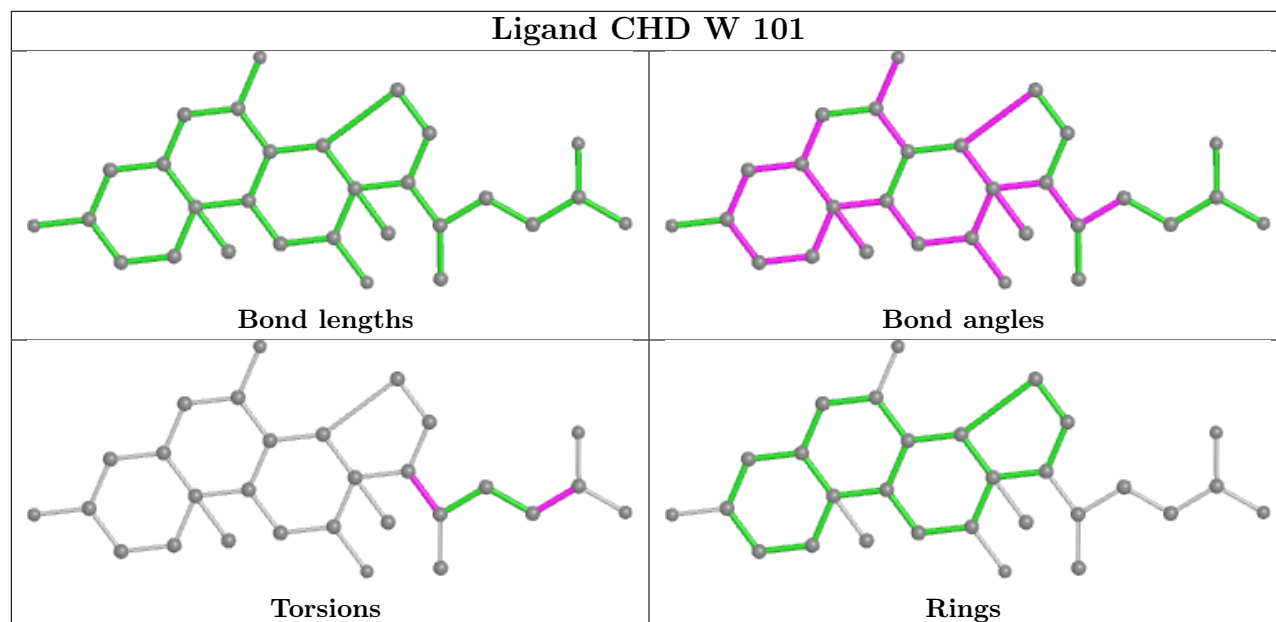
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	Q	201	PGV	6	0
14	A	601[B]	HEA	3	0
24	P	305	PEK	2	0
25	G	101	CDL	8	0
21	U	101	EDO	3	0
25	P	308	CDL	6	0
26	X	101	DMU	1	0
24	P	304	PEK	7	0
14	N	601[A]	HEA	4	0
26	X	103	DMU	4	0
26	Z	101	DMU	1	0
26	K	101	DMU	1	0
26	P	310	DMU	4	0
26	C	311	DMU	5	0
21	A	615	EDO	1	0
26	P	315	DMU	1	0
20	C	306	PGV	4	0
20	C	307	PGV	1	0
14	N	602[A]	HEA	4	0
25	T	102	CDL	15	0
23	C	309	CHD	5	0
14	A	602[C]	HEA	14	0
27	E	201	PSC	8	0
26	G	105	DMU	2	0
21	D	202	EDO	1	0
20	C	305	PGV	3	0
26	P	312	DMU	2	0
21	O	307	EDO	1	0
27	O	304	PSC	9	0
23	G	102	CHD	1	0
14	A	601[A]	HEA	4	0
19	D	201	TGL	7	0
26	J	101	DMU	3	0
20	N	607	PGV	4	0

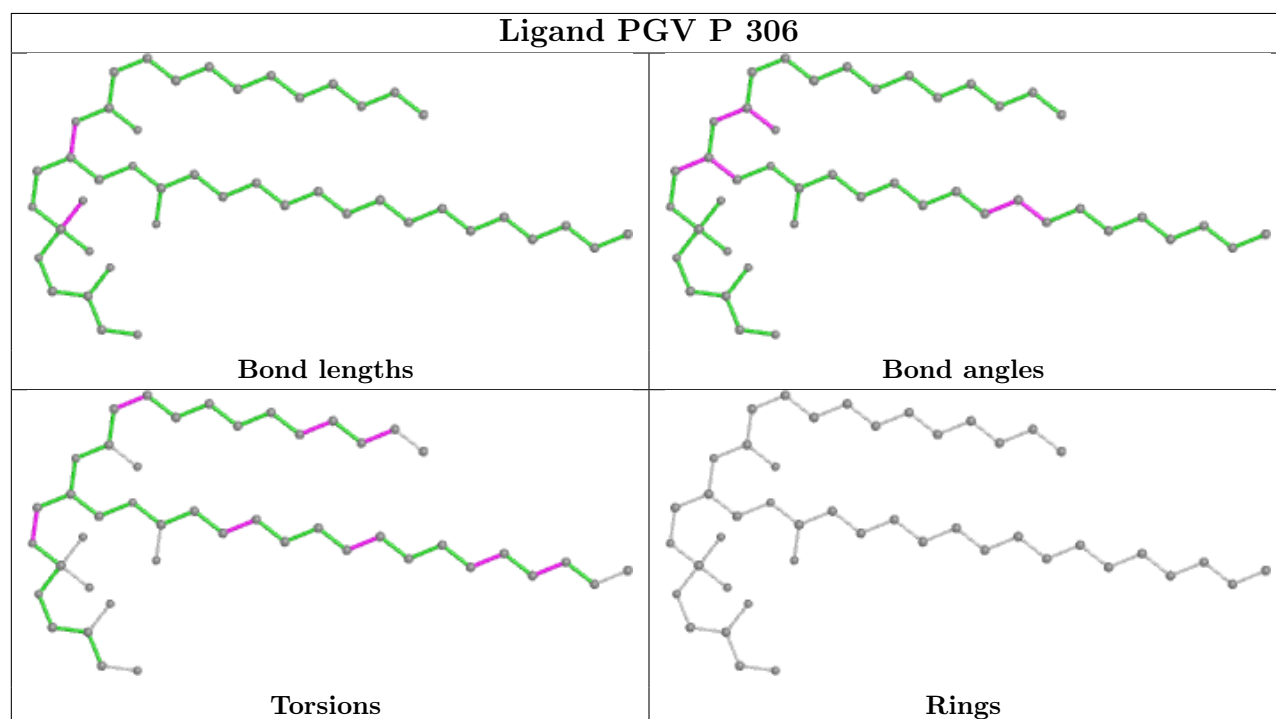
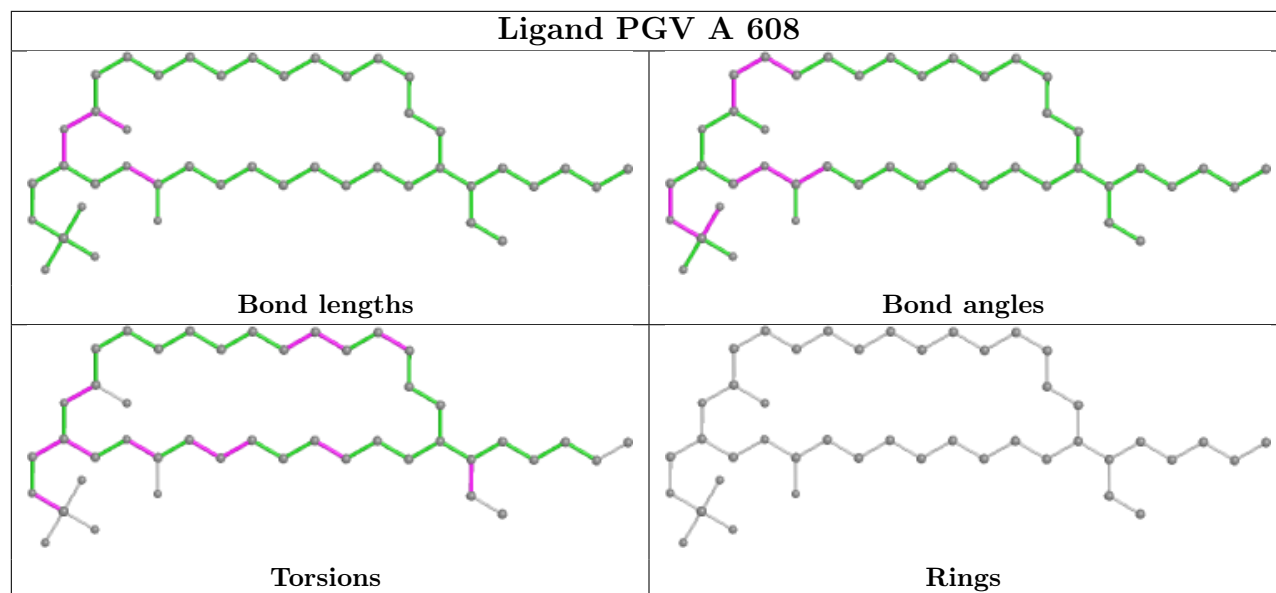
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

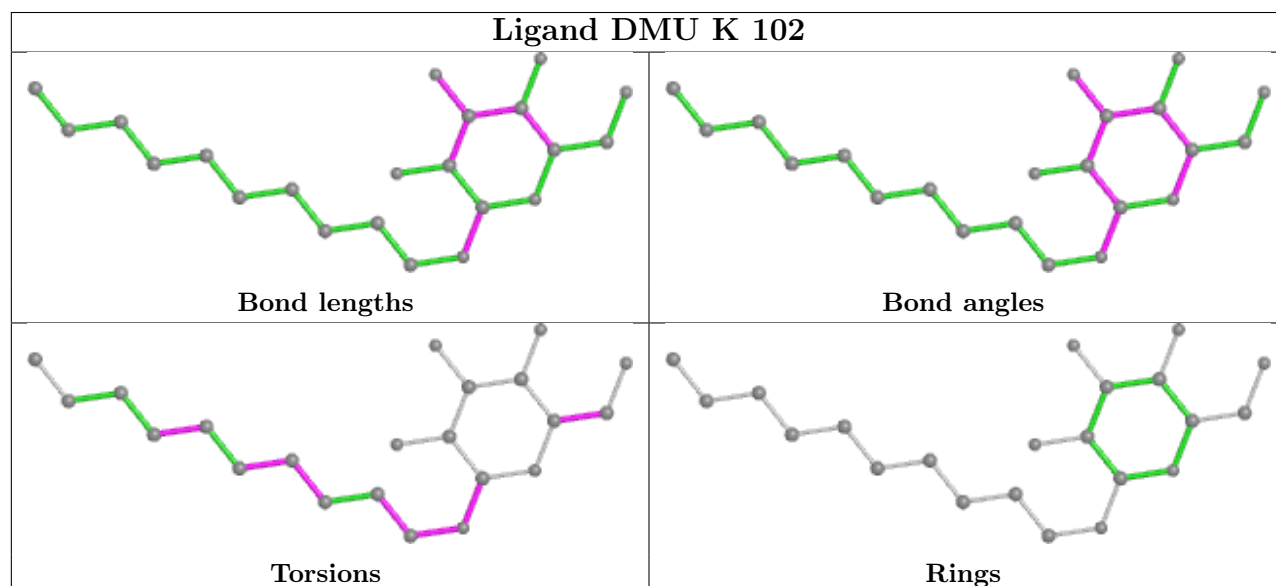
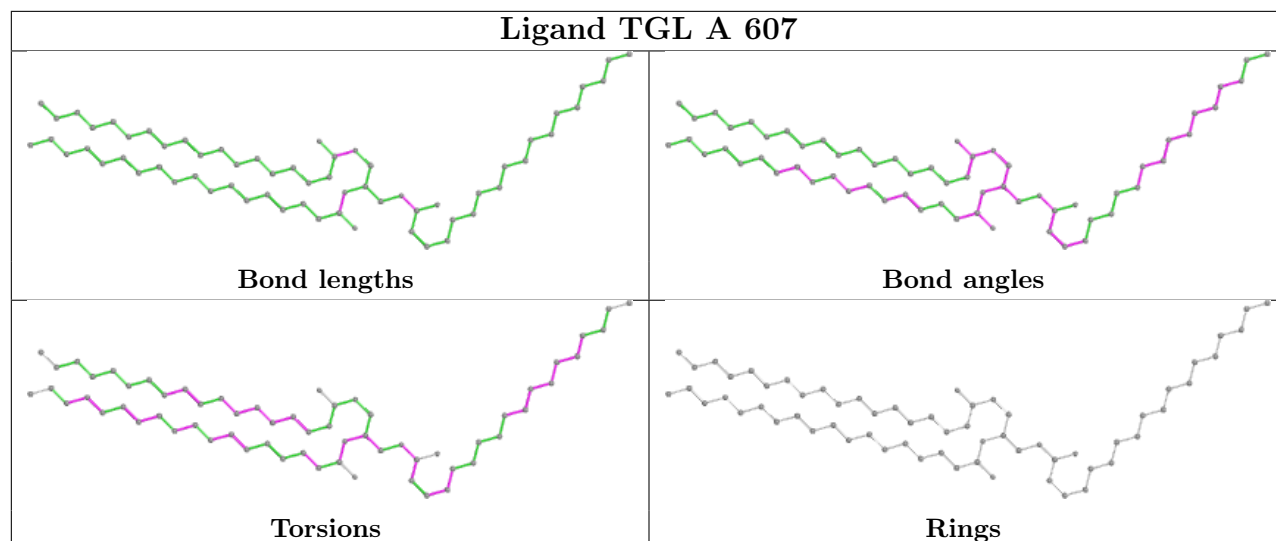
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

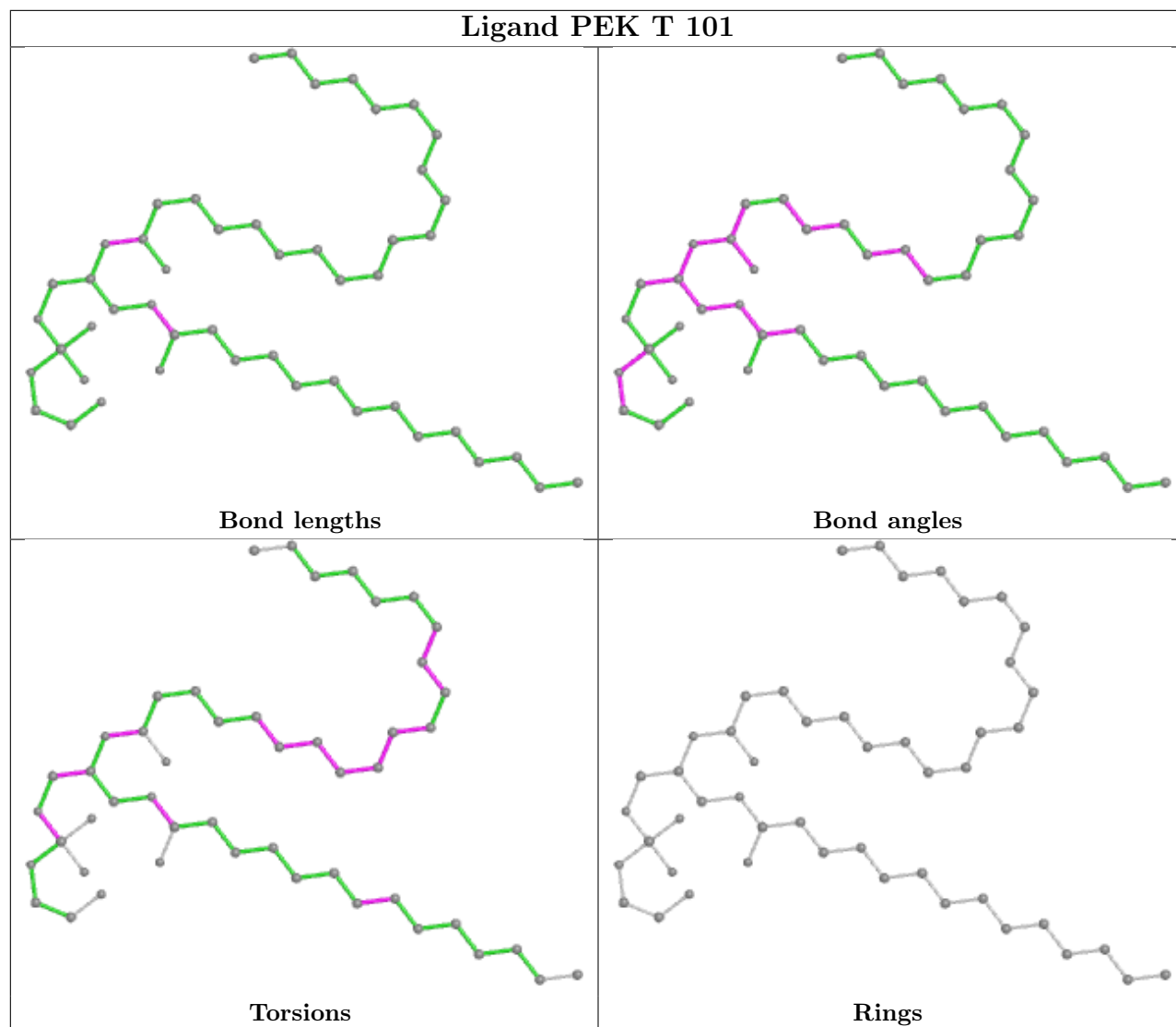


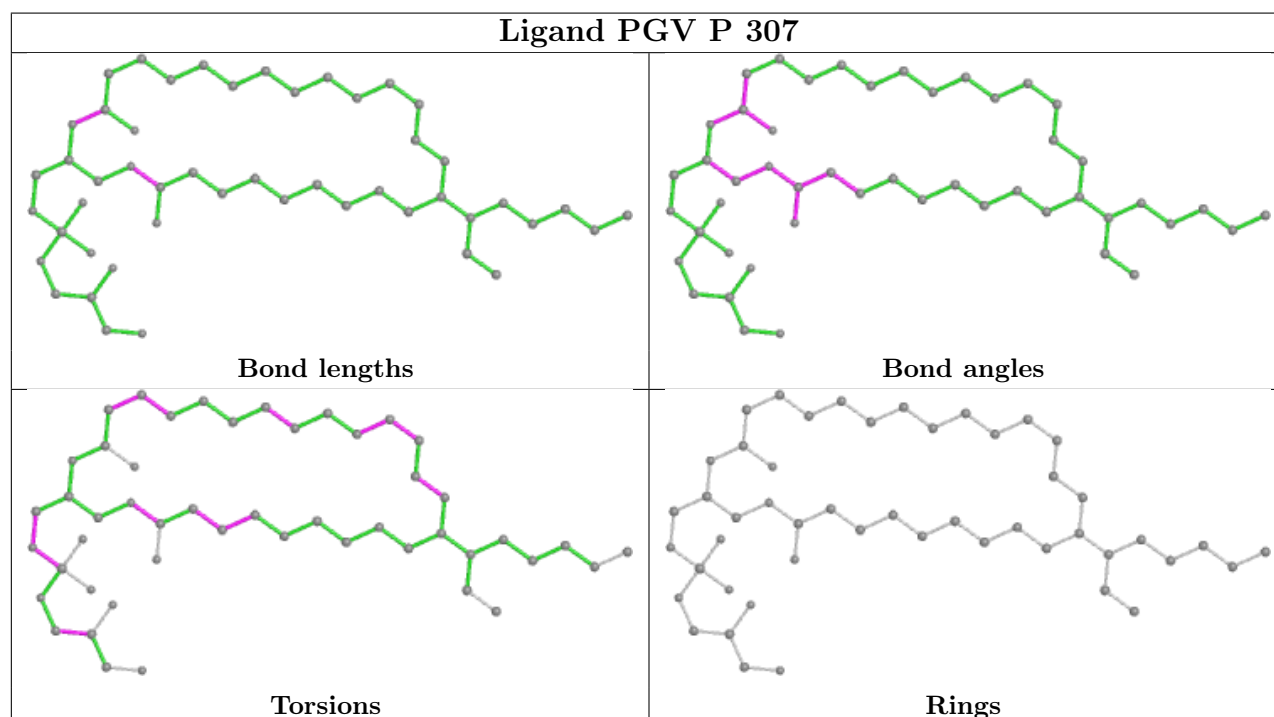
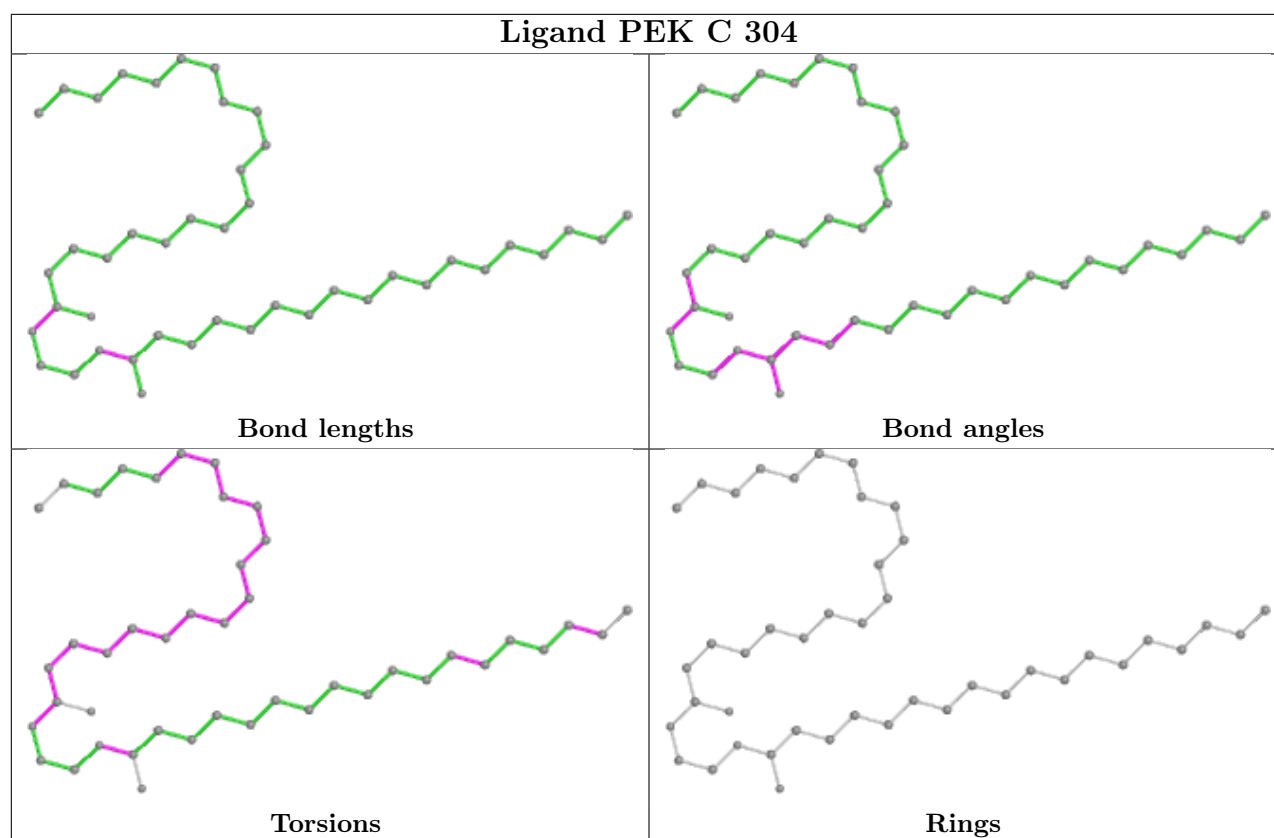


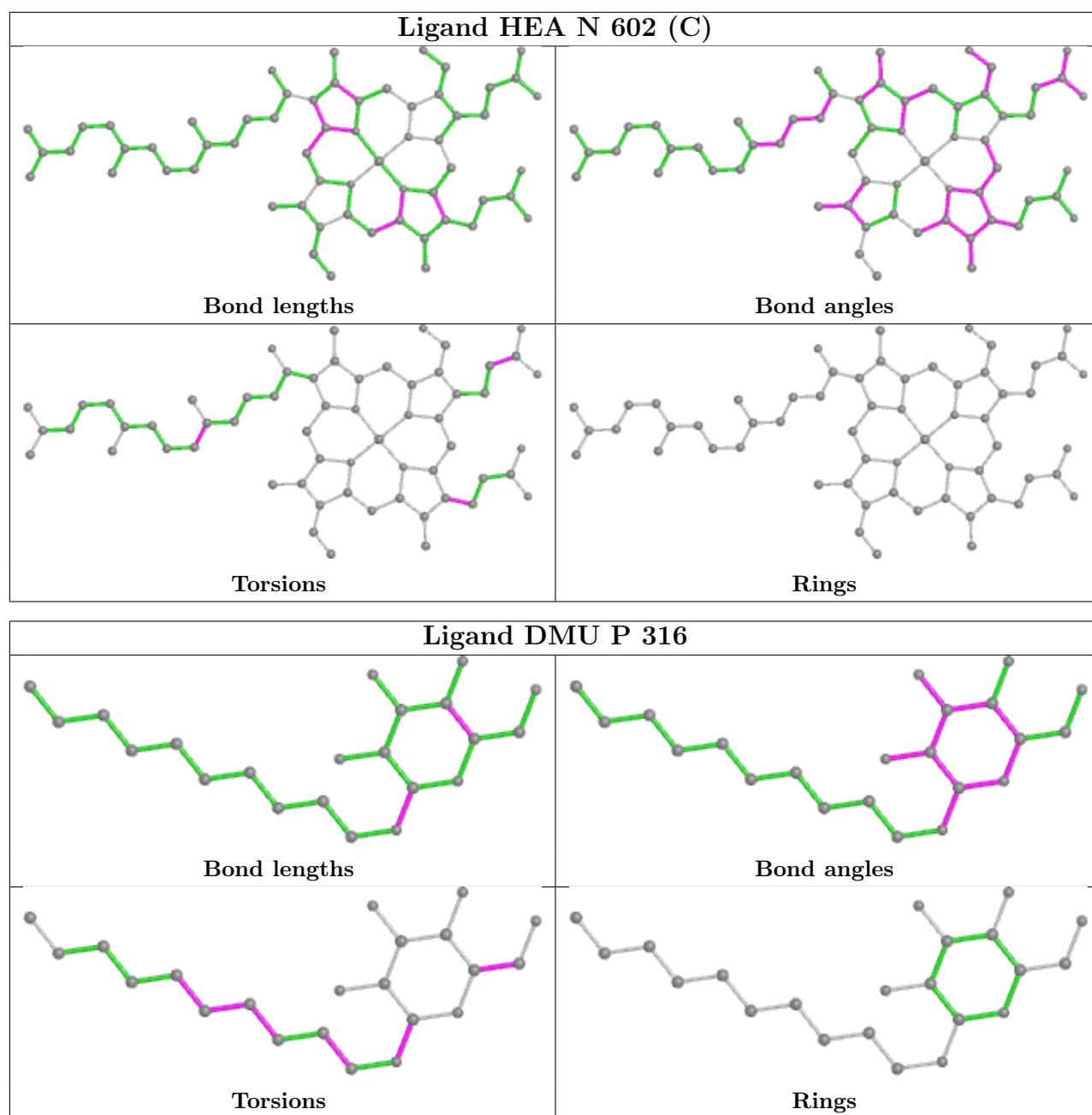


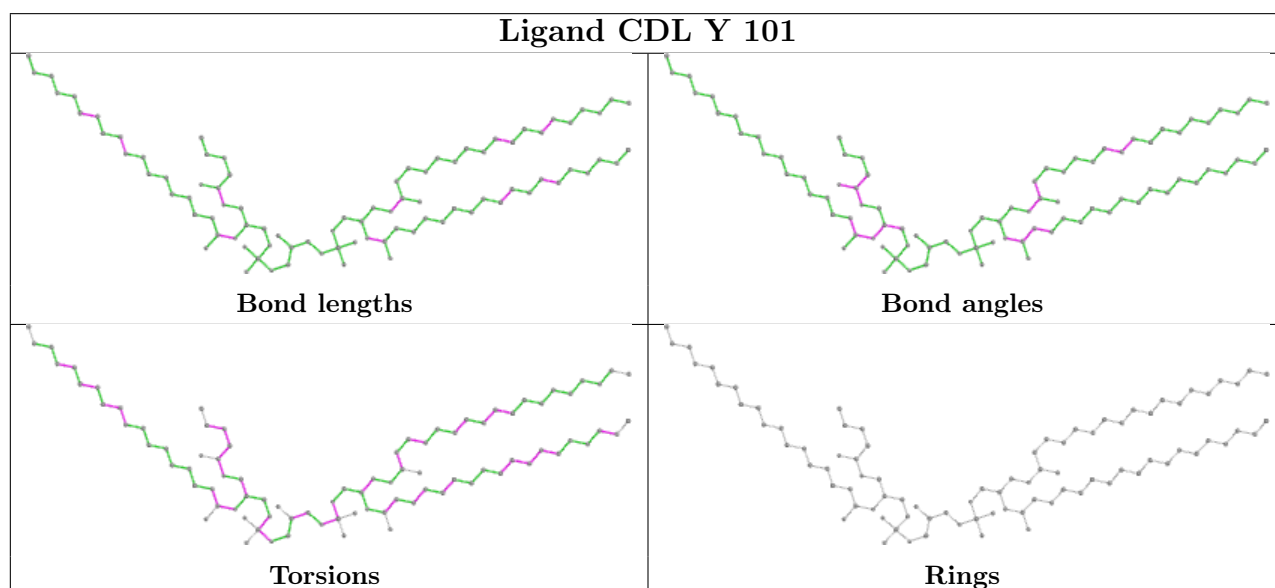
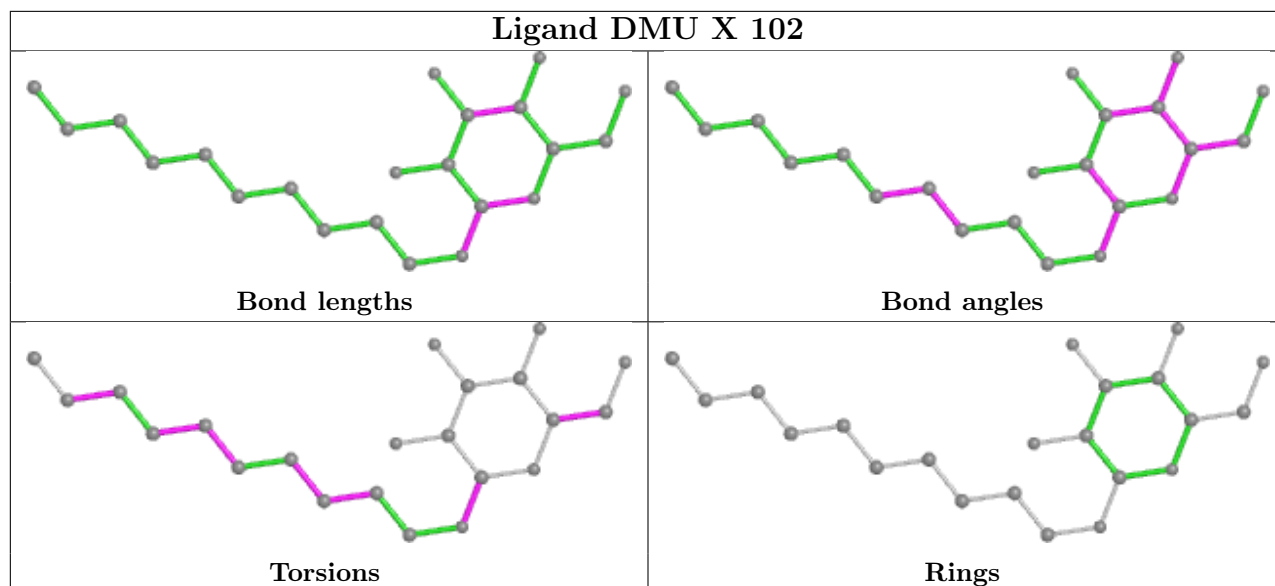


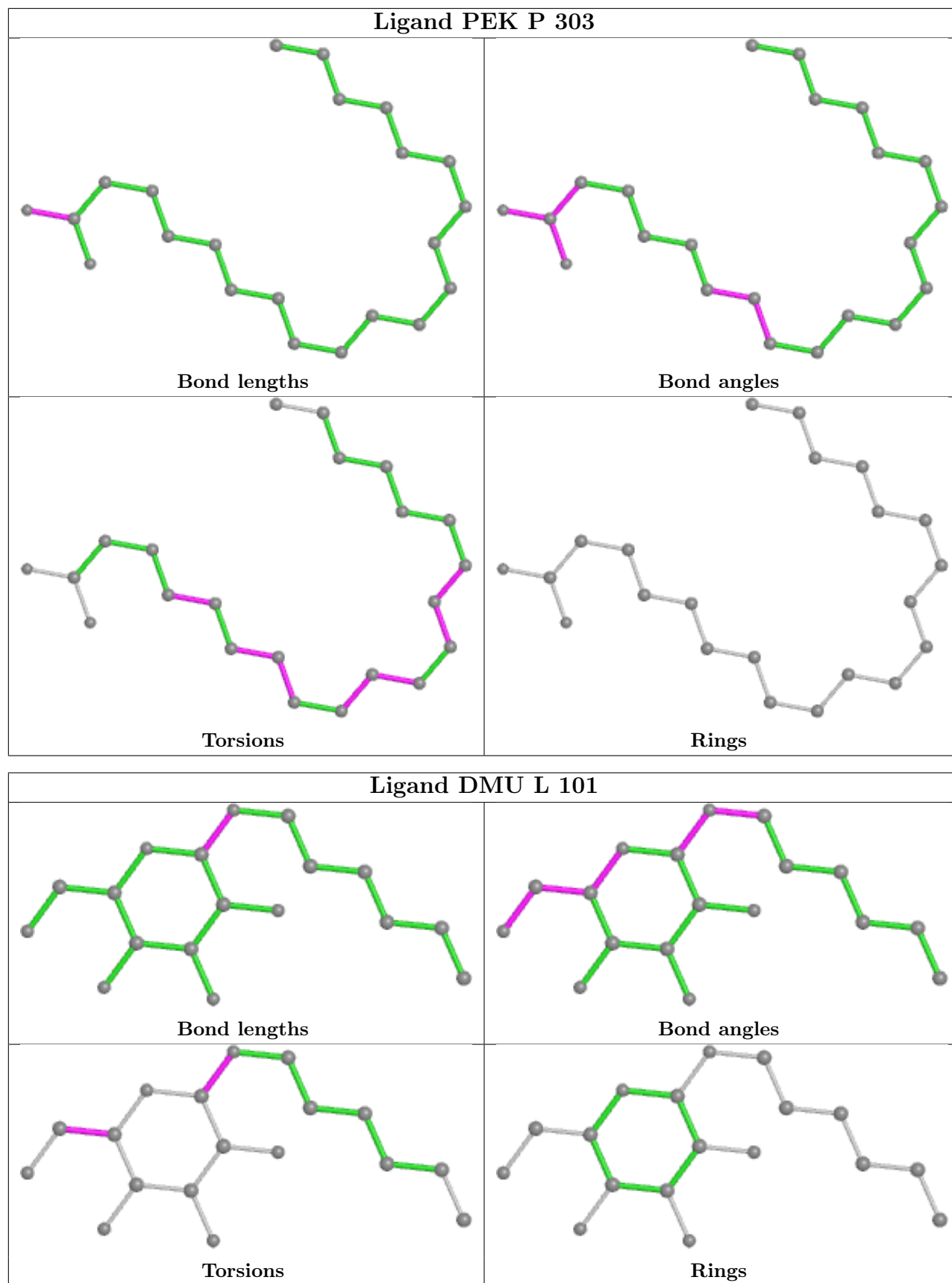


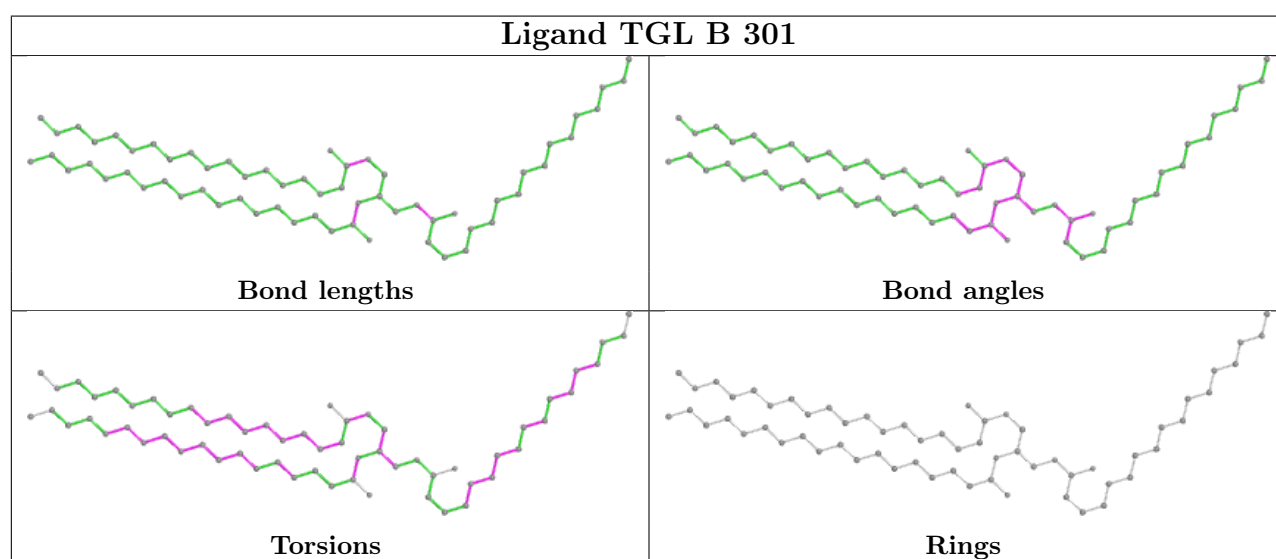
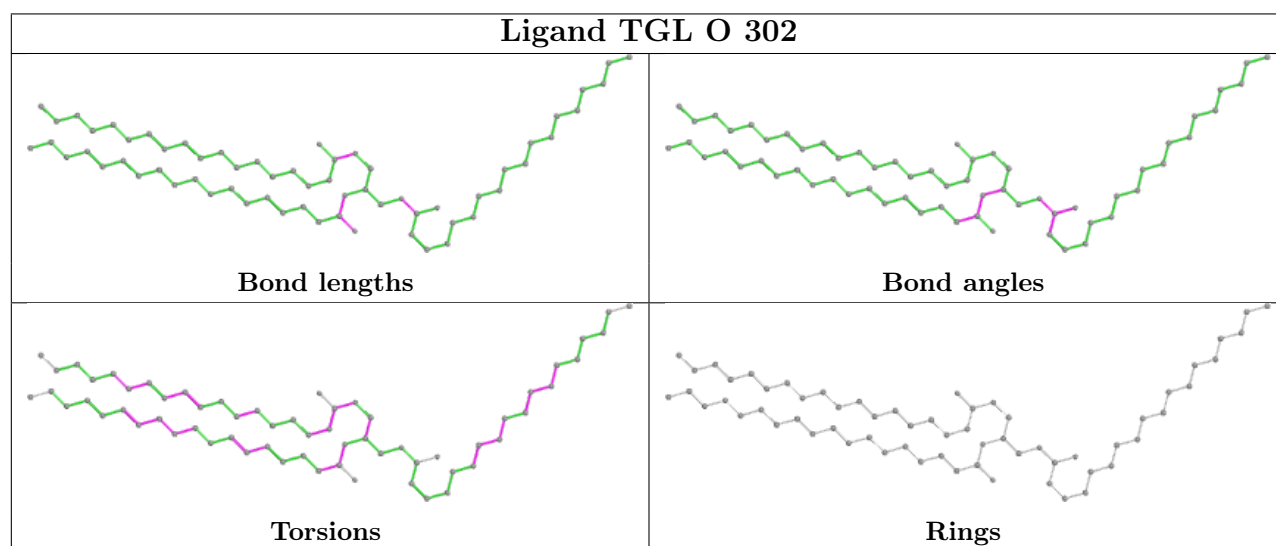
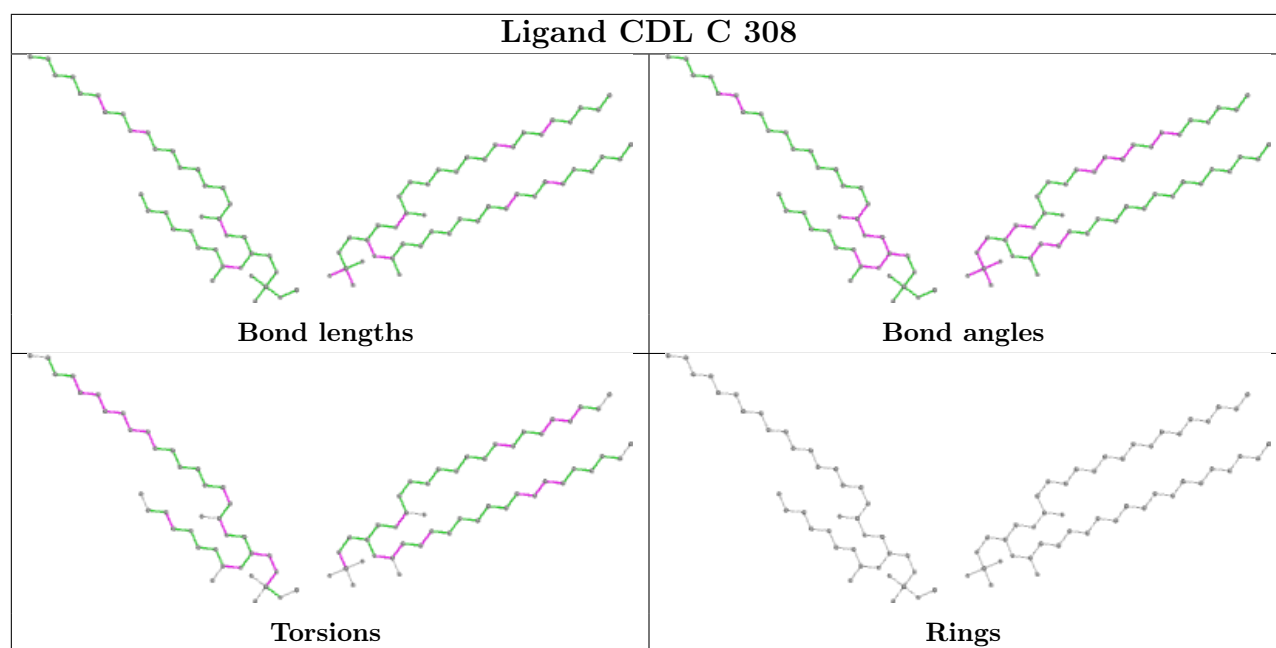


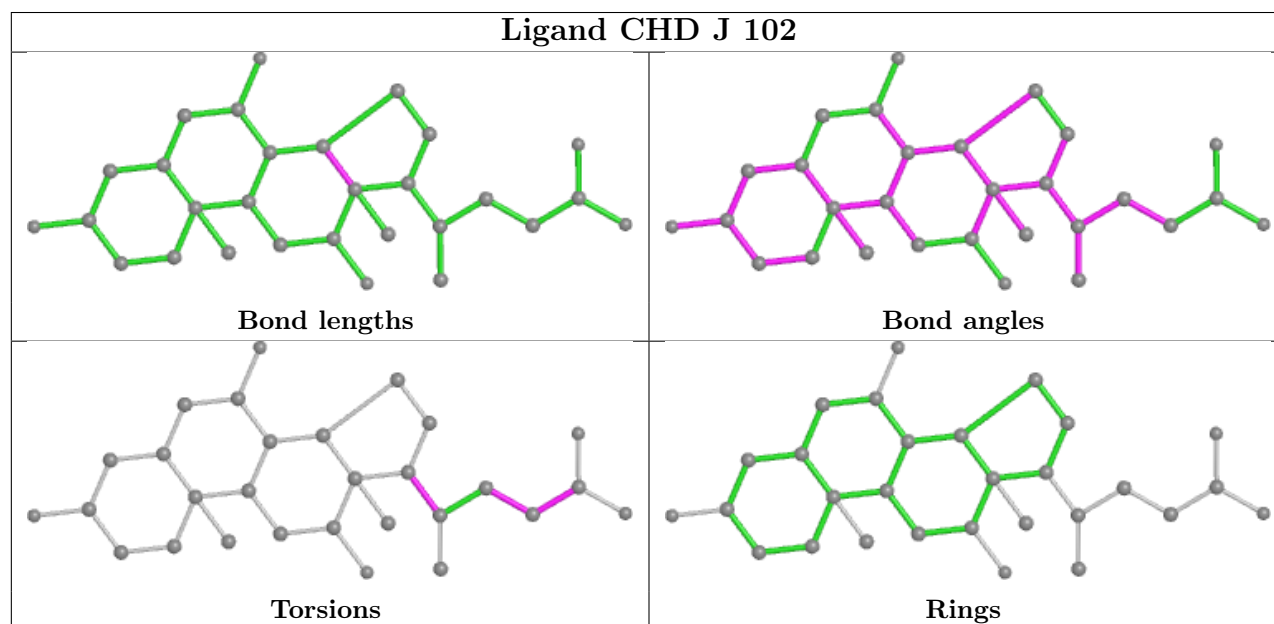
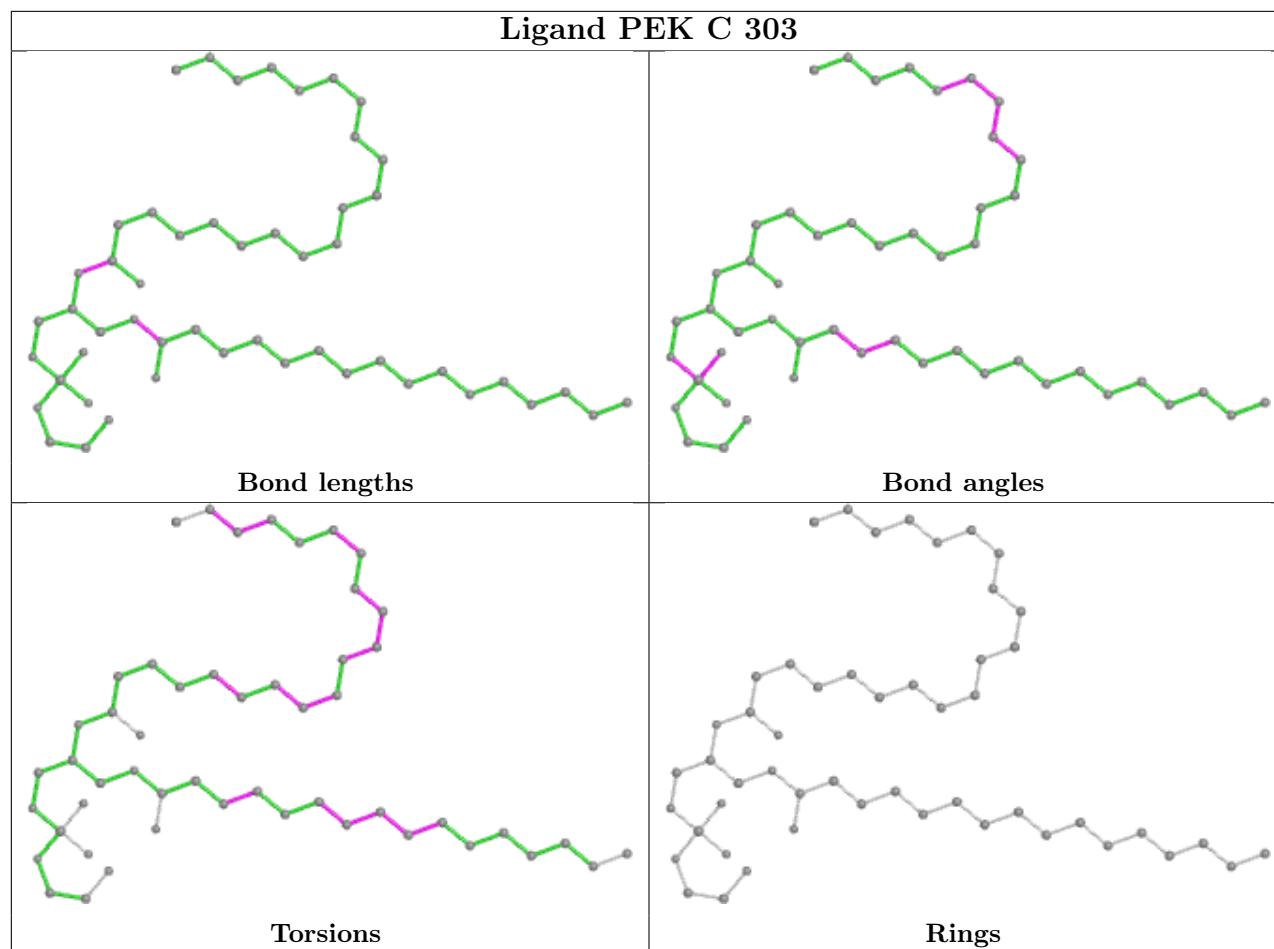


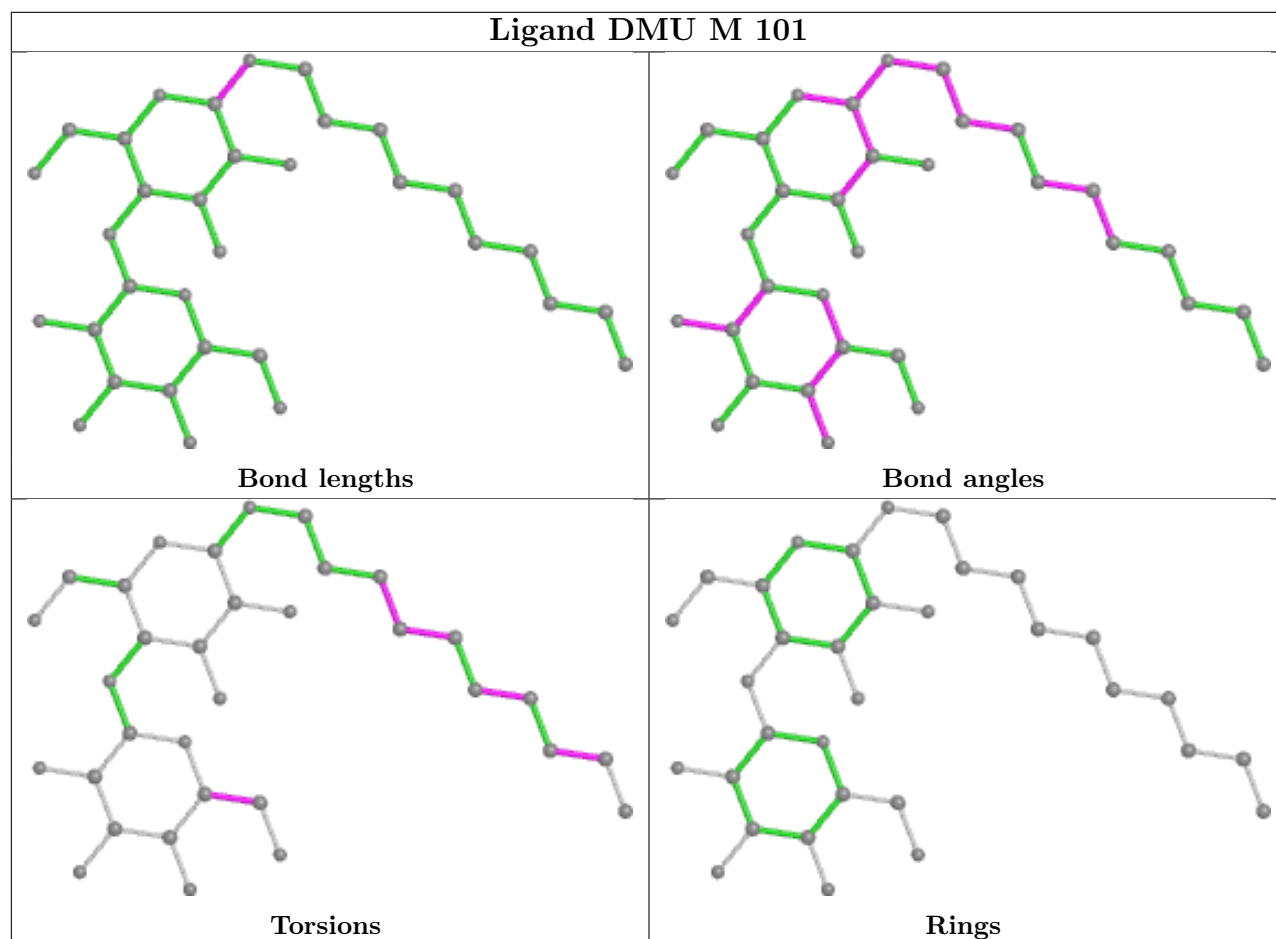
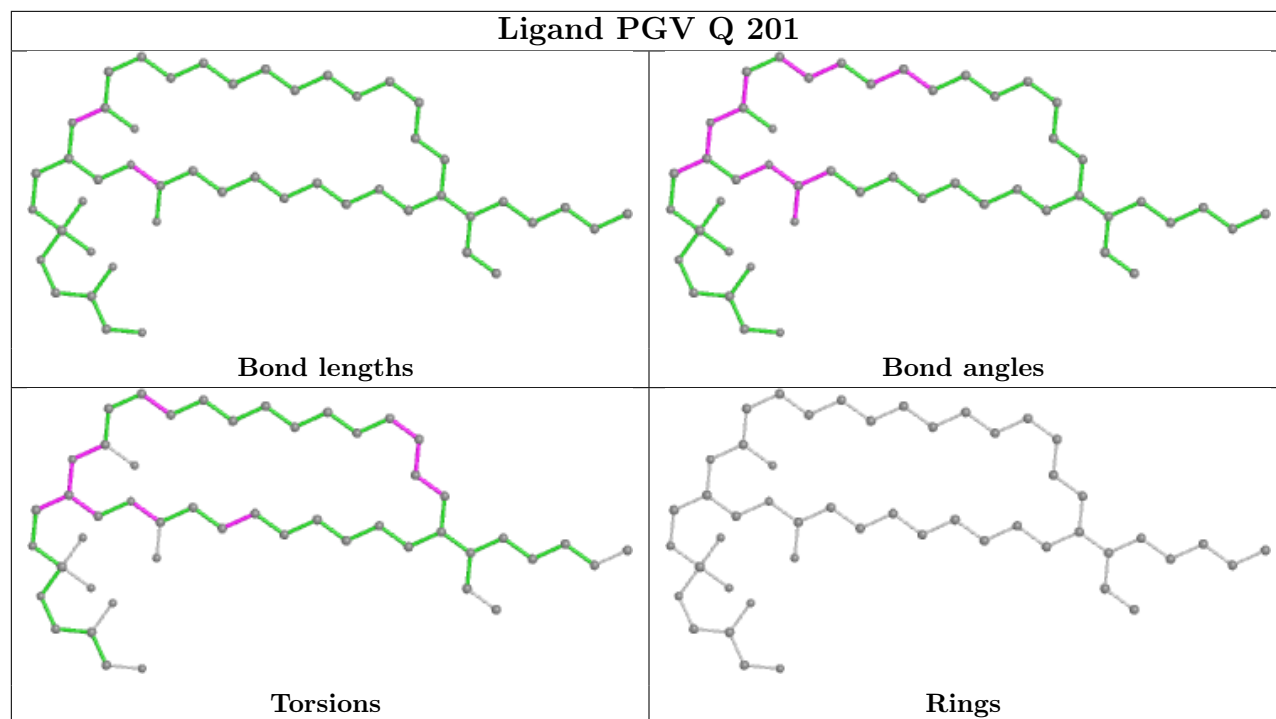


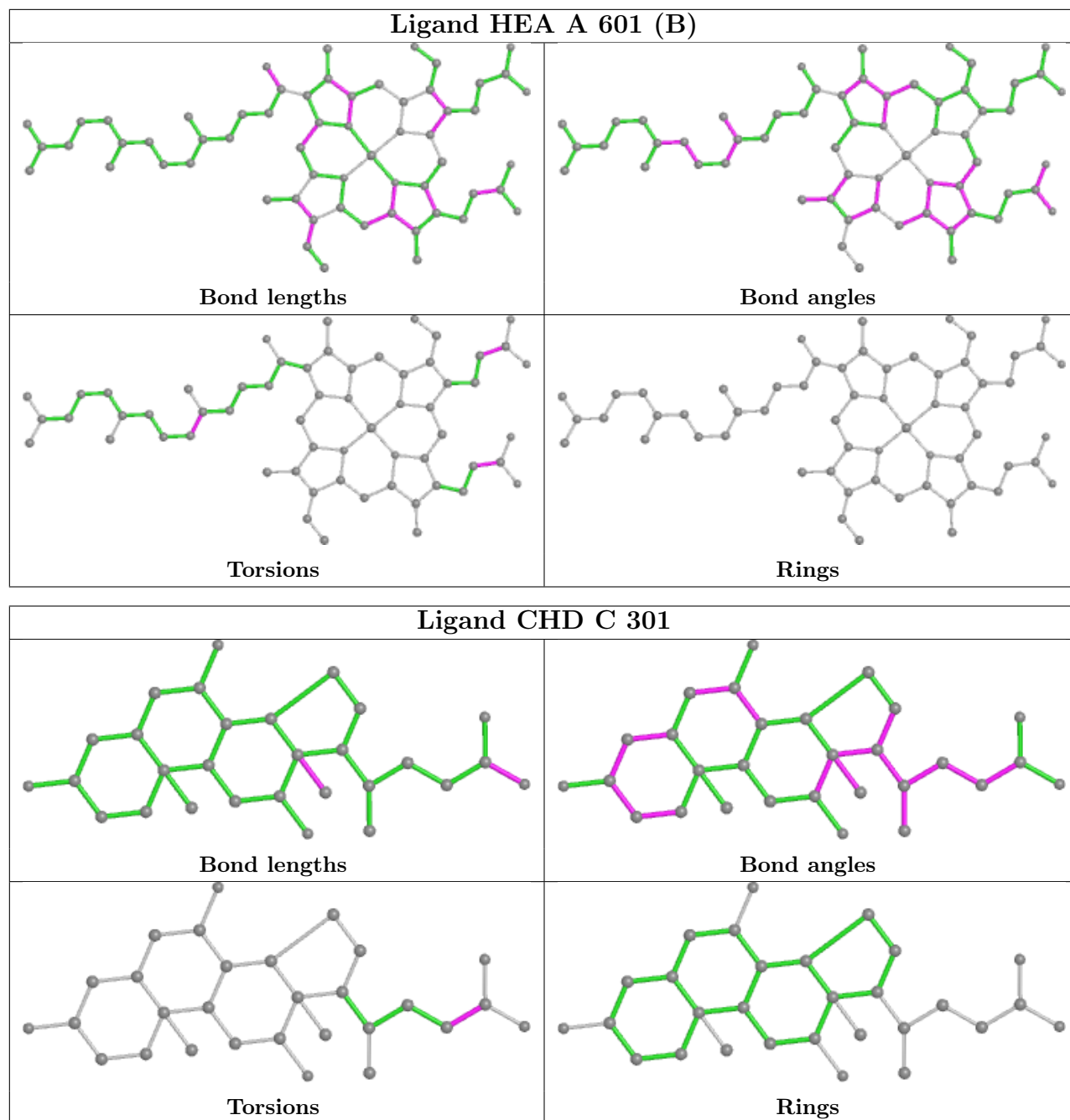


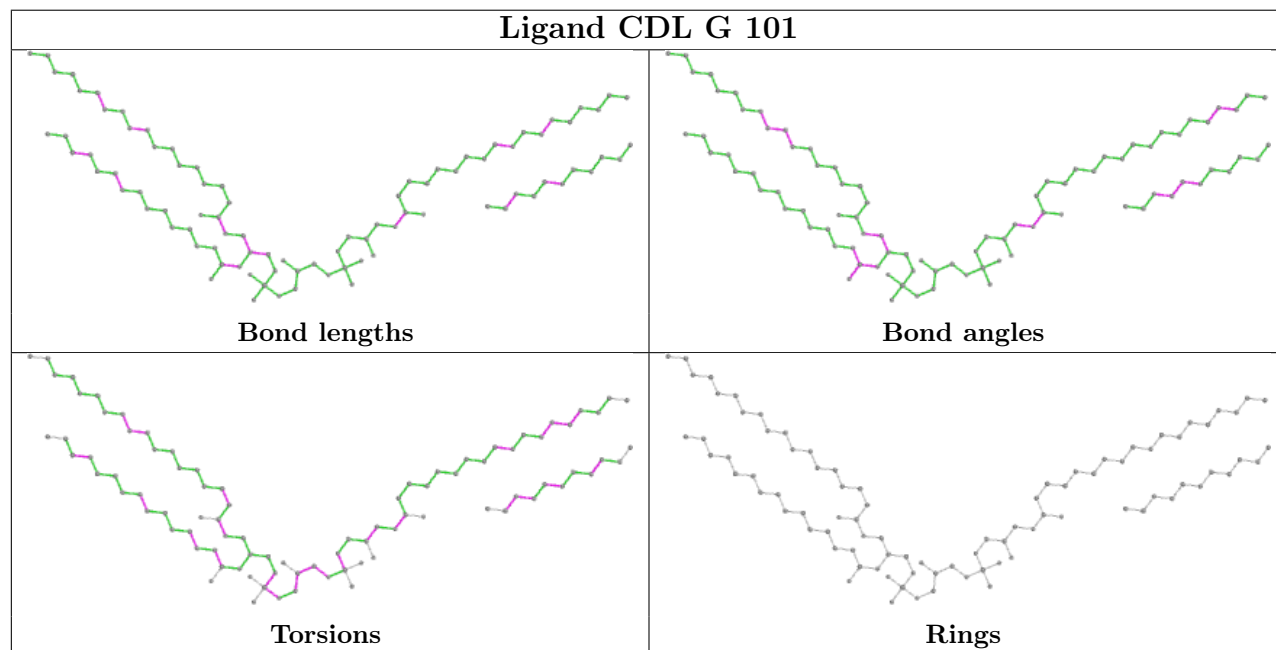
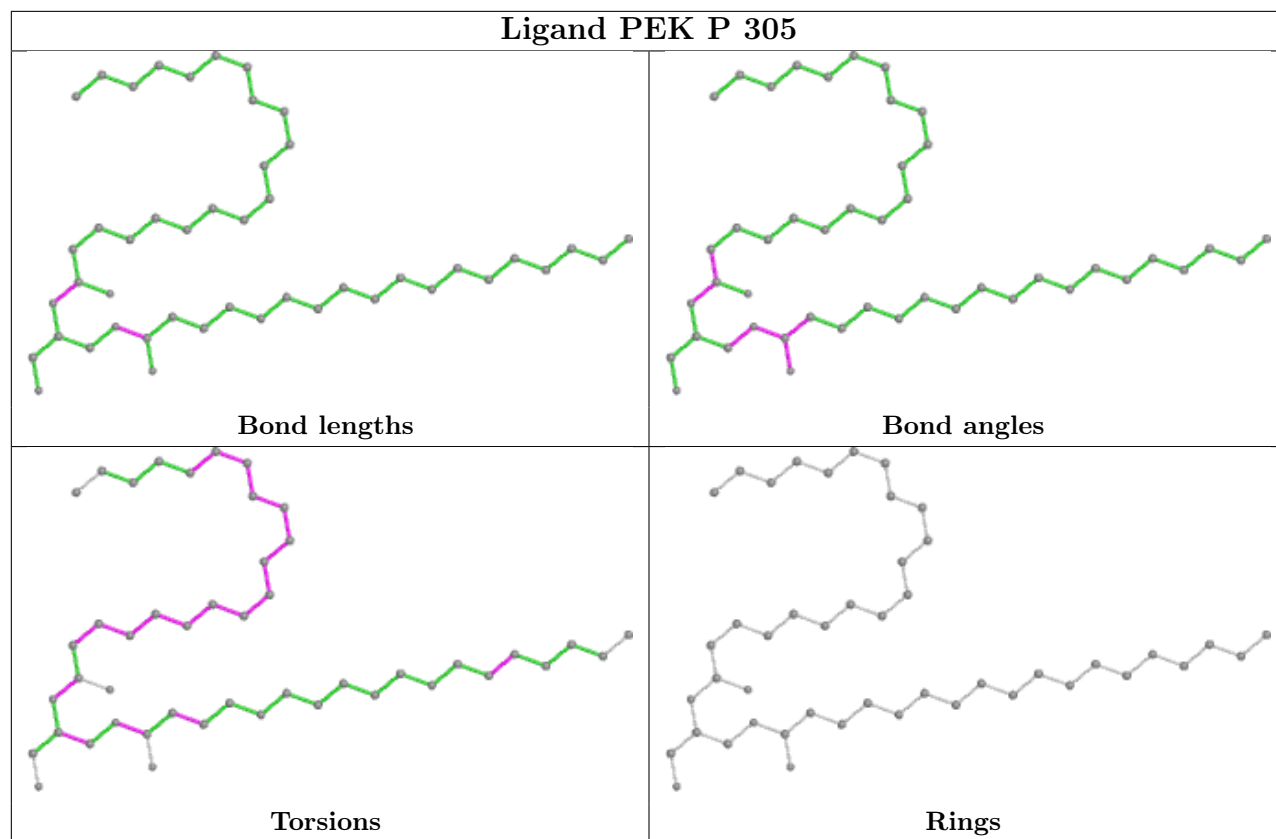


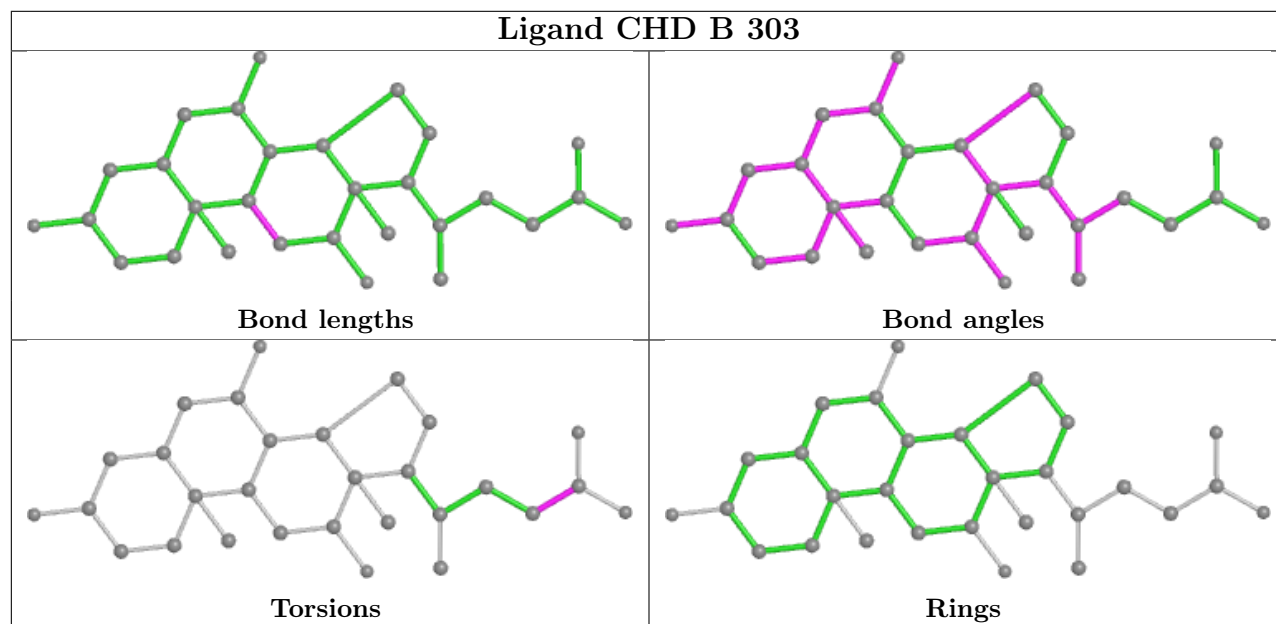
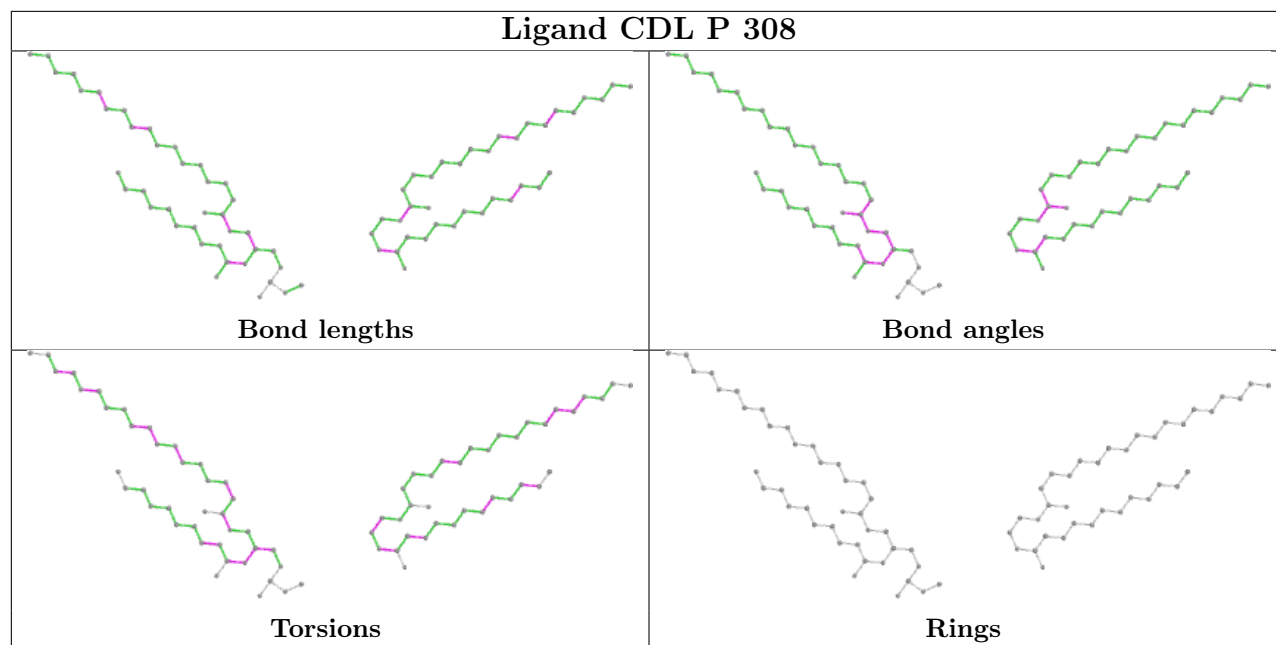


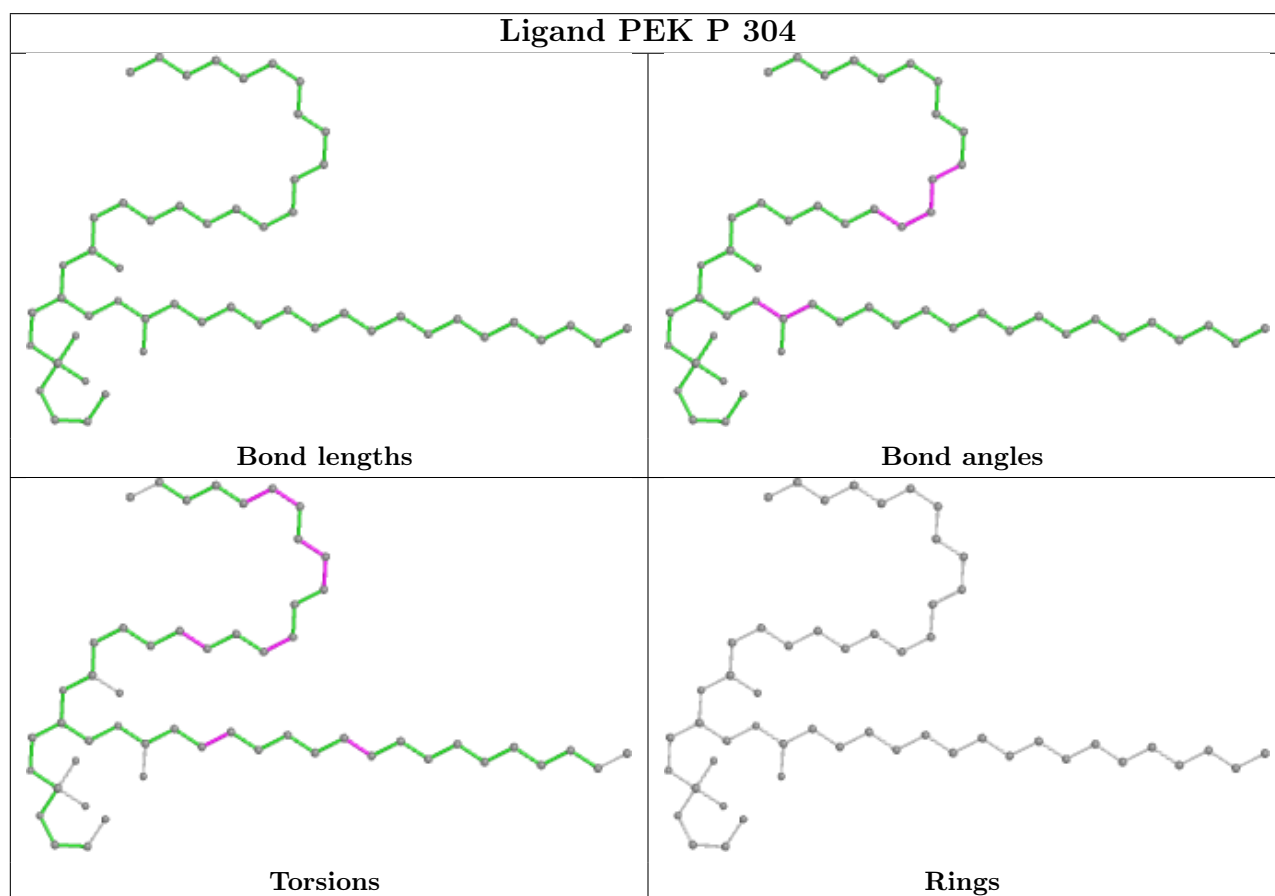
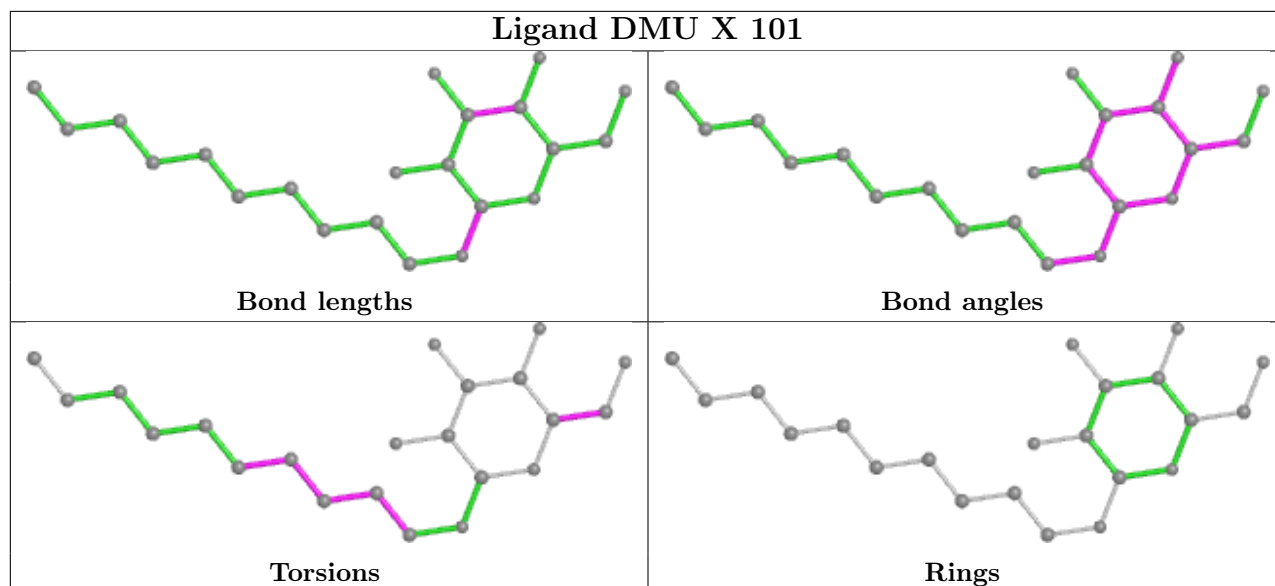


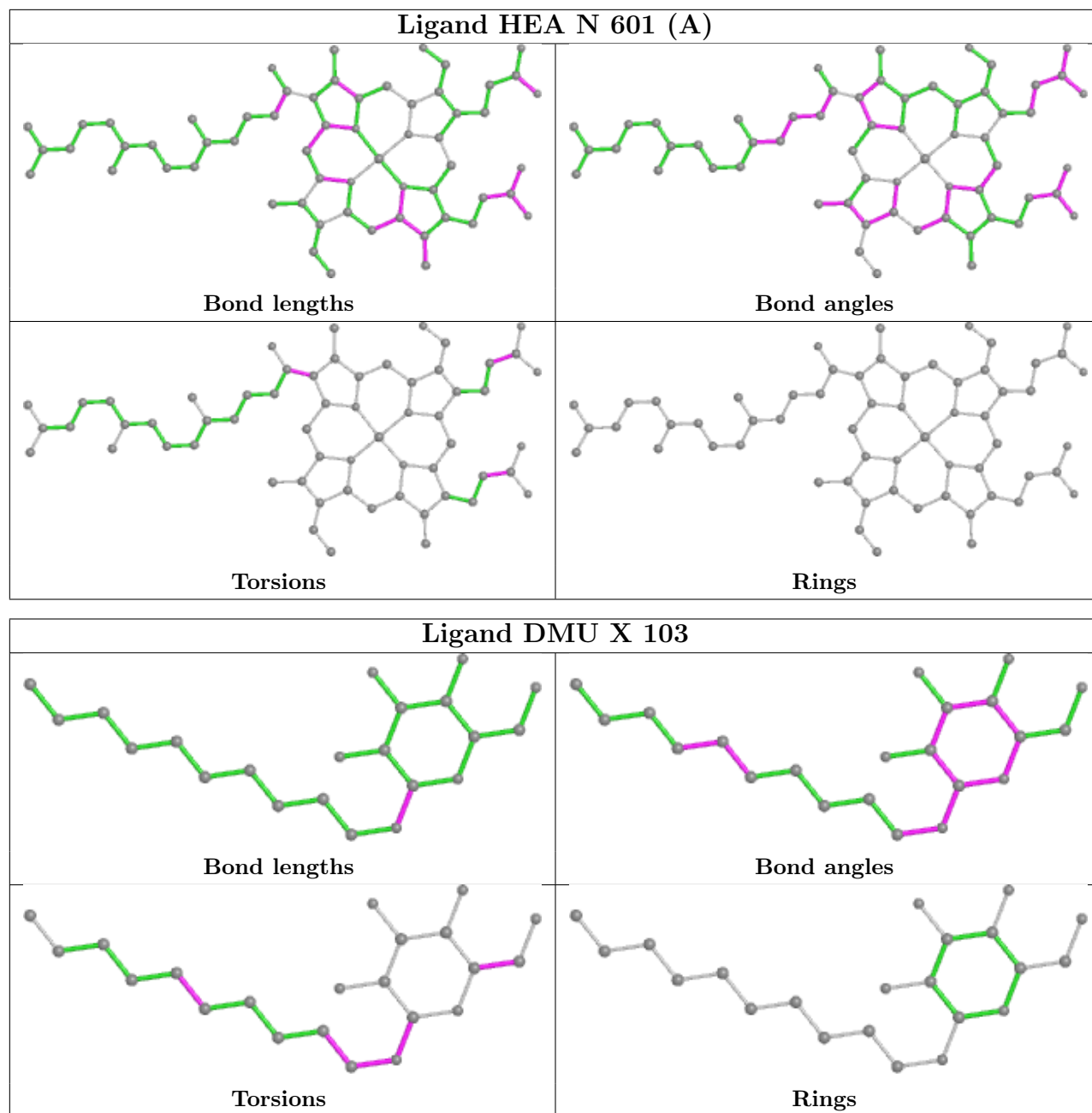


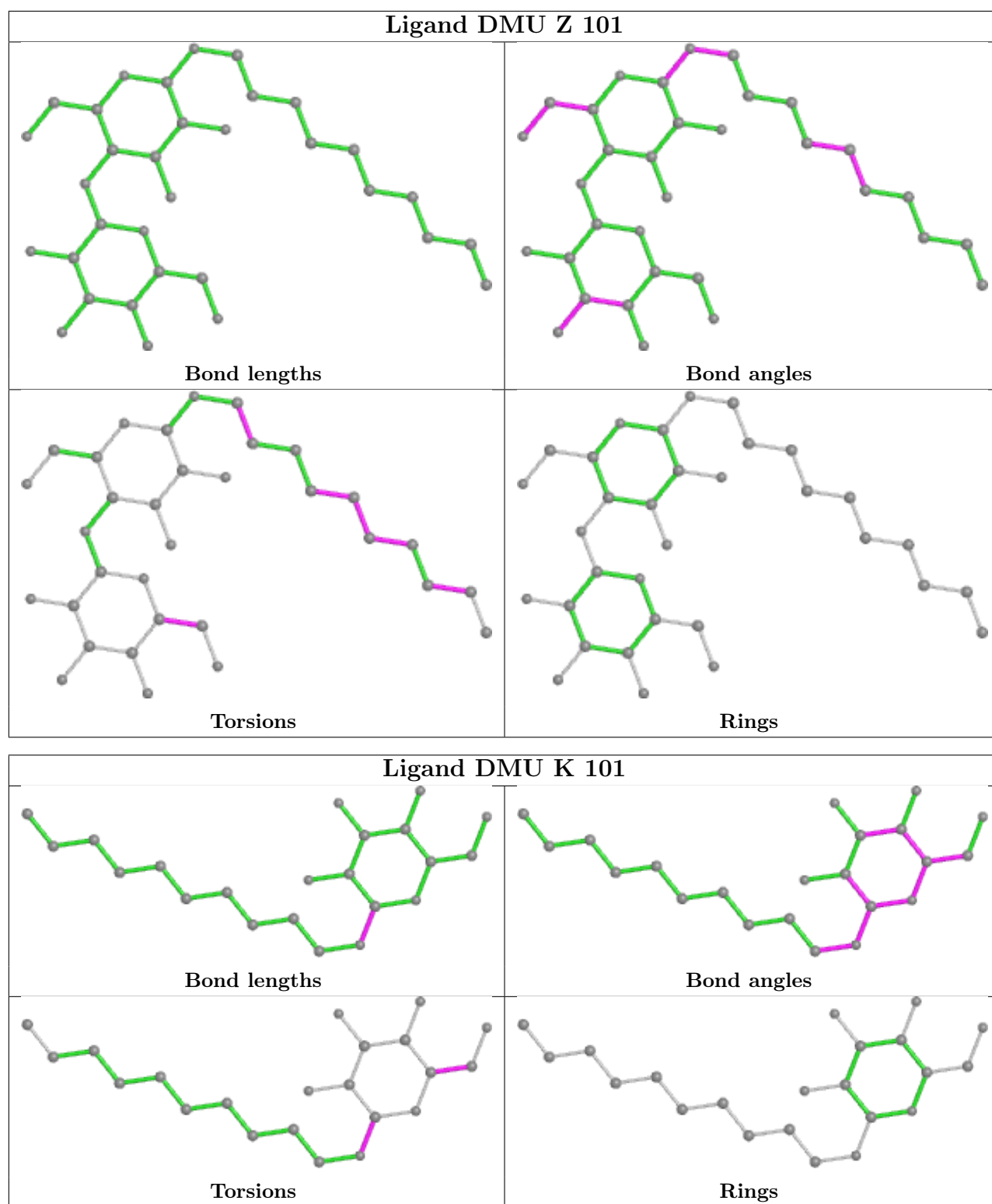


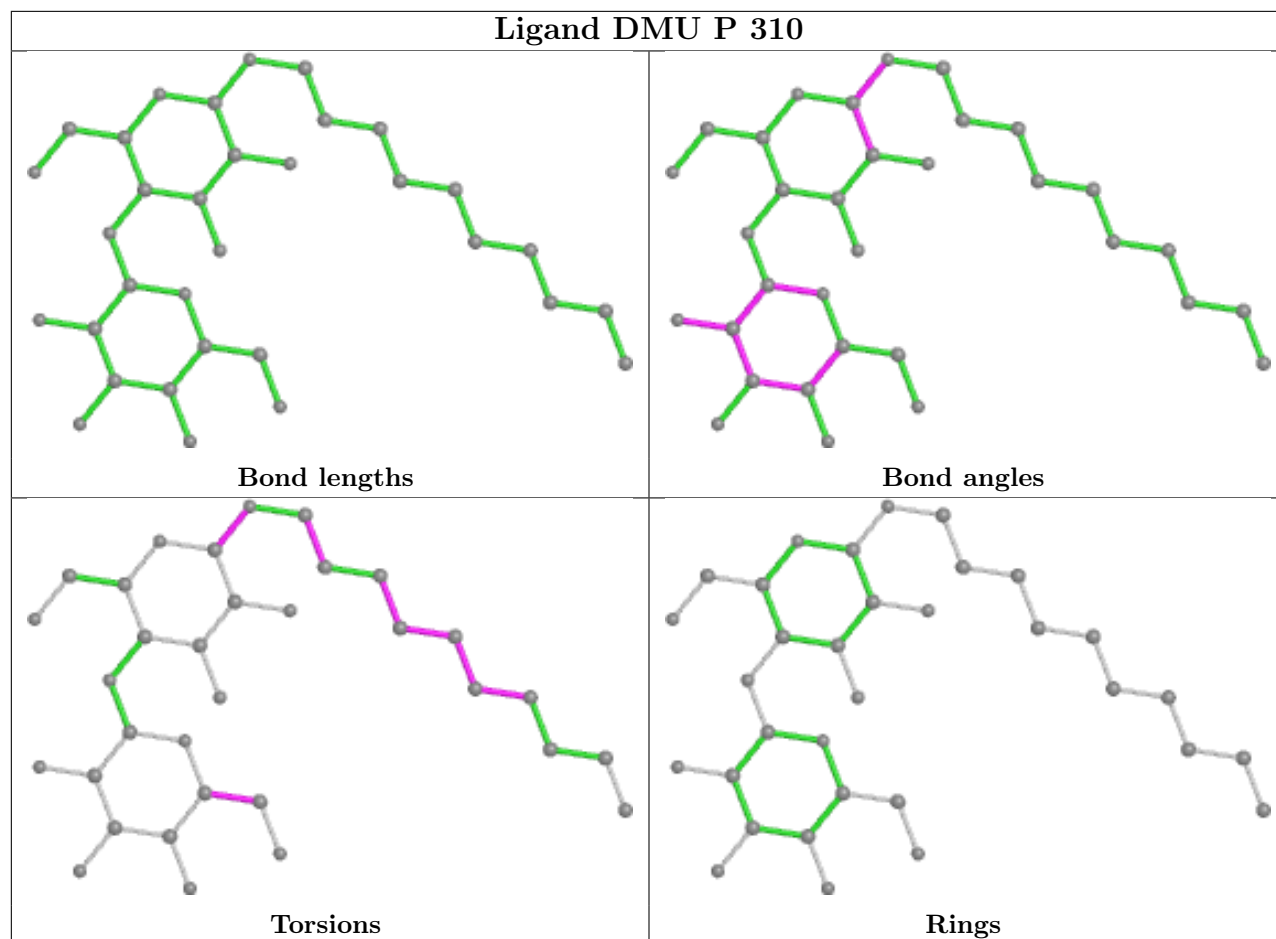


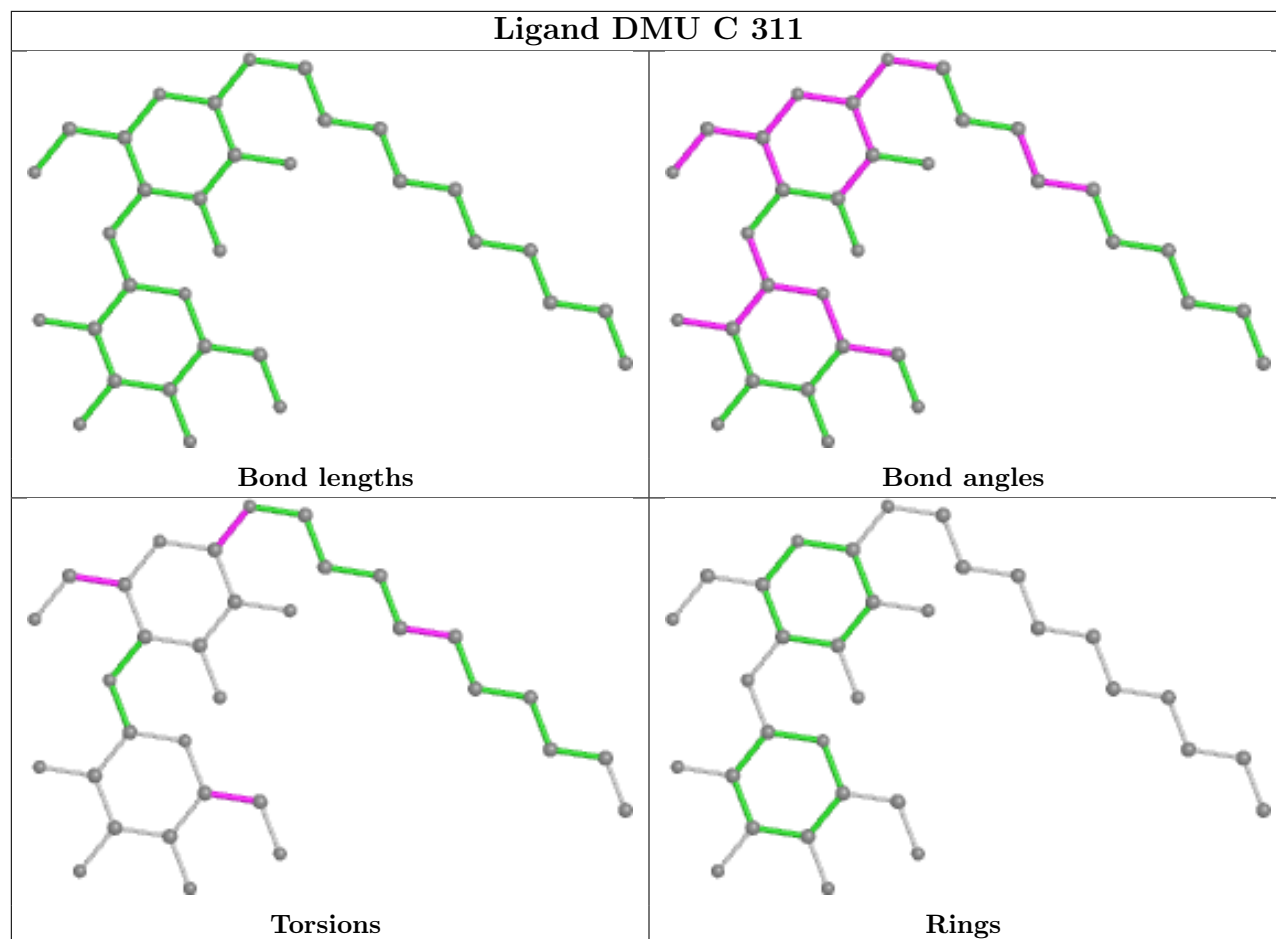


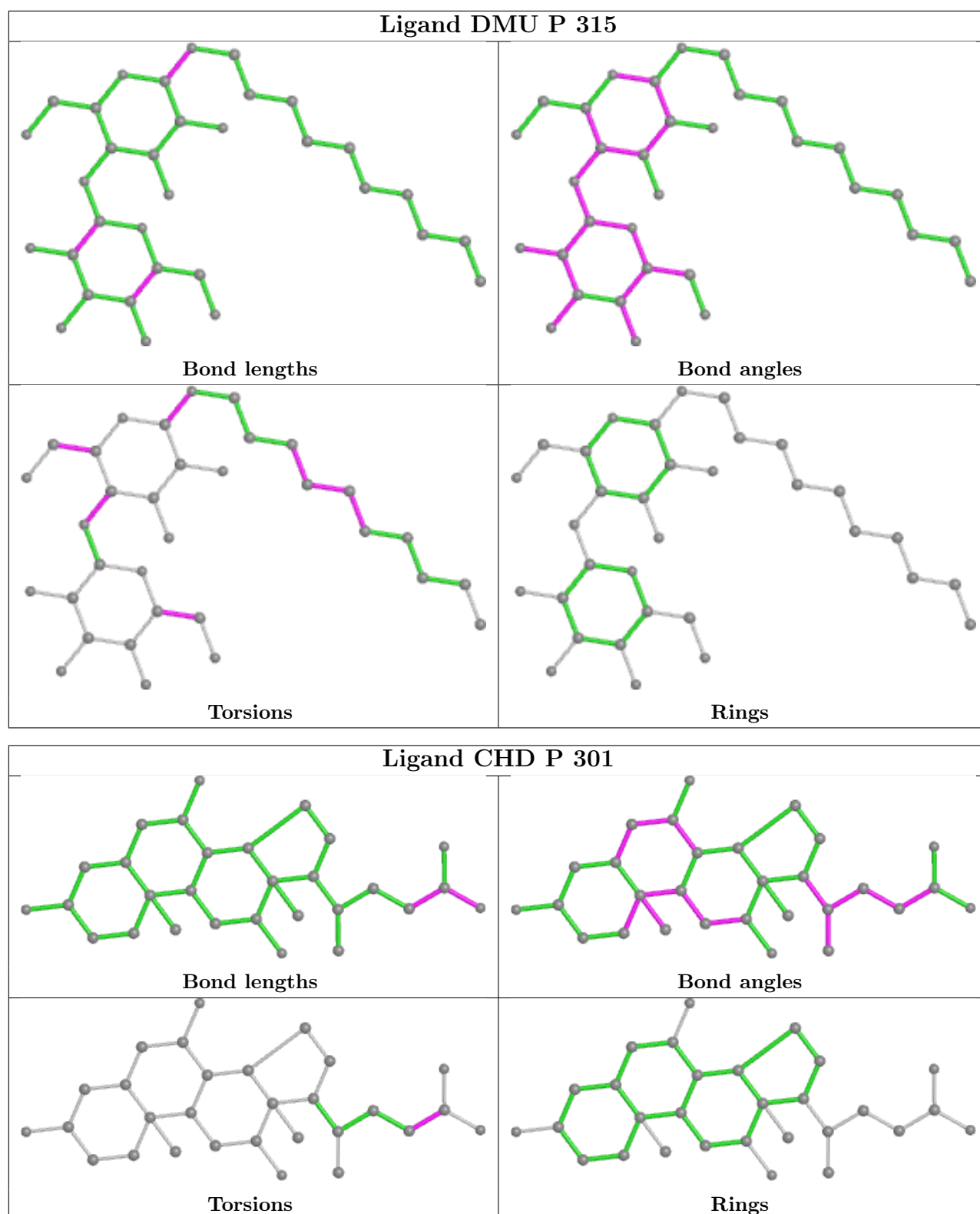


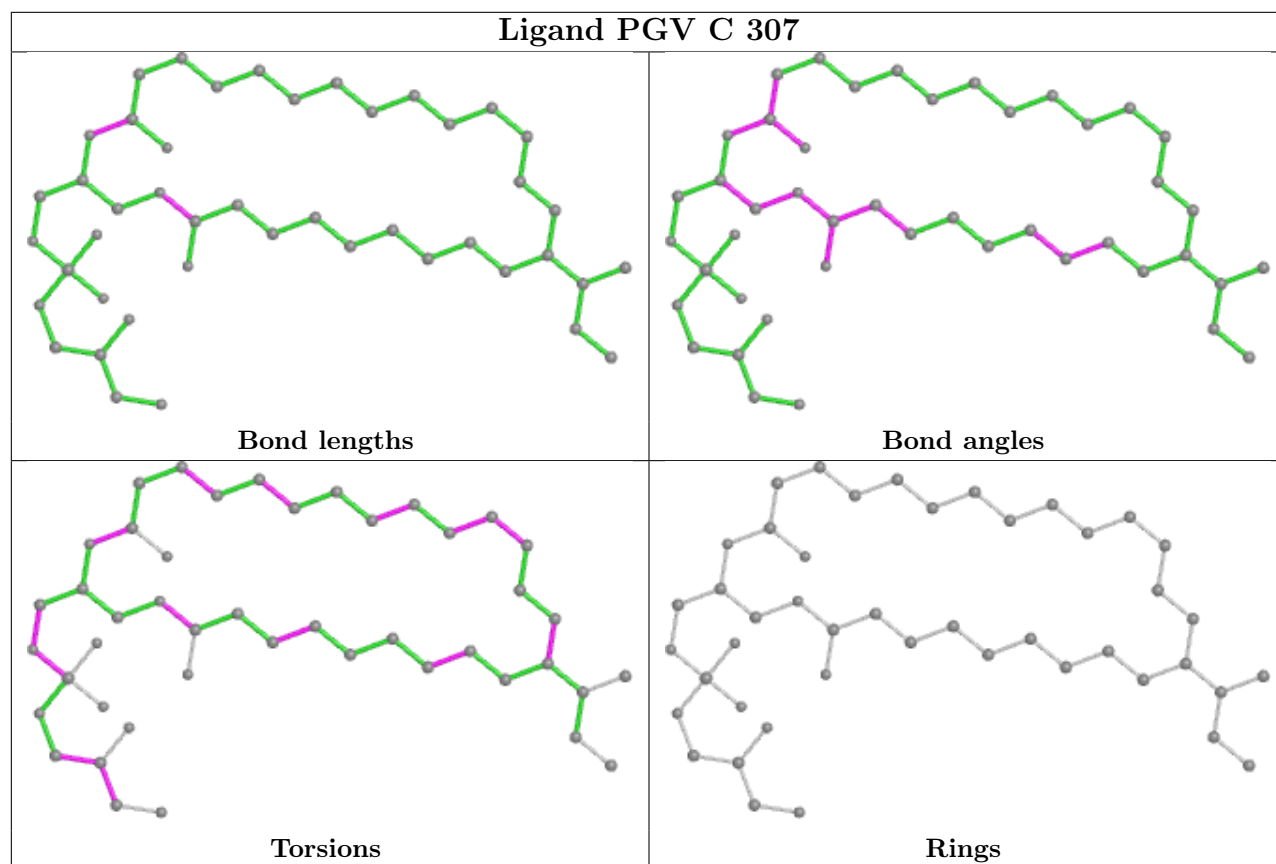
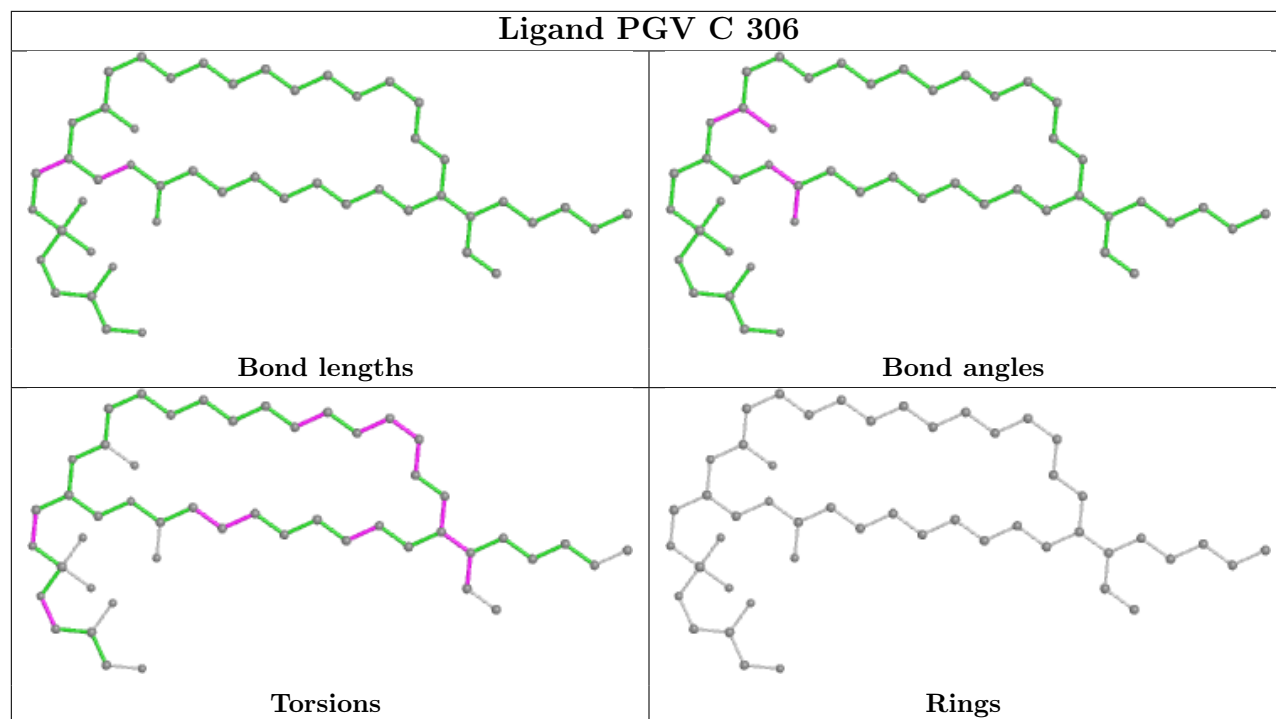


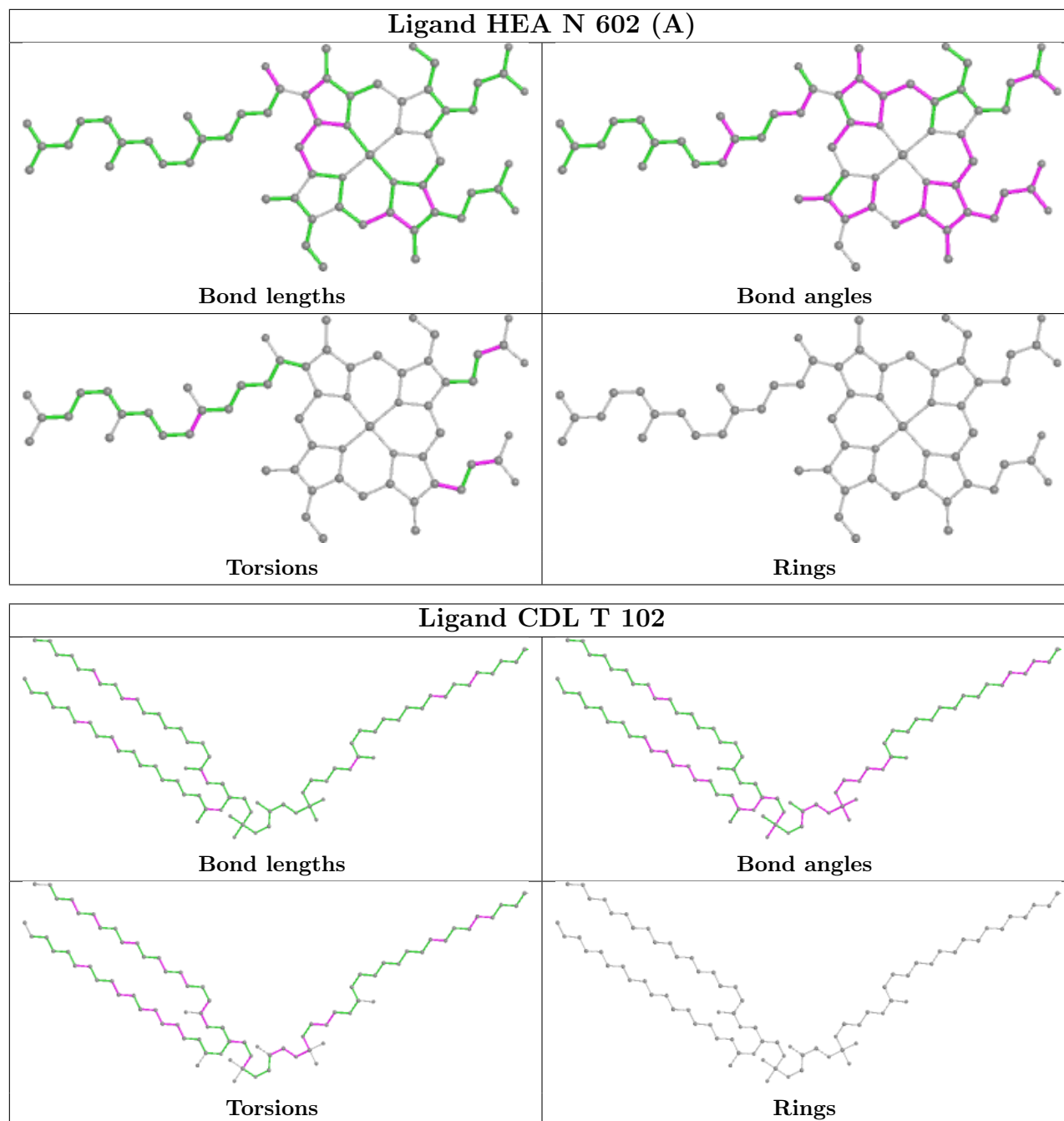


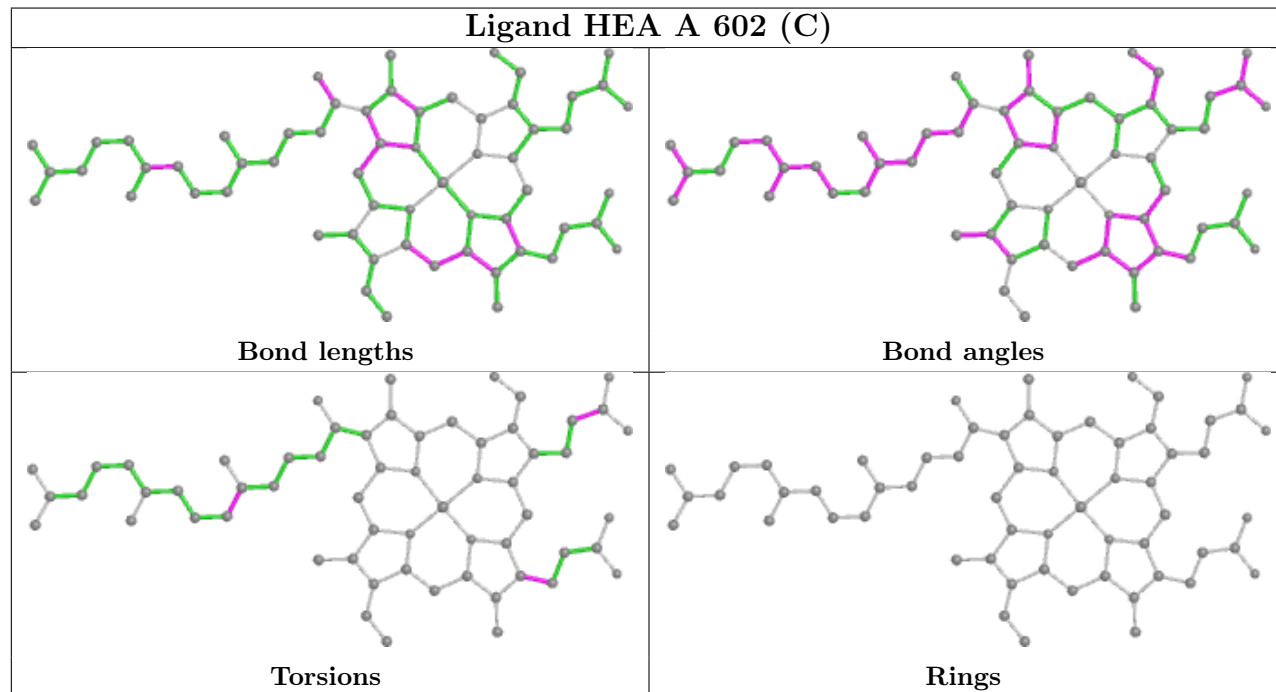
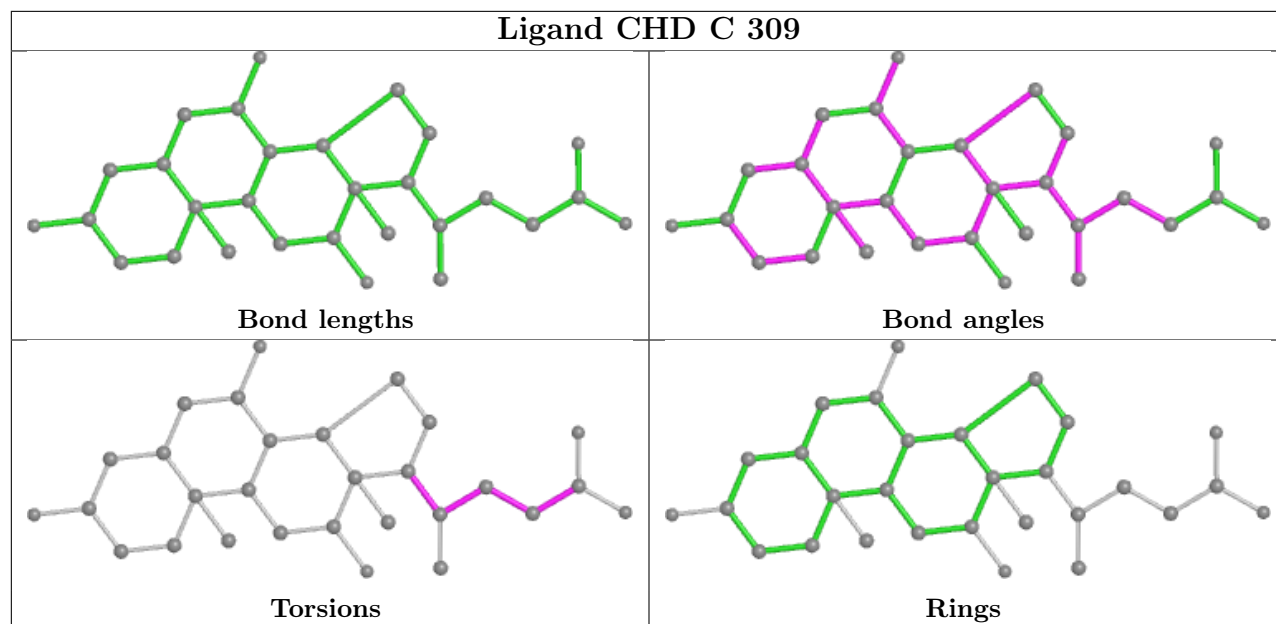


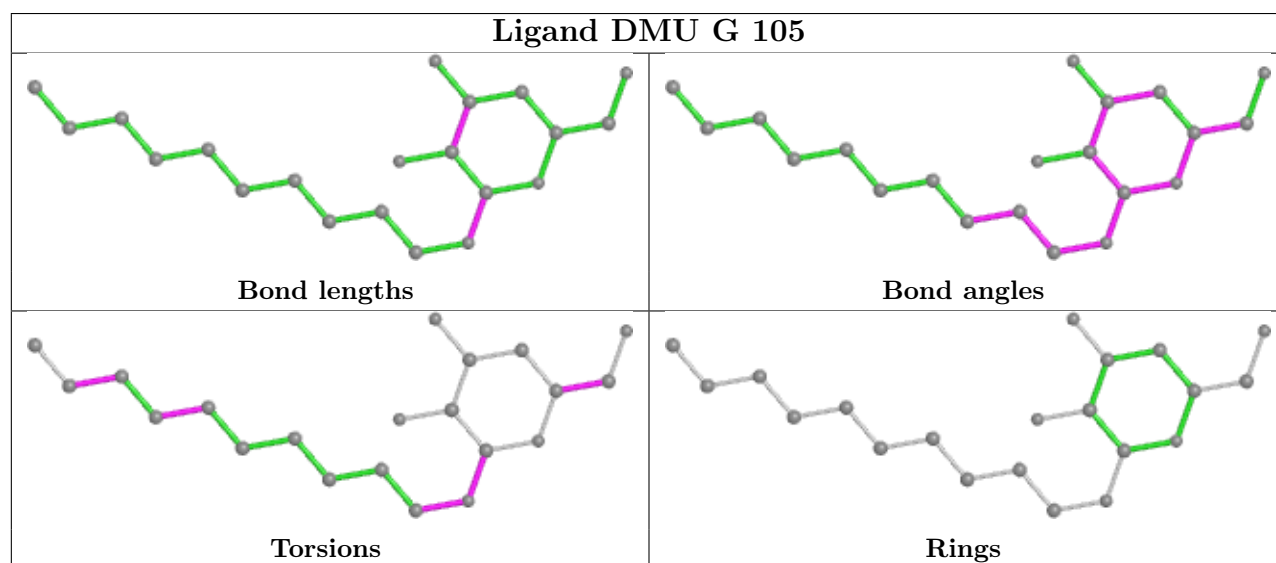
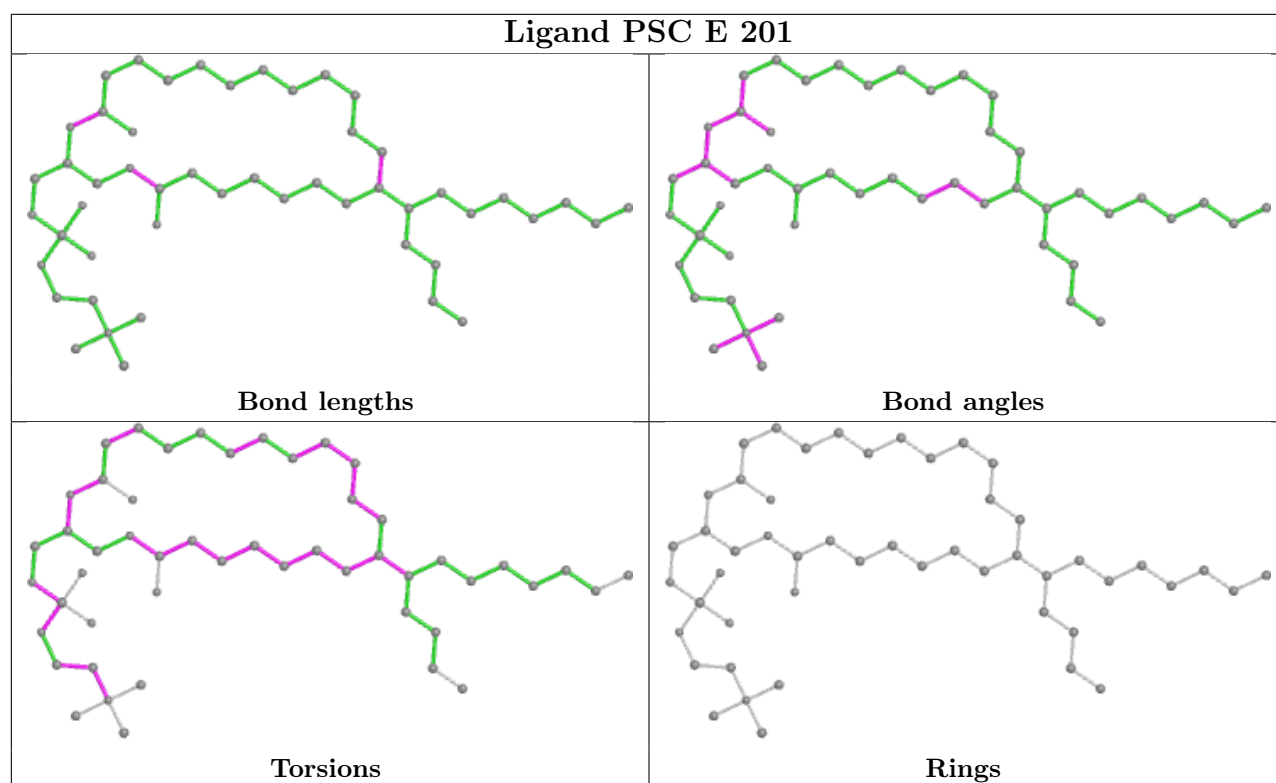


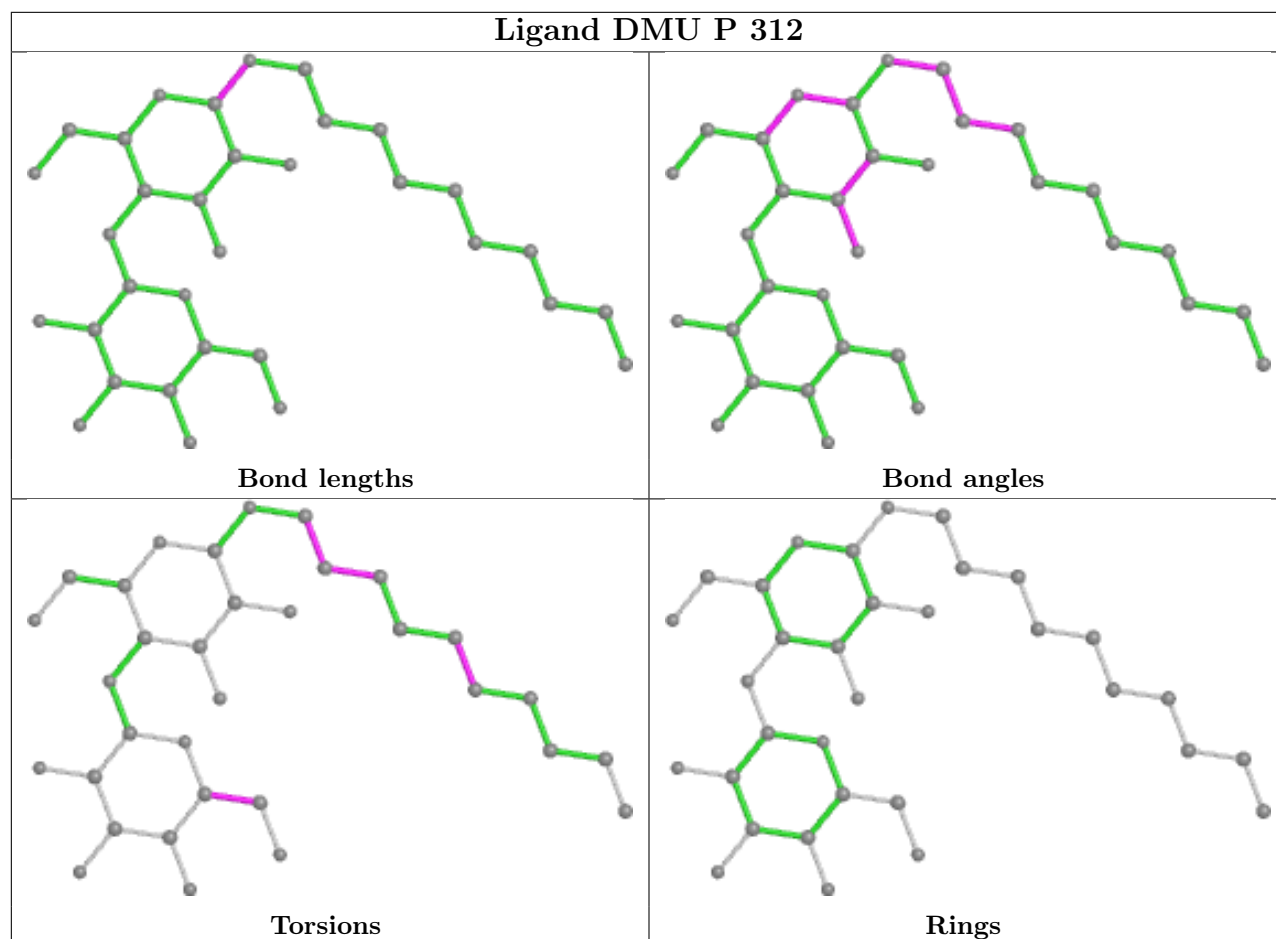
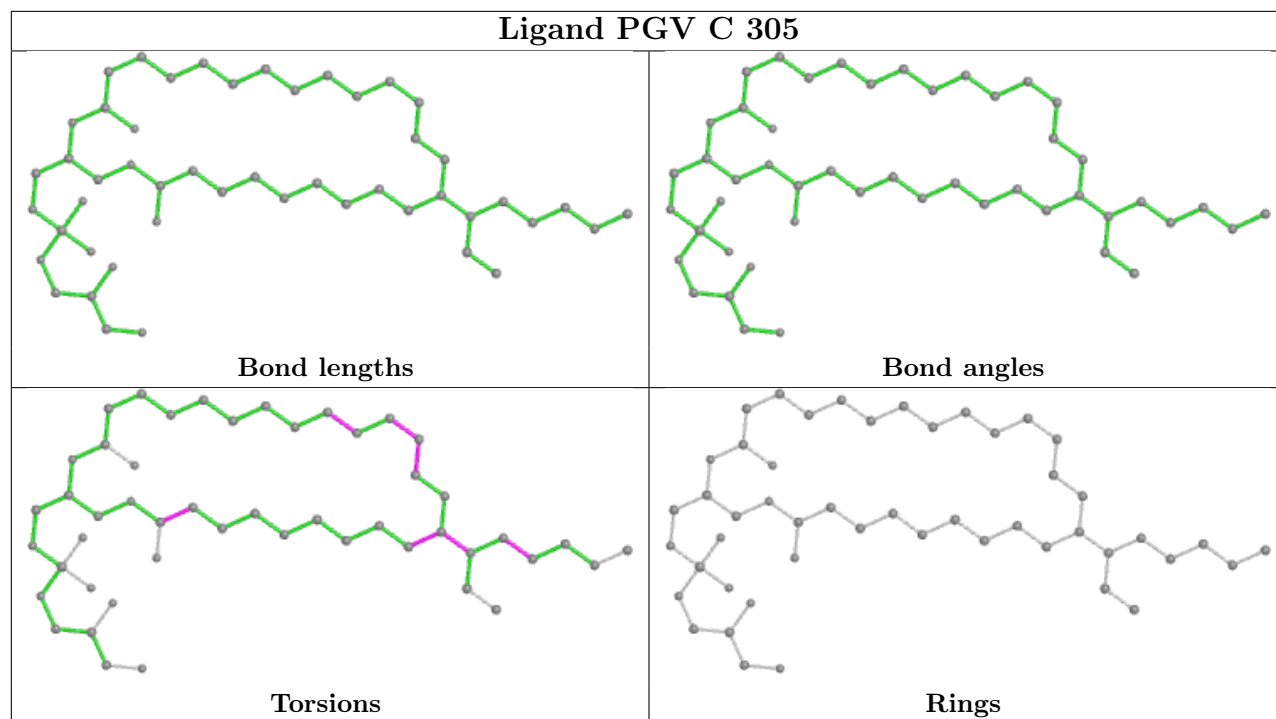


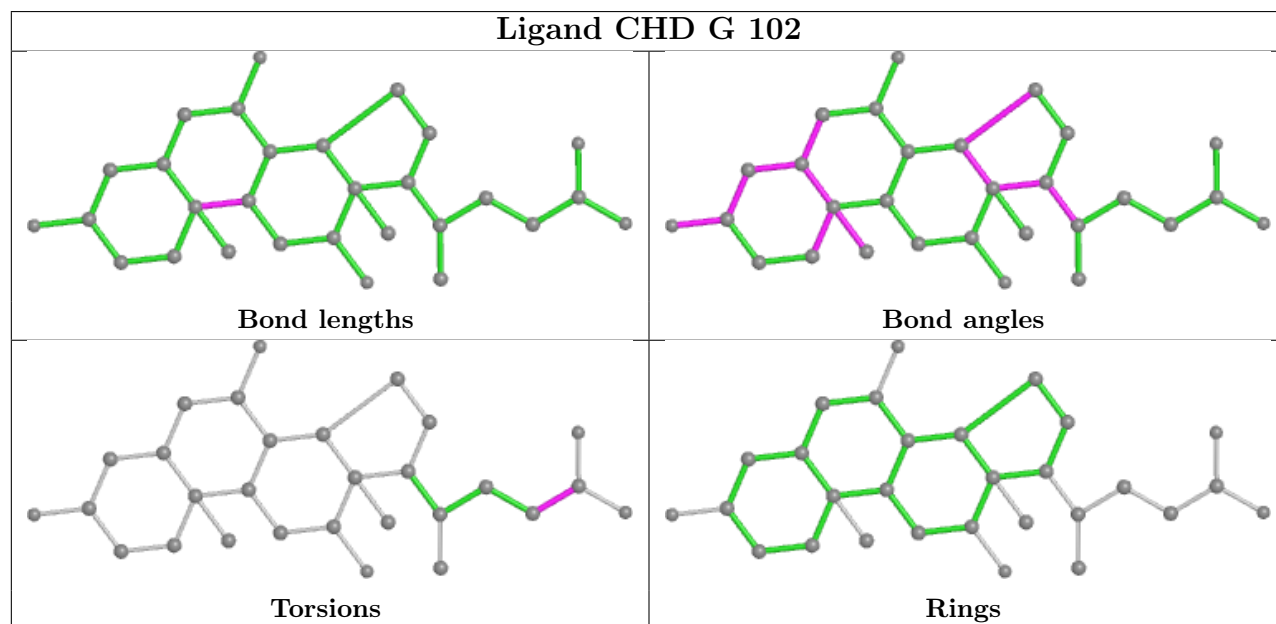
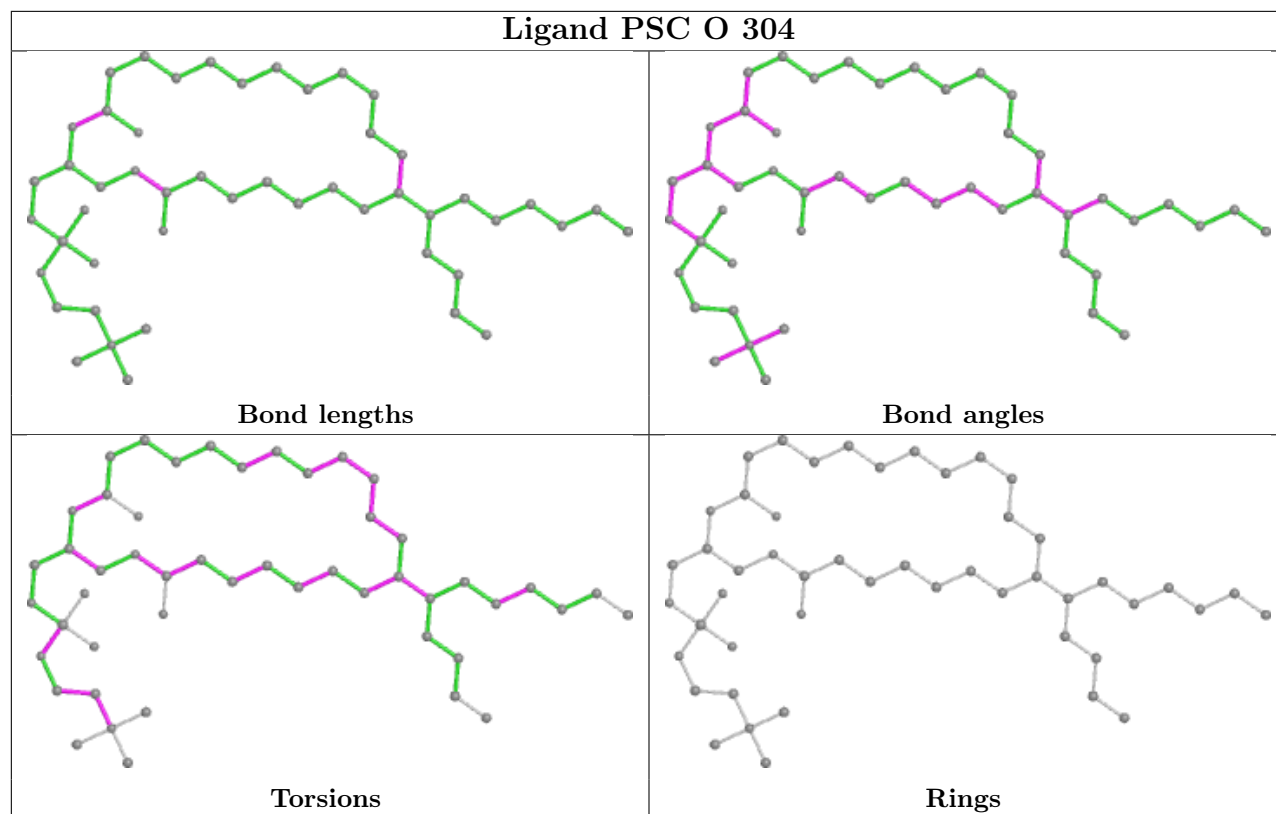


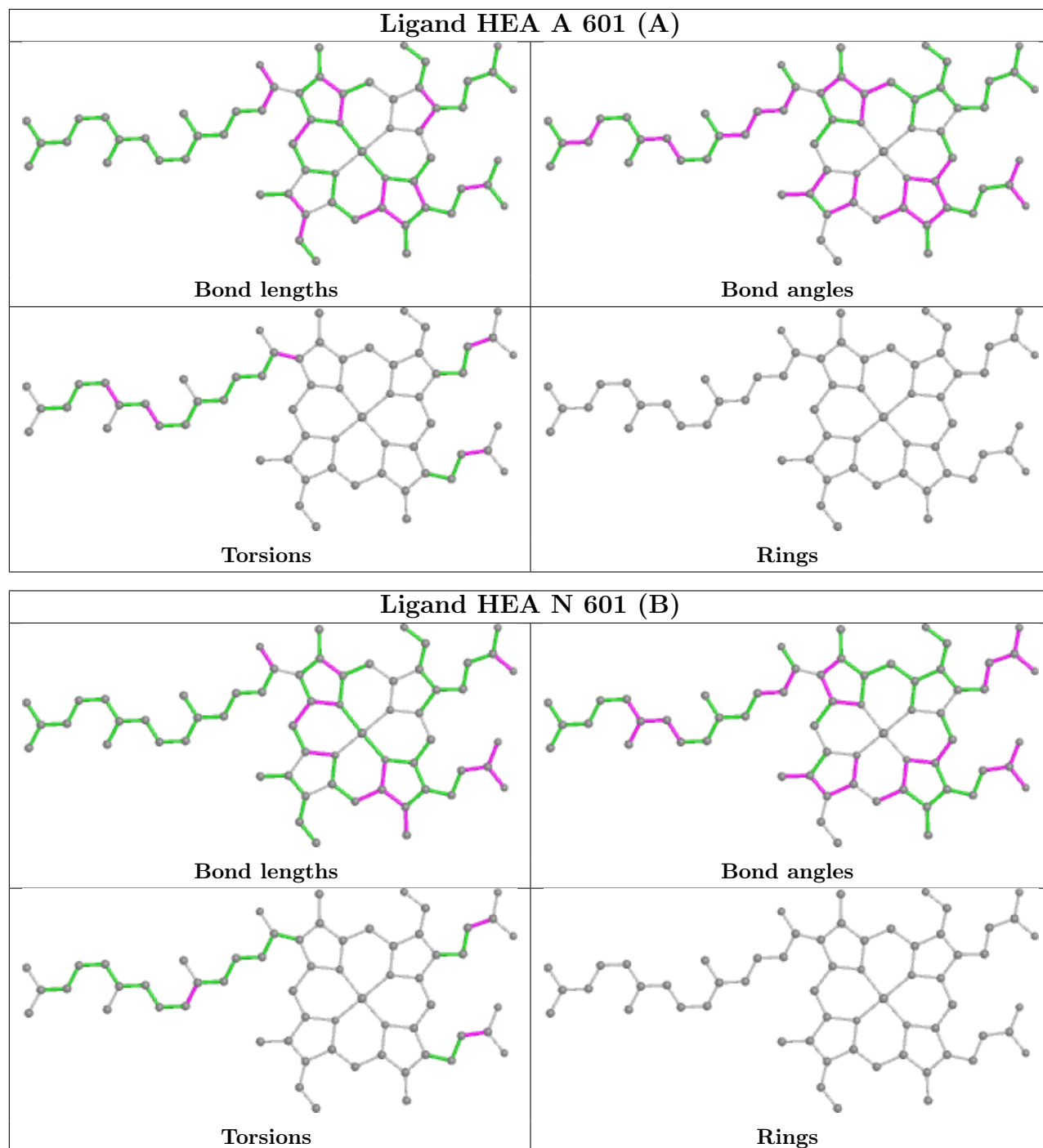


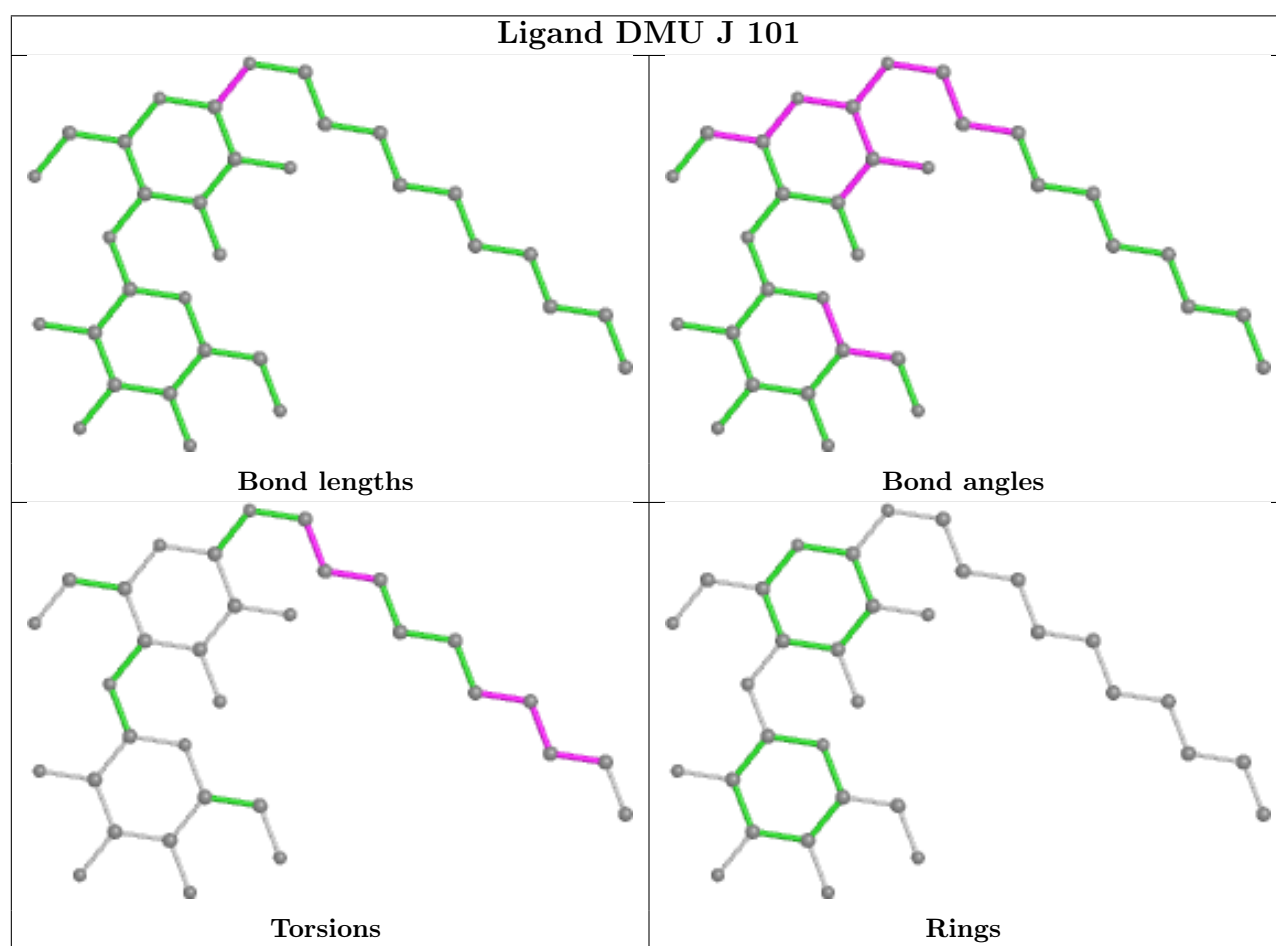
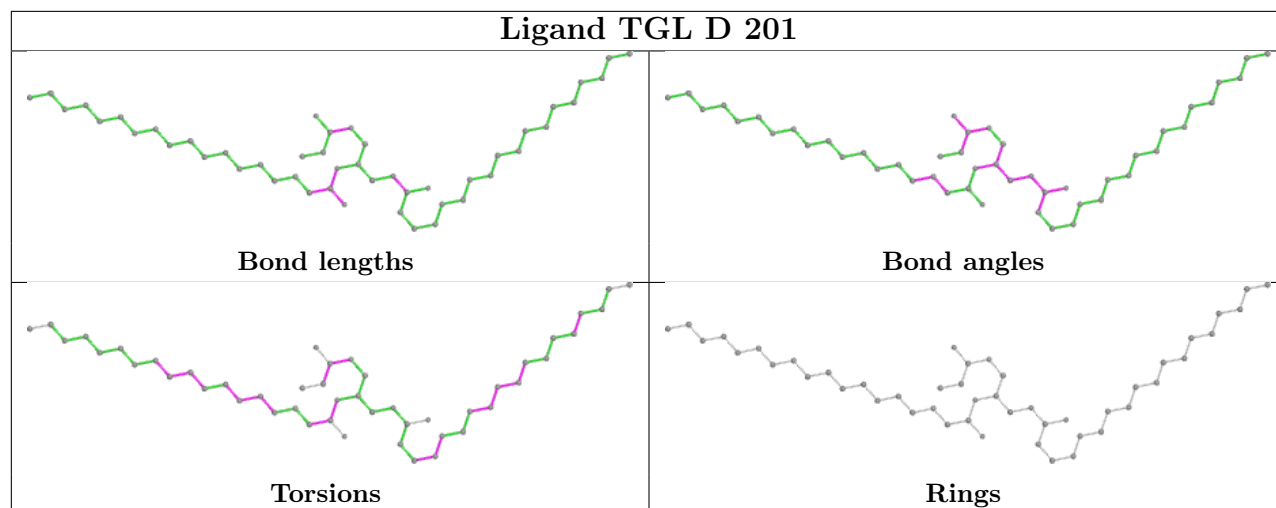


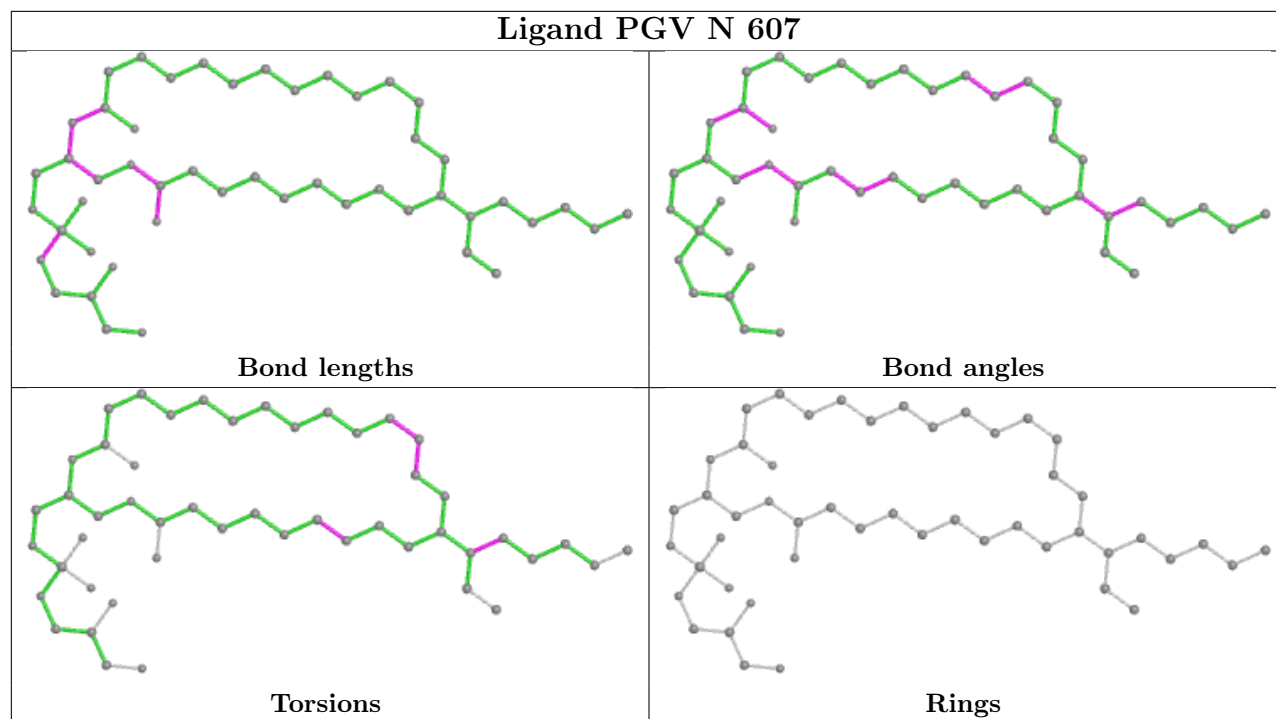












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	513/514 (99%)	-0.24	0 100 100	20, 24, 33, 97	0
1	N	513/514 (99%)	-0.31	0 100 100	21, 27, 36, 81	0
2	B	226/227 (99%)	-0.19	7 (3%) 49 52	23, 32, 65, 117	0
2	O	226/227 (99%)	-0.21	6 (2%) 54 56	26, 36, 72, 110	0
3	C	259/259 (100%)	-0.25	0 100 100	22, 28, 42, 81	0
3	P	259/259 (100%)	-0.27	2 (0%) 86 87	22, 28, 45, 110	0
4	D	144/144 (100%)	-0.38	1 (0%) 87 89	26, 33, 63, 101	0
4	Q	144/144 (100%)	0.30	6 (4%) 36 39	32, 47, 97, 205	0
5	E	104/104 (100%)	-0.36	0 100 100	26, 33, 61, 88	0
5	R	104/104 (100%)	-0.22	1 (0%) 82 84	30, 39, 67, 97	0
6	F	93/93 (100%)	-0.27	3 (3%) 47 50	23, 32, 63, 111	0
6	S	93/93 (100%)	-0.20	4 (4%) 35 38	24, 32, 63, 108	0
7	G	80/84 (95%)	0.71	15 (18%) 1 1	26, 37, 97, 117	0
7	T	84/84 (100%)	0.76	16 (19%) 1 1	25, 38, 125, 148	0
8	H	79/79 (100%)	0.18	8 (10%) 7 8	27, 37, 112, 130	0
8	U	79/79 (100%)	0.08	9 (11%) 5 5	31, 43, 132, 178	0
9	I	72/73 (98%)	0.44	7 (9%) 7 9	30, 46, 114, 194	0
9	V	72/73 (98%)	0.41	7 (9%) 7 9	30, 56, 98, 182	0
10	J	57/57 (100%)	-0.05	4 (7%) 16 18	28, 37, 78, 102	0
10	W	57/57 (100%)	-0.07	3 (5%) 26 29	28, 39, 80, 144	0
11	K	49/49 (100%)	-0.34	0 100 100	30, 37, 59, 72	0
11	X	49/49 (100%)	-0.08	0 100 100	36, 47, 84, 104	0
12	L	46/46 (100%)	-0.16	2 (4%) 35 38	24, 29, 50, 115	0
12	Y	46/46 (100%)	-0.13	2 (4%) 35 38	29, 34, 69, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	41/41 (100%)	-0.21	1 (2%) 59 61	26, 29, 58, 81	0
13	Z	41/41 (100%)	-0.03	2 (4%) 29 32	33, 38, 77, 122	0
All	All	3530/3540 (99%)	-0.13	106 (3%) 50 53	20, 31, 76, 209	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	4	SER	17.4
4	Q	5	VAL	14.0
4	Q	6	VAL	13.9
7	T	8	HIS	11.6
12	Y	47	LYS	9.8
7	G	8	HIS	9.4
7	T	3	ALA	8.7
4	Q	8	SER	8.3
9	I	29	LEU	7.7
4	Q	7	LYS	7.2
7	G	9	GLY	6.5
2	O	90	ILE	6.5
7	G	36	TRP	6.4
7	T	10	GLY	6.4
9	I	25	PHE	6.3
7	T	42	ARG	6.1
6	F	2	SER	6.1
6	S	2	SER	6.0
7	T	36	TRP	6.0
9	V	37	PHE	6.0
7	G	10	GLY	5.7
8	H	45	ALA	5.5
7	G	11	THR	5.3
7	T	5	LYS	5.3
8	H	8	ILE	5.2
8	U	8	ILE	5.1
7	G	7	ASP	5.1
7	G	42	ARG	5.1
7	T	7	ASP	5.0
9	I	37	PHE	4.7
12	L	47	LYS	4.6
13	Z	40	TYR	4.6
9	I	30	GLY	4.5
10	J	1	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
8	H	46	LYS	4.3
7	T	11	THR	4.2
8	U	7	LYS	4.2
7	G	6	GLY	4.2
8	H	44	THR	4.1
5	R	109	VAL	4.0
8	U	46	LYS	3.9
6	F	94	HIS	3.9
7	T	40	GLY	3.9
10	W	57	HIS	3.9
12	L	2	HIS	3.9
7	T	1	ALA	3.8
6	S	94	HIS	3.8
10	J	57	HIS	3.7
7	G	40	GLY	3.7
7	T	39	SER	3.7
8	U	45	ALA	3.6
9	V	2	THR	3.5
2	B	90	ILE	3.5
8	U	47	GLY	3.4
9	V	34	PHE	3.4
9	I	34	PHE	3.3
2	B	61	VAL	3.2
13	M	40	TYR	3.2
6	F	3	GLY	3.2
7	G	39	SER	3.1
9	V	25	PHE	3.1
8	H	47	GLY	3.1
2	B	58	ALA	3.1
9	I	33	THR	3.1
8	H	48	GLY	3.0
10	W	52	TRP	3.0
2	B	55	THR	2.9
9	I	32	ALA	2.9
3	P	3	HIS	2.9
8	H	7	LYS	2.8
10	W	55	PHE	2.8
9	V	29	LEU	2.7
13	Z	41	LYS	2.7
8	U	44	THR	2.6
7	T	84	LYS	2.6
10	J	56	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	59	GLN	2.6
4	Q	51	LEU	2.6
3	P	37	PHE	2.5
7	G	5	LYS	2.5
6	S	93	PRO	2.4
7	G	84	LYS	2.4
8	U	48	GLY	2.4
6	S	3	GLY	2.4
2	O	91	ASN	2.3
2	O	227	LEU	2.3
4	D	4	SER	2.3
2	B	87	MET	2.3
8	H	42	ALA	2.2
7	T	38	HIS	2.2
7	T	37	LEU	2.2
2	O	113	TYR	2.2
12	Y	2	HIS	2.2
8	U	9	LYS	2.2
7	T	2	SER	2.2
2	O	32[A]	PHE	2.2
7	G	37	LEU	2.2
2	B	57	ASP	2.2
7	T	9	GLY	2.1
9	V	39	VAL	2.1
2	O	87[A]	MET	2.1
7	G	43	GLU	2.1
10	J	52	TRP	2.1
7	G	41	HIS	2.0
8	U	10	ASN	2.0
9	V	35	TYR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	SAC	V	1	9/10	0.45	0.42	261,280,298,300	0
9	SAC	I	1	9/10	0.83	0.18	123,141,157,179	0
1	FME	A	1	10/11	0.96	0.10	34,45,69,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FME	O	1	10/11	0.97	0.07	34,36,42,117	0
1	FME	N	1	10/11	0.97	0.09	35,42,79,80	0
2	FME	B	1	10/11	0.98	0.08	27,30,35,81	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	DMU	X	101	22/33	0.25	0.33	49,75,84,89	0
26	DMU	G	105	21/33	0.29	0.23	53,70,81,87	0
26	DMU	K	101	22/33	0.32	0.32	40,67,83,84	0
26	DMU	K	102	22/33	0.36	0.34	46,73,82,87	0
26	DMU	X	102	22/33	0.43	0.30	62,71,84,89	0
26	DMU	P	316	22/33	0.46	0.21	50,68,84,87	0
26	DMU	X	103	22/33	0.47	0.35	61,72,82,86	0
26	DMU	C	311	33/33	0.54	0.26	53,68,90,99	0
24	PEK	P	305	46/53	0.67	0.26	48,75,102,117	0
25	CDL	G	101	89/100	0.67	0.28	51,77,107,188	0
21	EDO	S	107	4/4	0.67	0.28	52,58,59,63	0
26	DMU	L	101	18/33	0.67	0.18	46,65,84,84	0
27	PSC	E	201	52/52	0.67	0.34	45,77,123,221	0
24	PEK	T	101	49/53	0.69	0.33	47,76,117,205	0
20	PGV	P	307	51/51	0.69	0.25	42,75,109,197	0
19	TGL	O	302	63/63	0.70	0.19	49,71,97,104	0
25	CDL	T	102	80/100	0.71	0.29	42,78,116,206	0
23	CHD	W	101	29/29	0.72	0.33	60,74,91,109	0
24	PEK	C	304	44/53	0.72	0.26	47,74,99,130	0
27	PSC	O	304	51/52	0.72	0.26	43,74,116,204	0
25	CDL	Y	101	87/100	0.73	0.26	38,78,116,159	0
26	DMU	P	310	33/33	0.74	0.21	61,75,97,110	0
26	DMU	P	311	33/33	0.74	0.28	57,85,99,101	0
26	DMU	P	312	33/33	0.74	0.26	38,75,97,106	0
20	PGV	Q	201	51/51	0.75	0.27	47,72,111,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
20	PGV	C	307	47/51	0.75	0.23	39,73,103,206	0
26	DMU	K	103	17/33	0.75	0.27	55,70,77,89	0
26	DMU	P	315	33/33	0.75	0.26	41,67,84,90	0
21	EDO	S	108	4/4	0.75	0.11	49,55,62,64	0
25	CDL	P	308	76/100	0.76	0.22	31,74,108,157	0
25	CDL	C	308	86/100	0.77	0.21	29,73,103,171	0
17	NA	P	302	1/1	0.79	0.08	38,38,38,38	0
26	DMU	J	101	33/33	0.79	0.25	31,70,97,106	0
19	TGL	D	201	48/63	0.81	0.14	30,59,91,127	0
24	PEK	P	303	22/53	0.81	0.11	51,60,86,98	0
23	CHD	P	309	29/29	0.82	0.18	47,59,82,103	0
21	EDO	S	104	4/4	0.83	0.15	43,45,55,57	0
19	TGL	O	301	63/63	0.84	0.18	37,74,90,106	0
23	CHD	J	102	29/29	0.84	0.24	50,74,103,112	0
23	CHD	C	309	29/29	0.86	0.18	45,58,84,85	0
19	TGL	A	607	63/63	0.86	0.20	32,62,96,123	0
20	PGV	A	608	46/51	0.86	0.21	33,67,110,193	0
21	EDO	B	308	4/4	0.87	0.18	31,34,38,43	0
26	DMU	Z	101	33/33	0.87	0.10	38,46,63,74	0
29	PO4	U	102	5/5	0.87	0.26	53,58,65,65	0
19	TGL	B	301	62/63	0.88	0.14	28,65,88,98	0
21	EDO	A	614	4/4	0.88	0.14	37,39,42,46	0
21	EDO	G	104	4/4	0.89	0.14	42,62,72,77	0
21	EDO	B	306	4/4	0.89	0.14	29,45,56,75	0
26	DMU	M	101	33/33	0.89	0.09	33,39,56,71	0
21	EDO	A	610	4/4	0.90	0.10	29,29,30,31	0
21	EDO	A	613	4/4	0.90	0.12	39,39,41,56	0
21	EDO	O	308	4/4	0.91	0.17	38,46,48,51	0
21	EDO	N	614	4/4	0.92	0.08	38,41,41,41	0
21	EDO	A	616	4/4	0.92	0.11	38,38,40,41	0
21	EDO	P	314	4/4	0.92	0.15	47,58,60,61	0
21	EDO	N	610	4/4	0.93	0.13	31,50,52,52	0
21	EDO	U	101	4/4	0.93	0.34	35,37,62,63	0
21	EDO	Y	102	4/4	0.93	0.20	53,55,61,65	0
21	EDO	N	612	4/4	0.93	0.09	42,42,45,46	0
21	EDO	A	617	4/4	0.93	0.12	31,37,41,65	0
21	EDO	O	306	4/4	0.93	0.12	34,36,42,46	0
18	CYN	N	606[A]	2/2	0.94	0.22	26,26,26,28	2
18	CYN	N	606[C]	2/2	0.94	0.22	20,20,20,24	2
17	NA	C	302	1/1	0.94	0.09	38,38,38,38	0
21	EDO	D	202	4/4	0.94	0.11	42,45,53,61	0
23	CHD	P	301	29/29	0.94	0.07	27,30,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	EDO	E	203	4/4	0.94	0.08	49,50,54,58	0
21	EDO	B	304	4/4	0.95	0.20	35,39,40,43	0
21	EDO	B	305	4/4	0.95	0.26	30,31,38,43	0
21	EDO	S	105	4/4	0.95	0.09	28,30,31,33	0
17	NA	N	605	1/1	0.95	0.06	29,29,29,29	0
21	EDO	N	615	4/4	0.95	0.08	38,39,40,43	0
21	EDO	T	104	4/4	0.95	0.16	37,44,47,59	0
21	EDO	F	103	4/4	0.95	0.08	36,36,40,55	0
21	EDO	O	307	4/4	0.95	0.08	35,42,48,60	0
23	CHD	C	301	29/29	0.95	0.07	25,30,35,36	0
21	EDO	B	307	4/4	0.95	0.10	25,25,26,28	0
23	CHD	G	102	29/29	0.95	0.07	26,29,33,41	0
21	EDO	O	305	4/4	0.96	0.08	29,30,31,31	0
21	EDO	T	103	4/4	0.96	0.07	31,31,36,37	0
21	EDO	Q	202	4/4	0.96	0.14	30,49,53,65	0
21	EDO	C	310	4/4	0.96	0.06	29,30,30,31	0
21	EDO	A	612	4/4	0.96	0.19	41,53,56,68	0
24	PEK	C	303	51/53	0.96	0.12	27,43,85,92	0
21	EDO	S	106	4/4	0.96	0.35	40,49,50,52	0
21	EDO	N	611	4/4	0.96	0.08	37,38,41,44	0
24	PEK	P	304	53/53	0.96	0.11	28,46,85,94	0
20	PGV	N	607	51/51	0.97	0.10	22,29,75,83	0
21	EDO	F	104	4/4	0.97	0.07	31,31,31,32	0
20	PGV	P	306	45/51	0.97	0.09	24,29,58,76	0
21	EDO	N	608	4/4	0.97	0.10	28,29,30,31	0
21	EDO	N	609	4/4	0.97	0.07	26,27,29,30	0
20	PGV	C	306	51/51	0.97	0.09	23,29,83,91	0
21	EDO	P	313	4/4	0.97	0.11	33,35,38,38	0
20	PGV	C	305	51/51	0.97	0.10	22,28,72,81	0
21	EDO	A	615	4/4	0.97	0.18	32,48,68,71	0
23	CHD	B	303	29/29	0.97	0.07	26,29,38,54	0
21	EDO	R	201	4/4	0.97	0.08	38,40,41,43	0
21	EDO	S	103	4/4	0.97	0.07	33,34,37,38	0
14	HEA	A	601[C]	43/60	0.98	0.09	19,21,23,28	1
18	CYN	A	606[A]	2/2	0.98	0.25	24,24,24,25	2
18	CYN	A	606[C]	2/2	0.98	0.25	17,17,17,18	2
14	HEA	A	602[A]	60/60	0.98	0.10	17,22,37,43	51
21	EDO	N	613	4/4	0.98	0.14	32,34,35,39	0
14	HEA	A	602[C]	60/60	0.98	0.10	16,21,37,43	51
14	HEA	N	601[A]	60/60	0.98	0.08	21,25,32,35	18
21	EDO	A	609	4/4	0.98	0.14	29,33,34,38	0
14	HEA	N	601[B]	60/60	0.98	0.08	23,25,34,44	18

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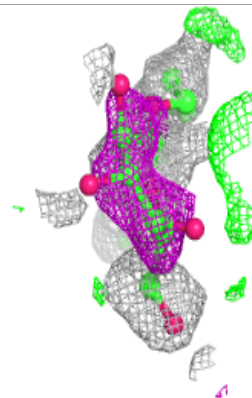
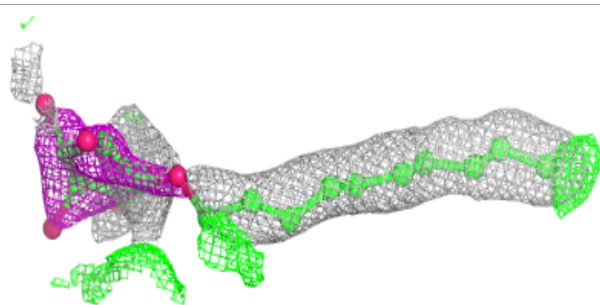
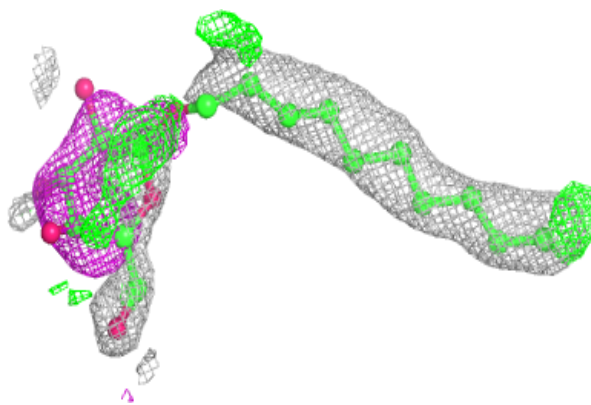
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
21	EDO	E	202	4/4	0.98	0.07	36,37,39,40	0
14	HEA	N	601[C]	43/60	0.98	0.08	23,25,27,28	1
14	HEA	N	602[A]	60/60	0.98	0.09	19,23,35,39	51
14	HEA	N	602[C]	60/60	0.98	0.09	19,24,35,39	51
21	EDO	G	103	4/4	0.98	0.06	30,32,33,36	0
14	HEA	A	601[A]	60/60	0.98	0.09	12,22,31,33	18
14	HEA	A	601[B]	60/60	0.98	0.09	19,22,30,46	18
21	EDO	S	102	4/4	0.99	0.08	24,24,24,26	0
16	MG	N	604	1/1	0.99	0.04	23,23,23,23	0
17	NA	A	605	1/1	0.99	0.05	25,25,25,25	0
21	EDO	A	611	4/4	0.99	0.09	23,24,24,27	0
28	ZN	F	101	1/1	0.99	0.13	29,29,29,29	0
21	EDO	F	102	4/4	0.99	0.07	23,24,24,25	0
15	CU	A	603	1/1	1.00	0.13	23,23,23,23	0
15	CU	N	603	1/1	1.00	0.12	25,25,25,25	0
16	MG	A	604	1/1	1.00	0.07	22,22,22,22	0
22	CUA	B	302	2/2	1.00	0.12	24,24,24,24	0
28	ZN	S	101	1/1	1.00	0.13	28,28,28,28	0
22	CUA	O	303	2/2	1.00	0.10	27,27,27,28	0

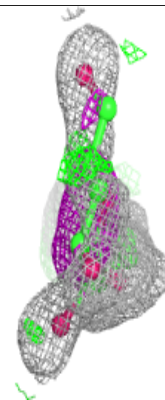
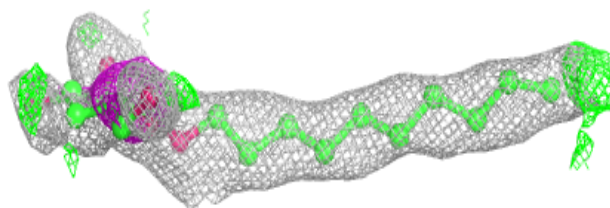
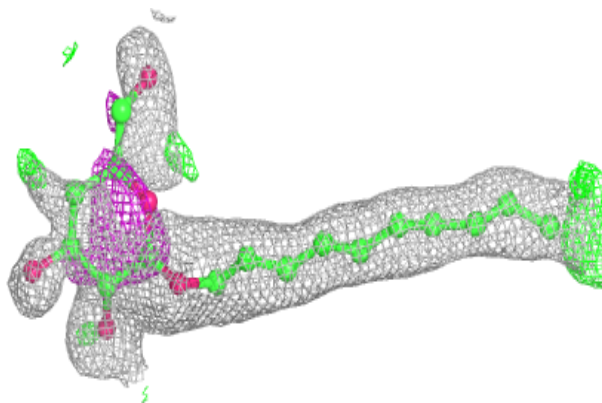
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

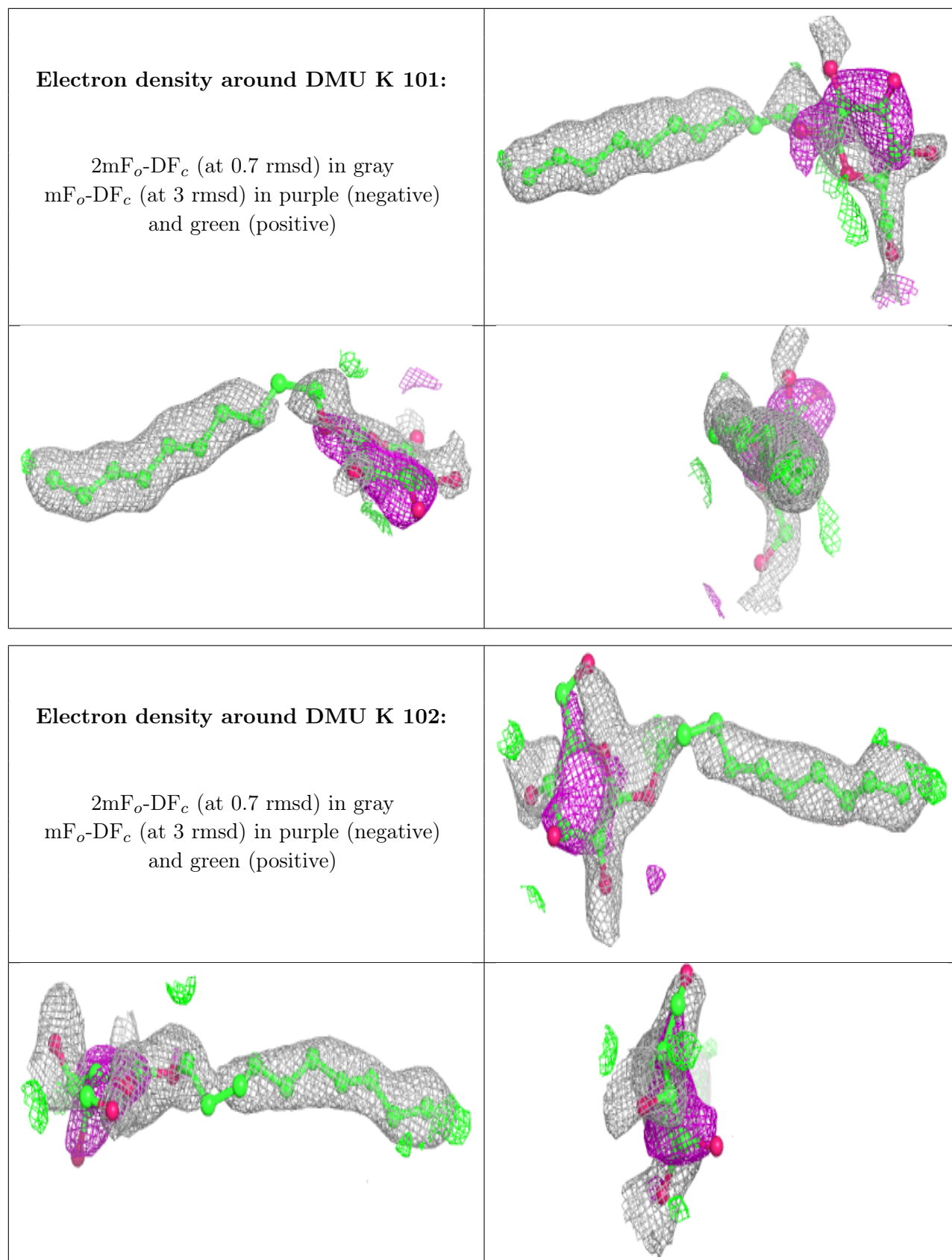
Electron density around DMU X 101:

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

**Electron density around DMU G 105:**

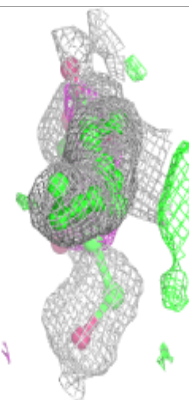
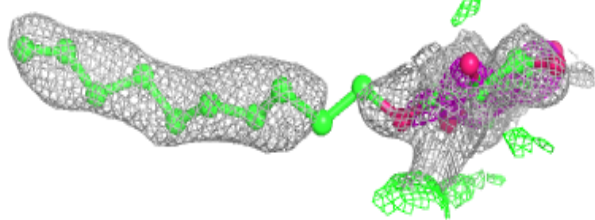
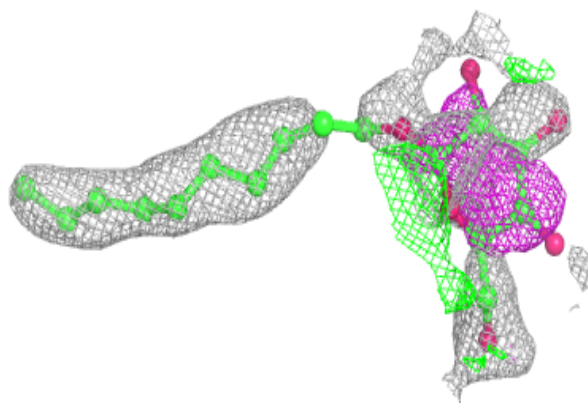
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



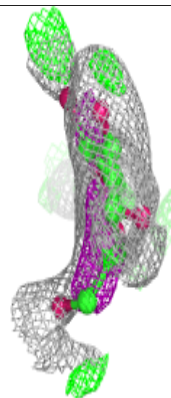
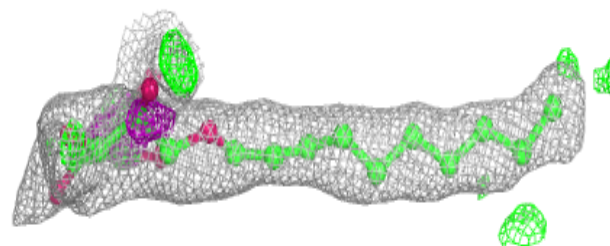
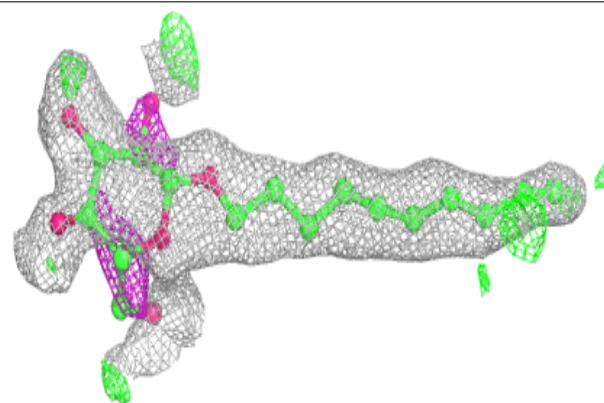


Electron density around DMU X 102:

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

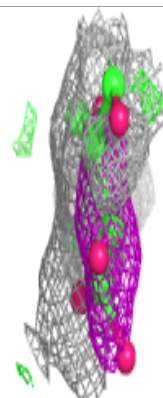
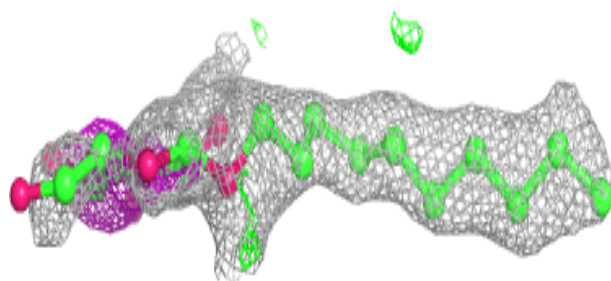
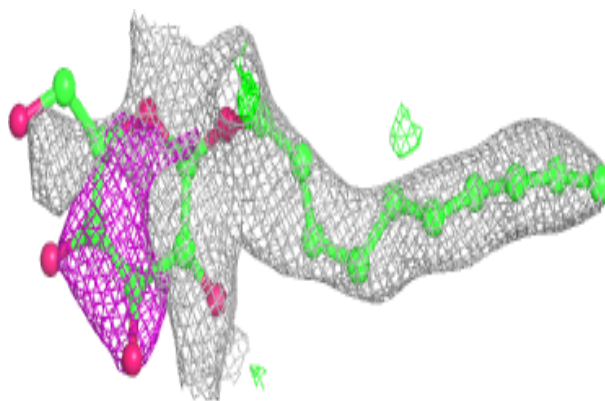
**Electron density around DMU P 316:**

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

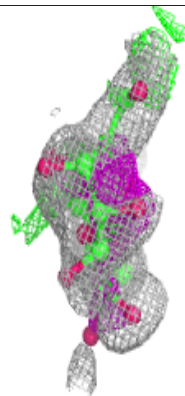
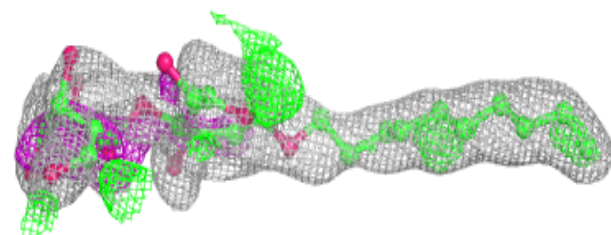
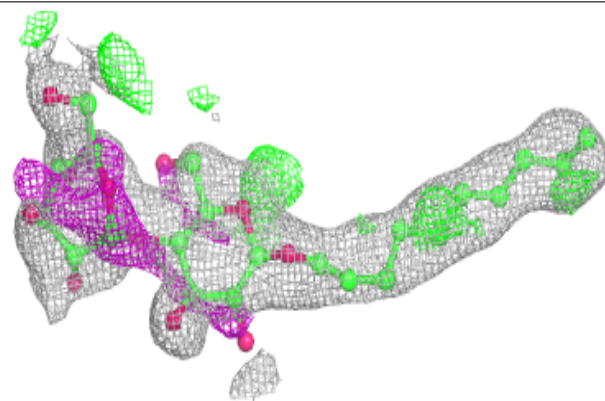


Electron density around DMU X 103:

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

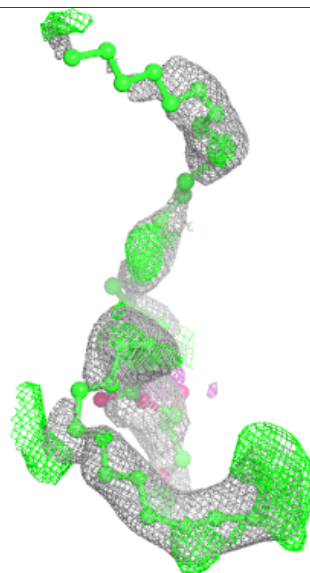
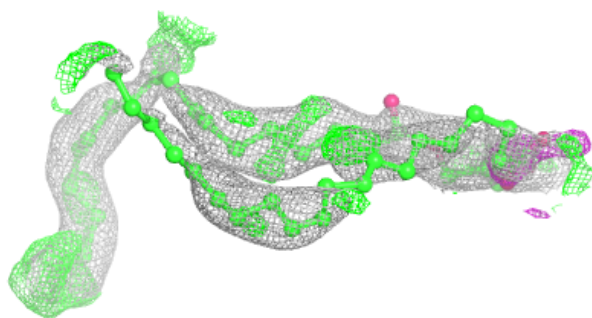
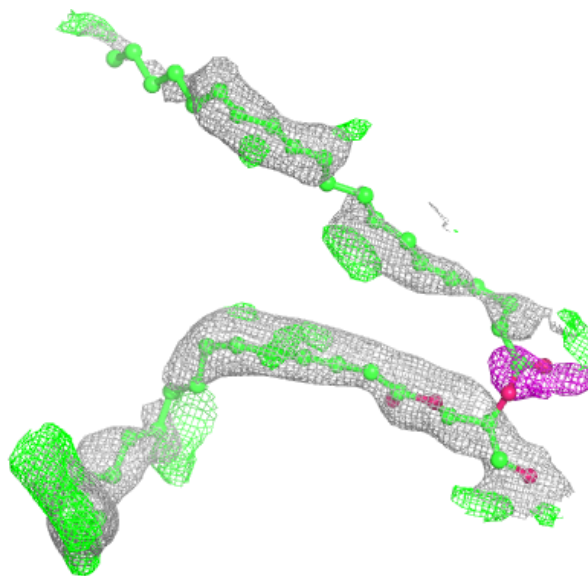
**Electron density around DMU C 311:**

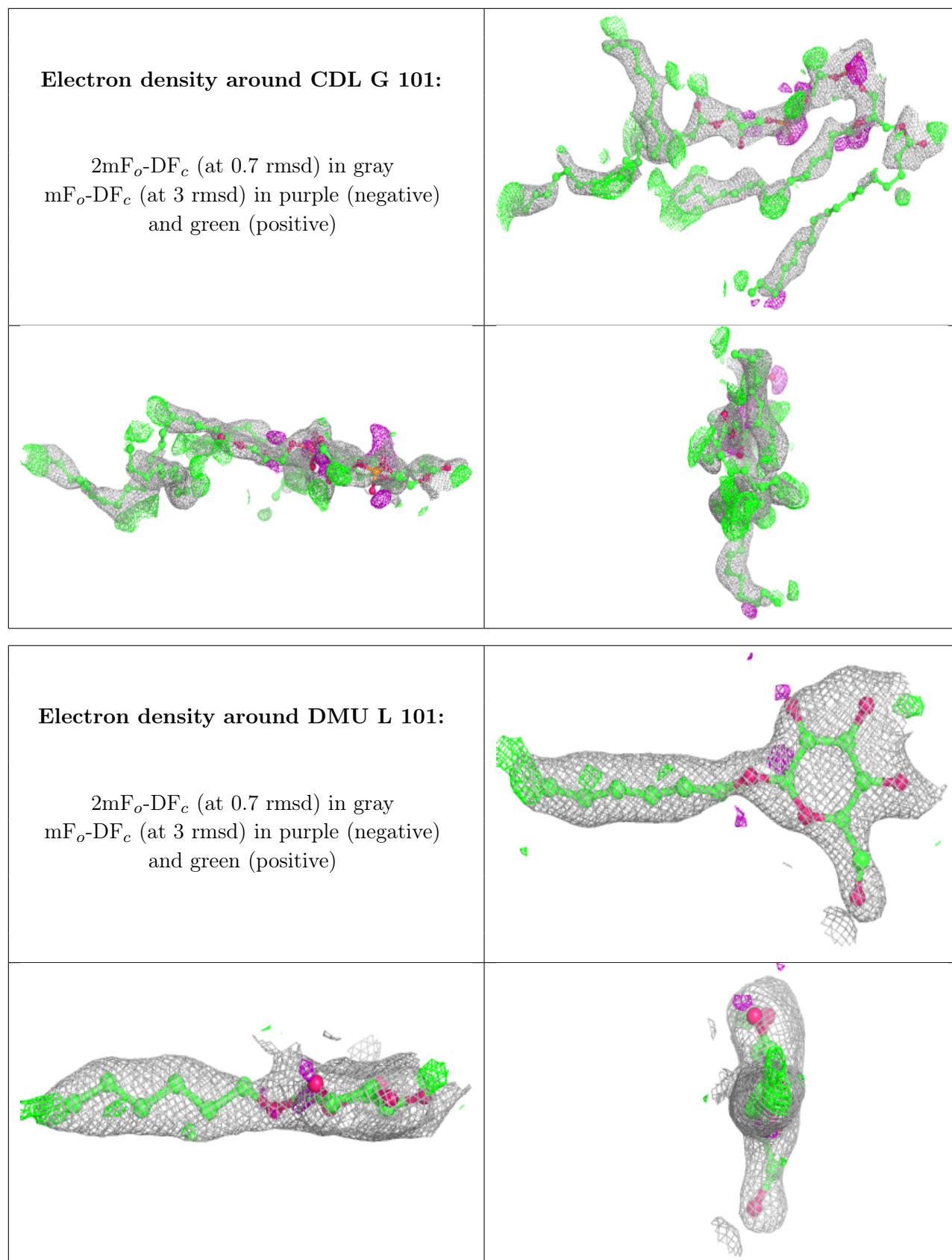
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PEK P 305:

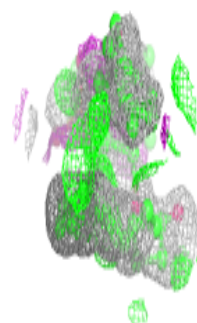
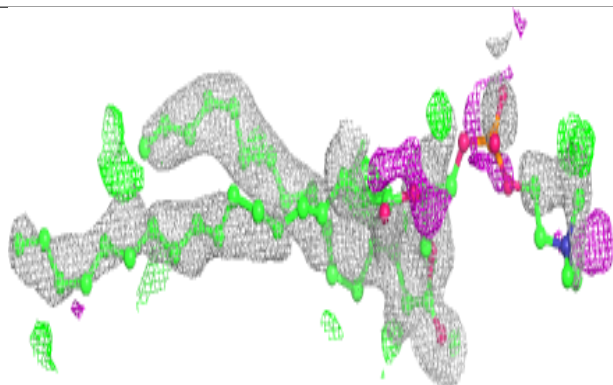
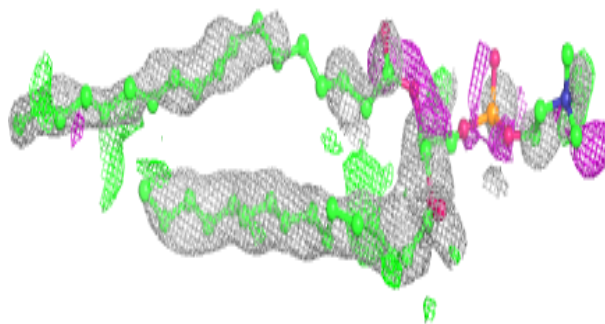
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

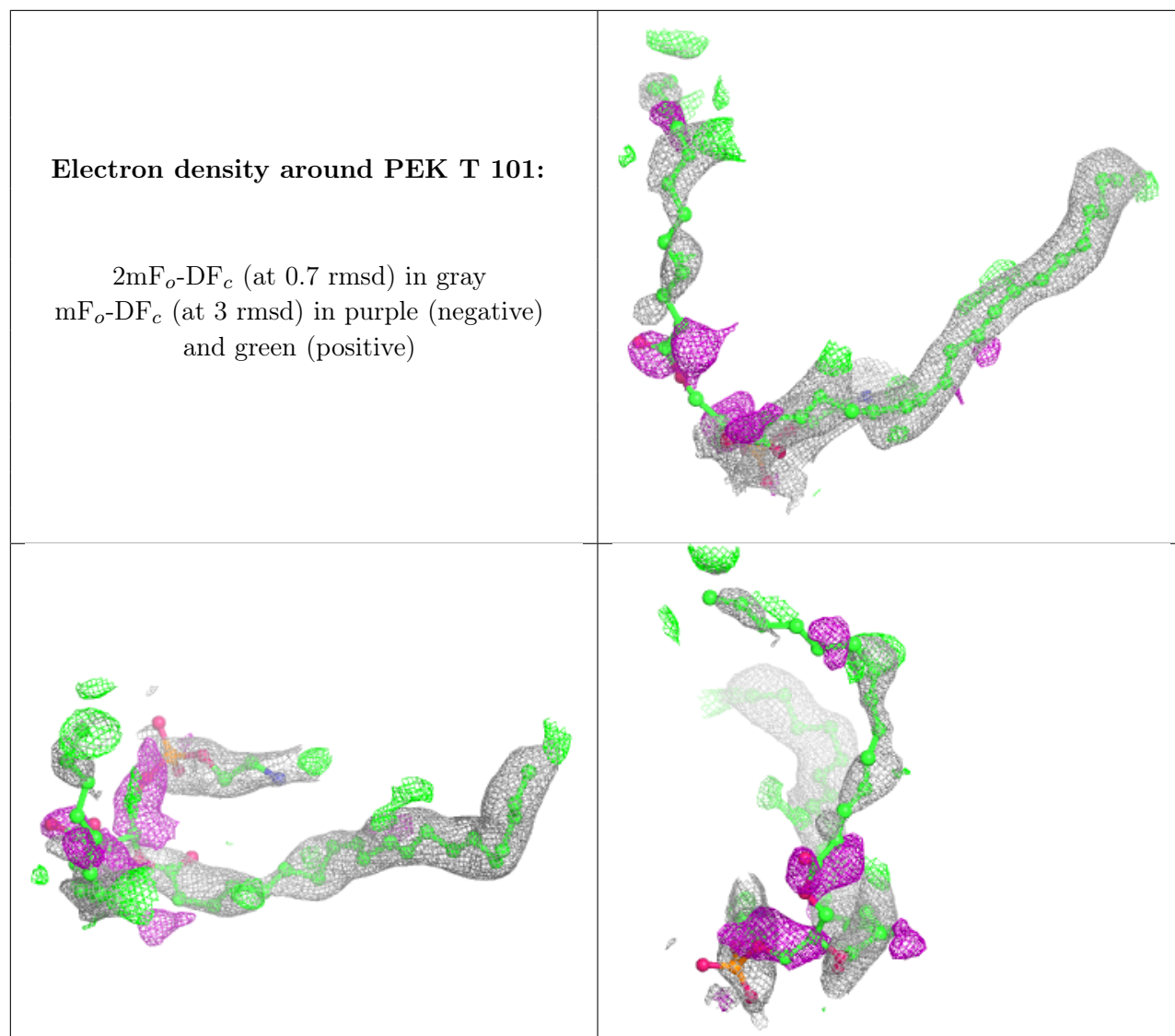


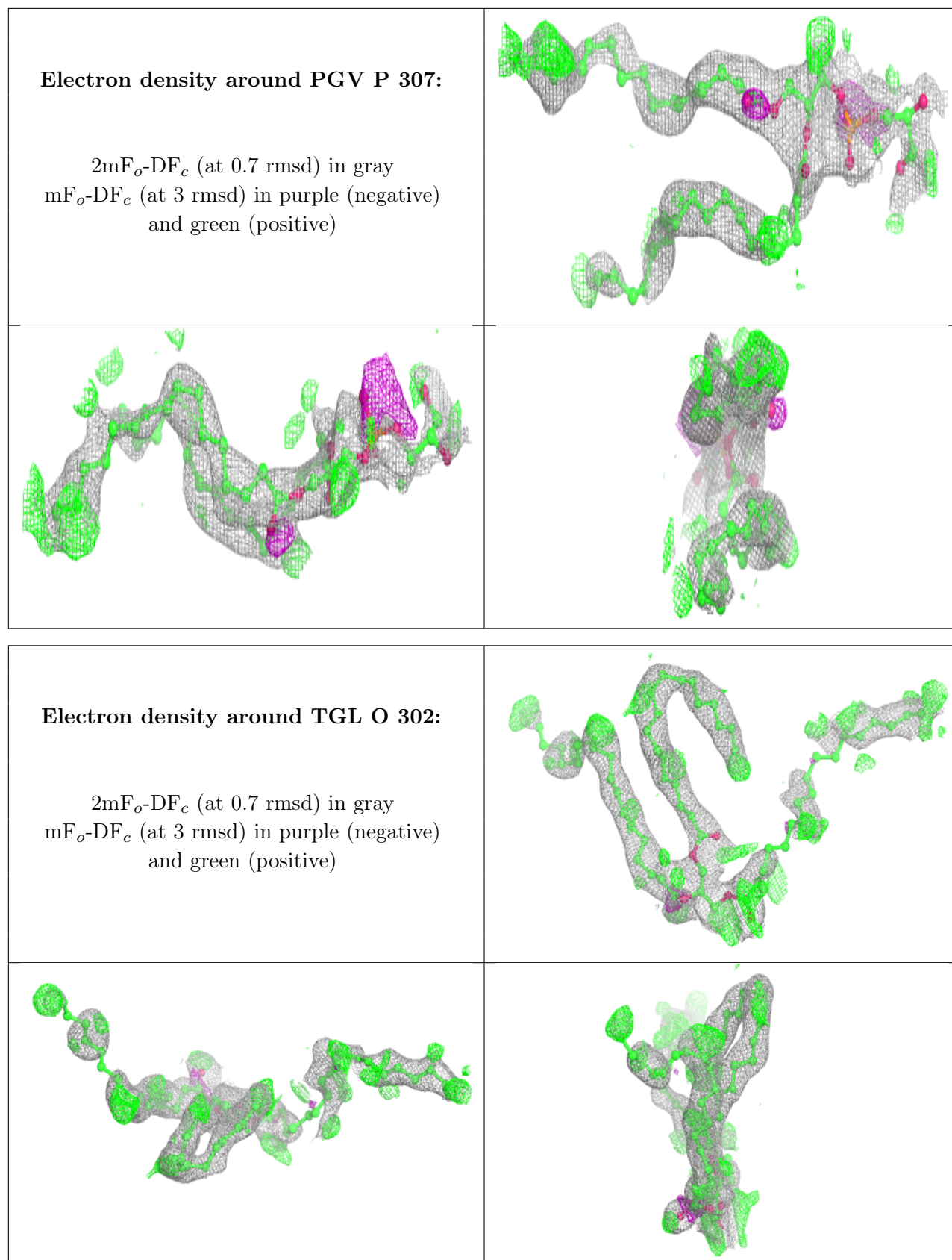


Electron density around PSC E 201:

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

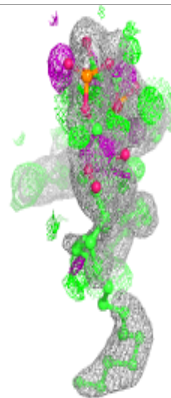
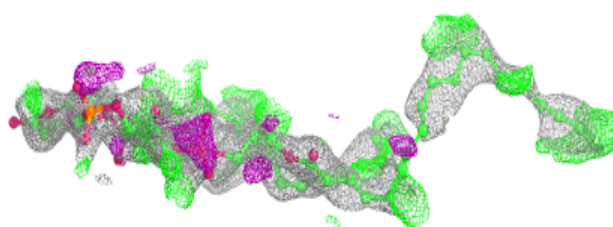
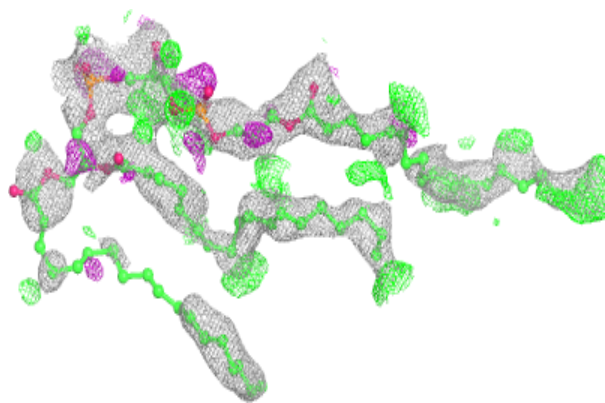




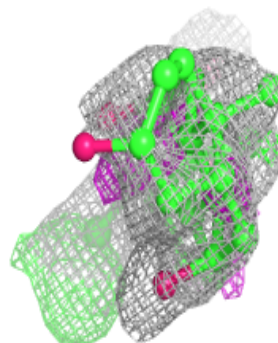
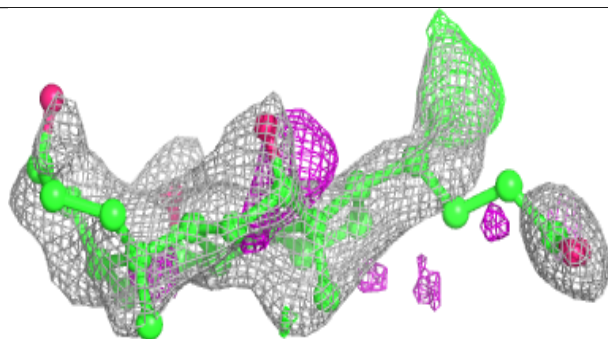
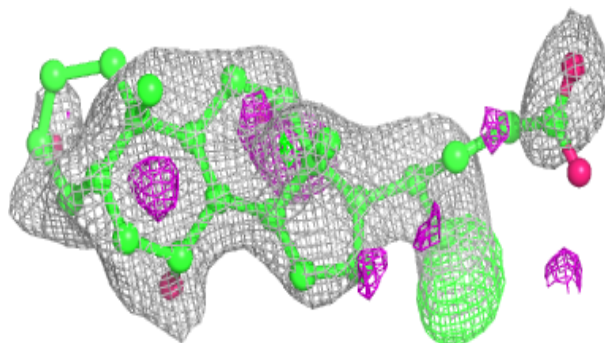


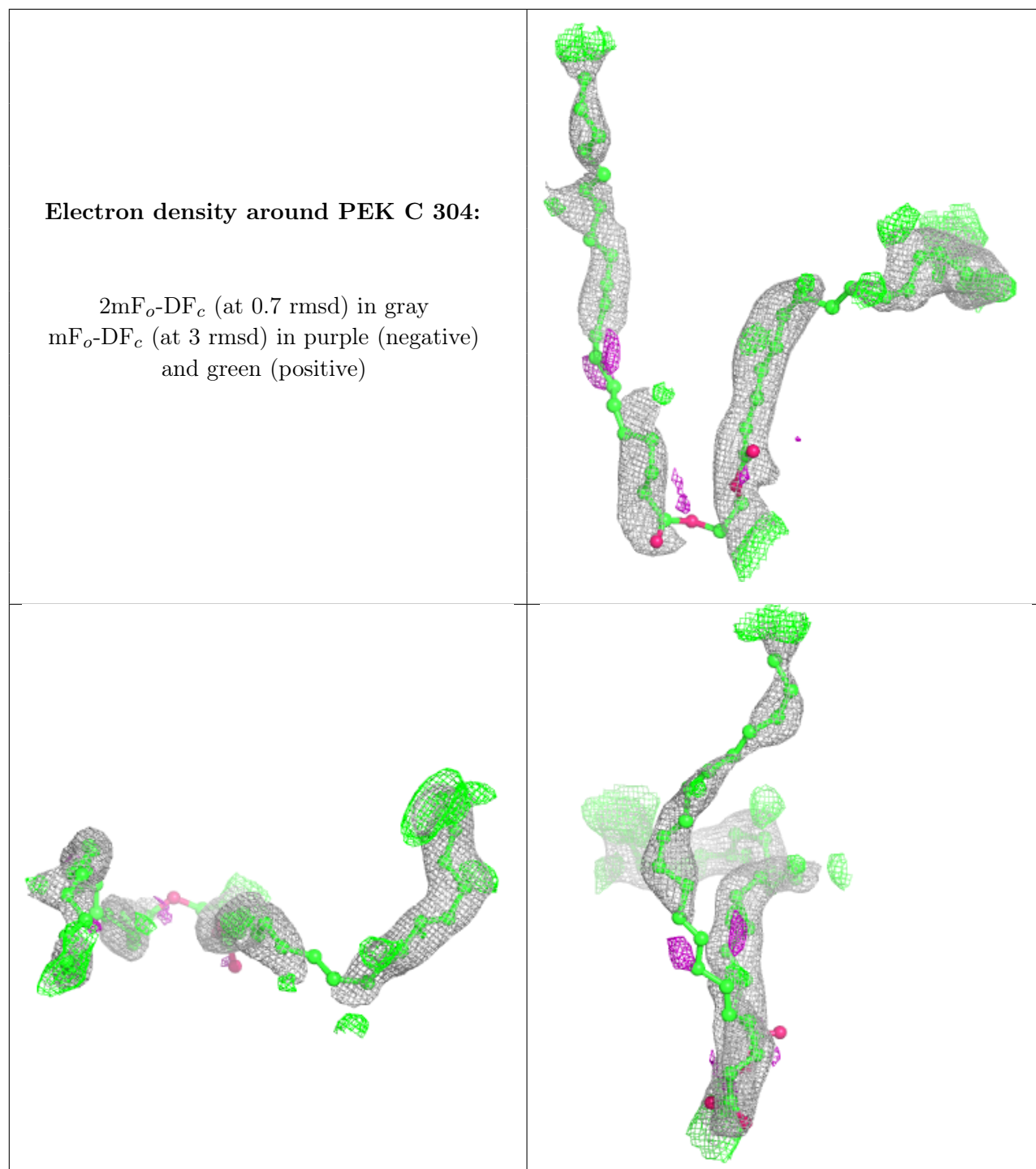
Electron density around CDL T 102:

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

**Electron density around CHD W 101:**

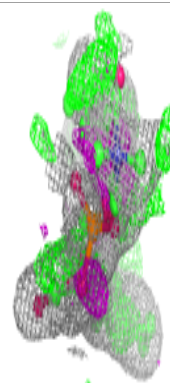
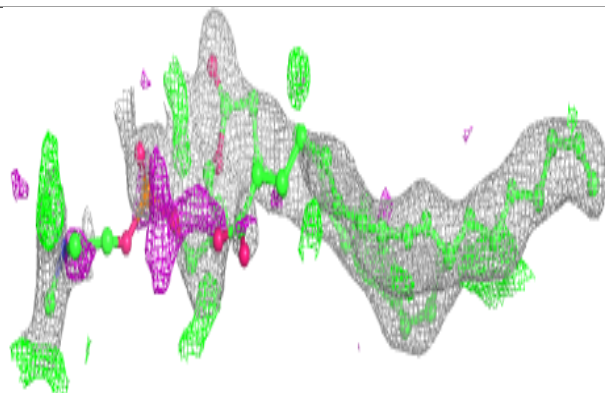
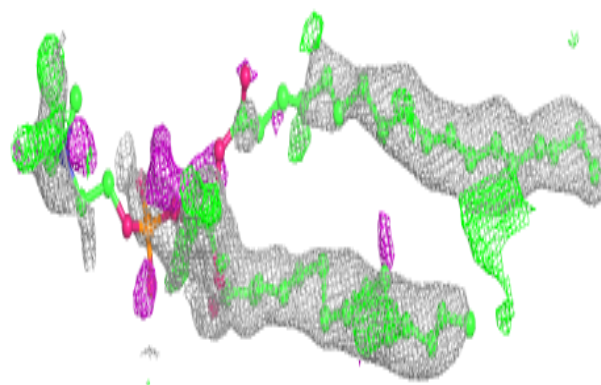
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





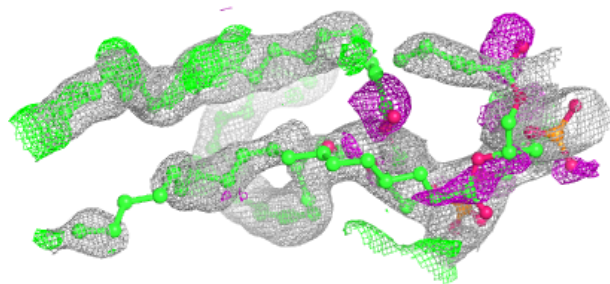
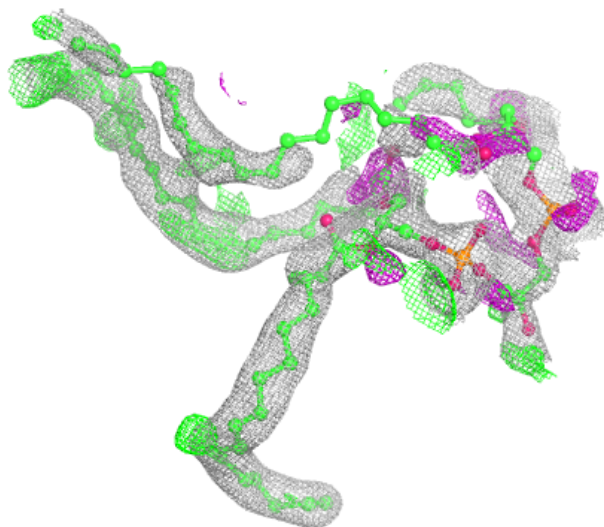
Electron density around PSC O 304:

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



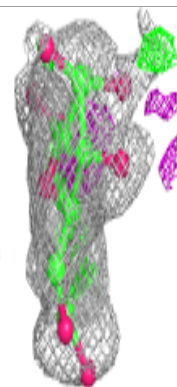
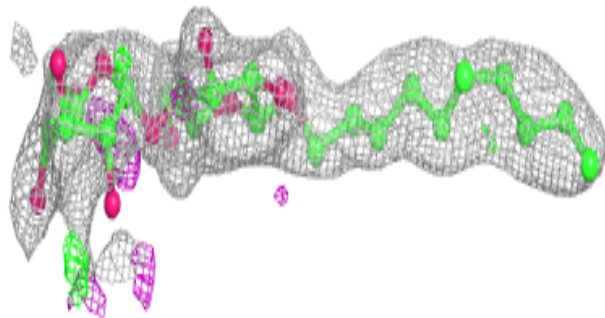
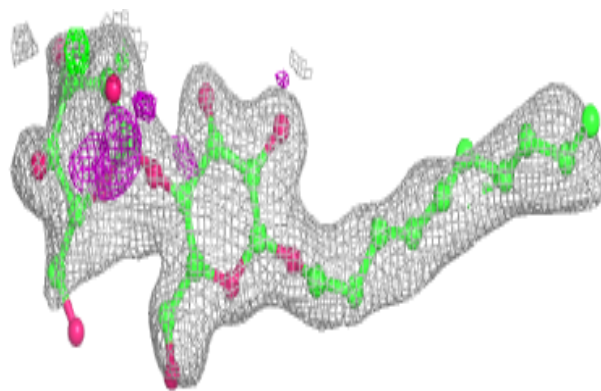
Electron density around CDL Y 101:

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

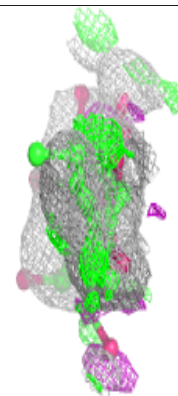
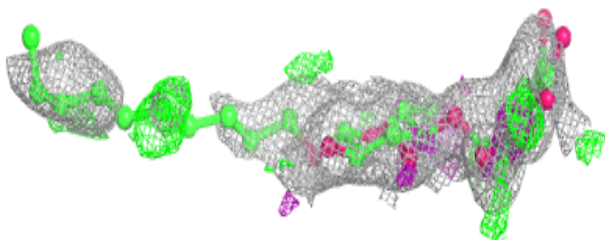
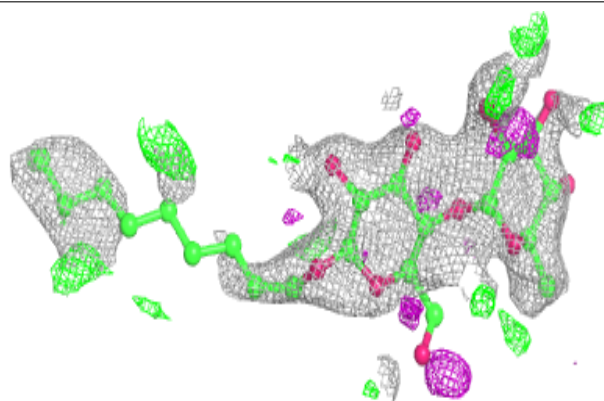


Electron density around DMU P 310:

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

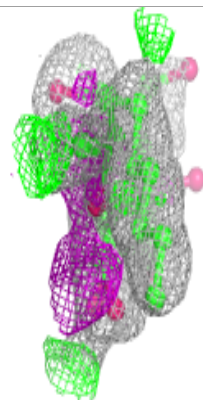
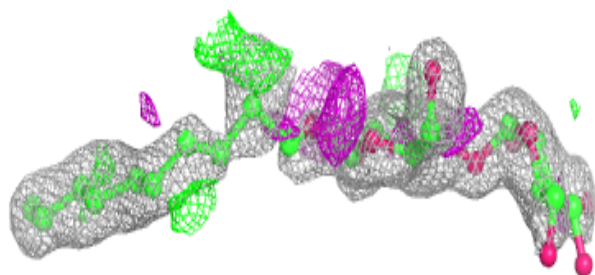
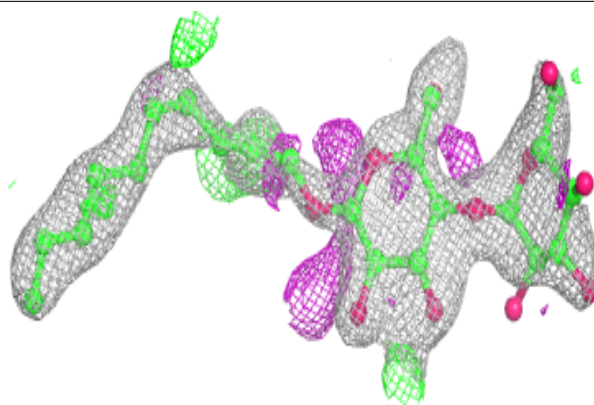
**Electron density around DMU P 311:**

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

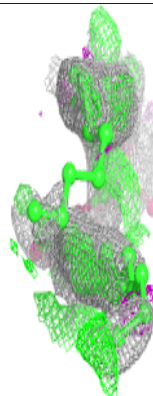
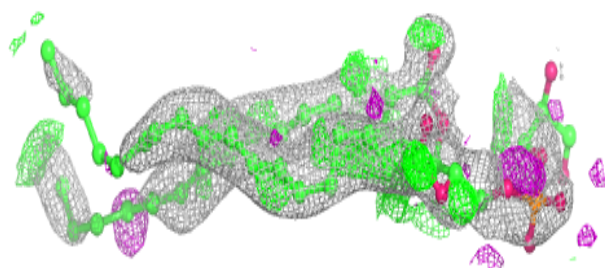
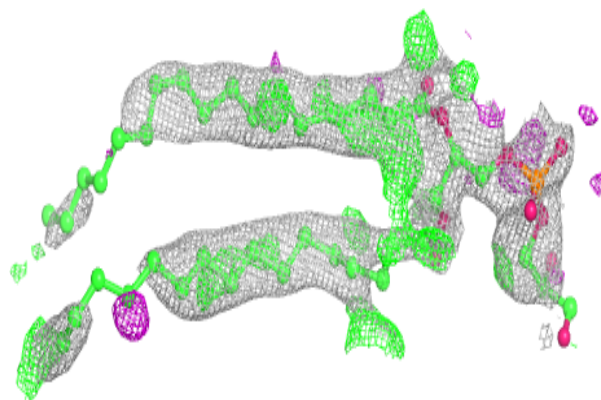


Electron density around DMU P 312:

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

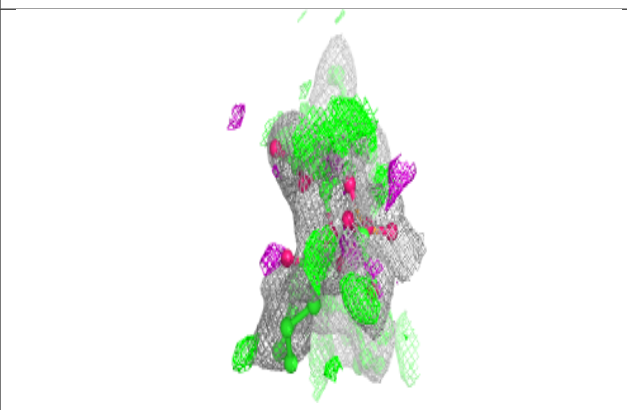
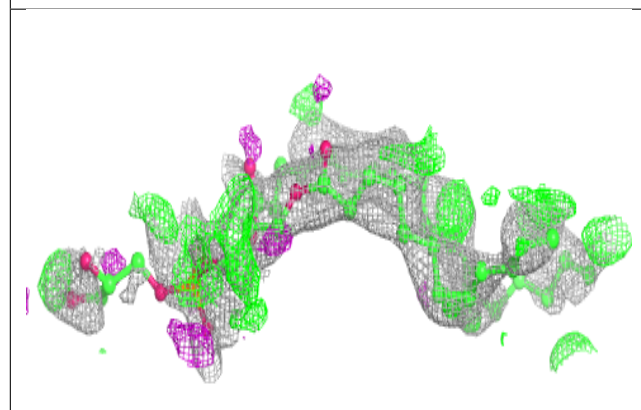
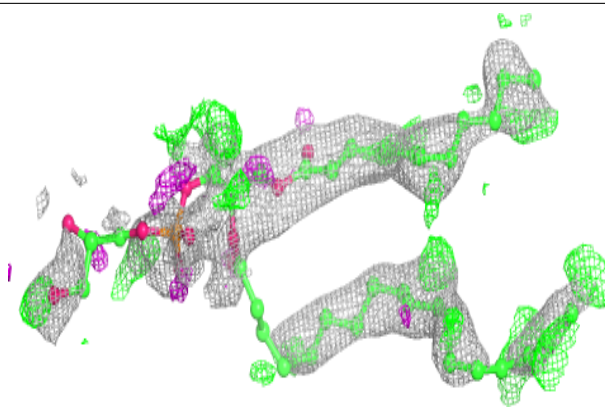
**Electron density around PGV Q 201:**

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

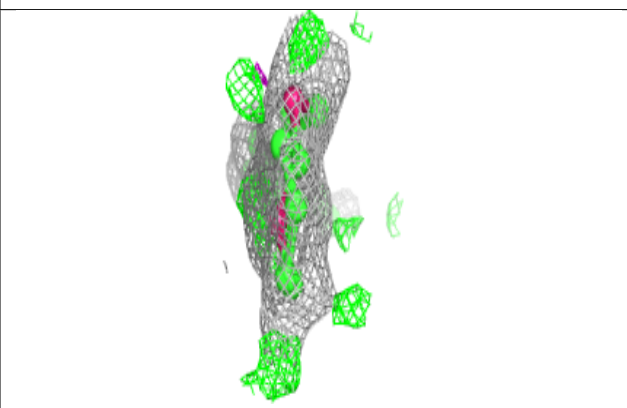
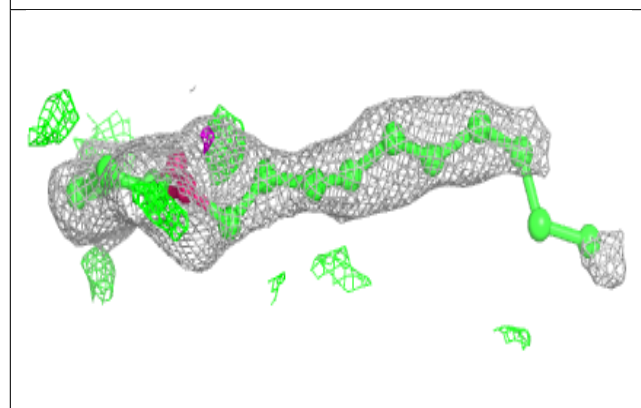
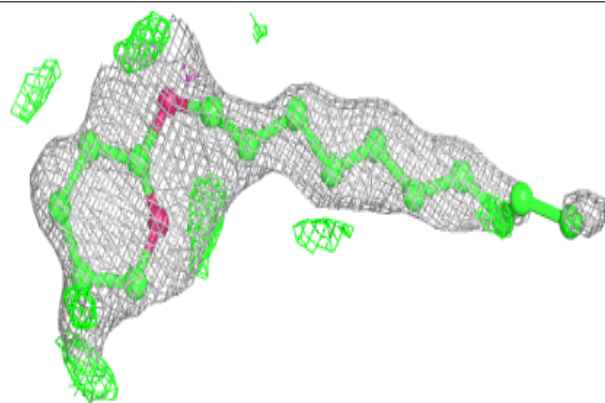


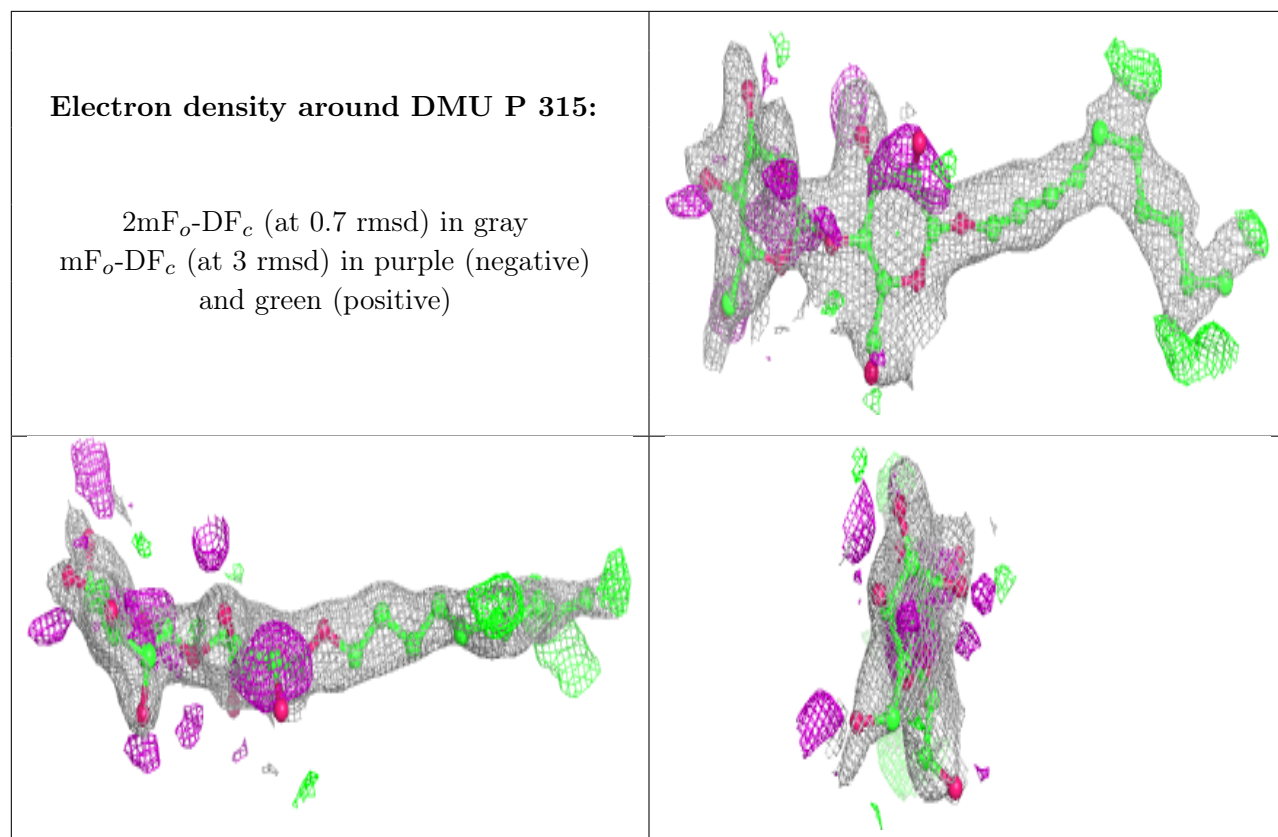
Electron density around PGV C 307:

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

**Electron density around DMU K 103:**

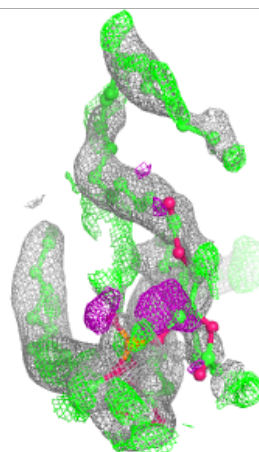
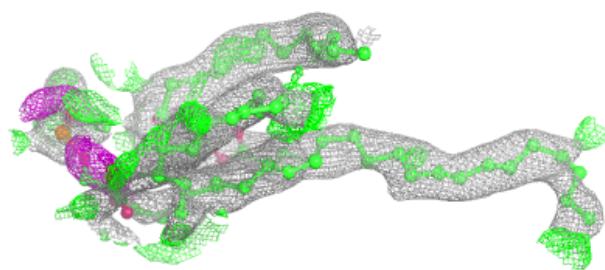
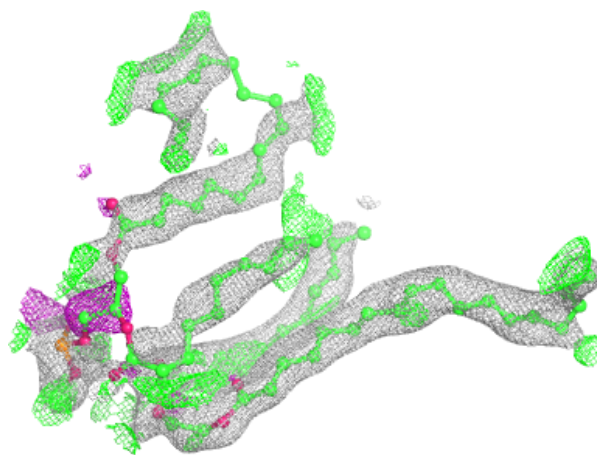
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

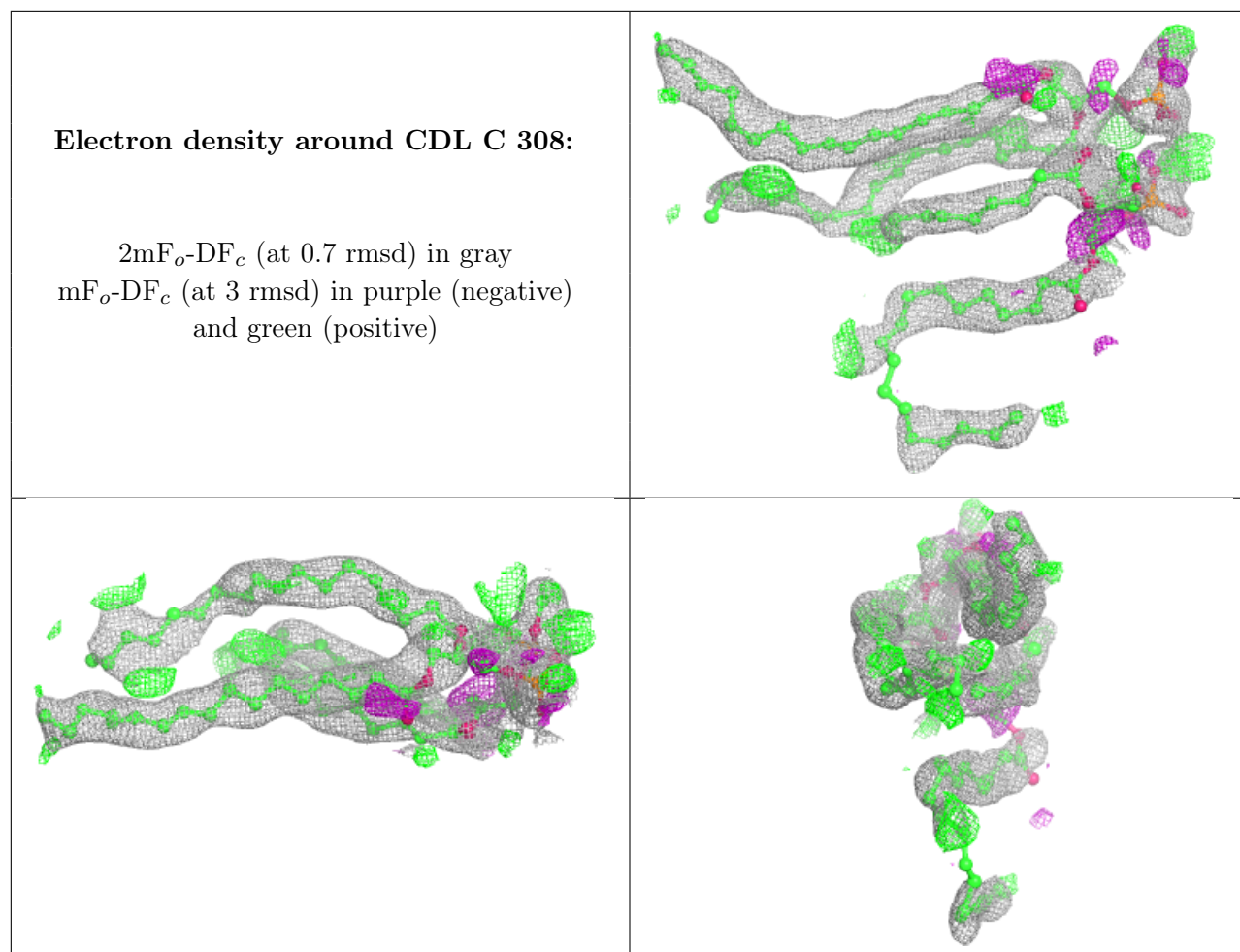


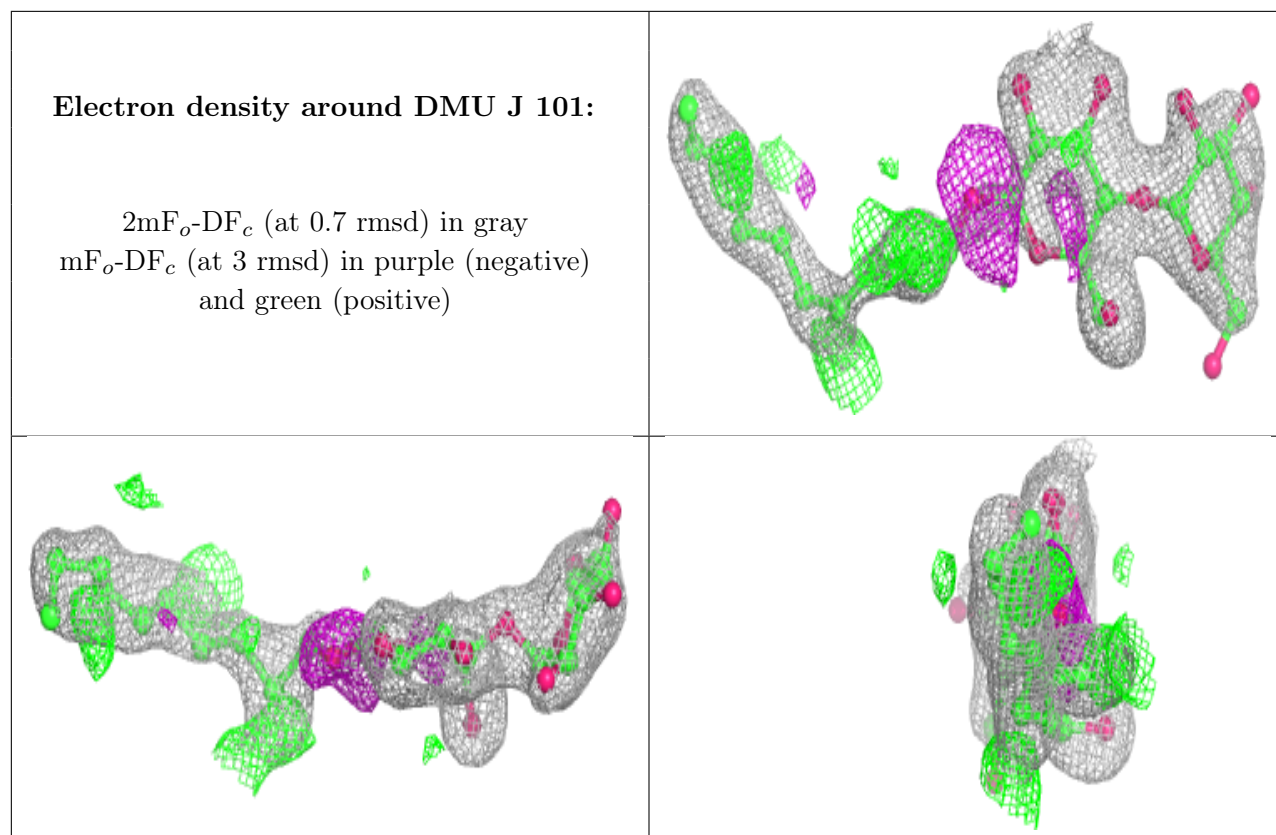


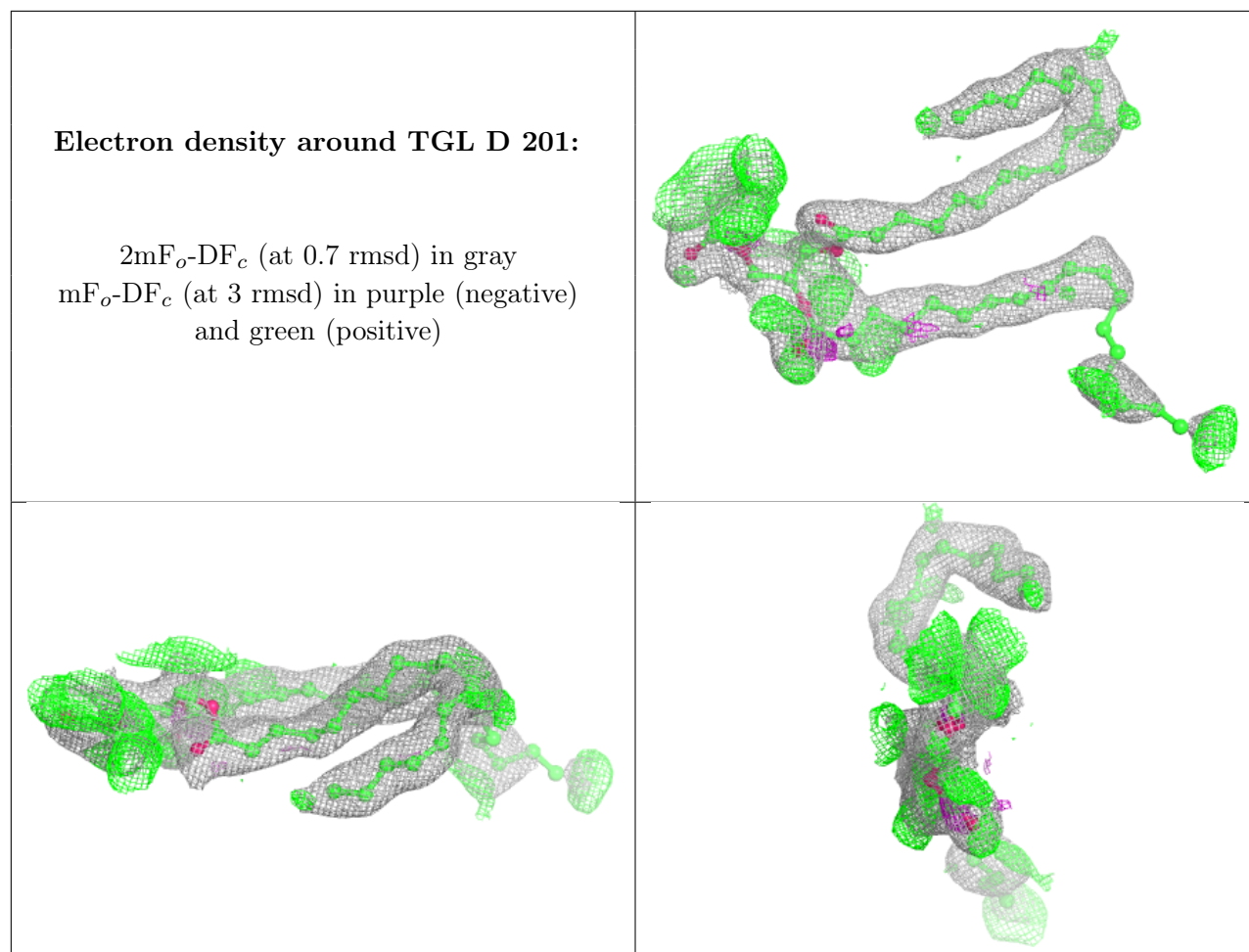
Electron density around CDL P 308:

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



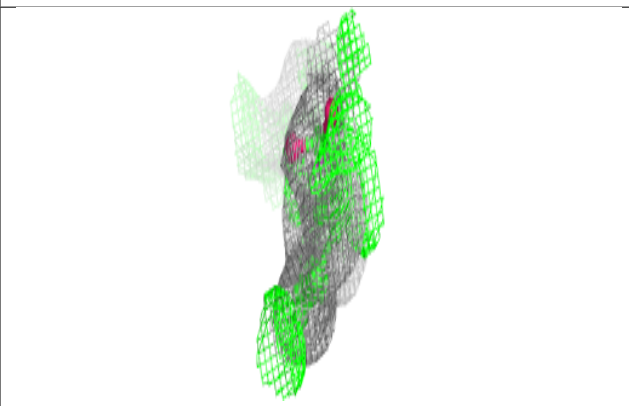
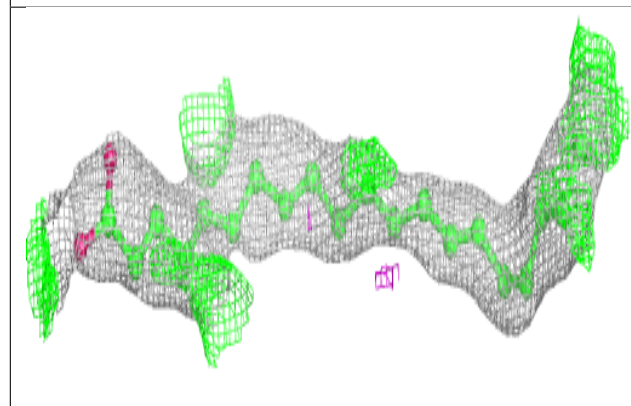
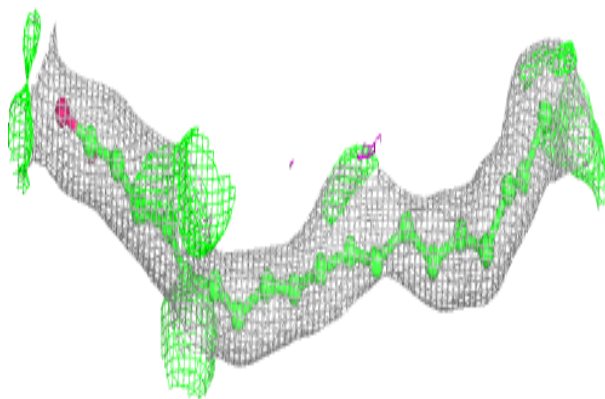




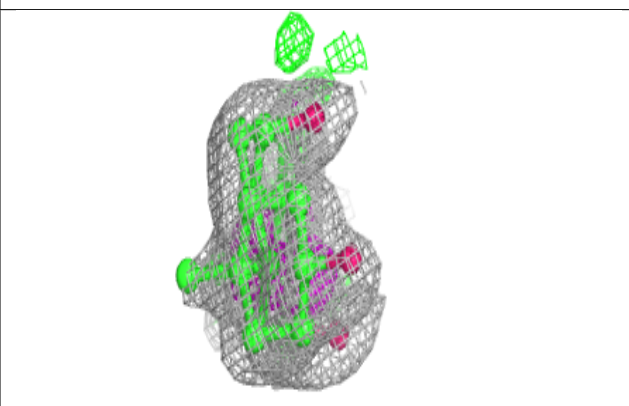
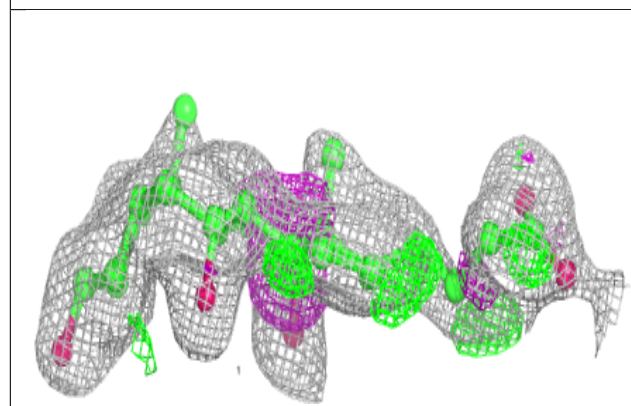
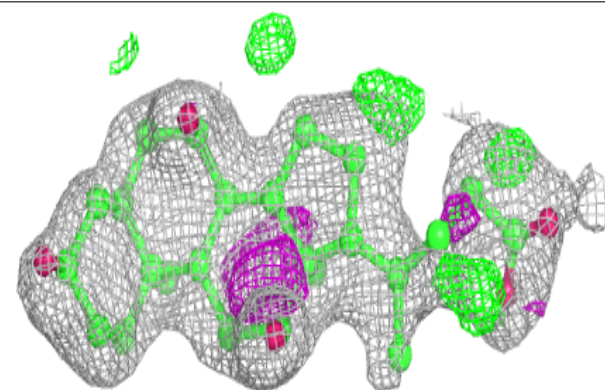


Electron density around PEK P 303:

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

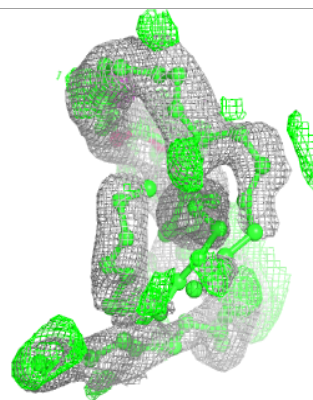
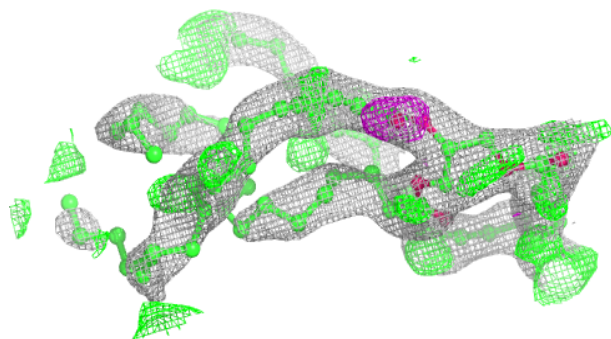
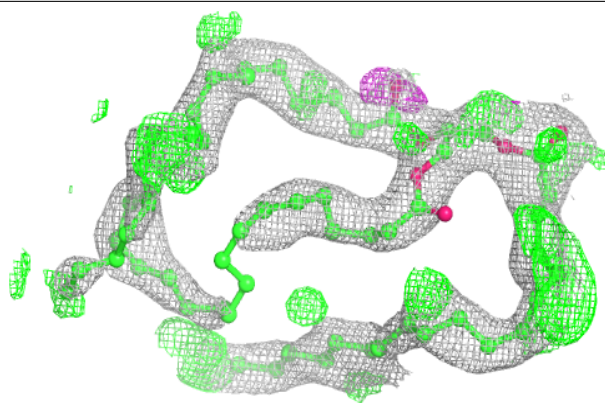
**Electron density around CHD P 309:**

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

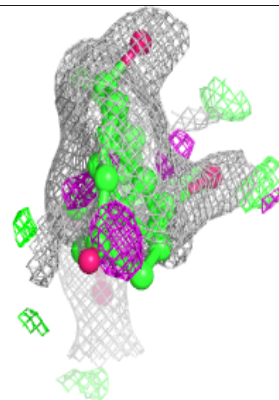
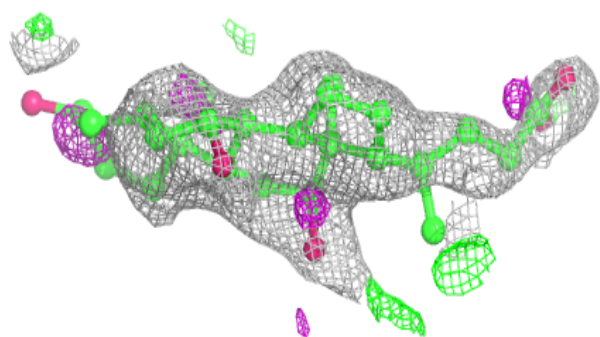
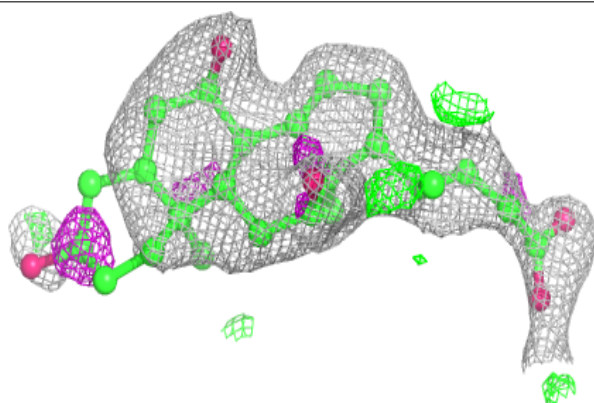


Electron density around TGL O 301:

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

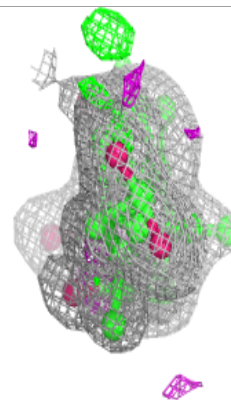
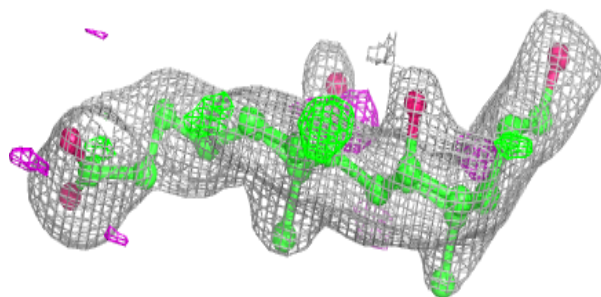
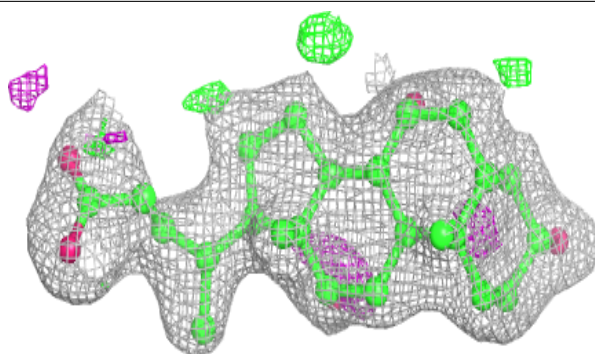
**Electron density around CHD J 102:**

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

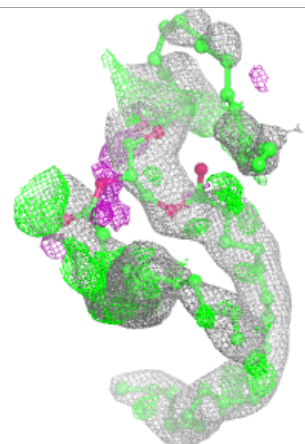
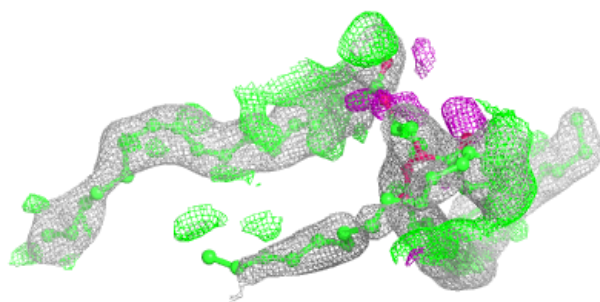
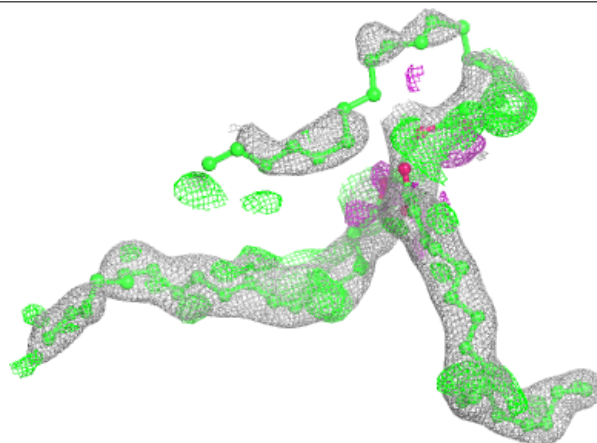


Electron density around CHD C 309:

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

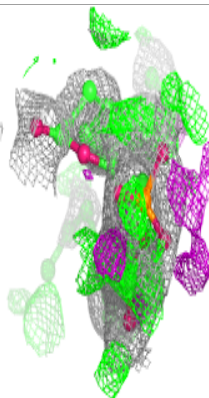
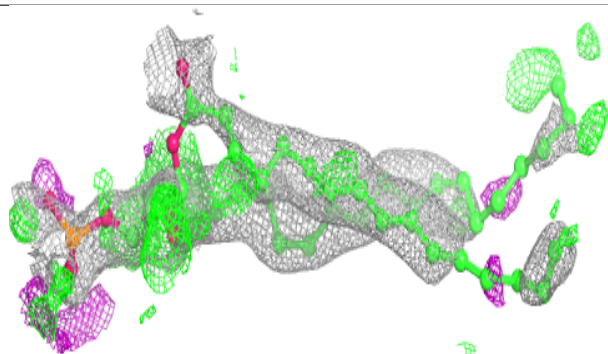
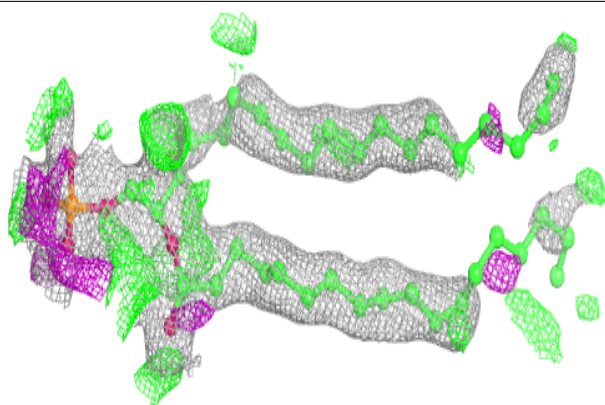
**Electron density around TGL A 607:**

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

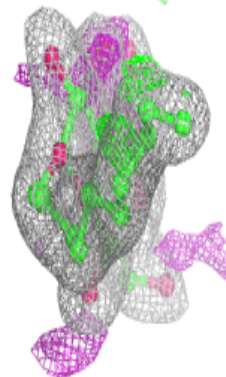
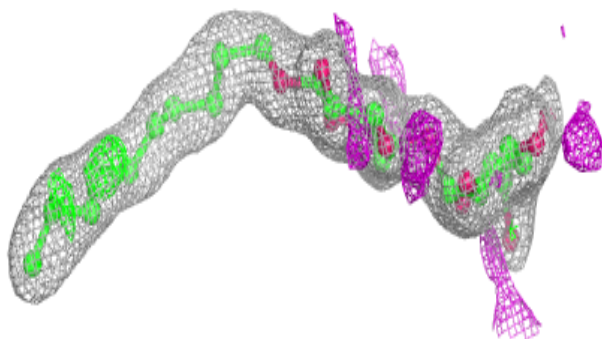
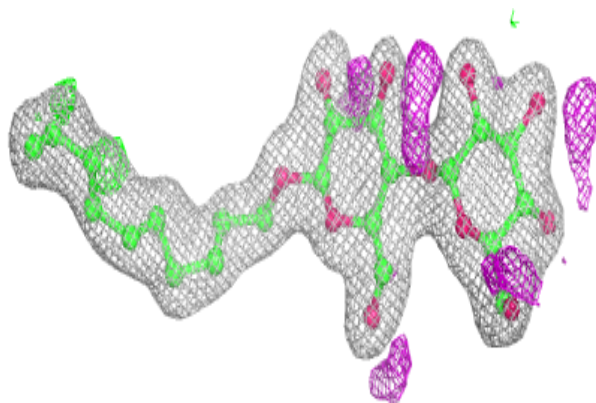


Electron density around PGV A 608:

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

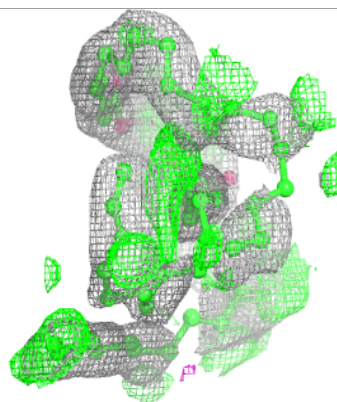
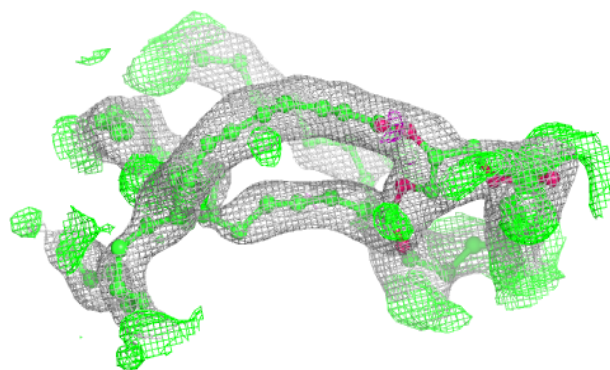
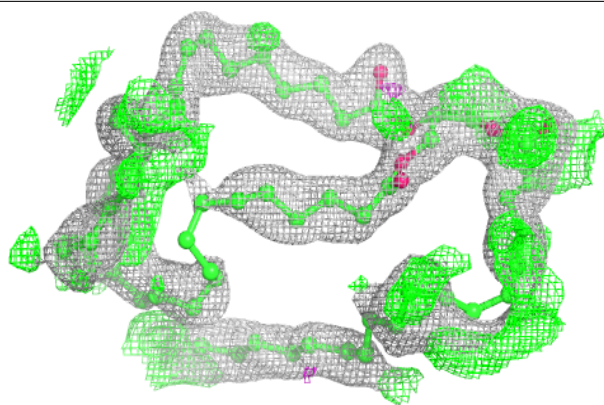
**Electron density around DMU Z 101:**

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

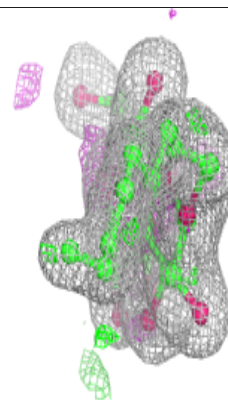
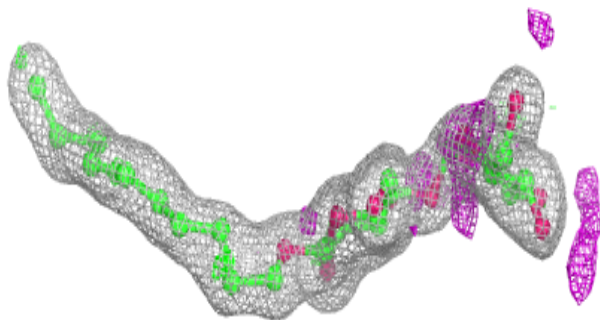
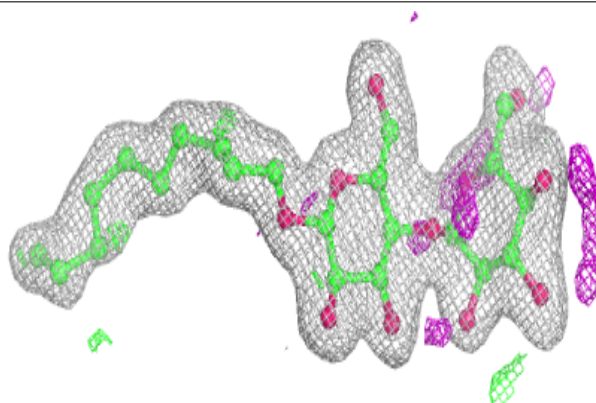


Electron density around TGL B 301:

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

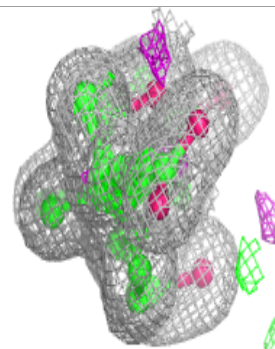
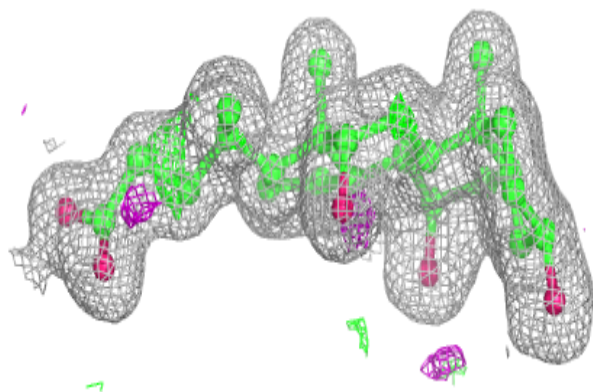
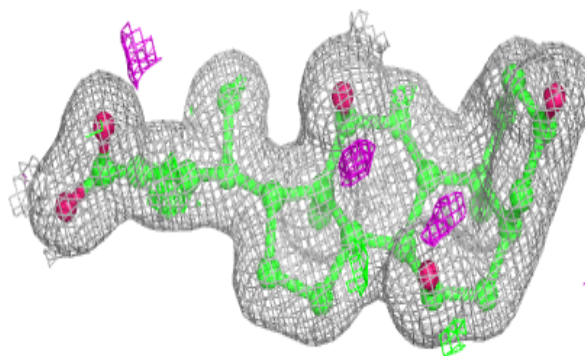
**Electron density around DMU M 101:**

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

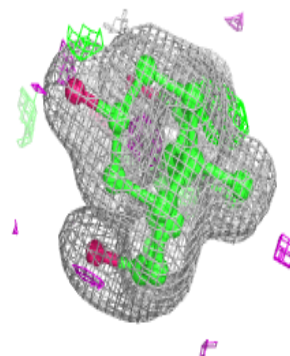
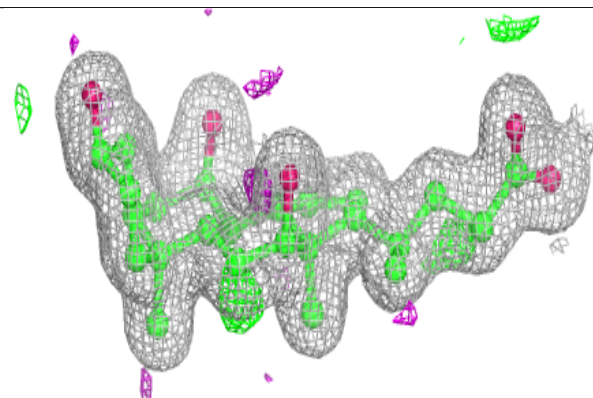
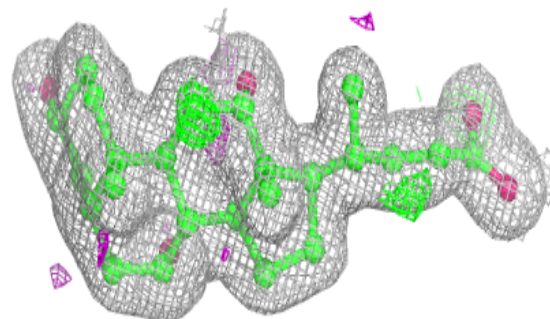


Electron density around CHD P 301:

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

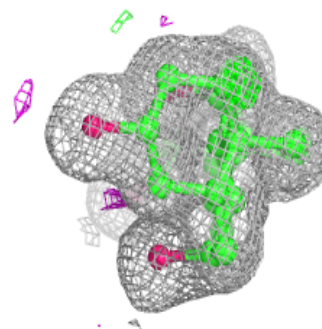
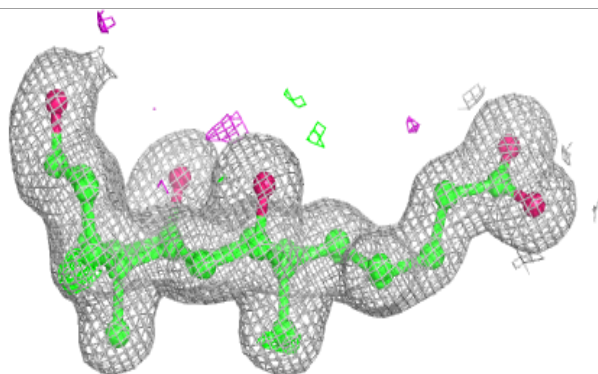
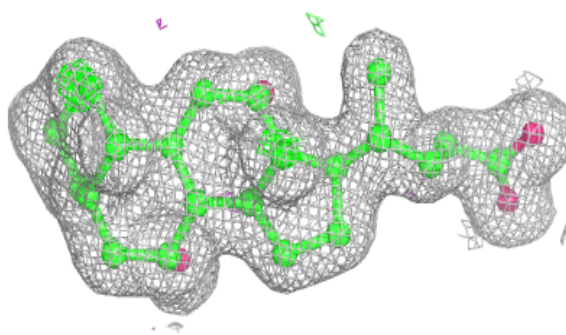
**Electron density around CHD C 301:**

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

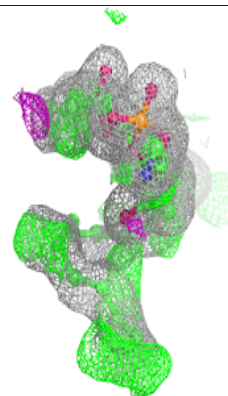
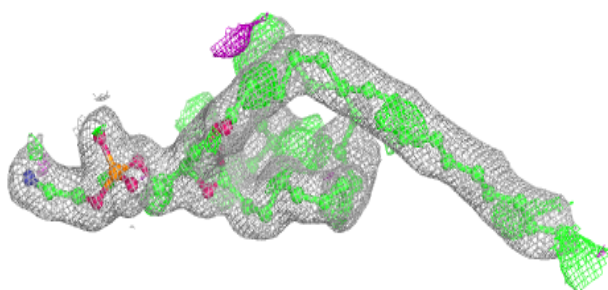
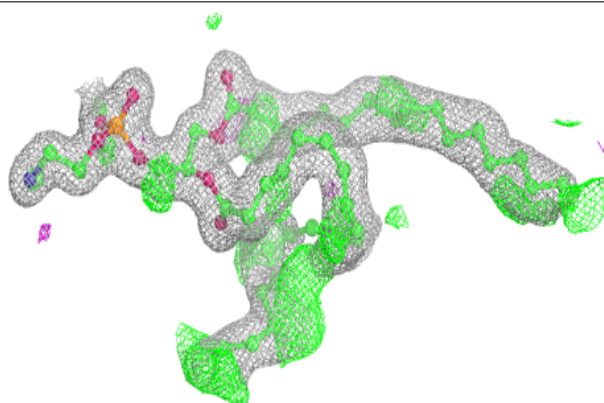


Electron density around CHD G 102:

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

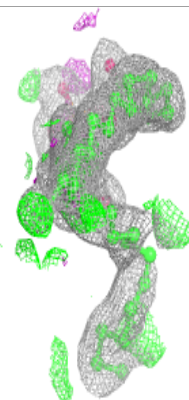
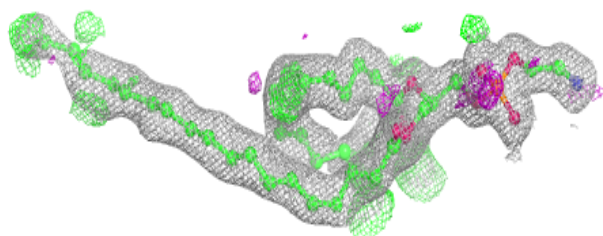
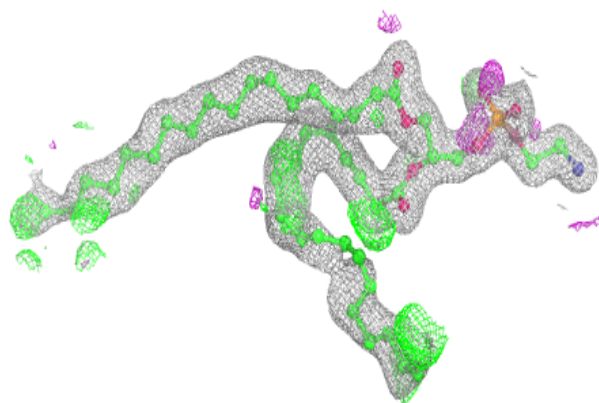
**Electron density around PEK C 303:**

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

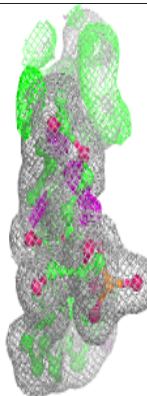
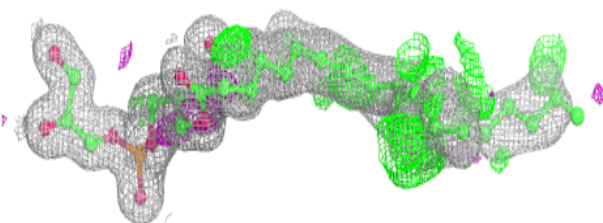
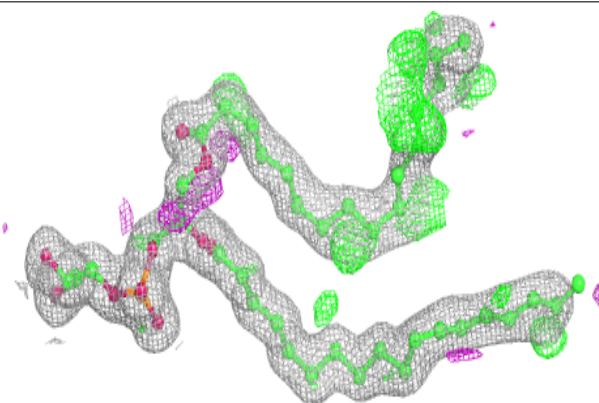


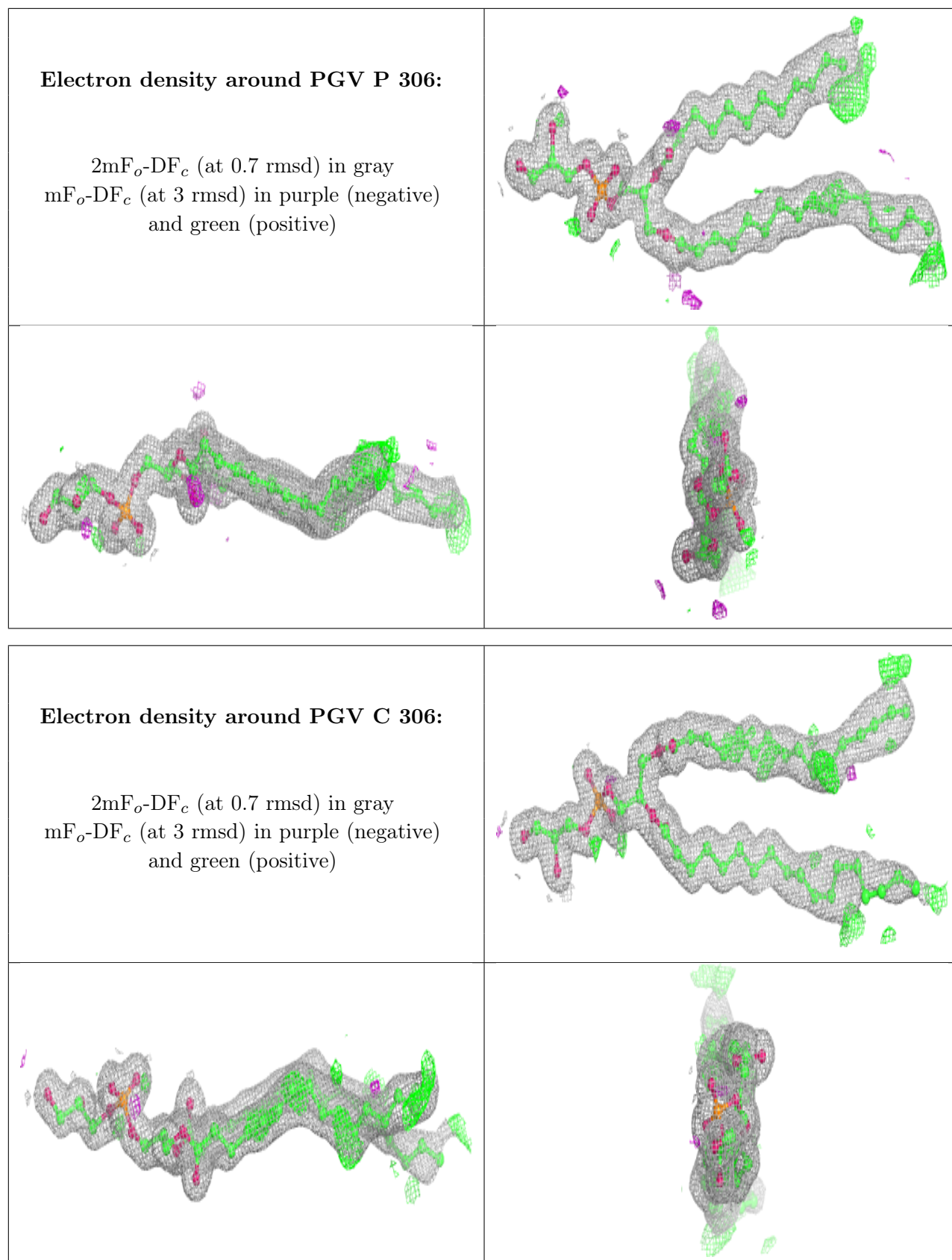
Electron density around PEK P 304:

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

**Electron density around PGV N 607:**

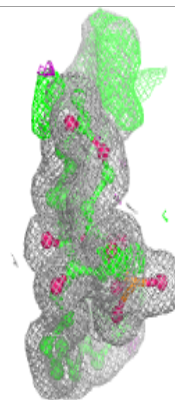
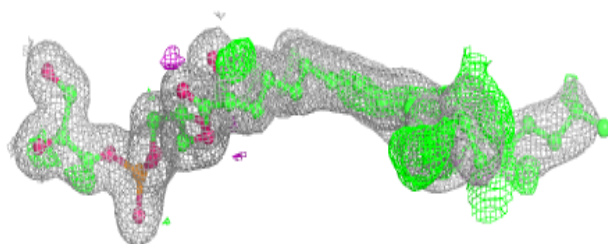
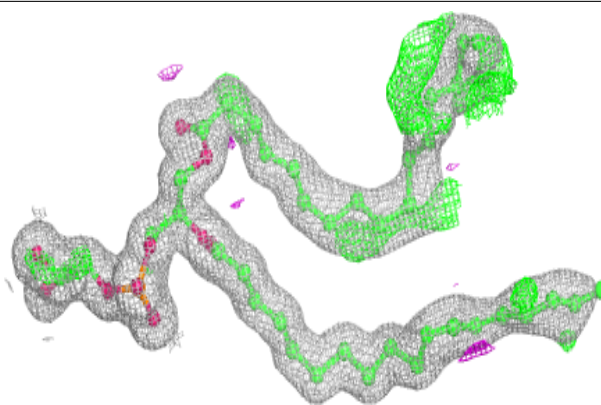
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



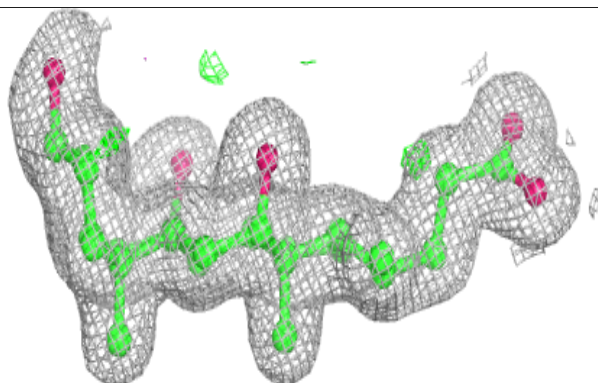
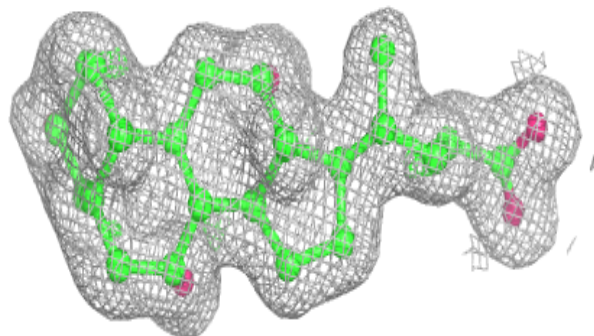


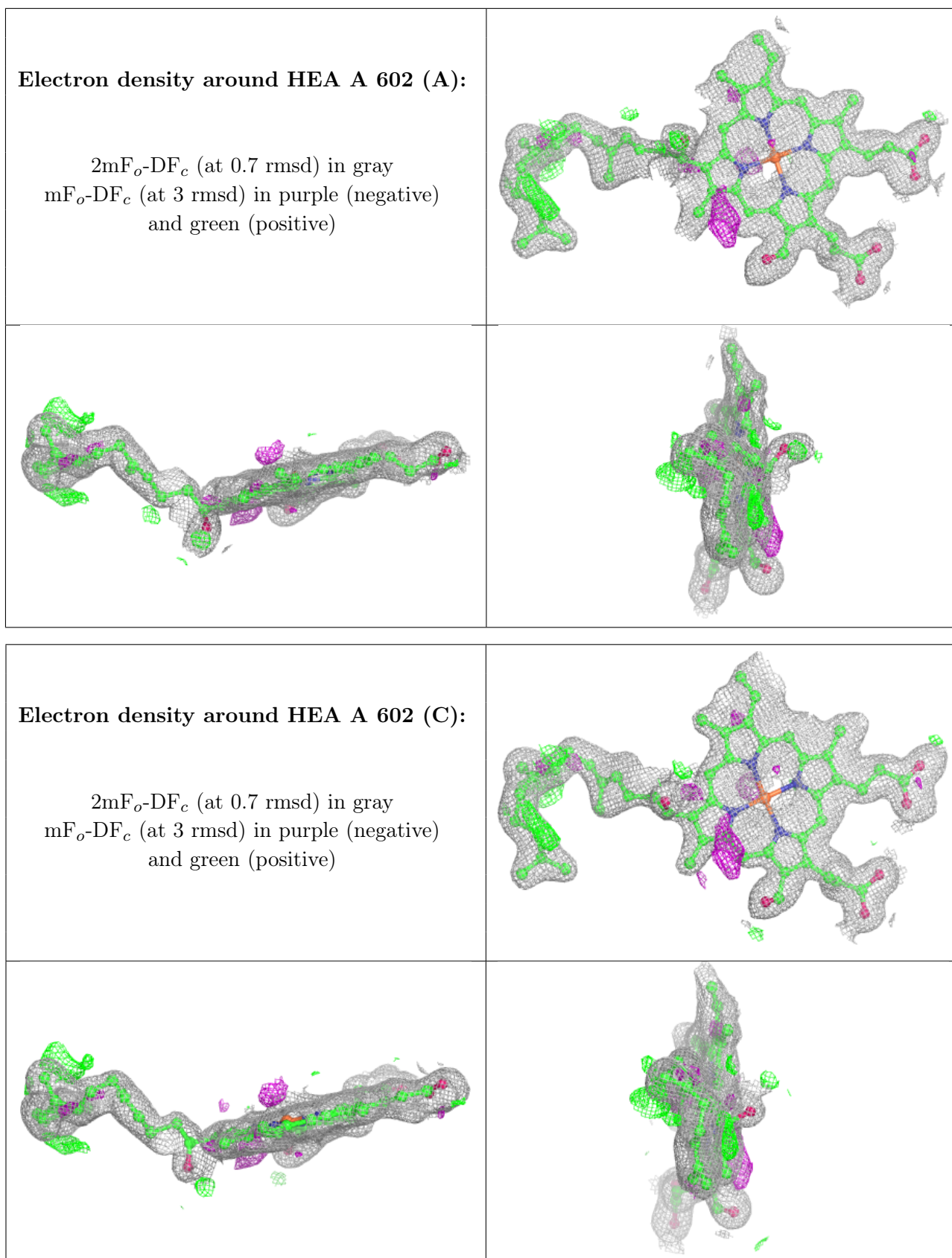
Electron density around PGV C 305:

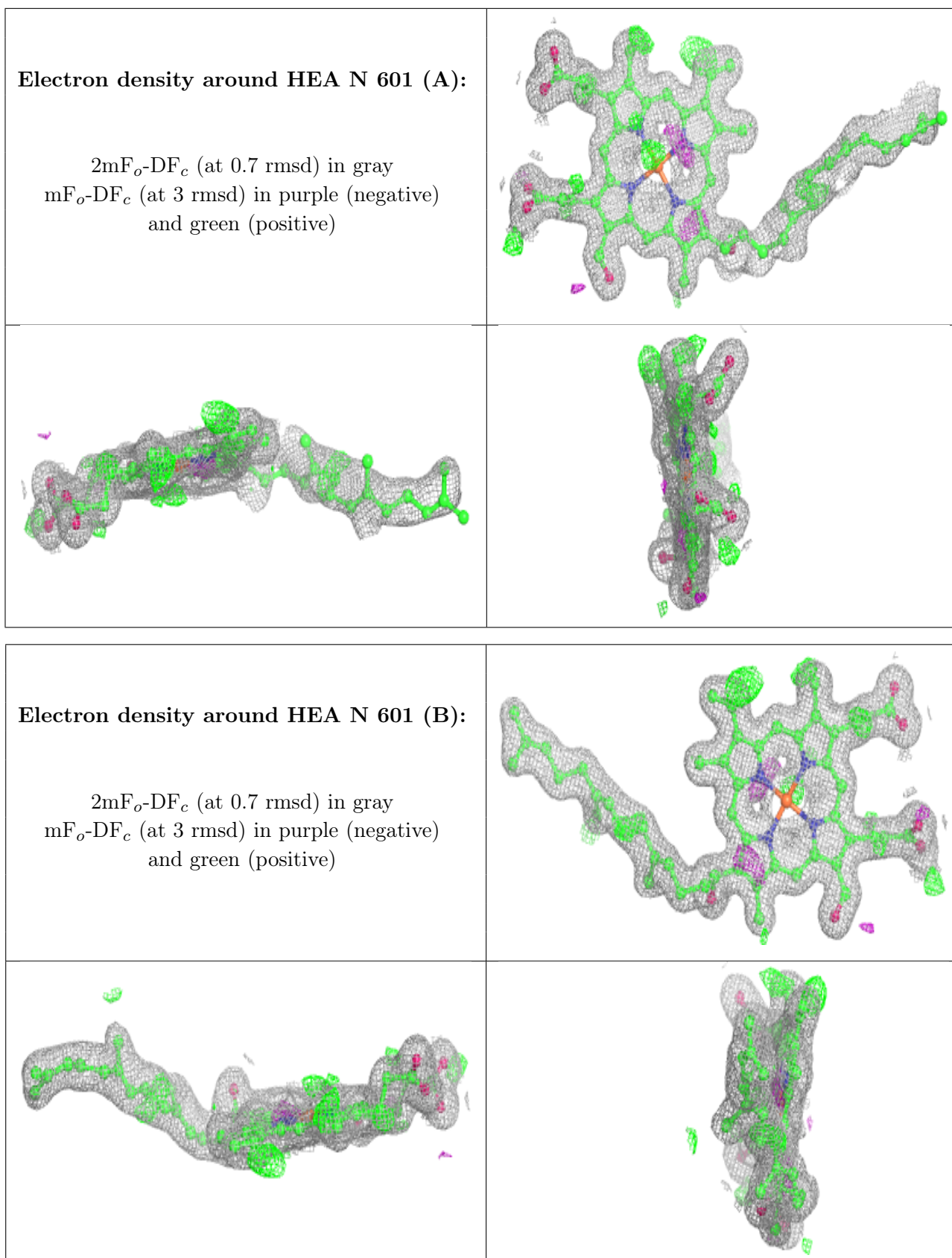
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

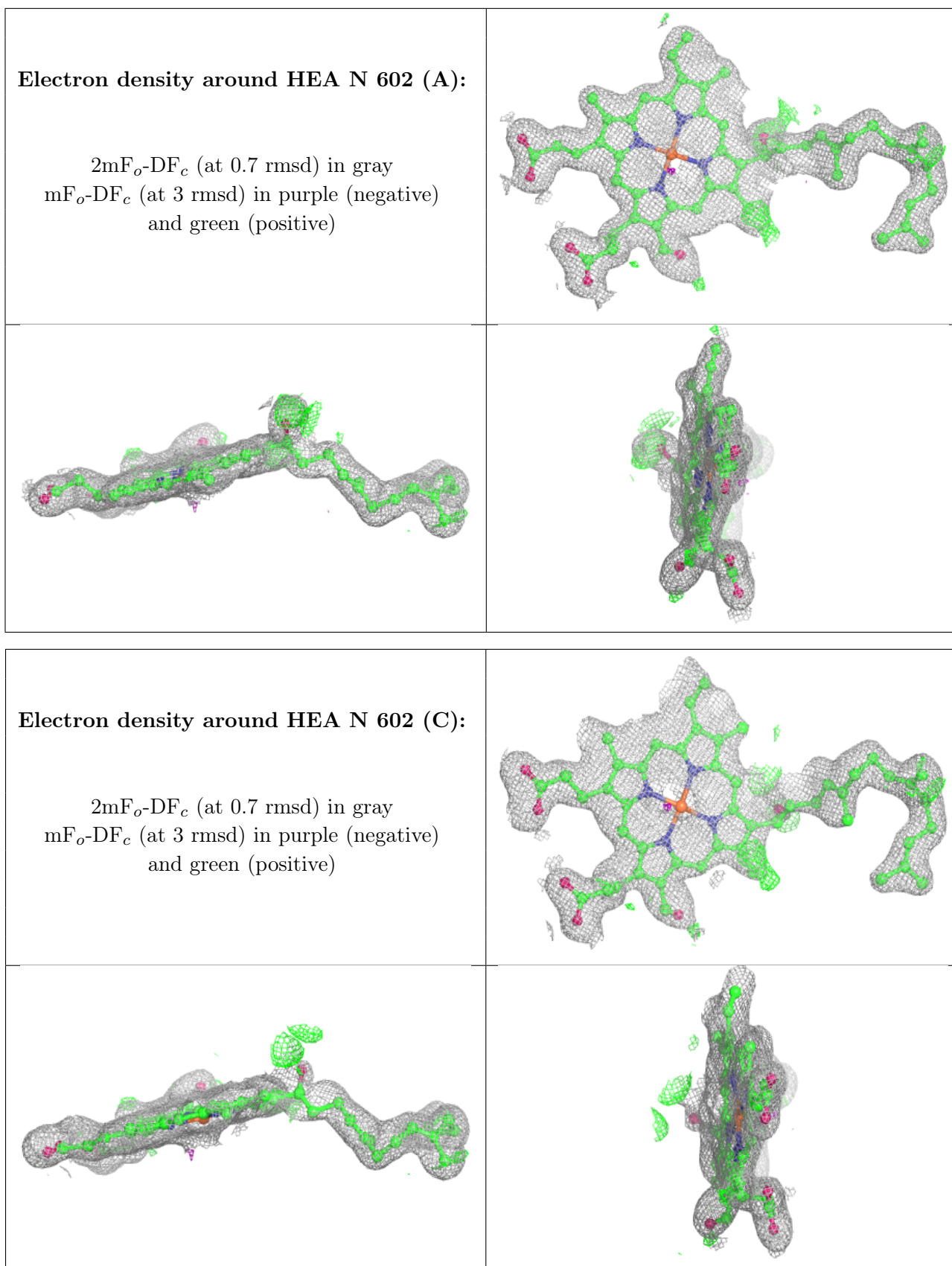
**Electron density around CHD B 303:**

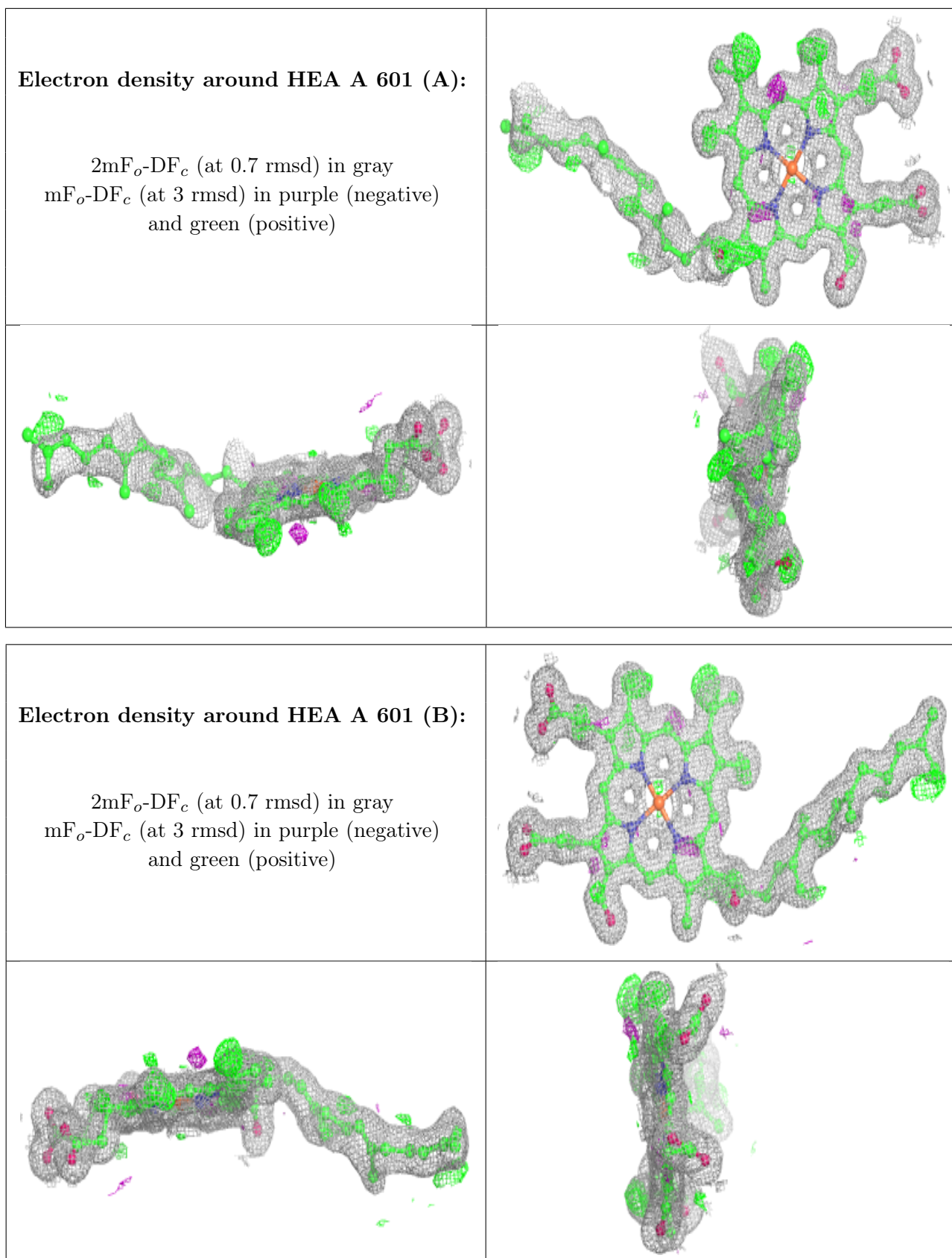
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)











6.5 Other polymers [i](#)

There are no such residues in this entry.