



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2019 – 03:00 PM EDT

PDB ID : 5H2F
Title : Crystal structure of the PsbM-deletion mutant of photosystem II
Authors : Uto, S.; Kawakami, K.; Umena, Y.; Iwai, M.; Ikeuchi, M.; Shen, J.R.; Kamiya, N.
Deposited on : 2016-10-15
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

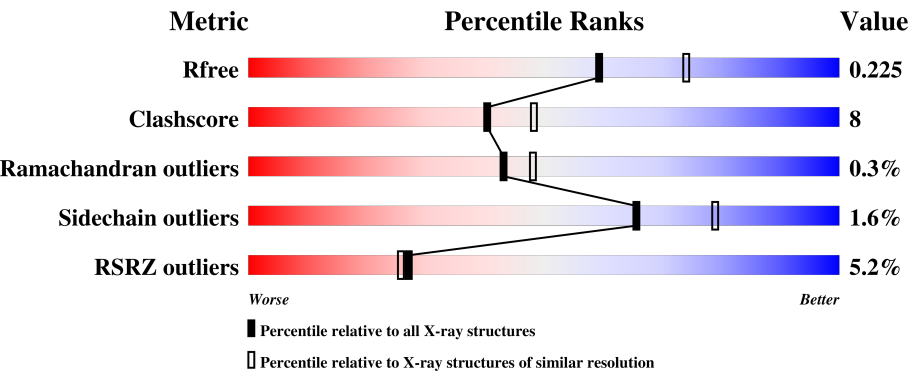
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.4
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

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 2.20 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.



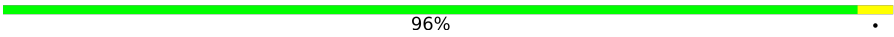

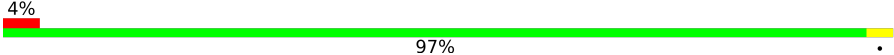

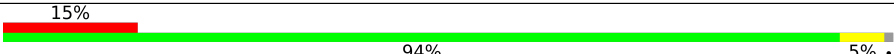
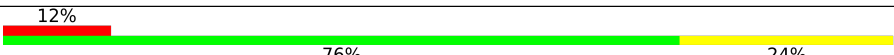
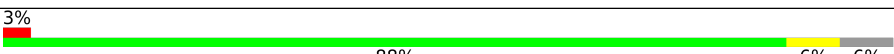
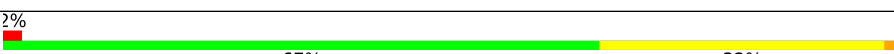
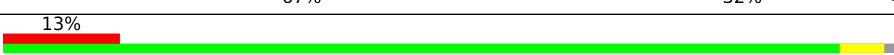
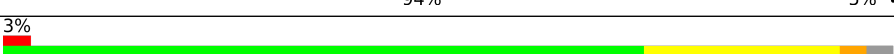
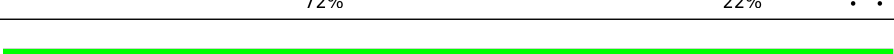
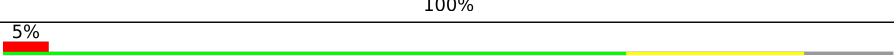

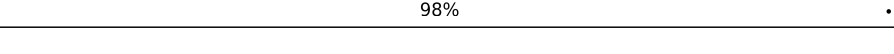
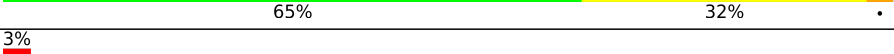
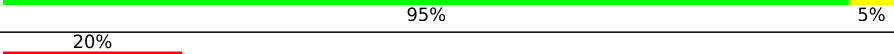

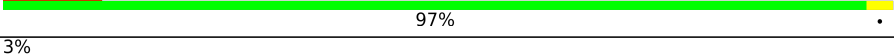

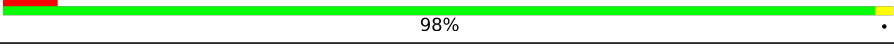
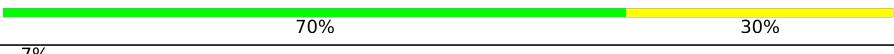
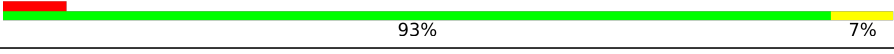
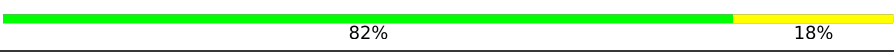
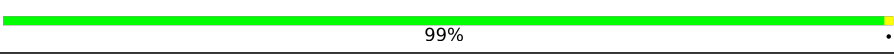

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	334	<div><div>4%</div><div>83%16%</div><div></div></div>
1	a	334	<div><div>10%</div><div>98%</div><div></div></div>
2	B	505	<div><div>7%</div><div>78%21%</div><div></div></div>
2	b	505	<div><div>4%</div><div>94%</div><div></div></div>
3	C	455	<div><div>3%</div><div>80%18%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	c	455	 96% .
4	D	342	 78% 21% .
4	d	342	 97% .
5	E	80	 13% 75% 23% ..
5	e	80	 15% 94% 5% .
6	F	33	 12% 76% 24%
6	f	33	 3% 88% 6% 6%
7	H	63	 2% 67% 32% .
7	h	63	 13% 94% 5% .
8	I	36	 3% 72% 22% . .
8	i	36	 100%
9	J	40	 5% 70% 20% 10%
9	j	40	 15% 98% .
10	K	37	 65% 32% .
10	k	37	 3% 95% 5%
11	L	35	 20% 86% 14%
11	l	35	 11% 97% .
12	O	243	 3% 78% 21%
12	o	243	 6% 98% .
13	T	30	 70% 30%
13	t	30	 7% 93% 7%
14	U	97	 82% 18%
14	u	97	 99% .
15	V	137	 84% 15% .
15	v	137	 2% 97% ..

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Mol	Chain	Length	Quality of chain
16	Y	29	
16	y	29	
17	X	37	
17	x	37	
18	Z	62	
18	z	62	

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
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	408	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	B	617	X	-	-	-
22	CLA	C	502	X	-	-	-
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	D	401	X	-	-	-
22	CLA	D	403	X	-	-	-
22	CLA	D	404	X	-	-	-
22	CLA	a	407	X	-	-	-
22	CLA	a	408	X	-	-	-
22	CLA	a	409	X	-	-	-
22	CLA	b	602	X	-	-	-
22	CLA	b	603	X	-	-	-
22	CLA	b	604	X	-	-	-
22	CLA	b	605	X	-	-	-
22	CLA	b	606	X	-	-	-
22	CLA	b	607	X	-	-	-
22	CLA	b	608	X	-	-	-
22	CLA	b	609	X	-	-	-
22	CLA	b	610	X	-	-	-
22	CLA	b	611	X	-	-	-
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22	CLA	b	613	X	-	-	-
22	CLA	b	614	X	-	-	-
22	CLA	b	615	X	-	-	-
22	CLA	b	616	X	-	-	-
22	CLA	b	617	X	-	-	-
22	CLA	c	902	X	-	-	-
22	CLA	c	903	X	-	-	-
22	CLA	c	904	X	-	-	-
22	CLA	c	905	X	-	-	-
22	CLA	c	906	X	-	-	-
22	CLA	c	907	X	-	-	-
22	CLA	c	908	X	-	-	-
22	CLA	c	909	X	-	-	-
22	CLA	c	910	X	-	-	-
22	CLA	c	911	X	-	-	-
22	CLA	c	912	X	-	-	-
22	CLA	c	913	X	-	-	-
22	CLA	c	914	X	-	-	-
22	CLA	d	402	X	-	-	-
22	CLA	d	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LMT	f	102	-	-	-	X
30	UNL	a	417	-	-	-	X
31	DMS	B	638	-	-	X	-
31	DMS	B	639	-	-	-	X
31	DMS	O	304	-	-	X	-
31	DMS	O	310	-	-	X	-
31	DMS	V	212	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 51892 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 Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2598	1706	428	449	15			
1	a	334	Total	C	N	O	S	0	1	0
			2555	1675	427	438	15			

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	3	0
			3950	2596	661	680	13			
2	b	483	Total	C	N	O	S	0	1	0
			3780	2484	631	652	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	0	0
			3470	2274	580	603	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	3	0
			2732	1814	442	464	12			
4	d	341	Total	C	N	O	S	0	2	0
			2717	1805	441	459	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	79	Total	C	N	O	0	0	0
			635	417	101	117			
5	e	79	Total	C	N	O	0	0	0
			636	418	101	117			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			269	184	44	40	1			
6	f	31	Total	C	N	O	S	0	0	0
			250	170	42	37	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	3	0
			522	347	87	86	2			
7	h	62	Total	C	N	O	S	0	1	0
			501	335	82	82	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			288	196	45	46	1			
8	i	36	Total	C	N	O	S	0	0	0
			293	199	46	47	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			277	186	41	49	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			286	198	42	46			

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	35	Total	C	N	O	0	0	0
			287	192	46	49			
11	l	35	Total	C	N	O	0	0	0
			287	192	46	49			

- Molecule 12 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	O	243	Total	C	N	O	S	0	1	0
			1853	1160	311	378	4			
12	o	243	Total	C	N	O	S	0	0	0
			1833	1149	305	375	4			

- Molecule 13 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	T	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			
13	t	30	Total	C	N	O	S	0	0	0
			253	177	36	38	2			

- Molecule 14 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	U	97	Total	C	N	O	0	1	0
			782	496	132	154			
14	u	97	Total	C	N	O	0	0	0
			766	487	129	150			

- Molecule 15 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	V	137	Total	C	N	O	S	0	1	0
			1066	677	177	208	4			
15	v	137	Total	C	N	O	S	0	1	0
			1058	671	175	208	4			

- Molecule 16 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
16	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

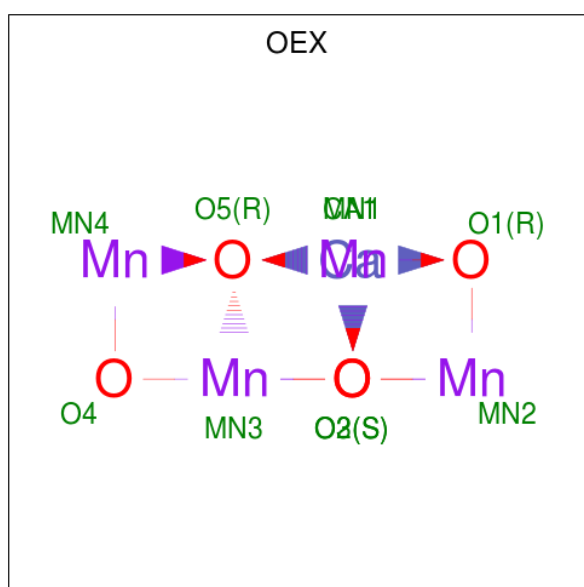
- Molecule 17 is a protein called Photosystem II reaction center X protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	37	Total	C	N	O	0	1	0
			269	183	40	46			
17	x	36	Total	C	N	O	0	0	0
			253	172	37	44			

- Molecule 18 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			453	311	68	72	2			
18	z	61	Total	C	N	O	S	0	0	0
			436	299	67	69	1			

- Molecule 19 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
19	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

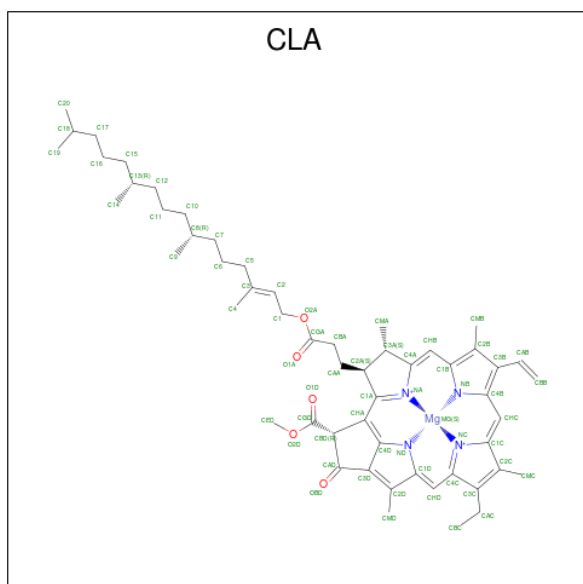
- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	1	Total	Fe	0	0
			1	1		
20	a	1	Total	Fe	0	0
			1	1		

- Molecule 21 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	Cl	0	0
			2	2		
21	a	2	Total	Cl	0	0
			2	2		

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			61	51	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			53	43	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	C	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
22	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	a	1	Total 61	C 51	Mg 1	N 4	O 5	0	0
22	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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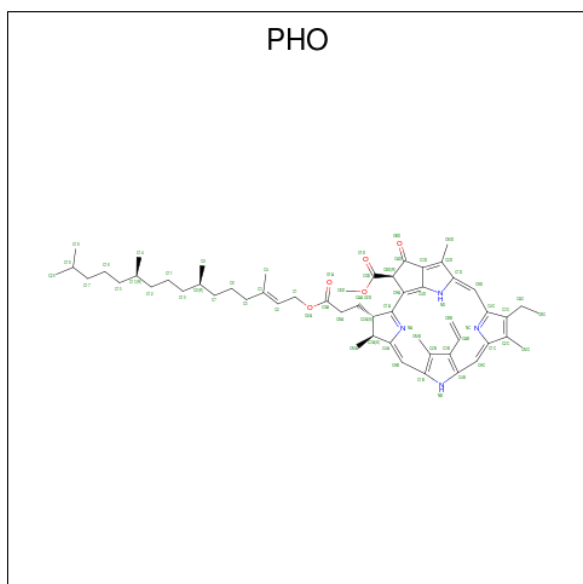
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 59	C 49	Mg 1	N 4	O 5	0	0
22	b	1	Total 52	C 42	Mg 1	N 4	O 5	0	0
22	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	b	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
22	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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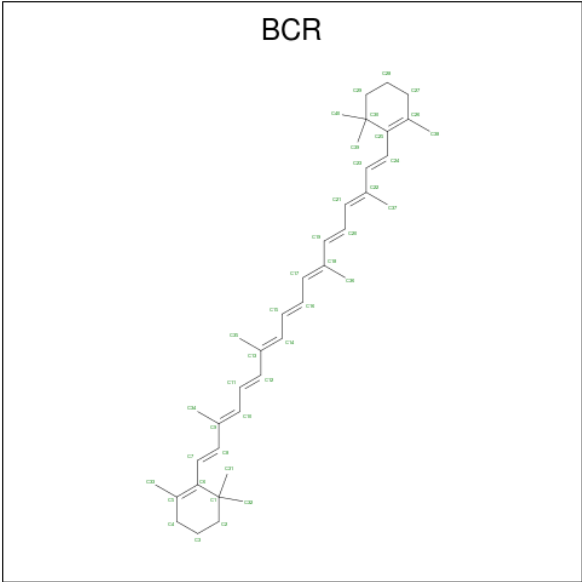
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
22	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 23 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	N	O	0	0
			64	55	4	5		
23	D	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		
23	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 24 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



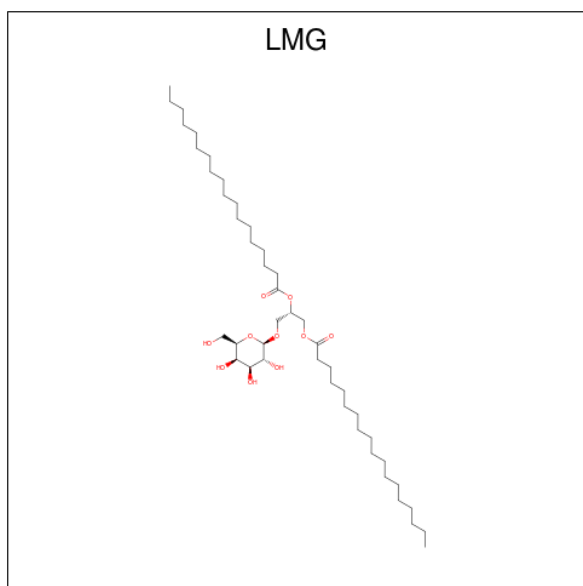
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 19 19	0	0
24	B	1	Total C 30 30	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	Y	1	Total C 39 39	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 20 20	0	0
24	b	1	Total C 31 31	0	0
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



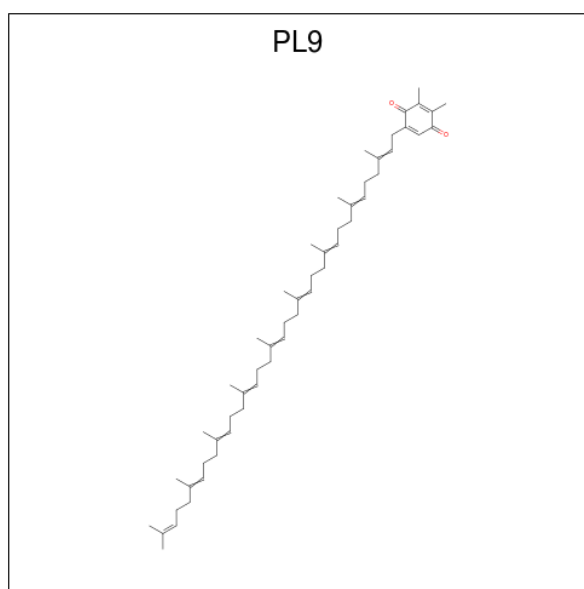
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 51 41 10	0	0
25	B	1	Total C O 40 30 10	0	0
25	C	1	Total C O 51 41 10	0	0
25	C	1	Total C O 40 30 10	0	0
25	D	1	Total C O 46 36 10	0	0
25	J	1	Total C O 45 35 10	0	0
25	b	1	Total C O 43 33 10	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	c	1	Total	C	O	0	0
			51	41	10		
25	c	1	Total	C	O	0	0
			49	39	10		
25	d	1	Total	C	O	0	0
			47	37	10		
25	i	1	Total	C	O	0	0
			51	41	10		
25	j	1	Total	C	O	0	0
			47	37	10		

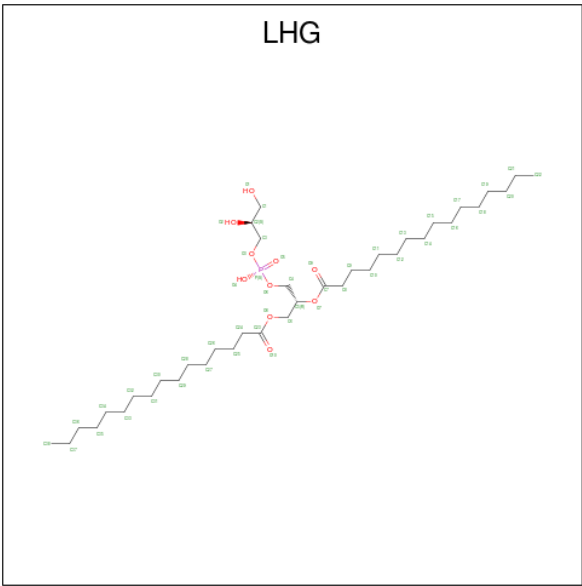
- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			55	53	2		
26	D	1	Total	C	O	0	0
			55	53	2		
26	a	1	Total	C	O	0	0
			55	53	2		
26	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code:

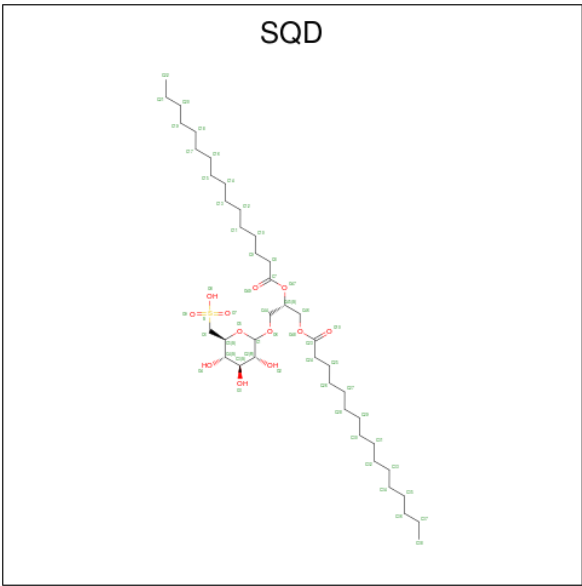
LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	O	P	0	0
			31	22	8	1		
27	C	1	Total	C	O	P	0	0
			30	21	8	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			49	38	10	1		
27	D	1	Total	C	O	P	0	0
			45	34	10	1		
27	L	1	Total	C	O	P	0	0
			40	29	10	1		
27	a	1	Total	C	O	P	0	0
			49	38	10	1		
27	a	1	Total	C	O	P	0	0
			45	34	10	1		
27	d	1	Total	C	O	P	0	0
			33	24	8	1		
27	d	1	Total	C	O	P	0	0
			49	38	10	1		
27	d	1	Total	C	O	P	0	0
			46	35	10	1		
27	l	1	Total	C	O	P	0	0
			49	38	10	1		

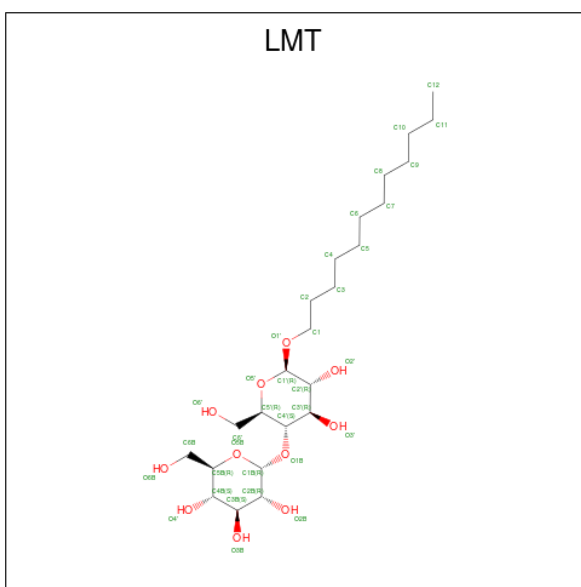
- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			49	36	12	1		
28	C	1	Total	C	O	S	0	0
			54	41	12	1		
28	D	1	Total	C	O	S	0	0
			20	9	10	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			51	38	12	1		
28	b	1	Total	C	O	S	0	0
			38	26	11	1		
28	f	1	Total	C	O	S	0	0
			14	6	7	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total 35	C 24	O 11	0	0
29	B	1	Total 24	C 18	O 6	0	0
29	E	1	Total 24	C 18	O 6	0	0
29	I	1	Total 35	C 24	O 11	0	0
29	T	1	Total 24	C 18	O 6	0	0
29	Z	1	Total 35	C 24	O 11	0	0
29	a	1	Total 35	C 24	O 11	0	0
29	c	1	Total 35	C 24	O 11	0	0
29	c	1	Total 24	C 18	O 6	0	0
29	f	1	Total 25	C 19	O 6	0	0
29	t	1	Total 24	C 18	O 6	0	0

- Molecule 30 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

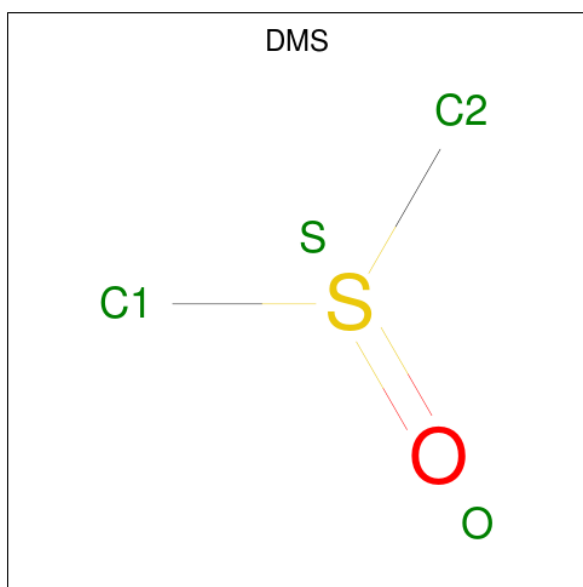
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	J	1	Total C 16 16	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	i	4	Total C 58 58	0	0
30	D	1	Total C 16 16	0	0
30	d	1	Total C 16 16	0	0
30	B	2	Total C 23 23	0	0
30	I	3	Total C 45 45	0	0
30	c	1	Total C 10 10	0	0
30	a	2	Total C 16 16	0	0
30	j	1	Total C 16 16	0	0
30	x	1	Total C 15 15	0	0
30	Z	1	Total C 9 9	0	0
30	A	1	Total C 5 5	0	0
30	T	1	Total C 13 13	0	0
30	U	1	Total C 14 14	0	0
30	X	1	Total C 16 16	0	0
30	O	1	Total C 16 16	0	0
30	t	1	Total C 16 16	0	0
30	u	1	Total C 11 11	0	0
30	b	2	Total C 27 27	0	0

- Molecule 31 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	I	1	Total 4	C 2	O 1	S 1	0	0
31	L	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0

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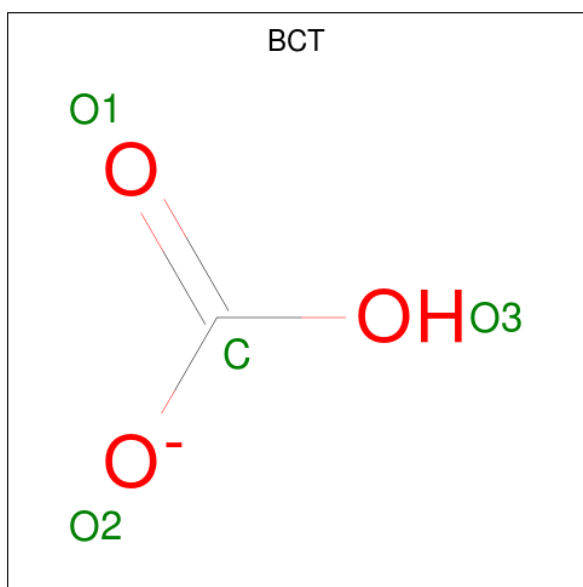
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	f	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	t	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	t	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).

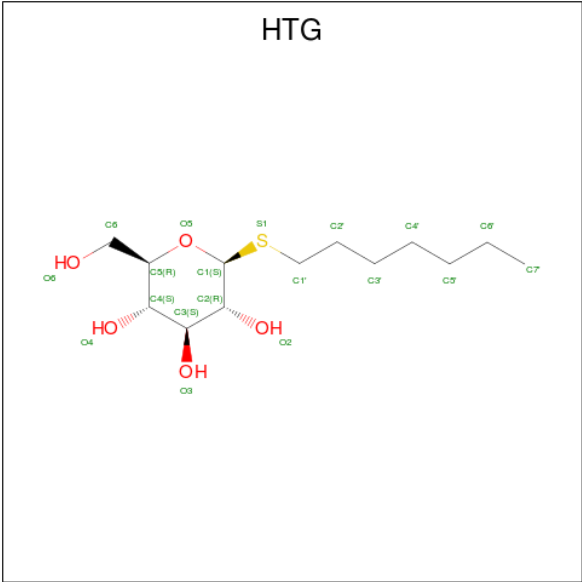


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			8	2	6		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	o	1	Total	Ca	0	0
			1	1		
33	O	1	Total	Ca	0	0
			1	1		
33	B	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		

- Molecule 34 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



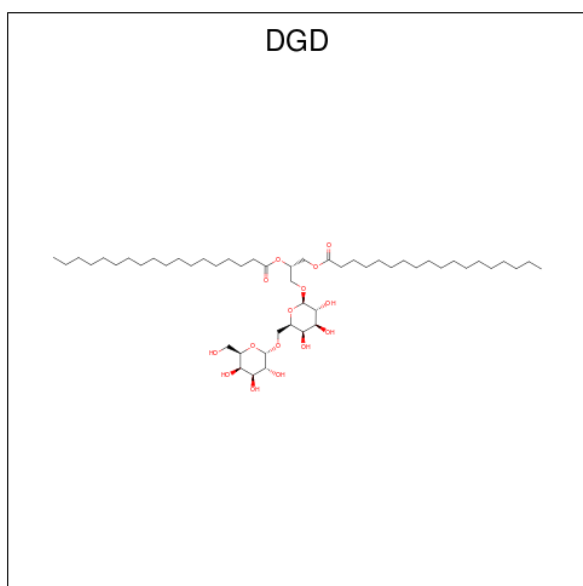
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	C	1	Total	C	S		0	0
			9	8	1			
34	C	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			19	13	5	1		
34	D	1	Total	C	O	S	0	0
			19	13	5	1		
34	V	1	Total	C	O	S	0	0
			14	8	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		
34	b	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	c	1	Total	C	O	S	0	0
			19	13	5	1		
34	l	1	Total	C	O	S	0	0
			19	13	5	1		
34	v	1	Total	C	O	S	0	0
			16	10	5	1		

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



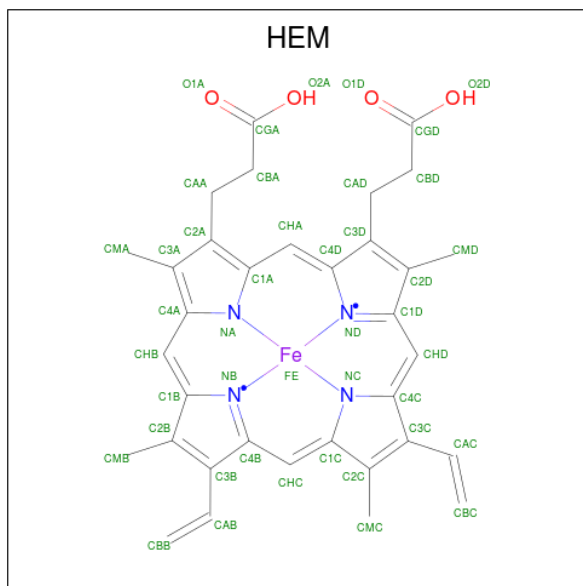
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	C	1	Total	C	O		0	0
			62	47	15			
35	D	1	Total	C	O		0	0
			50	41	9			
35	H	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			
35	c	1	Total	C	O		0	0
			62	47	15			

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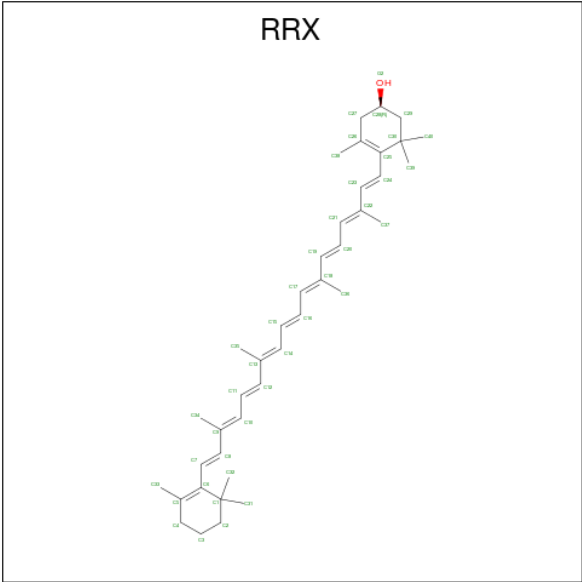
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			43	37	6		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
36	e	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 37 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).

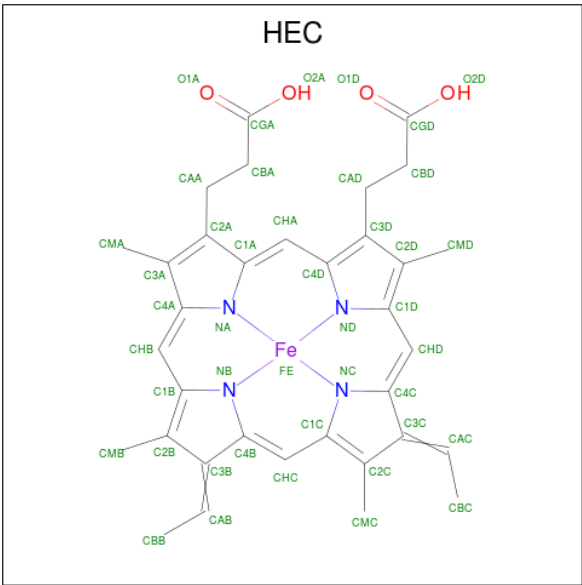


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	H	1	Total	C	O	0	0
			41	40	1		
37	h	1	Total	C	O	0	0
			41	40	1		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	J	1	Total	Mg	0	0
			1	1		
38	j	1	Total	Mg	0	0
			1	1		
38	K	1	Total	Mg	0	0
			1	1		
38	k	1	Total	Mg	0	0
			1	1		

- Molecule 39 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
39	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
39	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	132	Total	O	0	0
			132	132		
40	B	256	Total	O	0	6
			262	262		
40	C	174	Total	O	0	4
			178	178		
40	D	130	Total	O	0	1
			131	131		
40	E	33	Total	O	0	2
			35	35		
40	F	4	Total	O	0	0
			4	4		
40	H	39	Total	O	0	0
			39	39		
40	I	5	Total	O	0	0
			5	5		
40	J	15	Total	O	0	1
			16	16		
40	K	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	L	18	Total O 19 19	0	1
40	O	161	Total O 166 166	0	5
40	T	12	Total O 12 12	0	0
40	U	72	Total O 74 74	0	2
40	V	110	Total O 113 113	0	3
40	Y	7	Total O 8 8	0	1
40	X	15	Total O 16 16	0	1
40	Z	5	Total O 5 5	0	0
40	a	122	Total O 123 123	0	1
40	b	251	Total O 261 261	0	10
40	c	216	Total O 220 220	0	4
40	d	115	Total O 115 115	0	0
40	e	16	Total O 17 17	0	1
40	f	4	Total O 4 4	0	0
40	h	31	Total O 31 31	0	0
40	i	5	Total O 5 5	0	0
40	j	10	Total O 10 10	0	0
40	k	9	Total O 10 10	0	1
40	l	14	Total O 15 15	0	1
40	o	153	Total O 156 156	0	3
40	t	10	Total O 10 10	0	0

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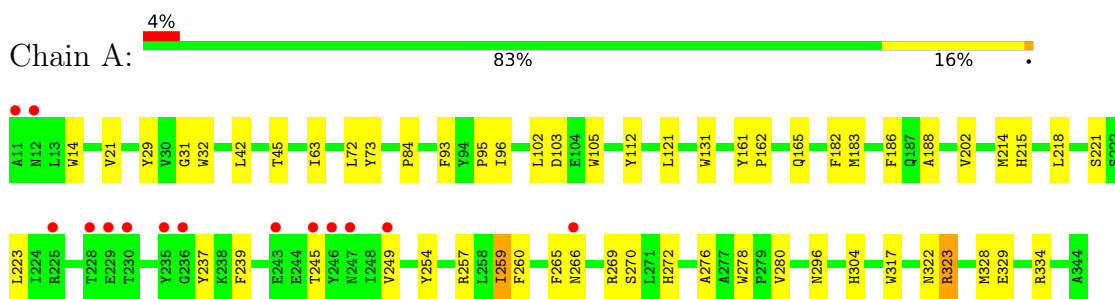
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	u	75	Total 75	O 75	0	0
40	v	77	Total 82	O 82	0	5
40	y	1	Total 1	O 1	0	0
40	x	5	Total 5	O 5	0	0
40	z	8	Total 8	O 8	0	0

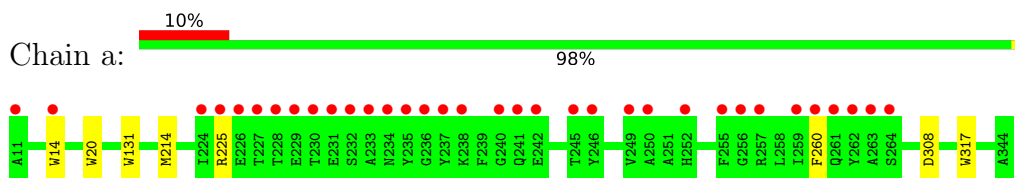
3 Residue-property plots [i](#)

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

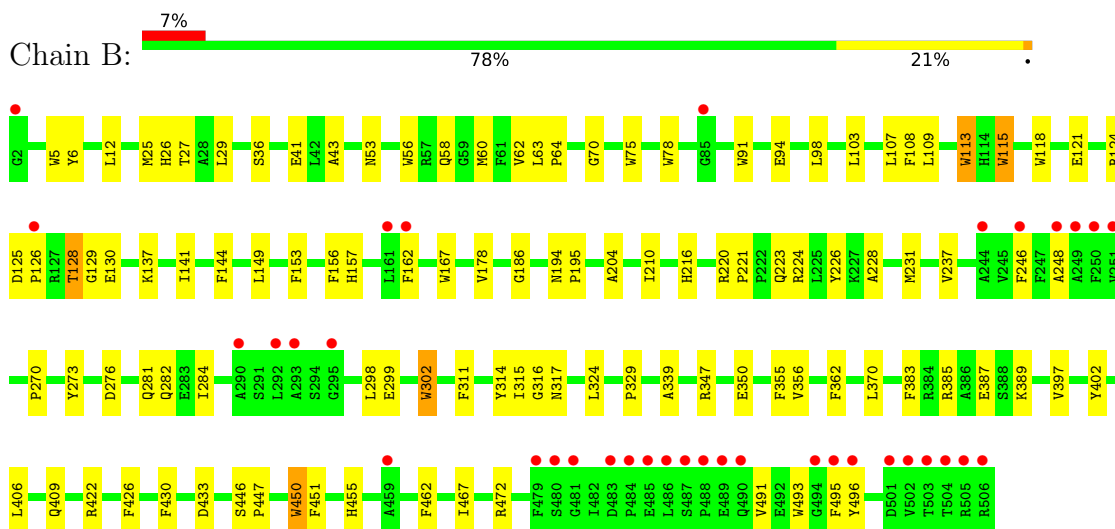
- Molecule 1: Photosystem II protein D1 1



- Molecule 1: Photosystem II protein D1 1

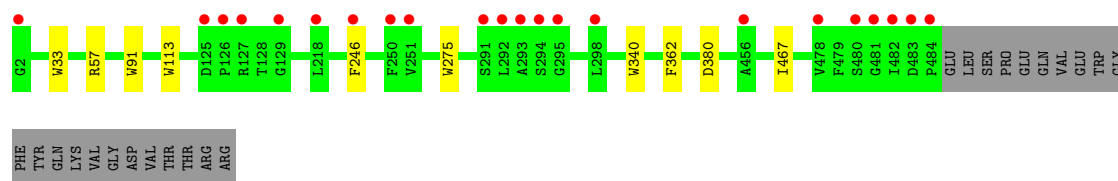


- Molecule 2: Photosystem II CP47 reaction center protein

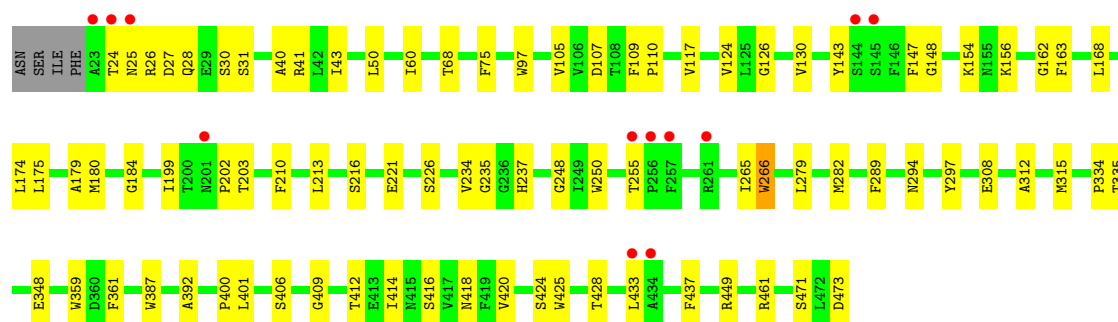
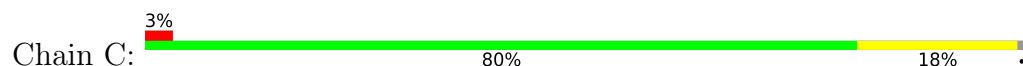


- Molecule 2: Photosystem II CP47 reaction center protein





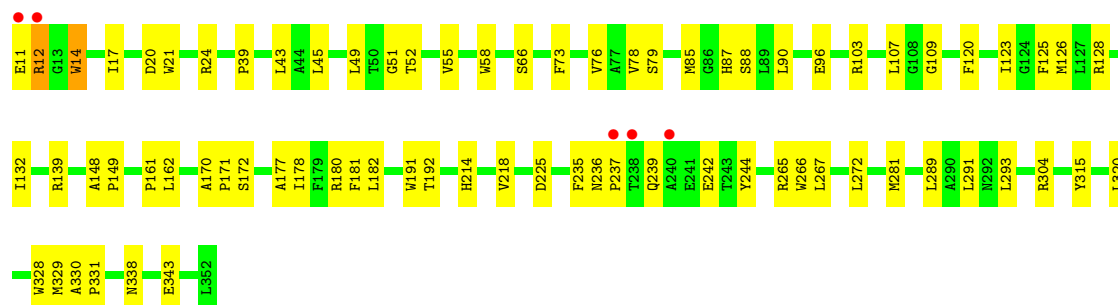
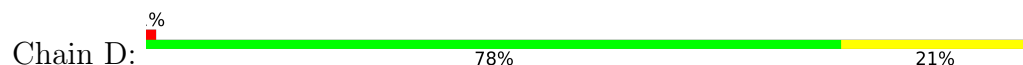
• Molecule 3: Photosystem II CP43 reaction center protein



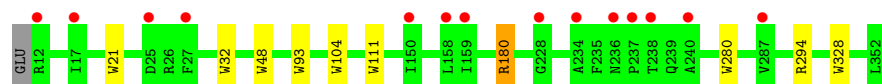
• Molecule 3: Photosystem II CP43 reaction center protein



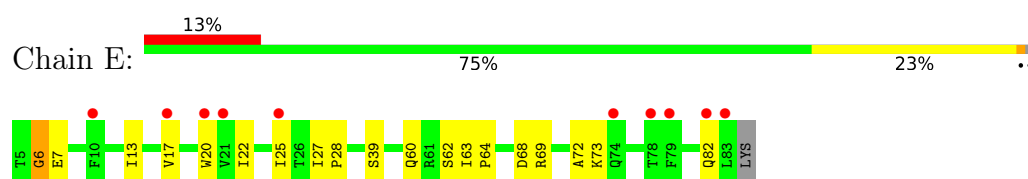
• Molecule 4: Photosystem II D2 protein



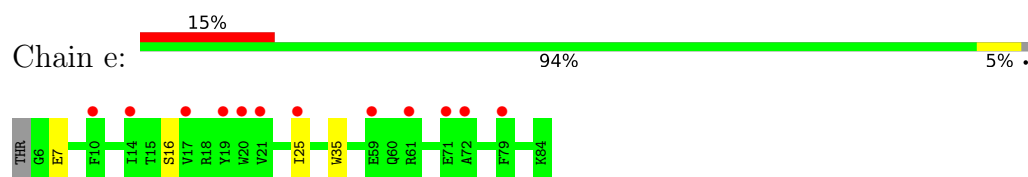
• Molecule 4: Photosystem II D2 protein



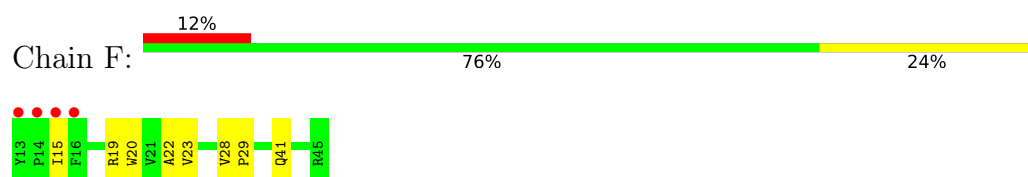
• Molecule 5: Cytochrome b559 subunit alpha



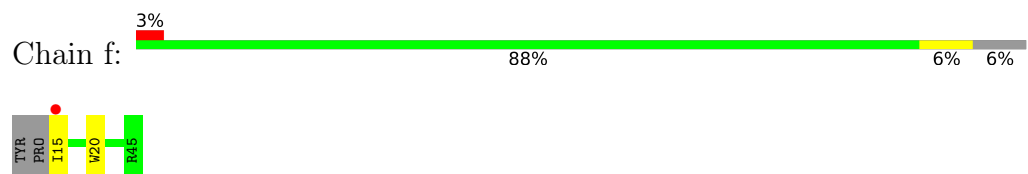
- Molecule 5: Cytochrome b559 subunit alpha



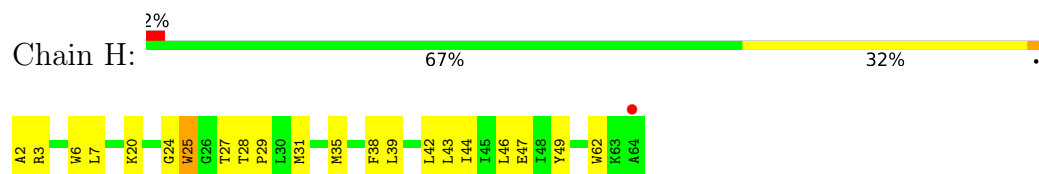
- Molecule 6: Cytochrome b559 subunit beta



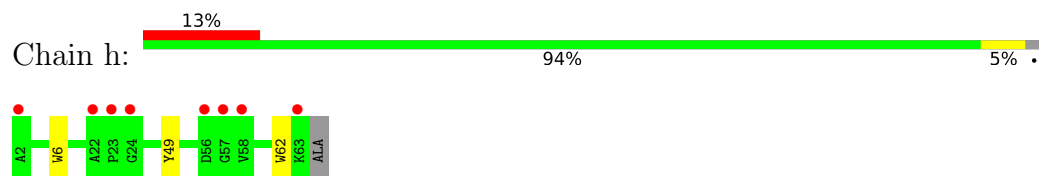
- Molecule 6: Cytochrome b559 subunit beta



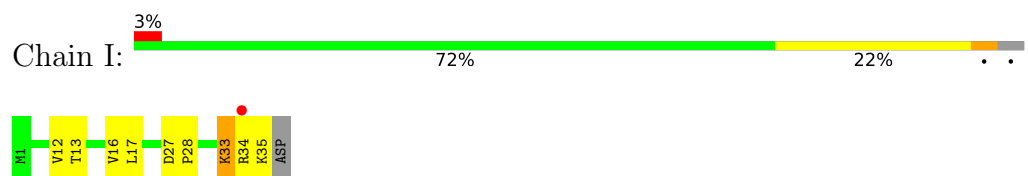
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  100%

There are no outlier residues recorded for this chain.

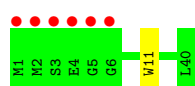
- Molecule 9: Photosystem II reaction center protein J

Chain J:  5% 70% 20% 10%



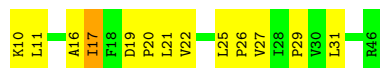
- Molecule 9: Photosystem II reaction center protein J

Chain j:  15% 98% .



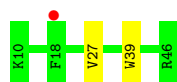
- Molecule 10: Photosystem II reaction center protein K

Chain K:  65% 32% .




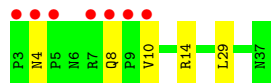
- Molecule 10: Photosystem II reaction center protein K

Chain k:  3% 95% 5%



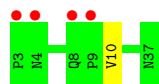
- Molecule 11: Photosystem II reaction center protein L

Chain L:  20% 86% 14%




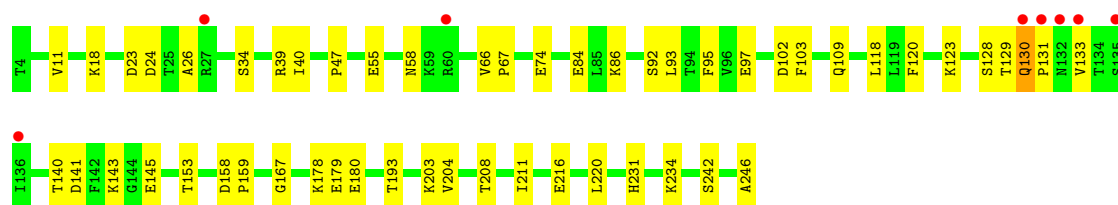
- Molecule 11: Photosystem II reaction center protein L

Chain l:  11% 97% .

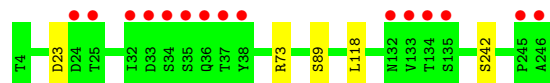


- Molecule 12: Photosystem II manganese-stabilizing polypeptide

Chain O:  3% 78% 21%



- Molecule 12: Photosystem II manganese-stabilizing polypeptide



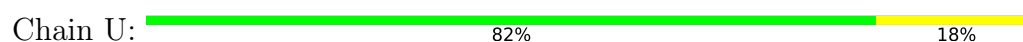
- Molecule 13: Photosystem II reaction center protein T



- Molecule 13: Photosystem II reaction center protein T



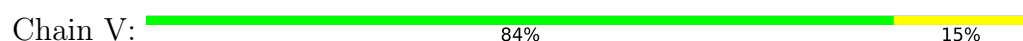
- Molecule 14: Photosystem II 12 kDa extrinsic protein



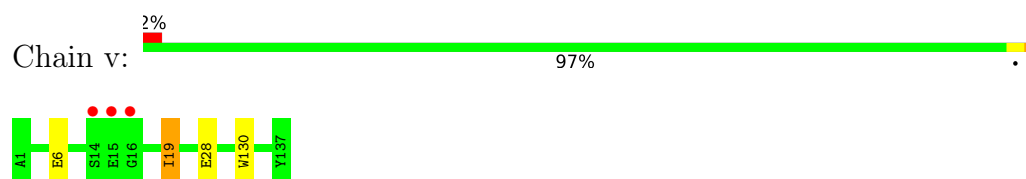
- Molecule 14: Photosystem II 12 kDa extrinsic protein



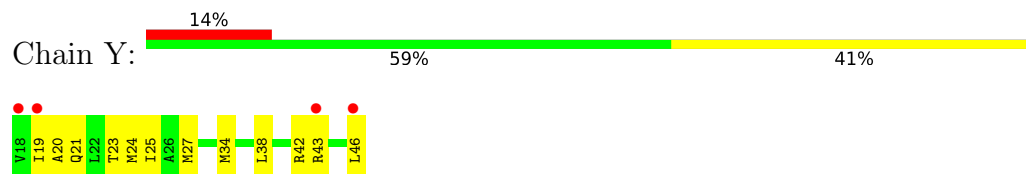
- Molecule 15: Cytochrome c-550



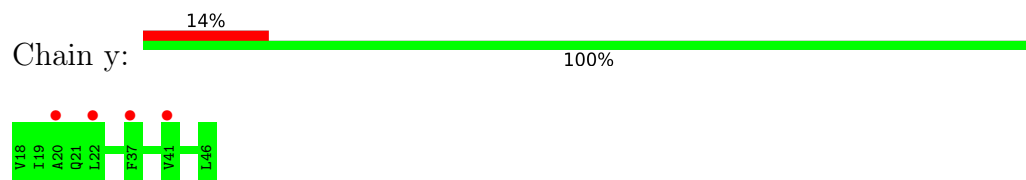
- Molecule 15: Cytochrome c-550



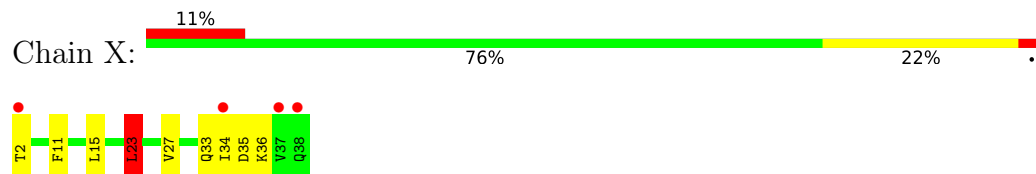
- Molecule 16: Photosystem II reaction center protein Ycf12



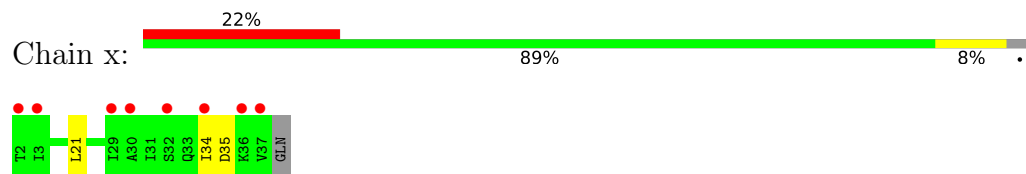
- Molecule 16: Photosystem II reaction center protein Ycf12



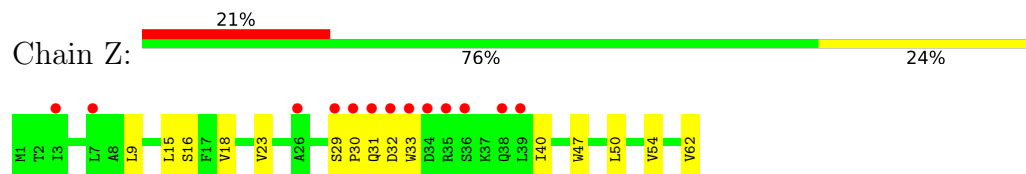
- Molecule 17: Photosystem II reaction center X protein



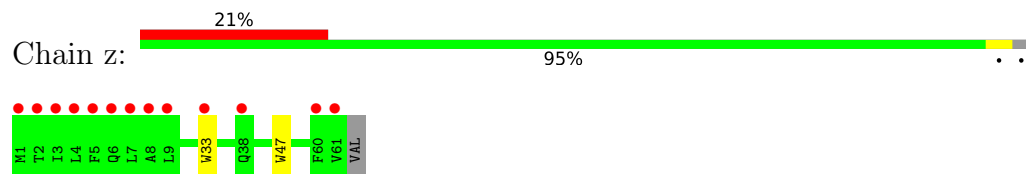
- Molecule 17: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center protein Z



- Molecule 18: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.95Å 226.99Å 285.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 46.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-2.20) 96.3 (46.79-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.174 , 0.226 0.174 , 0.225	Depositor DCC
R_{free} test set	19307 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51892	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, DMS, BCT, BCR, DGD, FE2, RRX, LHG, CL, CA, CLA, HEC, HEM, FME, UNL, HTG, MG, OEX, PHO, LMT, SQD, LMG

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	0.86	3/2686 (0.1%)	0.76	2/3666 (0.1%)
1	a	0.87	4/2640 (0.2%)	0.77	1/3604 (0.0%)
2	B	0.87	10/4099 (0.2%)	0.77	5/5591 (0.1%)
2	b	0.85	5/3917 (0.1%)	0.78	3/5342 (0.1%)
3	C	0.85	6/3583 (0.2%)	0.76	1/4880 (0.0%)
3	c	0.83	9/3638 (0.2%)	0.76	1/4953 (0.0%)
4	D	0.91	5/2836 (0.2%)	0.77	0/3866
4	d	0.88	8/2818 (0.3%)	0.75	2/3842 (0.1%)
5	E	0.73	0/654	0.73	0/895
5	e	0.71	1/655 (0.2%)	0.72	0/896
6	F	0.83	1/278 (0.4%)	0.62	0/379
6	f	0.78	1/257 (0.4%)	0.66	0/349
7	H	0.83	3/541 (0.6%)	0.74	0/737
7	h	0.80	2/517 (0.4%)	0.68	0/704
8	I	0.67	0/285	0.67	0/385
8	i	0.63	0/290	0.64	0/392
9	J	0.80	1/257 (0.4%)	0.72	0/349
9	j	0.79	1/283 (0.4%)	0.67	0/384
10	K	0.71	0/303	0.73	0/416
10	k	0.74	1/296 (0.3%)	0.70	0/408
11	L	0.74	0/294	0.73	0/399
11	l	0.72	0/294	0.71	0/399
12	O	0.69	0/1887	0.80	0/2561
12	o	0.63	0/1864	0.78	1/2535 (0.0%)
13	T	0.79	0/252	0.72	0/342
13	t	0.74	0/252	0.69	0/342
14	U	0.76	0/796	0.82	0/1078
14	u	0.71	0/777	0.79	0/1054
15	V	0.78	0/1090	0.78	0/1480
15	v	0.69	1/1082 (0.1%)	0.75	0/1472
16	Y	0.54	0/216	0.72	0/289

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	y	0.48	0/208	0.67	0/278
17	X	0.55	0/275	0.68	1/373 (0.3%)
17	x	0.56	0/256	0.65	0/349
18	Z	0.69	1/463 (0.2%)	0.67	0/636
18	z	0.65	2/447 (0.4%)	0.62	0/614
All	All	0.81	65/41286 (0.2%)	0.76	17/56239 (0.0%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	387	TRP	CD2-CE2	7.25	1.50	1.41
2	B	78	TRP	CD2-CE2	6.94	1.49	1.41
1	A	317	TRP	CD2-CE2	6.86	1.49	1.41
3	c	365	TRP	CD2-CE2	6.65	1.49	1.41
1	A	278	TRP	CD2-CE2	6.57	1.49	1.41
2	b	33	TRP	CD2-CE2	6.42	1.49	1.41
2	b	275	TRP	CD2-CE2	6.39	1.49	1.41
2	B	56	TRP	CD2-CE2	6.37	1.49	1.41
4	d	48	TRP	CD2-CE2	6.21	1.48	1.41
4	D	58	TRP	CD2-CE2	6.12	1.48	1.41
4	d	93	TRP	CD2-CE2	6.10	1.48	1.41
2	B	5	TRP	CD2-CE2	6.04	1.48	1.41
2	B	167	TRP	CD2-CE2	6.00	1.48	1.41
3	c	250	TRP	CD2-CE2	5.98	1.48	1.41
3	c	387	TRP	CD2-CE2	5.95	1.48	1.41
15	v	130	TRP	CD2-CE2	5.90	1.48	1.41
3	c	443	TRP	CD2-CE2	5.86	1.48	1.41
2	B	450	TRP	CD2-CE2	5.84	1.48	1.41
4	d	104	TRP	CD2-CE2	5.80	1.48	1.41
7	H	62	TRP	CD2-CE2	5.74	1.48	1.41
3	C	266	TRP	CD2-CE2	5.69	1.48	1.41
1	A	14	TRP	CD2-CE2	5.68	1.48	1.41
2	B	302	TRP	CD2-CE2	5.62	1.48	1.41
10	k	39	TRP	CD2-CE2	5.62	1.48	1.41
3	C	425	TRP	CD2-CE2	5.58	1.48	1.41
7	H	25	TRP	CD2-CE2	5.57	1.48	1.41
4	d	21	TRP	CD2-CE2	5.56	1.48	1.41
6	f	20	TRP	CD2-CE2	5.56	1.48	1.41
18	z	33	TRP	CD2-CE2	5.55	1.48	1.41
2	B	115	TRP	CD2-CE2	5.52	1.48	1.41
1	a	131	TRP	CD2-CE2	5.46	1.48	1.41
3	C	250	TRP	CD2-CE2	5.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	11	TRP	CD2-CE2	5.44	1.47	1.41
4	d	32	TRP	CD2-CE2	5.39	1.47	1.41
1	a	14	TRP	CD2-CE2	5.38	1.47	1.41
3	c	359	TRP	CD2-CE2	5.37	1.47	1.41
2	b	91	TRP	CD2-CE2	5.37	1.47	1.41
2	B	91	TRP	CD2-CE2	5.37	1.47	1.41
6	F	20	TRP	CD2-CE2	5.35	1.47	1.41
3	C	359	TRP	CD2-CE2	5.34	1.47	1.41
3	c	35	TRP	CD2-CE2	5.32	1.47	1.41
2	b	340	TRP	CD2-CE2	5.32	1.47	1.41
2	B	493	TRP	CD2-CE2	5.29	1.47	1.41
1	a	20	TRP	CD2-CE2	5.27	1.47	1.41
4	D	21	TRP	CD2-CE2	5.25	1.47	1.41
1	a	317	TRP	CD2-CE2	5.25	1.47	1.41
4	D	87	HIS	CG-CD2	5.25	1.44	1.35
4	d	328	TRP	CD2-CE2	5.23	1.47	1.41
2	b	113	TRP	CD2-CE2	5.22	1.47	1.41
4	D	14	TRP	CD2-CE2	5.19	1.47	1.41
3	c	259	TRP	CD2-CE2	5.19	1.47	1.41
18	z	47	TRP	CD2-CE2	5.18	1.47	1.41
18	Z	33	TRP	CD2-CE2	5.16	1.47	1.41
7	h	6	TRP	CD2-CE2	5.16	1.47	1.41
2	B	113	TRP	CD2-CE2	5.13	1.47	1.41
4	d	280	TRP	CD2-CE2	5.12	1.47	1.41
4	D	328	TRP	CD2-CE2	5.08	1.47	1.41
3	c	36	TRP	CD2-CE2	5.05	1.47	1.41
9	j	11	TRP	CD2-CE2	5.04	1.47	1.41
3	C	97	TRP	CD2-CE2	5.04	1.47	1.41
4	d	111	TRP	CD2-CE2	5.04	1.47	1.41
3	c	97	TRP	CD2-CE2	5.04	1.47	1.41
5	e	35	TRP	CD2-CE2	5.04	1.47	1.41
7	H	6	TRP	CD2-CE2	5.03	1.47	1.41
7	h	62	TRP	CD2-CE2	5.02	1.47	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	57	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	b	57	ARG	NE-CZ-NH1	6.84	123.72	120.30
3	C	473	ASP	CB-CG-OD1	6.78	124.40	118.30
4	d	180	ARG	NE-CZ-NH1	-5.99	117.31	120.30
2	B	433	ASP	CB-CG-OD1	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	385	ARG	NE-CZ-NH2	-5.71	117.44	120.30
12	o	73	ARG	NE-CZ-NH1	-5.58	117.51	120.30
4	d	294	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	B	298	LEU	CA-CB-CG	5.32	127.54	115.30
2	B	422	ARG	NE-CZ-NH2	-5.28	117.66	120.30
17	X	23	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	131	TRP	CA-CB-CG	-5.24	103.75	113.70
2	b	380	ASP	CB-CG-OD2	-5.18	113.63	118.30
2	B	433	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	A	323	ARG	NE-CZ-NH1	5.10	122.85	120.30
3	c	357	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	a	308	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2598	0	2484	59	0
1	a	2555	0	2420	0	0
2	B	3950	0	3776	101	0
2	b	3780	0	3636	0	0
3	C	3470	0	3380	56	0
3	c	3521	0	3439	0	0
4	D	2732	0	2640	74	0
4	d	2717	0	2628	0	0
5	E	635	0	613	14	0
5	e	636	0	609	0	0
6	F	269	0	277	7	0
6	f	250	0	261	0	0
7	H	522	0	547	20	0
7	h	501	0	526	0	0
8	I	288	0	307	5	0
8	i	293	0	309	0	0
9	J	251	0	257	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	277	0	0
10	K	293	0	305	15	0
10	k	286	0	285	0	0
11	L	287	0	299	5	0
11	l	287	0	299	0	0
12	O	1853	0	1819	48	0
12	o	1833	0	1783	0	0
13	T	253	0	247	6	0
13	t	253	0	247	0	0
14	U	782	0	786	12	0
14	u	766	0	765	0	0
15	V	1066	0	1075	26	0
15	v	1058	0	1053	0	0
16	Y	215	0	246	12	0
16	y	207	0	221	0	0
17	X	269	0	297	6	0
17	x	253	0	274	0	0
18	Z	453	0	471	8	0
18	z	436	0	431	0	0
19	A	10	0	0	0	0
19	a	10	0	0	0	0
20	A	1	0	0	0	0
20	a	1	0	0	0	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	185	0	193	15	0
22	B	1014	0	1091	72	0
22	C	836	0	915	39	0
22	D	195	0	216	7	0
22	a	256	0	277	0	0
22	b	1016	0	1096	0	0
22	c	845	0	936	0	0
22	d	130	0	144	0	0
23	A	64	0	74	1	0
23	D	64	0	74	5	0
23	a	128	0	148	0	0
24	A	40	0	56	0	0
24	B	89	0	121	11	0
24	C	80	0	112	5	0
24	D	40	0	56	1	0
24	K	40	0	56	2	0
24	Y	39	0	53	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	0	0
24	b	91	0	123	0	0
24	c	80	0	112	0	0
24	d	40	0	56	0	0
24	k	40	0	56	0	0
24	y	40	0	56	0	0
25	A	51	0	72	2	0
25	B	40	0	50	3	0
25	C	91	0	122	3	0
25	D	46	0	62	5	0
25	J	45	0	60	2	0
25	b	43	0	56	0	0
25	c	100	0	140	0	0
25	d	47	0	64	0	0
25	i	51	0	72	0	0
25	j	47	0	64	0	0
26	A	55	0	80	11	0
26	D	55	0	80	5	0
26	a	55	0	80	0	0
26	d	55	0	80	0	0
27	A	31	0	36	1	0
27	C	30	0	33	1	0
27	D	143	0	211	18	0
27	L	40	0	53	7	0
27	a	94	0	137	0	0
27	d	128	0	178	0	0
27	l	49	0	74	0	0
28	A	49	0	64	2	0
28	C	54	0	78	6	0
28	D	20	0	16	0	0
28	a	105	0	147	0	0
28	b	38	0	47	0	0
28	f	14	0	8	0	0
28	l	54	0	78	0	0
29	A	35	0	46	6	0
29	B	24	0	35	3	0
29	E	24	0	35	1	0
29	I	35	0	46	0	0
29	T	24	0	35	1	0
29	Z	35	0	46	1	0
29	a	35	0	46	0	0
29	c	59	0	81	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	f	25	0	35	0	0
29	t	24	0	35	0	0
30	A	5	0	0	0	0
30	B	23	0	0	0	0
30	D	16	0	0	0	0
30	I	45	0	0	1	0
30	J	16	0	0	1	0
30	O	16	0	0	0	0
30	T	13	0	0	0	0
30	U	14	0	0	1	0
30	X	16	0	0	1	0
30	Z	9	0	0	0	0
30	a	16	0	0	0	0
30	b	27	0	0	0	0
30	c	10	0	0	0	0
30	d	16	0	0	0	0
30	i	58	0	0	0	0
30	j	16	0	0	0	0
30	t	16	0	0	0	0
30	u	11	0	0	0	0
30	x	15	0	0	0	0
31	A	20	0	30	2	0
31	B	60	0	90	15	0
31	C	60	0	90	3	0
31	D	12	0	18	0	0
31	F	4	0	6	0	0
31	H	4	0	6	0	0
31	I	8	0	12	0	0
31	L	4	0	6	0	0
31	O	48	0	72	24	0
31	U	8	0	12	1	0
31	V	40	0	60	19	0
31	a	20	0	30	0	0
31	b	36	0	54	0	0
31	c	76	0	114	0	0
31	d	20	0	30	0	0
31	f	4	0	6	0	0
31	i	4	0	6	0	0
31	l	12	0	18	0	0
31	o	28	0	42	0	0
31	t	12	0	18	0	0
31	u	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	v	36	0	54	0	0
32	A	8	0	0	1	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	57	0	78	4	0
34	C	47	0	67	2	0
34	D	38	0	52	10	0
34	V	14	0	13	0	0
34	b	95	0	130	0	0
34	c	19	0	26	0	0
34	l	19	0	26	0	0
34	v	16	0	17	0	0
35	C	186	0	246	3	0
35	D	50	0	69	0	0
35	H	62	0	82	4	0
35	c	186	0	246	0	0
35	d	43	0	62	0	0
35	h	62	0	82	0	0
36	E	43	0	30	1	0
36	e	43	0	30	0	0
37	H	41	0	56	12	0
37	h	41	0	56	0	0
38	J	1	0	0	0	0
38	K	1	0	0	0	0
38	j	1	0	0	0	0
38	k	1	0	0	0	0
39	V	43	0	30	4	0
39	v	43	0	30	0	0
40	A	132	0	0	1	0
40	B	262	0	0	13	0
40	C	178	0	0	3	0
40	D	131	0	0	5	0
40	E	35	0	0	1	0
40	F	4	0	0	0	0
40	H	39	0	0	1	0
40	I	5	0	0	0	0
40	J	16	0	0	0	0
40	K	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	L	19	0	0	0	0
40	O	166	0	0	13	0
40	T	12	0	0	0	0
40	U	74	0	0	3	0
40	V	113	0	0	7	0
40	X	16	0	0	0	0
40	Y	8	0	0	0	0
40	Z	5	0	0	1	0
40	a	123	0	0	0	0
40	b	261	0	0	0	0
40	c	220	0	0	0	0
40	d	115	0	0	0	0
40	e	17	0	0	0	0
40	f	4	0	0	0	0
40	h	31	0	0	0	0
40	i	5	0	0	0	0
40	j	10	0	0	0	0
40	k	10	0	0	0	0
40	l	15	0	0	0	0
40	o	156	0	0	0	0
40	t	10	0	0	0	0
40	u	75	0	0	0	0
40	v	82	0	0	0	0
40	x	5	0	0	0	0
40	y	1	0	0	0	0
40	z	8	0	0	0	0
All	All	51892	0	50274	593	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 (593) 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)
22:B:608:CLA:H52	22:B:608:CLA:H92	2.73	1.10
22:B:608:CLA:H52	22:B:608:CLA:C9	3.21	1.05
2:B:125:ASP:HB3	2:B:128:THR:CG2	4.42	1.05
12:O:66:VAL:HG13	12:O:67:PRO:HD2	1.37	1.05
26:D:406:PL9:C33	27:L:101:LHG:H223	1.87	1.04
1:A:214:MET:HG2	26:A:411:PL9:H102	1.37	1.02
2:B:356:VAL:H	31:B:638:DMS:H21	18.54	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:HD12	10:K:17:ILE:H	1.27	0.96
22:B:608:CLA:H92	22:B:608:CLA:C5	3.22	0.96
2:B:125:ASP:HB3	2:B:128:THR:HG22	5.00	0.92
31:O:310:DMS:H12	40:O:501:HOH:O	1.69	0.91
27:D:411:LHG:H161	27:D:411:LHG:H322	1.52	0.91
1:A:304:HIS:HE1	31:V:212:DMS:H13	1.35	0.90
12:O:133:VAL:HG22	31:O:304:DMS:C2	2.02	0.90
2:B:347[A]:ARG:NH2	40:B:701:HOH:O	2.09	0.86
12:O:66:VAL:CG1	12:O:67:PRO:HD2	2.04	0.86
10:K:17:ILE:H	10:K:17:ILE:CD1	1.88	0.85
24:B:620:BCR:H331	24:B:620:BCR:HC8	2.39	0.84
31:B:628:DMS:H13	40:B:711:HOH:O	1.75	0.84
22:A:405:CLA:HMB1	22:A:405:CLA:HBB1	1.57	0.84
4:D:338:ASN:HB3	40:D:614:HOH:O	1.77	0.83
10:K:17:ILE:HD12	10:K:17:ILE:N	1.93	0.83
27:A:412:LHG:H352	30:I:105:UNL:C3	2.09	0.82
10:K:21:LEU:HD13	16:Y:24:MET:HE3	2.14	0.82
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.61	0.81
1:A:214:MET:HG2	26:A:411:PL9:C10	2.10	0.81
28:C:501:SQD:H381	9:J:22:ILE:HD11	1.63	0.81
1:A:304:HIS:HE1	31:V:212:DMS:C1	1.95	0.80
22:B:614:CLA:HMB1	22:B:614:CLA:HBB1	1.80	0.80
3:C:148:GLY:O	3:C:156:LYS:NZ	2.50	0.79
31:B:642:DMS:H13	40:B:853:HOH:O	1.83	0.78
13:T:2:GLU:HG2	13:T:6:TYR:CE2	2.43	0.78
22:D:401:CLA:HMB1	22:D:401:CLA:HBB1	1.66	0.78
24:B:620:BCR:H331	24:B:620:BCR:C8	2.48	0.78
4:D:242:GLU:HG3	4:D:244:TYR:O	3.24	0.77
12:O:133:VAL:HG22	31:O:304:DMS:H21	1.64	0.77
12:O:208:THR:O	31:O:305:DMS:C1	9.83	0.77
10:K:19:ASP:HB3	10:K:20:PRO:HD3	1.67	0.76
3:C:40:ALA:O	3:C:43:ILE:HG13	1.86	0.76
15:V:129[B]:LYS:HB3	31:V:210:DMS:S	26.59	0.76
14:U:9:LEU:HA	40:U:332:HOH:O	38.51	0.75
1:A:304:HIS:CE1	31:V:212:DMS:H13	2.21	0.75
27:D:411:LHG:H142	27:D:411:LHG:H331	1.68	0.74
4:D:343[B]:GLU:OE2	34:D:415:HTG:H2	1.87	0.74
29:A:414:LMT:H2B	4:D:304:ARG:HH22	1.53	0.74
4:D:85:MET:HE2	4:D:90[A]:LEU:HD21	1.83	0.74
27:D:409:LHG:O9	27:L:101:LHG:HC81	1.88	0.73
2:B:125:ASP:CB	2:B:128:THR:HG22	5.94	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:612:CLA:HMB1	22:B:612:CLA:HBB1	1.92	0.73
2:B:125:ASP:HB3	2:B:128:THR:HG23	4.94	0.72
12:O:208:THR:O	31:O:305:DMS:H12	9.78	0.72
15:V:126:LEU:O	15:V:129[A]:LYS:HD2	1.89	0.72
22:B:608:CLA:H203	27:D:409:LHG:H122	1.71	0.72
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.25	0.71
15:V:27:LEU:HD21	31:V:206:DMS:C1	2.20	0.71
2:B:125:ASP:OD2	2:B:128:THR:HG22	6.31	0.71
2:B:299:GLU:HG3	40:B:879:HOH:O	5.52	0.71
22:C:507:CLA:HBB1	22:C:507:CLA:HMB1	1.70	0.71
31:O:312:DMS:H21	40:O:467:HOH:O	1.89	0.71
12:O:179:GLU:HG3	31:O:312:DMS:H11	1.73	0.70
2:B:282:GLN:NE2	40:B:701:HOH:O	19.94	0.70
2:B:467:ILE:HG13	4:D:126:MET:HE2	2.74	0.70
2:B:383:PHE:CZ	12:O:167:GLY:HA2	2.62	0.70
3:C:461:ARG:HG3	40:D:534:HOH:O	1.91	0.70
1:A:183:MET:HA	22:A:405:CLA:HMD2	1.75	0.69
4:D:14:TRP:CD1	34:D:414:HTG:H61	2.28	0.69
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.75	0.68
2:B:446:SER:HB2	2:B:447:PRO:CD	2.22	0.68
1:A:304:HIS:CE1	31:V:212:DMS:C1	2.76	0.68
1:A:121[A]:LEU:HD23	25:A:410:LMG:H202	1.74	0.68
2:B:36:SER:OG	24:B:619:BCR:H362	2.38	0.68
4:D:343[A]:GLU:OE2	40:D:501:HOH:O	2.11	0.68
15:V:27:LEU:HD21	31:V:206:DMS:H13	1.76	0.68
3:C:279:LEU:HD22	22:C:510:CLA:HED2	1.76	0.67
12:O:133:VAL:HG22	31:O:304:DMS:H23	1.74	0.67
10:K:16:ALA:O	10:K:19:ASP:HB2	1.94	0.67
7:H:2:ALA:N	40:H:201:HOH:O	2.28	0.67
2:B:467:ILE:HG13	4:D:126:MET:CE	2.92	0.66
12:O:178:LYS:HG2	31:O:304:DMS:C2	61.65	0.66
15:V:124:LYS:HE2	40:V:356:HOH:O	20.05	0.66
5:E:68:ASP:O	5:E:72:ALA:HB2	1.96	0.66
27:D:409:LHG:HC12	27:L:101:LHG:O5	1.96	0.65
2:B:356:VAL:N	31:B:638:DMS:H21	17.72	0.65
25:B:621:LMG:H112	25:B:621:LMG:H312	1.79	0.65
2:B:26:HIS:HB2	22:B:613:CLA:HMB2	1.79	0.65
27:D:411:LHG:H331	27:D:411:LHG:C14	2.25	0.65
22:B:605:CLA:H43	22:B:606:CLA:H2	1.80	0.64
3:C:279:LEU:HD12	3:C:282:MET:CE	2.27	0.64
18:Z:50:LEU:O	18:Z:54:VAL:HG23	2.57	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:A:408:CLA:HBB1	22:A:408:CLA:HMB1	2.01	0.64
22:D:403:CLA:HMB1	22:D:403:CLA:HBB1	2.15	0.64
2:B:462:PHE:CE1	22:B:614:CLA:HMB3	2.45	0.63
22:C:510:CLA:HBB1	22:C:510:CLA:HMB1	1.81	0.63
37:H:101:RRX:H46	37:H:101:RRX:H55	1.95	0.63
4:D:85:MET:CE	4:D:96:GLU:HG2	2.28	0.63
14:U:9:LEU:HA	40:U:301:HOH:O	1.98	0.63
3:C:179:ALA:O	3:C:184:GLY:HA2	2.21	0.62
2:B:350:GLU:HG3	31:B:631:DMS:C1	2.30	0.62
22:D:404:CLA:HBB1	22:D:404:CLA:HMB1	1.81	0.62
12:O:74[A]:GLU:OE2	40:O:401:HOH:O	2.16	0.62
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.82	0.61
26:A:411:PL9:H403	6:F:22:ALA:HB2	1.82	0.61
5:E:22:ILE:O	5:E:25:ILE:HG22	4.25	0.61
12:O:102:ASP:OD1	12:O:123:LYS:NZ	2.85	0.61
1:A:265:PHE:HE2	26:A:411:PL9:H122	1.64	0.61
1:A:215:HIS:HA	26:A:411:PL9:O1	2.01	0.60
6:F:15:ILE:O	6:F:15:ILE:HG23	3.17	0.60
5:E:20:TRP:CD1	9:J:8:ILE:HD13	2.35	0.60
34:D:415:HTG:H3	15:V:55:ARG:HH12	1.66	0.60
22:C:507:CLA:HMC2	22:C:508:CLA:H102	1.83	0.60
37:H:101:RRX:H46	37:H:101:RRX:C33	2.62	0.60
22:C:512:CLA:HMB1	22:C:512:CLA:HBB1	1.83	0.60
12:O:18:LYS:HE3	40:O:490:HOH:O	52.84	0.60
4:D:85:MET:CE	4:D:90[A]:LEU:HD21	2.38	0.60
22:C:511:CLA:HMB1	22:C:511:CLA:HBB1	1.83	0.59
2:B:350:GLU:HG3	31:B:631:DMS:H12	1.84	0.59
25:D:412:LMG:H352	34:D:414:HTG:H6'2	1.84	0.59
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.59
1:A:223:LEU:HD22	4:D:265:ARG:HG2	1.84	0.59
17:X:34:ILE:C	17:X:36:LYS:H	3.45	0.58
22:B:606:CLA:C14	22:B:611:CLA:HED2	2.33	0.58
26:D:406:PL9:C32	27:L:101:LHG:H223	2.32	0.58
22:B:615:CLA:HED3	11:L:8:GLN:O	2.44	0.58
12:O:47:PRO:HG3	12:O:120:PHE:CE1	2.38	0.58
7:H:3[A]:ARG:HB2	7:H:3[A]:ARG:HH11	4.79	0.58
7:H:3[A]:ARG:HB2	7:H:3[A]:ARG:NH1	5.31	0.58
4:D:85:MET:HE3	4:D:96:GLU:HG2	1.96	0.58
4:D:49:LEU:HD21	25:J:101:LMG:H341	1.84	0.58
1:A:265:PHE:O	26:A:411:PL9:H531	2.04	0.58
2:B:137:LYS:O	2:B:141:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:606:CLA:HBB1	22:B:606:CLA:HHC	2.81	0.57
2:B:223:GLN:NE2	40:B:703:HOH:O	2.37	0.57
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.86	0.57
37:H:101:RRX:C23	37:H:101:RRX:H17	2.69	0.57
15:V:78:ASN:OD1	15:V:96:ARG:NH1	2.77	0.57
24:B:620:BCR:HC8	24:B:620:BCR:C33	2.93	0.57
27:D:409:LHG:HC92	27:L:101:LHG:HC92	1.86	0.57
22:C:502:CLA:HMD2	22:C:503:CLA:H101	1.87	0.57
29:A:414:LMT:H2B	4:D:304:ARG:NH2	2.18	0.57
2:B:356:VAL:HG23	31:B:638:DMS:H22	18.55	0.57
22:B:615:CLA:HBB1	22:B:615:CLA:HMB1	1.86	0.57
31:O:310:DMS:C1	40:O:427:HOH:O	2.52	0.56
12:O:39:ARG:HD3	40:O:413:HOH:O	2.04	0.56
2:B:29:LEU:HD11	24:B:618:BCR:H12C	2.65	0.56
26:A:411:PL9:H221	23:D:402:PHO:HMA2	1.87	0.56
10:K:21:LEU:HB2	16:Y:24:MET:HE3	3.90	0.56
1:A:322:ASN:OD1	3:C:412:THR:HA	2.23	0.56
1:A:329:GLU:HG3	40:A:617:HOH:O	23.17	0.56
1:A:96:ILE:HD12	22:A:408:CLA:HMD1	1.86	0.56
2:B:248:ALA:HB2	22:B:604:CLA:H51	1.87	0.56
34:D:415:HTG:C3	15:V:55:ARG:HH12	2.19	0.56
4:D:90[B]:LEU:HG	4:D:109:GLY:HA2	2.06	0.56
23:A:407:PHO:HBB1	23:A:407:PHO:HMB1	1.87	0.56
12:O:39:ARG:NH1	40:O:404:HOH:O	2.39	0.56
2:B:103:LEU:HD21	22:B:606:CLA:HMC3	1.96	0.56
22:B:609:CLA:H203	22:B:610:CLA:H191	2.63	0.56
3:C:437:PHE:CE1	22:C:511:CLA:HMB3	2.41	0.56
22:D:401:CLA:HMC1	22:D:401:CLA:HBC2	1.88	0.56
29:B:622:LMT:H11	25:D:412:LMG:HC92	1.88	0.55
9:J:18:GLY:HA3	24:Y:101:BCR:H371	2.11	0.55
2:B:339:ALA:HB2	12:O:58:ASN:HB3	45.08	0.55
2:B:125:ASP:CB	2:B:128:THR:CG2	5.31	0.55
24:C:515:BCR:H331	24:C:515:BCR:C8	2.36	0.55
16:Y:20:ALA:O	16:Y:24:MET:HG2	2.07	0.55
22:B:611:CLA:HBB1	22:B:611:CLA:HHC	1.87	0.55
2:B:281:GLN:NE2	40:B:702:HOH:O	48.71	0.55
12:O:208:THR:O	31:O:305:DMS:H13	8.97	0.55
3:C:126:GLY:O	3:C:130:VAL:HG23	2.54	0.55
8:I:13:THR:O	8:I:17:LEU:HG	2.07	0.55
15:V:129[B]:LYS:HB3	31:V:212:DMS:S	2.47	0.55
2:B:63:LEU:N	2:B:64:PRO:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:20:PRO:HB3	16:Y:21:GLN:HG3	1.88	0.55
2:B:389:LYS:NZ	34:D:415:HTG:H2'2	2.22	0.54
27:D:411:LHG:H161	27:D:411:LHG:C32	2.32	0.54
1:A:265:PHE:CE2	26:A:411:PL9:H122	2.42	0.54
2:B:324:LEU:HA	4:D:293[B]:LEU:HG	5.32	0.54
2:B:128:THR:HG23	2:B:130:GLU:H	4.46	0.54
4:D:192:THR:HG23	22:D:403:CLA:HBC2	1.90	0.54
15:V:27:LEU:HD21	31:V:206:DMS:H11	1.88	0.54
28:A:413:SQD:H272	2:B:109:LEU:HD13	60.26	0.54
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.88	0.54
22:B:611:CLA:OBD	22:B:611:CLA:H152	2.18	0.54
12:O:216:GLU:CD	12:O:234:LYS:HD2	2.28	0.54
28:C:501:SQD:H302	22:C:509:CLA:H71	1.90	0.54
12:O:66:VAL:CG1	12:O:67:PRO:CD	2.83	0.54
22:B:608:CLA:H191	26:D:406:PL9:H303	1.89	0.54
9:J:18:GLY:O	9:J:22:ILE:HD12	2.08	0.54
12:O:55:GLU:OE2	12:O:231:HIS:CD2	4.77	0.54
4:D:11:GLU:O	4:D:12:ARG:CB	2.56	0.53
1:A:334:ARG:HD3	4:D:320:LEU:HD13	2.09	0.53
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.53
2:B:314:TYR:CE1	2:B:316:GLY:HA3	2.43	0.53
22:C:505:CLA:H112	35:C:519:DGD:HBF1	1.89	0.53
24:C:516:BCR:H331	24:C:516:BCR:C8	2.39	0.53
15:V:129[A]:LYS:HB3	31:V:210:DMS:S	27.15	0.53
29:B:622:LMT:H11	25:D:412:LMG:C9	2.39	0.53
16:Y:23:THR:HG22	16:Y:27:MET:CE	3.21	0.53
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.90	0.53
14:U:58:VAL:HG12	14:U:79:LEU:HD22	2.27	0.53
17:X:23:LEU:O	17:X:27:VAL:HG23	2.08	0.53
1:A:221:SER:HB2	4:D:139:ARG:O	2.09	0.53
18:Z:9:LEU:HD13	18:Z:54:VAL:HG11	2.54	0.53
22:A:406:CLA:HMD3	4:D:182:LEU:HD11	1.89	0.53
27:D:410:LHG:H171	27:L:101:LHG:H201	1.91	0.53
15:V:126:LEU:O	15:V:129[A]:LYS:CD	2.56	0.53
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.64	0.53
2:B:355:PHE:O	2:B:370:LEU:HA	2.32	0.53
22:B:603:CLA:H201	35:H:102:DGD:HBT1	3.13	0.53
30:U:201:UNL:C4	40:U:346:HOH:O	2.57	0.53
22:B:616:CLA:H161	7:H:7:LEU:HD21	2.30	0.52
14:U:38:TYR:HB2	14:U:41:LEU:HD12	1.91	0.52
2:B:41:GLU:HB3	2:B:60:MET:SD	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:33:LYS:O	8:I:35:LYS:HG3	2.33	0.52
3:C:28:GLN:NE2	28:C:501:SQD:O7	2.36	0.52
22:C:505:CLA:H42	35:C:518:DGD:HB42	1.91	0.52
1:A:266:ASN:HD22	4:D:237:PRO:HG3	4.70	0.52
10:K:21:LEU:HD13	16:Y:24:MET:CE	2.54	0.52
12:O:158:ASP:HB2	12:O:159:PRO:CD	2.39	0.52
5:E:7:GLU:HG2	6:F:19:ARG:CZ	4.04	0.52
25:D:412:LMG:O9	25:D:412:LMG:O2	2.19	0.52
4:D:123:ILE:HD11	35:H:102:DGD:HAW1	4.10	0.52
34:D:415:HTG:H7'3	14:U:37:GLN:HE22	1.74	0.52
22:C:514:CLA:C4B	24:C:515:BCR:H383	2.40	0.52
12:O:40:ILE:HD12	12:O:95:PHE:CD2	2.73	0.52
3:C:437:PHE:CZ	22:C:511:CLA:HMB3	2.46	0.51
22:B:605:CLA:HMD2	22:B:613:CLA:H203	1.91	0.51
12:O:39:ARG:HG3	12:O:246:ALA:HB2	4.01	0.51
1:A:63:ILE:HB	3:C:335:THR:HG21	1.92	0.51
2:B:125:ASP:CG	2:B:128:THR:HG22	6.43	0.51
22:B:614:CLA:HMB1	22:B:614:CLA:CBB	2.65	0.51
22:B:608:CLA:H193	4:D:281:MET:SD	2.50	0.51
8:I:12:VAL:O	8:I:16:VAL:HG23	2.11	0.51
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.93	0.51
22:B:602:CLA:C9	37:H:101:RRX:H25	3.02	0.51
12:O:133:VAL:HG13	31:O:304:DMS:H23	1.93	0.51
31:C:530:DMS:H11	40:C:737:HOH:O	2.09	0.51
34:D:415:HTG:H62	40:V:301:HOH:O	2.11	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.54	0.51
2:B:128:THR:HB	2:B:130:GLU:H	1.75	0.51
2:B:355:PHE:HA	31:B:638:DMS:C2	17.76	0.51
3:C:143:TYR:HE2	34:C:532:HTG:H61	1.76	0.51
24:K:101:BCR:H331	24:K:101:BCR:C8	2.65	0.51
3:C:147:PHE:CD2	22:C:514:CLA:H3A	2.46	0.51
14:U:45:LEU:HD21	14:U:71:GLN:HB3	2.42	0.50
2:B:299:GLU:HG2	2:B:402:TYR:HD1	2.04	0.50
2:B:121:GLU:HA	7:H:2:ALA:HB1	1.93	0.50
3:C:334:PRO:HA	12:O:153:THR:OG1	2.11	0.50
31:O:310:DMS:H11	40:O:427:HOH:O	2.10	0.50
2:B:115:TRP:CD2	24:B:618:BCR:HC21	2.47	0.50
29:A:414:LMT:H12	34:B:623:HTG:H5	48.98	0.50
3:C:279:LEU:HD12	3:C:282:MET:HE1	1.92	0.50
3:C:60:ILE:HG22	22:C:504:CLA:HHD	1.94	0.50
12:O:178:LYS:HG2	31:O:304:DMS:H23	62.04	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LEU:CD2	4:D:265:ARG:HG2	2.42	0.50
10:K:25:LEU:N	10:K:26:PRO:CD	2.98	0.50
12:O:103:PHE:HA	12:O:120:PHE:O	2.21	0.50
29:A:414:LMT:H32	2:B:43:ALA:HA	42.43	0.49
22:B:609:CLA:H111	4:D:120:PHE:CE1	3.14	0.49
23:D:402:PHO:HMB1	23:D:402:PHO:HBB1	1.93	0.49
22:B:606:CLA:HHC	22:B:606:CLA:CBB	2.82	0.49
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.47	0.49
39:V:202:HEC:HMD2	40:V:360:HOH:O	2.12	0.49
2:B:221:PRO:HA	22:B:610:CLA:HED3	2.14	0.49
3:C:180:MET:HG2	3:C:199:ILE:O	2.12	0.49
16:Y:38:LEU:O	16:Y:42:ARG:HG2	4.41	0.49
1:A:103:ASP:OD1	31:A:419:DMS:H21	2.13	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.49
35:C:519:DGD:HBN1	27:D:411:LHG:H222	1.95	0.49
2:B:462:PHE:CZ	22:B:614:CLA:HMB3	2.75	0.49
2:B:62:VAL:HB	22:B:606:CLA:HED3	2.11	0.49
22:B:606:CLA:HBB1	22:B:607:CLA:C5	2.43	0.49
3:C:308:GLU:HB2	3:C:361:PHE:CE2	2.47	0.49
12:O:129:THR:HA	12:O:141:ASP:O	2.13	0.49
1:A:237:TYR:CB	4:D:265:ARG:HD2	2.43	0.49
4:D:272:LEU:HD23	4:D:272:LEU:C	2.34	0.48
22:B:615:CLA:OBD	11:L:10:VAL:CG2	4.65	0.48
1:A:121[B]:LEU:HD11	22:C:506:CLA:H152	1.94	0.48
26:A:411:PL9:H251	26:A:411:PL9:H272	1.66	0.48
31:B:638:DMS:H13	40:B:778:HOH:O	2.13	0.48
3:C:162:GLY:HA2	3:C:248:GLY:HA2	2.29	0.48
3:C:31:SER:CB	3:C:41:ARG:HG2	2.53	0.48
26:D:406:PL9:H401	11:L:29:LEU:HD23	1.94	0.48
26:A:411:PL9:H301	4:D:45:LEU:HD22	1.96	0.48
2:B:12:LEU:HB2	22:B:613:CLA:HMC2	2.24	0.48
1:A:249:VAL:HG12	2:B:491:VAL:HG23	1.95	0.48
3:C:117:VAL:HG12	25:C:531:LMG:H222	1.95	0.48
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.14	0.48
12:O:193:THR:HG21	12:O:220:LEU:HD12	2.15	0.48
12:O:145:GLU:CB	31:O:303:DMS:H23	2.43	0.48
15:V:72:LEU:HD12	15:V:120:LEU:HD11	2.93	0.48
1:A:304:HIS:CE1	31:V:212:DMS:H12	2.47	0.48
2:B:355:PHE:HA	31:B:638:DMS:H21	18.51	0.48
22:C:502:CLA:H42	22:C:503:CLA:HMD1	1.95	0.48
3:C:174:LEU:HB3	22:C:503:CLA:H161	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:D:410:LHG:HB2	13:T:17:PHE:HZ	1.79	0.48
31:V:207:DMS:H22	40:V:380:HOH:O	2.14	0.48
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.95	0.48
4:D:73:PHE:CZ	25:J:101:LMG:H182	5.49	0.48
18:Z:23:VAL:HG22	18:Z:40:ILE:HG12	2.61	0.48
2:B:162:PHE:O	22:B:607:CLA:HHD	2.17	0.47
22:B:610:CLA:H42	25:D:412:LMG:H171	1.95	0.47
3:C:461:ARG:HD2	4:D:225:ASP:OD1	2.14	0.47
4:D:51:GLY:HA3	4:D:78:VAL:HG22	2.01	0.47
16:Y:42:ARG:HD2	18:Z:29:SER:OG	4.07	0.47
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.49	0.47
4:D:236:ASN:O	4:D:239:GLN:HG2	2.19	0.47
7:H:38:PHE:HB2	37:H:101:RRX:C10	2.59	0.47
12:O:55:GLU:OE2	12:O:231:HIS:HD2	5.61	0.47
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.47
22:B:604:CLA:H18	22:B:610:CLA:H91	2.67	0.47
22:B:609:CLA:H142	7:H:39:LEU:HD21	2.54	0.47
22:B:609:CLA:HMB1	22:B:609:CLA:HBB1	1.95	0.47
3:C:202:PRO:HB3	3:C:234:VAL:HG12	2.44	0.47
14:U:27:LEU:HD22	14:U:49:ILE:HG21	2.06	0.47
3:C:414:ILE:HD13	31:V:212:DMS:C1	2.44	0.47
17:X:34:ILE:O	17:X:36:LYS:N	3.96	0.47
2:B:228:ALA:HB2	29:B:622:LMT:H21	1.96	0.47
7:H:28:THR:HB	7:H:29:PRO:HD3	2.26	0.47
24:B:618:BCR:C8	24:B:618:BCR:H331	2.43	0.47
1:A:223:LEU:HD12	4:D:139:ARG:HH12	1.79	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.96	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.57	0.47
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.96	0.47
22:D:401:CLA:CMC	22:D:401:CLA:HBC2	2.45	0.47
40:B:829:HOH:O	31:O:304:DMS:H11	83.40	0.47
3:C:75:PHE:HZ	3:C:105:VAL:HG21	2.10	0.47
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.97	0.47
24:Y:101:BCR:H312	18:Z:16:SER:HB3	1.96	0.47
31:B:638:DMS:C1	40:B:778:HOH:O	2.63	0.47
12:O:145:GLU:HB2	31:O:303:DMS:H23	1.96	0.47
18:Z:47:TRP:CD2	29:Z:101:LMT:H111	2.50	0.47
1:A:257:ARG:O	4:D:128:ARG:NH2	3.15	0.47
1:A:270:SER:HB2	28:C:501:SQD:O49	2.16	0.47
2:B:451:PHE:CD1	2:B:451:PHE:C	2.99	0.47
24:K:101:BCR:H371	24:K:101:BCR:H24C	1.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:O:303:DMS:H11	40:O:550:HOH:O	2.14	0.47
1:A:237:TYR:HD2	1:A:245:THR:HB	1.78	0.46
1:A:73:TYR:CD1	29:A:414:LMT:H3B	2.50	0.46
4:D:52:THR:HB	4:D:76:VAL:CG2	2.45	0.46
5:E:63:ILE:HG23	5:E:64:PRO:HD2	1.97	0.46
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.20	0.46
31:O:310:DMS:H13	40:O:427:HOH:O	2.13	0.46
1:A:29:TYR:CE1	1:A:31:GLY:HA3	2.66	0.46
4:D:343[B]:GLU:HG3	40:V:301:HOH:O	2.14	0.46
27:D:411:LHG:H111	27:D:411:LHG:H162	1.96	0.46
4:D:343[B]:GLU:CD	34:D:415:HTG:H2	2.36	0.46
3:C:265:ILE:HD11	3:C:449:ARG:HD3	1.98	0.46
4:D:178:ILE:O	4:D:181:PHE:HB3	2.15	0.46
2:B:450:TRP:CZ3	4:D:293[B]:LEU:HD21	4.66	0.46
22:C:505:CLA:H201	27:D:411:LHG:C34	2.46	0.46
22:C:511:CLA:H192	22:C:511:CLA:HBC3	1.98	0.46
4:D:170:ALA:HB1	4:D:171:PRO:CD	2.45	0.46
22:C:509:CLA:C2B	22:C:511:CLA:HBA1	2.45	0.46
2:B:216:HIS:HE1	22:B:610:CLA:C1A	2.40	0.46
22:C:513:CLA:C11	22:C:514:CLA:H141	2.46	0.46
15:V:79:PRO:HD3	15:V:94:SER:HB3	1.97	0.46
22:C:503:CLA:H61	22:C:513:CLA:H42	1.98	0.46
22:C:513:CLA:H92	22:C:514:CLA:H203	1.97	0.46
17:X:11:PHE:O	17:X:15[A]:LEU:HG	2.16	0.46
2:B:276:ASP:OD1	31:B:641:DMS:H22	2.15	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	2.22	0.46
22:C:505:CLA:H191	27:D:411:LHG:C34	2.46	0.46
4:D:55:VAL:O	4:D:66:SER:HB3	2.15	0.46
37:H:101:RRX:H48	37:H:101:RRX:H47	2.05	0.46
4:D:162:LEU:HD21	35:H:102:DGD:HA21	1.97	0.46
2:B:350:GLU:HG3	31:B:631:DMS:S	2.56	0.46
1:A:269:ARG:HD2	4:D:235:PHE:HB2	2.58	0.46
2:B:406:LEU:O	2:B:409:GLN:HG3	2.88	0.45
2:B:186:GLY:HA3	40:B:839:HOH:O	57.46	0.45
22:B:602:CLA:H203	22:B:602:CLA:H151	5.79	0.45
4:D:39:PRO:O	4:D:43:LEU:HG	2.17	0.45
2:B:25:MET:HE3	24:B:618:BCR:H333	3.52	0.45
3:C:154:LYS:HG2	3:C:266:TRP:CE3	3.14	0.45
22:B:610:CLA:HMC2	37:H:101:RRX:H44	1.99	0.45
22:B:602:CLA:HMC1	7:H:44:ILE:HG21	2.30	0.45
22:B:607:CLA:H102	22:B:607:CLA:H61	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:608:CLA:HBB1	22:B:608:CLA:HMB1	1.97	0.45
22:B:602:CLA:H161	37:H:101:RRX:C16	5.62	0.45
12:O:93:LEU:O	12:O:128:SER:HA	2.51	0.45
15:V:129[B]:LYS:HE3	15:V:136:TYR:O	3.74	0.45
22:B:605:CLA:C3B	22:B:614:CLA:HMC3	2.65	0.45
22:C:514:CLA:NB	24:C:515:BCR:H383	2.31	0.45
15:V:30:LYS:HG3	15:V:118:HIS:CE1	2.52	0.45
22:B:605:CLA:HBB1	22:B:605:CLA:HMB1	1.99	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.45
9:J:26:GLY:HA2	30:J:103:UNL:C10	3.43	0.45
12:O:92:SER:HB3	12:O:131:PRO:HA	1.99	0.45
3:C:294:ASN:HA	3:C:297:TYR:O	2.17	0.45
3:C:400:PRO:C	3:C:401:LEU:HD12	2.64	0.45
4:D:79:SER:HA	4:D:172:SER:HB3	1.97	0.45
5:E:20:TRP:HD1	9:J:8:ILE:HD13	1.82	0.45
26:D:406:PL9:H322	27:L:101:LHG:H223	1.98	0.45
16:Y:23:THR:HG22	16:Y:27:MET:HE1	3.26	0.45
22:B:606:CLA:HBB1	22:B:607:CLA:H51	1.99	0.45
4:D:52:THR:HB	4:D:76:VAL:HG21	1.97	0.45
22:B:609:CLA:C14	7:H:39:LEU:HD21	2.79	0.45
12:O:86:LYS:HE3	40:O:549:HOH:O	2.15	0.45
14:U:53:ALA:HB1	14:U:54:PRO:HA	2.12	0.45
18:Z:62:VAL:C	40:Z:203:HOH:O	2.55	0.45
4:D:266:TRP:CG	27:D:410:LHG:HC2	2.51	0.45
2:B:495:PHE:C	2:B:496:TYR:HD1	2.21	0.44
22:B:611:CLA:CBB	22:B:611:CLA:HHC	2.46	0.44
22:B:616:CLA:HMB1	22:B:616:CLA:HBB1	2.29	0.44
15:V:41:HIS:HA	15:V:45:ILE:O	2.17	0.44
22:A:408:CLA:HBA1	22:A:408:CLA:C4A	2.69	0.44
22:B:612:CLA:H72	22:B:612:CLA:H112	1.68	0.44
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.44
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.52	0.44
15:V:118:HIS:CE1	15:V:122:GLU:HG2	2.53	0.44
3:C:266:TRP:CZ3	22:C:508:CLA:HAC2	2.52	0.44
25:C:520:LMG:H241	9:J:22:ILE:HG12	1.99	0.44
25:C:531:LMG:HC8	25:C:531:LMG:HC1	1.77	0.44
3:C:68:THR:OG1	22:C:504:CLA:HED1	2.17	0.44
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.44
5:E:39:SER:HB3	29:E:101:LMT:H6E	1.99	0.44
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.84	0.44
5:E:60:GLN:NE2	5:E:62:SER:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:97:GLU:OE2	12:O:102:ASP:OD2	2.36	0.44
4:D:24:ARG:NH2	17:X:35:ASP:OD2	2.51	0.44
1:A:121[B]:LEU:CD2	22:A:408:CLA:HMB3	2.47	0.44
2:B:237:VAL:HG11	22:B:611:CLA:H201	3.16	0.44
22:B:602:CLA:H91	37:H:101:RRX:H25	2.10	0.44
22:A:408:CLA:H203	22:C:507:CLA:H101	2.00	0.44
2:B:226:TYR:HA	2:B:231:MET:HG3	1.99	0.44
22:B:606:CLA:H141	22:B:611:CLA:HED2	1.98	0.44
3:C:50:LEU:HD12	22:C:513:CLA:HMD3	1.98	0.44
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.48	0.44
39:V:202:HEC:HMD2	40:V:329:HOH:O	32.06	0.44
2:B:315:ILE:HG22	2:B:426:PHE:HB3	2.00	0.44
22:B:603:CLA:H41	7:H:46:LEU:HA	1.98	0.44
22:B:606:CLA:H122	22:B:611:CLA:HMA2	2.00	0.44
28:C:501:SQD:H111	27:C:522:LHG:H261	2.00	0.44
22:C:504:CLA:HBB1	22:C:504:CLA:HMB1	1.99	0.44
37:H:101:RRX:H47	37:H:101:RRX:H43	1.77	0.44
7:H:43:LEU:O	7:H:47:GLU:HG3	2.37	0.44
3:C:348:GLU:OE2	12:O:11:VAL:HA	2.17	0.44
15:V:2:GLU:OE2	31:V:207:DMS:C1	2.66	0.44
7:H:3[A]:ARG:CB	7:H:3[A]:ARG:HH11	4.72	0.43
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.99	0.43
22:A:408:CLA:H162	22:A:408:CLA:H203	4.19	0.43
28:C:501:SQD:H132	28:C:501:SQD:H162	1.40	0.43
4:D:90[A]:LEU:HA	4:D:90[A]:LEU:HD23	1.41	0.43
22:B:610:CLA:HMD1	7:H:27:THR:HB	2.25	0.43
40:D:630:HOH:O	30:X:101:UNL:C1	2.66	0.43
1:A:202:VAL:HG11	22:A:406:CLA:C3D	2.47	0.43
22:B:617:CLA:HBB1	22:B:617:CLA:HMB1	1.99	0.43
22:B:614:CLA:H121	25:B:621:LMG:H232	1.99	0.43
4:D:267:LEU:HD23	4:D:267:LEU:C	2.53	0.43
5:E:17:VAL:HG23	9:J:7:ARG:CB	2.49	0.43
16:Y:23:THR:HG22	16:Y:27:MET:HE2	4.13	0.43
22:B:608:CLA:H112	22:B:608:CLA:H91	1.76	0.43
22:C:503:CLA:H193	34:C:521:HTG:H2'1	2.00	0.43
9:J:18:GLY:O	9:J:22:ILE:CD1	2.67	0.43
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.09	0.43
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.53	0.43
23:D:402:PHO:HBC2	23:D:402:PHO:HHD	2.01	0.43
15:V:41:HIS:CD2	39:V:202:HEC:NB	3.02	0.43
32:A:421[B]:BCT:O3	4:D:214:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.43
12:O:178:LYS:HG2	31:O:304:DMS:H21	60.99	0.43
1:A:102:LEU:HD23	1:A:102:LEU:HA	2.31	0.43
2:B:153:PHE:O	2:B:157:HIS:HB3	2.19	0.43
12:O:204:VAL:HG13	12:O:211:ILE:HG22	2.53	0.43
1:A:161:TYR:CZ	1:A:165:GLN:HG3	2.60	0.43
4:D:170:ALA:HB1	4:D:171:PRO:HD2	2.01	0.43
31:B:628:DMS:C1	40:D:502:HOH:O	2.66	0.43
5:E:13:ILE:HG21	36:E:102:HEM:HAD2	2.00	0.43
18:Z:15:LEU:O	18:Z:18:VAL:HG22	2.19	0.43
1:A:103:ASP:OD1	31:A:419:DMS:C2	2.66	0.43
22:B:615:CLA:OBD	11:L:10:VAL:HG22	5.40	0.43
3:C:163:PHE:CD2	22:C:513:CLA:HAB	2.54	0.43
3:C:414:ILE:HD13	31:V:212:DMS:H11	2.01	0.43
5:E:6:GLY:HA2	40:E:216:HOH:O	51.11	0.43
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.70	0.42
22:B:602:CLA:H72	22:B:602:CLA:H2	4.71	0.42
1:A:239:PHE:O	13:T:29:ILE:HA	3.23	0.42
2:B:284:ILE:CG2	2:B:302:TRP:CZ3	3.34	0.42
25:A:410:LMG:H291	3:C:216:SER:HA	2.01	0.42
3:C:312:ALA:HB1	3:C:392:ALA:O	2.19	0.42
3:C:424:SER:O	3:C:428:THR:HG23	2.38	0.42
27:D:409:LHG:HC82	27:D:409:LHG:H361	2.00	0.42
2:B:108:PHE:HE2	24:B:618:BCR:H333	2.05	0.42
3:C:124:VAL:HB	24:C:515:BCR:H362	2.00	0.42
4:D:171:PRO:HG3	4:D:181:PHE:CZ	2.55	0.42
14:U:87:VAL:HG22	31:U:203:DMS:H13	2.01	0.42
3:C:210:PHE:HA	3:C:213:LEU:HD12	3.05	0.42
4:D:291:LEU:HD21	35:H:102:DGD:CGB	2.50	0.42
15:V:31:ARG:HG2	15:V:31:ARG:HH11	2.69	0.42
22:B:616:CLA:H112	22:B:616:CLA:H152	4.01	0.42
31:C:540:DMS:H11	40:C:638:HOH:O	2.19	0.42
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.07	0.42
2:B:144:PHE:CE2	2:B:210:ILE:HG23	2.67	0.42
27:D:409:LHG:H332	27:D:409:LHG:H121	2.00	0.42
12:O:140:THR:HG23	31:O:304:DMS:H22	2.00	0.42
1:A:218:LEU:HD12	26:A:411:PL9:C3	2.49	0.42
2:B:94:GLU:HG2	34:B:623:HTG:H2'1	4.71	0.42
10:K:19:ASP:HB3	10:K:20:PRO:CD	2.45	0.42
14:U:36:ILE:HG13	14:U:42:TYR:CG	2.55	0.42
15:V:26:TYR:CE2	15:V:118:HIS:HD2	6.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:HD1	29:A:414:LMT:H3B	1.83	0.42
2:B:113:TRP:CD1	22:B:617:CLA:HBA2	3.16	0.42
2:B:98:LEU:HB2	34:B:623:HTG:H7'3	2.02	0.42
22:D:401:CLA:H162	22:D:401:CLA:H203	1.75	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.56	0.42
12:O:23:ASP:O	12:O:203:LYS:HE3	4.65	0.42
1:A:45:THR:HG23	22:A:408:CLA:H201	26.36	0.42
2:B:387:GLU:HG2	34:D:415:HTG:H5'1	2.02	0.42
22:B:606:CLA:H143	22:B:611:CLA:HED2	2.18	0.42
3:C:409:GLY:HA2	31:V:201:DMS:S	2.59	0.42
22:A:408:CLA:C20	22:C:507:CLA:H101	2.49	0.42
37:H:101:RRX:H3	17:X:2:THR:N	2.18	0.42
7:H:42:LEU:HD23	7:H:42:LEU:HA	1.93	0.42
6:F:19:ARG:O	6:F:23:VAL:HG23	2.51	0.42
1:A:323:ARG:HB3	4:D:329:MET:HA	2.02	0.41
22:B:610:CLA:HMB2	22:B:611:CLA:C2B	2.54	0.41
12:O:180:GLU:H	12:O:180:GLU:CD	2.24	0.41
3:C:26:ARG:NH2	16:Y:46:LEU:OXT	2.82	0.41
22:A:406:CLA:HAB	22:A:406:CLA:HHC	1.80	0.41
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.84	0.41
3:C:25:ASN:HA	3:C:30:SER:CB	2.50	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.41
31:B:629:DMS:H11	40:B:734:HOH:O	59.94	0.41
8:I:27:ASP:N	8:I:28:PRO:CD	3.09	0.41
24:Y:101:BCR:HC8	24:Y:101:BCR:H311	2.61	0.41
1:A:21:VAL:HG11	1:A:32:TRP:CE3	2.88	0.41
1:A:259:ILE:HG22	1:A:260:PHE:N	2.87	0.41
24:B:618:BCR:H332	13:T:19:PHE:CZ	34.86	0.41
13:T:28:ARG:HA	13:T:28:ARG:HD3	1.87	0.41
22:A:405:CLA:H193	22:A:405:CLA:H161	1.70	0.41
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.55	0.41
2:B:75:TRP:CH2	34:B:626:HTG:H2'1	2.80	0.41
37:H:101:RRX:H28	37:H:101:RRX:H32	1.89	0.41
2:B:124:ARG:HD2	2:B:129:GLY:O	2.20	0.41
2:B:467:ILE:HG13	4:D:126:MET:HE1	2.29	0.41
2:B:6:TYR:OH	27:D:409:LHG:HC11	2.21	0.41
3:C:168:LEU:HD21	22:C:510:CLA:H62	2.02	0.41
3:C:433:LEU:HD13	22:C:503:CLA:CHC	2.50	0.41
22:C:507:CLA:HBB1	22:C:507:CLA:CMB	2.47	0.41
15:V:118:HIS:CE1	15:V:122:GLU:CG	3.04	0.41
2:B:156:PHE:HB3	2:B:162:PHE:HB3	2.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:608:CLA:H2	25:B:621:LMG:H161	2.01	0.41
2:B:270:PRO:HG2	2:B:317:ASN:O	2.70	0.41
2:B:446:SER:CB	2:B:447:PRO:CD	2.91	0.41
22:C:508:CLA:HMB1	22:C:508:CLA:HBB1	2.02	0.41
23:D:402:PHO:ND	23:D:402:PHO:NC	2.68	0.41
24:D:405:BCR:C8	24:D:405:BCR:H331	2.50	0.41
7:H:31:MET:O	7:H:35:MET:HG3	2.54	0.41
10:K:31:LEU:HD23	10:K:31:LEU:HA	2.25	0.41
15:V:5:PRO:HD3	31:V:205:DMS:C1	2.50	0.41
1:A:182:PHE:O	1:A:186:PHE:HB2	2.28	0.41
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.50	0.41
14:U:45:LEU:O	14:U:49:ILE:HG13	2.20	0.41
1:A:21:VAL:HG11	1:A:32:TRP:CZ3	3.12	0.41
12:O:143:LYS:HE3	31:O:306:DMS:C2	2.51	0.41
2:B:137:LYS:NZ	40:B:709:HOH:O	59.82	0.41
10:K:21:LEU:O	10:K:25:LEU:HG	2.53	0.41
31:O:312:DMS:C2	40:O:467:HOH:O	2.59	0.41
1:A:42:LEU:HD23	28:A:413:SQD:H192	2.02	0.40
2:B:224:ARG:HG2	7:H:24:GLY:O	2.22	0.40
2:B:273:TYR:HA	2:B:276:ASP:HB2	2.03	0.40
3:C:109:PHE:N	3:C:110:PRO:CD	2.97	0.40
2:B:121:GLU:CA	7:H:2:ALA:HB1	2.50	0.40
2:B:339:ALA:CB	12:O:58:ASN:HB3	45.19	0.40
22:B:609:CLA:HMB3	4:D:126:MET:HG2	2.51	0.40
22:B:613:CLA:HHC	22:B:613:CLA:HAB	1.91	0.40
2:B:115:TRP:CZ3	24:B:618:BCR:H322	2.57	0.40
31:C:536:DMS:H22	40:C:750:HOH:O	2.21	0.40
4:D:103:ARG:O	4:D:107:LEU:HG	2.34	0.40
12:O:130:GLN:NE2	12:O:141:ASP:H	2.20	0.40
12:O:179:GLU:HA	31:O:307:DMS:H12	35.72	0.40
1:A:72:LEU:HD21	29:T:102:LMT:H41	2.03	0.40
2:B:194:ASN:HA	2:B:195:PRO:HD2	1.90	0.40
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.09	0.40
13:T:20:ALA:O	13:T:24:ARG:HB3	2.21	0.40
15:V:124:LYS:CE	40:V:356:HOH:O	19.87	0.40
15:V:129[A]:LYS:HB3	31:V:212:DMS:S	2.61	0.40
1:A:276:ALA:O	1:A:280:VAL:HG23	2.41	0.40
2:B:41:GLU:OE1	2:B:63:LEU:HB2	2.21	0.40
12:O:130:GLN:HG2	40:O:480:HOH:O	26.57	0.40
14:U:83:THR:OG1	14:U:84:VAL:N	2.74	0.40
16:Y:34:MET:HE2	16:Y:34:MET:HA	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:HB3	3:C:401:LEU:HA	2.03	0.40
22:A:408:CLA:H41	22:A:408:CLA:H61	1.70	0.40
2:B:149:LEU:HB2	22:B:605:CLA:H171	2.22	0.40
2:B:204:ALA:CB	22:B:603:CLA:HAB	2.61	0.40
3:C:107:ASP:O	3:C:110:PRO:HD2	2.30	0.40
3:C:221:GLU:O	3:C:226:SER:HB3	2.27	0.40
4:D:125:PHE:CE1	23:D:402:PHO:HBD	2.57	0.40
4:D:17:ILE:O	4:D:20:ASP:HB2	2.22	0.40
6:F:15:ILE:O	6:F:15:ILE:CG2	3.28	0.40
39:V:202:HEC:HMB1	39:V:202:HEC:HBB3	2.58	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	333/334 (100%)	326 (98%)	6 (2%)	1 (0%)	43	48
1	a	333/334 (100%)	321 (96%)	11 (3%)	1 (0%)	43	48
2	B	506/505 (100%)	495 (98%)	11 (2%)	0	100	100
2	b	482/505 (95%)	465 (96%)	17 (4%)	0	100	100
3	C	449/455 (99%)	434 (97%)	13 (3%)	2 (0%)	36	39
3	c	454/455 (100%)	435 (96%)	18 (4%)	1 (0%)	49	57
4	D	343/342 (100%)	336 (98%)	6 (2%)	1 (0%)	43	48
4	d	341/342 (100%)	333 (98%)	8 (2%)	0	100	100
5	E	77/80 (96%)	75 (97%)	1 (1%)	1 (1%)	13	10
5	e	77/80 (96%)	75 (97%)	2 (3%)	0	100	100
6	F	31/33 (94%)	31 (100%)	0	0	100	100
6	f	29/33 (88%)	29 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	64/63 (102%)	60 (94%)	4 (6%)	0	100	100
7	h	61/63 (97%)	58 (95%)	3 (5%)	0	100	100
8	I	33/36 (92%)	31 (94%)	2 (6%)	0	100	100
8	i	34/36 (94%)	30 (88%)	4 (12%)	0	100	100
9	J	34/40 (85%)	33 (97%)	0	1 (3%)	5	2
9	j	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	33/35 (94%)	33 (100%)	0	0	100	100
11	l	33/35 (94%)	33 (100%)	0	0	100	100
12	O	242/243 (100%)	228 (94%)	12 (5%)	2 (1%)	21	20
12	o	241/243 (99%)	231 (96%)	10 (4%)	0	100	100
13	T	28/30 (93%)	28 (100%)	0	0	100	100
13	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
14	U	96/97 (99%)	92 (96%)	4 (4%)	0	100	100
14	u	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
15	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
15	v	136/137 (99%)	126 (93%)	9 (7%)	1 (1%)	24	23
16	Y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
16	y	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
17	X	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
17	x	34/37 (92%)	31 (91%)	1 (3%)	2 (6%)	2	0
18	Z	60/62 (97%)	56 (93%)	1 (2%)	3 (5%)	2	1
18	z	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
All	All	5100/5190 (98%)	4921 (96%)	163 (3%)	16 (0%)	43	48

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
3	C	24	THR
3	C	416	SER
5	E	6	GLY
18	Z	31	GLN

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Mol	Chain	Res	Type
18	Z	32	ASP
3	c	416	SER
15	v	19	ILE
17	x	35	ASP
9	J	6	GLY
12	O	34	SER
18	Z	30	PRO
1	a	225	ARG
12	O	26	ALA
1	A	259	ILE
17	x	34	ILE

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/270 (97%)	263 (100%)	0	100	100
1	a	252/270 (93%)	250 (99%)	2 (1%)	83	91
2	B	391/403 (97%)	386 (99%)	5 (1%)	71	83
2	b	378/403 (94%)	375 (99%)	3 (1%)	83	91
3	C	347/356 (98%)	341 (98%)	6 (2%)	63	77
3	c	356/356 (100%)	350 (98%)	6 (2%)	63	77
4	D	278/277 (100%)	276 (99%)	2 (1%)	85	93
4	d	276/277 (100%)	275 (100%)	1 (0%)	92	96
5	E	68/71 (96%)	67 (98%)	1 (2%)	67	80
5	e	67/71 (94%)	64 (96%)	3 (4%)	30	37
6	F	27/27 (100%)	27 (100%)	0	100	100
6	f	25/27 (93%)	24 (96%)	1 (4%)	34	43
7	H	56/53 (106%)	55 (98%)	1 (2%)	62	75
7	h	54/53 (102%)	53 (98%)	1 (2%)	60	74
8	I	31/32 (97%)	30 (97%)	1 (3%)	42	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	31/32 (97%)	31 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
9	j	25/28 (89%)	25 (100%)	0	100	100
10	K	30/30 (100%)	27 (90%)	3 (10%)	8	7
10	k	28/30 (93%)	27 (96%)	1 (4%)	38	48
11	L	33/33 (100%)	32 (97%)	1 (3%)	44	56
11	l	33/33 (100%)	32 (97%)	1 (3%)	44	56
12	O	203/206 (98%)	197 (97%)	6 (3%)	44	56
12	o	199/206 (97%)	195 (98%)	4 (2%)	58	72
13	T	24/26 (92%)	23 (96%)	1 (4%)	32	41
13	t	24/26 (92%)	22 (92%)	2 (8%)	12	12
14	U	85/84 (101%)	85 (100%)	0	100	100
14	u	82/84 (98%)	81 (99%)	1 (1%)	74	85
15	V	117/117 (100%)	113 (97%)	4 (3%)	40	50
15	v	115/117 (98%)	112 (97%)	3 (3%)	49	62
16	Y	22/22 (100%)	19 (86%)	3 (14%)	4	3
16	y	19/22 (86%)	19 (100%)	0	100	100
17	X	29/30 (97%)	27 (93%)	2 (7%)	17	18
17	x	27/30 (90%)	26 (96%)	1 (4%)	37	47
18	Z	45/52 (86%)	45 (100%)	0	100	100
18	z	40/52 (77%)	40 (100%)	0	100	100
All	All	4103/4234 (97%)	4037 (98%)	66 (2%)	65	79

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	128	THR
2	B	246	PHE
2	B	362	PHE
2	B	472	ARG
3	C	27	ASP
3	C	255	THR
3	C	289	PHE
3	C	315	MET

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Mol	Chain	Res	Type
3	C	418	ASN
3	C	471	SER
4	D	180	ARG
4	D	315	TYR
5	E	82	GLN
7	H	49	TYR
8	I	33	LYS
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
11	L	14	ARG
12	O	24	ASP
12	O	84	GLU
12	O	109	GLN
12	O	118	LEU
12	O	130	GLN
12	O	242	SER
13	T	25	GLU
15	V	30	LYS
15	V	110	LYS
15	V	129[A]	LYS
15	V	129[B]	LYS
16	Y	19	ILE
16	Y	25	ILE
16	Y	43	ARG
17	X	23	LEU
17	X	33	GLN
1	a	214	MET
1	a	260	PHE
2	b	246	PHE
2	b	362	PHE
2	b	467	ILE
3	c	78	GLU
3	c	156	LYS
3	c	289	PHE
3	c	334	PRO
3	c	381	LYS
3	c	418	ASN
4	d	180	ARG
5	e	7	GLU
5	e	16	SER
5	e	25	ILE

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Mol	Chain	Res	Type
6	f	15	ILE
7	h	49	TYR
10	k	27	VAL
11	l	10	VAL
12	o	23	ASP
12	o	89	SER
12	o	118	LEU
12	o	242	SER
13	t	25	GLU
13	t	28	ARG
14	u	39	ARG
15	v	6	GLU
15	v	19	ILE
15	v	28	GLU
17	x	21	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	HIS
2	B	53	ASN
2	B	331	ASN
6	F	44	GLN
12	O	58	ASN
12	O	104	GLN
12	O	130	GLN
14	U	37	GLN
15	V	34	GLN
1	a	266	ASN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
3	c	201	ASN
12	o	58	ASN
12	o	82	GLN
12	o	104	GLN
12	o	231	HIS
14	u	73	GLN
15	v	34	GLN
15	v	118	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
8	FME	I	1	8	9,9,10	0.93	0	6,9,11	1.44	2 (33%)
13	FME	T	1	13	9,9,10	0.90	1 (11%)	6,9,11	1.34	2 (33%)
8	FME	i	1	8	9,9,10	0.52	0	6,9,11	1.55	1 (16%)
13	FME	t	1	13	9,9,10	1.18	1 (11%)	6,9,11	1.90	2 (33%)

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
8	FME	I	1	8	-	1/6/9/11	-
13	FME	T	1	13	-	2/6/9/11	-
8	FME	i	1	8	-	2/6/9/11	-
13	FME	t	1	13	-	2/6/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	t	1	FME	CA-C	3.10	1.54	1.50
13	T	1	FME	CA-C	2.05	1.52	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	t	1	FME	CE-SD-CG	3.84	113.85	100.42
8	i	1	FME	O-C-CA	-2.81	118.69	125.11
8	I	1	FME	O-C-CA	-2.43	119.54	125.11
13	T	1	FME	O-C-CA	-2.23	120.02	125.11
8	I	1	FME	CE-SD-CG	2.21	108.15	100.42
13	T	1	FME	CE-SD-CG	2.19	108.08	100.42
13	t	1	FME	O-C-CA	-2.13	120.23	125.11

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	1	FME	O1-CN-N-CA
13	T	1	FME	CA-CB-CG-SD
8	I	1	FME	O1-CN-N-CA
13	t	1	FME	O1-CN-N-CA
13	t	1	FME	CA-CB-CG-SD
8	i	1	FME	O1-CN-N-CA
8	i	1	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 352 ligands modelled in this entry, 27 are unknown and 15 are monoatomic - leaving 310 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
19	OEX	A	401	1,3,40	0,15,15	0.00	-	-		
22	CLA	A	405	-	57,73,73	2.42	13 (22%)	66,113,113	1.80	18 (27%)
22	CLA	A	406	40	47,63,73	2.11	12 (25%)	54,101,113	2.36	22 (40%)
23	PHO	A	407	-	67,69,69	2.06	15 (22%)	86,99,99	1.90	18 (20%)
22	CLA	A	408	-	57,73,73	2.07	14 (24%)	66,113,113	1.89	17 (25%)
24	BCR	A	409	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	5 (8%)
25	LMG	A	410	-	51,51,55	0.94	2 (3%)	59,59,63	1.07	5 (8%)
26	PL9	A	411	-	55,55,55	0.96	3 (5%)	68,69,69	1.70	14 (20%)
27	LHG	A	412	-	30,30,48	1.37	2 (6%)	33,35,54	1.41	4 (12%)
28	SQD	A	413	-	48,49,54	1.06	3 (6%)	57,60,65	1.72	9 (15%)
29	LMT	A	414	-	36,36,36	0.79	0	47,47,47	1.13	4 (8%)
31	DMS	A	416	-	3,3,3	2.69	1 (33%)	3,3,3	1.04	0
31	DMS	A	417	-	3,3,3	2.69	1 (33%)	3,3,3	0.47	0
31	DMS	A	418	-	3,3,3	2.43	1 (33%)	3,3,3	1.24	0
31	DMS	A	419	-	3,3,3	2.69	1 (33%)	3,3,3	0.81	0
31	DMS	A	420	-	3,3,3	2.76	1 (33%)	3,3,3	1.33	0
32	BCT	A	421[A]	20	0,3,3	0.00	-	0,3,3	0.00	-
32	BCT	A	421[B]	20	0,3,3	0.00	-	0,3,3	0.00	-
22	CLA	B	602	40	57,73,73	2.84	15 (26%)	66,113,113	2.27	16 (24%)
22	CLA	B	603	-	57,73,73	2.29	16 (28%)	66,113,113	2.18	25 (37%)
22	CLA	B	604	-	57,73,73	2.25	15 (26%)	66,113,113	2.07	23 (34%)
22	CLA	B	605	-	57,73,73	1.99	14 (24%)	66,113,113	2.16	20 (30%)
22	CLA	B	606	-	57,73,73	2.72	13 (22%)	66,113,113	2.21	19 (28%)
22	CLA	B	607	-	57,73,73	2.42	13 (22%)	66,113,113	2.20	19 (28%)
22	CLA	B	608	40	57,73,73	2.13	14 (24%)	66,113,113	1.96	22 (33%)
22	CLA	B	609	-	57,73,73	2.16	14 (24%)	66,113,113	2.06	18 (27%)
22	CLA	B	610	-	57,73,73	2.07	13 (22%)	66,113,113	2.03	15 (22%)
22	CLA	B	611	40	57,73,73	2.47	14 (24%)	66,113,113	2.20	16 (24%)
22	CLA	B	612	-	57,73,73	2.17	12 (21%)	66,113,113	1.91	17 (25%)
22	CLA	B	613	-	57,73,73	2.50	14 (24%)	66,113,113	1.78	19 (28%)
22	CLA	B	614	-	53,69,73	2.35	13 (24%)	61,108,113	1.79	18 (29%)
22	CLA	B	615	-	45,61,73	2.80	15 (33%)	51,98,113	2.60	21 (41%)
22	CLA	B	616	-	57,73,73	2.41	15 (26%)	66,113,113	2.04	16 (24%)
22	CLA	B	617	-	47,63,73	2.23	13 (27%)	54,101,113	2.53	22 (40%)
24	BCR	B	618	-	18,19,41	0.87	0	24,26,56	1.42	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	619	-	30,30,41	0.92	0	39,39,56	1.32	7 (17%)
24	BCR	B	620	-	41,41,41	0.96	2 (4%)	56,56,56	1.49	11 (19%)
25	LMG	B	621	-	40,40,55	1.24	3 (7%)	48,48,63	1.38	8 (16%)
29	LMT	B	622	-	24,24,36	0.63	1 (4%)	29,29,47	0.84	1 (3%)
34	HTG	B	623	-	19,19,19	1.15	1 (5%)	23,24,24	1.77	3 (13%)
34	HTG	B	626	-	19,19,19	0.72	0	23,24,24	1.82	5 (21%)
34	HTG	B	627	-	19,19,19	0.99	1 (5%)	23,24,24	2.01	4 (17%)
31	DMS	B	628	-	3,3,3	2.83	1 (33%)	3,3,3	0.77	0
31	DMS	B	629	-	3,3,3	2.57	1 (33%)	3,3,3	1.17	0
31	DMS	B	630	-	3,3,3	2.84	1 (33%)	3,3,3	0.90	0
31	DMS	B	631	-	3,3,3	2.58	1 (33%)	3,3,3	0.61	0
31	DMS	B	632	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
31	DMS	B	633	-	3,3,3	2.69	1 (33%)	3,3,3	0.45	0
31	DMS	B	634	-	3,3,3	2.83	1 (33%)	3,3,3	0.64	0
31	DMS	B	635	-	3,3,3	2.80	1 (33%)	3,3,3	0.68	0
31	DMS	B	636	-	3,3,3	2.62	1 (33%)	3,3,3	0.62	0
31	DMS	B	637	-	3,3,3	2.80	1 (33%)	3,3,3	0.70	0
31	DMS	B	638	-	3,3,3	2.67	1 (33%)	3,3,3	0.39	0
31	DMS	B	639	-	3,3,3	2.78	1 (33%)	3,3,3	0.70	0
31	DMS	B	640	-	3,3,3	2.65	1 (33%)	3,3,3	0.61	0
31	DMS	B	641	-	3,3,3	2.78	1 (33%)	3,3,3	0.82	0
31	DMS	B	642	-	3,3,3	2.68	1 (33%)	3,3,3	1.04	0
28	SQD	C	501	-	53,54,54	1.03	3 (5%)	62,65,65	1.93	14 (22%)
22	CLA	C	502	-	57,73,73	2.05	15 (26%)	66,113,113	2.19	17 (25%)
22	CLA	C	503	-	57,73,73	2.31	13 (22%)	66,113,113	1.88	16 (24%)
22	CLA	C	504	-	57,73,73	2.67	15 (26%)	66,113,113	2.12	21 (31%)
22	CLA	C	505	40	57,73,73	2.78	14 (24%)	66,113,113	1.98	14 (21%)
22	CLA	C	506	-	57,73,73	2.57	15 (26%)	66,113,113	2.12	16 (24%)
22	CLA	C	507	-	57,73,73	2.25	15 (26%)	66,113,113	2.01	15 (22%)
22	CLA	C	508	40	57,73,73	2.36	15 (26%)	66,113,113	2.12	16 (24%)
22	CLA	C	509	-	57,73,73	2.46	15 (26%)	66,113,113	1.92	14 (21%)
22	CLA	C	510	-	57,73,73	2.15	12 (21%)	66,113,113	2.08	17 (25%)
22	CLA	C	511	-	57,73,73	2.33	14 (24%)	66,113,113	1.88	15 (22%)
22	CLA	C	512	3	57,73,73	2.53	16 (28%)	66,113,113	2.02	17 (25%)
22	CLA	C	513	-	48,64,73	2.73	15 (31%)	55,102,113	2.23	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	C	514	-	57,73,73	2.68	14 (24%)	66,113,113	2.12	17 (25%)
24	BCR	C	515	-	41,41,41	0.80	1 (2%)	56,56,56	1.48	9 (16%)
24	BCR	C	516	-	41,41,41	0.90	0	56,56,56	1.36	8 (14%)
35	DGD	C	517	-	63,63,67	0.84	3 (4%)	77,77,81	1.32	11 (14%)
35	DGD	C	518	-	63,63,67	0.95	3 (4%)	77,77,81	1.27	10 (12%)
35	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.19	8 (10%)
25	LMG	C	520	-	51,51,55	1.07	2 (3%)	59,59,63	1.21	5 (8%)
34	HTG	C	521	-	19,19,19	0.93	2 (10%)	23,24,24	1.64	2 (8%)
27	LHG	C	522	-	29,29,48	1.29	2 (6%)	33,34,54	1.37	4 (12%)
34	HTG	C	523	-	8,8,19	0.38	0	7,7,24	1.40	1 (14%)
31	DMS	C	524	-	3,3,3	2.50	1 (33%)	3,3,3	0.86	0
31	DMS	C	525	-	3,3,3	2.46	1 (33%)	3,3,3	0.61	0
31	DMS	C	526	-	3,3,3	2.62	1 (33%)	3,3,3	0.55	0
31	DMS	C	527	-	3,3,3	2.68	1 (33%)	3,3,3	0.56	0
31	DMS	C	528	-	3,3,3	2.65	1 (33%)	3,3,3	0.57	0
31	DMS	C	529	-	3,3,3	2.70	1 (33%)	3,3,3	0.54	0
31	DMS	C	530	-	3,3,3	2.70	1 (33%)	3,3,3	0.85	0
25	LMG	C	531	-	40,40,55	1.17	3 (7%)	48,48,63	1.11	3 (6%)
34	HTG	C	532	-	19,19,19	1.13	2 (10%)	23,24,24	1.90	1 (4%)
31	DMS	C	533	-	3,3,3	2.76	1 (33%)	3,3,3	0.74	0
31	DMS	C	534	-	3,3,3	2.72	1 (33%)	3,3,3	0.55	0
31	DMS	C	535	-	3,3,3	2.75	1 (33%)	3,3,3	0.77	0
31	DMS	C	536	-	3,3,3	2.71	1 (33%)	3,3,3	0.44	0
31	DMS	C	537	-	3,3,3	2.77	1 (33%)	3,3,3	0.69	0
31	DMS	C	538	-	3,3,3	2.69	1 (33%)	3,3,3	0.58	0
31	DMS	C	539	-	3,3,3	2.71	1 (33%)	3,3,3	0.60	0
31	DMS	C	540	-	3,3,3	2.80	1 (33%)	3,3,3	0.87	0
22	CLA	D	401	40	57,73,73	1.87	12 (21%)	66,113,113	2.21	21 (31%)
23	PHO	D	402	-	67,69,69	2.07	16 (23%)	86,99,99	2.03	21 (24%)
22	CLA	D	403	-	57,73,73	1.89	15 (26%)	66,113,113	2.39	20 (30%)
22	CLA	D	404	-	57,73,73	2.45	14 (24%)	66,113,113	1.77	15 (22%)
24	BCR	D	405	-	41,41,41	0.99	1 (2%)	56,56,56	1.98	15 (26%)
26	PL9	D	406	-	55,55,55	0.93	3 (5%)	68,69,69	1.53	14 (20%)
35	DGD	D	407	-	50,50,67	1.17	3 (6%)	58,58,81	1.30	6 (10%)
28	SQD	D	408	-	19,20,54	0.96	2 (10%)	26,29,65	1.92	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	D	409	-	48,48,48	1.01	2 (4%)	51,54,54	1.35	5 (9%)
27	LHG	D	410	-	48,48,48	0.78	2 (4%)	51,54,54	1.07	4 (7%)
27	LHG	D	411	-	44,44,48	0.96	2 (4%)	47,50,54	1.02	3 (6%)
25	LMG	D	412	-	46,46,55	1.12	3 (6%)	54,54,63	1.11	2 (3%)
34	HTG	D	414	-	19,19,19	0.85	1 (5%)	23,24,24	1.83	1 (4%)
34	HTG	D	415	-	19,19,19	1.15	1 (5%)	23,24,24	2.70	7 (30%)
31	DMS	D	416	-	3,3,3	2.52	1 (33%)	3,3,3	0.63	0
31	DMS	D	417	-	3,3,3	2.77	1 (33%)	3,3,3	0.59	0
31	DMS	D	418	-	3,3,3	2.42	1 (33%)	3,3,3	0.66	0
29	LMT	E	101	-	24,24,36	0.64	0	29,29,47	0.99	1 (3%)
36	HEM	E	102	5,6	27,50,50	2.06	6 (22%)	17,82,82	2.67	7 (41%)
31	DMS	F	101	-	3,3,3	2.68	1 (33%)	3,3,3	0.59	0
37	RRX	H	101	-	42,42,42	0.81	0	57,58,58	1.48	8 (14%)
35	DGD	H	102	-	63,63,67	1.01	3 (4%)	77,77,81	1.15	6 (7%)
31	DMS	H	103	-	3,3,3	2.94	1 (33%)	3,3,3	1.17	0
31	DMS	I	101	-	3,3,3	2.73	1 (33%)	3,3,3	0.68	0
29	LMT	I	102	-	36,36,36	0.68	1 (2%)	47,47,47	1.35	4 (8%)
31	DMS	I	106	-	3,3,3	2.70	1 (33%)	3,3,3	0.74	0
25	LMG	J	101	38	45,45,55	0.97	2 (4%)	53,53,63	1.02	5 (9%)
24	BCR	K	101	-	41,41,41	0.85	0	56,56,56	1.20	4 (7%)
27	LHG	L	101	-	39,39,48	1.03	2 (5%)	42,45,54	1.18	3 (7%)
31	DMS	L	102	-	3,3,3	2.77	1 (33%)	3,3,3	0.94	0
31	DMS	O	303	-	3,3,3	2.77	1 (33%)	3,3,3	0.76	0
31	DMS	O	304	-	3,3,3	2.59	1 (33%)	3,3,3	0.41	0
31	DMS	O	305	-	3,3,3	2.92	1 (33%)	3,3,3	0.83	0
31	DMS	O	306	-	3,3,3	2.72	1 (33%)	3,3,3	0.74	0
31	DMS	O	307	-	3,3,3	2.81	1 (33%)	3,3,3	0.91	0
31	DMS	O	308	-	3,3,3	2.81	1 (33%)	3,3,3	0.61	0
31	DMS	O	309	-	3,3,3	2.56	1 (33%)	3,3,3	0.58	0
31	DMS	O	310	-	3,3,3	2.65	1 (33%)	3,3,3	0.85	0
31	DMS	O	311	-	3,3,3	3.00	1 (33%)	3,3,3	0.90	0
31	DMS	O	312	-	3,3,3	2.65	1 (33%)	3,3,3	0.94	0
31	DMS	O	313	-	3,3,3	2.65	1 (33%)	3,3,3	0.47	0
31	DMS	O	314	-	3,3,3	2.76	1 (33%)	3,3,3	0.75	0
29	LMT	T	102	-	24,24,36	0.73	1 (4%)	29,29,47	1.26	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	U	202	-	3,3,3	2.79	1 (33%)	3,3,3	1.27	0
31	DMS	U	203	-	3,3,3	2.80	1 (33%)	3,3,3	1.24	0
31	DMS	V	201	-	3,3,3	2.66	1 (33%)	3,3,3	0.88	0
39	HEC	V	202	15	26,50,50	2.23	7 (26%)	18,82,82	1.93	5 (27%)
34	HTG	V	203	-	14,14,19	0.68	0	18,19,24	3.09	7 (38%)
31	DMS	V	204	-	3,3,3	2.75	1 (33%)	3,3,3	0.80	0
31	DMS	V	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.63	0
31	DMS	V	206	-	3,3,3	2.73	1 (33%)	3,3,3	0.55	0
31	DMS	V	207	-	3,3,3	2.77	1 (33%)	3,3,3	0.88	0
31	DMS	V	208	-	3,3,3	2.62	1 (33%)	3,3,3	0.39	0
31	DMS	V	209	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
31	DMS	V	210	-	3,3,3	2.79	1 (33%)	3,3,3	0.88	0
31	DMS	V	211	-	3,3,3	2.84	1 (33%)	3,3,3	0.76	0
31	DMS	V	212	-	3,3,3	2.80	1 (33%)	3,3,3	1.17	0
24	BCR	Y	101	-	39,40,41	0.87	1 (2%)	51,54,56	1.71	15 (29%)
29	LMT	Z	101	-	36,36,36	0.67	1 (2%)	47,47,47	1.15	3 (6%)
31	DMS	a	401	-	3,3,3	2.77	1 (33%)	3,3,3	0.79	0
31	DMS	a	402	-	3,3,3	2.41	1 (33%)	3,3,3	0.72	0
19	OEX	a	403	1,3,40	0,15,15	0.00	-	-	-	-
22	CLA	a	407	-	57,73,73	2.22	15 (26%)	66,113,113	1.93	21 (31%)
22	CLA	a	408	40	57,73,73	2.01	14 (24%)	66,113,113	2.08	19 (28%)
22	CLA	a	409	40	53,69,73	1.92	12 (22%)	61,108,113	2.35	22 (36%)
23	PHO	a	410	-	67,69,69	1.94	17 (25%)	86,99,99	1.91	20 (23%)
23	PHO	a	411	-	67,69,69	2.02	15 (22%)	86,99,99	2.21	22 (25%)
22	CLA	a	412	-	57,73,73	1.99	12 (21%)	66,113,113	2.15	21 (31%)
24	BCR	a	413	-	41,41,41	1.13	2 (4%)	56,56,56	1.15	8 (14%)
28	SQD	a	414	-	53,54,54	1.07	3 (5%)	62,65,65	1.98	12 (19%)
26	PL9	a	415	-	55,55,55	0.94	3 (5%)	68,69,69	1.47	11 (16%)
27	LHG	a	416	-	48,48,48	1.12	2 (4%)	51,54,54	1.17	4 (7%)
28	SQD	a	418	-	50,51,54	1.14	3 (6%)	59,62,65	1.46	8 (13%)
29	LMT	a	419	-	36,36,36	0.78	0	47,47,47	1.36	5 (10%)
31	DMS	a	421	-	3,3,3	2.68	1 (33%)	3,3,3	0.60	0
32	BCT	a	422	20	0,3,3	0.00	-	0,3,3	0.00	-
27	LHG	a	423	-	44,44,48	1.01	2 (4%)	47,50,54	1.07	4 (8%)
31	DMS	a	424	-	3,3,3	2.73	1 (33%)	3,3,3	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	a	425	-	3,3,3	3.04	1 (33%)	3,3,3	0.88	0
22	CLA	b	602	40	57,73,73	3.40	14 (24%)	66,113,113	2.37	18 (27%)
22	CLA	b	603	-	57,73,73	2.73	13 (22%)	66,113,113	2.06	20 (30%)
22	CLA	b	604	-	57,73,73	2.55	13 (22%)	66,113,113	2.22	22 (33%)
22	CLA	b	605	-	57,73,73	2.17	13 (22%)	66,113,113	2.00	15 (22%)
22	CLA	b	606	-	57,73,73	1.86	12 (21%)	66,113,113	2.13	18 (27%)
22	CLA	b	607	-	57,73,73	2.16	15 (26%)	66,113,113	2.25	16 (24%)
22	CLA	b	608	40	57,73,73	2.40	14 (24%)	66,113,113	2.07	15 (22%)
22	CLA	b	609	-	57,73,73	2.13	13 (22%)	66,113,113	1.92	17 (25%)
22	CLA	b	610	-	57,73,73	2.39	16 (28%)	66,113,113	1.89	16 (24%)
22	CLA	b	611	40	57,73,73	2.22	13 (22%)	66,113,113	2.07	18 (27%)
22	CLA	b	612	-	57,73,73	2.13	12 (21%)	66,113,113	1.95	14 (21%)
22	CLA	b	613	-	57,73,73	2.57	14 (24%)	66,113,113	2.17	20 (30%)
22	CLA	b	614	-	51,67,73	2.41	16 (31%)	58,105,113	2.17	15 (25%)
22	CLA	b	615	-	44,60,73	2.85	16 (36%)	50,97,113	2.29	21 (42%)
22	CLA	b	616	-	57,73,73	2.44	13 (22%)	66,113,113	1.99	19 (28%)
22	CLA	b	617	-	52,68,73	2.99	13 (25%)	60,107,113	2.36	20 (33%)
24	BCR	b	618	-	20,20,41	0.93	1 (5%)	27,27,56	1.74	5 (18%)
24	BCR	b	619	-	31,31,41	1.09	2 (6%)	40,40,56	1.34	8 (20%)
24	BCR	b	620	-	41,41,41	0.84	0	56,56,56	1.35	8 (14%)
28	SQD	b	621	-	37,38,54	1.03	2 (5%)	45,48,65	1.49	8 (17%)
25	LMG	b	622	-	43,43,55	1.34	4 (9%)	51,51,63	1.88	12 (23%)
34	HTG	b	623	-	19,19,19	1.09	1 (5%)	23,24,24	1.31	4 (17%)
34	HTG	b	624	-	19,19,19	1.05	1 (5%)	23,24,24	2.19	6 (26%)
34	HTG	b	626	-	19,19,19	0.83	1 (5%)	23,24,24	1.61	5 (21%)
34	HTG	b	627	-	19,19,19	1.01	2 (10%)	23,24,24	1.84	3 (13%)
31	DMS	b	629	-	3,3,3	2.30	1 (33%)	3,3,3	1.09	0
31	DMS	b	630	-	3,3,3	2.69	1 (33%)	3,3,3	0.29	0
31	DMS	b	631	-	3,3,3	2.70	1 (33%)	3,3,3	0.53	0
34	HTG	b	632	-	19,19,19	1.07	2 (10%)	23,24,24	2.52	7 (30%)
31	DMS	b	633	-	3,3,3	2.69	1 (33%)	3,3,3	0.55	0
31	DMS	b	634	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
31	DMS	b	635	-	3,3,3	2.78	1 (33%)	3,3,3	0.55	0
31	DMS	b	636	-	3,3,3	2.69	1 (33%)	3,3,3	0.69	0
31	DMS	b	637	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	b	638	-	3,3,3	3.00	1 (33%)	3,3,3	0.68	0
22	CLA	c	902	-	57,73,73	2.29	13 (22%)	66,113,113	1.97	12 (18%)
22	CLA	c	903	-	57,73,73	2.02	14 (24%)	66,113,113	2.13	20 (30%)
22	CLA	c	904	-	57,73,73	2.63	15 (26%)	66,113,113	2.16	19 (28%)
22	CLA	c	905	40	57,73,73	2.69	14 (24%)	66,113,113	2.05	15 (22%)
22	CLA	c	906	-	57,73,73	2.36	15 (26%)	66,113,113	1.90	16 (24%)
22	CLA	c	907	-	57,73,73	2.17	13 (22%)	66,113,113	1.91	15 (22%)
22	CLA	c	908	40	57,73,73	2.76	14 (24%)	66,113,113	2.26	14 (21%)
22	CLA	c	909	-	57,73,73	2.74	15 (26%)	66,113,113	2.11	18 (27%)
22	CLA	c	910	-	57,73,73	2.22	13 (22%)	66,113,113	1.99	20 (30%)
22	CLA	c	911	-	57,73,73	2.19	14 (24%)	66,113,113	1.95	17 (25%)
22	CLA	c	912	3	57,73,73	2.98	15 (26%)	66,113,113	1.98	14 (21%)
22	CLA	c	913	-	57,73,73	2.40	15 (26%)	66,113,113	1.99	17 (25%)
22	CLA	c	914	-	57,73,73	2.38	15 (26%)	66,113,113	2.00	19 (28%)
24	BCR	c	915	-	41,41,41	0.83	1 (2%)	56,56,56	1.39	8 (14%)
24	BCR	c	916	-	41,41,41	0.85	0	56,56,56	1.55	10 (17%)
35	DGD	c	917	-	63,63,67	0.96	3 (4%)	77,77,81	0.99	3 (3%)
35	DGD	c	918	-	63,63,67	0.93	4 (6%)	77,77,81	1.02	4 (5%)
35	DGD	c	919	-	63,63,67	0.97	4 (6%)	77,77,81	1.14	6 (7%)
25	LMG	c	920	-	51,51,55	0.98	2 (3%)	59,59,63	1.08	5 (8%)
29	LMT	c	921	-	36,36,36	0.67	1 (2%)	47,47,47	1.02	4 (8%)
34	HTG	c	922	-	19,19,19	0.83	1 (5%)	23,24,24	1.69	2 (8%)
31	DMS	c	923	-	3,3,3	2.52	1 (33%)	3,3,3	0.40	0
31	DMS	c	924	-	3,3,3	2.84	1 (33%)	3,3,3	1.30	1 (33%)
31	DMS	c	925	-	3,3,3	2.68	1 (33%)	3,3,3	1.09	0
31	DMS	c	926	-	3,3,3	2.62	1 (33%)	3,3,3	0.77	0
31	DMS	c	927	-	3,3,3	2.67	1 (33%)	3,3,3	0.42	0
31	DMS	c	928	-	3,3,3	2.72	1 (33%)	3,3,3	0.76	0
31	DMS	c	929	-	3,3,3	2.83	1 (33%)	3,3,3	0.83	0
25	LMG	c	930	-	49,49,55	1.09	3 (6%)	57,57,63	1.05	4 (7%)
29	LMT	c	931	-	24,24,36	0.79	1 (4%)	29,29,47	0.86	2 (6%)
31	DMS	c	933	-	3,3,3	2.86	1 (33%)	3,3,3	0.90	0
31	DMS	c	934	-	3,3,3	2.68	1 (33%)	3,3,3	0.67	0
31	DMS	c	935	-	3,3,3	2.68	1 (33%)	3,3,3	0.88	0
31	DMS	c	936	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	c	937	-	3,3,3	2.90	1 (33%)	3,3,3	0.81	0
31	DMS	c	938	-	3,3,3	2.79	1 (33%)	3,3,3	0.82	0
31	DMS	c	939	-	3,3,3	2.78	1 (33%)	3,3,3	0.64	0
31	DMS	c	940	-	3,3,3	2.75	1 (33%)	3,3,3	0.57	0
31	DMS	c	941	-	3,3,3	2.62	1 (33%)	3,3,3	0.52	0
31	DMS	c	942	-	3,3,3	2.76	1 (33%)	3,3,3	0.71	0
31	DMS	c	943	-	3,3,3	2.72	1 (33%)	3,3,3	0.79	0
31	DMS	c	944	-	3,3,3	2.74	1 (33%)	3,3,3	0.77	0
27	LHG	d	401	-	32,32,48	1.22	2 (6%)	36,37,54	1.17	4 (11%)
22	CLA	d	402	-	57,73,73	2.05	13 (22%)	66,113,113	1.94	16 (24%)
22	CLA	d	403	-	57,73,73	2.74	16 (28%)	66,113,113	1.87	13 (19%)
24	BCR	d	404	-	41,41,41	1.04	3 (7%)	56,56,56	1.78	13 (23%)
26	PL9	d	405	-	55,55,55	1.02	4 (7%)	68,69,69	1.45	9 (13%)
35	DGD	d	406	-	42,42,67	1.23	3 (7%)	44,45,81	1.08	3 (6%)
27	LHG	d	407	-	48,48,48	0.75	2 (4%)	51,54,54	1.05	3 (5%)
27	LHG	d	408	-	45,45,48	1.02	2 (4%)	48,51,54	0.72	0
25	LMG	d	409	-	47,47,55	1.08	3 (6%)	55,55,63	1.45	8 (14%)
31	DMS	d	411	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
31	DMS	d	412	-	3,3,3	2.58	1 (33%)	3,3,3	0.82	0
31	DMS	d	413	-	3,3,3	2.57	1 (33%)	3,3,3	0.39	0
31	DMS	d	414	-	3,3,3	2.72	1 (33%)	3,3,3	0.57	0
31	DMS	d	415	-	3,3,3	2.64	1 (33%)	3,3,3	0.60	0
36	HEM	e	101	5,6	27,50,50	2.11	9 (33%)	17,82,82	2.15	4 (23%)
28	SQD	f	101	-	13,13,54	2.15	1 (7%)	15,16,65	1.28	2 (13%)
29	LMT	f	102	-	25,25,36	1.01	1 (4%)	30,30,47	1.21	5 (16%)
31	DMS	f	103	-	3,3,3	2.73	1 (33%)	3,3,3	0.90	0
37	RRX	h	101	-	42,42,42	0.96	0	57,58,58	1.19	5 (8%)
35	DGD	h	102	-	63,63,67	0.97	3 (4%)	77,77,81	1.12	5 (6%)
25	LMG	i	101	-	51,51,55	0.97	2 (3%)	59,59,63	1.16	7 (11%)
31	DMS	i	106	-	3,3,3	2.65	1 (33%)	3,3,3	0.55	0
25	LMG	j	101	38	47,47,55	1.00	2 (4%)	55,55,63	1.17	9 (16%)
24	BCR	k	101	-	41,41,41	0.90	0	56,56,56	1.23	6 (10%)
28	SQD	l	101	-	53,54,54	1.11	4 (7%)	62,65,65	1.46	7 (11%)
27	LHG	l	102	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	2 (3%)
31	DMS	l	103	-	3,3,3	2.73	1 (33%)	3,3,3	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	DMS	l	104	-	3,3,3	2.79	1 (33%)	3,3,3	0.56	0
31	DMS	l	105	-	3,3,3	2.76	1 (33%)	3,3,3	0.71	0
34	HTG	l	106	-	19,19,19	1.00	2 (10%)	23,24,24	2.09	3 (13%)
31	DMS	o	302	-	3,3,3	2.70	1 (33%)	3,3,3	0.95	0
31	DMS	o	303	-	3,3,3	2.72	1 (33%)	3,3,3	0.80	0
31	DMS	o	304	-	3,3,3	2.84	1 (33%)	3,3,3	1.13	0
31	DMS	o	305	-	3,3,3	2.62	1 (33%)	3,3,3	0.65	0
31	DMS	o	306	-	3,3,3	2.67	1 (33%)	3,3,3	0.59	0
31	DMS	o	307	-	3,3,3	2.62	1 (33%)	3,3,3	0.57	0
31	DMS	o	308	-	3,3,3	2.81	1 (33%)	3,3,3	0.82	0
29	LMT	t	101	-	24,24,36	0.45	0	29,29,47	1.33	4 (13%)
31	DMS	t	103	-	3,3,3	2.73	1 (33%)	3,3,3	0.63	0
31	DMS	t	104	-	3,3,3	2.73	1 (33%)	3,3,3	0.58	0
31	DMS	t	105	-	3,3,3	2.73	1 (33%)	3,3,3	0.60	0
31	DMS	u	202	-	3,3,3	2.64	1 (33%)	3,3,3	1.04	0
31	DMS	u	203	-	3,3,3	2.75	1 (33%)	3,3,3	0.75	0
31	DMS	u	204	-	3,3,3	2.82	1 (33%)	3,3,3	0.80	0
31	DMS	u	205	-	3,3,3	3.10	1 (33%)	3,3,3	1.18	0
31	DMS	v	201	-	3,3,3	2.61	1 (33%)	3,3,3	0.84	0
39	HEC	v	202	15	26,50,50	2.43	8 (30%)	18,82,82	2.05	5 (27%)
34	HTG	v	203	-	16,16,19	1.04	1 (6%)	20,21,24	3.05	7 (35%)
31	DMS	v	204	-	3,3,3	2.69	1 (33%)	3,3,3	0.68	0
31	DMS	v	205	-	3,3,3	2.68	1 (33%)	3,3,3	0.82	0
31	DMS	v	206	-	3,3,3	2.71	1 (33%)	3,3,3	0.72	0
31	DMS	v	207	-	3,3,3	2.74	1 (33%)	3,3,3	0.64	0
31	DMS	v	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.52	0
31	DMS	v	209	-	3,3,3	2.66	1 (33%)	3,3,3	0.62	0
31	DMS	v	210	-	3,3,3	2.86	1 (33%)	3,3,3	0.77	0
31	DMS	v	211	-	3,3,3	2.78	1 (33%)	3,3,3	0.75	0
24	BCR	y	101	-	41,41,41	0.89	0	56,56,56	1.60	14 (25%)

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
22	CLA	A	405	-	2/2/20/25	7/37/135/135	-
22	CLA	A	406	40	2/2/18/25	5/25/123/135	-
23	PHO	A	407	-	-	1/53/103/103	0/5/6/6
22	CLA	A	408	-	2/2/20/25	13/37/135/135	-
24	BCR	A	409	-	-	2/29/63/63	0/2/2/2
25	LMG	A	410	-	-	28/46/66/70	0/1/1/1
26	PL9	A	411	-	-	12/53/73/73	0/1/1/1
27	LHG	A	412	-	-	14/33/33/53	-
28	SQD	A	413	-	-	26/44/64/69	0/1/1/1
29	LMT	A	414	-	-	14/21/61/61	0/2/2/2
22	CLA	B	602	40	3/3/20/25	23/37/135/135	-
22	CLA	B	603	-	3/3/20/25	8/37/135/135	-
22	CLA	B	604	-	3/3/20/25	7/37/135/135	-
22	CLA	B	605	-	3/3/20/25	9/37/135/135	-
22	CLA	B	606	-	2/2/20/25	9/37/135/135	-
22	CLA	B	607	-	3/3/20/25	14/37/135/135	-
22	CLA	B	608	40	3/3/20/25	7/37/135/135	-
22	CLA	B	609	-	1/1/20/25	2/37/135/135	-
22	CLA	B	610	-	3/3/20/25	2/37/135/135	-
22	CLA	B	611	40	3/3/20/25	8/37/135/135	-
22	CLA	B	612	-	3/3/20/25	11/37/135/135	-
22	CLA	B	613	-	3/3/20/25	4/37/135/135	-
22	CLA	B	614	-	3/3/19/25	6/33/131/135	-
22	CLA	B	615	-	3/3/17/25	11/23/121/135	-
22	CLA	B	616	-	3/3/20/25	12/37/135/135	-
22	CLA	B	617	-	3/3/18/25	5/25/123/135	-
24	BCR	B	618	-	-	0/11/28/63	0/1/1/2
24	BCR	B	619	-	-	1/24/41/63	0/1/1/2
24	BCR	B	620	-	-	0/29/63/63	0/2/2/2
25	LMG	B	621	-	-	23/35/55/70	0/1/1/1
29	LMT	B	622	-	-	8/15/35/61	0/1/1/2
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
34	HTG	B	626	-	-	2/10/30/30	0/1/1/1
34	HTG	B	627	-	-	7/10/30/30	0/1/1/1
28	SQD	C	501	-	-	26/49/69/69	0/1/1/1
22	CLA	C	502	-	3/3/20/25	5/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	C	503	-	3/3/20/25	7/37/135/135	-
22	CLA	C	504	-	1/1/20/25	3/37/135/135	-
22	CLA	C	505	40	2/2/20/25	6/37/135/135	-
22	CLA	C	506	-	2/2/20/25	5/37/135/135	-
22	CLA	C	507	-	3/3/20/25	11/37/135/135	-
22	CLA	C	508	40	3/3/20/25	11/37/135/135	-
22	CLA	C	509	-	3/3/20/25	11/37/135/135	-
22	CLA	C	510	-	3/3/20/25	13/37/135/135	-
22	CLA	C	511	-	3/3/20/25	14/37/135/135	-
22	CLA	C	512	3	2/2/20/25	1/37/135/135	-
22	CLA	C	513	-	3/3/18/25	9/27/125/135	-
22	CLA	C	514	-	2/2/20/25	18/37/135/135	-
24	BCR	C	515	-	-	4/29/63/63	0/2/2/2
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
35	DGD	C	517	-	-	18/51/91/95	0/2/2/2
35	DGD	C	518	-	-	23/51/91/95	0/2/2/2
35	DGD	C	519	-	-	29/51/91/95	0/2/2/2
25	LMG	C	520	-	-	19/46/66/70	0/1/1/1
34	HTG	C	521	-	-	4/10/30/30	0/1/1/1
27	LHG	C	522	-	-	15/31/31/53	-
34	HTG	C	523	-	-	1/6/6/30	-
25	LMG	C	531	-	-	14/35/55/70	0/1/1/1
34	HTG	C	532	-	-	7/10/30/30	0/1/1/1
22	CLA	D	401	40	1/1/20/25	6/37/135/135	-
23	PHO	D	402	-	-	8/53/103/103	0/5/6/6
22	CLA	D	403	-	2/2/20/25	0/37/135/135	-
22	CLA	D	404	-	3/3/20/25	13/37/135/135	-
24	BCR	D	405	-	-	4/29/63/63	0/2/2/2
26	PL9	D	406	-	-	8/53/73/73	0/1/1/1
35	DGD	D	407	-	-	29/44/64/95	0/1/1/2
28	SQD	D	408	-	-	3/12/32/69	0/1/1/1
27	LHG	D	409	-	-	15/53/53/53	-
27	LHG	D	410	-	-	12/53/53/53	-
27	LHG	D	411	-	-	12/49/49/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	D	412	-	-	14/41/61/70	0/1/1/1
34	HTG	D	414	-	-	3/10/30/30	0/1/1/1
34	HTG	D	415	-	-	8/10/30/30	0/1/1/1
29	LMT	E	101	-	-	9/15/35/61	0/1/1/2
36	HEM	E	102	5,6	-	0/6/54/54	-
37	RRX	H	101	-	-	1/29/65/65	0/2/2/2
35	DGD	H	102	-	-	17/51/91/95	0/2/2/2
29	LMT	I	102	-	-	11/21/61/61	0/2/2/2
25	LMG	J	101	38	-	9/40/60/70	0/1/1/1
24	BCR	K	101	-	-	3/29/63/63	0/2/2/2
27	LHG	L	101	-	-	20/44/44/53	-
29	LMT	T	102	-	-	10/15/35/61	0/1/1/2
39	HEC	V	202	15	-	0/6/54/54	-
34	HTG	V	203	-	-	0/5/25/30	0/1/1/1
24	BCR	Y	101	-	-	6/29/60/63	0/2/2/2
29	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
22	CLA	a	407	-	3/3/20/25	7/37/135/135	-
22	CLA	a	408	40	3/3/20/25	6/37/135/135	-
22	CLA	a	409	40	2/2/19/25	10/33/131/135	-
23	PHO	a	410	-	-	1/53/103/103	0/5/6/6
23	PHO	a	411	-	-	7/53/103/103	0/5/6/6
22	CLA	a	412	-	-	12/37/135/135	-
24	BCR	a	413	-	-	2/29/63/63	0/2/2/2
28	SQD	a	414	-	-	27/49/69/69	0/1/1/1
26	PL9	a	415	-	-	15/53/73/73	0/1/1/1
27	LHG	a	416	-	-	28/53/53/53	-
28	SQD	a	418	-	-	23/46/66/69	0/1/1/1
29	LMT	a	419	-	-	14/21/61/61	0/2/2/2
27	LHG	a	423	-	-	22/49/49/53	-
22	CLA	b	602	40	2/2/20/25	21/37/135/135	-
22	CLA	b	603	-	1/1/20/25	3/37/135/135	-
22	CLA	b	604	-	2/2/20/25	10/37/135/135	-
22	CLA	b	605	-	3/3/20/25	11/37/135/135	-
22	CLA	b	606	-	3/3/20/25	3/37/135/135	-
22	CLA	b	607	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	608	40	3/3/20/25	15/37/135/135	-
22	CLA	b	609	-	2/2/20/25	7/37/135/135	-
22	CLA	b	610	-	1/1/20/25	1/37/135/135	-
22	CLA	b	611	40	3/3/20/25	6/37/135/135	-
22	CLA	b	612	-	2/2/20/25	10/37/135/135	-
22	CLA	b	613	-	3/3/20/25	6/37/135/135	-
22	CLA	b	614	-	3/3/18/25	6/30/128/135	-
22	CLA	b	615	-	3/3/17/25	6/22/120/135	-
22	CLA	b	616	-	3/3/20/25	9/37/135/135	-
22	CLA	b	617	-	3/3/19/25	7/31/129/135	-
24	BCR	b	618	-	-	7/13/30/63	0/1/1/2
24	BCR	b	619	-	-	4/26/43/63	0/1/1/2
24	BCR	b	620	-	-	0/29/63/63	0/2/2/2
28	SQD	b	621	-	-	16/32/52/69	0/1/1/1
25	LMG	b	622	-	-	20/38/58/70	0/1/1/1
34	HTG	b	623	-	-	6/10/30/30	0/1/1/1
34	HTG	b	624	-	-	4/10/30/30	0/1/1/1
34	HTG	b	626	-	-	6/10/30/30	0/1/1/1
34	HTG	b	627	-	-	3/10/30/30	0/1/1/1
34	HTG	b	632	-	-	6/10/30/30	0/1/1/1
22	CLA	c	902	-	3/3/20/25	3/37/135/135	-
22	CLA	c	903	-	3/3/20/25	10/37/135/135	-
22	CLA	c	904	-	1/1/20/25	7/37/135/135	-
22	CLA	c	905	40	2/2/20/25	15/37/135/135	-
22	CLA	c	906	-	1/1/20/25	9/37/135/135	-
22	CLA	c	907	-	3/3/20/25	11/37/135/135	-
22	CLA	c	908	40	3/3/20/25	11/37/135/135	-
22	CLA	c	909	-	2/2/20/25	12/37/135/135	-
22	CLA	c	910	-	3/3/20/25	15/37/135/135	-
22	CLA	c	911	-	3/3/20/25	7/37/135/135	-
22	CLA	c	912	3	2/2/20/25	4/37/135/135	-
22	CLA	c	913	-	2/2/20/25	19/37/135/135	-
22	CLA	c	914	-	2/2/20/25	16/37/135/135	-
24	BCR	c	915	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	916	-	-	4/29/63/63	0/2/2/2
35	DGD	c	917	-	-	21/51/91/95	0/2/2/2
35	DGD	c	918	-	-	22/51/91/95	0/2/2/2
35	DGD	c	919	-	-	19/51/91/95	0/2/2/2
25	LMG	c	920	-	-	21/46/66/70	0/1/1/1
29	LMT	c	921	-	-	11/21/61/61	0/2/2/2
34	HTG	c	922	-	-	6/10/30/30	0/1/1/1
25	LMG	c	930	-	-	12/44/64/70	0/1/1/1
29	LMT	c	931	-	-	11/15/35/61	0/1/1/2
27	LHG	d	401	-	-	15/34/34/53	-
22	CLA	d	402	-	2/2/20/25	8/37/135/135	-
22	CLA	d	403	-	2/2/20/25	10/37/135/135	-
24	BCR	d	404	-	-	4/29/63/63	0/2/2/2
26	PL9	d	405	-	-	6/53/73/73	0/1/1/1
35	DGD	d	406	-	-	30/44/44/95	-
27	LHG	d	407	-	-	20/53/53/53	-
27	LHG	d	408	-	-	17/50/50/53	-
25	LMG	d	409	-	-	28/42/62/70	0/1/1/1
36	HEM	e	101	5,6	-	2/6/54/54	-
28	SQD	f	101	-	-	4/12/12/69	-
29	LMT	f	102	-	-	10/17/37/61	0/1/1/2
37	RRX	h	101	-	-	8/29/65/65	0/2/2/2
35	DGD	h	102	-	-	18/51/91/95	0/2/2/2
25	LMG	i	101	-	-	25/46/66/70	0/1/1/1
25	LMG	j	101	38	-	13/42/62/70	0/1/1/1
24	BCR	k	101	-	-	4/29/63/63	0/2/2/2
28	SQD	l	101	-	-	32/49/69/69	0/1/1/1
27	LHG	l	102	-	-	26/53/53/53	-
34	HTG	l	106	-	-	6/10/30/30	0/1/1/1
29	LMT	t	101	-	-	10/15/35/61	0/1/1/2
39	HEC	v	202	15	-	0/6/54/54	-
34	HTG	v	203	-	-	4/7/27/30	0/1/1/1
24	BCR	y	101	-	-	5/29/63/63	0/2/2/2

All (1366) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	602	CLA	MG-NA	19.40	2.52	2.06
22	B	606	CLA	MG-NA	15.87	2.44	2.06
22	b	617	CLA	MG-NA	15.18	2.42	2.06
22	c	912	CLA	MG-NA	14.71	2.41	2.06
22	B	602	CLA	MG-NA	14.39	2.40	2.06
22	b	603	CLA	MG-NA	14.14	2.39	2.06
22	C	505	CLA	MG-NA	13.78	2.39	2.06
22	b	604	CLA	MG-NA	13.69	2.38	2.06
22	c	908	CLA	MG-NA	13.08	2.37	2.06
22	c	905	CLA	MG-NA	12.88	2.36	2.06
22	c	904	CLA	MG-NA	12.83	2.36	2.06
22	B	613	CLA	MG-NA	12.32	2.35	2.06
22	b	613	CLA	MG-NA	12.17	2.35	2.06
22	A	405	CLA	MG-NC	11.62	2.33	2.06
22	C	506	CLA	MG-NA	11.61	2.33	2.06
22	c	909	CLA	MG-NA	11.40	2.33	2.06
22	C	512	CLA	MG-NA	11.28	2.33	2.06
22	B	611	CLA	MG-NC	11.25	2.33	2.06
22	C	514	CLA	MG-NA	10.98	2.32	2.06
22	D	404	CLA	MG-NC	10.68	2.31	2.06
22	b	615	CLA	MG-NA	10.66	2.31	2.06
22	B	616	CLA	MG-NA	10.56	2.31	2.06
22	C	503	CLA	MG-NA	10.17	2.30	2.06
22	c	902	CLA	MG-NA	9.92	2.29	2.06
22	C	504	CLA	MG-NC	9.77	2.29	2.06
22	b	610	CLA	MG-NA	9.74	2.29	2.06
22	C	513	CLA	MG-NA	9.70	2.29	2.06
22	b	614	CLA	MG-NA	9.53	2.28	2.06
22	b	608	CLA	MG-NA	9.39	2.28	2.06
22	B	615	CLA	MG-NC	9.39	2.28	2.06
22	b	616	CLA	MG-NA	9.38	2.28	2.06
22	b	605	CLA	MG-NA	9.04	2.27	2.06
22	d	403	CLA	MG-NC	9.04	2.27	2.06
22	C	509	CLA	MG-NA	8.92	2.27	2.06
22	B	614	CLA	MG-NA	8.89	2.27	2.06
22	b	612	CLA	MG-NA	8.87	2.27	2.06
22	B	608	CLA	MG-NA	8.51	2.26	2.06
22	c	914	CLA	MG-NC	8.49	2.26	2.06
22	d	403	CLA	MG-NA	8.48	2.26	2.06
22	b	607	CLA	MG-NA	8.43	2.26	2.06
22	B	604	CLA	MG-NA	8.37	2.26	2.06
22	b	611	CLA	MG-NC	8.35	2.26	2.06
22	c	906	CLA	MG-NA	8.26	2.25	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	504	CLA	MG-NA	8.13	2.25	2.06
22	B	612	CLA	MG-NA	8.10	2.25	2.06
22	C	508	CLA	MG-NA	8.09	2.25	2.06
22	c	912	CLA	MG-NC	8.05	2.25	2.06
22	B	607	CLA	MG-NA	8.00	2.25	2.06
22	B	607	CLA	MG-NC	7.92	2.25	2.06
22	C	511	CLA	MG-NA	7.83	2.24	2.06
22	a	407	CLA	MG-NA	7.78	2.24	2.06
22	B	609	CLA	MG-NC	7.71	2.24	2.06
22	C	507	CLA	MG-NA	7.71	2.24	2.06
22	c	907	CLA	MG-NA	7.68	2.24	2.06
22	c	913	CLA	MG-NC	7.66	2.24	2.06
22	D	403	CLA	MG-NA	7.55	2.24	2.06
22	c	909	CLA	MG-NC	7.45	2.24	2.06
22	C	509	CLA	MG-NC	7.29	2.23	2.06
28	f	101	SQD	C6-S	-7.16	1.67	1.77
22	C	514	CLA	MG-NC	7.15	2.23	2.06
22	b	609	CLA	MG-NA	7.07	2.23	2.06
22	A	406	CLA	MG-NA	7.05	2.23	2.06
22	C	505	CLA	MG-NC	6.94	2.22	2.06
22	c	911	CLA	MG-NA	6.94	2.22	2.06
22	c	905	CLA	MG-NC	6.93	2.22	2.06
22	B	605	CLA	MG-NA	6.88	2.22	2.06
22	C	511	CLA	OBD-CAD	6.73	1.31	1.22
22	c	908	CLA	C3B-C2B	6.73	1.49	1.40
22	B	603	CLA	MG-NA	6.71	2.22	2.06
22	B	617	CLA	MG-NA	6.58	2.21	2.06
22	C	510	CLA	MG-NA	6.53	2.21	2.06
22	c	913	CLA	MG-NA	6.53	2.21	2.06
22	B	603	CLA	MG-NC	6.45	2.21	2.06
22	d	403	CLA	OBD-CAD	6.41	1.31	1.22
22	b	617	CLA	C3B-C2B	6.31	1.49	1.40
22	b	616	CLA	C3B-C2B	6.29	1.49	1.40
22	C	508	CLA	MG-NC	6.27	2.21	2.06
39	V	202	HEC	C3B-C2B	-6.25	1.34	1.40
22	C	513	CLA	MG-NC	6.22	2.21	2.06
22	C	514	CLA	C3B-C2B	6.14	1.48	1.40
22	C	508	CLA	C3B-C2B	6.13	1.48	1.40
22	a	412	CLA	C3C-C2C	6.12	1.49	1.36
22	B	607	CLA	C3B-C2B	6.11	1.48	1.40
22	c	910	CLA	OBD-CAD	6.10	1.31	1.22
22	c	910	CLA	MG-NA	6.08	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	909	CLA	C3C-C2C	6.05	1.49	1.36
22	b	602	CLA	C3B-C2B	6.04	1.48	1.40
23	a	410	PHO	CHB-C1B	6.04	1.50	1.38
39	v	202	HEC	C3B-C2B	-6.01	1.34	1.40
22	b	603	CLA	C3C-C2C	5.98	1.49	1.36
22	c	913	CLA	C3B-C2B	5.94	1.48	1.40
22	b	602	CLA	C3C-C2C	5.91	1.49	1.36
22	B	616	CLA	O2D-CGD	5.89	1.47	1.33
22	c	908	CLA	C3C-C2C	5.89	1.49	1.36
22	a	409	CLA	MG-NA	5.88	2.20	2.06
22	D	401	CLA	OBD-CAD	5.87	1.30	1.22
22	B	611	CLA	C3C-C2C	5.87	1.49	1.36
22	d	402	CLA	MG-NA	5.86	2.20	2.06
23	A	407	PHO	C1A-NA	-5.85	1.25	1.37
22	c	913	CLA	C3C-C2C	5.83	1.49	1.36
23	D	402	PHO	C3B-C2B	5.81	1.49	1.37
22	C	513	CLA	C3C-C2C	5.80	1.49	1.36
22	b	608	CLA	MG-NC	5.78	2.20	2.06
22	C	503	CLA	C3C-C2C	5.76	1.48	1.36
22	B	603	CLA	C3C-C2C	5.76	1.48	1.36
22	c	904	CLA	C3C-C2C	5.76	1.48	1.36
22	b	608	CLA	C3C-C2C	5.74	1.48	1.36
22	C	504	CLA	C3B-C2B	5.71	1.48	1.40
22	A	408	CLA	C3C-C2C	5.68	1.48	1.36
22	b	609	CLA	C3C-C2C	5.68	1.48	1.36
22	B	610	CLA	CHC-C1C	5.65	1.50	1.35
22	b	606	CLA	MG-NA	5.65	2.19	2.06
22	C	504	CLA	CHC-C1C	5.64	1.50	1.35
22	B	614	CLA	CHC-C1C	5.64	1.50	1.35
22	b	616	CLA	C3C-C2C	5.63	1.48	1.36
22	C	514	CLA	C3C-C2C	5.63	1.48	1.36
22	B	602	CLA	C3B-C2B	5.63	1.48	1.40
23	A	407	PHO	CHB-C1B	5.62	1.49	1.38
23	a	411	PHO	C3C-C2C	5.62	1.48	1.36
22	b	617	CLA	C3C-C2C	5.61	1.48	1.36
22	a	408	CLA	C3B-C2B	5.61	1.48	1.40
22	B	610	CLA	MG-NA	5.60	2.19	2.06
22	B	609	CLA	C3C-C2C	5.57	1.48	1.36
23	D	402	PHO	CHB-C1B	5.56	1.49	1.38
22	c	908	CLA	CHC-C1C	5.56	1.50	1.35
22	b	604	CLA	C3C-C2C	5.56	1.48	1.36
23	D	402	PHO	O2D-CGD	5.56	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	905	CLA	O2D-CGD	5.54	1.46	1.33
22	b	602	CLA	O2D-CGD	5.54	1.46	1.33
22	b	615	CLA	C3C-C2C	5.53	1.48	1.36
22	A	408	CLA	MG-NA	5.53	2.19	2.06
22	C	505	CLA	C3B-C2B	5.53	1.48	1.40
22	c	905	CLA	C3C-C2C	5.52	1.48	1.36
22	c	906	CLA	C3B-C2B	5.51	1.48	1.40
22	C	506	CLA	CHC-C1C	5.50	1.49	1.35
22	C	509	CLA	C3C-C2C	5.48	1.48	1.36
22	C	505	CLA	C3C-C2C	5.47	1.48	1.36
23	D	402	PHO	CHC-C1C	5.47	1.49	1.38
22	B	605	CLA	OBD-CAD	5.47	1.30	1.22
22	c	909	CLA	O2D-CGD	5.46	1.46	1.33
22	B	612	CLA	C3C-C2C	5.46	1.48	1.36
23	a	411	PHO	CHB-C1B	5.46	1.49	1.38
22	B	615	CLA	O2A-CGA	5.44	1.49	1.33
22	b	602	CLA	CHC-C1C	5.43	1.49	1.35
22	B	615	CLA	CHC-C1C	5.42	1.49	1.35
22	d	402	CLA	C3B-C2B	5.41	1.47	1.40
22	c	903	CLA	MG-NC	5.41	2.19	2.06
22	C	512	CLA	C3C-C2C	5.41	1.48	1.36
36	e	101	HEM	C3D-C2D	5.41	1.53	1.37
22	c	914	CLA	O2D-CGD	5.40	1.46	1.33
22	b	602	CLA	O2A-CGA	5.40	1.49	1.33
36	E	102	HEM	C3D-C2D	5.40	1.53	1.37
22	c	914	CLA	MG-NA	5.38	2.19	2.06
22	B	617	CLA	C3C-C2C	5.37	1.48	1.36
22	c	912	CLA	CHC-C1C	5.36	1.49	1.35
22	C	506	CLA	C3C-C2C	5.36	1.48	1.36
39	v	202	HEC	C3D-C2D	5.35	1.53	1.37
22	D	404	CLA	C3C-C2C	5.34	1.48	1.36
22	B	603	CLA	C3B-C2B	5.34	1.47	1.40
22	c	912	CLA	O2D-CGD	5.34	1.46	1.33
22	b	603	CLA	O2D-CGD	5.34	1.46	1.33
22	c	902	CLA	CHC-C1C	5.33	1.49	1.35
22	C	504	CLA	C3C-C2C	5.32	1.48	1.36
22	c	912	CLA	C3B-C2B	5.32	1.47	1.40
22	c	906	CLA	CHC-C1C	5.32	1.49	1.35
22	D	404	CLA	OBD-CAD	5.32	1.29	1.22
22	C	513	CLA	O2D-CGD	5.31	1.46	1.33
22	B	611	CLA	CHC-C1C	5.31	1.49	1.35
22	C	508	CLA	C3C-C2C	5.30	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	412	CLA	O2D-CGD	5.30	1.46	1.33
22	c	907	CLA	C3B-C2B	5.29	1.47	1.40
22	b	611	CLA	CHC-C1C	5.29	1.49	1.35
22	A	405	CLA	C3C-C2C	5.29	1.47	1.36
22	c	904	CLA	OBD-CAD	5.29	1.29	1.22
22	A	405	CLA	OBD-CAD	5.29	1.29	1.22
22	c	910	CLA	C3B-C2B	5.28	1.47	1.40
22	D	401	CLA	C3C-C2C	5.28	1.47	1.36
22	B	610	CLA	MG-NC	5.27	2.18	2.06
22	C	510	CLA	C3C-C2C	5.25	1.47	1.36
22	a	407	CLA	O2D-CGD	5.24	1.46	1.33
22	b	617	CLA	CHC-C1C	5.24	1.49	1.35
22	B	602	CLA	O2D-CGD	5.24	1.46	1.33
22	b	611	CLA	C3C-C2C	5.24	1.47	1.36
22	B	615	CLA	C3C-C2C	5.23	1.47	1.36
22	b	606	CLA	CHC-C1C	5.23	1.49	1.35
23	a	411	PHO	CHC-C1C	5.23	1.48	1.38
23	a	411	PHO	C3B-C2B	5.21	1.47	1.37
27	A	412	LHG	O7-C7	5.21	1.47	1.35
22	C	514	CLA	CHC-C1C	5.21	1.49	1.35
22	c	911	CLA	C3D-C2D	5.21	1.49	1.39
22	C	513	CLA	C3B-C2B	5.21	1.47	1.40
22	b	606	CLA	C3C-C2C	5.20	1.47	1.36
31	u	205	DMS	O-S	5.20	1.85	1.50
22	C	510	CLA	O2D-CGD	5.20	1.46	1.33
22	b	604	CLA	O2D-CGD	5.19	1.46	1.33
22	b	603	CLA	CHC-C1C	5.18	1.49	1.35
22	B	607	CLA	C3C-C2C	5.18	1.47	1.36
23	A	407	PHO	C3B-C2B	5.18	1.47	1.37
22	b	608	CLA	O2D-CGD	5.18	1.46	1.33
22	C	511	CLA	C3B-C2B	5.17	1.47	1.40
23	A	407	PHO	CHD-C1D	5.17	1.48	1.38
22	c	907	CLA	O2D-CGD	5.16	1.46	1.33
22	d	403	CLA	C3B-C2B	5.16	1.47	1.40
22	D	404	CLA	CHC-C1C	5.16	1.49	1.35
22	B	604	CLA	C3C-C2C	5.16	1.47	1.36
22	a	412	CLA	MG-NC	5.15	2.18	2.06
22	c	906	CLA	C3C-C2C	5.15	1.47	1.36
22	c	902	CLA	C3C-C2C	5.15	1.47	1.36
22	d	403	CLA	O2A-CGA	5.15	1.48	1.33
22	C	513	CLA	CHC-C1C	5.15	1.49	1.35
22	b	610	CLA	CHC-C1C	5.15	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	CHC-C1C	5.15	1.49	1.35
22	B	617	CLA	C3B-C2B	5.14	1.47	1.40
22	C	502	CLA	MG-NA	5.14	2.18	2.06
22	d	403	CLA	CHC-C1C	5.13	1.48	1.35
22	c	907	CLA	C3C-C2C	5.13	1.47	1.36
22	b	615	CLA	O2D-CGD	5.13	1.45	1.33
22	c	910	CLA	O2D-CGD	5.13	1.45	1.33
31	a	425	DMS	O-S	5.12	1.84	1.50
22	B	616	CLA	CHC-C1C	5.12	1.48	1.35
22	b	613	CLA	CHC-C1C	5.12	1.48	1.35
22	c	909	CLA	CHC-C1C	5.12	1.48	1.35
22	d	403	CLA	C3C-C2C	5.12	1.47	1.36
22	C	502	CLA	C3C-C2C	5.11	1.47	1.36
31	O	311	DMS	O-S	5.11	1.84	1.50
31	b	638	DMS	O-S	5.10	1.84	1.50
22	b	608	CLA	C3D-C2D	5.10	1.49	1.39
22	d	403	CLA	C3D-C2D	5.09	1.49	1.39
22	b	616	CLA	OBD-CAD	5.09	1.29	1.22
22	A	406	CLA	OBD-CAD	5.07	1.29	1.22
22	C	512	CLA	O2D-CGD	5.07	1.45	1.33
22	c	909	CLA	C3B-C2B	5.07	1.47	1.40
22	a	412	CLA	CHC-C1C	5.07	1.48	1.35
22	b	614	CLA	CHC-C1C	5.06	1.48	1.35
22	c	914	CLA	C3B-C2B	5.06	1.47	1.40
22	b	613	CLA	C3B-C2B	5.06	1.47	1.40
22	C	503	CLA	CHC-C1C	5.05	1.48	1.35
22	B	612	CLA	O2D-CGD	5.05	1.45	1.33
22	b	614	CLA	C3C-C2C	5.05	1.47	1.36
22	b	607	CLA	C3C-C2C	5.05	1.47	1.36
22	B	615	CLA	OBD-CAD	5.05	1.29	1.22
22	b	609	CLA	CHC-C1C	5.04	1.48	1.35
22	C	508	CLA	CHC-C1C	5.04	1.48	1.35
22	C	510	CLA	OBD-CAD	5.04	1.29	1.22
22	B	602	CLA	C3C-C2C	5.04	1.47	1.36
22	b	602	CLA	C3D-C2D	5.03	1.49	1.39
22	c	912	CLA	C3C-C2C	5.03	1.47	1.36
22	C	507	CLA	O2D-CGD	5.03	1.45	1.33
22	c	903	CLA	C3B-C2B	5.02	1.47	1.40
22	C	510	CLA	C3D-C2D	5.02	1.49	1.39
22	d	402	CLA	CHC-C1C	5.01	1.48	1.35
22	a	407	CLA	CHC-C1C	5.01	1.48	1.35
22	A	406	CLA	O2D-CGD	5.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	509	CLA	C3D-C2D	5.00	1.49	1.39
22	C	507	CLA	CHC-C1C	5.00	1.48	1.35
22	C	512	CLA	C3B-C2B	5.00	1.47	1.40
22	C	502	CLA	CHC-C1C	4.99	1.48	1.35
22	B	609	CLA	C3B-C2B	4.99	1.47	1.40
22	c	902	CLA	C3B-C2B	4.98	1.47	1.40
22	c	914	CLA	C3C-C2C	4.98	1.47	1.36
22	b	613	CLA	O2D-CGD	4.97	1.45	1.33
22	C	505	CLA	CHC-C1C	4.97	1.48	1.35
22	B	604	CLA	O2D-CGD	4.97	1.45	1.33
22	b	610	CLA	OBD-CAD	4.97	1.29	1.22
22	B	616	CLA	C3C-C2C	4.97	1.47	1.36
22	a	408	CLA	CHC-C1C	4.96	1.48	1.35
22	b	603	CLA	C3B-C2B	4.96	1.47	1.40
39	v	202	HEC	C3C-C2C	-4.96	1.35	1.40
22	c	914	CLA	CHC-C1C	4.96	1.48	1.35
35	D	407	DGD	O2G-C1B	4.95	1.48	1.34
22	b	611	CLA	C3B-C2B	4.95	1.47	1.40
22	B	612	CLA	C3B-C2B	4.95	1.47	1.40
27	a	416	LHG	O8-C23	4.94	1.48	1.33
22	c	904	CLA	CHC-C1C	4.94	1.48	1.35
22	b	613	CLA	OBD-CAD	4.94	1.29	1.22
22	c	909	CLA	OBD-CAD	4.93	1.29	1.22
22	B	607	CLA	CHC-C1C	4.93	1.48	1.35
22	a	408	CLA	C3C-C2C	4.93	1.47	1.36
22	B	615	CLA	O2D-CGD	4.93	1.45	1.33
22	B	612	CLA	OBD-CAD	4.92	1.29	1.22
22	b	611	CLA	O2D-CGD	4.92	1.45	1.33
22	B	606	CLA	CHC-C1C	4.91	1.48	1.35
22	B	614	CLA	C3B-C2B	4.90	1.47	1.40
22	b	614	CLA	O2D-CGD	4.90	1.45	1.33
22	c	911	CLA	CHC-C1C	4.90	1.48	1.35
22	c	911	CLA	OBD-CAD	4.90	1.29	1.22
22	C	509	CLA	CHC-C1C	4.90	1.48	1.35
25	b	622	LMG	O8-C28	4.89	1.47	1.33
22	B	614	CLA	OBD-CAD	4.89	1.29	1.22
22	b	616	CLA	O2D-CGD	4.89	1.45	1.33
22	B	608	CLA	OBD-CAD	4.89	1.29	1.22
31	H	103	DMS	O-S	4.88	1.82	1.50
22	B	609	CLA	CHC-C1C	4.88	1.48	1.35
22	b	605	CLA	C3C-C2C	4.88	1.47	1.36
22	B	616	CLA	C3B-C2B	4.88	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	615	CLA	C3D-C2D	4.88	1.49	1.39
22	A	408	CLA	O2D-CGD	4.88	1.45	1.33
31	O	305	DMS	O-S	4.87	1.82	1.50
31	c	937	DMS	O-S	4.87	1.82	1.50
22	C	511	CLA	MG-NC	4.87	2.17	2.06
22	C	514	CLA	O2D-CGD	4.86	1.45	1.33
22	B	613	CLA	C3C-C2C	4.86	1.47	1.36
22	c	913	CLA	CHC-C1C	4.85	1.48	1.35
22	b	615	CLA	C3B-C2B	4.85	1.47	1.40
31	B	628	DMS	O-S	4.85	1.82	1.50
22	B	603	CLA	CHC-C1C	4.85	1.48	1.35
22	b	610	CLA	O2D-CGD	4.85	1.45	1.33
22	B	613	CLA	O2D-CGD	4.85	1.45	1.33
22	C	511	CLA	O2D-CGD	4.85	1.45	1.33
22	B	602	CLA	O2A-CGA	4.84	1.47	1.33
22	B	613	CLA	C3B-C2B	4.84	1.47	1.40
22	c	903	CLA	CHC-C1C	4.83	1.48	1.35
22	B	617	CLA	C3D-C2D	4.83	1.48	1.39
22	d	402	CLA	C3C-C2C	4.83	1.46	1.36
31	c	933	DMS	O-S	4.83	1.82	1.50
31	v	210	DMS	O-S	4.82	1.82	1.50
31	c	924	DMS	O-S	4.82	1.82	1.50
35	d	406	DGD	O2G-C1B	4.82	1.48	1.34
23	A	407	PHO	CHC-C1C	4.82	1.48	1.38
22	a	409	CLA	C3B-C2B	4.82	1.47	1.40
22	c	908	CLA	OBD-CAD	4.82	1.29	1.22
25	D	412	LMG	O8-C28	4.81	1.47	1.33
22	c	903	CLA	C3C-C2C	4.81	1.46	1.36
31	B	630	DMS	O-S	4.81	1.82	1.50
22	b	610	CLA	C3C-C2C	4.80	1.46	1.36
22	c	905	CLA	CHC-C1C	4.79	1.48	1.35
31	o	304	DMS	O-S	4.79	1.82	1.50
22	C	507	CLA	C3B-C2B	4.79	1.47	1.40
22	b	607	CLA	CHC-C1C	4.79	1.48	1.35
22	B	604	CLA	C3B-C2B	4.78	1.47	1.40
22	B	604	CLA	MG-NC	4.77	2.17	2.06
22	B	611	CLA	C3D-C2D	4.77	1.48	1.39
23	A	407	PHO	C3C-C2C	4.77	1.46	1.36
22	c	905	CLA	C3D-C2D	4.77	1.48	1.39
35	d	406	DGD	O1G-C1A	4.76	1.47	1.33
22	a	408	CLA	OBD-CAD	4.75	1.29	1.22
22	C	510	CLA	CHC-C1C	4.75	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	609	CLA	OBD-CAD	4.75	1.29	1.22
31	B	634	DMS	O-S	4.74	1.82	1.50
31	V	211	DMS	O-S	4.74	1.82	1.50
31	c	929	DMS	O-S	4.74	1.82	1.50
22	b	617	CLA	O2D-CGD	4.74	1.44	1.33
22	C	504	CLA	C3D-C2D	4.73	1.48	1.39
25	B	621	LMG	O8-C28	4.73	1.47	1.33
25	D	412	LMG	O7-C10	4.73	1.47	1.34
31	B	635	DMS	O-S	4.72	1.81	1.50
22	A	408	CLA	MG-NC	4.72	2.17	2.06
22	C	502	CLA	MG-NC	4.72	2.17	2.06
22	C	512	CLA	OBD-CAD	4.72	1.29	1.22
22	C	507	CLA	C3C-C2C	4.71	1.46	1.36
31	o	308	DMS	O-S	4.71	1.81	1.50
31	B	637	DMS	O-S	4.71	1.81	1.50
25	C	531	LMG	O7-C10	4.70	1.47	1.34
31	O	308	DMS	O-S	4.69	1.81	1.50
25	c	930	LMG	O7-C10	4.69	1.47	1.34
22	B	613	CLA	CHC-C1C	4.69	1.47	1.35
31	O	307	DMS	O-S	4.68	1.81	1.50
31	B	641	DMS	O-S	4.68	1.81	1.50
31	c	939	DMS	O-S	4.68	1.81	1.50
31	V	212	DMS	O-S	4.68	1.81	1.50
31	V	210	DMS	O-S	4.68	1.81	1.50
31	b	635	DMS	O-S	4.68	1.81	1.50
22	b	612	CLA	O2D-CGD	4.68	1.44	1.33
31	C	540	DMS	O-S	4.68	1.81	1.50
31	u	204	DMS	O-S	4.68	1.81	1.50
22	B	615	CLA	C3B-C2B	4.68	1.46	1.40
22	C	512	CLA	O2A-CGA	4.68	1.47	1.33
31	v	211	DMS	O-S	4.67	1.81	1.50
22	b	616	CLA	CHC-C1C	4.67	1.47	1.35
22	a	407	CLA	C3B-C2B	4.67	1.46	1.40
22	B	614	CLA	C3C-C2C	4.67	1.46	1.36
31	l	104	DMS	O-S	4.67	1.81	1.50
23	a	410	PHO	C3C-C2C	4.67	1.46	1.36
22	D	404	CLA	C3B-C2B	4.66	1.46	1.40
22	C	504	CLA	OBD-CAD	4.66	1.28	1.22
22	C	506	CLA	OBD-CAD	4.66	1.28	1.22
31	c	938	DMS	O-S	4.66	1.81	1.50
27	a	416	LHG	O7-C7	4.66	1.47	1.34
22	A	405	CLA	CHC-C1C	4.65	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	520	LMG	O8-C28	4.65	1.47	1.33
31	O	303	DMS	O-S	4.65	1.81	1.50
22	C	510	CLA	O2A-CGA	4.65	1.47	1.33
35	D	407	DGD	O1G-C1A	4.64	1.47	1.33
22	B	610	CLA	C3C-C2C	4.64	1.46	1.36
31	U	203	DMS	O-S	4.64	1.81	1.50
31	D	417	DMS	O-S	4.64	1.81	1.50
31	V	206	DMS	O-S	4.64	1.81	1.50
22	b	602	CLA	OBD-CAD	4.63	1.28	1.22
22	B	612	CLA	CHC-C1C	4.63	1.47	1.35
22	B	607	CLA	O2D-CGD	4.63	1.44	1.33
31	C	537	DMS	O-S	4.63	1.81	1.50
31	V	207	DMS	O-S	4.62	1.81	1.50
22	b	613	CLA	C3C-C2C	4.62	1.46	1.36
27	C	522	LHG	O7-C7	4.62	1.47	1.34
31	I	101	DMS	O-S	4.62	1.81	1.50
22	b	607	CLA	C3B-C2B	4.62	1.46	1.40
31	B	639	DMS	O-S	4.62	1.81	1.50
22	b	607	CLA	O2D-CGD	4.62	1.44	1.33
22	C	509	CLA	C3B-C2B	4.61	1.46	1.40
22	B	608	CLA	O2D-CGD	4.61	1.44	1.33
31	C	533	DMS	O-S	4.61	1.81	1.50
25	i	101	LMG	O8-C28	4.61	1.47	1.33
22	C	506	CLA	C3B-C2B	4.60	1.46	1.40
31	a	401	DMS	O-S	4.60	1.81	1.50
31	C	535	DMS	O-S	4.60	1.81	1.50
31	l	105	DMS	O-S	4.60	1.81	1.50
31	O	314	DMS	O-S	4.60	1.81	1.50
31	c	942	DMS	O-S	4.60	1.81	1.50
25	c	920	LMG	O8-C28	4.60	1.47	1.33
22	D	404	CLA	O2D-CGD	4.59	1.44	1.33
31	L	102	DMS	O-S	4.59	1.81	1.50
22	c	903	CLA	C3D-C2D	4.59	1.48	1.39
22	b	609	CLA	C3B-C2B	4.59	1.46	1.40
22	c	913	CLA	O2D-CGD	4.59	1.44	1.33
31	a	424	DMS	O-S	4.59	1.81	1.50
22	C	503	CLA	C3D-C2D	4.59	1.48	1.39
31	b	637	DMS	O-S	4.59	1.81	1.50
22	c	911	CLA	C3C-C2C	4.59	1.46	1.36
31	c	940	DMS	O-S	4.59	1.80	1.50
31	b	634	DMS	O-S	4.59	1.80	1.50
31	u	203	DMS	O-S	4.59	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	407	CLA	MG-NC	4.58	2.17	2.06
22	c	910	CLA	C3D-C2D	4.58	1.48	1.39
31	U	202	DMS	O-S	4.58	1.80	1.50
31	V	204	DMS	O-S	4.58	1.80	1.50
31	d	411	DMS	O-S	4.58	1.80	1.50
31	O	306	DMS	O-S	4.58	1.80	1.50
31	C	536	DMS	O-S	4.58	1.80	1.50
22	B	605	CLA	C3C-C2C	4.58	1.46	1.36
31	f	103	DMS	O-S	4.58	1.80	1.50
22	C	512	CLA	CHC-C1C	4.57	1.47	1.35
31	b	630	DMS	O-S	4.57	1.80	1.50
31	t	104	DMS	O-S	4.57	1.80	1.50
22	a	407	CLA	C3C-C2C	4.57	1.46	1.36
22	b	616	CLA	MG-NC	4.57	2.17	2.06
31	A	419	DMS	O-S	4.57	1.80	1.50
31	c	928	DMS	O-S	4.57	1.80	1.50
31	c	944	DMS	O-S	4.57	1.80	1.50
27	d	401	LHG	O8-C23	4.57	1.46	1.33
31	t	103	DMS	O-S	4.56	1.80	1.50
23	a	410	PHO	CHC-C1C	4.56	1.47	1.38
31	B	633	DMS	O-S	4.56	1.80	1.50
22	b	613	CLA	C3D-C2D	4.56	1.48	1.39
31	t	105	DMS	O-S	4.56	1.80	1.50
31	l	103	DMS	O-S	4.56	1.80	1.50
31	o	302	DMS	O-S	4.56	1.80	1.50
22	B	609	CLA	C3D-C2D	4.56	1.48	1.39
28	a	414	SQD	O48-C23	4.56	1.46	1.33
31	c	943	DMS	O-S	4.55	1.80	1.50
22	c	904	CLA	C3B-C2B	4.55	1.46	1.40
31	v	207	DMS	O-S	4.55	1.80	1.50
22	b	615	CLA	O2A-CGA	4.55	1.46	1.33
22	c	910	CLA	MG-NC	4.55	2.17	2.06
31	A	420	DMS	O-S	4.55	1.80	1.50
31	o	303	DMS	O-S	4.54	1.80	1.50
31	C	534	DMS	O-S	4.54	1.80	1.50
25	B	621	LMG	O7-C10	4.54	1.47	1.34
31	b	631	DMS	O-S	4.54	1.80	1.50
31	d	414	DMS	O-S	4.54	1.80	1.50
31	c	936	DMS	O-S	4.53	1.80	1.50
22	c	908	CLA	C3D-C2D	4.53	1.48	1.39
22	C	505	CLA	O2D-CGD	4.53	1.44	1.33
31	c	925	DMS	O-S	4.53	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	539	DMS	O-S	4.53	1.80	1.50
31	v	206	DMS	O-S	4.53	1.80	1.50
31	C	527	DMS	O-S	4.53	1.80	1.50
31	C	530	DMS	O-S	4.52	1.80	1.50
22	A	408	CLA	OBD-CAD	4.52	1.28	1.22
31	I	106	DMS	O-S	4.52	1.80	1.50
22	A	408	CLA	CHC-C1C	4.52	1.47	1.35
22	B	604	CLA	CHC-C1C	4.51	1.47	1.35
31	A	417	DMS	O-S	4.51	1.80	1.50
31	b	633	DMS	O-S	4.51	1.80	1.50
31	B	642	DMS	O-S	4.51	1.80	1.50
23	a	410	PHO	C3B-C2B	4.51	1.46	1.37
22	B	615	CLA	MG-NA	4.51	2.17	2.06
23	D	402	PHO	C3C-C2C	4.50	1.46	1.36
39	V	202	HEC	C3D-C2D	4.50	1.51	1.37
31	C	529	DMS	O-S	4.50	1.80	1.50
22	B	609	CLA	O2D-CGD	4.50	1.44	1.33
22	c	910	CLA	O2A-CGA	4.50	1.46	1.33
22	C	502	CLA	C3D-C2D	4.50	1.48	1.39
22	b	605	CLA	O2D-CGD	4.49	1.44	1.33
22	A	406	CLA	CHC-C1C	4.49	1.47	1.35
22	b	615	CLA	CHC-C1C	4.49	1.47	1.35
31	A	416	DMS	O-S	4.49	1.80	1.50
31	b	636	DMS	O-S	4.49	1.80	1.50
22	d	402	CLA	O2A-CGA	4.49	1.46	1.33
31	V	209	DMS	O-S	4.49	1.80	1.50
25	C	520	LMG	O7-C10	4.49	1.47	1.34
31	v	204	DMS	O-S	4.49	1.80	1.50
31	c	927	DMS	O-S	4.49	1.80	1.50
31	C	538	DMS	O-S	4.48	1.80	1.50
31	F	101	DMS	O-S	4.48	1.80	1.50
31	c	934	DMS	O-S	4.48	1.80	1.50
22	B	608	CLA	CHC-C1C	4.48	1.47	1.35
31	B	638	DMS	O-S	4.48	1.80	1.50
22	b	608	CLA	C3B-C2B	4.48	1.46	1.40
31	c	935	DMS	O-S	4.48	1.80	1.50
27	A	412	LHG	O8-C23	4.48	1.46	1.33
22	B	610	CLA	C3D-C2D	4.48	1.48	1.39
28	a	418	SQD	O48-C23	4.47	1.46	1.33
31	a	421	DMS	O-S	4.46	1.80	1.50
31	O	310	DMS	O-S	4.46	1.80	1.50
22	c	914	CLA	O2A-CGA	4.46	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	506	CLA	O2D-CGD	4.46	1.44	1.33
22	c	907	CLA	OBD-CAD	4.46	1.28	1.22
22	b	608	CLA	CHC-C1C	4.46	1.47	1.35
22	b	606	CLA	O2D-CGD	4.46	1.44	1.33
31	B	632	DMS	O-S	4.45	1.80	1.50
22	d	403	CLA	O2D-CGD	4.45	1.44	1.33
22	a	409	CLA	CHC-C1C	4.45	1.47	1.35
31	o	306	DMS	O-S	4.45	1.80	1.50
22	c	913	CLA	C3D-C2D	4.45	1.48	1.39
31	i	106	DMS	O-S	4.44	1.80	1.50
31	v	209	DMS	O-S	4.44	1.80	1.50
31	O	312	DMS	O-S	4.44	1.80	1.50
23	A	407	PHO	O2D-CGD	4.44	1.44	1.33
31	C	526	DMS	O-S	4.44	1.79	1.50
22	C	504	CLA	O2D-CGD	4.44	1.44	1.33
31	C	528	DMS	O-S	4.44	1.79	1.50
31	v	205	DMS	O-S	4.44	1.79	1.50
31	c	926	DMS	O-S	4.44	1.79	1.50
31	O	313	DMS	O-S	4.44	1.79	1.50
22	C	506	CLA	MG-NC	4.44	2.16	2.06
22	c	906	CLA	O2D-CGD	4.44	1.44	1.33
22	B	605	CLA	CHC-C1C	4.43	1.47	1.35
22	c	907	CLA	CHC-C1C	4.43	1.47	1.35
22	c	903	CLA	O2D-CGD	4.43	1.44	1.33
31	v	208	DMS	O-S	4.43	1.79	1.50
28	l	101	SQD	O47-C7	4.43	1.46	1.34
22	c	902	CLA	OBD-CAD	4.42	1.28	1.22
28	a	418	SQD	O47-C7	4.42	1.46	1.34
31	V	205	DMS	O-S	4.42	1.79	1.50
31	o	307	DMS	O-S	4.42	1.79	1.50
23	a	411	PHO	O2D-CGD	4.42	1.44	1.33
22	c	913	CLA	OBD-CAD	4.42	1.28	1.22
22	C	504	CLA	O2A-CGA	4.41	1.46	1.33
28	l	101	SQD	O48-C23	4.41	1.46	1.33
22	B	610	CLA	O2D-CGD	4.41	1.44	1.33
35	H	102	DGD	O1G-C1A	4.41	1.46	1.33
28	b	621	SQD	O48-C23	4.41	1.46	1.33
22	B	606	CLA	C3C-C2C	4.41	1.46	1.36
22	D	403	CLA	C3C-C2C	4.41	1.46	1.36
22	A	408	CLA	C3B-C2B	4.41	1.46	1.40
22	C	503	CLA	O2D-CGD	4.41	1.44	1.33
35	c	919	DGD	O1G-C1A	4.40	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	510	CLA	C3B-C2B	4.40	1.46	1.40
31	o	305	DMS	O-S	4.40	1.79	1.50
22	b	612	CLA	CHC-C1C	4.40	1.46	1.35
27	D	409	LHG	O8-C23	4.40	1.46	1.33
22	b	610	CLA	C3D-C2D	4.39	1.48	1.39
22	b	604	CLA	CHC-C1C	4.39	1.46	1.35
31	B	640	DMS	O-S	4.39	1.79	1.50
22	B	617	CLA	CHC-C1C	4.39	1.46	1.35
22	B	611	CLA	O2D-CGD	4.39	1.44	1.33
31	V	201	DMS	O-S	4.38	1.79	1.50
39	V	202	HEC	C3C-C2C	-4.38	1.36	1.40
31	V	208	DMS	O-S	4.38	1.79	1.50
22	b	605	CLA	MG-NC	4.37	2.16	2.06
22	c	906	CLA	C3D-C2D	4.37	1.48	1.39
31	d	415	DMS	O-S	4.37	1.79	1.50
22	B	606	CLA	C3B-C2B	4.37	1.46	1.40
25	j	101	LMG	O8-C28	4.37	1.46	1.33
31	c	941	DMS	O-S	4.37	1.79	1.50
22	c	904	CLA	O2D-CGD	4.37	1.44	1.33
28	C	501	SQD	O47-C7	4.37	1.46	1.34
22	D	401	CLA	O2D-CGD	4.37	1.44	1.33
31	u	202	DMS	O-S	4.37	1.79	1.50
25	b	622	LMG	O7-C10	4.36	1.46	1.34
22	c	911	CLA	O2D-CGD	4.36	1.44	1.33
31	O	304	DMS	O-S	4.36	1.79	1.50
22	A	405	CLA	O2D-CGD	4.35	1.44	1.33
22	c	908	CLA	O2D-CGD	4.35	1.44	1.33
31	B	636	DMS	O-S	4.35	1.79	1.50
22	c	913	CLA	O2A-CGA	4.35	1.46	1.33
25	d	409	LMG	O8-C28	4.34	1.46	1.33
22	c	910	CLA	C3C-C2C	4.34	1.45	1.36
25	C	531	LMG	O8-C28	4.34	1.46	1.33
31	B	629	DMS	O-S	4.34	1.79	1.50
23	a	410	PHO	O2D-CGD	4.34	1.43	1.33
22	b	605	CLA	CHC-C1C	4.33	1.46	1.35
27	a	423	LHG	O8-C23	4.33	1.46	1.33
34	B	623	HTG	C1'-S1	-4.33	1.75	1.81
22	b	604	CLA	C3D-C2D	4.33	1.47	1.39
22	C	514	CLA	O2A-CGA	4.32	1.46	1.33
25	A	410	LMG	O8-C28	4.32	1.46	1.33
22	c	911	CLA	MG-NC	4.32	2.16	2.06
22	b	617	CLA	C3D-C2D	4.32	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	v	201	DMS	O-S	4.31	1.79	1.50
22	a	409	CLA	O2D-CGD	4.31	1.43	1.33
31	d	413	DMS	O-S	4.31	1.79	1.50
22	C	507	CLA	MG-NC	4.31	2.16	2.06
22	C	511	CLA	CHC-C1C	4.31	1.46	1.35
22	b	605	CLA	C3D-C2D	4.31	1.47	1.39
22	D	401	CLA	C3D-C2D	4.30	1.47	1.39
25	c	930	LMG	O8-C28	4.30	1.46	1.33
22	C	511	CLA	C3C-C2C	4.29	1.45	1.36
22	b	612	CLA	C3C-C2C	4.29	1.45	1.36
31	B	631	DMS	O-S	4.29	1.78	1.50
27	C	522	LHG	O8-C23	4.28	1.46	1.33
31	d	412	DMS	O-S	4.28	1.78	1.50
22	B	611	CLA	C3B-C2B	4.28	1.46	1.40
22	b	610	CLA	C3B-C2B	4.28	1.46	1.40
22	c	906	CLA	MG-NC	4.28	2.16	2.06
22	C	513	CLA	OBD-CAD	4.28	1.28	1.22
22	c	914	CLA	C3D-C2D	4.27	1.47	1.39
23	a	411	PHO	C1A-NA	-4.27	1.28	1.37
35	C	518	DGD	O1G-C1A	4.26	1.46	1.33
22	B	603	CLA	OBD-CAD	4.26	1.28	1.22
22	c	908	CLA	O2A-CGA	4.26	1.46	1.33
22	c	911	CLA	C3B-C2B	4.26	1.46	1.40
31	O	309	DMS	O-S	4.26	1.78	1.50
31	c	923	DMS	O-S	4.26	1.78	1.50
22	C	512	CLA	C3D-C2D	4.26	1.47	1.39
22	b	617	CLA	OBD-CAD	4.25	1.28	1.22
22	b	613	CLA	O2A-CGA	4.25	1.46	1.33
23	a	411	PHO	CHD-C1D	4.25	1.46	1.38
22	c	912	CLA	OBD-CAD	4.25	1.28	1.22
22	C	508	CLA	O2D-CGD	4.25	1.43	1.33
31	D	416	DMS	O-S	4.25	1.78	1.50
35	h	102	DGD	O1G-C1A	4.25	1.46	1.33
22	b	603	CLA	O2A-CGA	4.25	1.45	1.33
22	A	405	CLA	C3D-C2D	4.25	1.47	1.39
22	C	514	CLA	C3D-C2D	4.24	1.47	1.39
22	B	616	CLA	C3D-C2D	4.24	1.47	1.39
22	B	614	CLA	MG-NC	4.24	2.16	2.06
22	B	607	CLA	O2A-CGA	4.24	1.45	1.33
22	C	503	CLA	OBD-CAD	4.24	1.28	1.22
22	D	404	CLA	C3D-C2D	4.23	1.47	1.39
22	D	404	CLA	C4C-C3C	4.23	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	OBD-CAD	4.23	1.28	1.22
22	C	509	CLA	O2D-CGD	4.23	1.43	1.33
22	b	610	CLA	O2A-CGA	4.22	1.45	1.33
23	D	402	PHO	O2A-CGA	4.22	1.45	1.33
22	B	608	CLA	C3B-C2B	4.22	1.46	1.40
22	B	614	CLA	C3D-C2D	4.22	1.47	1.39
22	c	904	CLA	O2A-CGA	4.22	1.45	1.33
22	C	507	CLA	O2A-CGA	4.21	1.45	1.33
27	d	401	LHG	O7-C7	4.21	1.46	1.34
25	i	101	LMG	O7-C10	4.20	1.46	1.34
22	a	407	CLA	C3D-C2D	4.19	1.47	1.39
22	b	612	CLA	C3D-C2D	4.19	1.47	1.39
22	a	412	CLA	C3B-C2B	4.19	1.46	1.40
35	h	102	DGD	O2G-C1B	4.18	1.46	1.34
22	B	609	CLA	O2A-CGA	4.18	1.45	1.33
22	B	602	CLA	C3D-C2D	4.17	1.47	1.39
22	B	617	CLA	O2D-CGD	4.17	1.43	1.33
28	a	414	SQD	O47-C7	4.17	1.46	1.34
22	D	401	CLA	MG-NA	4.17	2.16	2.06
31	C	524	DMS	O-S	4.16	1.78	1.50
22	B	607	CLA	C4B-CHC	4.15	1.51	1.40
22	B	617	CLA	O2A-CGA	4.15	1.45	1.33
22	d	402	CLA	O2D-CGD	4.14	1.43	1.33
27	l	102	LHG	O7-C7	4.13	1.46	1.34
22	C	511	CLA	C3D-C2D	4.12	1.47	1.39
22	b	614	CLA	C3B-C2B	4.12	1.46	1.40
22	B	615	CLA	C3D-C2D	4.11	1.47	1.39
22	B	604	CLA	O2A-CGA	4.11	1.45	1.33
25	c	920	LMG	O7-C10	4.11	1.46	1.34
22	B	610	CLA	C3B-C2B	4.11	1.46	1.40
22	B	608	CLA	C3C-C2C	4.11	1.45	1.36
22	c	907	CLA	O2A-CGA	4.10	1.45	1.33
22	b	617	CLA	O2A-CGA	4.10	1.45	1.33
22	C	508	CLA	OBD-CAD	4.09	1.28	1.22
22	c	902	CLA	O2D-CGD	4.09	1.43	1.33
22	a	408	CLA	C3D-C2D	4.08	1.47	1.39
27	d	408	LHG	O8-C23	4.08	1.45	1.33
22	C	506	CLA	C3D-C2D	4.07	1.47	1.39
23	D	402	PHO	C1A-NA	-4.07	1.29	1.37
22	C	502	CLA	O2D-CGD	4.07	1.43	1.33
22	C	514	CLA	C4B-CHC	4.07	1.50	1.40
25	d	409	LMG	O7-C10	4.07	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	906	CLA	O2A-CGA	4.07	1.45	1.33
22	b	611	CLA	C3D-C2D	4.06	1.47	1.39
22	C	507	CLA	C3D-C2D	4.06	1.47	1.39
23	A	407	PHO	O2A-CGA	4.06	1.45	1.33
22	a	408	CLA	O2D-CGD	4.06	1.43	1.33
22	D	403	CLA	O2A-CGA	4.05	1.45	1.33
31	a	402	DMS	O-S	4.04	1.77	1.50
22	b	609	CLA	O2A-CGA	4.04	1.45	1.33
22	c	914	CLA	OBD-CAD	4.04	1.28	1.22
22	B	605	CLA	O2D-CGD	4.04	1.43	1.33
36	E	102	HEM	C3C-CAC	4.04	1.56	1.47
28	A	413	SQD	O48-C23	4.04	1.45	1.33
22	b	612	CLA	O2A-CGA	4.03	1.45	1.33
31	A	418	DMS	O-S	4.03	1.77	1.50
25	A	410	LMG	O7-C10	4.03	1.45	1.34
22	B	610	CLA	O2A-CGA	4.02	1.45	1.33
31	C	525	DMS	O-S	4.01	1.77	1.50
31	D	418	DMS	O-S	4.01	1.77	1.50
22	C	505	CLA	C3D-C2D	4.00	1.47	1.39
22	C	513	CLA	C3D-C2D	3.98	1.47	1.39
22	C	506	CLA	O2A-CGA	3.98	1.45	1.33
22	b	616	CLA	C3D-C2D	3.97	1.47	1.39
22	b	606	CLA	O2A-CGA	3.97	1.45	1.33
35	C	519	DGD	O1G-C1A	3.97	1.45	1.33
22	b	616	CLA	O2A-CGA	3.96	1.45	1.33
22	B	613	CLA	C3D-C2D	3.95	1.47	1.39
35	H	102	DGD	O2G-C1B	3.95	1.45	1.34
25	J	101	LMG	O7-C10	3.94	1.45	1.34
22	b	610	CLA	MG-NC	3.94	2.15	2.06
22	B	612	CLA	C3D-C2D	3.94	1.47	1.39
22	a	412	CLA	O2A-CGA	3.93	1.45	1.33
22	b	608	CLA	OBD-CAD	3.92	1.27	1.22
22	c	912	CLA	C3D-C2D	3.92	1.47	1.39
22	C	513	CLA	O2A-CGA	3.91	1.44	1.33
22	c	910	CLA	CHC-C1C	3.91	1.45	1.35
22	C	503	CLA	C3B-C2B	3.91	1.45	1.40
22	a	407	CLA	OBD-CAD	3.91	1.27	1.22
22	C	502	CLA	C3B-C2B	3.90	1.45	1.40
22	C	508	CLA	C3D-C2D	3.90	1.47	1.39
22	b	602	CLA	C1B-CHB	3.90	1.50	1.40
22	c	903	CLA	MG-NA	3.90	2.15	2.06
22	b	609	CLA	C3D-C2D	3.89	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	603	CLA	O2D-CGD	3.89	1.42	1.33
22	A	405	CLA	C3B-C2B	3.88	1.45	1.40
23	a	410	PHO	C1A-NA	-3.88	1.29	1.37
28	A	413	SQD	O47-C7	3.87	1.45	1.34
25	J	101	LMG	O8-C28	3.87	1.44	1.33
22	C	502	CLA	O2A-CGA	3.87	1.44	1.33
22	c	909	CLA	C3D-C2D	3.86	1.47	1.39
22	B	608	CLA	C3D-C2D	3.86	1.47	1.39
22	B	614	CLA	O2D-CGD	3.86	1.42	1.33
22	B	614	CLA	O2A-CGA	3.86	1.44	1.33
27	L	101	LHG	O8-C23	3.85	1.44	1.33
22	b	606	CLA	C3D-C2D	3.85	1.47	1.39
35	c	918	DGD	O1G-C1A	3.85	1.44	1.33
22	d	402	CLA	OBD-CAD	3.84	1.27	1.22
22	B	613	CLA	OBD-CAD	3.84	1.27	1.22
22	B	611	CLA	OBD-CAD	3.84	1.27	1.22
27	l	102	LHG	O8-C23	3.84	1.44	1.33
27	D	411	LHG	O7-C7	3.84	1.45	1.34
22	b	612	CLA	C1B-CHB	3.84	1.50	1.40
36	E	102	HEM	C3B-CAB	3.84	1.55	1.47
22	a	408	CLA	O2A-CGA	3.83	1.44	1.33
35	c	917	DGD	O2G-C1B	3.83	1.45	1.34
22	B	602	CLA	C4C-C3C	3.83	1.51	1.45
22	a	409	CLA	O2A-CGA	3.83	1.44	1.33
22	a	412	CLA	OBD-CAD	3.82	1.27	1.22
27	a	423	LHG	O7-C7	3.82	1.45	1.34
23	a	411	PHO	OBD-CAD	3.82	1.29	1.22
22	b	603	CLA	C3D-C2D	3.82	1.46	1.39
22	D	404	CLA	O2A-CGA	3.81	1.44	1.33
22	C	507	CLA	OBD-CAD	3.81	1.27	1.22
22	C	504	CLA	C4B-CHC	3.81	1.50	1.40
36	e	101	HEM	C3B-CAB	3.81	1.55	1.47
27	L	101	LHG	O7-C7	3.80	1.45	1.34
31	b	629	DMS	O-S	3.80	1.75	1.50
28	C	501	SQD	O48-C23	3.79	1.44	1.33
27	D	409	LHG	O7-C7	3.79	1.45	1.34
22	B	606	CLA	O2D-CGD	3.78	1.42	1.33
22	B	603	CLA	O2A-CGA	3.78	1.44	1.33
23	A	407	PHO	CHD-C4C	3.76	1.49	1.40
34	C	532	HTG	C1'-S1	-3.75	1.76	1.81
22	b	609	CLA	O2D-CGD	3.75	1.42	1.33
22	B	616	CLA	O2A-CGA	3.74	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	909	CLA	O2A-CGA	3.74	1.44	1.33
22	c	908	CLA	C1B-CHB	3.74	1.50	1.40
22	C	509	CLA	O2A-CGA	3.74	1.44	1.33
22	C	503	CLA	O2A-CGA	3.73	1.44	1.33
22	b	614	CLA	OBD-CAD	3.72	1.27	1.22
22	B	615	CLA	C1B-CHB	3.72	1.50	1.40
22	C	506	CLA	C4C-C3C	3.72	1.51	1.45
25	j	101	LMG	O7-C10	3.72	1.44	1.34
22	C	509	CLA	OBD-CAD	3.71	1.27	1.22
22	b	616	CLA	C1B-CHB	3.70	1.50	1.40
22	a	409	CLA	C3D-C2D	3.70	1.46	1.39
22	c	914	CLA	C1B-CHB	3.70	1.50	1.40
22	c	904	CLA	C3D-C2D	3.69	1.46	1.39
22	B	612	CLA	O2A-CGA	3.69	1.44	1.33
22	b	614	CLA	C3D-C2D	3.68	1.46	1.39
34	b	623	HTG	C1'-S1	-3.68	1.76	1.81
35	c	919	DGD	O2G-C1B	3.67	1.44	1.34
22	a	409	CLA	C3C-C2C	3.67	1.44	1.36
22	c	908	CLA	C4B-CHC	3.67	1.49	1.40
22	C	502	CLA	OBD-CAD	3.66	1.27	1.22
22	C	514	CLA	C1B-CHB	3.66	1.49	1.40
22	a	409	CLA	OBD-CAD	3.66	1.27	1.22
22	d	403	CLA	C4C-C3C	3.65	1.51	1.45
22	B	607	CLA	C3D-C2D	3.65	1.46	1.39
22	C	514	CLA	OBD-CAD	3.64	1.27	1.22
22	b	614	CLA	O2A-CGA	3.63	1.44	1.33
22	D	403	CLA	O2D-CGD	3.63	1.42	1.33
35	c	917	DGD	O1G-C1A	3.62	1.44	1.33
22	c	905	CLA	C3B-C2B	3.61	1.45	1.40
22	B	605	CLA	C3B-C2B	3.61	1.45	1.40
22	c	906	CLA	OBD-CAD	3.61	1.27	1.22
27	D	411	LHG	O8-C23	3.60	1.44	1.33
22	B	604	CLA	C3D-C2D	3.60	1.46	1.39
23	D	402	PHO	OBD-CAD	3.60	1.28	1.22
22	c	911	CLA	C4B-CHC	3.60	1.49	1.40
22	a	412	CLA	C3D-C2D	3.60	1.46	1.39
39	v	202	HEC	CBC-CAC	-3.60	1.35	1.49
23	a	411	PHO	O2A-CGA	3.59	1.44	1.33
22	B	613	CLA	O2A-CGA	3.59	1.44	1.33
22	b	610	CLA	C1B-CHB	3.59	1.49	1.40
22	d	402	CLA	MG-NC	3.58	2.14	2.06
22	b	612	CLA	OBD-CAD	3.58	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	911	CLA	O2A-CGA	3.57	1.43	1.33
22	b	611	CLA	O2A-CGA	3.57	1.43	1.33
22	B	613	CLA	C4B-CHC	3.57	1.49	1.40
22	C	511	CLA	O2A-CGA	3.57	1.43	1.33
23	D	402	PHO	CHD-C1D	3.56	1.45	1.38
22	c	907	CLA	C3D-C2D	3.56	1.46	1.39
22	b	605	CLA	C3B-C2B	3.55	1.45	1.40
22	c	902	CLA	O2A-CGA	3.55	1.43	1.33
22	D	401	CLA	CHC-C1C	3.55	1.44	1.35
35	c	918	DGD	O2G-C1B	3.54	1.44	1.34
22	a	407	CLA	O2A-CGA	3.53	1.43	1.33
23	a	410	PHO	O2A-CGA	3.53	1.43	1.33
22	a	408	CLA	MG-NA	3.53	2.14	2.06
22	A	406	CLA	C3B-C2B	3.52	1.45	1.40
22	C	505	CLA	C1B-CHB	3.52	1.49	1.40
22	A	408	CLA	O2A-CGA	3.52	1.43	1.33
22	C	513	CLA	C1B-CHB	3.51	1.49	1.40
22	b	611	CLA	OBD-CAD	3.51	1.27	1.22
22	B	604	CLA	C1B-CHB	3.50	1.49	1.40
36	E	102	HEM	C3B-C2B	-3.50	1.35	1.40
23	a	411	PHO	CHC-C4B	3.49	1.48	1.40
27	d	408	LHG	O7-C7	3.49	1.44	1.34
22	b	605	CLA	O2A-CGA	3.48	1.43	1.33
36	e	101	HEM	C3C-CAC	3.48	1.55	1.47
22	A	406	CLA	O2A-CGA	3.47	1.43	1.33
22	c	903	CLA	O2A-CGA	3.47	1.43	1.33
22	c	909	CLA	C4B-CHC	3.47	1.49	1.40
22	b	615	CLA	C1B-CHB	3.47	1.49	1.40
22	b	607	CLA	O2A-CGA	3.47	1.43	1.33
22	b	602	CLA	C4B-CHC	3.46	1.49	1.40
25	b	622	LMG	O1-C1	3.46	1.46	1.40
22	C	512	CLA	C1B-CHB	3.46	1.49	1.40
22	c	910	CLA	C4C-C3C	3.45	1.51	1.45
22	B	611	CLA	O2A-CGA	3.45	1.43	1.33
22	c	912	CLA	C4B-CHC	3.45	1.49	1.40
22	c	906	CLA	C4B-CHC	3.45	1.49	1.40
34	v	203	HTG	C1'-S1	-3.45	1.77	1.81
22	B	605	CLA	O2A-CGA	3.45	1.43	1.33
22	b	615	CLA	OBD-CAD	3.45	1.27	1.22
22	b	609	CLA	MG-NC	3.44	2.14	2.06
22	c	905	CLA	O2A-CGA	3.44	1.43	1.33
22	B	611	CLA	C1B-CHB	3.44	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	O2A-CGA	3.43	1.43	1.33
22	a	407	CLA	C1B-CHB	3.43	1.49	1.40
26	A	411	PL9	C7-C3	3.42	1.54	1.51
22	B	605	CLA	C3D-C2D	3.42	1.46	1.39
22	b	612	CLA	C3B-C2B	3.41	1.45	1.40
22	B	606	CLA	C4B-CHC	3.41	1.49	1.40
22	b	615	CLA	C4C-C3C	3.41	1.50	1.45
22	b	611	CLA	C4C-C3C	3.41	1.50	1.45
23	a	410	PHO	CHD-C1D	3.39	1.45	1.38
22	C	508	CLA	C4B-CHC	3.38	1.49	1.40
22	c	912	CLA	C1B-CHB	3.38	1.49	1.40
22	b	604	CLA	C3B-C2B	3.38	1.45	1.40
22	b	603	CLA	C1B-CHB	3.38	1.49	1.40
22	C	508	CLA	O2A-CGA	3.36	1.43	1.33
22	b	607	CLA	C3D-C2D	3.36	1.46	1.39
35	C	517	DGD	O1G-C1A	3.36	1.43	1.33
22	D	403	CLA	C4C-C3C	3.35	1.50	1.45
22	b	617	CLA	C1C-NC	-3.35	1.32	1.37
22	D	404	CLA	C1B-CHB	3.34	1.49	1.40
22	B	602	CLA	C1B-CHB	3.34	1.49	1.40
22	c	912	CLA	O2A-CGA	3.34	1.43	1.33
34	l	106	HTG	C1'-S1	-3.34	1.77	1.81
22	B	616	CLA	C1B-CHB	3.34	1.49	1.40
22	b	611	CLA	C1B-CHB	3.33	1.49	1.40
22	B	604	CLA	OBD-CAD	3.33	1.27	1.22
22	C	511	CLA	C1B-CHB	3.33	1.49	1.40
22	d	403	CLA	C4B-CHC	3.32	1.49	1.40
22	B	611	CLA	C4C-C3C	3.32	1.50	1.45
22	A	406	CLA	C3D-C2D	3.32	1.46	1.39
22	b	608	CLA	O2A-CGA	3.32	1.43	1.33
22	B	616	CLA	OBD-CAD	3.32	1.27	1.22
22	b	603	CLA	OBD-CAD	3.32	1.27	1.22
22	c	909	CLA	C1B-CHB	3.31	1.48	1.40
22	B	611	CLA	C4B-CHC	3.31	1.48	1.40
22	B	606	CLA	C1B-CHB	3.31	1.48	1.40
22	C	509	CLA	C1C-NC	-3.30	1.32	1.37
23	a	410	PHO	CHD-C4C	3.30	1.48	1.40
39	V	202	HEC	CBB-CAB	-3.30	1.36	1.49
22	A	408	CLA	C3D-C2D	3.29	1.45	1.39
22	c	909	CLA	C4C-C3C	3.29	1.50	1.45
22	b	613	CLA	C4B-CHC	3.29	1.48	1.40
36	E	102	HEM	C3C-C2C	-3.29	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	e	101	HEM	C3B-C2B	-3.28	1.35	1.40
22	D	401	CLA	C4B-CHC	3.28	1.48	1.40
22	b	603	CLA	CHD-C4C	3.28	1.50	1.41
22	B	608	CLA	C1B-CHB	3.28	1.48	1.40
22	C	506	CLA	C4B-CHC	3.27	1.48	1.40
39	v	202	HEC	CBB-CAB	-3.27	1.37	1.49
22	B	603	CLA	C3D-C2D	3.27	1.45	1.39
27	D	410	LHG	O7-C7	3.27	1.43	1.34
22	c	905	CLA	C1B-CHB	3.27	1.48	1.40
22	C	511	CLA	C4C-C3C	3.26	1.50	1.45
22	b	604	CLA	OBD-CAD	3.25	1.26	1.22
22	C	505	CLA	O2A-CGA	3.25	1.43	1.33
22	b	614	CLA	C1B-CHB	3.24	1.48	1.40
22	C	507	CLA	C1B-CHB	3.24	1.48	1.40
22	C	505	CLA	CHD-C4C	3.23	1.50	1.41
22	C	512	CLA	C4C-C3C	3.23	1.50	1.45
22	C	508	CLA	C1B-CHB	3.22	1.48	1.40
22	B	606	CLA	C1C-C2C	3.21	1.50	1.44
27	D	410	LHG	O8-C23	3.21	1.42	1.33
39	V	202	HEC	CBC-CAC	-3.21	1.37	1.49
36	e	101	HEM	C3C-C2C	-3.20	1.35	1.40
22	b	617	CLA	C1B-CHB	3.20	1.48	1.40
22	d	402	CLA	C3D-C2D	3.20	1.45	1.39
22	a	408	CLA	C1D-C2D	3.20	1.49	1.42
22	B	610	CLA	C1B-CHB	3.19	1.48	1.40
22	B	616	CLA	C1C-NC	-3.19	1.33	1.37
34	D	415	HTG	C1'-S1	-3.18	1.77	1.81
22	B	605	CLA	C1B-CHB	3.18	1.48	1.40
22	c	905	CLA	C4C-C3C	3.18	1.50	1.45
22	b	616	CLA	C4C-C3C	3.18	1.50	1.45
22	d	403	CLA	C1B-CHB	3.18	1.48	1.40
34	b	624	HTG	C1'-S1	-3.17	1.77	1.81
22	c	903	CLA	OBD-CAD	3.16	1.26	1.22
22	d	402	CLA	C4C-C3C	3.16	1.50	1.45
22	b	608	CLA	C1B-CHB	3.16	1.48	1.40
22	b	615	CLA	MG-NC	3.15	2.13	2.06
22	C	513	CLA	C4B-CHC	3.15	1.48	1.40
22	D	403	CLA	MG-NC	3.15	2.13	2.06
22	b	610	CLA	C4B-CHC	3.14	1.48	1.40
22	c	913	CLA	C1B-CHB	3.13	1.48	1.40
22	c	905	CLA	C4B-CHC	3.13	1.48	1.40
22	c	906	CLA	C1B-CHB	3.13	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	605	CLA	C4C-C3C	3.12	1.50	1.45
22	B	614	CLA	C1B-CHB	3.11	1.48	1.40
23	D	402	PHO	CHC-C4B	3.11	1.47	1.40
22	a	412	CLA	C1B-CHB	3.10	1.48	1.40
22	C	514	CLA	C1C-C2C	3.10	1.50	1.44
22	C	502	CLA	C1B-CHB	3.09	1.48	1.40
22	c	906	CLA	CHD-C4C	3.09	1.50	1.41
22	b	606	CLA	C4B-CHC	3.09	1.48	1.40
22	b	605	CLA	C4B-CHC	3.09	1.48	1.40
22	C	509	CLA	C4B-CHC	3.09	1.48	1.40
22	C	507	CLA	C4B-CHC	3.08	1.48	1.40
22	C	503	CLA	C4B-CHC	3.08	1.48	1.40
22	A	405	CLA	O2A-CGA	3.08	1.42	1.33
22	b	614	CLA	C4B-CHC	3.08	1.48	1.40
22	D	403	CLA	CHC-C1C	3.07	1.43	1.35
22	B	603	CLA	C1B-CHB	3.07	1.48	1.40
22	B	602	CLA	C1C-NC	-3.07	1.33	1.37
22	C	510	CLA	C4C-C3C	3.06	1.50	1.45
22	D	403	CLA	C1B-CHB	3.06	1.48	1.40
22	b	607	CLA	MG-NC	3.06	2.13	2.06
22	B	602	CLA	C4B-CHC	3.04	1.48	1.40
22	B	616	CLA	MG-NC	3.04	2.13	2.06
22	C	505	CLA	C1C-NC	-3.04	1.33	1.37
22	c	907	CLA	C4C-C3C	3.04	1.50	1.45
23	A	407	PHO	C3D-C4D	-3.03	1.34	1.43
22	a	408	CLA	MG-NC	3.03	2.13	2.06
22	C	504	CLA	C1C-C2C	3.03	1.50	1.44
22	c	904	CLA	C1B-CHB	3.03	1.48	1.40
22	A	405	CLA	C4C-C3C	3.02	1.50	1.45
22	B	603	CLA	C1C-NC	-3.02	1.33	1.37
22	B	610	CLA	C4B-CHC	3.02	1.48	1.40
22	A	408	CLA	C4C-C3C	3.02	1.50	1.45
22	B	615	CLA	C4B-CHC	3.01	1.48	1.40
23	a	410	PHO	C3D-C2D	3.01	1.47	1.39
22	c	902	CLA	C1C-C2C	3.01	1.50	1.44
27	d	407	LHG	O7-C7	3.01	1.42	1.34
23	D	402	PHO	CHD-C4C	3.01	1.47	1.40
35	C	518	DGD	O3G-C1D	3.01	1.45	1.40
28	A	413	SQD	C6-S	-3.01	1.65	1.77
22	c	911	CLA	C1C-NC	-3.01	1.33	1.37
22	C	502	CLA	C4B-CHC	3.01	1.48	1.40
22	c	903	CLA	C1B-CHB	3.00	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	MG-NC	-2.99	1.99	2.06
35	C	517	DGD	O2G-C1B	2.99	1.42	1.34
22	c	902	CLA	C4B-CHC	2.99	1.48	1.40
22	d	403	CLA	C1D-C2D	2.98	1.49	1.42
22	A	406	CLA	C4B-CHC	2.98	1.48	1.40
29	f	102	LMT	O1'-C1'	2.98	1.45	1.40
22	c	906	CLA	C1C-NC	-2.98	1.33	1.37
22	D	401	CLA	C3B-C2B	2.98	1.44	1.40
22	b	611	CLA	C4B-CHC	2.97	1.48	1.40
22	C	509	CLA	C1B-CHB	2.97	1.48	1.40
22	B	608	CLA	O2A-CGA	2.97	1.42	1.33
22	b	607	CLA	C1C-C2C	2.97	1.50	1.44
22	b	607	CLA	C4B-CHC	2.96	1.48	1.40
22	b	608	CLA	C4B-CHC	2.96	1.48	1.40
22	c	902	CLA	C4C-C3C	2.95	1.50	1.45
22	B	605	CLA	MG-NC	2.95	2.13	2.06
22	d	403	CLA	C1C-NC	-2.95	1.33	1.37
22	B	606	CLA	OBD-CAD	2.95	1.26	1.22
22	B	615	CLA	C1C-C2C	2.95	1.50	1.44
22	C	504	CLA	C1B-CHB	2.95	1.48	1.40
22	C	505	CLA	C4B-CHC	2.95	1.48	1.40
22	b	606	CLA	C3B-C2B	2.95	1.44	1.40
23	D	402	PHO	C3D-C4D	-2.94	1.34	1.43
22	B	611	CLA	C1C-C2C	2.94	1.50	1.44
22	b	615	CLA	C1C-NC	-2.94	1.33	1.37
22	c	914	CLA	C4B-CHC	2.93	1.47	1.40
22	B	608	CLA	CHD-C4C	2.93	1.49	1.41
22	b	610	CLA	C1D-C2D	2.93	1.49	1.42
22	B	612	CLA	C1D-C2D	2.93	1.49	1.42
34	C	521	HTG	C1'-S1	-2.93	1.77	1.81
35	H	102	DGD	O5D-C1E	2.91	1.45	1.40
22	b	613	CLA	C1B-CHB	2.91	1.47	1.40
22	b	602	CLA	C1C-C2C	2.91	1.50	1.44
22	A	405	CLA	C4B-CHC	2.90	1.47	1.40
22	d	403	CLA	CHD-C4C	2.90	1.49	1.41
22	D	403	CLA	OBD-CAD	2.89	1.26	1.22
22	b	609	CLA	C4B-CHC	2.89	1.47	1.40
22	D	404	CLA	C4B-CHC	2.89	1.47	1.40
22	B	607	CLA	OBD-CAD	2.88	1.26	1.22
34	b	627	HTG	C1'-S1	-2.88	1.77	1.81
22	a	408	CLA	CHD-C4C	2.88	1.49	1.41
24	b	618	BCR	C14-C13	2.87	1.35	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	617	CLA	C4B-CHC	2.87	1.47	1.40
22	c	914	CLA	C1C-C2C	2.87	1.50	1.44
22	D	401	CLA	O2A-CGA	2.87	1.41	1.33
22	C	509	CLA	C1D-C2D	2.86	1.49	1.42
34	B	627	HTG	C1'-S1	-2.86	1.77	1.81
22	b	609	CLA	C1B-CHB	2.86	1.47	1.40
22	b	614	CLA	C4C-C3C	2.86	1.50	1.45
22	D	403	CLA	C3D-C2D	2.86	1.45	1.39
22	C	512	CLA	C1C-C2C	2.85	1.50	1.44
22	c	912	CLA	CHD-C4C	2.85	1.49	1.41
22	A	406	CLA	C3C-C2C	2.85	1.42	1.36
22	B	609	CLA	OBD-CAD	2.85	1.26	1.22
35	C	519	DGD	O2G-C1B	2.84	1.42	1.34
26	a	415	PL9	C6-C5	2.83	1.50	1.35
22	B	612	CLA	C4B-CHC	2.83	1.47	1.40
22	b	607	CLA	C1B-CHB	2.83	1.47	1.40
22	B	615	CLA	C1C-NC	-2.82	1.33	1.37
22	b	605	CLA	C1B-CHB	2.82	1.47	1.40
22	B	617	CLA	C1B-CHB	2.82	1.47	1.40
27	d	407	LHG	O8-C23	2.82	1.41	1.33
22	b	614	CLA	MG-NC	2.82	2.13	2.06
22	c	902	CLA	C3D-C2D	2.82	1.45	1.39
22	C	506	CLA	CHD-C4C	2.81	1.49	1.41
22	b	604	CLA	C1C-C2C	2.81	1.50	1.44
22	b	607	CLA	C1D-C2D	2.81	1.48	1.42
22	b	615	CLA	C1C-C2C	2.80	1.50	1.44
22	B	615	CLA	C4C-C3C	2.80	1.49	1.45
22	c	904	CLA	C1D-C2D	2.80	1.48	1.42
22	c	904	CLA	C1C-NC	-2.80	1.33	1.37
22	B	613	CLA	C1B-CHB	2.80	1.47	1.40
28	a	414	SQD	C6-S	-2.80	1.66	1.77
22	a	409	CLA	C1B-CHB	2.80	1.47	1.40
23	A	407	PHO	CHC-C4B	2.79	1.47	1.40
34	b	632	HTG	O5-C1	2.79	1.46	1.42
22	c	902	CLA	C1B-CHB	2.79	1.47	1.40
22	c	913	CLA	C4C-C3C	2.79	1.49	1.45
22	b	603	CLA	C1D-C2D	2.79	1.48	1.42
24	A	409	BCR	C19-C18	2.79	1.52	1.45
22	b	604	CLA	C4C-C3C	2.78	1.49	1.45
22	C	512	CLA	C4B-CHC	2.78	1.47	1.40
22	c	911	CLA	C1B-CHB	2.78	1.47	1.40
22	b	604	CLA	C4B-CHC	2.78	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	C4B-CHC	2.78	1.47	1.40
22	c	910	CLA	C1B-CHB	2.78	1.47	1.40
22	b	612	CLA	MG-NC	2.77	2.12	2.06
22	c	913	CLA	C4B-CHC	2.77	1.47	1.40
22	B	608	CLA	C4C-C3C	2.77	1.49	1.45
22	b	615	CLA	C4B-CHC	2.77	1.47	1.40
22	C	503	CLA	C1B-CHB	2.77	1.47	1.40
26	A	411	PL9	C2-C3	2.76	1.42	1.34
22	B	613	CLA	C4C-C3C	2.76	1.49	1.45
22	c	903	CLA	C4B-CHC	2.76	1.47	1.40
26	D	406	PL9	C7-C3	2.75	1.54	1.51
22	c	906	CLA	C1D-C2D	2.75	1.48	1.42
22	b	616	CLA	C4B-CHC	2.75	1.47	1.40
28	a	418	SQD	C6-S	-2.75	1.66	1.77
22	C	508	CLA	C1D-C2D	2.74	1.48	1.42
22	b	602	CLA	CHD-C4C	2.74	1.49	1.41
22	b	605	CLA	OBD-CAD	2.72	1.26	1.22
22	b	613	CLA	C1D-C2D	2.72	1.48	1.42
22	a	407	CLA	C4B-CHC	2.71	1.47	1.40
22	a	412	CLA	MG-NA	2.71	2.12	2.06
22	C	505	CLA	C1D-C2D	2.70	1.48	1.42
23	a	411	PHO	CHD-C4C	2.70	1.46	1.40
22	c	904	CLA	MG-NC	2.69	2.12	2.06
22	C	511	CLA	C4B-CHC	2.69	1.47	1.40
22	B	603	CLA	C4B-CHC	2.69	1.47	1.40
22	A	408	CLA	C4B-CHC	2.69	1.47	1.40
29	I	102	LMT	O1'-C1'	2.68	1.44	1.40
22	d	402	CLA	CHD-C4C	2.68	1.48	1.41
23	D	402	PHO	C3B-C4B	2.68	1.49	1.43
22	d	402	CLA	C1B-CHB	2.68	1.47	1.40
22	b	617	CLA	C1C-C2C	2.68	1.49	1.44
35	C	517	DGD	O5D-C1E	2.68	1.44	1.40
22	b	609	CLA	C1C-NC	-2.67	1.33	1.37
24	d	404	BCR	C12-C13	2.67	1.51	1.45
26	a	415	PL9	C7-C3	2.66	1.54	1.51
22	d	403	CLA	C1C-C2C	2.66	1.49	1.44
24	D	405	BCR	C8-C9	2.66	1.51	1.45
22	C	507	CLA	C4C-C3C	2.66	1.49	1.45
22	c	908	CLA	MG-NC	2.66	2.12	2.06
22	c	904	CLA	C4C-C3C	2.66	1.49	1.45
23	a	410	PHO	CHB-C4A	-2.66	1.33	1.40
22	c	907	CLA	C1D-C2D	2.65	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C4B-CHC	2.65	1.47	1.40
22	c	909	CLA	C1C-C2C	2.65	1.49	1.44
34	b	626	HTG	C1'-S1	-2.65	1.78	1.81
22	c	907	CLA	CHD-C4C	2.64	1.48	1.41
22	B	602	CLA	CHD-C4C	2.64	1.48	1.41
22	b	612	CLA	C4B-CHC	2.64	1.47	1.40
22	b	617	CLA	C4B-CHC	2.63	1.47	1.40
26	d	405	PL9	C6-C5	2.63	1.49	1.35
29	c	921	LMT	O1'-C1'	2.63	1.44	1.40
25	d	409	LMG	O1-C1	2.62	1.44	1.40
29	c	931	LMT	O1'-C1'	2.62	1.44	1.40
22	B	603	CLA	CHD-C4C	2.62	1.48	1.41
22	B	607	CLA	C1C-C2C	2.62	1.49	1.44
22	b	602	CLA	C4C-C3C	2.62	1.49	1.45
22	c	907	CLA	C4B-CHC	2.62	1.47	1.40
22	C	504	CLA	CHD-C4C	2.62	1.48	1.41
22	b	603	CLA	MG-NC	2.61	2.12	2.06
22	B	609	CLA	C1B-CHB	2.61	1.47	1.40
23	D	402	PHO	C3D-C2D	2.61	1.46	1.39
35	c	917	DGD	O5D-C1E	2.61	1.44	1.40
22	a	408	CLA	C4B-CHC	2.61	1.47	1.40
23	a	411	PHO	C3D-C2D	2.61	1.46	1.39
23	a	411	PHO	C4C-C3C	2.60	1.49	1.45
22	C	507	CLA	CHD-C4C	2.60	1.48	1.41
22	c	909	CLA	CHD-C4C	2.60	1.48	1.41
22	B	602	CLA	C1D-C2D	2.60	1.48	1.42
26	A	411	PL9	C6-C5	2.60	1.48	1.35
22	c	912	CLA	C1C-NC	-2.59	1.33	1.37
22	C	502	CLA	CHD-C4C	2.58	1.48	1.41
34	D	414	HTG	C1'-S1	-2.58	1.78	1.81
22	c	907	CLA	C1B-CHB	2.58	1.47	1.40
22	b	614	CLA	CHD-C4C	2.58	1.48	1.41
22	b	607	CLA	OBD-CAD	2.57	1.26	1.22
22	b	614	CLA	C1C-NC	-2.57	1.34	1.37
28	C	501	SQD	C6-S	-2.57	1.67	1.77
22	b	608	CLA	CHD-C4C	2.57	1.48	1.41
22	D	403	CLA	C3B-C2B	2.56	1.43	1.40
22	b	616	CLA	CHD-C4C	2.56	1.48	1.41
34	c	922	HTG	C1'-S1	-2.56	1.78	1.81
35	C	518	DGD	O2G-C1B	2.56	1.41	1.34
22	B	610	CLA	OBD-CAD	2.56	1.25	1.22
22	B	604	CLA	C1D-C2D	2.56	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	415	PL9	C2-C3	2.55	1.41	1.34
22	B	616	CLA	C4B-CHC	2.55	1.46	1.40
26	d	405	PL9	C18-C19	2.55	1.39	1.33
22	A	405	CLA	C1B-CHB	2.55	1.46	1.40
22	B	603	CLA	C1D-C2D	2.55	1.48	1.42
22	C	509	CLA	C4C-C3C	2.54	1.49	1.45
22	c	914	CLA	C1D-C2D	2.54	1.48	1.42
22	c	912	CLA	C4C-C3C	2.54	1.49	1.45
22	B	613	CLA	C1D-C2D	2.54	1.48	1.42
22	b	613	CLA	C1A-CHA	2.54	1.53	1.43
22	c	909	CLA	C1C-NC	-2.53	1.34	1.37
24	a	413	BCR	C5-C6	2.53	1.38	1.34
22	c	911	CLA	CHD-C4C	2.53	1.48	1.41
29	Z	101	LMT	O1'-C1'	2.53	1.44	1.40
23	a	410	PHO	C3D-C4D	-2.53	1.35	1.43
22	C	507	CLA	C1C-C2C	2.52	1.49	1.44
22	b	604	CLA	O2A-CGA	2.52	1.40	1.33
36	e	101	HEM	CAA-C2A	2.51	1.55	1.52
22	B	606	CLA	C1D-C2D	2.50	1.48	1.42
22	B	617	CLA	C1D-C2D	2.50	1.48	1.42
22	a	407	CLA	CHD-C4C	2.50	1.48	1.41
23	a	411	PHO	C3D-C4D	-2.50	1.35	1.43
22	c	908	CLA	C1D-C2D	2.49	1.48	1.42
22	b	608	CLA	C1D-C2D	2.49	1.48	1.42
22	a	408	CLA	C1B-CHB	2.49	1.46	1.40
23	A	407	PHO	OBD-CAD	2.49	1.26	1.22
22	B	606	CLA	C3D-C2D	2.49	1.44	1.39
22	C	510	CLA	MG-NC	2.48	2.12	2.06
22	b	614	CLA	C1D-C2D	2.48	1.48	1.42
22	B	602	CLA	C1C-C2C	2.48	1.49	1.44
22	b	605	CLA	C1C-NC	-2.48	1.34	1.37
22	A	408	CLA	C1D-C2D	2.48	1.48	1.42
22	B	616	CLA	CHD-C4C	2.47	1.48	1.41
22	B	606	CLA	C1C-NC	-2.47	1.34	1.37
22	C	502	CLA	C4C-C3C	2.47	1.49	1.45
22	b	606	CLA	MG-NC	2.47	2.12	2.06
22	A	405	CLA	C1D-C2D	2.46	1.48	1.42
22	B	607	CLA	C1B-CHB	2.46	1.46	1.40
24	A	409	BCR	C12-C13	2.46	1.51	1.45
22	b	613	CLA	C1C-NC	-2.46	1.34	1.37
22	a	412	CLA	CHD-C4C	2.46	1.48	1.41
22	B	604	CLA	CHD-C4C	2.46	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	C1C-C2C	2.45	1.49	1.44
22	b	614	CLA	C1C-C2C	2.44	1.49	1.44
23	a	410	PHO	OBD-CAD	2.44	1.26	1.22
35	c	919	DGD	O5D-C1E	2.44	1.44	1.40
22	b	615	CLA	C1D-C2D	2.44	1.48	1.42
22	B	603	CLA	C1C-C2C	2.44	1.49	1.44
22	b	605	CLA	C4C-C3C	2.43	1.49	1.45
22	C	513	CLA	C1C-C2C	2.43	1.49	1.44
22	c	902	CLA	C1D-C2D	2.43	1.48	1.42
22	C	509	CLA	CHD-C4C	2.43	1.48	1.41
22	D	403	CLA	C4B-CHC	2.42	1.46	1.40
22	c	904	CLA	C4B-CHC	2.42	1.46	1.40
22	B	605	CLA	CHD-C4C	2.42	1.48	1.41
22	b	607	CLA	C4C-C3C	2.41	1.49	1.45
22	B	604	CLA	C4B-CHC	2.41	1.46	1.40
24	d	404	BCR	C23-C22	2.41	1.51	1.45
22	b	615	CLA	CHD-C4C	2.40	1.48	1.41
22	D	404	CLA	CHD-C4C	2.39	1.48	1.41
28	b	621	SQD	C6-S	-2.39	1.68	1.77
22	B	612	CLA	C1B-CHB	2.39	1.46	1.40
22	C	507	CLA	C1C-NC	-2.39	1.34	1.37
22	C	508	CLA	C1C-C2C	2.38	1.49	1.44
22	b	609	CLA	C1D-C2D	2.38	1.48	1.42
22	B	609	CLA	C4C-C3C	2.38	1.49	1.45
22	B	611	CLA	CHD-C4C	2.38	1.48	1.41
22	B	609	CLA	C1C-C2C	2.38	1.49	1.44
22	C	512	CLA	CHD-C4C	2.38	1.48	1.41
22	A	406	CLA	MG-NC	-2.37	2.00	2.06
22	C	511	CLA	CHD-C4C	2.37	1.48	1.41
22	c	903	CLA	C1D-C2D	2.37	1.47	1.42
22	c	914	CLA	CHD-C4C	2.36	1.48	1.41
22	C	512	CLA	C1D-C2D	2.36	1.47	1.42
22	c	912	CLA	C1D-C2D	2.36	1.47	1.42
22	C	510	CLA	C4B-CHC	2.36	1.46	1.40
22	c	905	CLA	C1C-NC	-2.35	1.34	1.37
22	B	607	CLA	C4C-C3C	2.35	1.49	1.45
22	B	614	CLA	C4C-C3C	2.35	1.49	1.45
22	A	406	CLA	C1B-CHB	2.35	1.46	1.40
22	b	602	CLA	C1D-C2D	2.35	1.47	1.42
35	D	407	DGD	O3G-C1D	2.35	1.44	1.40
22	c	908	CLA	C4C-C3C	2.34	1.49	1.45
22	A	408	CLA	CHD-C4C	2.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	406	DGD	O3G-C1D	2.34	1.44	1.40
39	v	202	HEC	CMD-C2D	2.34	1.56	1.51
28	D	408	SQD	O6-C1	2.33	1.44	1.40
22	C	510	CLA	C1B-CHB	2.33	1.46	1.40
22	B	608	CLA	C4B-CHC	2.33	1.46	1.40
22	C	513	CLA	CHD-C4C	2.33	1.47	1.41
28	l	101	SQD	C6-S	-2.33	1.68	1.77
34	C	532	HTG	C1-S1	-2.32	1.77	1.80
24	d	404	BCR	C30-C25	-2.32	1.50	1.53
22	C	505	CLA	OBD-CAD	2.32	1.25	1.22
22	C	504	CLA	C1C-NC	-2.32	1.34	1.37
22	c	910	CLA	CHD-C4C	2.32	1.47	1.41
26	D	406	PL9	C6-C5	2.32	1.47	1.35
22	a	407	CLA	C1D-C2D	2.32	1.47	1.42
22	B	605	CLA	C4B-CHC	2.31	1.46	1.40
24	b	619	BCR	C12-C13	2.31	1.50	1.45
22	D	401	CLA	C1B-CHB	2.31	1.46	1.40
25	B	621	LMG	O1-C1	2.31	1.44	1.40
23	a	410	PHO	CHC-C4B	2.30	1.45	1.40
39	V	202	HEC	C3B-C4B	2.30	1.47	1.43
24	b	619	BCR	C8-C9	2.30	1.50	1.46
29	B	622	LMT	O1'-C1'	2.30	1.44	1.40
28	l	101	SQD	O6-C1	2.30	1.44	1.40
22	D	401	CLA	CHD-C4C	2.29	1.47	1.41
22	B	609	CLA	C1D-C2D	2.29	1.47	1.42
22	B	604	CLA	C1C-NC	-2.29	1.34	1.37
22	a	409	CLA	C4C-C3C	2.29	1.49	1.45
22	b	610	CLA	C1C-NC	-2.29	1.34	1.37
36	e	101	HEM	C1C-C2C	2.28	1.47	1.42
22	C	514	CLA	CHD-C4C	2.28	1.47	1.41
22	b	608	CLA	C4C-C3C	2.28	1.49	1.45
22	c	911	CLA	C1D-C2D	2.28	1.47	1.42
22	B	612	CLA	CHD-C4C	2.27	1.47	1.41
22	a	409	CLA	CHD-C4C	2.26	1.47	1.41
22	c	903	CLA	C4C-C3C	2.26	1.48	1.45
23	a	411	PHO	C3B-C4B	2.26	1.48	1.43
22	c	903	CLA	CHD-C4C	2.26	1.47	1.41
23	D	402	PHO	C1B-C2B	2.26	1.50	1.45
22	a	409	CLA	C4B-CHC	2.25	1.46	1.40
25	C	531	LMG	O1-C1	2.25	1.44	1.40
22	B	617	CLA	OBD-CAD	2.25	1.25	1.22
22	B	610	CLA	C1C-C2C	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	l	106	HTG	C1-S1	-2.25	1.77	1.80
23	a	410	PHO	C1B-C2B	2.24	1.50	1.45
36	E	102	HEM	CMA-C3A	2.24	1.56	1.51
22	C	503	CLA	C4C-C3C	2.24	1.48	1.45
22	c	904	CLA	CHD-C4C	2.24	1.47	1.41
22	b	604	CLA	C1B-CHB	2.24	1.46	1.40
24	a	413	BCR	C12-C13	2.24	1.50	1.45
22	c	908	CLA	CHD-C4C	2.24	1.47	1.41
22	b	610	CLA	C1C-C2C	2.23	1.48	1.44
24	C	515	BCR	C19-C18	2.23	1.50	1.45
22	A	406	CLA	CHD-C4C	2.23	1.47	1.41
22	C	508	CLA	CHD-C4C	2.23	1.47	1.41
22	b	606	CLA	C1C-NC	-2.23	1.34	1.37
23	A	407	PHO	C4C-C3C	2.23	1.49	1.45
22	b	606	CLA	CHD-C4C	2.23	1.47	1.41
22	C	506	CLA	C1B-CHB	2.22	1.46	1.40
22	A	408	CLA	C1B-CHB	2.22	1.46	1.40
22	c	913	CLA	CHD-C4C	2.22	1.47	1.41
22	c	905	CLA	C1D-C2D	2.22	1.47	1.42
22	c	914	CLA	C4C-C3C	2.22	1.48	1.45
22	C	511	CLA	C1C-C2C	2.22	1.48	1.44
22	A	405	CLA	C3A-C2A	-2.22	1.48	1.54
22	C	503	CLA	C1C-C2C	2.21	1.48	1.44
22	C	506	CLA	C1D-C2D	2.21	1.47	1.42
26	d	405	PL9	C7-C3	2.21	1.53	1.51
22	b	611	CLA	CHD-C4C	2.21	1.47	1.41
24	Y	101	BCR	C5-C6	2.20	1.36	1.33
22	a	407	CLA	C1C-NC	-2.20	1.34	1.37
36	e	101	HEM	CMD-C2D	2.19	1.56	1.51
22	B	617	CLA	CHD-C4C	2.19	1.47	1.41
22	D	404	CLA	C1C-C2C	2.19	1.48	1.44
22	B	615	CLA	CHD-C4C	2.19	1.47	1.41
34	b	632	HTG	C1'-S1	-2.19	1.78	1.81
22	b	604	CLA	CHD-C4C	2.18	1.47	1.41
28	D	408	SQD	C6-S	-2.18	1.69	1.77
22	b	607	CLA	O2A-C1	-2.18	1.39	1.46
22	B	608	CLA	C1C-NC	-2.17	1.34	1.37
39	v	202	HEC	C1D-ND	2.17	1.40	1.36
22	c	906	CLA	C4C-C3C	2.17	1.48	1.45
22	B	614	CLA	C4B-CHC	2.16	1.45	1.40
22	C	502	CLA	C1D-C2D	2.16	1.47	1.42
22	C	513	CLA	C4C-C3C	2.15	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	611	CLA	C1D-C2D	2.15	1.47	1.42
24	c	915	BCR	C23-C22	2.15	1.50	1.45
26	D	406	PL9	C2-C3	2.15	1.40	1.34
22	D	401	CLA	C1D-C2D	2.15	1.47	1.42
34	C	521	HTG	C1-S1	-2.15	1.77	1.80
22	C	502	CLA	C1C-C2C	2.14	1.48	1.44
22	C	513	CLA	C1D-C2D	2.14	1.47	1.42
22	c	913	CLA	C1C-C2C	2.14	1.48	1.44
23	A	407	PHO	C3D-C2D	2.14	1.45	1.39
22	B	608	CLA	C1D-C2D	2.14	1.47	1.42
22	B	613	CLA	CHD-C4C	2.14	1.47	1.41
22	C	514	CLA	C4C-C3C	2.14	1.48	1.45
22	d	402	CLA	C4B-CHC	2.13	1.45	1.40
22	B	609	CLA	CHD-C4C	2.12	1.47	1.41
26	d	405	PL9	C23-C24	2.12	1.38	1.33
22	C	508	CLA	C4C-C3C	2.11	1.48	1.45
23	D	402	PHO	C4D-CHA	2.11	1.49	1.43
24	B	620	BCR	C26-C25	2.11	1.38	1.34
29	T	102	LMT	O1'-C1'	2.11	1.43	1.40
23	a	410	PHO	C3B-C4B	2.11	1.47	1.43
39	V	202	HEC	CMC-C2C	2.11	1.56	1.51
22	B	605	CLA	C1D-C2D	2.10	1.47	1.42
35	c	918	DGD	O3G-C1D	2.09	1.43	1.40
22	D	403	CLA	C1C-C2C	2.09	1.48	1.44
22	b	613	CLA	C4C-C3C	2.08	1.48	1.45
22	c	905	CLA	OBD-CAD	2.08	1.25	1.22
35	c	918	DGD	O5D-C1E	2.08	1.43	1.40
22	B	610	CLA	C4C-C3C	2.08	1.48	1.45
22	B	614	CLA	C1C-C2C	2.08	1.48	1.44
22	a	412	CLA	C4B-CHC	2.07	1.45	1.40
22	C	503	CLA	C1C-NC	-2.07	1.34	1.37
22	c	913	CLA	C1D-C2D	2.07	1.47	1.42
22	b	617	CLA	C1D-C2D	2.07	1.47	1.42
22	D	403	CLA	C1D-C2D	2.06	1.47	1.42
22	b	606	CLA	C1B-CHB	2.06	1.45	1.40
36	e	101	HEM	C1D-ND	2.06	1.40	1.36
22	D	403	CLA	CHD-C4C	2.06	1.47	1.41
22	C	512	CLA	MG-NC	2.06	2.11	2.06
22	D	404	CLA	C1D-C2D	2.06	1.47	1.42
25	D	412	LMG	O1-C1	2.06	1.43	1.40
25	c	930	LMG	O1-C1	2.06	1.43	1.40
23	a	410	PHO	C1B-NB	-2.06	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	620	BCR	C19-C18	2.05	1.50	1.45
22	C	504	CLA	C4C-C3C	2.05	1.48	1.45
22	a	408	CLA	C4C-C3C	2.05	1.48	1.45
25	b	622	LMG	C4-C5	2.05	1.57	1.53
22	B	617	CLA	C1C-C2C	2.04	1.48	1.44
22	b	612	CLA	C1D-C2D	2.04	1.47	1.42
22	a	407	CLA	C4C-C3C	2.04	1.48	1.45
34	b	627	HTG	O5-C1	2.04	1.45	1.42
35	c	919	DGD	O2G-C2G	-2.04	1.41	1.46
22	B	604	CLA	C4C-C3C	2.04	1.48	1.45
22	C	512	CLA	C1C-NC	-2.02	1.34	1.37
39	v	202	HEC	C4D-ND	2.02	1.40	1.36
22	B	616	CLA	C1D-C2D	2.02	1.47	1.42
22	b	610	CLA	CHD-C4C	2.02	1.47	1.41
22	b	610	CLA	C4C-C3C	2.02	1.48	1.45
22	C	506	CLA	C1A-CHA	2.01	1.51	1.43
23	A	407	PHO	C1C-C2C	2.01	1.50	1.45
22	c	910	CLA	C4B-CHC	2.01	1.45	1.40
22	B	616	CLA	C4C-C3C	2.01	1.48	1.45
35	h	102	DGD	O5D-C1E	2.01	1.43	1.40
22	B	603	CLA	C4C-C3C	2.00	1.48	1.45

All (1909) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	602	CLA	C4A-NA-C1A	11.72	111.97	106.71
22	C	506	CLA	C4A-NA-C1A	11.20	111.74	106.71
22	B	602	CLA	C4A-NA-C1A	10.95	111.63	106.71
22	c	912	CLA	C4A-NA-C1A	10.35	111.36	106.71
22	c	909	CLA	C4A-NA-C1A	9.96	111.19	106.71
22	c	904	CLA	C4A-NA-C1A	9.82	111.12	106.71
22	b	608	CLA	C4A-NA-C1A	9.79	111.11	106.71
22	c	908	CLA	C4A-NA-C1A	9.69	111.06	106.71
22	C	514	CLA	C4A-NA-C1A	9.68	111.06	106.71
22	c	905	CLA	C4A-NA-C1A	9.23	110.85	106.71
34	V	203	HTG	O5-C1-C2	-9.01	98.98	110.31
22	B	606	CLA	C4A-NA-C1A	8.85	110.68	106.71
22	C	507	CLA	C4A-NA-C1A	8.72	110.63	106.71
22	B	615	CLA	C4A-NA-C1A	8.71	110.62	106.71
34	l	106	HTG	C1'-S1-C1	8.58	116.14	100.09
22	b	617	CLA	C4A-NA-C1A	8.54	110.54	106.71
22	B	616	CLA	C4A-NA-C1A	8.53	110.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	411	PHO	CMD-C2D-C1D	8.53	138.28	125.06
22	C	505	CLA	C4A-NA-C1A	8.46	110.51	106.71
22	C	504	CLA	C4A-NA-C1A	8.43	110.50	106.71
34	C	532	HTG	C1'-S1-C1	8.39	115.79	100.09
23	A	407	PHO	CMD-C2D-C1D	8.39	138.06	125.06
22	C	513	CLA	C4A-NA-C1A	8.39	110.48	106.71
28	a	414	SQD	O6-C1-C2	8.35	121.56	108.26
34	D	414	HTG	C1'-S1-C1	8.16	115.35	100.09
22	C	512	CLA	C4A-NA-C1A	8.08	110.34	106.71
22	B	611	CLA	O2D-CGD-CBD	8.05	125.33	111.25
22	b	614	CLA	C4A-NA-C1A	7.98	110.29	106.71
34	b	632	HTG	C1'-S1-C1	7.96	114.97	100.09
22	C	508	CLA	C4A-NA-C1A	7.91	110.26	106.71
22	D	403	CLA	C4A-NA-C1A	7.88	110.25	106.71
22	D	403	CLA	C2C-C1C-NC	7.75	117.24	109.97
34	v	203	HTG	O5-C1-C2	-7.74	100.58	110.31
34	b	624	HTG	C1'-S1-C1	7.69	114.47	100.09
36	E	102	HEM	CBD-CAD-C3D	-7.63	97.91	112.47
22	b	606	CLA	CHD-C4C-C3C	-7.63	113.75	124.87
22	b	605	CLA	C4A-NA-C1A	7.62	110.13	106.71
22	a	409	CLA	C2C-C1C-NC	7.61	117.10	109.97
34	D	415	HTG	C1'-S1-C1	7.58	114.27	100.09
22	d	403	CLA	C4A-NA-C1A	7.56	110.11	106.71
22	b	615	CLA	C4A-NA-C1A	7.49	110.07	106.71
22	B	605	CLA	C4A-NA-C1A	7.48	110.07	106.71
22	B	604	CLA	O2D-CGD-CBD	7.42	124.23	111.25
34	v	203	HTG	C1'-S1-C1	7.39	113.91	100.09
22	b	603	CLA	O2D-CGD-CBD	7.34	124.10	111.25
22	b	616	CLA	C4A-NA-C1A	7.33	110.00	106.71
23	a	411	PHO	C1-C2-C3	-7.29	113.43	126.04
22	B	612	CLA	C4A-NA-C1A	7.24	109.96	106.71
23	a	410	PHO	CMD-C2D-C1D	7.18	136.19	125.06
22	C	509	CLA	C4A-NA-C1A	7.17	109.93	106.71
34	B	627	HTG	C1'-S1-C1	7.17	113.50	100.09
34	b	627	HTG	C1'-S1-C1	7.09	113.35	100.09
23	D	402	PHO	CMD-C2D-C1D	7.06	136.01	125.06
22	b	612	CLA	C4A-NA-C1A	7.01	109.86	106.71
22	B	611	CLA	C4A-NA-C1A	6.96	109.84	106.71
22	B	610	CLA	C4A-NA-C1A	6.93	109.82	106.71
22	C	502	CLA	O2D-CGD-O1D	-6.89	110.22	123.83
28	a	414	SQD	O9-S-C6	6.88	115.12	106.94
22	b	602	CLA	O2D-CGD-CBD	6.84	123.22	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	902	CLA	C4A-NA-C1A	6.81	109.77	106.71
22	C	510	CLA	C2C-C1C-NC	6.73	116.28	109.97
22	A	406	CLA	C2C-C1C-NC	6.72	116.27	109.97
34	D	415	HTG	O5-C1-C2	-6.70	101.88	110.31
22	D	401	CLA	C2C-C1C-NC	6.69	116.24	109.97
34	B	623	HTG	C1'-S1-C1	6.69	112.61	100.09
22	C	508	CLA	O2D-CGD-CBD	6.68	122.94	111.25
28	C	501	SQD	O6-C1-C2	6.68	118.90	108.26
22	c	913	CLA	C4A-NA-C1A	6.60	109.67	106.71
22	C	502	CLA	O2D-CGD-CBD	6.59	122.79	111.25
22	D	403	CLA	C1C-C2C-C3C	-6.58	99.97	106.95
22	C	502	CLA	C4A-NA-C1A	6.51	109.63	106.71
34	c	922	HTG	C1'-S1-C1	6.50	112.25	100.09
34	C	521	HTG	C1'-S1-C1	6.49	112.23	100.09
22	b	613	CLA	CHD-C4C-C3C	-6.42	115.50	124.87
22	B	614	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	B	615	CLA	CHD-C4C-C3C	-6.38	115.56	124.87
22	a	409	CLA	C1C-C2C-C3C	-6.37	100.19	106.95
22	B	610	CLA	CHD-C4C-C3C	-6.32	115.65	124.87
22	B	609	CLA	O2D-CGD-CBD	6.32	122.32	111.25
22	D	401	CLA	C1C-C2C-C3C	-6.32	100.25	106.95
22	b	607	CLA	CHD-C4C-C3C	-6.32	115.66	124.87
22	b	604	CLA	C2C-C1C-NC	6.27	115.84	109.97
22	B	617	CLA	O2D-CGD-CBD	6.24	122.17	111.25
22	B	605	CLA	C2C-C1C-NC	6.23	115.81	109.97
34	B	626	HTG	C1'-S1-C1	6.22	111.73	100.09
22	a	408	CLA	CHD-C4C-C3C	-6.22	115.81	124.87
22	A	406	CLA	C1C-C2C-C3C	-6.19	100.39	106.95
22	B	617	CLA	CHD-C4C-C3C	-6.18	115.86	124.87
22	b	607	CLA	O2D-CGD-CBD	6.17	122.06	111.25
24	D	405	BCR	C24-C23-C22	-6.16	116.96	126.21
22	c	914	CLA	C4A-NA-C1A	6.14	109.47	106.71
22	a	412	CLA	O2D-CGD-CBD	6.14	121.99	111.25
36	e	101	HEM	CBD-CAD-C3D	-6.13	100.77	112.47
22	c	910	CLA	C2C-C1C-NC	6.06	115.65	109.97
28	C	501	SQD	O9-S-C6	6.02	114.09	106.94
22	b	607	CLA	C4A-NA-C1A	6.01	109.41	106.71
22	b	617	CLA	O2D-CGD-CBD	6.00	121.75	111.25
22	B	602	CLA	O2D-CGD-CBD	6.00	121.74	111.25
22	b	612	CLA	CHD-C4C-C3C	-5.98	116.15	124.87
22	B	607	CLA	O2D-CGD-O1D	-5.97	112.03	123.83
22	c	907	CLA	C2C-C1C-NC	5.93	115.53	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	622	LMG	O1-C1-C2	5.90	117.66	108.26
22	B	607	CLA	O2D-CGD-CBD	5.89	121.55	111.25
22	C	511	CLA	C2C-C1C-NC	5.82	115.43	109.97
22	b	604	CLA	CHD-C4C-C3C	-5.80	116.41	124.87
22	D	401	CLA	CHD-C4C-C3C	-5.80	116.41	124.87
22	b	611	CLA	O2D-CGD-CBD	5.79	121.38	111.25
22	B	607	CLA	CHD-C4C-C3C	-5.78	116.44	124.87
27	A	412	LHG	O7-C7-C8	5.77	121.88	111.09
22	b	613	CLA	C4A-NA-C1A	5.76	109.29	106.71
23	D	402	PHO	C4C-C3C-C2C	-5.76	100.39	106.79
23	a	411	PHO	O2D-CGD-CBD	5.75	121.31	111.25
22	b	611	CLA	C2C-C1C-NC	5.73	115.34	109.97
22	c	910	CLA	C4A-NA-C1A	5.73	109.28	106.71
22	A	405	CLA	C2C-C1C-NC	5.68	115.29	109.97
27	D	409	LHG	O7-C7-C8	5.63	123.81	111.51
22	b	607	CLA	O2D-CGD-O1D	-5.61	112.74	123.83
22	b	617	CLA	CHD-C4C-C3C	-5.61	116.69	124.87
22	A	408	CLA	C2C-C1C-NC	5.61	115.22	109.97
22	B	608	CLA	C2C-C1C-NC	5.60	115.22	109.97
22	B	617	CLA	C2C-C1C-NC	5.58	115.20	109.97
22	B	609	CLA	CHD-C4C-C3C	-5.56	116.76	124.87
22	B	607	CLA	C2C-C1C-NC	5.55	115.17	109.97
22	c	908	CLA	O2D-CGD-CBD	5.53	120.93	111.25
22	d	402	CLA	O2D-CGD-CBD	5.52	120.91	111.25
34	V	203	HTG	C1'-S1-C1	5.51	110.71	100.16
22	B	604	CLA	C2C-C1C-NC	5.50	115.12	109.97
25	d	409	LMG	O1-C1-C2	5.49	117.01	108.26
22	B	606	CLA	CHD-C4C-C3C	-5.49	116.86	124.87
34	b	626	HTG	C1'-S1-C1	5.49	110.35	100.09
22	c	914	CLA	CHD-C4C-C3C	-5.47	116.89	124.87
22	b	610	CLA	C1C-C2C-C3C	-5.47	101.16	106.95
25	b	622	LMG	O7-C10-C11	5.43	123.37	111.51
27	a	416	LHG	O7-C7-C8	5.42	123.33	111.51
22	B	609	CLA	C2C-C1C-NC	5.41	115.04	109.97
22	a	412	CLA	C1C-C2C-C3C	-5.41	101.22	106.95
22	a	408	CLA	C2C-C1C-NC	5.40	115.03	109.97
22	B	613	CLA	C4A-NA-C1A	5.40	109.13	106.71
22	B	603	CLA	C2C-C1C-NC	5.39	115.02	109.97
22	c	903	CLA	C4A-NA-C1A	5.36	109.12	106.71
22	c	903	CLA	C1-C2-C3	-5.36	116.77	126.04
22	b	611	CLA	C4A-NA-C1A	5.35	109.11	106.71
24	D	405	BCR	C7-C8-C9	-5.33	118.21	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	903	CLA	CHD-C4C-C3C	-5.32	117.11	124.87
22	b	611	CLA	CHD-C4C-C3C	-5.31	117.13	124.87
22	a	408	CLA	CHD-C4C-NC	5.31	132.56	124.20
28	A	413	SQD	O9-S-C6	5.30	113.24	106.94
22	b	610	CLA	C2C-C1C-NC	5.30	114.94	109.97
22	B	616	CLA	CHD-C4C-C3C	-5.28	117.16	124.87
22	a	412	CLA	C2C-C1C-NC	5.27	114.91	109.97
22	D	403	CLA	C1-C2-C3	-5.26	116.95	126.04
22	c	906	CLA	C4A-NA-C1A	5.25	109.06	106.71
22	D	404	CLA	C4A-NA-C1A	5.22	109.05	106.71
22	c	902	CLA	CHD-C4C-C3C	-5.22	117.26	124.87
23	D	402	PHO	C1-C2-C3	-5.22	117.02	126.04
22	a	408	CLA	C1C-C2C-C3C	-5.21	101.42	106.95
22	C	510	CLA	C4A-NA-C1A	5.21	109.05	106.71
34	b	632	HTG	O5-C5-C4	5.19	119.15	109.68
22	C	510	CLA	C1C-C2C-C3C	-5.18	101.47	106.95
22	b	605	CLA	C2C-C1C-NC	5.17	114.82	109.97
22	d	402	CLA	C2C-C1C-NC	5.17	114.82	109.97
22	c	913	CLA	C1-C2-C3	-5.17	117.10	126.04
22	c	913	CLA	O2D-CGD-CBD	5.17	120.30	111.25
22	B	605	CLA	C1C-C2C-C3C	-5.16	101.48	106.95
22	C	514	CLA	CHD-C4C-C3C	-5.16	117.34	124.87
22	b	604	CLA	O2D-CGD-CBD	5.16	120.28	111.25
22	a	407	CLA	C4A-NA-C1A	5.16	109.02	106.71
24	d	404	BCR	C7-C8-C9	-5.15	118.47	126.21
22	C	505	CLA	C2C-C1C-NC	5.13	114.78	109.97
22	c	902	CLA	C1C-C2C-C3C	-5.11	101.53	106.95
28	l	101	SQD	O6-C1-C2	5.11	116.40	108.26
22	C	507	CLA	C2C-C1C-NC	5.10	114.75	109.97
22	C	504	CLA	CHD-C4C-C3C	-5.10	117.44	124.87
35	d	406	DGD	O2G-C1B-C2B	5.09	122.63	111.51
22	c	911	CLA	CHD-C4C-C3C	-5.09	117.45	124.87
22	c	906	CLA	O2D-CGD-CBD	5.09	120.16	111.25
28	a	414	SQD	O47-C7-C8	5.06	122.56	111.51
22	c	911	CLA	C4A-NA-C1A	5.05	108.98	106.71
22	c	908	CLA	CHD-C4C-C3C	-5.05	117.51	124.87
22	b	608	CLA	C2C-C1C-NC	5.05	114.70	109.97
22	C	503	CLA	O2D-CGD-CBD	5.04	120.08	111.25
22	c	907	CLA	O2D-CGD-CBD	5.03	120.06	111.25
22	B	603	CLA	CHD-C4C-C3C	-5.03	117.54	124.87
24	b	618	BCR	C3-C4-C5	-5.02	105.25	113.99
22	C	502	CLA	C2C-C1C-NC	5.00	114.66	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	613	CLA	CAC-C3C-C4C	4.99	131.35	124.82
22	B	611	CLA	CHD-C4C-C3C	-4.99	117.60	124.87
22	b	606	CLA	CHD-C4C-NC	4.98	132.05	124.20
22	B	617	CLA	O2D-CGD-O1D	-4.98	114.00	123.83
22	A	406	CLA	CHD-C4C-C3C	-4.97	117.62	124.87
22	b	609	CLA	CHD-C4C-C3C	-4.96	117.63	124.87
22	c	903	CLA	O2D-CGD-O1D	-4.96	114.04	123.83
22	C	513	CLA	CHD-C4C-C3C	-4.96	117.64	124.87
22	b	607	CLA	C1-C2-C3	-4.94	117.50	126.04
22	c	904	CLA	C2C-C1C-NC	4.93	114.59	109.97
22	b	606	CLA	O2D-CGD-CBD	4.92	119.87	111.25
22	b	612	CLA	C2C-C1C-NC	4.92	114.58	109.97
22	C	503	CLA	C4A-NA-C1A	4.91	108.91	106.71
28	a	418	SQD	C1-O5-C5	-4.90	104.05	113.70
22	A	405	CLA	C1C-C2C-C3C	-4.88	101.78	106.95
22	C	503	CLA	O2D-CGD-O1D	-4.86	114.24	123.83
22	C	510	CLA	O2D-CGD-CBD	4.83	119.71	111.25
22	b	604	CLA	C1C-C2C-C3C	-4.83	101.83	106.95
22	C	507	CLA	CHD-C4C-C3C	-4.83	117.83	124.87
27	C	522	LHG	O7-C7-C8	4.82	122.04	111.51
23	a	411	PHO	O2D-CGD-O1D	-4.81	114.32	123.83
34	v	203	HTG	C1-C2-C3	-4.81	101.08	110.59
22	C	508	CLA	CHD-C4C-C3C	-4.81	117.85	124.87
39	V	202	HEC	CBD-CAD-C3D	-4.81	103.28	112.48
22	a	409	CLA	O2D-CGD-CBD	4.80	119.64	111.25
24	C	515	BCR	C33-C5-C6	-4.79	119.17	124.51
23	a	410	PHO	C4C-C3C-C2C	-4.79	101.46	106.79
22	c	903	CLA	C2C-C1C-NC	4.79	114.46	109.97
26	A	411	PL9	C7-C3-C4	4.79	120.77	116.88
28	D	408	SQD	O6-C1-C2	4.79	115.89	108.26
22	b	604	CLA	C4-C3-C5	4.79	123.53	115.29
22	B	611	CLA	O2D-CGD-O1D	-4.78	114.38	123.83
22	b	614	CLA	C2C-C1C-NC	4.77	114.44	109.97
22	d	403	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	c	902	CLA	C2C-C1C-NC	4.75	114.42	109.97
22	c	907	CLA	C4A-NA-C1A	4.74	108.84	106.71
22	a	407	CLA	O2D-CGD-CBD	4.73	119.54	111.25
23	D	402	PHO	C3D-C2D-C1D	-4.72	98.89	105.88
29	I	102	LMT	O1B-C4'-C3'	4.72	119.99	107.28
28	l	101	SQD	O47-C7-C8	4.71	121.80	111.51
22	C	513	CLA	O2D-CGD-CBD	4.71	119.49	111.25
22	b	610	CLA	CHD-C4C-C3C	-4.71	118.00	124.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	O2D-CGD-CBD	4.70	119.48	111.25
22	C	512	CLA	CHD-C4C-C3C	-4.69	118.03	124.87
22	c	908	CLA	O2D-CGD-O1D	-4.69	114.57	123.83
23	a	410	PHO	O2D-CGD-CBD	4.69	119.45	111.25
35	c	919	DGD	O2G-C1B-C2B	4.69	121.74	111.51
22	C	505	CLA	O2D-CGD-CBD	4.68	119.44	111.25
22	b	606	CLA	C2C-C1C-NC	4.68	114.36	109.97
22	B	612	CLA	CHD-C4C-C3C	-4.67	118.06	124.87
22	B	615	CLA	O2D-CGD-CBD	4.67	119.43	111.25
22	a	409	CLA	CHD-C4C-C3C	-4.67	118.06	124.87
22	b	607	CLA	C2C-C1C-NC	4.66	114.34	109.97
22	B	607	CLA	C1C-C2C-C3C	-4.66	102.01	106.95
22	C	505	CLA	C1C-C2C-C3C	-4.65	102.02	106.95
22	B	603	CLA	C4A-NA-C1A	4.65	108.80	106.71
22	A	408	CLA	C1C-C2C-C3C	-4.64	102.03	106.95
22	B	605	CLA	O2D-CGD-CBD	4.63	119.36	111.25
22	B	604	CLA	C1C-C2C-C3C	-4.61	102.07	106.95
28	A	413	SQD	O48-C23-C24	4.60	126.72	111.93
24	Y	101	BCR	C38-C26-C25	-4.60	119.39	124.51
22	a	412	CLA	C4-C3-C5	4.60	123.21	115.29
22	C	511	CLA	C1C-C2C-C3C	-4.60	102.08	106.95
28	C	501	SQD	O8-S-C6	4.60	113.06	105.74
24	y	101	BCR	C33-C5-C6	-4.59	119.39	124.51
22	b	609	CLA	C2C-C1C-NC	4.58	114.26	109.97
24	d	404	BCR	C38-C26-C25	-4.58	119.41	124.51
23	A	407	PHO	O2D-CGD-CBD	4.58	119.27	111.25
22	B	613	CLA	C2C-C1C-NC	4.58	114.26	109.97
28	l	101	SQD	O7-S-C6	4.58	112.38	106.94
22	C	512	CLA	C2C-C1C-NC	4.58	114.26	109.97
23	a	410	PHO	C3C-C4C-NC	4.58	117.39	110.28
22	B	611	CLA	C2C-C1C-NC	4.57	114.25	109.97
22	D	401	CLA	CHD-C4C-NC	4.57	131.40	124.20
22	b	615	CLA	C2C-C1C-NC	4.57	114.25	109.97
23	a	410	PHO	C3D-C2D-C1D	-4.57	99.12	105.88
22	C	502	CLA	CHD-C4C-C3C	-4.56	118.22	124.87
22	d	403	CLA	C1C-C2C-C3C	-4.55	102.13	106.95
22	A	408	CLA	C4A-NA-C1A	4.54	108.75	106.71
22	b	614	CLA	CHD-C4C-C3C	-4.54	118.24	124.87
23	a	411	PHO	C3D-C2D-C1D	-4.54	99.16	105.88
22	d	402	CLA	C1C-C2C-C3C	-4.54	102.14	106.95
29	I	102	LMT	C1'-O5'-C5'	4.54	122.64	113.70
22	b	609	CLA	C4A-NA-C1A	4.53	108.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	406	CLA	C4-C3-C5	4.53	123.09	115.29
28	a	418	SQD	O6-C1-C2	4.52	115.47	108.26
22	c	905	CLA	C2C-C1C-NC	4.52	114.20	109.97
22	C	503	CLA	CHD-C4C-C3C	-4.51	118.30	124.87
23	A	407	PHO	C3D-C2D-C1D	-4.51	99.21	105.88
22	c	909	CLA	O2D-CGD-CBD	4.49	119.11	111.25
34	V	203	HTG	O2-C2-C1	4.49	118.51	110.27
22	D	404	CLA	O2D-CGD-CBD	4.48	119.10	111.25
22	B	610	CLA	C2C-C1C-NC	4.48	114.17	109.97
22	c	909	CLA	C1C-C2C-C3C	-4.46	102.23	106.95
22	c	914	CLA	C1C-C2C-C3C	-4.45	102.23	106.95
22	b	614	CLA	CAC-C3C-C4C	4.45	130.63	124.82
22	B	608	CLA	C1C-C2C-C3C	-4.45	102.24	106.95
23	A	407	PHO	C2C-C1C-NC	4.44	116.52	109.79
22	B	612	CLA	C2C-C1C-NC	4.42	114.12	109.97
22	c	902	CLA	O2D-CGD-CBD	4.42	119.00	111.25
22	a	412	CLA	CMD-C2D-C3D	4.42	133.09	124.80
22	C	511	CLA	CHD-C4C-C3C	-4.41	118.44	124.87
22	b	613	CLA	O2D-CGD-CBD	4.41	118.97	111.25
28	C	501	SQD	C1-O5-C5	-4.41	105.01	113.70
22	b	603	CLA	C4A-NA-C1A	4.41	108.69	106.71
22	a	407	CLA	CAC-C3C-C4C	4.40	130.57	124.82
22	c	910	CLA	CAC-C3C-C4C	4.39	130.56	124.82
22	b	615	CLA	O2D-CGD-CBD	4.39	118.94	111.25
24	c	916	BCR	C15-C14-C13	-4.39	121.04	127.31
22	B	603	CLA	C1C-C2C-C3C	-4.39	102.30	106.95
22	B	605	CLA	CHD-C4C-C3C	-4.39	118.47	124.87
28	A	413	SQD	O6-C1-C2	4.39	115.25	108.26
22	c	907	CLA	C1C-C2C-C3C	-4.39	102.30	106.95
28	C	501	SQD	C1-C2-C3	-4.39	100.83	109.98
22	b	605	CLA	O2D-CGD-CBD	4.38	118.92	111.25
22	c	910	CLA	C1C-C2C-C3C	-4.37	102.32	106.95
22	B	615	CLA	C2C-C1C-NC	4.36	114.06	109.97
22	c	908	CLA	C1C-C2C-C3C	-4.36	102.33	106.95
22	B	617	CLA	C1C-C2C-C3C	-4.35	102.34	106.95
23	A	407	PHO	C1C-C2C-C3C	-4.35	101.47	106.50
22	B	610	CLA	CHD-C4C-NC	4.35	131.05	124.20
23	a	411	PHO	C4C-C3C-C2C	-4.34	101.97	106.79
35	D	407	DGD	C4D-C3D-C2D	4.34	118.44	110.82
23	D	402	PHO	C4-C3-C5	4.34	122.76	115.29
22	B	609	CLA	C1C-C2C-C3C	-4.33	102.37	106.95
22	c	908	CLA	CHD-C4C-NC	4.32	131.00	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	O2D-CGD-CBD	4.31	118.80	111.25
22	b	613	CLA	CMD-C2D-C3D	4.31	132.88	124.80
22	B	611	CLA	C1C-C2C-C3C	-4.30	102.39	106.95
22	b	617	CLA	CBC-CAC-C3C	-4.30	100.49	112.43
22	B	603	CLA	O2D-CGD-CBD	4.29	118.76	111.25
24	c	915	BCR	C33-C5-C6	-4.29	119.74	124.51
22	c	914	CLA	C2C-C1C-NC	4.29	113.99	109.97
35	H	102	DGD	O1G-C1A-O1A	-4.28	112.61	123.56
22	B	602	CLA	O2D-CGD-O1D	-4.28	115.37	123.83
22	c	911	CLA	CHD-C4C-NC	4.28	130.95	124.20
22	B	606	CLA	CMC-C2C-C1C	4.28	131.53	125.03
35	D	407	DGD	O2G-C1B-C2B	4.27	120.82	111.51
22	b	602	CLA	C1C-C2C-C3C	-4.26	102.44	106.95
28	a	414	SQD	C1-C2-C3	-4.26	101.10	109.98
22	a	408	CLA	O2D-CGD-CBD	4.25	118.70	111.25
27	l	102	LHG	O7-C7-C8	4.25	120.78	111.51
22	c	907	CLA	CHD-C4C-C3C	-4.24	118.68	124.87
22	B	617	CLA	CHD-C4C-NC	4.24	130.89	124.20
25	D	412	LMG	O7-C10-C11	4.24	120.76	111.51
22	c	906	CLA	CHD-C4C-C3C	-4.23	118.69	124.87
25	d	409	LMG	O7-C10-C11	4.23	120.75	111.51
22	C	506	CLA	C2C-C1C-NC	4.23	113.94	109.97
22	D	401	CLA	CMD-C2D-C3D	4.23	132.74	124.80
34	D	415	HTG	O5-C5-C4	4.23	117.40	109.68
22	b	602	CLA	CHD-C4C-C3C	-4.23	118.70	124.87
37	H	101	RRX	C24-C23-C22	-4.23	119.86	126.21
35	C	517	DGD	O3G-C3G-C2G	-4.22	100.71	110.90
22	C	512	CLA	C1-O2A-CGA	4.22	128.08	116.54
22	c	911	CLA	CMC-C2C-C1C	4.22	131.44	125.03
22	c	905	CLA	C1C-C2C-C3C	-4.21	102.49	106.95
22	B	610	CLA	C1C-C2C-C3C	-4.21	102.49	106.95
22	B	613	CLA	CHD-C4C-C3C	-4.21	118.73	124.87
22	c	913	CLA	C1C-C2C-C3C	-4.20	102.50	106.95
22	a	407	CLA	C2C-C1C-NC	4.20	113.91	109.97
22	A	408	CLA	C4-C3-C5	4.20	122.52	115.29
22	C	504	CLA	O2D-CGD-O1D	-4.20	115.53	123.83
22	c	913	CLA	C2C-C1C-NC	4.20	113.90	109.97
22	b	617	CLA	C2C-C1C-NC	4.20	113.90	109.97
22	C	508	CLA	C1C-C2C-C3C	-4.20	102.50	106.95
25	B	621	LMG	O7-C10-C11	4.19	120.65	111.51
22	b	612	CLA	C1C-C2C-C3C	-4.19	102.51	106.95
22	B	606	CLA	CHC-C1C-NC	-4.18	117.86	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	411	PL9	C53-C6-C1	4.18	123.60	114.98
22	d	403	CLA	C1-O2A-CGA	4.17	127.95	116.54
25	C	520	LMG	O8-C28-C29	4.17	125.33	111.93
28	C	501	SQD	O47-C7-C8	4.16	120.60	111.51
22	b	611	CLA	C1C-C2C-C3C	-4.16	102.54	106.95
23	D	402	PHO	C4A-NA-C1A	4.16	111.50	108.14
23	a	410	PHO	C2C-C1C-NC	4.16	116.10	109.79
22	C	508	CLA	C2C-C1C-NC	4.16	113.87	109.97
22	c	905	CLA	CHD-C4C-C3C	-4.16	118.81	124.87
22	a	407	CLA	C1C-C2C-C3C	-4.16	102.55	106.95
22	C	506	CLA	CAC-C3C-C4C	4.15	130.25	124.82
22	C	511	CLA	O2D-CGD-O1D	-4.15	115.63	123.83
28	A	413	SQD	O47-C7-C8	4.15	120.57	111.51
22	b	608	CLA	C1C-C2C-C3C	-4.15	102.56	106.95
22	C	507	CLA	C1C-C2C-C3C	-4.14	102.56	106.95
22	b	616	CLA	CHD-C4C-C3C	-4.14	118.83	124.87
22	c	904	CLA	C1C-C2C-C3C	-4.13	102.57	106.95
22	B	602	CLA	CAC-C3C-C4C	4.13	130.22	124.82
22	d	403	CLA	O2D-CGD-CBD	4.12	118.45	111.25
22	C	514	CLA	O2D-CGD-O1D	-4.11	115.70	123.83
35	c	917	DGD	O2G-C1B-C2B	4.11	120.49	111.51
22	a	409	CLA	C4A-NA-C1A	4.11	108.56	106.71
24	b	618	BCR	C33-C5-C6	-4.11	119.94	124.51
22	B	617	CLA	O2A-CGA-CBA	4.11	125.11	111.93
22	b	606	CLA	O2D-CGD-O1D	-4.10	115.73	123.83
22	b	613	CLA	C2C-C1C-NC	4.10	113.81	109.97
22	C	502	CLA	C1C-C2C-C3C	-4.10	102.61	106.95
22	b	615	CLA	CHD-C4C-C3C	-4.09	118.90	124.87
22	D	404	CLA	C2C-C1C-NC	4.09	113.81	109.97
22	c	911	CLA	O2D-CGD-CBD	4.09	118.41	111.25
22	b	607	CLA	C1C-C2C-C3C	-4.09	102.62	106.95
22	B	604	CLA	CHD-C4C-C3C	-4.09	118.91	124.87
39	v	202	HEC	CBD-CAD-C3D	-4.09	104.67	112.48
22	c	903	CLA	O2D-CGD-CBD	4.08	118.39	111.25
23	a	410	PHO	O2D-CGD-O1D	-4.08	115.78	123.83
25	C	520	LMG	O7-C10-C11	4.08	120.41	111.51
22	a	412	CLA	O2D-CGD-O1D	-4.07	115.78	123.83
23	D	402	PHO	C3C-C4C-NC	4.07	116.61	110.28
22	D	404	CLA	CAC-C3C-C4C	4.07	130.14	124.82
22	c	913	CLA	CHD-C4C-C3C	-4.07	118.93	124.87
22	b	603	CLA	CMB-C2B-C3B	4.07	132.44	124.80
22	B	616	CLA	C2C-C1C-NC	4.07	113.78	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	615	CLA	CHD-C4C-NC	4.06	130.60	124.20
22	B	609	CLA	O2D-CGD-O1D	-4.06	115.81	123.83
22	b	602	CLA	C1-O2A-CGA	4.05	127.61	116.54
22	B	616	CLA	O2D-CGD-CBD	4.05	118.33	111.25
22	B	616	CLA	CHD-C4C-NC	4.05	130.58	124.20
27	d	407	LHG	O8-C23-O10	-4.05	113.22	123.56
22	B	617	CLA	C1-O2A-CGA	4.04	127.59	116.54
22	B	606	CLA	O2D-CGD-O1D	-4.04	115.85	123.83
22	c	906	CLA	C2C-C1C-NC	4.04	113.76	109.97
26	D	406	PL9	C40-C39-C41	4.04	122.24	115.29
34	b	632	HTG	C1-O5-C5	4.03	120.17	112.58
26	d	405	PL9	C35-C34-C36	4.02	122.22	115.29
28	b	621	SQD	O7-S-C6	4.02	111.72	106.94
22	C	511	CLA	C4A-NA-C1A	4.02	108.51	106.71
22	B	615	CLA	C1C-C2C-C3C	-4.02	102.69	106.95
22	a	412	CLA	CHD-C4C-C3C	-4.02	119.01	124.87
22	c	914	CLA	CMC-C2C-C1C	4.01	131.14	125.03
22	B	613	CLA	CAC-C3C-C4C	4.01	130.07	124.82
22	b	605	CLA	CHD-C4C-C3C	-4.01	119.02	124.87
22	B	604	CLA	O2D-CGD-O1D	-4.01	115.92	123.83
22	b	616	CLA	CMD-C2D-C3D	4.01	132.31	124.80
22	C	514	CLA	O2D-CGD-CBD	3.99	118.23	111.25
23	a	411	PHO	C4-C3-C5	3.98	122.15	115.29
22	b	605	CLA	C1C-C2C-C3C	-3.98	102.73	106.95
22	b	610	CLA	CMC-C2C-C1C	3.98	131.09	125.03
22	B	602	CLA	O1D-CGD-CBD	-3.98	116.23	124.48
22	C	506	CLA	C1C-C2C-C3C	-3.98	102.73	106.95
27	D	409	LHG	O7-C7-O9	-3.98	113.94	123.71
22	a	409	CLA	C3B-C4B-NB	3.98	114.35	109.21
22	c	913	CLA	O2D-CGD-O1D	-3.97	115.99	123.83
22	B	602	CLA	C2C-C1C-NC	3.97	113.69	109.97
22	b	612	CLA	CHD-C4C-NC	3.97	130.46	124.20
22	A	408	CLA	O2D-CGD-CBD	3.97	118.19	111.25
22	b	617	CLA	C3C-C4C-NC	3.96	115.02	110.57
22	d	402	CLA	O2D-CGD-O1D	-3.96	116.00	123.83
22	b	616	CLA	C2C-C1C-NC	3.96	113.68	109.97
22	C	513	CLA	C1-O2A-CGA	3.96	127.36	116.54
22	C	503	CLA	C1C-C2C-C3C	-3.95	102.76	106.95
37	H	101	RRX	C31-C1-C6	-3.94	103.93	110.30
22	B	607	CLA	C4-C3-C5	3.94	122.08	115.29
34	V	203	HTG	C1-C2-C3	-3.94	102.81	110.59
36	E	102	HEM	CBA-CAA-C2A	-3.94	104.95	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	909	CLA	C2C-C1C-NC	3.93	113.66	109.97
22	b	603	CLA	C1C-C2C-C3C	-3.93	102.78	106.95
34	b	624	HTG	O5-C1-C2	3.93	115.25	110.31
22	B	612	CLA	C1C-C2C-C3C	-3.92	102.79	106.95
23	D	402	PHO	C2D-C1D-ND	3.92	115.73	109.79
25	C	531	LMG	O7-C10-C11	3.92	120.07	111.51
22	c	910	CLA	O2D-CGD-CBD	3.92	118.11	111.25
28	A	413	SQD	O48-C23-O10	-3.91	113.57	123.56
22	B	608	CLA	O2D-CGD-CBD	3.91	118.09	111.25
22	B	605	CLA	CMC-C2C-C1C	3.90	130.97	125.03
22	b	608	CLA	CGD-CBD-CAD	-3.89	98.13	110.73
22	c	909	CLA	CHD-C4C-C3C	-3.89	119.20	124.87
34	B	627	HTG	O5-C1-C2	3.89	115.21	110.31
26	d	405	PL9	O1-C4-C3	-3.89	116.36	120.71
22	C	511	CLA	O2D-CGD-CBD	3.88	118.05	111.25
29	a	419	LMT	C4B-C3B-C2B	-3.87	104.02	110.82
25	b	622	LMG	C7-O1-C1	3.87	121.53	113.75
35	C	517	DGD	C3G-C2G-C1G	-3.87	102.56	111.79
22	B	610	CLA	O2D-CGD-CBD	3.87	118.03	111.25
29	T	102	LMT	C1'-C2'-C3'	3.87	118.06	109.98
26	a	415	PL9	C53-C6-C1	3.87	122.96	114.98
22	C	513	CLA	C1C-C2C-C3C	-3.87	102.85	106.95
23	D	402	PHO	CAC-C3C-C4C	3.86	129.44	125.22
22	a	408	CLA	C4A-NA-C1A	3.86	108.44	106.71
22	b	603	CLA	O2D-CGD-O1D	-3.86	116.21	123.83
22	b	610	CLA	C4A-NA-C1A	3.86	108.44	106.71
22	A	406	CLA	CMC-C2C-C1C	3.86	130.90	125.03
22	B	603	CLA	O2D-CGD-O1D	-3.86	116.22	123.83
22	C	509	CLA	CHD-C4C-C3C	-3.85	119.25	124.87
34	B	627	HTG	C1-O5-C5	3.85	119.84	112.58
22	b	611	CLA	CMD-C2D-C3D	3.85	132.02	124.80
22	c	903	CLA	C1C-C2C-C3C	-3.85	102.87	106.95
22	a	409	CLA	C4-C3-C5	3.85	121.91	115.29
22	B	608	CLA	CGD-CBD-CAD	-3.85	98.27	110.73
23	a	411	PHO	C2B-C1B-NB	3.84	115.62	109.79
25	c	930	LMG	O7-C10-C11	3.84	119.90	111.51
22	c	914	CLA	O2D-CGD-O1D	-3.84	116.24	123.83
22	c	912	CLA	C1C-C2C-C3C	-3.84	102.88	106.95
22	C	508	CLA	O2D-CGD-O1D	-3.84	116.25	123.83
27	a	423	LHG	O7-C7-C8	3.83	119.88	111.51
22	C	504	CLA	O2D-CGD-CBD	3.83	117.96	111.25
22	b	616	CLA	C1C-C2C-C3C	-3.83	102.89	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	408	CLA	CED-O2D-CGD	3.83	124.69	115.95
22	b	611	CLA	O2D-CGD-O1D	-3.82	116.28	123.83
22	b	614	CLA	O2D-CGD-CBD	3.82	117.94	111.25
22	C	512	CLA	C1C-C2C-C3C	-3.81	102.91	106.95
22	b	613	CLA	CHD-C4C-NC	3.81	130.20	124.20
24	B	620	BCR	C2-C1-C6	3.81	116.37	110.48
22	C	514	CLA	C1C-C2C-C3C	-3.81	102.92	106.95
22	d	402	CLA	O2A-CGA-CBA	3.80	124.14	111.93
24	d	404	BCR	C30-C25-C26	-3.80	117.28	122.59
26	D	406	PL9	C7-C8-C9	-3.80	120.47	126.79
22	B	604	CLA	C4A-NA-C1A	3.79	108.41	106.71
22	C	503	CLA	CMD-C2D-C3D	3.79	131.91	124.80
22	b	604	CLA	CMC-C2C-C1C	3.79	130.80	125.03
24	Y	101	BCR	C16-C15-C14	-3.79	115.54	123.51
39	v	202	HEC	CMC-C2C-C1C	-3.79	122.64	128.46
22	c	906	CLA	C1C-C2C-C3C	-3.79	102.93	106.95
22	c	904	CLA	C1-C2-C3	-3.78	119.50	126.04
22	B	612	CLA	O2D-CGD-O1D	-3.78	116.36	123.83
25	b	622	LMG	C3-C4-C5	3.78	117.02	110.23
22	A	408	CLA	CHD-C4C-C3C	-3.78	119.36	124.87
24	c	915	BCR	C15-C14-C13	-3.78	121.92	127.31
22	C	505	CLA	CHD-C4C-C3C	-3.77	119.37	124.87
22	B	606	CLA	CAC-C3C-C4C	3.77	129.75	124.82
22	b	607	CLA	CHD-C4C-NC	3.77	130.14	124.20
22	B	609	CLA	CAC-C3C-C4C	3.76	129.73	124.82
22	c	905	CLA	C3B-C4B-NB	3.75	114.06	109.21
22	a	407	CLA	C4-C3-C5	3.75	121.75	115.29
26	a	415	PL9	C7-C3-C4	3.74	119.92	116.88
22	B	608	CLA	CBC-CAC-C3C	-3.74	102.04	112.43
24	B	618	BCR	C3-C4-C5	-3.74	107.48	113.99
22	c	906	CLA	CMD-C2D-C3D	3.73	131.80	124.80
23	a	411	PHO	C2D-C1D-ND	3.73	115.45	109.79
22	c	903	CLA	C1D-CHD-C4C	-3.73	117.39	122.48
22	c	914	CLA	CHD-C4C-NC	3.73	130.08	124.20
22	B	614	CLA	CHD-C4C-C3C	-3.72	119.44	124.87
22	c	908	CLA	C2C-C1C-NC	3.72	113.45	109.97
22	B	614	CLA	C2C-C1C-NC	3.71	113.45	109.97
22	b	602	CLA	C2C-C1C-NC	3.71	113.45	109.97
35	h	102	DGD	O1G-C1A-C2A	3.71	123.84	111.93
22	D	401	CLA	CBC-CAC-C3C	-3.70	102.16	112.43
22	C	509	CLA	O2D-CGD-O1D	-3.70	116.53	123.83
22	D	404	CLA	C1C-C2C-C3C	-3.70	103.03	106.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	604	CLA	C4A-NA-C1A	3.69	108.36	106.71
22	C	503	CLA	C2C-C1C-NC	3.69	113.43	109.97
35	H	102	DGD	O1G-C1A-C2A	3.69	123.76	111.93
22	c	911	CLA	O2D-CGD-O1D	-3.68	116.55	123.83
22	c	902	CLA	O2D-CGD-O1D	-3.68	116.55	123.83
22	C	509	CLA	C2C-C1C-NC	3.67	113.41	109.97
22	b	614	CLA	CMB-C2B-C1B	3.67	134.11	128.46
25	c	920	LMG	O8-C28-C29	3.67	123.72	111.93
22	c	902	CLA	CHD-C4C-NC	3.67	129.98	124.20
23	D	402	PHO	O2D-CGD-CBD	3.67	117.67	111.25
24	k	101	BCR	C24-C23-C22	-3.67	120.70	126.21
22	b	607	CLA	C1-O2A-CGA	3.66	126.55	116.54
22	B	608	CLA	C4A-NA-C1A	3.66	108.35	106.71
22	c	911	CLA	C1C-C2C-C3C	-3.65	103.08	106.95
22	D	401	CLA	C1D-CHD-C4C	-3.65	117.49	122.48
22	b	616	CLA	O2D-CGD-CBD	3.65	117.64	111.25
22	b	604	CLA	CHD-C4C-NC	3.65	129.96	124.20
24	C	515	BCR	C38-C26-C25	-3.65	120.45	124.51
22	A	406	CLA	C1D-CHD-C4C	-3.65	117.50	122.48
22	D	403	CLA	C3B-C4B-NB	3.64	113.92	109.21
22	B	607	CLA	C4A-NA-C1A	3.64	108.34	106.71
24	D	405	BCR	C28-C27-C26	-3.64	107.65	113.99
22	B	614	CLA	C1C-C2C-C3C	-3.64	103.09	106.95
24	b	620	BCR	C7-C8-C9	-3.64	120.74	126.21
22	b	606	CLA	C4A-NA-C1A	3.64	108.34	106.71
22	B	605	CLA	CAC-C3C-C4C	3.64	129.57	124.82
24	d	404	BCR	C16-C15-C14	-3.63	115.88	123.51
22	B	606	CLA	C2C-C1C-NC	3.62	113.37	109.97
22	b	602	CLA	O2D-CGD-O1D	-3.62	116.67	123.83
22	B	611	CLA	O2A-CGA-CBA	3.62	123.56	111.93
24	A	409	BCR	C15-C16-C17	-3.62	115.90	123.51
22	d	402	CLA	CHD-C4C-C3C	-3.62	119.59	124.87
22	C	507	CLA	O2D-CGD-CBD	3.62	117.59	111.25
22	C	509	CLA	C1C-C2C-C3C	-3.62	103.12	106.95
22	b	617	CLA	O2D-CGD-O1D	-3.62	116.69	123.83
22	B	608	CLA	C4-C3-C5	3.61	121.51	115.29
34	b	624	HTG	C1-C2-C3	3.61	117.72	110.59
22	B	603	CLA	C7-C6-C5	-3.61	103.55	113.25
28	a	418	SQD	O47-C7-C8	3.61	119.39	111.51
22	B	613	CLA	C1C-C2C-C3C	-3.61	103.13	106.95
22	b	604	CLA	CMD-C2D-C3D	3.60	131.56	124.80
22	D	401	CLA	O2D-CGD-CBD	3.60	117.55	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	406	CLA	CHD-C4C-NC	3.60	129.87	124.20
22	D	403	CLA	C2A-C1A-CHA	-3.60	117.57	123.86
39	v	202	HEC	C1D-C2D-C3D	-3.60	104.49	107.00
22	C	510	CLA	CHD-C4C-C3C	-3.60	119.63	124.87
22	B	617	CLA	C4A-NA-C1A	3.59	108.32	106.71
22	a	409	CLA	CMB-C2B-C3B	3.59	131.53	124.80
26	d	405	PL9	C7-C8-C9	-3.59	120.82	126.79
25	b	622	LMG	O6-C1-O1	3.59	118.41	109.94
22	B	617	CLA	CMD-C2D-C3D	3.58	131.51	124.80
22	b	608	CLA	O2D-CGD-CBD	3.58	117.52	111.25
22	b	606	CLA	C4-C3-C5	3.58	121.45	115.29
27	D	411	LHG	O8-C23-O10	-3.58	114.42	123.56
22	B	616	CLA	C1C-C2C-C3C	-3.57	103.16	106.95
22	b	608	CLA	O2D-CGD-O1D	-3.57	116.78	123.83
22	b	614	CLA	C1C-C2C-C3C	-3.57	103.17	106.95
22	C	514	CLA	CHD-C4C-NC	3.56	129.82	124.20
22	c	903	CLA	CHD-C4C-NC	3.56	129.81	124.20
22	D	403	CLA	CHD-C4C-C3C	-3.56	119.68	124.87
22	B	614	CLA	O2D-CGD-O1D	-3.56	116.81	123.83
23	A	407	PHO	C2B-C1B-NB	3.56	115.18	109.79
22	c	904	CLA	CHD-C4C-C3C	-3.55	119.69	124.87
22	d	402	CLA	C4-C3-C5	3.55	121.40	115.29
36	E	102	HEM	CAD-CBD-CGD	3.55	118.73	112.66
22	B	615	CLA	C4-C3-C5	3.55	121.40	115.29
22	b	608	CLA	CHD-C4C-C3C	-3.55	119.70	124.87
22	a	409	CLA	C1-C2-C3	-3.55	119.91	126.04
35	C	519	DGD	O6D-C1D-O3G	-3.53	101.59	109.94
35	c	918	DGD	O2G-C1B-C2B	3.53	119.22	111.51
22	B	615	CLA	C1-O2A-CGA	3.53	126.19	116.54
22	b	605	CLA	CMD-C2D-C3D	3.53	131.41	124.80
22	b	613	CLA	C4-C3-C5	3.52	121.36	115.29
27	d	401	LHG	O7-C7-C8	3.52	119.19	111.51
22	c	904	CLA	O2A-CGA-CBA	3.52	123.22	111.93
22	b	603	CLA	C2C-C1C-NC	3.52	113.27	109.97
24	c	916	BCR	C33-C5-C6	-3.51	120.60	124.51
22	b	605	CLA	O2D-CGD-O1D	-3.51	116.90	123.83
22	c	908	CLA	C4-C3-C5	3.51	121.33	115.29
22	D	403	CLA	CMD-C2D-C3D	3.50	131.37	124.80
35	h	102	DGD	O2G-C1B-C2B	3.50	119.16	111.51
29	a	419	LMT	C2'-C3'-C4'	3.50	117.68	109.67
22	c	906	CLA	CMB-C2B-C3B	3.50	131.37	124.80
22	C	514	CLA	CMC-C2C-C1C	3.50	130.36	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	414	SQD	C1-O5-C5	-3.50	106.80	113.70
22	D	403	CLA	O2D-CGD-CBD	3.50	117.38	111.25
27	L	101	LHG	O7-C7-C8	3.50	119.14	111.51
22	c	910	CLA	C2A-C1A-CHA	-3.49	117.75	123.86
24	K	101	BCR	C24-C23-C22	-3.49	120.96	126.21
22	A	405	CLA	CMD-C2D-C3D	3.49	131.35	124.80
22	a	409	CLA	CMC-C2C-C1C	3.49	130.34	125.03
22	b	609	CLA	O2D-CGD-O1D	-3.49	116.94	123.83
22	C	507	CLA	CAC-C3C-C4C	3.48	129.37	124.82
35	h	102	DGD	O1G-C1A-O1A	-3.48	114.66	123.56
22	b	615	CLA	C1C-C2C-C3C	-3.47	103.27	106.95
22	c	912	CLA	O2D-CGD-CBD	3.47	117.32	111.25
34	v	203	HTG	O4-C4-C3	-3.47	102.30	110.34
26	D	406	PL9	C53-C6-C1	3.46	122.13	114.98
22	C	505	CLA	CHD-C4C-NC	3.46	129.66	124.20
22	b	610	CLA	CHD-C4C-NC	3.46	129.65	124.20
35	C	518	DGD	O5D-C6D-C5D	3.46	115.73	109.14
34	C	523	HTG	C1-S1-C1'	3.45	112.50	100.42
25	b	622	LMG	C4-C3-C2	3.45	116.88	110.82
22	b	617	CLA	C1C-C2C-C3C	-3.45	103.30	106.95
24	y	101	BCR	C21-C20-C19	-3.44	112.96	123.31
22	B	611	CLA	O2A-CGA-O1A	-3.44	114.78	123.56
22	B	613	CLA	C2A-C1A-CHA	-3.44	117.85	123.86
22	c	906	CLA	C1-O2A-CGA	3.43	125.92	116.54
22	c	908	CLA	CMB-C2B-C3B	3.43	131.24	124.80
29	E	101	LMT	O5'-C5'-C6'	3.43	114.98	106.43
22	B	607	CLA	C1-C2-C3	-3.43	120.11	126.04
22	B	606	CLA	C3C-C4C-NC	3.42	114.41	110.57
22	C	513	CLA	C2C-C1C-NC	3.42	113.17	109.97
22	C	504	CLA	C1C-C2C-C3C	-3.42	103.33	106.95
22	C	514	CLA	O2A-CGA-CBA	3.41	122.88	111.93
25	A	410	LMG	O7-C10-C11	3.40	118.93	111.51
22	C	513	CLA	O1D-CGD-CBD	-3.40	117.44	124.48
22	b	616	CLA	CHD-C4C-NC	3.39	129.55	124.20
22	c	911	CLA	CMD-C2D-C3D	3.39	131.16	124.80
22	C	513	CLA	O2D-CGD-O1D	-3.39	117.14	123.83
22	b	617	CLA	CMD-C2D-C3D	3.39	131.16	124.80
26	D	406	PL9	C20-C19-C21	3.39	121.12	115.29
22	b	613	CLA	C4C-C3C-C2C	-3.39	101.99	106.89
22	C	506	CLA	O2D-CGD-CBD	3.38	117.17	111.25
22	b	615	CLA	CAC-C3C-C4C	3.38	129.24	124.82
22	b	605	CLA	C3C-C4C-NC	3.38	114.36	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	406	CLA	C4A-NA-C1A	3.38	108.22	106.71
35	C	518	DGD	O2G-C1B-C2B	3.37	118.87	111.51
22	B	615	CLA	CMD-C2D-C3D	3.37	131.12	124.80
22	C	502	CLA	CAC-C3C-C4C	3.37	129.22	124.82
22	C	504	CLA	C2C-C1C-NC	3.37	113.12	109.97
25	b	622	LMG	O6-C5-C6	3.37	114.82	106.43
22	c	908	CLA	CBC-CAC-C3C	-3.36	103.09	112.43
22	B	606	CLA	O2D-CGD-CBD	3.36	117.13	111.25
22	c	907	CLA	C3B-C4B-NB	3.36	113.55	109.21
22	a	409	CLA	CHD-C4C-NC	3.36	129.49	124.20
22	b	603	CLA	CHD-C4C-C3C	-3.36	119.98	124.87
22	b	617	CLA	C4C-C3C-C2C	-3.35	102.04	106.89
22	b	609	CLA	C3C-C4C-NC	3.35	114.33	110.57
22	D	401	CLA	CMC-C2C-C1C	3.35	130.12	125.03
22	B	603	CLA	OBD-CAD-CBD	3.35	130.83	125.91
27	D	411	LHG	O8-C23-C24	3.35	122.67	111.93
22	B	607	CLA	CHC-C1C-NC	-3.35	119.13	124.20
22	b	602	CLA	O2A-CGA-CBA	3.34	122.66	111.93
24	D	405	BCR	C29-C30-C25	3.34	115.65	110.48
22	B	603	CLA	CHC-C1C-NC	-3.34	119.14	124.20
22	b	614	CLA	C4-C3-C5	3.34	121.03	115.29
29	Z	101	LMT	C3B-C4B-C5B	3.33	116.22	110.23
23	A	407	PHO	CMB-C2B-C1B	3.33	130.23	125.06
22	B	615	CLA	CED-O2D-CGD	3.33	123.56	115.95
22	B	608	CLA	CAC-C3C-C4C	3.33	129.17	124.82
22	b	614	CLA	CAA-CBA-CGA	-3.33	103.45	113.26
37	H	101	RRX	C7-C8-C9	-3.33	121.21	126.21
22	b	609	CLA	C1C-C2C-C3C	-3.33	103.43	106.95
27	D	409	LHG	O8-C23-C24	3.32	122.60	111.93
22	c	912	CLA	O2A-CGA-O1A	-3.32	115.08	123.56
29	f	102	LMT	O1'-C1'-C2'	3.32	113.55	108.26
22	B	602	CLA	C1-O2A-CGA	3.32	125.61	116.54
35	C	519	DGD	O2G-C1B-C2B	3.32	118.75	111.51
24	y	101	BCR	C24-C23-C22	-3.32	121.23	126.21
22	c	912	CLA	C2C-C1C-NC	3.32	113.08	109.97
22	c	914	CLA	O2D-CGD-CBD	3.31	117.05	111.25
22	c	905	CLA	O2D-CGD-CBD	3.31	117.04	111.25
22	a	408	CLA	CBC-CAC-C3C	-3.30	103.25	112.43
22	C	510	CLA	CHB-C4A-NA	3.30	129.08	124.51
22	b	604	CLA	O2A-CGA-O1A	-3.30	115.12	123.56
23	D	402	PHO	CMB-C2B-C1B	3.30	130.18	125.06
22	C	513	CLA	CHD-C4C-NC	3.30	129.40	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	C1C-C2C-C3C	-3.30	103.46	106.95
22	b	617	CLA	O1D-CGD-CBD	-3.29	117.65	124.48
22	A	406	CLA	O2D-CGD-CBD	3.29	117.02	111.25
22	C	508	CLA	CHD-C4C-NC	3.29	129.39	124.20
22	B	607	CLA	C3C-C4C-NC	3.29	114.26	110.57
28	D	408	SQD	O7-S-C6	3.29	110.85	106.94
22	C	507	CLA	CMC-C2C-C1C	3.29	130.03	125.03
22	b	613	CLA	C3C-C4C-NC	3.28	114.25	110.57
35	C	519	DGD	O1G-C1A-C2A	3.28	122.47	111.93
35	D	407	DGD	C3D-C4D-C5D	3.28	114.88	109.74
22	B	612	CLA	C2A-C1A-CHA	-3.28	118.13	123.86
22	B	605	CLA	CHD-C4C-NC	3.27	129.36	124.20
28	a	418	SQD	O48-C23-C24	3.27	122.43	111.93
22	B	603	CLA	C3B-C4B-NB	3.27	113.44	109.21
22	d	402	CLA	O2A-CGA-O1A	-3.27	115.20	123.56
22	b	611	CLA	C3C-C4C-NC	3.27	114.24	110.57
22	b	606	CLA	C1-C2-C3	-3.27	120.39	126.04
22	C	507	CLA	CMD-C2D-C3D	3.26	130.92	124.80
22	d	403	CLA	CHD-C4C-C3C	-3.26	120.11	124.87
22	B	602	CLA	CHD-C4C-C3C	-3.26	120.11	124.87
22	b	616	CLA	CED-O2D-CGD	3.26	123.40	115.95
22	C	514	CLA	CHC-C1C-NC	-3.26	119.26	124.20
22	b	612	CLA	C7-C6-C5	-3.25	104.51	113.25
23	a	411	PHO	C3C-C4C-NC	3.24	115.32	110.28
22	c	907	CLA	CHD-C4C-NC	3.24	129.31	124.20
22	C	504	CLA	CMB-C2B-C3B	3.24	130.87	124.80
22	A	408	CLA	O2D-CGD-O1D	-3.24	117.44	123.83
23	a	411	PHO	CMB-C2B-C1B	3.24	130.08	125.06
28	D	408	SQD	O8-S-C6	3.23	110.89	105.74
22	d	402	CLA	C3B-C4B-NB	3.23	113.39	109.21
22	d	403	CLA	O2D-CGD-O1D	-3.23	117.45	123.83
34	D	415	HTG	O5-C1-S1	3.23	118.01	109.90
24	y	101	BCR	C38-C26-C25	-3.22	120.92	124.51
28	f	101	SQD	O8-S-C6	3.22	110.97	105.77
24	b	619	BCR	C29-C30-C25	3.22	115.46	110.48
22	D	403	CLA	CMC-C2C-C1C	3.22	129.93	125.03
22	c	902	CLA	C4-C3-C5	3.21	120.82	115.29
22	B	617	CLA	C3B-C4B-NB	3.21	113.36	109.21
22	C	509	CLA	O2A-CGA-O1A	-3.21	115.37	123.56
22	b	603	CLA	C4-C3-C5	3.20	120.80	115.29
22	b	607	CLA	C3C-C4C-NC	3.20	114.16	110.57
22	a	407	CLA	O2D-CGD-O1D	-3.20	117.51	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	C1C-C2C-C3C	-3.20	103.56	106.95
22	C	504	CLA	C3C-C4C-NC	3.20	114.16	110.57
22	B	615	CLA	O2A-CGA-CBA	3.19	122.18	111.93
22	b	606	CLA	C3C-C4C-NC	3.18	114.14	110.57
22	B	607	CLA	CHD-C4C-NC	3.18	129.21	124.20
37	h	101	RRX	C7-C8-C9	-3.17	121.44	126.21
28	D	408	SQD	O6-C44-C45	3.17	114.96	108.82
22	B	612	CLA	O2D-CGD-CBD	3.17	116.81	111.25
22	b	610	CLA	CBC-CAC-C3C	-3.17	103.62	112.43
22	C	512	CLA	O2D-CGD-O1D	-3.17	117.57	123.83
22	b	603	CLA	C1-C2-C3	-3.17	120.56	126.04
22	c	912	CLA	C4-C3-C5	3.17	120.75	115.29
22	B	611	CLA	CHD-C4C-NC	3.17	129.19	124.20
22	B	609	CLA	CHD-C4C-NC	3.16	129.19	124.20
22	C	503	CLA	CAC-C3C-C4C	3.16	128.95	124.82
22	B	608	CLA	C3B-C4B-NB	3.16	113.30	109.21
22	a	408	CLA	CMB-C2B-C3B	3.16	130.72	124.80
26	a	415	PL9	C35-C34-C36	3.16	120.73	115.29
28	b	621	SQD	O5-C1-C2	-3.16	103.61	110.35
22	b	613	CLA	C11-C12-C13	-3.16	105.92	115.77
22	b	609	CLA	CMB-C2B-C3B	3.15	130.71	124.80
22	b	606	CLA	CMD-C2D-C3D	3.15	130.71	124.80
22	b	605	CLA	CAC-C3C-C4C	3.15	128.93	124.82
22	b	616	CLA	O2D-CGD-O1D	-3.15	117.61	123.83
34	V	203	HTG	O5-C1-S1	3.15	117.80	109.90
34	v	203	HTG	O3-C3-C2	3.14	117.64	110.34
22	B	607	CLA	OBD-CAD-C3D	-3.14	122.47	128.04
22	c	905	CLA	CHD-C4C-NC	3.14	129.15	124.20
22	a	412	CLA	C1-C2-C3	-3.14	120.61	126.04
27	a	423	LHG	O8-C23-C24	3.14	122.00	111.93
22	A	405	CLA	CHD-C4C-C3C	-3.13	120.30	124.87
22	B	616	CLA	CMD-C2D-C3D	3.13	130.67	124.80
22	c	905	CLA	C5-C3-C2	-3.13	114.68	121.11
22	B	603	CLA	OBD-CAD-C3D	-3.13	122.50	128.04
23	D	402	PHO	C2C-C1C-NC	3.13	114.53	109.79
24	d	404	BCR	C21-C20-C19	-3.13	113.90	123.31
22	B	617	CLA	CMB-C2B-C3B	3.13	130.66	124.80
22	c	911	CLA	CMB-C2B-C3B	3.12	130.66	124.80
22	c	910	CLA	CMC-C2C-C1C	3.12	129.78	125.03
22	D	403	CLA	CHC-C1C-NC	-3.12	119.47	124.20
22	B	603	CLA	C1-C2-C3	-3.12	120.65	126.04
22	B	615	CLA	O1D-CGD-CBD	-3.12	118.02	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	t	101	LMT	C1'-C2'-C3'	-3.12	103.48	109.98
36	e	101	HEM	C1D-C2D-C3D	-3.11	104.83	107.00
22	C	504	CLA	C4-C3-C5	3.11	120.65	115.29
22	B	609	CLA	C3C-C4C-NC	3.11	114.06	110.57
25	c	920	LMG	O7-C10-C11	3.11	118.29	111.51
25	C	520	LMG	O8-C28-O10	-3.11	115.62	123.56
22	C	509	CLA	CMD-C2D-C3D	3.10	130.62	124.80
35	c	919	DGD	O1G-C1A-C2A	3.10	121.90	111.93
22	b	604	CLA	C2A-C3A-C4A	-3.10	96.86	101.87
24	B	620	BCR	C38-C26-C25	-3.10	121.06	124.51
36	e	101	HEM	CAD-CBD-CGD	3.10	117.96	112.66
22	b	604	CLA	CMB-C2B-C3B	3.10	130.61	124.80
35	c	919	DGD	O2G-C1B-O1B	-3.10	116.10	123.71
22	c	910	CLA	O2A-CGA-CBA	3.10	121.88	111.93
24	d	404	BCR	C37-C22-C21	-3.10	118.58	122.92
22	B	609	CLA	CMD-C2D-C3D	3.10	130.61	124.80
22	a	409	CLA	O2D-CGD-O1D	-3.09	117.72	123.83
22	b	612	CLA	CAC-C3C-C4C	3.09	128.86	124.82
22	b	602	CLA	CMD-C2D-C3D	3.09	130.60	124.80
28	b	621	SQD	O6-C1-C2	3.09	113.19	108.26
37	h	101	RRX	C11-C10-C9	-3.09	122.91	127.31
22	C	506	CLA	CMD-C2D-C3D	3.09	130.59	124.80
23	a	411	PHO	CAC-C3C-C4C	3.08	128.59	125.22
22	c	905	CLA	C4-C3-C5	3.08	120.60	115.29
29	t	101	LMT	O5'-C5'-C4'	3.08	115.30	109.68
24	B	618	BCR	C2-C3-C4	-3.08	104.43	111.37
22	b	602	CLA	CHD-C4C-NC	3.08	129.05	124.20
22	c	904	CLA	CAC-C3C-C4C	3.08	128.84	124.82
22	c	910	CLA	C1-O2A-CGA	3.07	124.94	116.54
22	c	904	CLA	C7-C6-C5	-3.07	105.00	113.25
22	a	409	CLA	C2A-C1A-CHA	-3.07	118.49	123.86
22	B	603	CLA	O2A-CGA-CBA	3.07	121.78	111.93
22	D	401	CLA	C3B-C4B-NB	3.07	113.17	109.21
22	B	617	CLA	O2A-CGA-O1A	-3.07	115.72	123.56
24	C	516	BCR	C7-C8-C9	-3.06	121.61	126.21
22	b	609	CLA	C4C-C3C-C2C	-3.06	102.45	106.89
27	d	407	LHG	O8-C23-C24	3.06	121.76	111.93
22	B	602	CLA	C1C-C2C-C3C	-3.06	103.71	106.95
22	a	408	CLA	CHB-C4A-NA	3.06	128.74	124.51
22	C	511	CLA	O2A-CGA-O1A	-3.05	115.75	123.56
22	c	910	CLA	C3B-C4B-NB	3.05	113.16	109.21
23	a	410	PHO	C2D-C1D-ND	3.05	114.41	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	C4-C3-C5	3.05	120.54	115.29
22	b	604	CLA	O2D-CGD-O1D	-3.05	117.81	123.83
36	E	102	HEM	C1D-C2D-C3D	-3.04	104.88	107.00
23	a	411	PHO	C4D-ND-C1D	-3.04	101.27	106.79
22	b	609	CLA	C4-C3-C5	3.04	120.52	115.29
22	B	610	CLA	CMC-C2C-C1C	3.04	129.65	125.03
22	D	403	CLA	O2D-CGD-O1D	-3.03	117.84	123.83
22	C	513	CLA	C4-C3-C5	3.03	120.51	115.29
22	b	615	CLA	C4-C3-C5	3.03	120.51	115.29
22	C	505	CLA	O2D-CGD-O1D	-3.03	117.85	123.83
22	A	405	CLA	O2A-CGA-O1A	-3.03	115.83	123.56
34	v	203	HTG	O5-C1-S1	3.03	117.50	109.90
22	b	610	CLA	CHC-C1C-NC	-3.03	119.61	124.20
23	D	402	PHO	C4D-ND-C1D	-3.02	101.30	106.79
22	c	911	CLA	CAC-C3C-C4C	3.02	128.77	124.82
24	B	620	BCR	C7-C8-C9	-3.02	121.67	126.21
24	C	515	BCR	C7-C8-C9	-3.02	121.67	126.21
22	B	605	CLA	O2D-CGD-O1D	-3.02	117.86	123.83
26	A	411	PL9	C22-C23-C24	-3.02	120.25	127.67
24	B	620	BCR	C32-C1-C6	-3.02	105.42	110.30
37	H	101	RRX	C10-C11-C12	-3.02	114.22	123.31
22	c	911	CLA	C2C-C1C-NC	3.02	112.80	109.97
22	b	613	CLA	O2A-CGA-CBA	3.02	121.62	111.93
22	c	904	CLA	OBD-CAD-C3D	-3.02	122.69	128.04
37	H	101	RRX	C16-C17-C18	-3.01	123.01	127.31
26	A	411	PL9	C32-C33-C34	-3.01	120.27	127.67
22	C	510	CLA	O2A-CGA-CBA	3.01	121.61	111.93
22	A	405	CLA	C7-C6-C5	-3.01	105.15	113.25
22	a	412	CLA	C3B-C4B-NB	3.01	113.10	109.21
24	D	405	BCR	C33-C5-C6	-3.01	121.16	124.51
22	c	909	CLA	CHD-C4C-NC	3.01	128.95	124.20
25	B	621	LMG	O8-C28-C29	3.01	121.59	111.93
22	a	412	CLA	OBD-CAD-C3D	-3.01	122.71	128.04
23	D	402	PHO	C2B-C1B-NB	3.01	114.35	109.79
35	C	518	DGD	O6E-C1E-C2E	3.01	116.75	110.35
22	C	511	CLA	CAC-C3C-C4C	3.00	128.75	124.82
22	b	610	CLA	C1-C2-C3	-3.00	120.86	126.04
24	y	101	BCR	C16-C15-C14	-3.00	117.21	123.51
22	C	509	CLA	CHB-C4A-NA	3.00	128.66	124.51
22	b	612	CLA	C3B-C4B-NB	3.00	113.08	109.21
24	B	619	BCR	C28-C27-C26	-2.99	108.78	113.99
22	B	610	CLA	CBC-CAC-C3C	-2.99	104.12	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	516	BCR	C11-C10-C9	-2.99	123.04	127.31
22	C	504	CLA	C1D-CHD-C4C	-2.99	118.40	122.48
22	D	404	CLA	O2D-CGD-O1D	-2.99	117.94	123.83
24	D	405	BCR	C38-C26-C25	-2.98	121.19	124.51
26	A	411	PL9	C45-C44-C46	2.98	120.42	115.29
34	b	632	HTG	C3-C4-C5	2.98	115.59	110.23
22	b	607	CLA	C3B-C4B-NB	2.98	113.06	109.21
22	b	608	CLA	C4-C3-C5	2.97	120.41	115.29
24	Y	101	BCR	C37-C22-C23	2.97	122.80	118.09
22	b	606	CLA	CMC-C2C-C1C	2.97	129.55	125.03
28	A	413	SQD	C1-O5-C5	-2.96	107.86	113.70
35	H	102	DGD	O2G-C1B-C2B	2.96	117.98	111.51
28	A	413	SQD	O3-C3-C2	2.96	117.22	110.34
22	A	405	CLA	CMB-C2B-C3B	2.96	130.35	124.80
24	c	915	BCR	C7-C8-C9	-2.96	121.77	126.21
22	C	510	CLA	C1-C2-C3	-2.96	120.93	126.04
22	C	510	CLA	C3B-C4B-NB	2.96	113.03	109.21
22	c	909	CLA	O2D-CGD-O1D	-2.95	118.00	123.83
22	C	511	CLA	CHD-C4C-NC	2.95	128.86	124.20
34	b	623	HTG	C2'-C1'-S1	-2.95	102.86	112.40
22	B	605	CLA	C6-C5-C3	-2.95	105.92	113.01
24	c	916	BCR	C11-C10-C9	-2.95	123.10	127.31
28	l	101	SQD	O48-C23-C24	2.95	121.39	111.93
23	a	411	PHO	C4A-NA-C1A	2.95	110.52	108.14
34	c	922	HTG	C1-O5-C5	2.94	118.13	112.58
22	B	610	CLA	C1-C2-C3	-2.94	120.95	126.04
34	b	632	HTG	O5-C1-S1	2.94	117.29	109.90
22	B	617	CLA	CBC-CAC-C3C	-2.94	104.28	112.43
28	b	621	SQD	O48-C23-C24	2.94	121.36	111.93
24	c	916	BCR	C38-C26-C25	-2.93	121.24	124.51
23	A	407	PHO	C3C-C4C-NC	2.93	114.84	110.28
22	B	614	CLA	O2D-CGD-CBD	2.93	116.39	111.25
22	C	509	CLA	CHD-C4C-NC	2.93	128.82	124.20
22	a	407	CLA	CMB-C2B-C3B	2.93	130.29	124.80
28	C	501	SQD	O48-C23-O10	-2.93	116.08	123.56
27	D	409	LHG	C5-O7-C7	-2.93	110.52	117.82
22	C	512	CLA	C3B-C4B-NB	2.92	112.99	109.21
22	c	914	CLA	CHC-C1C-NC	-2.92	119.77	124.20
27	a	416	LHG	O8-C23-C24	2.92	121.32	111.93
22	a	412	CLA	CHD-C4C-NC	2.92	128.81	124.20
22	B	607	CLA	CMB-C2B-C3B	2.92	130.27	124.80
37	h	101	RRX	C16-C17-C18	-2.91	123.15	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	C4-C3-C5	2.91	120.30	115.29
22	B	615	CLA	C3C-C4C-NC	2.91	113.84	110.57
22	C	506	CLA	C1-O2A-CGA	2.91	124.49	116.54
22	a	412	CLA	CBC-CAC-C3C	-2.91	104.35	112.43
26	D	406	PL9	C10-C9-C11	2.91	120.29	115.29
22	C	510	CLA	O2D-CGD-O1D	-2.91	118.09	123.83
22	b	615	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
22	c	905	CLA	CAC-C3C-C4C	2.90	128.62	124.82
29	A	414	LMT	C1'-C2'-C3'	-2.90	103.92	109.98
22	A	405	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
22	C	502	CLA	CMD-C2D-C3D	2.90	130.23	124.80
24	d	404	BCR	C35-C13-C14	-2.90	118.87	122.92
28	a	414	SQD	O48-C23-C24	2.90	121.23	111.93
22	C	504	CLA	CMD-C2D-C3D	2.90	130.23	124.80
22	b	613	CLA	CED-O2D-CGD	2.89	122.56	115.95
22	b	617	CLA	CAC-C3C-C4C	2.89	128.60	124.82
22	b	605	CLA	C4C-C3C-C2C	-2.89	102.70	106.89
22	D	401	CLA	O2D-CGD-O1D	-2.89	118.12	123.83
22	c	903	CLA	CMD-C2D-C3D	2.89	130.22	124.80
22	c	914	CLA	C1-O2A-CGA	2.89	124.43	116.54
24	K	101	BCR	C33-C5-C6	-2.89	121.30	124.51
25	C	531	LMG	O8-C28-C29	2.89	121.19	111.93
22	c	904	CLA	OBD-CAD-CBD	2.88	130.15	125.91
24	B	620	BCR	C23-C24-C25	-2.88	119.20	127.28
22	B	606	CLA	C4-C3-C5	2.88	120.25	115.29
25	J	101	LMG	O8-C28-O10	-2.88	116.20	123.56
23	a	411	PHO	C2C-C1C-NC	2.88	114.16	109.79
22	B	603	CLA	CHD-C4C-NC	2.88	128.74	124.20
25	j	101	LMG	C7-O1-C1	-2.88	107.96	113.75
22	d	402	CLA	C2A-C1A-CHA	-2.88	118.82	123.86
22	B	608	CLA	CMD-C2D-C3D	2.88	130.19	124.80
24	d	404	BCR	C37-C22-C23	2.88	122.65	118.09
27	D	410	LHG	O8-C6-C5	-2.87	100.04	108.43
22	b	609	CLA	O2A-CGA-O1A	-2.87	116.22	123.56
22	a	407	CLA	CHD-C4C-C3C	-2.87	120.68	124.87
22	C	503	CLA	CHD-C4C-NC	2.87	128.73	124.20
25	A	410	LMG	O8-C28-C29	2.87	121.15	111.93
29	t	101	LMT	O1'-C1'-C2'	2.87	112.83	108.26
35	C	518	DGD	O3G-C1D-C2D	2.87	112.83	108.26
22	D	404	CLA	C1-O2A-CGA	2.87	124.38	116.54
22	B	606	CLA	CHD-C4C-NC	2.87	128.72	124.20
22	c	913	CLA	CMB-C2B-C3B	2.87	130.18	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	514	CLA	C2C-C1C-NC	2.86	112.65	109.97
22	A	406	CLA	CAC-C3C-C4C	2.86	128.56	124.82
22	B	602	CLA	CMC-C2C-C1C	2.86	129.38	125.03
22	c	913	CLA	CHD-C4C-NC	2.86	128.71	124.20
22	B	609	CLA	CHB-C4A-NA	2.86	128.46	124.51
22	b	609	CLA	CAC-C3C-C4C	2.86	128.56	124.82
22	C	507	CLA	C3C-C4C-NC	2.86	113.77	110.57
22	c	908	CLA	CED-O2D-CGD	-2.85	109.43	115.95
22	c	906	CLA	CHD-C4C-NC	2.85	128.70	124.20
22	A	408	CLA	O2A-CGA-O1A	-2.85	116.27	123.56
24	k	101	BCR	C32-C1-C6	-2.85	105.69	110.30
24	Y	101	BCR	C24-C23-C22	-2.85	121.93	126.21
22	D	403	CLA	C4-C3-C5	2.85	120.19	115.29
26	A	411	PL9	C20-C19-C21	2.84	120.19	115.29
26	d	405	PL9	C53-C6-C1	2.84	120.85	114.98
22	b	615	CLA	C1-O2A-CGA	2.84	124.30	116.54
22	B	614	CLA	CMD-C2D-C3D	2.84	130.12	124.80
22	C	508	CLA	CMB-C2B-C3B	2.84	130.12	124.80
39	V	202	HEC	CMB-C2B-C1B	-2.84	124.10	128.46
26	A	411	PL9	C37-C36-C34	-2.84	103.56	112.98
34	B	626	HTG	O5-C1-C2	-2.84	106.75	110.31
24	b	618	BCR	C11-C10-C9	-2.83	123.26	127.31
22	B	617	CLA	CAC-C3C-C4C	2.83	128.52	124.82
24	A	409	BCR	C38-C26-C25	-2.83	121.36	124.51
24	D	405	BCR	C16-C17-C18	-2.83	123.27	127.31
24	D	405	BCR	C10-C11-C12	-2.83	114.80	123.31
22	a	409	CLA	C1-O2A-CGA	2.83	124.27	116.54
27	A	412	LHG	O8-C23-C24	2.82	121.00	111.93
22	B	610	CLA	CMD-C2D-C3D	2.82	130.09	124.80
22	C	502	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
22	B	605	CLA	CGD-CBD-CAD	-2.82	101.60	110.73
22	b	615	CLA	CED-O2D-CGD	2.81	122.38	115.95
22	B	612	CLA	C7-C6-C5	-2.81	105.69	113.25
25	J	101	LMG	C7-O1-C1	-2.81	108.10	113.75
23	a	411	PHO	C4D-C3D-CAD	2.81	110.50	105.39
26	a	415	PL9	C42-C43-C44	-2.81	120.78	127.67
22	C	510	CLA	CAC-C3C-C4C	2.81	128.49	124.82
22	c	911	CLA	O2A-CGA-O1A	-2.81	116.39	123.56
22	C	509	CLA	C5-C3-C2	-2.81	115.35	121.11
22	c	910	CLA	CHD-C4C-C3C	-2.80	120.78	124.87
29	Z	101	LMT	O5B-C5B-C4B	2.80	114.80	109.68
22	b	604	CLA	C1D-CHD-C4C	-2.80	118.65	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	603	CLA	O2A-CGA-CBA	2.80	120.93	111.93
22	b	611	CLA	CHD-C4C-NC	2.80	128.62	124.20
22	B	617	CLA	O2A-C1-C2	2.80	115.99	108.64
23	a	410	PHO	C7-C6-C5	-2.80	105.73	113.25
22	b	612	CLA	CMC-C2C-C1C	2.80	129.29	125.03
22	b	603	CLA	OBD-CAD-C3D	-2.80	123.08	128.04
34	D	415	HTG	C3-C4-C5	2.80	115.25	110.23
26	a	415	PL9	C20-C19-C21	2.80	120.10	115.29
22	B	603	CLA	C3C-C4C-NC	2.79	113.70	110.57
22	B	608	CLA	CED-O2D-CGD	2.79	122.33	115.95
22	c	903	CLA	CMB-C2B-C3B	2.79	130.04	124.80
24	c	916	BCR	C35-C13-C14	-2.79	119.01	122.92
25	B	621	LMG	C3-C4-C5	2.79	115.24	110.23
22	B	608	CLA	CHD-C4C-C3C	-2.79	120.80	124.87
22	A	408	CLA	C3B-C4B-NB	2.79	112.81	109.21
22	c	912	CLA	CHD-C4C-C3C	-2.79	120.81	124.87
22	B	604	CLA	C2A-C3A-C4A	-2.78	97.37	101.87
22	B	612	CLA	CHD-C4C-NC	2.78	128.59	124.20
25	b	622	LMG	O8-C28-C29	2.78	120.86	111.93
34	C	521	HTG	C1-O5-C5	2.78	117.82	112.58
22	B	608	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
22	C	513	CLA	CMD-C2D-C3D	2.78	130.01	124.80
22	D	401	CLA	C1-C2-C3	-2.78	121.24	126.04
22	c	913	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
22	a	412	CLA	C2A-C1A-CHA	-2.77	119.02	123.86
24	b	620	BCR	C24-C23-C22	-2.77	122.05	126.21
22	b	616	CLA	CMB-C2B-C3B	2.77	129.99	124.80
22	C	504	CLA	C4C-C3C-C2C	-2.77	102.88	106.89
35	D	407	DGD	O1G-C1A-C2A	2.77	120.81	111.93
22	b	606	CLA	C4C-C3C-C2C	-2.76	102.89	106.89
26	A	411	PL9	C25-C24-C26	2.76	120.05	115.29
28	C	501	SQD	O5-C1-C2	-2.76	104.46	110.35
22	a	409	CLA	CAC-C3C-C4C	2.76	128.43	124.82
22	B	604	CLA	CMB-C2B-C3B	2.76	129.97	124.80
22	D	403	CLA	CMB-C2B-C3B	2.76	129.97	124.80
22	B	616	CLA	O2A-CGA-O1A	-2.76	116.52	123.56
22	C	504	CLA	OBD-CAD-C3D	-2.75	123.16	128.04
28	b	621	SQD	O48-C23-O10	-2.75	116.54	123.56
25	i	101	LMG	O6-C1-C2	-2.75	104.49	110.35
22	b	607	CLA	C14-C13-C12	-2.75	101.29	111.30
22	C	505	CLA	C7-C6-C5	-2.75	105.86	113.25
36	E	102	HEM	CMC-C2C-C3C	2.75	129.95	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	606	CLA	OBD-CAD-C3D	-2.75	123.17	128.04
22	C	502	CLA	CHD-C4C-NC	2.75	128.53	124.20
22	c	903	CLA	C6-C5-C3	-2.74	106.41	113.01
22	B	609	CLA	C11-C12-C13	-2.74	107.21	115.77
34	b	627	HTG	C3-C4-C5	2.74	115.16	110.23
27	L	101	LHG	C6-C5-C4	-2.74	105.25	111.79
22	c	909	CLA	C1-C2-C3	-2.74	121.30	126.04
29	c	931	LMT	O5'-C5'-C6'	2.74	113.26	106.43
34	B	626	HTG	C3-C4-C5	2.74	115.15	110.23
22	b	616	CLA	CMC-C2C-C1C	2.74	129.20	125.03
22	c	903	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
23	A	407	PHO	C4A-NA-C1A	2.73	110.35	108.14
22	b	604	CLA	C3C-C4C-NC	2.73	113.63	110.57
22	b	606	CLA	CAC-C3C-C4C	2.73	128.39	124.82
27	d	401	LHG	O8-C23-C24	2.73	120.70	111.93
22	B	607	CLA	CBC-CAC-C3C	-2.73	104.85	112.43
25	i	101	LMG	O8-C28-C29	2.73	120.69	111.93
34	D	415	HTG	C1-C2-C3	-2.73	105.20	110.59
22	B	615	CLA	CHC-C1C-NC	-2.73	120.07	124.20
22	c	906	CLA	O2D-CGD-O1D	-2.72	118.45	123.83
22	B	604	CLA	CHC-C1C-NC	-2.72	120.07	124.20
22	c	907	CLA	O2D-CGD-O1D	-2.72	118.45	123.83
24	C	516	BCR	C37-C22-C23	2.72	122.40	118.09
24	Y	101	BCR	C1-C6-C7	2.72	123.51	115.78
22	c	911	CLA	CBC-CAC-C3C	-2.72	104.88	112.43
24	b	620	BCR	C3-C4-C5	-2.72	109.26	113.99
22	a	407	CLA	O2A-CGA-O1A	-2.72	116.61	123.56
39	V	202	HEC	C1D-C2D-C3D	-2.72	105.11	107.00
27	D	411	LHG	O7-C7-C8	2.72	117.44	111.51
24	d	404	BCR	C30-C25-C24	2.72	123.50	115.78
22	A	405	CLA	CHC-C1C-NC	-2.71	120.08	124.20
22	C	514	CLA	O2A-CGA-O1A	-2.71	116.62	123.56
22	B	616	CLA	C6-C7-C8	-2.71	107.30	115.77
22	C	513	CLA	C1-C2-C3	-2.71	121.35	126.04
22	b	616	CLA	O2A-CGA-O1A	-2.71	116.63	123.56
22	B	613	CLA	O2D-CGD-CBD	2.71	116.00	111.25
22	a	408	CLA	CMD-C2D-C3D	2.71	129.88	124.80
28	a	414	SQD	O9-S-O7	-2.71	104.57	113.95
24	D	405	BCR	C29-C28-C27	-2.71	105.27	111.37
22	A	406	CLA	O2A-CGA-O1A	-2.71	116.64	123.56
22	b	617	CLA	CMB-C2B-C3B	2.71	129.88	124.80
24	D	405	BCR	C38-C26-C27	2.71	118.64	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	613	CLA	CMC-C2C-C1C	2.71	129.15	125.03
28	l	101	SQD	O5-C1-C2	-2.71	104.58	110.35
22	b	609	CLA	C1D-CHD-C4C	-2.70	118.79	122.48
25	d	409	LMG	C8-O7-C10	-2.70	111.08	117.82
22	b	602	CLA	CED-O2D-CGD	2.70	122.12	115.95
25	i	101	LMG	O7-C10-C11	2.70	117.40	111.51
28	b	621	SQD	O9-S-C6	2.70	110.14	106.94
22	b	615	CLA	CMD-C2D-C3D	2.69	129.85	124.80
22	B	615	CLA	C4C-C3C-C2C	-2.69	102.99	106.89
22	b	613	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
22	C	508	CLA	C4-C3-C5	2.69	119.92	115.29
22	b	609	CLA	C11-C12-C13	-2.69	107.37	115.77
22	a	412	CLA	C1D-CHD-C4C	-2.69	118.81	122.48
29	c	921	LMT	O2'-C2'-C3'	-2.69	104.10	110.34
22	a	408	CLA	C2A-C1A-CHA	-2.69	119.16	123.86
22	B	613	CLA	C1-O2A-CGA	2.69	123.89	116.54
22	C	512	CLA	CHD-C4C-NC	2.69	128.44	124.20
22	b	613	CLA	CHB-C4A-NA	2.69	128.23	124.51
22	b	610	CLA	C7-C6-C5	-2.68	106.04	113.25
22	b	611	CLA	O2A-CGA-CBA	2.68	120.55	111.93
24	C	515	BCR	C29-C30-C25	2.68	114.63	110.48
22	B	606	CLA	C7-C6-C5	-2.68	106.05	113.25
22	c	912	CLA	O2A-CGA-CBA	2.68	120.53	111.93
35	C	517	DGD	O2G-C1B-O1B	-2.68	117.14	123.71
23	a	410	PHO	C1C-C2C-C3C	-2.68	103.40	106.50
22	B	616	CLA	O1D-CGD-CBD	-2.67	118.94	124.48
24	a	413	BCR	C28-C27-C26	-2.67	109.34	113.99
22	A	408	CLA	CHD-C4C-NC	2.67	128.41	124.20
22	b	611	CLA	C4C-C3C-C2C	-2.67	103.02	106.89
22	d	402	CLA	CMA-C3A-C2A	-2.67	103.02	113.78
26	D	406	PL9	C50-C49-C48	-2.67	114.78	122.65
22	A	406	CLA	O1D-CGD-CBD	-2.67	118.95	124.48
22	B	602	CLA	C4C-C3C-C2C	-2.67	103.03	106.89
22	D	404	CLA	C2A-C1A-CHA	-2.67	119.19	123.86
23	A	407	PHO	C2D-C1D-ND	2.67	113.83	109.79
24	k	101	BCR	C2-C1-C6	2.67	114.61	110.48
29	c	921	LMT	O1'-C1'-C2'	2.67	112.51	108.26
39	v	202	HEC	CMC-C2C-C3C	2.67	128.95	125.82
22	C	504	CLA	CHD-C4C-NC	2.67	128.40	124.20
24	C	516	BCR	C33-C5-C6	-2.66	121.54	124.51
22	c	909	CLA	C1-O2A-CGA	2.66	123.81	116.54
22	b	616	CLA	O1D-CGD-CBD	-2.66	118.97	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	623	HTG	O4-C4-C3	-2.66	104.17	110.34
24	d	404	BCR	C24-C23-C22	-2.65	122.22	126.21
22	C	507	CLA	CHD-C4C-NC	2.65	128.39	124.20
35	C	517	DGD	O5D-C6D-C5D	-2.65	104.07	109.14
34	b	626	HTG	C3-C4-C5	2.65	115.00	110.23
28	a	414	SQD	O2-C2-C1	2.65	116.53	110.06
22	a	409	CLA	CMD-C2D-C3D	2.65	129.77	124.80
22	c	908	CLA	C1-C2-C3	-2.65	121.46	126.04
22	B	604	CLA	O2A-CGA-CBA	2.65	120.44	111.93
22	C	507	CLA	C4-C3-C5	2.65	119.85	115.29
27	a	423	LHG	O8-C23-O10	-2.65	116.79	123.56
22	b	613	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
23	a	410	PHO	C2B-C1B-NB	2.65	113.81	109.79
22	c	902	CLA	CMC-C2C-C1C	2.65	129.06	125.03
22	c	908	CLA	O2A-CGA-CBA	2.64	120.41	111.93
22	A	408	CLA	C5-C3-C2	-2.64	115.69	121.11
22	c	903	CLA	O2A-CGA-O1A	-2.64	116.81	123.56
26	d	405	PL9	C22-C23-C24	-2.64	121.19	127.67
39	V	202	HEC	CMC-C2C-C1C	-2.64	124.41	128.46
22	B	610	CLA	C1-O2A-CGA	2.64	123.75	116.54
22	c	902	CLA	C1-O2A-CGA	2.64	123.75	116.54
22	A	406	CLA	C1-C2-C3	-2.64	121.48	126.04
24	y	101	BCR	C1-C6-C7	2.64	123.28	115.78
22	b	606	CLA	C3B-C4B-NB	2.64	112.62	109.21
22	C	512	CLA	C3C-C4C-NC	2.63	113.53	110.57
27	D	409	LHG	O8-C23-O10	-2.63	116.83	123.56
24	C	515	BCR	C8-C7-C6	-2.63	119.90	127.28
22	b	610	CLA	O2D-CGD-CBD	2.63	115.86	111.25
35	C	517	DGD	O6E-C1E-C2E	-2.63	104.73	110.35
23	a	410	PHO	C4A-NA-C1A	2.63	110.27	108.14
22	B	602	CLA	O2A-CGA-CBA	2.63	120.38	111.93
22	b	614	CLA	CHD-C4C-NC	2.63	128.35	124.20
22	d	403	CLA	CHD-C4C-NC	2.63	128.34	124.20
22	c	907	CLA	O2A-CGA-CBA	2.63	120.36	111.93
22	b	615	CLA	C6-C5-C3	2.63	119.12	114.63
35	C	518	DGD	O1G-C1A-O1A	-2.63	116.85	123.56
22	C	511	CLA	O1D-CGD-CBD	-2.62	119.04	124.48
22	a	407	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
28	a	414	SQD	C44-O6-C1	-2.62	108.48	113.75
22	C	502	CLA	CMC-C2C-C1C	2.62	129.02	125.03
22	D	404	CLA	C4-C3-C5	2.62	119.80	115.29
23	A	407	PHO	CED-O2D-CGD	2.62	121.94	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	918	DGD	O1G-C1A-C2A	2.62	120.34	111.93
25	j	101	LMG	C9-C8-C7	-2.62	105.54	111.79
22	b	605	CLA	CMB-C2B-C3B	2.62	129.71	124.80
25	b	622	LMG	O7-C10-O9	-2.62	117.28	123.71
22	b	609	CLA	C1-C2-C3	-2.62	121.52	126.04
22	B	607	CLA	O1D-CGD-CBD	-2.62	119.06	124.48
22	b	613	CLA	C1-C2-C3	-2.62	121.52	126.04
35	C	519	DGD	O3G-C3G-C2G	-2.62	104.59	110.90
22	b	608	CLA	OBD-CAD-C3D	-2.61	123.41	128.04
22	C	504	CLA	CMC-C2C-C1C	2.61	129.00	125.03
22	b	615	CLA	C3B-C4B-NB	2.61	112.58	109.21
22	b	608	CLA	CHD-C4C-NC	2.61	128.31	124.20
22	C	504	CLA	O2A-CGA-CBA	2.61	120.31	111.93
22	B	613	CLA	CHD-C4C-NC	2.61	128.31	124.20
35	c	919	DGD	O1G-C1A-O1A	-2.61	116.90	123.56
22	b	616	CLA	O2A-CGA-CBA	2.61	120.30	111.93
25	d	409	LMG	O2-C2-C1	2.61	116.41	110.06
22	c	903	CLA	CMC-C2C-C1C	2.60	128.99	125.03
22	B	609	CLA	C6-C5-C3	-2.60	106.75	113.01
26	D	406	PL9	C37-C38-C39	-2.60	121.28	127.67
22	b	614	CLA	CED-O2D-CGD	2.60	121.89	115.95
24	b	618	BCR	C7-C8-C9	-2.60	122.30	126.21
22	c	914	CLA	O1D-CGD-CBD	-2.60	119.09	124.48
22	a	412	CLA	CMC-C2C-C1C	2.60	128.99	125.03
22	D	404	CLA	CMB-C2B-C3B	2.60	129.67	124.80
22	b	614	CLA	C4C-C3C-C2C	-2.60	103.13	106.89
28	D	408	SQD	C3-C4-C5	2.59	114.89	110.23
39	v	202	HEC	CMB-C2B-C1B	-2.59	124.48	128.46
22	C	508	CLA	CBC-CAC-C3C	-2.59	105.23	112.43
22	b	617	CLA	CHD-C4C-NC	2.59	128.29	124.20
22	b	604	CLA	O1D-CGD-CBD	-2.59	119.11	124.48
28	f	101	SQD	O7-S-C6	2.59	110.03	106.92
22	b	602	CLA	C4-C3-C5	2.59	119.75	115.29
22	C	508	CLA	O2A-CGA-CBA	2.59	120.24	111.93
22	D	401	CLA	CHB-C4A-NA	2.59	128.09	124.51
26	D	406	PL9	C12-C13-C14	-2.59	121.32	127.67
26	a	415	PL9	C10-C9-C11	2.58	119.74	115.29
24	K	101	BCR	C20-C21-C22	-2.58	123.62	127.31
22	C	511	CLA	C1D-CHD-C4C	-2.58	118.96	122.48
22	c	906	CLA	CAC-C3C-C4C	2.58	128.19	124.82
24	D	405	BCR	C15-C14-C13	-2.58	123.63	127.31
22	B	606	CLA	C4C-C3C-C2C	-2.58	103.16	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	C3B-C4B-NB	2.58	112.54	109.21
29	a	419	LMT	O5B-C5B-C6B	2.58	112.86	106.43
22	c	906	CLA	O2A-CGA-CBA	2.58	120.21	111.93
25	j	101	LMG	O7-C10-C11	2.58	117.14	111.51
22	B	612	CLA	CHB-C4A-NA	2.58	128.07	124.51
22	c	911	CLA	O2A-CGA-CBA	2.57	120.19	111.93
22	c	909	CLA	OBD-CAD-C3D	-2.57	123.48	128.04
22	c	912	CLA	O2A-C1-C2	-2.57	101.88	108.64
22	B	604	CLA	CMD-C2D-C3D	2.57	129.62	124.80
22	c	907	CLA	C4-C3-C5	2.57	119.71	115.29
22	A	408	CLA	CMC-C2C-C1C	2.57	128.94	125.03
22	B	616	CLA	C3B-C4B-NB	2.57	112.53	109.21
24	A	409	BCR	C36-C18-C17	-2.56	119.33	122.92
26	D	406	PL9	C25-C24-C26	2.56	119.70	115.29
22	c	904	CLA	C4C-C3C-C2C	-2.56	103.18	106.89
22	B	614	CLA	O2A-CGA-CBA	2.56	120.16	111.93
34	D	415	HTG	O2-C2-C3	2.56	116.28	110.34
22	B	613	CLA	O2A-CGA-CBA	2.56	120.14	111.93
22	C	502	CLA	C1-O2A-CGA	2.56	123.53	116.54
22	A	406	CLA	CMB-C2B-C3B	2.56	129.59	124.80
24	D	405	BCR	C36-C18-C19	2.56	122.14	118.09
22	C	512	CLA	C4C-C3C-C2C	-2.56	103.19	106.89
29	f	102	LMT	C3'-C4'-C5'	-2.56	105.03	110.92
22	b	602	CLA	CHC-C1C-NC	-2.55	120.33	124.20
22	C	510	CLA	C3C-C4C-NC	2.55	113.44	110.57
22	D	401	CLA	CMB-C2B-C1B	2.55	132.39	128.46
22	B	610	CLA	O2D-CGD-O1D	-2.55	118.79	123.83
22	C	506	CLA	C4-C3-C5	2.55	119.68	115.29
35	C	518	DGD	O2G-C1B-O1B	-2.55	117.45	123.71
26	a	415	PL9	C40-C39-C41	2.55	119.68	115.29
22	b	610	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
22	B	613	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
23	a	410	PHO	C1C-NC-C4C	-2.55	101.63	106.50
25	d	409	LMG	O7-C10-O9	-2.54	117.46	123.71
25	j	101	LMG	O8-C28-C29	2.54	120.10	111.93
28	l	101	SQD	O9-S-C6	2.54	109.96	106.94
22	c	914	CLA	CED-O2D-CGD	2.54	121.76	115.95
22	d	403	CLA	CED-O2D-CGD	2.54	121.75	115.95
22	C	509	CLA	C4C-C3C-C2C	-2.54	103.21	106.89
22	c	914	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	d	409	LMG	C3-C4-C5	2.54	114.79	110.23
35	C	518	DGD	C3B-C2B-C1B	-2.54	104.45	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	411	PL9	C3-C4-C5	2.54	121.97	118.62
22	b	610	CLA	CAC-C3C-C4C	2.54	128.13	124.82
24	B	620	BCR	C10-C11-C12	-2.54	115.68	123.31
25	i	101	LMG	C31-C30-C29	-2.54	104.06	113.20
22	b	604	CLA	CHC-C1C-NC	-2.54	120.36	124.20
22	c	912	CLA	CMC-C2C-C1C	2.53	128.89	125.03
22	b	603	CLA	CAA-CBA-CGA	-2.53	105.80	113.26
22	B	614	CLA	C1-C2-C3	-2.53	121.66	126.04
22	B	612	CLA	C3B-C4B-NB	2.53	112.48	109.21
24	c	916	BCR	C16-C17-C18	-2.53	123.70	127.31
22	b	614	CLA	C3C-C4C-NC	2.53	113.41	110.57
22	b	611	CLA	O2A-CGA-O1A	-2.53	117.09	123.56
25	i	101	LMG	C1-O6-C5	-2.53	108.71	113.70
22	c	913	CLA	CMD-C2D-C3D	2.53	129.54	124.80
22	C	509	CLA	O2A-CGA-CBA	2.53	120.05	111.93
24	Y	101	BCR	C8-C9-C10	-2.53	115.06	118.94
22	a	412	CLA	CED-O2D-CGD	2.53	121.72	115.95
22	A	405	CLA	CAA-CBA-CGA	-2.53	105.81	113.26
26	D	406	PL9	C51-C49-C50	2.53	120.27	114.59
26	a	415	PL9	C32-C33-C34	-2.53	121.47	127.67
28	a	414	SQD	O47-C7-O49	-2.52	117.52	123.71
24	K	101	BCR	C16-C17-C18	-2.52	123.71	127.31
22	B	603	CLA	C5-C3-C2	-2.52	115.93	121.11
22	a	412	CLA	O2A-CGA-CBA	2.52	120.02	111.93
22	b	608	CLA	CMD-C2D-C3D	2.52	129.53	124.80
35	D	407	DGD	O1G-C1G-C2G	2.52	115.78	108.43
22	b	612	CLA	CBC-CAC-C3C	-2.52	105.44	112.43
26	A	411	PL9	C37-C38-C39	-2.52	121.49	127.67
22	C	503	CLA	CMC-C2C-C1C	2.51	128.86	125.03
22	b	607	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
22	b	603	CLA	C1-O2A-CGA	2.51	123.41	116.54
26	A	411	PL9	C30-C29-C31	2.51	119.61	115.29
29	f	102	LMT	O5'-C5'-C6'	2.51	112.69	106.43
22	b	607	CLA	CMB-C2B-C3B	2.51	129.51	124.80
28	D	408	SQD	C4-C3-C2	2.51	115.23	110.82
22	a	408	CLA	C3B-C4B-NB	2.51	112.45	109.21
22	c	907	CLA	CHB-C4A-NA	2.51	127.98	124.51
28	C	501	SQD	O48-C23-C24	2.50	119.97	111.93
22	a	407	CLA	CMC-C2C-C1C	2.50	128.84	125.03
24	k	101	BCR	C11-C10-C9	-2.50	123.74	127.31
22	C	510	CLA	C1-O2A-CGA	2.50	123.38	116.54
22	D	403	CLA	O2A-CGA-CBA	2.50	119.96	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	O2A-CGA-CBA	2.50	119.96	111.93
22	b	612	CLA	C3C-C4C-NC	2.50	113.37	110.57
22	C	510	CLA	C11-C10-C8	-2.50	107.98	115.77
22	B	604	CLA	O1D-CGD-CBD	-2.50	119.31	124.48
22	B	616	CLA	CHB-C4A-NA	2.49	127.96	124.51
27	D	410	LHG	C14-C13-C12	-2.49	101.55	114.44
24	Y	101	BCR	C7-C8-C9	-2.49	122.46	126.21
25	j	101	LMG	O2-C2-C1	-2.49	103.98	110.06
22	d	402	CLA	CAC-C3C-C4C	2.49	128.08	124.82
28	l	101	SQD	O47-C7-O49	-2.49	117.59	123.71
22	B	610	CLA	CAC-C3C-C4C	2.49	128.08	124.82
22	c	914	CLA	O2A-CGA-CBA	2.49	119.93	111.93
23	A	407	PHO	C4C-C3C-C2C	-2.49	104.02	106.79
22	B	616	CLA	O2D-CGD-O1D	-2.49	118.91	123.83
22	B	609	CLA	CMB-C2B-C3B	2.49	129.47	124.80
35	h	102	DGD	C3D-C4D-C5D	-2.49	105.76	110.23
22	c	914	CLA	CMD-C2D-C3D	2.49	129.46	124.80
22	c	902	CLA	C3B-C4B-NB	2.49	112.42	109.21
22	B	608	CLA	C1-O2A-CGA	2.48	123.33	116.54
27	a	423	LHG	O7-C7-O9	-2.48	117.61	123.71
22	C	502	CLA	O1D-CGD-CBD	-2.48	119.33	124.48
22	C	512	CLA	C1D-CHD-C4C	-2.48	119.09	122.48
27	d	401	LHG	O4-P-O5	2.48	120.33	110.53
27	L	101	LHG	O7-C7-O9	-2.48	117.61	123.71
24	C	516	BCR	C38-C26-C25	-2.48	121.75	124.51
22	d	402	CLA	CMD-C2D-C3D	2.48	129.45	124.80
22	B	603	CLA	C4C-C3C-C2C	-2.48	103.30	106.89
24	B	619	BCR	C15-C16-C17	-2.47	118.31	123.51
22	c	906	CLA	CBC-CAC-C3C	-2.47	105.56	112.43
25	D	412	LMG	O8-C28-C29	2.47	119.87	111.93
28	C	501	SQD	O9-S-O7	-2.47	105.39	113.95
22	B	616	CLA	O2A-CGA-CBA	2.47	119.87	111.93
22	c	910	CLA	CMD-C2D-C3D	2.47	129.44	124.80
22	B	604	CLA	O2A-CGA-O1A	-2.47	117.25	123.56
24	y	101	BCR	C7-C6-C5	-2.47	115.48	121.48
22	A	405	CLA	O2D-CGD-O1D	-2.47	118.96	123.83
22	c	904	CLA	CAA-CBA-CGA	-2.47	105.99	113.26
22	C	512	CLA	O2D-CGD-CBD	2.46	115.57	111.25
22	B	614	CLA	C3B-C4B-NB	2.46	112.40	109.21
35	D	407	DGD	C1D-C2D-C3D	2.46	115.13	109.98
22	D	401	CLA	C4-C3-C5	2.46	119.53	115.29
24	Y	101	BCR	C34-C9-C8	2.46	121.99	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	CHC-C1C-NC	-2.46	120.47	124.20
22	C	508	CLA	O1D-CGD-CBD	-2.46	119.39	124.48
22	c	903	CLA	O2A-CGA-CBA	2.46	119.82	111.93
22	D	403	CLA	C4-C3-C2	-2.46	117.29	123.68
28	C	501	SQD	O2-C2-C1	2.46	116.05	110.06
22	B	604	CLA	CMC-C2C-C1C	2.45	128.77	125.03
35	c	919	DGD	C2G-O2G-C1B	-2.45	111.70	117.82
22	B	611	CLA	O1D-CGD-CBD	-2.45	119.40	124.48
22	B	617	CLA	C4-C3-C5	2.45	119.51	115.29
22	B	605	CLA	CHB-C4A-NA	2.45	127.90	124.51
22	a	409	CLA	O2A-CGA-O1A	-2.45	117.30	123.56
22	a	408	CLA	O2D-CGD-O1D	-2.45	118.99	123.83
22	A	408	CLA	CAC-C3C-C4C	2.45	128.02	124.82
26	A	411	PL9	C26-C27-C28	2.45	119.98	111.88
22	A	405	CLA	C3C-C4C-NC	2.45	113.31	110.57
22	b	615	CLA	O2D-CGD-O1D	-2.45	119.00	123.83
22	B	612	CLA	C3C-C4C-NC	2.45	113.31	110.57
22	a	407	CLA	O2A-CGA-CBA	2.44	119.78	111.93
24	D	405	BCR	C32-C1-C6	2.44	114.26	110.30
22	C	504	CLA	CHC-C1C-NC	-2.44	120.50	124.20
34	l	106	HTG	O5-C1-C2	-2.44	107.24	110.31
22	c	914	CLA	CAC-C3C-C4C	2.44	128.01	124.82
22	B	603	CLA	CMB-C2B-C3B	2.44	129.37	124.80
22	b	610	CLA	C16-C15-C13	-2.44	108.16	115.77
22	D	404	CLA	CBC-CAC-C3C	-2.44	105.66	112.43
22	B	617	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	b	613	CLA	O2A-CGA-O1A	-2.44	117.33	123.56
37	H	101	RRX	C38-C26-C25	-2.44	121.80	124.51
22	c	911	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
22	B	610	CLA	C3C-C4C-NC	2.43	113.30	110.57
22	b	609	CLA	CHD-C4C-NC	2.43	128.03	124.20
28	b	621	SQD	C3-C4-C5	2.43	114.60	110.23
22	B	606	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
22	C	508	CLA	O2A-CGA-O1A	-2.43	117.35	123.56
25	c	930	LMG	O8-C28-C29	2.43	119.73	111.93
22	b	617	CLA	C1-O2A-CGA	2.43	123.18	116.54
22	b	611	CLA	CMB-C2B-C3B	2.43	129.35	124.80
22	C	505	CLA	C3B-C4B-NB	2.42	112.34	109.21
22	B	605	CLA	C4-C3-C5	2.42	119.46	115.29
35	C	518	DGD	C6D-C5D-C4D	2.42	117.31	112.14
22	b	615	CLA	C3C-C4C-NC	2.42	113.28	110.57
24	B	620	BCR	C33-C5-C6	-2.42	121.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	v	203	HTG	O2-C2-C1	2.42	114.71	110.27
22	B	604	CLA	C6-C5-C3	2.42	118.81	113.01
25	A	410	LMG	C8-O7-C10	-2.42	111.79	117.82
23	D	402	PHO	CHD-C4C-C3C	-2.42	119.57	124.48
22	B	613	CLA	C3B-C4B-NB	2.41	112.33	109.21
23	A	407	PHO	C4D-C3D-CAD	2.41	109.77	105.39
22	B	615	CLA	O2D-CGD-O1D	-2.41	119.07	123.83
22	c	905	CLA	CMD-C2D-C3D	2.41	129.32	124.80
22	B	611	CLA	CMB-C2B-C3B	2.41	129.32	124.80
24	a	413	BCR	C40-C30-C25	-2.41	106.41	110.30
22	B	604	CLA	C3C-C4C-NC	2.41	113.27	110.57
35	c	917	DGD	O2G-C1B-O1B	-2.41	117.80	123.71
22	c	912	CLA	CHC-C1C-NC	-2.41	120.55	124.20
23	a	410	PHO	O2A-CGA-CBA	2.40	119.65	111.93
22	B	615	CLA	C3B-C4B-NB	2.40	112.32	109.21
23	a	411	PHO	C1C-C2C-C3C	-2.40	103.72	106.50
24	a	413	BCR	C23-C24-C25	-2.40	120.56	127.28
22	C	510	CLA	C4-C3-C5	2.40	119.42	115.29
24	c	915	BCR	C38-C26-C25	-2.40	121.84	124.51
25	B	621	LMG	O7-C10-O9	-2.40	117.82	123.71
22	B	613	CLA	CMB-C2B-C3B	2.40	129.30	124.80
22	a	407	CLA	CMD-C2D-C3D	2.40	129.29	124.80
22	C	504	CLA	C5-C3-C2	-2.40	116.19	121.11
22	B	609	CLA	O2A-CGA-CBA	2.40	119.62	111.93
24	Y	101	BCR	C15-C14-C13	-2.40	123.89	127.31
28	C	501	SQD	C45-O47-C7	-2.40	111.84	117.82
22	B	612	CLA	CAC-C3C-C4C	2.39	127.95	124.82
22	b	617	CLA	C4-C3-C5	2.39	119.41	115.29
22	b	602	CLA	CMB-C2B-C3B	2.39	129.29	124.80
22	b	610	CLA	CMD-C2D-C3D	2.39	129.29	124.80
24	D	405	BCR	C30-C25-C24	2.39	122.58	115.78
35	c	919	DGD	O2E-C2E-C3E	-2.39	104.79	110.34
24	A	409	BCR	C33-C5-C6	-2.39	121.85	124.51
22	B	609	CLA	CMC-C2C-C1C	2.39	128.67	125.03
22	b	612	CLA	O2D-CGD-O1D	-2.39	119.11	123.83
22	B	603	CLA	C1-O2A-CGA	2.39	123.07	116.54
26	D	406	PL9	C40-C39-C38	-2.39	117.47	123.68
22	c	912	CLA	CAC-C3C-C4C	2.39	127.94	124.82
22	B	617	CLA	C3C-C4C-NC	2.39	113.25	110.57
22	C	502	CLA	C3C-C4C-NC	2.39	113.25	110.57
24	a	413	BCR	C8-C7-C6	-2.38	120.60	127.28
22	a	407	CLA	O1D-CGD-CBD	-2.38	119.54	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	514	CLA	OBD-CAD-C3D	-2.38	123.82	128.04
22	b	615	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
27	d	401	LHG	O8-C23-O10	-2.38	117.47	123.56
22	b	611	CLA	CMC-C2C-C1C	2.38	128.66	125.03
23	D	402	PHO	CHD-C1D-ND	-2.38	119.61	124.58
24	d	404	BCR	C15-C14-C13	-2.38	123.91	127.31
22	b	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
22	c	904	CLA	C3B-C4B-NB	2.38	112.29	109.21
22	C	505	CLA	O1D-CGD-CBD	-2.38	119.55	124.48
34	l	106	HTG	C1-C2-C3	-2.38	105.89	110.59
35	c	918	DGD	O1G-C1A-O1A	-2.38	117.49	123.56
22	A	405	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
22	C	505	CLA	C6-C5-C3	2.38	118.71	113.01
22	B	602	CLA	CHC-C1C-NC	-2.37	120.60	124.20
25	J	101	LMG	O3-C3-C2	-2.37	104.83	110.34
22	b	617	CLA	O2A-CGA-CBA	2.37	119.55	111.93
35	C	519	DGD	O2G-C1B-O1B	-2.37	117.89	123.71
22	B	604	CLA	CBC-CAC-C3C	-2.37	105.86	112.43
35	C	517	DGD	O2G-C1B-C2B	2.36	116.67	111.51
22	B	608	CLA	C1-C2-C3	-2.36	121.95	126.04
23	a	410	PHO	C4D-C3D-CAD	2.36	109.68	105.39
22	b	616	CLA	CAC-C3C-C4C	2.36	127.91	124.82
29	c	931	LMT	O1'-C1'-C2'	2.36	112.02	108.26
23	A	407	PHO	CHB-C1B-NB	-2.36	119.65	124.58
36	E	102	HEM	CMA-C3A-C4A	-2.36	124.84	128.46
22	a	412	CLA	CMB-C2B-C3B	2.36	129.23	124.80
25	c	930	LMG	O7-C10-O9	-2.36	117.92	123.71
22	b	605	CLA	CGD-CBD-CAD	-2.36	103.10	110.73
22	d	402	CLA	CMC-C2C-C1C	2.36	128.62	125.03
35	d	406	DGD	O2G-C1B-O1B	-2.36	117.93	123.71
25	C	531	LMG	O6-C5-C6	2.35	112.30	106.43
22	b	607	CLA	O2A-CGA-O1A	-2.35	117.55	123.56
22	c	906	CLA	C4C-C3C-C2C	-2.35	103.48	106.89
34	b	623	HTG	C1-O5-C5	2.35	117.01	112.58
22	a	408	CLA	O2A-CGA-CBA	2.35	119.48	111.93
29	c	921	LMT	C1B-O1B-C4'	-2.35	112.11	117.97
22	B	602	CLA	CED-O2D-CGD	2.35	121.31	115.95
22	b	613	CLA	CMC-C2C-C1C	2.35	128.60	125.03
22	b	617	CLA	C3B-C4B-NB	2.35	112.24	109.21
22	c	905	CLA	CED-O2D-CGD	2.34	121.30	115.95
22	C	506	CLA	O2D-CGD-O1D	-2.34	119.20	123.83
23	a	410	PHO	CMB-C2B-C1B	2.34	128.69	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	O2A-CGA-O1A	-2.34	117.58	123.56
22	B	611	CLA	C3C-C4C-NC	2.34	113.19	110.57
22	b	604	CLA	C3B-C4B-NB	2.34	112.23	109.21
22	C	507	CLA	C4C-C3C-C2C	-2.34	103.50	106.89
22	b	603	CLA	O1D-CGD-CBD	-2.34	119.63	124.48
24	B	619	BCR	C23-C24-C25	-2.34	120.73	127.28
22	B	603	CLA	CMD-C2D-C3D	2.34	129.18	124.80
25	d	409	LMG	O8-C28-C29	2.34	119.43	111.93
22	C	512	CLA	C3A-C2A-C1A	2.33	104.83	101.34
28	D	408	SQD	C1-O5-C5	-2.33	109.10	113.70
24	B	619	BCR	C24-C23-C22	-2.33	122.71	126.21
29	T	102	LMT	O5'-C1'-C2'	2.33	115.32	110.35
22	C	514	CLA	CMD-C2D-C3D	2.33	129.17	124.80
22	b	617	CLA	C4-C3-C2	-2.33	117.62	123.68
22	c	904	CLA	O2D-CGD-O1D	-2.33	119.23	123.83
22	c	910	CLA	C3C-C4C-NC	2.33	113.18	110.57
37	h	101	RRX	C10-C11-C12	-2.33	116.31	123.31
22	b	615	CLA	CHC-C1C-NC	-2.33	120.67	124.20
25	c	930	LMG	C1-O6-C5	2.32	118.28	113.70
23	a	411	PHO	C11-C12-C13	-2.32	108.52	115.77
22	b	606	CLA	C3D-CAD-CBD	2.32	110.74	107.61
22	a	407	CLA	C7-C6-C5	-2.32	107.01	113.25
22	B	605	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
22	D	404	CLA	O2A-CGA-O1A	-2.32	117.63	123.56
24	d	404	BCR	C10-C11-C12	-2.32	116.33	123.31
22	C	503	CLA	C4C-C3C-C2C	-2.32	103.53	106.89
22	C	506	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	a	407	CLA	C5-C3-C2	-2.32	116.35	121.11
22	B	603	CLA	C6-C7-C8	-2.32	108.54	115.77
24	Y	101	BCR	C24-C25-C26	-2.32	115.86	121.48
22	c	909	CLA	CMC-C2C-C3C	2.31	132.42	126.11
24	B	620	BCR	C40-C30-C25	-2.31	106.56	110.30
22	b	615	CLA	O2A-CGA-CBA	2.31	119.36	111.93
25	B	621	LMG	O6-C5-C4	2.31	113.90	109.68
24	B	620	BCR	C15-C14-C13	-2.31	124.01	127.31
34	b	623	HTG	O5-C1-C2	2.31	113.22	110.31
24	c	916	BCR	C36-C18-C19	2.31	121.75	118.09
22	B	607	CLA	CMC-C2C-C1C	2.31	128.55	125.03
22	d	403	CLA	C3B-C4B-NB	2.31	112.20	109.21
27	a	416	LHG	O7-C7-O9	-2.31	118.05	123.71
24	y	101	BCR	C15-C14-C13	-2.31	124.02	127.31
22	B	606	CLA	CMD-C2D-C3D	2.31	129.13	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C6-C5-C3	-2.31	107.47	113.01
27	a	416	LHG	C6-O8-C23	2.30	125.69	117.13
22	C	507	CLA	CMB-C2B-C3B	2.30	129.12	124.80
22	c	910	CLA	O2D-CGD-O1D	-2.30	119.28	123.83
22	c	910	CLA	CMB-C2B-C3B	2.30	129.12	124.80
22	b	609	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
22	b	605	CLA	C3B-C4B-NB	2.30	112.19	109.21
22	C	507	CLA	O2D-CGD-O1D	-2.30	119.29	123.83
25	B	621	LMG	C4-C3-C2	2.30	114.86	110.82
22	D	403	CLA	C3C-C4C-NC	2.30	113.15	110.57
22	B	611	CLA	CMD-C2D-C3D	2.30	129.11	124.80
22	c	909	CLA	CAC-C3C-C2C	2.30	131.46	127.53
22	C	510	CLA	CMD-C2D-C3D	2.30	129.11	124.80
35	H	102	DGD	C3B-C2B-C1B	-2.30	105.32	113.62
24	B	619	BCR	C20-C21-C22	-2.30	124.03	127.31
22	B	608	CLA	CMC-C2C-C1C	2.30	128.53	125.03
24	b	620	BCR	C33-C5-C6	-2.29	121.95	124.51
22	B	608	CLA	C4-C3-C2	-2.29	117.71	123.68
22	c	907	CLA	CAC-C3C-C4C	2.29	127.82	124.82
22	A	406	CLA	CED-O2D-CGD	2.29	121.19	115.95
22	C	508	CLA	CHC-C1C-NC	-2.29	120.72	124.20
22	b	604	CLA	C5-C3-C2	-2.29	116.40	121.11
22	a	407	CLA	C3C-C4C-NC	2.29	113.14	110.57
28	C	501	SQD	O7-S-C6	-2.29	104.22	106.94
22	C	506	CLA	CHD-C4C-C3C	-2.29	121.53	124.87
25	J	101	LMG	O8-C28-C29	2.29	119.28	111.93
28	a	418	SQD	C44-O6-C1	-2.29	109.15	113.75
22	b	614	CLA	C3B-C4B-NB	2.29	112.17	109.21
22	a	412	CLA	C5-C3-C2	-2.29	116.41	121.11
22	A	408	CLA	O2A-CGA-CBA	2.29	119.28	111.93
22	D	401	CLA	CAC-C3C-C4C	2.29	127.81	124.82
22	B	604	CLA	CHD-C4C-NC	2.29	127.81	124.20
25	i	101	LMG	O1-C1-C2	2.29	111.90	108.26
22	D	403	CLA	CAC-C3C-C4C	2.29	127.81	124.82
22	C	505	CLA	C1-O2A-CGA	2.29	122.79	116.54
22	C	511	CLA	C3B-C4B-NB	2.28	112.16	109.21
22	b	607	CLA	C4C-C3C-C2C	-2.28	103.58	106.89
22	a	412	CLA	CHC-C1C-C2C	-2.28	120.41	126.71
22	A	406	CLA	C5-C3-C2	-2.28	116.42	121.11
22	C	506	CLA	CMB-C2B-C3B	2.28	129.08	124.80
22	C	512	CLA	C6-C7-C8	-2.28	108.65	115.77
22	B	613	CLA	C4C-C3C-C2C	-2.28	103.59	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	V	203	HTG	C1-O5-C5	-2.28	108.28	112.58
23	D	402	PHO	C4D-C3D-CAD	2.28	109.53	105.39
22	B	608	CLA	O1D-CGD-CBD	-2.28	119.75	124.48
22	B	602	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
22	B	613	CLA	CHC-C1C-NC	-2.28	120.75	124.20
22	c	907	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
22	B	608	CLA	CHB-C4A-NA	2.28	127.66	124.51
26	d	405	PL9	C42-C43-C44	-2.28	122.08	127.67
22	c	905	CLA	C7-C6-C5	-2.28	107.14	113.25
22	c	913	CLA	C6-C5-C3	-2.27	107.54	113.01
22	C	503	CLA	CMB-C2B-C1B	2.27	131.96	128.46
22	c	913	CLA	C1-O2A-CGA	2.27	122.75	116.54
22	b	617	CLA	CHC-C1C-NC	-2.27	120.76	124.20
28	a	414	SQD	O5-C1-C2	-2.27	105.50	110.35
22	b	612	CLA	C1-C2-C3	-2.27	122.11	126.04
35	C	517	DGD	O3D-C3D-C2D	-2.27	105.07	110.34
22	b	611	CLA	C3B-C4B-NB	2.27	112.14	109.21
22	B	612	CLA	CBC-CAC-C3C	-2.27	106.13	112.43
26	a	415	PL9	C51-C49-C50	2.27	119.69	114.59
22	b	612	CLA	O2A-CGA-CBA	2.27	119.21	111.93
22	d	402	CLA	CHD-C4C-NC	2.27	127.78	124.20
22	B	604	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
23	a	411	PHO	CMD-C2D-C3D	-2.26	122.53	127.71
22	b	615	CLA	CHD-C4C-NC	2.26	127.77	124.20
22	D	401	CLA	O2A-CGA-O1A	-2.26	117.78	123.56
22	c	912	CLA	O2D-CGD-O1D	-2.26	119.36	123.83
26	A	411	PL9	C10-C9-C11	2.26	119.18	115.29
22	B	605	CLA	O2A-CGA-CBA	2.26	119.18	111.93
22	C	511	CLA	CBC-CAC-C3C	-2.26	106.16	112.43
22	C	506	CLA	CMC-C2C-C1C	2.26	128.46	125.03
29	I	102	LMT	C2'-C3'-C4'	-2.25	104.51	109.67
24	B	620	BCR	C15-C16-C17	-2.25	118.77	123.51
22	c	907	CLA	O2A-CGA-O1A	-2.25	117.80	123.56
22	a	407	CLA	C11-C10-C8	-2.25	108.74	115.77
24	Y	101	BCR	C21-C20-C19	-2.25	116.53	123.31
24	a	413	BCR	C24-C23-C22	-2.25	122.83	126.21
22	A	405	CLA	O2A-CGA-CBA	2.25	119.15	111.93
24	y	101	BCR	C10-C11-C12	-2.25	116.54	123.31
22	b	602	CLA	OBD-CAD-C3D	-2.25	124.06	128.04
22	b	616	CLA	C6-C7-C8	-2.25	108.76	115.77
22	c	911	CLA	C16-C15-C13	-2.25	108.76	115.77
22	C	502	CLA	O2A-CGA-O1A	-2.25	117.82	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	101	BCR	C10-C11-C12	-2.25	116.55	123.31
22	C	507	CLA	C1-O2A-CGA	2.25	122.68	116.54
22	B	616	CLA	C4C-C3C-C2C	-2.25	103.64	106.89
22	B	602	CLA	CHD-C4C-NC	2.25	127.74	124.20
22	B	615	CLA	CMC-C2C-C1C	2.24	128.44	125.03
35	C	519	DGD	O4D-C4D-C3D	-2.24	105.14	110.34
22	B	609	CLA	C3B-C4B-NB	2.24	112.11	109.21
22	B	607	CLA	C4C-C3C-C2C	-2.24	103.64	106.89
22	c	909	CLA	CMD-C2D-C3D	2.24	129.00	124.80
22	c	904	CLA	C4-C3-C5	2.24	119.15	115.29
24	c	916	BCR	C21-C20-C19	-2.24	116.57	123.31
25	B	621	LMG	O1-C1-C2	2.24	111.83	108.26
22	B	614	CLA	CMB-C2B-C3B	2.24	129.00	124.80
22	b	614	CLA	O2A-CGA-CBA	2.24	119.12	111.93
22	C	510	CLA	O2A-CGA-O1A	-2.24	117.84	123.56
22	b	604	CLA	CAC-C3C-C4C	2.24	127.75	124.82
22	a	408	CLA	C6-C5-C3	-2.24	107.63	113.01
22	b	615	CLA	CMB-C2B-C3B	2.24	129.00	124.80
22	b	606	CLA	CHC-C1C-NC	-2.24	120.81	124.20
22	A	406	CLA	C3B-C4B-NB	2.23	112.10	109.21
31	c	924	DMS	O-S-C2	2.23	118.11	106.56
22	C	506	CLA	C3A-C2A-C1A	2.23	104.68	101.34
22	C	508	CLA	CMC-C2C-C1C	2.23	128.43	125.03
23	a	411	PHO	CHD-C4C-NC	-2.23	120.25	124.94
22	b	616	CLA	CHB-C4A-NA	2.23	127.60	124.51
22	a	409	CLA	CHC-C1C-C2C	-2.23	120.56	126.71
22	d	403	CLA	CAC-C3C-C4C	2.23	127.73	124.82
23	a	411	PHO	CHD-C1D-ND	-2.23	119.93	124.58
22	D	401	CLA	C6-C5-C3	-2.23	107.65	113.01
22	C	511	CLA	O2A-CGA-CBA	2.23	119.08	111.93
24	c	915	BCR	C8-C7-C6	-2.23	121.04	127.28
22	a	409	CLA	CHB-C4A-NA	2.23	127.59	124.51
24	c	916	BCR	C7-C8-C9	-2.22	122.87	126.21
22	c	913	CLA	CBC-CAC-C3C	-2.22	106.26	112.43
25	B	621	LMG	O6-C1-O1	2.22	115.19	109.94
34	b	632	HTG	C4-C3-C2	-2.22	106.92	110.82
23	D	402	PHO	O2D-CGD-O1D	-2.22	119.44	123.83
36	E	102	HEM	CMB-C2B-C3B	2.22	128.97	124.80
22	B	617	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
22	C	514	CLA	C1-O2A-CGA	2.22	122.61	116.54
22	C	511	CLA	CMC-C2C-C1C	2.22	128.41	125.03
22	B	607	CLA	O2A-CGA-O1A	-2.22	117.89	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	505	CLA	CMB-C2B-C3B	2.22	128.96	124.80
27	D	410	LHG	O8-C23-O10	-2.22	117.89	123.56
34	b	627	HTG	C1-O5-C5	2.22	116.76	112.58
22	B	603	CLA	O2A-CGA-O1A	-2.22	117.90	123.56
24	B	619	BCR	C11-C12-C13	-2.21	120.21	126.42
22	C	512	CLA	CED-O2D-CGD	2.21	121.00	115.95
24	C	516	BCR	C37-C22-C21	-2.21	119.83	122.92
22	B	614	CLA	CHD-C4C-NC	2.21	127.69	124.20
24	b	618	BCR	C1-C6-C7	2.21	122.06	115.78
22	c	903	CLA	C3C-C4C-NC	2.21	113.05	110.57
22	C	506	CLA	C3B-C4B-NB	2.21	112.06	109.21
24	k	101	BCR	C38-C26-C25	-2.21	122.05	124.51
34	b	626	HTG	C2'-C1'-S1	-2.21	105.27	112.40
22	b	605	CLA	O2A-CGA-CBA	2.21	119.01	111.93
34	b	624	HTG	C1-O5-C5	2.21	116.74	112.58
34	b	632	HTG	O2-C2-C3	2.20	115.46	110.34
22	c	910	CLA	CED-O2D-CGD	2.20	120.98	115.95
25	d	409	LMG	O6-C5-C6	2.20	111.92	106.43
22	B	614	CLA	C7-C6-C5	-2.20	107.33	113.25
27	C	522	LHG	O8-C23-C24	2.20	119.00	111.93
25	C	520	LMG	O8-C9-C8	2.20	114.86	108.43
28	a	418	SQD	O5-C1-O6	2.20	115.14	109.94
22	b	611	CLA	C9-C8-C10	-2.20	103.28	111.30
37	h	101	RRX	C2-C1-C6	2.20	113.89	110.48
22	B	606	CLA	O2A-CGA-O1A	-2.20	117.94	123.56
22	b	610	CLA	O2A-CGA-O1A	-2.20	117.94	123.56
29	f	102	LMT	C1-O1'-C1'	2.20	117.49	113.83
22	c	906	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
35	H	102	DGD	C2G-O2G-C1B	-2.19	112.34	117.82
22	B	615	CLA	CAA-CBA-CGA	-2.19	106.79	113.26
22	a	408	CLA	C4-C3-C5	2.19	119.07	115.29
22	D	404	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
22	C	513	CLA	CED-O2D-CGD	2.19	120.96	115.95
22	c	914	CLA	C3C-C4C-NC	2.19	113.03	110.57
22	C	508	CLA	C3B-C4B-NB	2.19	112.04	109.21
35	C	517	DGD	C4E-C3E-C2E	-2.19	106.97	110.82
22	C	504	CLA	CED-O2D-CGD	2.19	120.95	115.95
22	c	910	CLA	C1D-CHD-C4C	-2.19	119.49	122.48
24	b	620	BCR	C16-C17-C18	-2.19	124.19	127.31
25	c	920	LMG	O8-C9-C8	2.19	114.82	108.43
22	A	406	CLA	CHC-C1C-C2C	-2.19	120.68	126.71
22	c	903	CLA	C16-C15-C13	-2.19	108.95	115.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	408	CLA	CMC-C2C-C3C	2.19	132.07	126.11
22	B	617	CLA	C1-C2-C3	-2.18	122.27	126.04
22	c	903	CLA	OBD-CAD-C3D	-2.18	124.17	128.04
24	Y	101	BCR	C36-C18-C19	2.18	121.55	118.09
34	b	624	HTG	O5-C5-C6	2.18	111.87	106.43
23	A	407	PHO	CMD-C2D-C3D	-2.18	122.73	127.71
22	B	613	CLA	CBA-CAA-C2A	-2.18	107.37	113.85
23	a	410	PHO	CAC-C3C-C2C	2.18	131.25	127.53
35	C	519	DGD	O6E-C5E-C6E	2.18	111.85	106.43
25	j	101	LMG	O4-C4-C5	-2.17	103.85	109.29
35	C	519	DGD	O1G-C1A-O1A	-2.17	118.01	123.56
22	a	412	CLA	CAC-C3C-C4C	2.17	127.66	124.82
22	b	604	CLA	O2A-CGA-CBA	2.17	118.90	111.93
22	c	906	CLA	O2A-CGA-O1A	-2.17	118.01	123.56
22	B	609	CLA	C1-O2A-CGA	2.17	122.47	116.54
22	c	912	CLA	CHD-C4C-NC	2.17	127.62	124.20
22	B	610	CLA	C3B-C4B-NB	2.17	112.01	109.21
22	B	605	CLA	C5-C3-C2	-2.17	116.66	121.11
24	y	101	BCR	C8-C9-C10	-2.17	115.61	118.94
22	B	608	CLA	CHD-C4C-NC	2.17	127.62	124.20
36	e	101	HEM	CMB-C2B-C3B	2.17	128.86	124.80
22	c	914	CLA	OBD-CAD-C3D	-2.17	124.20	128.04
26	D	406	PL9	C22-C23-C24	-2.17	122.35	127.67
22	b	608	CLA	C3B-C4B-NB	2.17	112.01	109.21
22	A	408	CLA	CHC-C1C-NC	-2.16	120.92	124.20
22	c	911	CLA	CHB-C4A-NA	2.16	127.50	124.51
22	b	603	CLA	C4C-C3C-C2C	-2.16	103.76	106.89
22	c	904	CLA	C3C-C4C-NC	2.16	112.99	110.57
22	c	913	CLA	O2A-CGA-CBA	2.16	118.85	111.93
22	b	602	CLA	CMC-C2C-C1C	2.15	128.31	125.03
24	y	101	BCR	C23-C24-C25	-2.15	121.25	127.28
23	A	407	PHO	C7-C6-C5	-2.15	107.46	113.25
26	d	405	PL9	C10-C9-C11	2.15	119.00	115.29
25	i	101	LMG	C6-C5-C4	2.15	118.06	113.00
24	C	515	BCR	C24-C23-C22	-2.15	122.98	126.21
22	A	408	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
24	b	620	BCR	C15-C14-C13	-2.15	124.24	127.31
22	c	910	CLA	C4C-C3C-C2C	-2.15	103.77	106.89
24	B	620	BCR	C33-C5-C4	2.15	117.60	113.57
22	b	608	CLA	CBC-CAC-C3C	-2.15	106.46	112.43
24	b	620	BCR	C32-C1-C6	-2.15	106.83	110.30
34	B	626	HTG	O5-C5-C4	2.15	113.60	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	513	CLA	C4C-C3C-C2C	-2.15	103.78	106.89
22	C	514	CLA	C2A-C1A-CHA	-2.15	120.11	123.86
22	b	603	CLA	C3B-C4B-NB	2.14	111.98	109.21
25	c	920	LMG	O3-C3-C4	-2.14	105.37	110.34
22	a	409	CLA	O2A-CGA-CBA	2.14	118.81	111.93
24	y	101	BCR	C34-C9-C8	2.14	121.49	118.09
25	j	101	LMG	O8-C28-O10	-2.14	118.09	123.56
22	b	603	CLA	CAC-C3C-C4C	2.14	127.61	124.82
24	y	101	BCR	C35-C13-C14	-2.14	119.93	122.92
22	B	609	CLA	O2A-CGA-O1A	-2.14	118.10	123.56
34	b	623	HTG	C4'-C3'-C2'	-2.14	103.41	114.44
24	b	619	BCR	C35-C13-C14	-2.14	119.93	122.92
34	B	626	HTG	O5-C5-C6	2.14	111.75	106.43
22	C	503	CLA	C3C-C4C-NC	2.13	112.97	110.57
23	a	410	PHO	CHB-C1B-NB	-2.13	120.13	124.58
22	A	406	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
26	D	406	PL9	C36-C37-C38	-2.13	104.82	111.88
22	D	403	CLA	CED-O2D-CGD	2.13	120.82	115.95
22	B	605	CLA	C6-C7-C8	-2.13	109.12	115.77
24	C	515	BCR	C36-C18-C19	2.13	121.47	118.09
22	D	404	CLA	CMC-C2C-C1C	2.13	128.27	125.03
25	b	622	LMG	C9-O8-C28	2.13	125.04	117.13
29	A	414	LMT	O3B-C3B-C2B	2.13	115.29	110.34
22	D	403	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
22	B	615	CLA	CMB-C2B-C3B	2.13	128.79	124.80
35	C	517	DGD	O6D-C1D-O3G	-2.13	104.92	109.94
22	c	909	CLA	CHC-C1C-NC	-2.13	120.98	124.20
22	c	904	CLA	C6-C5-C3	-2.12	107.90	113.01
23	A	407	PHO	C4D-ND-C1D	-2.12	102.94	106.79
22	B	614	CLA	C2A-C1A-CHA	-2.12	120.14	123.86
26	D	406	PL9	C42-C43-C44	-2.12	122.46	127.67
22	C	512	CLA	CMD-C2D-C3D	2.12	128.78	124.80
28	A	413	SQD	C45-O47-C7	-2.12	112.52	117.82
23	D	402	PHO	CED-O2D-CGD	2.12	120.80	115.95
22	B	613	CLA	C3C-C4C-NC	2.12	112.95	110.57
27	A	412	LHG	C6-O8-C23	2.12	124.99	117.13
22	C	513	CLA	C3C-C4C-NC	2.12	112.94	110.57
22	c	909	CLA	OBD-CAD-CBD	2.11	129.02	125.91
24	b	619	BCR	C30-C25-C24	2.11	121.79	115.78
22	a	407	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
22	b	611	CLA	C2A-C1A-CHA	-2.11	120.16	123.86
22	b	602	CLA	O1D-CGD-CBD	-2.11	120.10	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	C16-C15-C13	-2.11	109.19	115.77
27	C	522	LHG	O4-P-O5	2.11	118.86	110.53
24	Y	101	BCR	C11-C12-C13	-2.11	120.49	126.42
26	d	405	PL9	C22-C21-C19	2.11	119.97	112.98
28	a	418	SQD	O48-C23-O10	-2.11	118.17	123.56
37	H	101	RRX	C20-C21-C22	-2.11	124.30	127.31
29	A	414	LMT	O1'-C1'-C2'	2.11	111.62	108.26
39	V	202	HEC	CBA-CAA-C2A	-2.11	108.45	112.47
24	b	619	BCR	C23-C24-C25	-2.11	121.38	127.28
24	C	515	BCR	C11-C12-C13	-2.10	120.50	126.42
24	d	404	BCR	C12-C13-C14	2.10	122.17	118.94
34	V	203	HTG	O5-C5-C6	2.10	111.67	106.43
35	d	406	DGD	O1G-C1A-C2A	2.10	118.68	111.93
22	C	504	CLA	O2A-CGA-O1A	-2.10	118.19	123.56
27	C	522	LHG	P-O6-C4	2.10	124.08	118.30
22	C	512	CLA	CHB-C4A-NA	2.10	127.42	124.51
24	b	619	BCR	C24-C25-C26	-2.10	116.38	121.48
22	a	407	CLA	C4C-C3C-C2C	-2.10	103.85	106.89
23	a	410	PHO	CMC-C2C-C1C	2.10	128.31	125.06
22	B	612	CLA	O1D-CGD-CBD	-2.10	120.14	124.48
22	B	608	CLA	O2A-CGA-O1A	-2.10	118.21	123.56
22	b	613	CLA	C3B-C4B-NB	2.10	111.92	109.21
22	B	611	CLA	CMC-C2C-C1C	2.09	128.22	125.03
22	C	504	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
22	D	401	CLA	O2A-CGA-CBA	2.09	118.65	111.93
27	l	102	LHG	C6-O8-C23	2.09	124.90	117.13
25	A	410	LMG	O8-C28-O10	-2.09	118.22	123.56
29	Z	101	LMT	O3B-C3B-C2B	-2.09	105.49	110.34
28	A	413	SQD	C1-C2-C3	-2.09	105.62	109.98
22	a	408	CLA	CBA-CAA-C2A	-2.09	107.64	113.85
22	B	612	CLA	C1-C2-C3	-2.09	122.43	126.04
22	b	615	CLA	OBD-CAD-C3D	-2.09	124.34	128.04
22	A	405	CLA	C4C-C3C-C2C	-2.09	103.87	106.89
27	D	410	LHG	C34-C33-C32	-2.09	103.67	114.44
27	d	407	LHG	O7-C7-C8	2.08	116.06	111.51
22	c	904	CLA	O2A-C1-C2	2.08	114.11	108.64
24	a	413	BCR	C32-C1-C31	-2.08	102.04	108.51
25	c	920	LMG	O4-C4-C3	-2.08	105.51	110.34
22	c	903	CLA	C3B-C4B-NB	2.08	111.90	109.21
22	d	403	CLA	CHC-C1C-NC	-2.08	121.05	124.20
22	c	907	CLA	CHC-C1C-C2C	-2.08	120.98	126.71
25	A	410	LMG	O6-C1-C2	-2.08	105.92	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	621	SQD	C1-C2-C3	-2.08	105.65	109.98
24	k	101	BCR	C15-C16-C17	-2.08	119.14	123.51
22	C	503	CLA	C16-C15-C13	-2.08	109.29	115.77
22	B	611	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
22	B	607	CLA	C1-O2A-CGA	2.08	122.22	116.54
35	h	102	DGD	C3G-O3G-C1D	-2.08	109.58	113.75
29	a	419	LMT	O4'-C4B-C5B	2.08	114.48	109.29
22	b	602	CLA	C5-C3-C2	-2.07	116.85	121.11
24	A	409	BCR	C35-C13-C12	2.07	121.38	118.09
24	c	915	BCR	C35-C13-C14	-2.07	120.02	122.92
24	b	619	BCR	C37-C22-C21	-2.07	120.02	122.92
24	D	405	BCR	C2-C1-C6	2.07	113.69	110.48
24	c	916	BCR	C37-C22-C21	-2.07	120.02	122.92
24	B	618	BCR	C32-C1-C6	-2.07	106.96	110.30
29	c	921	LMT	C1B-O5B-C5B	2.07	117.77	113.70
35	c	918	DGD	C3A-C2A-C1A	-2.07	106.16	113.62
22	A	405	CLA	CHB-C4A-NA	2.07	127.37	124.51
22	c	913	CLA	C4C-C3C-C2C	-2.07	103.90	106.89
23	A	407	PHO	CHD-C1D-ND	-2.06	120.27	124.58
22	B	616	CLA	CMB-C2B-C3B	2.06	128.67	124.80
22	B	604	CLA	C1D-CHD-C4C	-2.06	119.67	122.48
22	b	604	CLA	OBD-CAD-C3D	-2.06	124.39	128.04
29	B	622	LMT	O5'-C5'-C4'	2.06	113.44	109.68
22	B	611	CLA	CAA-CBA-CGA	-2.06	107.19	113.26
22	b	603	CLA	CED-O2D-CGD	2.06	120.65	115.95
22	c	909	CLA	O2A-CGA-CBA	2.06	118.53	111.93
22	d	403	CLA	O2A-CGA-CBA	2.06	118.53	111.93
22	A	406	CLA	CBC-CAC-C3C	-2.06	106.72	112.43
34	b	624	HTG	C4-C3-C2	2.05	114.43	110.82
37	H	101	RRX	C33-C5-C6	-2.05	122.22	124.51
22	c	913	CLA	O1D-CGD-CBD	-2.05	120.22	124.48
24	Y	101	BCR	C30-C25-C24	2.05	121.62	115.78
29	T	102	LMT	O1'-C1-C2	2.05	116.87	109.59
22	B	614	CLA	C4C-C3C-C2C	-2.05	103.92	106.89
24	B	618	BCR	C1-C6-C5	-2.05	119.72	122.59
24	a	413	BCR	C16-C15-C14	-2.05	119.20	123.51
24	b	619	BCR	C20-C21-C22	-2.05	124.38	127.31
22	C	505	CLA	CMC-C2C-C3C	2.05	131.70	126.11
34	b	626	HTG	C4'-C3'-C2'	-2.05	103.86	114.44
22	D	401	CLA	C16-C15-C13	-2.05	109.38	115.77
35	c	917	DGD	O4D-C4D-C5D	-2.05	104.17	109.29
35	C	517	DGD	O6E-C5E-C6E	2.05	111.53	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	405	PL9	C31-C32-C33	-2.05	105.11	111.88
24	B	619	BCR	C15-C14-C13	-2.04	124.39	127.31
22	B	604	CLA	CAC-C3C-C4C	2.04	127.49	124.82
35	H	102	DGD	C1D-O6D-C5D	-2.04	109.67	113.70
22	a	409	CLA	CED-O2D-CGD	2.04	120.62	115.95
22	A	405	CLA	C3B-C4B-NB	2.04	111.85	109.21
23	D	402	PHO	C4-C3-C2	-2.04	118.37	123.68
22	c	909	CLA	C4C-C3C-C2C	-2.04	103.93	106.89
22	b	608	CLA	CMC-C2C-C3C	2.04	131.68	126.11
24	a	413	BCR	C15-C16-C17	-2.04	119.22	123.51
22	B	614	CLA	C3C-C4C-NC	2.04	112.86	110.57
25	C	520	LMG	O6-C5-C6	2.04	111.52	106.43
22	c	905	CLA	C4C-C3C-C2C	-2.04	103.94	106.89
34	B	623	HTG	C2'-C1'-S1	-2.04	105.81	112.40
24	c	915	BCR	C15-C16-C17	-2.04	119.22	123.51
22	b	605	CLA	C1-O2A-CGA	2.04	122.11	116.54
22	b	603	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
24	C	516	BCR	C8-C7-C6	-2.04	121.57	127.28
29	f	102	LMT	O1B-C4'-C5'	2.04	116.04	108.87
25	b	622	LMG	O8-C9-C8	2.04	114.38	108.43
22	B	603	CLA	CAC-C3C-C2C	2.04	131.01	127.53
29	I	102	LMT	C3'-C4'-C5'	-2.04	106.23	110.92
22	B	615	CLA	OBD-CAD-CBD	2.04	128.90	125.91
22	c	910	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
22	B	604	CLA	CED-O2D-CGD	2.03	120.59	115.95
22	C	514	CLA	C4C-C3C-C2C	-2.03	103.94	106.89
24	b	620	BCR	C23-C24-C25	-2.03	121.58	127.28
26	a	415	PL9	C46-C47-C48	-2.03	105.15	111.88
34	b	626	HTG	O5-C1-C2	-2.03	107.76	110.31
24	C	516	BCR	C23-C24-C25	-2.03	121.59	127.28
23	D	402	PHO	C1C-NC-C4C	-2.03	102.61	106.50
22	B	612	CLA	C4C-C3C-C2C	-2.03	103.95	106.89
25	j	101	LMG	O3-C3-C4	2.03	115.06	110.34
22	B	614	CLA	O2A-CGA-O1A	-2.03	118.37	123.56
22	B	605	CLA	CMD-C2D-C3D	2.03	128.61	124.80
22	D	404	CLA	C3B-C4B-NB	2.03	111.83	109.21
29	A	414	LMT	O2B-C2B-C3B	2.03	115.05	110.34
22	B	604	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
35	C	518	DGD	O1G-C1A-C2A	2.03	118.44	111.93
22	a	409	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
22	c	904	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
22	C	502	CLA	C3B-C4B-NB	2.03	111.83	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	518	DGD	O3D-C3D-C2D	-2.03	105.64	110.34
23	a	411	PHO	C16-C15-C13	-2.03	109.45	115.77
25	b	622	LMG	O6-C5-C4	2.02	113.38	109.68
27	A	412	LHG	O7-C7-O9	-2.02	118.87	122.95
28	C	501	SQD	C44-O6-C1	-2.02	109.69	113.75
28	a	418	SQD	C4-C3-C2	2.02	114.38	110.82
34	B	627	HTG	O5-C1-S1	-2.02	104.83	109.90
22	d	402	CLA	OBD-CAD-C3D	-2.02	124.46	128.04
28	a	414	SQD	O48-C23-O10	-2.02	118.39	123.56
22	B	603	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
22	c	905	CLA	CMC-C2C-C1C	2.02	128.11	125.03
22	B	608	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
22	C	503	CLA	C3B-C4B-NB	2.02	111.82	109.21
22	A	406	CLA	CHB-C4A-NA	2.02	127.30	124.51
22	A	406	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
29	t	101	LMT	C1-O1'-C1'	-2.02	110.47	113.83
22	A	408	CLA	CMD-C2D-C3D	2.02	128.58	124.80
22	D	401	CLA	C4A-NA-C1A	2.02	107.61	106.71
22	C	514	CLA	C3C-C4C-NC	2.02	112.83	110.57
24	y	101	BCR	C35-C13-C12	2.01	121.29	118.09
22	C	506	CLA	C7-C6-C5	-2.01	107.84	113.25
35	C	517	DGD	O1G-C1A-O1A	-2.01	118.42	123.56
22	b	608	CLA	C1-O2A-CGA	2.01	122.04	116.54
24	C	515	BCR	C36-C18-C17	-2.01	120.10	122.92
22	B	606	CLA	OBD-CAD-C3D	-2.01	124.47	128.04
22	B	613	CLA	C4-C3-C5	2.01	118.75	115.29
22	c	910	CLA	C4-C3-C5	2.01	118.75	115.29
22	b	603	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
22	B	614	CLA	CAC-C3C-C4C	2.01	127.45	124.82
22	c	914	CLA	CMB-C2B-C3B	2.01	128.57	124.80
23	a	410	PHO	CHD-C1D-ND	-2.01	120.39	124.58
22	B	603	CLA	CAA-CBA-CGA	-2.01	107.33	113.26
29	a	419	LMT	O3B-C3B-C2B	2.01	115.01	110.34
22	B	617	CLA	CMC-C2C-C1C	2.01	128.09	125.03
24	b	619	BCR	C38-C26-C25	-2.01	122.28	124.51
26	A	411	PL9	C35-C34-C36	2.01	118.74	115.29
25	j	101	LMG	C31-C30-C29	-2.01	105.97	113.20
22	b	616	CLA	OBD-CAD-C3D	-2.00	124.49	128.04
24	c	915	BCR	C24-C23-C22	-2.00	123.20	126.21
22	c	902	CLA	O2A-CGA-O1A	-2.00	118.44	123.56
22	c	909	CLA	C3B-C4B-NB	2.00	111.80	109.21
26	a	415	PL9	C7-C8-C9	-2.00	123.46	126.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	908	CLA	CMD-C2D-C3D	2.00	128.56	124.80
25	J	101	LMG	C9-C8-C7	-2.00	107.02	111.79

All (172) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	503	CLA	NC
22	C	503	CLA	ND
22	C	503	CLA	NA
22	C	510	CLA	NC
22	C	510	CLA	NA
22	C	510	CLA	ND
22	A	406	CLA	NC
22	A	406	CLA	NA
22	d	402	CLA	ND
22	d	402	CLA	NA
22	B	615	CLA	NC
22	B	615	CLA	ND
22	B	615	CLA	NA
22	c	906	CLA	ND
22	c	905	CLA	NC
22	c	905	CLA	NA
22	b	612	CLA	NC
22	b	612	CLA	NA
22	B	606	CLA	NC
22	B	606	CLA	NA
22	C	506	CLA	ND
22	C	506	CLA	NA
22	b	602	CLA	ND
22	b	602	CLA	NA
22	c	912	CLA	NC
22	c	912	CLA	NA
22	b	609	CLA	NC
22	b	609	CLA	NA
22	C	505	CLA	NC
22	C	505	CLA	NA
22	B	610	CLA	NC
22	B	610	CLA	ND
22	B	610	CLA	NA
22	B	605	CLA	NC
22	B	605	CLA	ND
22	B	605	CLA	NA

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Mol	Chain	Res	Type	Atom
22	A	408	CLA	NC
22	A	408	CLA	ND
22	b	613	CLA	NA
22	b	613	CLA	NC
22	b	613	CLA	ND
22	C	513	CLA	NC
22	C	513	CLA	ND
22	C	513	CLA	NA
22	B	612	CLA	NC
22	B	612	CLA	ND
22	B	612	CLA	NA
22	C	514	CLA	NC
22	C	514	CLA	NA
22	D	403	CLA	ND
22	D	403	CLA	NA
22	b	615	CLA	NC
22	b	615	CLA	ND
22	b	615	CLA	NA
22	D	404	CLA	NC
22	D	404	CLA	ND
22	D	404	CLA	NA
22	d	403	CLA	NC
22	d	403	CLA	NA
22	a	408	CLA	NC
22	a	408	CLA	ND
22	a	408	CLA	NA
22	B	604	CLA	NC
22	B	604	CLA	ND
22	B	604	CLA	NA
22	B	613	CLA	NA
22	B	613	CLA	NC
22	B	613	CLA	ND
22	a	407	CLA	NC
22	a	407	CLA	ND
22	a	407	CLA	NA
22	c	914	CLA	NC
22	c	914	CLA	NA
22	c	902	CLA	NC
22	c	902	CLA	ND
22	c	902	CLA	NA
22	b	610	CLA	NA
22	B	607	CLA	NC

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Mol	Chain	Res	Type	Atom
22	B	607	CLA	ND
22	B	607	CLA	NA
22	b	614	CLA	NC
22	b	614	CLA	ND
22	b	614	CLA	NA
22	C	508	CLA	NC
22	C	508	CLA	ND
22	C	508	CLA	NA
22	c	908	CLA	NC
22	c	908	CLA	ND
22	c	908	CLA	NA
22	B	616	CLA	NC
22	B	616	CLA	ND
22	B	616	CLA	NA
22	B	611	CLA	NC
22	B	611	CLA	ND
22	B	611	CLA	NA
22	b	616	CLA	NC
22	b	616	CLA	ND
22	b	616	CLA	NA
22	b	603	CLA	ND
22	B	609	CLA	NC
22	b	608	CLA	NC
22	b	608	CLA	ND
22	b	608	CLA	NA
22	a	409	CLA	NC
22	a	409	CLA	NA
22	c	909	CLA	NC
22	c	909	CLA	NA
22	b	605	CLA	NC
22	b	605	CLA	ND
22	b	605	CLA	NA
22	b	606	CLA	NC
22	b	606	CLA	ND
22	b	606	CLA	NA
22	b	611	CLA	NC
22	b	611	CLA	ND
22	b	611	CLA	NA
22	c	910	CLA	NC
22	c	910	CLA	ND
22	c	910	CLA	NA
22	b	604	CLA	NC

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Mol	Chain	Res	Type	Atom
22	b	604	CLA	ND
22	C	511	CLA	NA
22	C	511	CLA	NC
22	C	511	CLA	ND
22	C	509	CLA	NC
22	C	509	CLA	ND
22	C	509	CLA	NA
22	c	904	CLA	NC
22	c	913	CLA	NC
22	c	913	CLA	ND
22	B	614	CLA	NC
22	B	614	CLA	ND
22	B	614	CLA	NA
22	b	617	CLA	NC
22	b	617	CLA	NA
22	b	617	CLA	ND
22	B	602	CLA	NC
22	B	602	CLA	ND
22	B	602	CLA	NA
22	c	911	CLA	NC
22	c	911	CLA	ND
22	c	911	CLA	NA
22	C	502	CLA	NC
22	C	502	CLA	ND
22	C	502	CLA	NA
22	C	504	CLA	NC
22	B	608	CLA	NC
22	B	608	CLA	ND
22	B	608	CLA	NA
22	B	603	CLA	NC
22	B	603	CLA	ND
22	B	603	CLA	NA
22	b	607	CLA	NC
22	b	607	CLA	ND
22	b	607	CLA	NA
22	A	405	CLA	NC
22	A	405	CLA	ND
22	c	903	CLA	NC
22	c	903	CLA	ND
22	c	903	CLA	NA
22	D	401	CLA	NA
22	c	907	CLA	NC

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Mol	Chain	Res	Type	Atom
22	c	907	CLA	ND
22	c	907	CLA	NA
22	C	512	CLA	NC
22	C	512	CLA	NA
22	B	617	CLA	NC
22	B	617	CLA	ND
22	B	617	CLA	NA
22	C	507	CLA	NC
22	C	507	CLA	ND
22	C	507	CLA	NA

All (1754) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	a	415	PL9	C14-C16-C17-C18
26	a	415	PL9	C35-C34-C36-C37
27	d	407	LHG	C3-O3-P-O5
27	d	407	LHG	C3-O3-P-O6
27	d	407	LHG	C4-O6-P-O4
27	D	409	LHG	O1-C1-C2-C3
22	C	503	CLA	CHA-CBD-CGD-O1D
22	C	503	CLA	CAD-CBD-CGD-O1D
22	B	615	CLA	C2-C1-O2A-CGA
22	B	615	CLA	CHA-CBD-CGD-O2D
22	B	615	CLA	CAD-CBD-CGD-O2D
22	B	606	CLA	C2-C3-C5-C6
22	B	606	CLA	C4-C3-C5-C6
22	b	602	CLA	C2-C1-O2A-CGA
22	b	602	CLA	CHA-CBD-CGD-O1D
22	b	602	CLA	CHA-CBD-CGD-O2D
24	D	405	BCR	C21-C22-C23-C24
24	D	405	BCR	C37-C22-C23-C24
24	D	405	BCR	C23-C24-C25-C30
34	B	627	HTG	C2-C1-S1-C1'
34	B	627	HTG	O5-C1-S1-C1'
27	a	423	LHG	O1-C1-C2-C3
27	a	423	LHG	C4-O6-P-O5
34	b	632	HTG	O5-C1-S1-C1'
34	C	532	HTG	O5-C1-S1-C1'
22	A	408	CLA	C4-C3-C5-C6
24	b	618	BCR	C7-C8-C9-C10
24	b	618	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	CHA-CBD-CGD-O1D
34	c	922	HTG	C2-C1-S1-C1'
34	c	922	HTG	O5-C1-S1-C1'
28	D	408	SQD	O6-C44-C45-C46
28	D	408	SQD	O6-C44-C45-O47
22	b	615	CLA	CHA-CBD-CGD-O1D
22	b	615	CLA	CHA-CBD-CGD-O2D
28	A	413	SQD	C2-C1-O6-C44
28	A	413	SQD	C5-C6-S-O7
28	A	413	SQD	C5-C6-S-O8
28	A	413	SQD	C5-C6-S-O9
22	a	408	CLA	CHA-CBD-CGD-O2D
24	y	101	BCR	C7-C8-C9-C10
24	y	101	BCR	C7-C8-C9-C34
24	y	101	BCR	C37-C22-C23-C24
25	D	412	LMG	C11-C10-O7-C8
22	c	914	CLA	C11-C12-C13-C15
29	t	101	LMT	C2-C1-O1'-C1'
34	D	415	HTG	C2-C1-S1-C1'
34	D	415	HTG	O5-C1-S1-C1'
34	D	415	HTG	C2'-C1'-S1-C1
22	C	508	CLA	CHA-CBD-CGD-O1D
24	b	619	BCR	C7-C8-C9-C10
24	b	619	BCR	C7-C8-C9-C34
29	f	102	LMT	C2'-C1'-O1'-C1
29	f	102	LMT	O5'-C1'-O1'-C1
28	C	501	SQD	C5-C6-S-O8
26	A	411	PL9	C9-C11-C12-C13
26	A	411	PL9	C25-C24-C26-C27
26	A	411	PL9	C26-C27-C28-C29
25	C	531	LMG	C8-C7-O1-C1
29	I	102	LMT	O5'-C1'-O1'-C1
34	l	106	HTG	C2-C1-S1-C1'
34	l	106	HTG	O5-C1-S1-C1'
23	a	411	PHO	CHA-CBD-CGD-O2D
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C21-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
36	e	101	HEM	C1A-C2A-CAA-CBA
36	e	101	HEM	C3A-C2A-CAA-CBA
29	a	419	LMT	O5'-C1'-O1'-C1
27	A	412	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
27	A	412	LHG	C4-O6-P-O4
27	A	412	LHG	C4-O6-P-O5
22	a	409	CLA	CHA-CBD-CGD-O1D
35	d	406	DGD	C2B-C1B-O2G-C2G
22	c	909	CLA	CHA-CBD-CGD-O1D
22	c	909	CLA	CHA-CBD-CGD-O2D
37	h	101	RRX	C7-C8-C9-C10
37	h	101	RRX	C7-C8-C9-C34
24	k	101	BCR	C11-C12-C13-C35
29	E	101	LMT	C2'-C1'-O1'-C1
22	b	606	CLA	C4-C3-C5-C6
35	D	407	DGD	O1G-C1G-C2G-O2G
35	D	407	DGD	C2D-C1D-O3G-C3G
35	D	407	DGD	O6D-C1D-O3G-C3G
25	d	409	LMG	C2-C1-O1-C7
25	d	409	LMG	O6-C1-O1-C7
27	a	416	LHG	C3-O3-P-O5
27	a	416	LHG	C3-O3-P-O6
27	a	416	LHG	C4-O6-P-O5
28	a	418	SQD	C2-C1-O6-C44
28	a	418	SQD	O6-C44-C45-O47
28	l	101	SQD	O5-C5-C6-S
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	c	904	CLA	C1A-C2A-CAA-CBA
28	a	414	SQD	C5-C6-S-O7
28	a	414	SQD	C5-C6-S-O8
28	a	414	SQD	C5-C6-S-O9
29	c	931	LMT	C2'-C1'-O1'-C1
29	c	931	LMT	O5'-C1'-O1'-C1
22	B	602	CLA	CAD-CBD-CGD-O2D
22	B	602	CLA	O2A-C1-C2-C3
22	B	602	CLA	C11-C10-C8-C9
25	B	621	LMG	C2-C1-O1-C7
27	d	401	LHG	C4-O6-P-O3
27	d	401	LHG	C4-O6-P-O4
27	d	401	LHG	C5-C4-O6-P
27	d	401	LHG	O10-C23-O8-C6
27	d	401	LHG	C24-C23-O8-C6
29	B	622	LMT	C2-C1-O1'-C1'
24	d	404	BCR	C21-C22-C23-C24
24	d	404	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	d	404	BCR	C23-C24-C25-C26
22	b	607	CLA	CHA-CBD-CGD-O1D
22	c	903	CLA	CHA-CBD-CGD-O1D
22	c	903	CLA	CAD-CBD-CGD-O1D
22	D	401	CLA	CHA-CBD-CGD-O1D
34	C	521	HTG	O5-C1-S1-C1'
27	l	102	LHG	O1-C1-C2-C3
27	l	102	LHG	C3-O3-P-O4
34	v	203	HTG	C2'-C1'-S1-C1
29	I	102	LMT	C3'-C4'-O1B-C1B
27	A	412	LHG	C8-C7-O7-C5
27	A	412	LHG	O9-C7-O7-C5
23	a	411	PHO	O1D-CGD-O2D-CED
22	C	514	CLA	O1D-CGD-O2D-CED
22	C	510	CLA	C3-C5-C6-C7
22	c	912	CLA	CBD-CGD-O2D-CED
22	C	514	CLA	CBD-CGD-O2D-CED
23	a	411	PHO	CBD-CGD-O2D-CED
22	c	913	CLA	CBD-CGD-O2D-CED
22	b	602	CLA	O1A-CGA-O2A-C1
28	l	101	SQD	O10-C23-O48-C46
25	B	621	LMG	O10-C28-O8-C9
25	A	410	LMG	O10-C28-O8-C9
22	B	617	CLA	O1A-CGA-O2A-C1
22	b	608	CLA	C5-C6-C7-C8
22	c	914	CLA	O1D-CGD-O2D-CED
22	b	617	CLA	O1D-CGD-O2D-CED
25	D	412	LMG	O9-C10-O7-C8
22	C	513	CLA	C3-C5-C6-C7
22	c	913	CLA	C3-C5-C6-C7
22	b	617	CLA	C3-C5-C6-C7
29	c	921	LMT	C4'-C5'-C6'-O6'
22	b	602	CLA	CBA-CGA-O2A-C1
35	d	406	DGD	C2A-C1A-O1G-C1G
28	l	101	SQD	C24-C23-O48-C46
22	c	910	CLA	CBD-CGD-O2D-CED
34	c	922	HTG	O5-C5-C6-O6
29	A	414	LMT	O5B-C5B-C6B-O6B
29	c	921	LMT	O5'-C5'-C6'-O6'
22	B	615	CLA	C4-C3-C5-C6
26	a	415	PL9	C33-C34-C36-C37
22	B	615	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	A	408	CLA	C2-C3-C5-C6
26	A	411	PL9	C23-C24-C26-C27
22	b	606	CLA	C2-C3-C5-C6
22	A	408	CLA	C3-C5-C6-C7
22	b	605	CLA	C3-C5-C6-C7
22	B	602	CLA	C3-C5-C6-C7
25	B	621	LMG	C29-C28-O8-C9
25	A	410	LMG	C29-C28-O8-C9
28	b	621	SQD	C24-C23-O48-C46
22	B	617	CLA	CBA-CGA-O2A-C1
23	a	411	PHO	C2C-C3C-CAC-CBC
34	b	624	HTG	S1-C1'-C2'-C3'
22	b	617	CLA	CBD-CGD-O2D-CED
25	D	412	LMG	O6-C5-C6-O5
29	t	101	LMT	O5'-C5'-C6'-O6'
34	b	627	HTG	O5-C5-C6-O6
25	b	622	LMG	O9-C10-O7-C8
35	d	406	DGD	O1B-C1B-O2G-C2G
34	b	626	HTG	C4-C5-C6-O6
29	a	419	LMT	C4'-C5'-C6'-O6'
29	c	931	LMT	C4'-C5'-C6'-O6'
22	B	615	CLA	O1A-CGA-O2A-C1
25	D	412	LMG	O10-C28-O8-C9
28	b	621	SQD	O10-C23-O48-C46
25	d	409	LMG	C8-C9-O8-C28
29	a	419	LMT	O5'-C5'-C6'-O6'
22	a	407	CLA	C2C-C3C-CAC-CBC
22	c	902	CLA	CBD-CGD-O2D-CED
22	a	412	CLA	C3-C5-C6-C7
29	c	931	LMT	O5'-C5'-C6'-O6'
25	D	412	LMG	C4-C5-C6-O5
29	f	102	LMT	C4'-C5'-C6'-O6'
35	d	406	DGD	O1A-C1A-O1G-C1G
22	C	513	CLA	O1D-CGD-O2D-CED
27	C	522	LHG	C8-C7-O7-C5
25	b	622	LMG	C11-C10-O7-C8
25	d	409	LMG	C11-C10-O7-C8
34	D	415	HTG	O5-C5-C6-O6
35	c	918	DGD	C8B-C9B-CAB-CBB
28	C	501	SQD	C13-C14-C15-C16
27	d	408	LHG	C11-C12-C13-C14
28	a	414	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	D	407	DGD	CCB-CDB-CEB-CFB
34	b	626	HTG	O5-C5-C6-O6
34	c	922	HTG	C4-C5-C6-O6
34	C	532	HTG	S1-C1'-C2'-C3'
34	l	106	HTG	S1-C1'-C2'-C3'
29	I	102	LMT	O5B-C5B-C6B-O6B
34	b	627	HTG	C4-C5-C6-O6
22	B	615	CLA	CBA-CGA-O2A-C1
25	D	412	LMG	C29-C28-O8-C9
29	T	102	LMT	C4'-C5'-C6'-O6'
29	A	414	LMT	C4B-C5B-C6B-O6B
34	l	106	HTG	C4-C5-C6-O6
26	a	415	PL9	C9-C11-C12-C13
26	a	415	PL9	C34-C36-C37-C38
26	D	406	PL9	C39-C41-C42-C43
29	t	101	LMT	C4'-C5'-C6'-O6'
22	b	616	CLA	O1D-CGD-O2D-CED
28	A	413	SQD	O5-C1-O6-C44
28	b	621	SQD	O5-C1-O6-C44
22	c	907	CLA	C5-C6-C7-C8
34	C	532	HTG	C4-C5-C6-O6
27	a	423	LHG	C1-C2-C3-O3
22	b	612	CLA	C13-C15-C16-C17
34	v	203	HTG	C1'-C2'-C3'-C4'
25	i	101	LMG	C29-C28-O8-C9
25	C	531	LMG	C29-C28-O8-C9
25	b	622	LMG	C29-C28-O8-C9
35	D	407	DGD	C2A-C1A-O1G-C1G
22	c	913	CLA	CBA-CGA-O2A-C1
22	B	602	CLA	CBA-CGA-O2A-C1
34	b	624	HTG	C1'-C2'-C3'-C4'
34	l	106	HTG	C1'-C2'-C3'-C4'
22	c	911	CLA	O1D-CGD-O2D-CED
35	c	917	DGD	C1B-C2B-C3B-C4B
22	C	502	CLA	C13-C15-C16-C17
29	T	102	LMT	O5'-C5'-C6'-O6'
29	f	102	LMT	O5'-C5'-C6'-O6'
22	B	607	CLA	O1D-CGD-O2D-CED
28	l	101	SQD	C23-C24-C25-C26
22	C	510	CLA	C14-C13-C15-C16
22	c	905	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	c	912	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C10-C8-C9
22	b	608	CLA	C6-C7-C8-C9
22	c	910	CLA	C11-C10-C8-C9
22	c	913	CLA	C6-C7-C8-C9
22	B	602	CLA	C14-C13-C15-C16
29	A	414	LMT	C4'-C5'-C6'-O6'
35	H	102	DGD	C6B-C7B-C8B-C9B
22	C	505	CLA	C8-C10-C11-C12
22	c	910	CLA	C13-C15-C16-C17
22	b	617	CLA	C5-C6-C7-C8
24	c	916	BCR	C37-C22-C23-C24
25	D	412	LMG	C2-C1-O1-C7
24	Y	101	BCR	C36-C18-C19-C20
24	K	101	BCR	C11-C12-C13-C35
37	h	101	RRX	C37-C22-C23-C24
24	A	409	BCR	C36-C18-C19-C20
22	c	913	CLA	O1A-CGA-O2A-C1
24	b	618	BCR	C11-C12-C13-C14
22	b	612	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	O1D-CGD-O2D-CED
22	D	401	CLA	C2C-C3C-CAC-CBC
27	D	411	LHG	C12-C13-C14-C15
22	c	905	CLA	C4-C3-C5-C6
22	C	510	CLA	C10-C11-C12-C13
22	C	510	CLA	C15-C16-C17-C18
22	B	606	CLA	C13-C15-C16-C17
22	b	609	CLA	C13-C15-C16-C17
22	B	605	CLA	C13-C15-C16-C17
22	A	408	CLA	C13-C15-C16-C17
22	B	607	CLA	C13-C15-C16-C17
22	B	616	CLA	C8-C10-C11-C12
23	a	411	PHO	C4C-C3C-CAC-CBC
22	b	604	CLA	C5-C6-C7-C8
28	C	501	SQD	C7-C8-C9-C10
27	a	416	LHG	C7-C8-C9-C10
25	C	531	LMG	O10-C28-O8-C9
22	D	404	CLA	C15-C16-C17-C18
22	B	607	CLA	C15-C16-C17-C18
22	A	405	CLA	C15-C16-C17-C18
22	C	507	CLA	C10-C11-C12-C13
35	c	918	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
35	c	918	DGD	C1B-C2B-C3B-C4B
25	c	920	LMG	C28-C29-C30-C31
35	C	518	DGD	C1A-C2A-C3A-C4A
25	A	410	LMG	C28-C29-C30-C31
27	a	423	LHG	C24-C23-O8-C6
22	b	612	CLA	C10-C11-C12-C13
22	b	602	CLA	C10-C11-C12-C13
22	d	403	CLA	C8-C10-C11-C12
22	B	616	CLA	C5-C6-C7-C8
25	c	930	LMG	O6-C5-C6-O5
34	l	106	HTG	O5-C5-C6-O6
35	C	517	DGD	O6E-C5E-C6E-O5E
25	j	101	LMG	O6-C5-C6-O5
28	f	101	SQD	O6-C1-O5-C5
27	a	423	LHG	O1-C1-C2-O2
22	C	504	CLA	O1D-CGD-O2D-CED
27	a	423	LHG	C23-C24-C25-C26
28	A	413	SQD	C23-C24-C25-C26
35	d	406	DGD	C1B-C2B-C3B-C4B
25	d	409	LMG	C10-C11-C12-C13
25	C	520	LMG	C10-C11-C12-C13
35	C	518	DGD	C1B-C2B-C3B-C4B
28	b	621	SQD	C23-C24-C25-C26
35	H	102	DGD	C2B-C3B-C4B-C5B
25	b	622	LMG	O10-C28-O8-C9
27	C	522	LHG	O9-C7-O7-C5
25	d	409	LMG	O9-C10-O7-C8
29	t	101	LMT	O1'-C1-C2-C3
22	B	602	CLA	C13-C15-C16-C17
22	c	910	CLA	C2-C1-O2A-CGA
27	C	522	LHG	C7-C8-C9-C10
25	c	930	LMG	C10-C11-C12-C13
27	A	412	LHG	C23-C24-C25-C26
22	c	909	CLA	C11-C10-C8-C7
22	B	614	CLA	C11-C10-C8-C7
22	A	408	CLA	C10-C11-C12-C13
22	C	503	CLA	O1D-CGD-O2D-CED
22	C	512	CLA	O1D-CGD-O2D-CED
24	k	101	BCR	C9-C10-C11-C12
22	b	616	CLA	C5-C6-C7-C8
22	B	609	CLA	C13-C15-C16-C17
22	b	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	i	101	LMG	O10-C28-O8-C9
25	b	622	LMG	C4-C5-C6-O5
26	a	415	PL9	C19-C21-C22-C23
26	a	415	PL9	C24-C26-C27-C28
26	a	415	PL9	C39-C41-C42-C43
26	a	415	PL9	C44-C46-C47-C48
34	b	623	HTG	S1-C1'-C2'-C3'
22	B	612	CLA	C15-C16-C17-C18
22	C	514	CLA	C15-C16-C17-C18
22	B	604	CLA	C5-C6-C7-C8
28	a	418	SQD	C32-C33-C34-C35
22	c	910	CLA	C15-C16-C17-C18
25	B	621	LMG	C28-C29-C30-C31
22	c	909	CLA	CBD-CGD-O2D-CED
29	E	101	LMT	O5'-C1'-O1'-C1
28	a	418	SQD	O5-C1-O6-C44
25	B	621	LMG	O6-C1-O1-C7
22	c	912	CLA	O1D-CGD-O2D-CED
22	A	408	CLA	C8-C10-C11-C12
22	c	908	CLA	C5-C6-C7-C8
22	B	611	CLA	C15-C16-C17-C18
22	b	608	CLA	C15-C16-C17-C18
35	C	519	DGD	O6E-C5E-C6E-O5E
29	f	102	LMT	O1'-C1-C2-C3
22	c	903	CLA	O1D-CGD-O2D-CED
27	L	101	LHG	C4-O6-P-O3
27	l	102	LHG	C3-O3-P-O6
35	D	407	DGD	O1A-C1A-O1G-C1G
22	B	602	CLA	O1A-CGA-O2A-C1
22	d	403	CLA	C15-C16-C17-C18
22	b	616	CLA	C10-C11-C12-C13
22	b	605	CLA	C13-C15-C16-C17
22	C	509	CLA	C13-C15-C16-C17
34	B	623	HTG	C4-C5-C6-O6
27	d	401	LHG	C8-C7-O7-C5
27	D	409	LHG	C23-C24-C25-C26
25	C	531	LMG	C28-C29-C30-C31
27	d	408	LHG	C31-C32-C33-C34
34	B	627	HTG	S1-C1'-C2'-C3'
22	c	905	CLA	C10-C11-C12-C13
22	c	909	CLA	C10-C11-C12-C13
22	B	608	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	d	401	LHG	O9-C7-O7-C5
22	B	607	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	CBD-CGD-O2D-CED
22	c	914	CLA	C4-C3-C5-C6
35	c	918	DGD	C3A-C4A-C5A-C6A
25	c	920	LMG	C15-C16-C17-C18
25	J	101	LMG	C30-C31-C32-C33
25	c	930	LMG	C35-C36-C37-C38
25	d	409	LMG	C20-C21-C22-C23
34	C	532	HTG	O5-C5-C6-O6
27	d	407	LHG	C14-C15-C16-C17
27	a	423	LHG	C26-C27-C28-C29
28	C	501	SQD	C17-C18-C19-C20
25	C	531	LMG	C13-C14-C15-C16
25	b	622	LMG	C19-C20-C21-C22
35	d	406	DGD	CAA-CBA-CCA-CDA
35	d	406	DGD	CBB-CCB-CDB-CEB
35	C	519	DGD	C5B-C6B-C7B-C8B
25	d	409	LMG	C19-C20-C21-C22
28	l	101	SQD	C17-C18-C19-C20
35	C	517	DGD	C2B-C3B-C4B-C5B
35	C	517	DGD	C5B-C6B-C7B-C8B
25	j	101	LMG	C30-C31-C32-C33
29	B	622	LMT	C6-C7-C8-C9
34	C	521	HTG	C1'-C2'-C3'-C4'
25	b	622	LMG	C10-C11-C12-C13
24	b	618	BCR	C9-C10-C11-C12
25	i	101	LMG	C11-C12-C13-C14
35	h	102	DGD	C8A-C9A-CAA-CBA
35	D	407	DGD	C8B-C9B-CAB-CBB
27	l	102	LHG	C10-C11-C12-C13
27	l	102	LHG	C26-C27-C28-C29
35	D	407	DGD	C2B-C1B-O2G-C2G
35	H	102	DGD	CCB-CDB-CEB-CFB
34	b	632	HTG	C2'-C3'-C4'-C5'
35	C	519	DGD	CAB-CBB-CCB-CDB
28	a	418	SQD	C13-C14-C15-C16
28	l	101	SQD	C24-C25-C26-C27
28	l	101	SQD	C34-C35-C36-C37
35	D	407	DGD	O1B-C1B-O2G-C2G
22	B	608	CLA	O1D-CGD-O2D-CED
22	c	906	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	a	407	CLA	C16-C17-C18-C19
22	c	914	CLA	C16-C17-C18-C19
22	C	508	CLA	C16-C17-C18-C20
22	c	913	CLA	C16-C17-C18-C19
22	c	907	CLA	C16-C17-C18-C19
22	C	507	CLA	C16-C17-C18-C20
28	A	413	SQD	C9-C10-C11-C12
35	h	102	DGD	C5B-C6B-C7B-C8B
35	d	406	DGD	C5B-C6B-C7B-C8B
28	a	418	SQD	C12-C13-C14-C15
28	a	418	SQD	C15-C16-C17-C18
28	a	418	SQD	C27-C28-C29-C30
25	B	621	LMG	C14-C15-C16-C17
25	A	410	LMG	C16-C17-C18-C19
27	l	102	LHG	C7-C8-C9-C10
29	T	102	LMT	O1'-C1-C2-C3
29	I	102	LMT	C5-C6-C7-C8
27	d	408	LHG	C10-C11-C12-C13
35	C	519	DGD	C7B-C8B-C9B-CAB
25	d	409	LMG	C12-C13-C14-C15
28	a	418	SQD	C24-C25-C26-C27
28	a	414	SQD	C15-C16-C17-C18
25	A	410	LMG	C29-C30-C31-C32
35	c	917	DGD	C7B-C8B-C9B-CAB
27	l	102	LHG	C32-C33-C34-C35
25	d	409	LMG	C29-C28-O8-C9
35	c	918	DGD	C3B-C4B-C5B-C6B
25	c	930	LMG	C37-C38-C39-C40
28	A	413	SQD	C26-C27-C28-C29
28	C	501	SQD	C15-C16-C17-C18
25	b	622	LMG	C31-C32-C33-C34
35	d	406	DGD	C6A-C7A-C8A-C9A
25	d	409	LMG	C29-C30-C31-C32
27	a	416	LHG	C15-C16-C17-C18
28	l	101	SQD	C14-C15-C16-C17
35	C	518	DGD	CBB-CCB-CDB-CEB
27	d	401	LHG	C27-C28-C29-C30
27	a	423	LHG	O10-C23-O8-C6
34	b	624	HTG	C3'-C4'-C5'-C6'
35	C	519	DGD	C5A-C6A-C7A-C8A
27	a	416	LHG	C11-C12-C13-C14
27	a	416	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
25	C	520	LMG	C31-C32-C33-C34
28	l	101	SQD	C12-C13-C14-C15
25	A	410	LMG	C38-C39-C40-C41
25	A	410	LMG	C39-C40-C41-C42
28	b	621	SQD	C31-C32-C33-C34
27	d	407	LHG	C30-C31-C32-C33
25	c	920	LMG	C35-C36-C37-C38
27	C	522	LHG	C24-C25-C26-C27
25	c	930	LMG	C32-C33-C34-C35
35	c	919	DGD	C4A-C5A-C6A-C7A
35	D	407	DGD	C4A-C5A-C6A-C7A
25	C	520	LMG	C34-C35-C36-C37
28	a	414	SQD	C29-C30-C31-C32
34	C	523	HTG	C2'-C3'-C4'-C5'
25	j	101	LMG	C36-C37-C38-C39
25	j	101	LMG	C37-C38-C39-C40
22	c	908	CLA	C11-C10-C8-C9
22	B	611	CLA	C14-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C14
22	b	604	CLA	C6-C7-C8-C9
22	B	614	CLA	C11-C10-C8-C9
22	A	405	CLA	C14-C13-C15-C16
22	c	907	CLA	C14-C13-C15-C16
28	C	501	SQD	C9-C10-C11-C12
29	a	419	LMT	C11-C10-C9-C8
35	C	519	DGD	CBB-CCB-CDB-CEB
25	d	409	LMG	C34-C35-C36-C37
35	C	517	DGD	C4A-C5A-C6A-C7A
27	D	411	LHG	C13-C14-C15-C16
27	D	411	LHG	C18-C19-C20-C21
27	d	407	LHG	O1-C1-C2-C3
24	b	618	BCR	C11-C12-C13-C35
27	D	410	LHG	O1-C1-C2-C3
22	C	503	CLA	C16-C17-C18-C19
22	b	616	CLA	C16-C17-C18-C20
34	b	626	HTG	S1-C1'-C2'-C3'
25	c	920	LMG	C20-C21-C22-C23
35	h	102	DGD	CBB-CCB-CDB-CEB
25	b	622	LMG	C21-C22-C23-C24
29	Z	101	LMT	C4-C5-C6-C7
27	d	408	LHG	C15-C16-C17-C18
35	c	917	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
27	D	411	LHG	C29-C30-C31-C32
35	C	519	DGD	C1A-C2A-C3A-C4A
27	d	407	LHG	O2-C2-C3-O3
35	H	102	DGD	C7A-C8A-C9A-CAA
25	J	101	LMG	C12-C13-C14-C15
22	c	905	CLA	C15-C16-C17-C18
29	A	414	LMT	C6-C7-C8-C9
35	h	102	DGD	C2B-C3B-C4B-C5B
28	C	501	SQD	C14-C15-C16-C17
25	b	622	LMG	C17-C18-C19-C20
29	I	102	LMT	C6-C7-C8-C9
35	d	406	DGD	C3B-C4B-C5B-C6B
35	d	406	DGD	C4B-C5B-C6B-C7B
35	d	406	DGD	C8B-C9B-CAB-CBB
25	d	409	LMG	C32-C33-C34-C35
28	a	418	SQD	C28-C29-C30-C31
28	a	414	SQD	C16-C17-C18-C19
35	C	518	DGD	C2A-C3A-C4A-C5A
29	B	622	LMT	O1'-C1-C2-C3
29	c	921	LMT	C2-C3-C4-C5
25	A	410	LMG	C21-C22-C23-C24
27	l	102	LHG	C27-C28-C29-C30
28	l	101	SQD	O49-C7-O47-C45
25	B	621	LMG	O9-C10-O7-C8
26	d	405	PL9	C40-C39-C41-C42
22	B	612	CLA	C4-C3-C5-C6
26	a	415	PL9	C13-C14-C16-C17
26	d	405	PL9	C38-C39-C41-C42
22	c	914	CLA	C2-C3-C5-C6
25	i	101	LMG	C14-C15-C16-C17
35	h	102	DGD	C3B-C4B-C5B-C6B
35	c	919	DGD	C9A-CAA-CBA-CCA
29	f	102	LMT	C2-C3-C4-C5
25	b	622	LMG	C14-C15-C16-C17
29	a	419	LMT	C2-C3-C4-C5
35	C	519	DGD	C2A-C3A-C4A-C5A
27	a	416	LHG	C25-C26-C27-C28
25	C	520	LMG	C20-C21-C22-C23
25	A	410	LMG	C20-C21-C22-C23
27	l	102	LHG	C13-C14-C15-C16
25	B	621	LMG	C11-C10-O7-C8
22	b	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	I	102	LMT	C7-C8-C9-C10
35	D	407	DGD	CAA-CBA-CCA-CDA
28	a	418	SQD	C29-C30-C31-C32
28	a	414	SQD	C13-C14-C15-C16
29	c	931	LMT	C7-C8-C9-C10
27	a	423	LHG	C7-C8-C9-C10
28	a	418	SQD	C7-C8-C9-C10
27	d	407	LHG	C26-C27-C28-C29
35	c	918	DGD	CAB-CBB-CCB-CDB
28	A	413	SQD	C28-C29-C30-C31
35	c	919	DGD	C6A-C7A-C8A-C9A
35	c	919	DGD	CCB-CDB-CEB-CFB
29	t	101	LMT	C7-C8-C9-C10
25	d	409	LMG	C11-C12-C13-C14
25	C	520	LMG	C15-C16-C17-C18
28	a	414	SQD	C32-C33-C34-C35
35	C	518	DGD	C7A-C8A-C9A-CAA
35	C	518	DGD	CCA-CDA-CEA-CFA
27	d	401	LHG	C11-C12-C13-C14
27	d	401	LHG	C26-C27-C28-C29
29	t	101	LMT	C1-C2-C3-C4
22	c	906	CLA	C16-C17-C18-C20
22	A	408	CLA	C16-C17-C18-C20
22	C	514	CLA	C16-C17-C18-C19
22	c	914	CLA	C16-C17-C18-C20
22	C	508	CLA	C16-C17-C18-C19
22	c	908	CLA	C16-C17-C18-C20
22	B	611	CLA	C16-C17-C18-C20
22	b	616	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C20
27	C	522	LHG	C26-C27-C28-C29
28	C	501	SQD	C18-C19-C20-C21
29	Z	101	LMT	C3-C4-C5-C6
35	d	406	DGD	CCA-CDA-CEA-CFA
28	a	418	SQD	C18-C19-C20-C21
28	a	414	SQD	C18-C19-C20-C21
25	C	520	LMG	C18-C19-C20-C21
28	a	414	SQD	C31-C32-C33-C34
25	A	410	LMG	C17-C18-C19-C20
27	l	102	LHG	C16-C17-C18-C19
29	I	102	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
22	c	910	CLA	O1D-CGD-O2D-CED
28	C	501	SQD	C30-C31-C32-C33
35	D	407	DGD	C2B-C3B-C4B-C5B
28	a	418	SQD	C17-C18-C19-C20
28	a	414	SQD	C27-C28-C29-C30
29	c	931	LMT	C2-C3-C4-C5
22	b	617	CLA	C10-C11-C12-C13
35	C	518	DGD	C6A-C7A-C8A-C9A
25	B	621	LMG	C15-C16-C17-C18
22	c	907	CLA	C15-C16-C17-C18
27	l	102	LHG	C28-C29-C30-C31
23	a	410	PHO	O2A-C1-C2-C3
29	A	414	LMT	C2-C1-O1'-C1'
29	f	102	LMT	C2-C1-O1'-C1'
28	C	501	SQD	O6-C44-C45-C46
29	c	931	LMT	C2-C1-O1'-C1'
25	c	920	LMG	C30-C31-C32-C33
35	c	919	DGD	C4B-C5B-C6B-C7B
35	D	407	DGD	C3B-C4B-C5B-C6B
27	a	416	LHG	C12-C13-C14-C15
25	C	520	LMG	C16-C17-C18-C19
29	B	622	LMT	C1-C2-C3-C4
34	D	415	HTG	C1'-C2'-C3'-C4'
35	c	918	DGD	CAA-CBA-CCA-CDA
25	J	101	LMG	C34-C35-C36-C37
25	i	101	LMG	C12-C13-C14-C15
27	A	412	LHG	C26-C27-C28-C29
27	a	416	LHG	C32-C33-C34-C35
22	A	405	CLA	C13-C15-C16-C17
27	l	102	LHG	C29-C30-C31-C32
27	C	522	LHG	C9-C10-C11-C12
28	a	414	SQD	C24-C25-C26-C27
22	B	606	CLA	C16-C17-C18-C20
22	A	408	CLA	C16-C17-C18-C19
22	a	407	CLA	C16-C17-C18-C20
22	c	909	CLA	C16-C17-C18-C19
35	H	102	DGD	CAB-CBB-CCB-CDB
25	b	622	LMG	C18-C19-C20-C21
27	d	408	LHG	C13-C14-C15-C16
27	a	416	LHG	C9-C10-C11-C12
25	d	409	LMG	C28-C29-C30-C31
22	B	605	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	i	101	LMG	C11-C10-O7-C8
27	a	416	LHG	C8-C7-O7-C5
28	l	101	SQD	C8-C7-O47-C45
25	A	410	LMG	C11-C10-O7-C8
35	c	919	DGD	C2A-C3A-C4A-C5A
22	B	614	CLA	O1D-CGD-O2D-CED
28	f	101	SQD	O5-C1-O6-C44
27	D	410	LHG	O1-C1-C2-O2
35	c	918	DGD	CBA-CCA-CDA-CEA
25	c	920	LMG	C18-C19-C20-C21
22	a	407	CLA	C4C-C3C-CAC-CBC
35	d	406	DGD	C9A-CAA-CBA-CCA
28	l	101	SQD	C27-C28-C29-C30
28	l	101	SQD	C28-C29-C30-C31
29	f	102	LMT	C11-C10-C9-C8
25	J	101	LMG	O6-C5-C6-O5
34	b	632	HTG	O5-C5-C6-O6
25	C	520	LMG	C28-C29-C30-C31
29	Z	101	LMT	C1-C2-C3-C4
25	c	930	LMG	C34-C35-C36-C37
22	B	605	CLA	C10-C11-C12-C13
35	D	407	DGD	C2A-C3A-C4A-C5A
22	c	913	CLA	C15-C16-C17-C18
28	b	621	SQD	C28-C29-C30-C31
22	B	612	CLA	C2-C3-C5-C6
22	A	406	CLA	C6-C7-C8-C9
22	C	507	CLA	C16-C17-C18-C19
28	A	413	SQD	C11-C12-C13-C14
28	A	413	SQD	C27-C28-C29-C30
28	C	501	SQD	C12-C13-C14-C15
35	D	407	DGD	C5A-C6A-C7A-C8A
28	a	418	SQD	C31-C32-C33-C34
28	l	101	SQD	C26-C27-C28-C29
35	C	517	DGD	C4B-C5B-C6B-C7B
35	C	518	DGD	C5A-C6A-C7A-C8A
24	Y	101	BCR	C1-C6-C7-C8
27	d	407	LHG	C1-C2-C3-O3
27	D	410	LHG	C14-C15-C16-C17
22	a	408	CLA	C15-C16-C17-C18
27	a	416	LHG	C29-C30-C31-C32
25	B	621	LMG	C12-C13-C14-C15
25	j	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	i	101	LMG	C10-C11-C12-C13
24	D	405	BCR	C23-C24-C25-C26
24	b	618	BCR	C1-C6-C7-C8
24	b	618	BCR	C5-C6-C7-C8
37	h	101	RRX	C1-C6-C7-C8
37	h	101	RRX	C5-C6-C7-C8
24	d	404	BCR	C23-C24-C25-C30
27	a	416	LHG	O9-C7-O7-C5
27	D	409	LHG	C10-C11-C12-C13
27	L	101	LHG	C13-C14-C15-C16
25	i	101	LMG	C34-C35-C36-C37
25	d	409	LMG	O10-C28-O8-C9
35	c	917	DGD	C8A-C9A-CAA-CBA
28	b	621	SQD	C29-C30-C31-C32
22	c	904	CLA	CBA-CGA-O2A-C1
27	D	409	LHG	C31-C32-C33-C34
25	c	920	LMG	C19-C20-C21-C22
35	D	407	DGD	C7B-C8B-C9B-CAB
27	a	416	LHG	C10-C11-C12-C13
28	a	418	SQD	C16-C17-C18-C19
22	C	510	CLA	C2-C1-O2A-CGA
27	a	423	LHG	C29-C30-C31-C32
35	C	518	DGD	CAA-CBA-CCA-CDA
35	C	518	DGD	C3B-C4B-C5B-C6B
27	l	102	LHG	C34-C35-C36-C37
22	b	610	CLA	C3-C5-C6-C7
22	B	603	CLA	C3-C5-C6-C7
22	C	514	CLA	C16-C17-C18-C20
22	b	612	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C15
22	A	408	CLA	C11-C12-C13-C15
22	D	404	CLA	C6-C7-C8-C10
22	d	403	CLA	C6-C7-C8-C10
22	c	908	CLA	C11-C10-C8-C7
22	B	611	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C15
22	b	608	CLA	C12-C13-C15-C16
22	a	409	CLA	C6-C7-C8-C10
22	a	412	CLA	C6-C7-C8-C10
22	b	604	CLA	C6-C7-C8-C10
22	C	509	CLA	C12-C13-C15-C16
22	c	913	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C6-C7-C8-C10
22	c	907	CLA	C12-C13-C15-C16
25	c	920	LMG	C11-C12-C13-C14
28	A	413	SQD	C17-C18-C19-C20
28	A	413	SQD	C18-C19-C20-C21
28	A	413	SQD	C25-C26-C27-C28
29	a	419	LMT	C6-C7-C8-C9
27	d	408	LHG	C28-C29-C30-C31
22	a	412	CLA	O1D-CGD-O2D-CED
22	B	602	CLA	O1D-CGD-O2D-CED
29	Z	101	LMT	O5B-C5B-C6B-O6B
27	D	409	LHG	C15-C16-C17-C18
27	D	409	LHG	C29-C30-C31-C32
28	A	413	SQD	C15-C16-C17-C18
22	B	607	CLA	C10-C11-C12-C13
25	C	520	LMG	C39-C40-C41-C42
22	b	607	CLA	C2A-CAA-CBA-CGA
25	i	101	LMG	O9-C10-O7-C8
34	b	626	HTG	C3'-C4'-C5'-C6'
25	i	101	LMG	C30-C31-C32-C33
35	C	517	DGD	C6A-C7A-C8A-C9A
25	A	410	LMG	C18-C19-C20-C21
29	a	419	LMT	C1-C2-C3-C4
22	B	606	CLA	C16-C17-C18-C19
28	l	101	SQD	C33-C34-C35-C36
29	c	921	LMT	C6-C7-C8-C9
22	B	608	CLA	C15-C16-C17-C18
28	b	621	SQD	C24-C25-C26-C27
22	c	904	CLA	O1A-CGA-O2A-C1
22	d	403	CLA	CBD-CGD-O2D-CED
26	a	415	PL9	C15-C14-C16-C17
26	A	411	PL9	C30-C29-C31-C32
27	D	409	LHG	C28-C29-C30-C31
27	L	101	LHG	C24-C25-C26-C27
25	i	101	LMG	C35-C36-C37-C38
27	D	410	LHG	C32-C33-C34-C35
22	c	905	CLA	C2-C3-C5-C6
22	B	612	CLA	C13-C15-C16-C17
35	d	406	DGD	C2A-C3A-C4A-C5A
22	C	502	CLA	C15-C16-C17-C18
27	a	423	LHG	O6-C4-C5-O7
22	A	406	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	J	101	LMG	C16-C17-C18-C19
27	C	522	LHG	C12-C13-C14-C15
28	a	414	SQD	C30-C31-C32-C33
29	c	921	LMT	C4-C5-C6-C7
22	a	409	CLA	C8-C10-C11-C12
29	E	101	LMT	C11-C10-C9-C8
35	D	407	DGD	C3A-C4A-C5A-C6A
22	c	904	CLA	C8-C10-C11-C12
29	I	102	LMT	C4-C5-C6-C7
35	D	407	DGD	C6B-C7B-C8B-C9B
28	A	413	SQD	O6-C44-C45-O47
28	C	501	SQD	O6-C44-C45-O47
35	d	406	DGD	O2G-C2G-C3G-O3G
28	a	414	SQD	O6-C44-C45-O47
25	c	920	LMG	C17-C18-C19-C20
22	c	906	CLA	C13-C15-C16-C17
35	c	919	DGD	C8A-C9A-CAA-CBA
22	c	908	CLA	C13-C15-C16-C17
25	C	520	LMG	C12-C13-C14-C15
28	l	101	SQD	C11-C12-C13-C14
25	A	410	LMG	O9-C10-O7-C8
35	c	917	DGD	O6E-C5E-C6E-O5E
29	c	921	LMT	C1-C2-C3-C4
25	C	531	LMG	C12-C13-C14-C15
28	l	101	SQD	C9-C10-C11-C12
28	a	414	SQD	C7-C8-C9-C10
25	i	101	LMG	C16-C17-C18-C19
28	A	413	SQD	C16-C17-C18-C19
35	D	407	DGD	CCA-CDA-CEA-CFA
22	b	612	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14
22	A	408	CLA	C11-C12-C13-C14
22	D	404	CLA	C6-C7-C8-C9
22	d	403	CLA	C6-C7-C8-C9
22	B	607	CLA	C11-C12-C13-C14
22	b	614	CLA	C11-C10-C8-C9
22	B	616	CLA	C11-C12-C13-C14
22	b	608	CLA	C14-C13-C15-C16
22	a	409	CLA	C6-C7-C8-C9
22	c	909	CLA	C11-C10-C8-C9
22	a	412	CLA	C6-C7-C8-C9
22	C	509	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	913	CLA	C14-C13-C15-C16
22	c	909	CLA	C1A-C2A-CAA-CBA
22	C	507	CLA	C1A-C2A-CAA-CBA
28	C	501	SQD	C28-C29-C30-C31
22	b	608	CLA	C8-C10-C11-C12
35	d	406	DGD	CAB-CBB-CCB-CDB
22	c	910	CLA	C8-C10-C11-C12
25	B	621	LMG	C13-C14-C15-C16
22	C	507	CLA	C5-C6-C7-C8
22	B	611	CLA	C16-C17-C18-C19
29	a	419	LMT	O5B-C5B-C6B-O6B
27	a	416	LHG	C4-O6-P-O3
27	D	409	LHG	C16-C17-C18-C19
28	C	501	SQD	C34-C35-C36-C37
25	A	410	LMG	C33-C34-C35-C36
34	D	414	HTG	C2'-C3'-C4'-C5'
27	L	101	LHG	C16-C17-C18-C19
29	T	102	LMT	C11-C10-C9-C8
25	i	101	LMG	C33-C34-C35-C36
29	t	101	LMT	C11-C10-C9-C8
27	A	412	LHG	C27-C28-C29-C30
35	C	519	DGD	C9A-CAA-CBA-CCA
35	C	519	DGD	C2B-C3B-C4B-C5B
22	a	412	CLA	C15-C16-C17-C18
35	c	917	DGD	C9A-CAA-CBA-CCA
35	c	919	DGD	C3B-C4B-C5B-C6B
35	c	919	DGD	C5B-C6B-C7B-C8B
23	D	402	PHO	C2C-C3C-CAC-CBC
22	D	404	CLA	C8-C10-C11-C12
27	d	408	LHG	C25-C26-C27-C28
25	A	410	LMG	C31-C32-C33-C34
26	A	411	PL9	C28-C29-C31-C32
28	C	501	SQD	C8-C7-O47-C45
25	c	920	LMG	C32-C33-C34-C35
27	d	408	LHG	C16-C17-C18-C19
35	C	519	DGD	C4A-C5A-C6A-C7A
25	d	409	LMG	C21-C22-C23-C24
35	C	517	DGD	CAA-CBA-CCA-CDA
34	B	623	HTG	O5-C5-C6-O6
22	D	401	CLA	O1D-CGD-O2D-CED
22	c	910	CLA	C10-C11-C12-C13
22	B	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	c	908	CLA	C16-C17-C18-C19
22	c	913	CLA	C16-C17-C18-C20
22	c	907	CLA	C16-C17-C18-C20
26	A	411	PL9	C4-C3-C7-C8
35	C	519	DGD	O6D-C5D-C6D-O5D
28	l	101	SQD	C31-C32-C33-C34
29	a	419	LMT	O5B-C1B-O1B-C4'
35	c	918	DGD	C8A-C9A-CAA-CBA
22	b	602	CLA	C13-C15-C16-C17
35	C	519	DGD	C9B-CAB-CBB-CCB
27	C	522	LHG	C23-C24-C25-C26
29	a	419	LMT	C2B-C1B-O1B-C4'
27	d	407	LHG	C12-C13-C14-C15
25	J	101	LMG	C17-C18-C19-C20
29	c	921	LMT	O1'-C1-C2-C3
25	c	920	LMG	C12-C13-C14-C15
34	b	623	HTG	C2'-C3'-C4'-C5'
27	l	102	LHG	C30-C31-C32-C33
22	A	406	CLA	C6-C7-C8-C10
29	E	101	LMT	O5'-C5'-C6'-O6'
27	L	101	LHG	C14-C15-C16-C17
28	a	414	SQD	C14-C15-C16-C17
25	A	410	LMG	C35-C36-C37-C38
35	c	917	DGD	C2A-C3A-C4A-C5A
28	C	501	SQD	C33-C34-C35-C36
25	C	520	LMG	C17-C18-C19-C20
25	C	520	LMG	C33-C34-C35-C36
28	A	413	SQD	O6-C44-C45-C46
25	D	412	LMG	O1-C7-C8-C9
27	d	408	LHG	C4-C5-C6-O8
35	D	407	DGD	C1G-C2G-C3G-O3G
25	d	409	LMG	C7-C8-C9-O8
28	a	414	SQD	O6-C44-C45-C46
25	B	621	LMG	C7-C8-C9-O8
35	C	518	DGD	O6D-C5D-C6D-O5D
35	c	919	DGD	C6B-C7B-C8B-C9B
22	c	911	CLA	C8-C10-C11-C12
25	A	410	LMG	C22-C23-C24-C25
35	H	102	DGD	CDB-CEB-CFB-CGB
27	a	423	LHG	C14-C15-C16-C17
25	b	622	LMG	C15-C16-C17-C18
25	i	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C10-C11-C12-C13
34	B	626	HTG	C2'-C3'-C4'-C5'
29	Z	101	LMT	C9-C10-C11-C12
35	c	917	DGD	C8B-C9B-CAB-CBB
27	L	101	LHG	C10-C11-C12-C13
28	A	413	SQD	C19-C20-C21-C22
25	C	531	LMG	C14-C15-C16-C17
29	I	102	LMT	C11-C10-C9-C8
29	I	102	LMT	C9-C10-C11-C12
25	C	520	LMG	C22-C23-C24-C25
22	b	605	CLA	C16-C17-C18-C19
28	l	101	SQD	C25-C26-C27-C28
35	h	102	DGD	CDB-CEB-CFB-CGB
25	b	622	LMG	C13-C14-C15-C16
28	l	101	SQD	C19-C20-C21-C22
35	C	517	DGD	C3B-C4B-C5B-C6B
25	A	410	LMG	C11-C12-C13-C14
34	D	415	HTG	C4'-C5'-C6'-C7'
27	A	412	LHG	C25-C26-C27-C28
22	B	612	CLA	C8-C10-C11-C12
25	b	622	LMG	C12-C13-C14-C15
34	B	626	HTG	C3'-C4'-C5'-C6'
29	Z	101	LMT	C11-C10-C9-C8
28	l	101	SQD	C10-C11-C12-C13
25	B	621	LMG	C17-C18-C19-C20
29	c	921	LMT	O5B-C5B-C6B-O6B
27	l	102	LHG	C9-C10-C11-C12
28	A	413	SQD	C30-C31-C32-C33
27	d	408	LHG	C19-C20-C21-C22
23	D	402	PHO	C8-C10-C11-C12
28	a	414	SQD	C35-C36-C37-C38
25	C	531	LMG	O6-C5-C6-O5
35	h	102	DGD	C6B-C7B-C8B-C9B
22	B	615	CLA	O1D-CGD-O2D-CED
35	c	918	DGD	C2B-C3B-C4B-C5B
35	C	517	DGD	C6B-C7B-C8B-C9B
27	L	101	LHG	O6-C4-C5-O7
22	C	503	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19
22	C	509	CLA	C16-C17-C18-C19
29	A	414	LMT	C9-C10-C11-C12
22	b	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
27	A	412	LHG	C32-C33-C34-C35
28	b	621	SQD	C35-C36-C37-C38
27	l	102	LHG	C35-C36-C37-C38
35	H	102	DGD	O2G-C1B-C2B-C3B
35	c	918	DGD	C2G-C3G-O3G-C1D
35	c	918	DGD	C5D-C6D-O5D-C1E
35	C	518	DGD	C2G-C3G-O3G-C1D
35	c	919	DGD	C8B-C9B-CAB-CBB
28	l	101	SQD	C13-C14-C15-C16
22	c	908	CLA	O1D-CGD-O2D-CED
25	c	920	LMG	C39-C40-C41-C42
22	b	613	CLA	C8-C10-C11-C12
27	d	408	LHG	C12-C13-C14-C15
35	C	518	DGD	C3A-C4A-C5A-C6A
22	C	513	CLA	CBA-CGA-O2A-C1
26	a	415	PL9	C45-C44-C46-C47
34	D	414	HTG	C1'-C2'-C3'-C4'
29	A	414	LMT	C11-C10-C9-C8
35	C	518	DGD	CDB-CEB-CFB-CGB
27	a	423	LHG	O7-C5-C6-O8
27	A	412	LHG	C3-O3-P-O5
25	c	930	LMG	C38-C39-C40-C41
25	i	101	LMG	C15-C16-C17-C18
22	B	614	CLA	C10-C11-C12-C13
29	T	102	LMT	C1-C2-C3-C4
27	d	407	LHG	C29-C30-C31-C32
27	d	407	LHG	C35-C36-C37-C38
25	i	101	LMG	C13-C14-C15-C16
35	d	406	DGD	C7B-C8B-C9B-CAB
22	c	909	CLA	C16-C17-C18-C20
22	d	402	CLA	C11-C12-C13-C15
22	c	905	CLA	C11-C10-C8-C7
22	c	905	CLA	C11-C12-C13-C15
22	B	605	CLA	C11-C12-C13-C15
22	B	612	CLA	C12-C13-C15-C16
22	a	407	CLA	C12-C13-C15-C16
22	B	607	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C10-C8-C7
22	c	908	CLA	C11-C12-C13-C15
22	B	616	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C12-C13-C15-C16
22	a	409	CLA	C11-C10-C8-C7
22	b	605	CLA	C6-C7-C8-C10
22	a	412	CLA	C11-C12-C13-C15
22	c	910	CLA	C11-C10-C8-C7
22	B	602	CLA	C11-C10-C8-C7
22	B	602	CLA	C12-C13-C15-C16
22	A	405	CLA	C12-C13-C15-C16
22	c	903	CLA	C11-C12-C13-C15
35	d	406	DGD	C2B-C3B-C4B-C5B
22	c	909	CLA	C13-C15-C16-C17
34	D	414	HTG	C4'-C5'-C6'-C7'
22	b	611	CLA	CBD-CGD-O2D-CED
27	L	101	LHG	C19-C20-C21-C22
27	D	410	LHG	C26-C27-C28-C29
35	c	919	DGD	CBB-CCB-CDB-CEB
28	C	501	SQD	C11-C12-C13-C14
29	a	419	LMT	O1'-C1-C2-C3
25	B	621	LMG	C29-C30-C31-C32
29	T	102	LMT	C9-C10-C11-C12
29	A	414	LMT	C4-C5-C6-C7
34	D	415	HTG	C3'-C4'-C5'-C6'
25	j	101	LMG	C16-C17-C18-C19
34	C	521	HTG	C2'-C3'-C4'-C5'
22	A	408	CLA	C11-C10-C8-C9
22	B	612	CLA	C14-C13-C15-C16
22	C	514	CLA	C11-C10-C8-C9
22	D	404	CLA	C14-C13-C15-C16
22	a	407	CLA	C14-C13-C15-C16
22	B	607	CLA	C14-C13-C15-C16
22	a	409	CLA	C11-C10-C8-C9
22	b	605	CLA	C6-C7-C8-C9
22	a	412	CLA	C11-C12-C13-C14
22	c	903	CLA	C11-C12-C13-C14
27	a	416	LHG	C33-C34-C35-C36
35	C	519	DGD	C4D-C5D-C6D-O5D
22	B	605	CLA	O1D-CGD-O2D-CED
34	b	627	HTG	C3'-C4'-C5'-C6'
22	C	504	CLA	C8-C10-C11-C12
25	b	622	LMG	C2-C1-O1-C7
29	A	414	LMT	C3-C4-C5-C6
29	A	414	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
34	b	624	HTG	C2'-C3'-C4'-C5'
22	d	403	CLA	C13-C15-C16-C17
22	b	603	CLA	C13-C15-C16-C17
25	d	409	LMG	C22-C23-C24-C25
29	c	931	LMT	C4-C5-C6-C7
25	c	920	LMG	C33-C34-C35-C36
25	c	930	LMG	C11-C12-C13-C14
25	i	101	LMG	C40-C41-C42-C43
29	A	414	LMT	C2-C3-C4-C5
35	h	102	DGD	CDA-CEA-CFA-CGA
35	C	517	DGD	CAB-CBB-CCB-CDB
27	a	416	LHG	C13-C14-C15-C16
22	c	904	CLA	C5-C6-C7-C8
25	b	622	LMG	C16-C17-C18-C19
25	B	621	LMG	C10-C11-C12-C13
22	b	604	CLA	C2-C3-C5-C6
25	A	410	LMG	C19-C20-C21-C22
27	l	102	LHG	C11-C10-C9-C8
27	L	101	LHG	O6-C4-C5-C6
22	c	914	CLA	CBA-CGA-O2A-C1
25	c	920	LMG	C31-C32-C33-C34
22	c	914	CLA	C5-C6-C7-C8
22	c	914	CLA	C13-C15-C16-C17
29	I	102	LMT	C4B-C5B-C6B-O6B
29	E	101	LMT	C3-C4-C5-C6
27	d	408	LHG	C2-C3-O3-P
22	a	408	CLA	C2C-C3C-CAC-CBC
22	B	609	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	O1D-CGD-O2D-CED
28	a	418	SQD	C24-C23-O48-C46
22	a	409	CLA	C10-C11-C12-C13
22	C	513	CLA	O1A-CGA-O2A-C1
35	c	917	DGD	O6D-C5D-C6D-O5D
35	c	918	DGD	CDA-CEA-CFA-CGA
25	i	101	LMG	O8-C28-C29-C30
35	c	918	DGD	C5B-C6B-C7B-C8B
25	b	622	LMG	C32-C33-C34-C35
35	C	519	DGD	CCB-CDB-CEB-CFB
27	a	416	LHG	C31-C32-C33-C34
25	C	520	LMG	C38-C39-C40-C41
25	j	101	LMG	C13-C14-C15-C16
22	C	514	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	A	407	PHO	O2A-C1-C2-C3
22	a	409	CLA	C14-C13-C15-C16
22	D	404	CLA	C3-C5-C6-C7
34	b	626	HTG	C2'-C3'-C4'-C5'
27	L	101	LHG	C15-C16-C17-C18
28	A	413	SQD	C11-C10-C9-C8
22	D	404	CLA	C16-C17-C18-C19
35	H	102	DGD	O1G-C1G-C2G-C3G
29	T	102	LMT	C2-C1-O1'-C1'
27	a	423	LHG	C4-C5-C6-O8
25	i	101	LMG	C7-C8-C9-O8
35	d	406	DGD	O1G-C1G-C2G-C3G
35	d	406	DGD	C1G-C2G-C3G-O3G
28	a	418	SQD	O6-C44-C45-C46
28	l	101	SQD	C44-C45-C46-O48
25	B	621	LMG	O1-C7-C8-C9
25	J	101	LMG	C35-C36-C37-C38
25	i	101	LMG	C22-C23-C24-C25
25	i	101	LMG	C29-C30-C31-C32
22	c	914	CLA	C10-C11-C12-C13
35	c	919	DGD	CDB-CEB-CFB-CGB
35	c	917	DGD	CDA-CEA-CFA-CGA
35	c	917	DGD	C4D-C5D-C6D-O5D
25	i	101	LMG	C31-C32-C33-C34
28	C	501	SQD	C27-C28-C29-C30
35	C	517	DGD	C5A-C6A-C7A-C8A
24	k	101	BCR	C19-C20-C21-C22
25	c	920	LMG	C21-C22-C23-C24
22	c	905	CLA	C8-C10-C11-C12
34	C	532	HTG	C2'-C3'-C4'-C5'
29	t	101	LMT	C9-C10-C11-C12
35	C	519	DGD	CDB-CEB-CFB-CGB
25	A	410	LMG	C36-C37-C38-C39
35	C	519	DGD	CBA-CCA-CDA-CEA
22	C	502	CLA	O1D-CGD-O2D-CED
27	L	101	LHG	O2-C2-C3-O3
27	a	423	LHG	O2-C2-C3-O3
28	C	501	SQD	C35-C36-C37-C38
35	d	406	DGD	CDB-CEB-CFB-CGB
25	D	412	LMG	C12-C13-C14-C15
28	a	418	SQD	C9-C10-C11-C12
22	c	903	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	f	102	LMT	C1-C2-C3-C4
27	A	412	LHG	C33-C34-C35-C36
35	d	406	DGD	C4A-C5A-C6A-C7A
25	B	621	LMG	C18-C19-C20-C21
35	c	917	DGD	C3B-C4B-C5B-C6B
27	D	411	LHG	C16-C17-C18-C19
25	d	409	LMG	C36-C37-C38-C39
22	B	615	CLA	C2A-CAA-CBA-CGA
28	f	101	SQD	O5-C5-C6-S
29	f	102	LMT	C9-C10-C11-C12
27	A	412	LHG	C24-C25-C26-C27
27	d	407	LHG	O1-C1-C2-O2
27	a	423	LHG	C28-C29-C30-C31
22	b	602	CLA	C16-C17-C18-C20
22	c	911	CLA	C16-C17-C18-C20
28	C	501	SQD	O49-C7-O47-C45
35	c	918	DGD	C6A-C7A-C8A-C9A
35	d	406	DGD	O1G-C1G-C2G-O2G
35	D	407	DGD	O2G-C2G-C3G-O3G
28	l	101	SQD	O47-C45-C46-O48
25	B	621	LMG	O7-C8-C9-O8
27	L	101	LHG	C11-C10-C9-C8
22	C	508	CLA	C5-C6-C7-C8
35	C	519	DGD	C2A-C1A-O1G-C1G
29	t	101	LMT	C3-C4-C5-C6
35	D	407	DGD	C5B-C6B-C7B-C8B
22	b	615	CLA	C4-C3-C5-C6
27	d	408	LHG	C32-C33-C34-C35
25	C	520	LMG	C37-C38-C39-C40
22	C	511	CLA	C8-C10-C11-C12
35	C	518	DGD	CDA-CEA-CFA-CGA
26	a	415	PL9	C43-C44-C46-C47
29	t	101	LMT	C2-C3-C4-C5
22	b	612	CLA	C16-C17-C18-C19
22	b	612	CLA	C16-C17-C18-C20
35	C	518	DGD	C9A-CAA-CBA-CCA
22	D	401	CLA	C4C-C3C-CAC-CBC
27	D	411	LHG	C2-C3-O3-P
28	C	501	SQD	C10-C11-C12-C13
35	C	518	DGD	CBA-CCA-CDA-CEA
27	L	101	LHG	C25-C26-C27-C28
24	c	916	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	B	612	CLA	C11-C12-C13-C14
22	c	914	CLA	C11-C12-C13-C14
24	b	619	BCR	C23-C24-C25-C26
24	b	619	BCR	C23-C24-C25-C30
22	c	908	CLA	C14-C13-C15-C16
22	B	611	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C12-C13-C14
24	C	515	BCR	C23-C24-C25-C26
24	C	515	BCR	C23-C24-C25-C30
22	B	614	CLA	C11-C12-C13-C14
22	B	603	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C12-C13-C14
27	a	416	LHG	C14-C15-C16-C17
35	c	917	DGD	C3A-C4A-C5A-C6A
24	y	101	BCR	C21-C22-C23-C24
37	h	101	RRX	C21-C22-C23-C24
35	c	918	DGD	O6E-C1E-O5D-C6D
35	c	917	DGD	O6E-C1E-O5D-C6D
34	b	632	HTG	C3'-C4'-C5'-C6'
28	C	501	SQD	C31-C32-C33-C34
22	C	507	CLA	C2-C1-O2A-CGA
22	b	613	CLA	O1D-CGD-O2D-CED
28	C	501	SQD	C24-C25-C26-C27
29	Z	101	LMT	C5-C6-C7-C8
27	d	401	LHG	C31-C32-C33-C34
22	b	605	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C19
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	918	DGD	C4A-C5A-C6A-C7A
22	b	602	CLA	C11-C12-C13-C15
22	B	605	CLA	C11-C10-C8-C7
22	A	408	CLA	C11-C10-C8-C7
22	C	514	CLA	C11-C10-C8-C7
22	D	404	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C10-C8-C7
22	c	914	CLA	C12-C13-C15-C16
23	D	402	PHO	C11-C12-C13-C15
22	b	604	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	c	913	CLA	C6-C7-C8-C10
22	c	913	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	B	602	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C12-C13-C15
22	c	907	CLA	C6-C7-C8-C10
22	C	507	CLA	C11-C12-C13-C15
22	C	514	CLA	CBA-CGA-O2A-C1
22	d	403	CLA	C10-C11-C12-C13
25	j	101	LMG	C35-C36-C37-C38
29	T	102	LMT	C5-C6-C7-C8
28	A	413	SQD	C13-C14-C15-C16
35	d	406	DGD	C9B-CAB-CBB-CCB
35	C	519	DGD	CAA-CBA-CCA-CDA
22	a	409	CLA	C12-C13-C15-C16
25	D	412	LMG	C35-C36-C37-C38
25	d	409	LMG	C13-C14-C15-C16
27	a	416	LHG	C30-C31-C32-C33
34	B	627	HTG	C2'-C1'-S1-C1
34	c	922	HTG	C2'-C1'-S1-C1
34	b	623	HTG	C2'-C1'-S1-C1
29	A	414	LMT	O5'-C5'-C6'-O6'
22	B	612	CLA	O1D-CGD-O2D-CED
24	c	915	BCR	C9-C10-C11-C12
25	c	930	LMG	C14-C15-C16-C17
35	c	919	DGD	CAA-CBA-CCA-CDA
35	C	518	DGD	C4D-C5D-C6D-O5D
22	C	509	CLA	C16-C17-C18-C20
25	C	520	LMG	C21-C22-C23-C24
22	c	913	CLA	C8-C10-C11-C12
22	B	603	CLA	C13-C15-C16-C17
22	C	507	CLA	C13-C15-C16-C17
22	C	513	CLA	CAD-CBD-CGD-O2D
22	b	615	CLA	CAD-CBD-CGD-O2D
22	d	403	CLA	CAD-CBD-CGD-O2D
22	b	605	CLA	CAD-CBD-CGD-O2D
23	D	402	PHO	CAD-CBD-CGD-O2D
22	c	904	CLA	CAD-CBD-CGD-O2D
22	c	913	CLA	CAD-CBD-CGD-O2D
22	B	617	CLA	CAD-CBD-CGD-O2D
29	T	102	LMT	C2-C3-C4-C5
25	c	930	LMG	C33-C34-C35-C36
22	B	617	CLA	O1D-CGD-O2D-CED
27	C	522	LHG	C4-C5-C6-O8
35	D	407	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
34	b	623	HTG	C4'-C5'-C6'-C7'
35	d	406	DGD	C3A-C4A-C5A-C6A
25	c	920	LMG	C34-C35-C36-C37
35	H	102	DGD	C7B-C8B-C9B-CAB
25	i	101	LMG	C36-C37-C38-C39
25	d	409	LMG	C15-C16-C17-C18
27	a	416	LHG	C27-C28-C29-C30
29	A	414	LMT	C1-C2-C3-C4
34	c	922	HTG	S1-C1'-C2'-C3'
35	D	407	DGD	C8A-C9A-CAA-CBA
35	C	517	DGD	C8B-C9B-CAB-CBB
35	C	518	DGD	C4B-C5B-C6B-C7B
22	C	508	CLA	C10-C11-C12-C13
27	l	102	LHG	C14-C15-C16-C17
22	c	914	CLA	O1A-CGA-O2A-C1
25	C	520	LMG	C14-C15-C16-C17
35	H	102	DGD	O1G-C1G-C2G-O2G
27	C	522	LHG	O7-C5-C6-O8
25	i	101	LMG	O7-C8-C9-O8
25	d	409	LMG	O7-C8-C9-O8
25	B	621	LMG	O1-C7-C8-O7
28	b	621	SQD	O47-C45-C46-O48
27	L	101	LHG	C1-C2-C3-O3
27	l	102	LHG	C1-C2-C3-O3
34	b	626	HTG	C4'-C5'-C6'-C7'
29	B	622	LMT	C4-C5-C6-C7
35	C	519	DGD	O6D-C1D-O3G-C3G
34	B	623	HTG	C1'-C2'-C3'-C4'
28	a	418	SQD	O10-C23-O48-C46
22	B	615	CLA	CHA-CBD-CGD-O1D
22	c	905	CLA	CHA-CBD-CGD-O1D
22	B	606	CLA	CHA-CBD-CGD-O1D
22	C	505	CLA	CHA-CBD-CGD-O1D
22	C	513	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O1D
22	C	508	CLA	CHA-CBD-CGD-O2D
22	c	908	CLA	CHA-CBD-CGD-O1D
22	b	608	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O1D
22	B	602	CLA	CHA-CBD-CGD-O2D
22	B	608	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
28	a	414	SQD	C11-C10-C9-C8
29	c	921	LMT	C9-C10-C11-C12
27	D	409	LHG	O1-C1-C2-O2
22	C	514	CLA	O1A-CGA-O2A-C1
27	D	410	LHG	C13-C14-C15-C16
28	a	414	SQD	C12-C13-C14-C15
22	c	906	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	B	605	CLA	C11-C10-C8-C9
23	D	402	PHO	C11-C12-C13-C14
22	C	509	CLA	C11-C10-C8-C9
22	c	913	CLA	C11-C12-C13-C14
22	c	903	CLA	C16-C17-C18-C19
27	D	410	LHG	C3-O3-P-O6
22	b	612	CLA	C8-C10-C11-C12
27	A	412	LHG	C28-C29-C30-C31
24	c	916	BCR	C21-C22-C23-C24
24	k	101	BCR	C11-C12-C13-C14
24	A	409	BCR	C17-C18-C19-C20
25	C	531	LMG	C29-C30-C31-C32
22	b	617	CLA	C8-C10-C11-C12
25	j	101	LMG	C34-C35-C36-C37
27	L	101	LHG	C4-O6-P-O5
27	a	416	LHG	C4-O6-P-O4
27	l	102	LHG	C3-O3-P-O5
25	b	622	LMG	C29-C30-C31-C32
29	E	101	LMT	C5-C6-C7-C8
25	d	409	LMG	C30-C31-C32-C33
22	b	609	CLA	C16-C17-C18-C20
28	a	414	SQD	C25-C26-C27-C28
27	d	401	LHG	C9-C10-C11-C12
22	c	906	CLA	C8-C10-C11-C12
35	D	407	DGD	CDA-CEA-CFA-CGA
29	c	921	LMT	C3-C4-C5-C6
27	a	423	LHG	O6-C4-C5-C6
27	a	416	LHG	O6-C4-C5-C6
25	c	930	LMG	C28-C29-C30-C31
27	d	407	LHG	C16-C17-C18-C19
22	B	615	CLA	CAD-CBD-CGD-O1D
22	c	905	CLA	CAD-CBD-CGD-O1D
22	B	606	CLA	CAD-CBD-CGD-O1D
22	b	602	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	CAD-CBD-CGD-O1D
22	C	513	CLA	CAD-CBD-CGD-O1D
22	b	615	CLA	CAD-CBD-CGD-O1D
22	b	608	CLA	CAD-CBD-CGD-O1D
22	B	602	CLA	CAD-CBD-CGD-O1D
22	B	608	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CAD-CBD-CGD-O1D
27	d	407	LHG	C34-C35-C36-C37
22	B	602	CLA	C16-C17-C18-C20
22	c	911	CLA	C16-C17-C18-C19
26	a	415	PL9	C4-C3-C7-C8
27	D	410	LHG	C30-C31-C32-C33
27	L	101	LHG	C26-C27-C28-C29
35	h	102	DGD	O2G-C1B-C2B-C3B
22	d	402	CLA	C2-C1-O2A-CGA
22	B	617	CLA	C2-C1-O2A-CGA
28	b	621	SQD	O5-C5-C6-S
35	h	102	DGD	CCB-CDB-CEB-CFB
22	C	510	CLA	C12-C13-C15-C16
22	c	906	CLA	C12-C13-C15-C16
22	c	905	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C7
22	c	912	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C10-C8-C7
22	b	609	CLA	C11-C12-C13-C15
22	C	505	CLA	C12-C13-C15-C16
22	C	514	CLA	C6-C7-C8-C10
22	C	514	CLA	C11-C12-C13-C15
22	B	604	CLA	C6-C7-C8-C10
22	B	604	CLA	C11-C10-C8-C7
22	B	616	CLA	C11-C10-C8-C7
22	b	608	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C10-C8-C7
22	c	909	CLA	C11-C12-C13-C15
22	c	910	CLA	C6-C7-C8-C10
22	B	602	CLA	C6-C7-C8-C10
22	B	603	CLA	C6-C7-C8-C10
22	c	907	CLA	C11-C12-C13-C15
34	b	623	HTG	C3'-C4'-C5'-C6'
25	j	101	LMG	C39-C40-C41-C42
27	a	416	LHG	C16-C17-C18-C19
29	B	622	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
25	d	409	LMG	C14-C15-C16-C17
29	B	622	LMT	C9-C10-C11-C12
35	C	519	DGD	O1A-C1A-O1G-C1G
22	b	604	CLA	C4-C3-C5-C6
25	J	101	LMG	C18-C19-C20-C21
22	c	906	CLA	C2-C3-C5-C6
22	b	611	CLA	C8-C10-C11-C12
28	a	414	SQD	C33-C34-C35-C36
35	C	517	DGD	CBB-CCB-CDB-CEB
25	A	410	LMG	C12-C13-C14-C15
35	c	919	DGD	C2A-C1A-O1G-C1G
27	D	411	LHG	C15-C16-C17-C18
22	c	905	CLA	C3-C5-C6-C7
22	C	514	CLA	C3-C5-C6-C7
35	C	519	DGD	C4E-C5E-C6E-O5E
25	A	410	LMG	O1-C7-C8-C9
25	c	930	LMG	O1-C7-C8-O7
25	D	412	LMG	O1-C7-C8-O7
28	l	101	SQD	O6-C44-C45-O47
25	A	410	LMG	O1-C7-C8-O7
25	A	410	LMG	O7-C8-C9-O8
28	b	621	SQD	O6-C44-C45-O47
35	H	102	DGD	C5B-C6B-C7B-C8B
26	a	415	PL9	C3-C7-C8-C9
25	c	920	LMG	C37-C38-C39-C40
27	d	401	LHG	C11-C10-C9-C8
35	c	917	DGD	C5B-C6B-C7B-C8B
28	l	101	SQD	C15-C16-C17-C18
22	c	914	CLA	CBD-CGD-O2D-CED
26	A	411	PL9	C39-C41-C42-C43
22	c	905	CLA	C11-C10-C8-C9
22	C	514	CLA	C6-C7-C8-C9
22	d	403	CLA	C11-C10-C8-C9
22	B	607	CLA	C11-C10-C8-C9
22	B	616	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C9
22	B	602	CLA	C11-C12-C13-C14
35	c	918	DGD	C2E-C1E-O5D-C6D
35	C	518	DGD	C2E-C1E-O5D-C6D
35	c	917	DGD	C2E-C1E-O5D-C6D
22	D	404	CLA	C16-C17-C18-C20
22	c	910	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
27	C	522	LHG	O7-C7-C8-C9
35	c	918	DGD	CCA-CDA-CEA-CFA
29	A	414	LMT	C7-C8-C9-C10
27	l	102	LHG	O1-C1-C2-O2
27	L	101	LHG	C5-C6-O8-C23
25	c	920	LMG	C36-C37-C38-C39
25	J	101	LMG	C14-C15-C16-C17
35	h	102	DGD	C9A-CAA-CBA-CCA
27	d	401	LHG	C4-C5-O7-C7
27	d	408	LHG	C29-C30-C31-C32
34	b	632	HTG	C4'-C5'-C6'-C7'
35	h	102	DGD	C7A-C8A-C9A-CAA
22	b	602	CLA	C4-C3-C5-C6
22	C	511	CLA	C2-C3-C5-C6
25	d	409	LMG	C18-C19-C20-C21
27	C	522	LHG	C13-C14-C15-C16
25	j	101	LMG	C18-C19-C20-C21
34	C	532	HTG	C1'-C2'-C3'-C4'
22	C	508	CLA	C2A-CAA-CBA-CGA
22	B	613	CLA	O1A-CGA-O2A-C1
22	b	605	CLA	C2C-C3C-CAC-CBC
24	a	413	BCR	C1-C6-C7-C8
24	c	916	BCR	C1-C6-C7-C8
35	D	407	DGD	C4B-C5B-C6B-C7B
25	b	622	LMG	C20-C21-C22-C23
22	C	510	CLA	O1D-CGD-O2D-CED
35	C	518	DGD	C5D-C6D-O5D-C1E
27	d	407	LHG	C4-O6-P-O3
27	a	423	LHG	C4-O6-P-O3
35	d	406	DGD	C7A-C8A-C9A-CAA
28	l	101	SQD	C7-C8-C9-C10
22	b	616	CLA	C4-C3-C5-C6
35	C	517	DGD	O6D-C5D-C6D-O5D
34	B	627	HTG	C1'-C2'-C3'-C4'
22	C	506	CLA	O1D-CGD-O2D-CED
35	h	102	DGD	O1G-C1G-C2G-O2G
27	d	408	LHG	O7-C5-C6-O8
35	c	918	DGD	C4B-C5B-C6B-C7B
25	C	531	LMG	C21-C22-C23-C24
22	b	602	CLA	C6-C7-C8-C10
22	C	511	CLA	C6-C7-C8-C10
27	a	416	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	C	517	DGD	CDA-CEA-CFA-CGA
25	C	531	LMG	O1-C7-C8-C9
25	A	410	LMG	C7-C8-C9-O8
28	b	621	SQD	C44-C45-C46-O48
27	a	423	LHG	C10-C11-C12-C13
29	a	419	LMT	C7-C8-C9-C10
27	l	102	LHG	C31-C32-C33-C34
34	b	623	HTG	C4-C5-C6-O6
22	C	510	CLA	C11-C12-C13-C14
22	d	402	CLA	C11-C12-C13-C14
22	c	905	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C12-C13-C14
22	c	914	CLA	C14-C13-C15-C16
22	c	908	CLA	C11-C12-C13-C14
23	D	402	PHO	C6-C7-C8-C9
22	b	611	CLA	C11-C12-C13-C14
22	c	907	CLA	C6-C7-C8-C9
22	b	615	CLA	C2-C3-C5-C6
27	D	409	LHG	C25-C26-C27-C28
35	C	517	DGD	C4D-C5D-C6D-O5D
22	a	408	CLA	C4C-C3C-CAC-CBC
35	h	102	DGD	CAA-CBA-CCA-CDA
29	E	101	LMT	C1-C2-C3-C4
35	c	918	DGD	C9A-CAA-CBA-CCA
29	B	622	LMT	C3-C4-C5-C6
24	C	515	BCR	C13-C14-C15-C16
27	a	416	LHG	C35-C36-C37-C38
29	c	921	LMT	C5-C6-C7-C8
25	C	531	LMG	C10-C11-C12-C13
22	B	606	CLA	C8-C10-C11-C12
22	B	616	CLA	C13-C15-C16-C17
22	c	902	CLA	C2A-CAA-CBA-CGA
25	B	621	LMG	C4-C5-C6-O5
27	D	410	LHG	C29-C30-C31-C32
28	a	414	SQD	C28-C29-C30-C31
27	d	407	LHG	C31-C32-C33-C34
22	b	606	CLA	O1D-CGD-O2D-CED
22	B	613	CLA	C8-C10-C11-C12
37	H	101	RRX	C9-C10-C11-C12
37	h	101	RRX	C9-C10-C11-C12
28	A	413	SQD	O47-C45-C46-O48
25	C	520	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	C16-C17-C18-C20
22	c	906	CLA	C4-C3-C5-C6
22	B	616	CLA	C4-C3-C5-C6
26	D	406	PL9	C43-C44-C46-C47
26	A	411	PL9	C13-C14-C16-C17
27	d	401	LHG	C25-C26-C27-C28
27	D	409	LHG	C11-C10-C9-C8
27	d	407	LHG	C28-C29-C30-C31
25	D	412	LMG	C21-C22-C23-C24
22	B	605	CLA	O2A-C1-C2-C3
28	A	413	SQD	C24-C23-O48-C46
25	j	101	LMG	C32-C33-C34-C35
34	v	203	HTG	S1-C1'-C2'-C3'
35	h	102	DGD	O1G-C1G-C2G-C3G
22	b	602	CLA	C2-C3-C5-C6
27	l	102	LHG	C23-C24-C25-C26
34	B	627	HTG	C4'-C5'-C6'-C7'
25	C	531	LMG	C17-C18-C19-C20
35	C	519	DGD	CDA-CEA-CFA-CGA
28	D	408	SQD	C2-C1-O6-C44
29	E	101	LMT	O1'-C1-C2-C3
22	C	510	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16
22	A	408	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C12-C13-C15
22	c	904	CLA	C6-C7-C8-C10
22	c	903	CLA	C12-C13-C15-C16
27	l	102	LHG	C17-C18-C19-C20
35	H	102	DGD	C5A-C6A-C7A-C8A
28	a	418	SQD	C10-C11-C12-C13
35	c	917	DGD	CAA-CBA-CCA-CDA
27	a	416	LHG	O2-C2-C3-O3
35	C	517	DGD	C8A-C9A-CAA-CBA
22	d	402	CLA	C15-C16-C17-C18
22	a	412	CLA	C10-C11-C12-C13
28	b	621	SQD	C34-C35-C36-C37
28	l	101	SQD	C11-C10-C9-C8
24	K	101	BCR	C9-C10-C11-C12
22	c	911	CLA	O1A-CGA-O2A-C1
34	v	203	HTG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	CCA-CDA-CEA-CFA
35	c	917	DGD	C6A-C7A-C8A-C9A
26	A	411	PL9	C15-C14-C16-C17
29	a	419	LMT	C4-C5-C6-C7
27	d	407	LHG	C11-C12-C13-C14
26	D	406	PL9	C34-C36-C37-C38
34	C	521	HTG	O5-C5-C6-O6
22	C	510	CLA	C2A-CAA-CBA-CGA
35	C	519	DGD	C4B-C5B-C6B-C7B
35	C	519	DGD	C6B-C7B-C8B-C9B
35	c	919	DGD	O1A-C1A-O1G-C1G
25	c	920	LMG	C22-C23-C24-C25
35	C	519	DGD	C8A-C9A-CAA-CBA
35	D	407	DGD	C6A-C7A-C8A-C9A
28	a	414	SQD	C10-C11-C12-C13
24	a	413	BCR	C5-C6-C7-C8
24	y	101	BCR	C23-C24-C25-C30
22	b	605	CLA	C11-C10-C8-C9
37	h	101	RRX	C19-C20-C21-C22
22	B	613	CLA	C10-C11-C12-C13
35	D	407	DGD	C9B-CAB-CBB-CCB
26	d	405	PL9	C35-C34-C36-C37
22	C	511	CLA	C4-C3-C5-C6
22	B	610	CLA	C2-C3-C5-C6
35	C	518	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	O1B-C1B-C2B-C3B
27	D	411	LHG	C26-C27-C28-C29
27	D	409	LHG	C19-C20-C21-C22
22	b	616	CLA	C8-C10-C11-C12
28	b	621	SQD	C44-C45-O47-C7
25	A	410	LMG	C15-C16-C17-C18
22	b	607	CLA	C16-C17-C18-C20
22	C	511	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C15
28	A	413	SQD	O10-C23-O48-C46
22	b	616	CLA	C2-C3-C5-C6
22	c	913	CLA	CAA-CBA-CGA-O2A
35	c	917	DGD	O2G-C1B-C2B-C3B
28	f	101	SQD	C45-C44-O6-C1
26	A	411	PL9	C2-C3-C7-C8
27	D	410	LHG	C35-C36-C37-C38
25	i	101	LMG	O10-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
22	d	402	CLA	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C19
22	B	604	CLA	C4-C3-C5-C6
26	d	405	PL9	C36-C37-C38-C39
28	l	101	SQD	O47-C7-C8-C9
28	a	414	SQD	O47-C7-C8-C9
22	B	616	CLA	C2-C3-C5-C6
29	c	931	LMT	O1'-C1-C2-C3
34	D	415	HTG	C4-C5-C6-O6
34	b	632	HTG	C2'-C1'-S1-C1
34	C	532	HTG	C2'-C1'-S1-C1
22	c	903	CLA	C16-C17-C18-C20
29	c	931	LMT	C9-C10-C11-C12
22	C	513	CLA	CAA-CBA-CGA-O2A
27	d	408	LHG	C27-C28-C29-C30
22	b	616	CLA	C3A-C2A-CAA-CBA
22	C	511	CLA	O1A-CGA-O2A-C1
22	c	911	CLA	CBA-CGA-O2A-C1
22	C	514	CLA	C10-C11-C12-C13
22	c	913	CLA	C10-C11-C12-C13
25	j	101	LMG	C40-C41-C42-C43
27	D	411	LHG	C31-C32-C33-C34
22	C	510	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	b	609	CLA	C11-C12-C13-C14
22	C	514	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C10-C8-C9
22	c	909	CLA	C11-C12-C13-C14
22	b	605	CLA	C11-C12-C13-C14
22	c	910	CLA	C11-C12-C13-C14
22	C	511	CLA	C11-C10-C8-C9
22	c	907	CLA	C11-C12-C13-C14
22	c	906	CLA	CAD-CBD-CGD-O2D
22	C	505	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	D	404	CLA	CAD-CBD-CGD-O2D
22	B	604	CLA	CAD-CBD-CGD-O2D
22	a	407	CLA	CAD-CBD-CGD-O2D
22	c	914	CLA	CAD-CBD-CGD-O2D
22	B	611	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	b	611	CLA	CAD-CBD-CGD-O2D
22	C	511	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	B	608	CLA	CAD-CBD-CGD-O2D
22	A	405	CLA	CAD-CBD-CGD-O2D
35	D	407	DGD	CBB-CCB-CDB-CEB
29	T	102	LMT	C7-C8-C9-C10
25	D	412	LMG	C34-C35-C36-C37
22	C	509	CLA	C5-C6-C7-C8
22	d	402	CLA	O2A-C1-C2-C3
22	D	404	CLA	O2A-C1-C2-C3
22	a	408	CLA	C16-C17-C18-C20
22	b	604	CLA	CBD-CGD-O2D-CED
27	d	408	LHG	C17-C18-C19-C20
25	d	409	LMG	O8-C28-C29-C30
22	B	602	CLA	CAA-CBA-CGA-O2A
24	Y	101	BCR	C17-C18-C19-C20
24	K	101	BCR	C11-C12-C13-C14
28	A	413	SQD	C44-C45-C46-O48
25	C	520	LMG	O1-C7-C8-C9
28	l	101	SQD	O6-C44-C45-C46
35	c	919	DGD	O6D-C5D-C6D-O5D
27	C	522	LHG	O6-C4-C5-O7
27	l	102	LHG	O6-C4-C5-O7
25	A	410	LMG	C40-C41-C42-C43
23	a	411	PHO	C5-C6-C7-C8
35	C	518	DGD	C2B-C3B-C4B-C5B
28	C	501	SQD	O47-C7-C8-C9
35	c	917	DGD	C5D-C6D-O5D-C1E
25	B	621	LMG	C20-C21-C22-C23
35	h	102	DGD	C7B-C8B-C9B-CAB
27	D	409	LHG	C30-C31-C32-C33
22	d	402	CLA	C16-C17-C18-C20
34	B	627	HTG	C4-C5-C6-O6
22	A	405	CLA	C2C-C3C-CAC-CBC
35	d	406	DGD	C8A-C9A-CAA-CBA
22	a	412	CLA	C4-C3-C5-C6
25	B	621	LMG	C16-C17-C18-C19
26	d	405	PL9	C33-C34-C36-C37
25	D	412	LMG	O7-C8-C9-O8
22	b	611	CLA	C16-C17-C18-C19
22	b	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
27	a	423	LHG	C12-C13-C14-C15
22	c	902	CLA	C13-C15-C16-C17
35	d	406	DGD	C2D-C1D-O3G-C3G
22	D	401	CLA	C15-C16-C17-C18
22	c	910	CLA	C11-C12-C13-C15
35	C	519	DGD	C6A-C7A-C8A-C9A
22	C	503	CLA	CHA-CBD-CGD-O2D
22	C	510	CLA	CHA-CBD-CGD-O2D
22	A	406	CLA	CHA-CBD-CGD-O2D
22	b	612	CLA	CHA-CBD-CGD-O2D
22	a	408	CLA	CHA-CBD-CGD-O1D
22	B	607	CLA	CHA-CBD-CGD-O2D
23	a	411	PHO	CHA-CBD-CGD-O1D
22	a	409	CLA	CHA-CBD-CGD-O2D
23	D	402	PHO	CHA-CBD-CGD-O1D
23	D	402	PHO	CHA-CBD-CGD-O2D
22	C	511	CLA	CHA-CBD-CGD-O1D
22	c	913	CLA	CHA-CBD-CGD-O1D
22	b	617	CLA	CHA-CBD-CGD-O2D
22	B	603	CLA	CHA-CBD-CGD-O1D
22	B	603	CLA	CHA-CBD-CGD-O2D
22	b	607	CLA	CHA-CBD-CGD-O2D
22	D	401	CLA	CHA-CBD-CGD-O2D
22	b	604	CLA	C2A-CAA-CBA-CGA
26	D	406	PL9	C11-C12-C13-C14
26	D	406	PL9	C28-C29-C31-C32
35	H	102	DGD	C8A-C9A-CAA-CBA
25	c	920	LMG	C40-C41-C42-C43
29	E	101	LMT	C4-C5-C6-C7
25	c	920	LMG	C13-C14-C15-C16
22	C	513	CLA	CAA-CBA-CGA-O1A
22	B	613	CLA	CBA-CGA-O2A-C1
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	602	CLA	C6-C7-C8-C9
22	b	609	CLA	C11-C10-C8-C9
22	B	604	CLA	C6-C7-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	a	412	CLA	C14-C13-C15-C16
22	c	910	CLA	C6-C7-C8-C9
22	c	910	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
22	B	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C6-C7-C8-C9
22	c	903	CLA	C14-C13-C15-C16
35	h	102	DGD	CAB-CBB-CCB-CDB
22	b	602	CLA	C1A-C2A-CAA-CBA
28	a	414	SQD	C19-C20-C21-C22
22	c	913	CLA	CAA-CBA-CGA-O1A
22	b	614	CLA	CAA-CBA-CGA-O2A
22	C	511	CLA	CAA-CBA-CGA-O2A
29	a	419	LMT	C5-C6-C7-C8
27	D	411	LHG	C30-C31-C32-C33
22	C	503	CLA	C15-C16-C17-C18
22	A	405	CLA	C4C-C3C-CAC-CBC
22	C	502	CLA	CAA-CBA-CGA-O2A
24	c	915	BCR	C11-C12-C13-C14
24	C	515	BCR	C21-C22-C23-C24
24	B	619	BCR	C11-C12-C13-C14
27	D	410	LHG	C25-C26-C27-C28
28	l	101	SQD	C16-C17-C18-C19
35	c	917	DGD	O1B-C1B-C2B-C3B
22	a	412	CLA	C8-C10-C11-C12
27	d	407	LHG	C4-O6-P-O5
27	L	101	LHG	C4-O6-P-O4
27	D	410	LHG	C4-O6-P-O5
29	Z	101	LMT	C7-C8-C9-C10
35	h	102	DGD	C1G-C2G-C3G-O3G
28	b	621	SQD	O6-C44-C45-C46
35	d	406	DGD	CDA-CEA-CFA-CGA
22	B	607	CLA	C16-C17-C18-C19
35	C	517	DGD	O6E-C1E-O5D-C6D
25	A	410	LMG	O6-C1-O1-C7
29	c	931	LMT	C5-C6-C7-C8
24	c	915	BCR	C23-C24-C25-C30
27	C	522	LHG	C27-C28-C29-C30
22	C	514	CLA	C4-C3-C5-C6
26	D	406	PL9	C45-C44-C46-C47
22	B	611	CLA	C4C-C3C-CAC-CBC
22	C	514	CLA	C8-C10-C11-C12
22	b	604	CLA	C10-C11-C12-C13
22	A	406	CLA	CAD-CBD-CGD-O1D
22	b	613	CLA	CAD-CBD-CGD-O1D
22	c	907	CLA	CAD-CBD-CGD-O1D
22	c	911	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
25	d	409	LMG	O10-C28-C29-C30
28	l	101	SQD	O49-C7-C8-C9
35	C	519	DGD	O1A-C1A-C2A-C3A
27	a	423	LHG	C30-C31-C32-C33
22	b	602	CLA	CAA-CBA-CGA-O2A
25	B	621	LMG	O8-C28-C29-C30
26	d	405	PL9	C4-C3-C7-C8
22	b	614	CLA	CAA-CBA-CGA-O1A
28	C	501	SQD	O49-C7-C8-C9
22	C	502	CLA	CAA-CBA-CGA-O1A
28	C	501	SQD	C32-C33-C34-C35
35	C	519	DGD	O1G-C1A-C2A-C3A
27	D	411	LHG	C11-C12-C13-C14
22	b	614	CLA	C2-C1-O2A-CGA
22	B	602	CLA	CAA-CBA-CGA-O1A
22	B	606	CLA	C10-C11-C12-C13
27	l	102	LHG	C11-C12-C13-C14
25	C	531	LMG	O8-C28-C29-C30
35	c	919	DGD	CCA-CDA-CEA-CFA
22	B	608	CLA	C13-C15-C16-C17
22	c	905	CLA	C6-C7-C8-C9
22	D	404	CLA	C11-C10-C8-C9
22	C	508	CLA	C11-C12-C13-C14
28	a	418	SQD	O10-C23-C24-C25
22	C	511	CLA	CAA-CBA-CGA-O1A
27	D	409	LHG	O7-C7-C8-C9
22	d	402	CLA	CAA-CBA-CGA-O2A
27	L	101	LHG	O7-C7-C8-C9
22	b	612	CLA	C6-C7-C8-C10
22	D	404	CLA	C11-C10-C8-C7
22	a	412	CLA	C12-C13-C15-C16
22	C	511	CLA	C11-C10-C8-C7
27	L	101	LHG	O9-C7-C8-C9
35	c	918	DGD	O2G-C1B-C2B-C3B
28	a	418	SQD	O48-C23-C24-C25
27	D	411	LHG	O8-C23-C24-C25
22	b	613	CLA	O1A-CGA-O2A-C1
35	H	102	DGD	C3B-C4B-C5B-C6B
35	c	919	DGD	O1A-C1A-C2A-C3A
22	B	610	CLA	C4-C3-C5-C6
26	D	406	PL9	C30-C29-C31-C32
26	D	406	PL9	C35-C34-C36-C37

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Mol	Chain	Res	Type	Atoms
26	A	411	PL9	C20-C19-C21-C22
27	C	522	LHG	O8-C23-C24-C25
27	a	423	LHG	O8-C23-C24-C25
27	D	409	LHG	O9-C7-C8-C9

There are no ring outliers.

78 monomers are involved in 246 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	405	CLA	3	0
22	A	406	CLA	3	0
23	A	407	PHO	1	0
22	A	408	CLA	9	0
25	A	410	LMG	2	0
26	A	411	PL9	11	0
27	A	412	LHG	1	0
28	A	413	SQD	2	0
29	A	414	LMT	6	0
22	B	602	CLA	6	0
22	B	603	CLA	3	0
22	B	604	CLA	2	0
22	B	605	CLA	5	0
22	B	606	CLA	11	0
22	B	607	CLA	4	0
22	B	608	CLA	9	0
22	B	609	CLA	6	0
22	B	610	CLA	8	0
22	B	611	CLA	9	0
22	B	612	CLA	2	0
22	B	613	CLA	4	0
22	B	614	CLA	6	0
22	B	615	CLA	4	0
22	B	616	CLA	3	0
22	B	617	CLA	2	0
24	B	618	BCR	7	0
24	B	619	BCR	1	0
24	B	620	BCR	3	0
25	B	621	LMG	3	0
29	B	622	LMT	3	0
34	B	623	HTG	3	0
34	B	626	HTG	1	0
28	C	501	SQD	6	0

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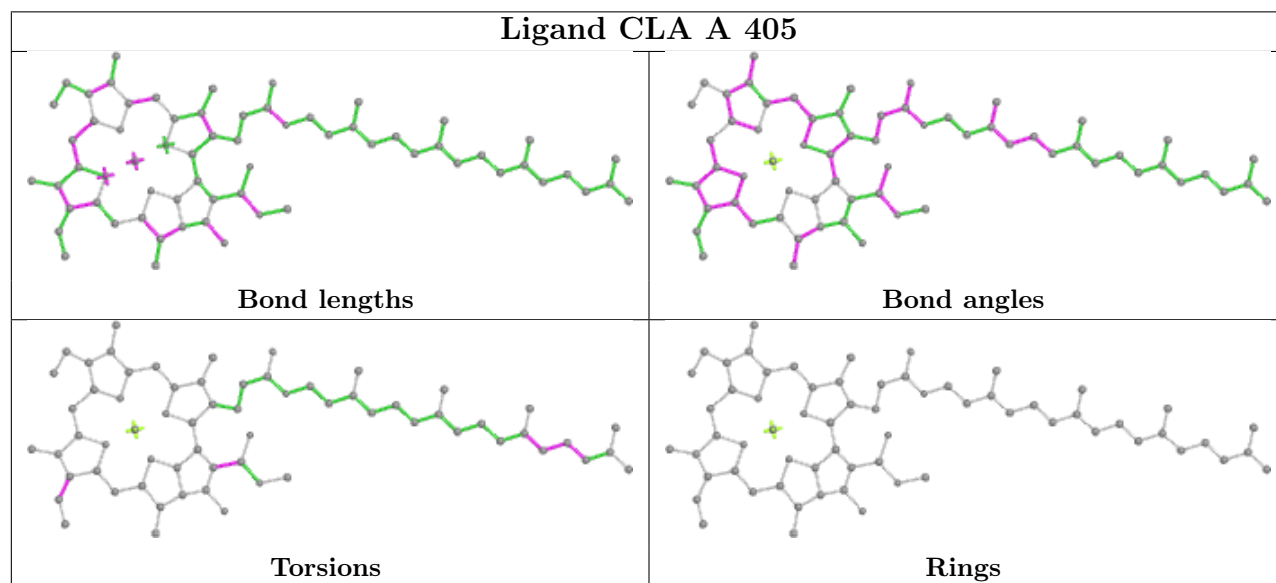
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	502	CLA	2	0
22	C	503	CLA	6	0
22	C	504	CLA	3	0
22	C	505	CLA	4	0
22	C	506	CLA	1	0
22	C	507	CLA	5	0
22	C	508	CLA	3	0
22	C	509	CLA	3	0
22	C	510	CLA	3	0
22	C	511	CLA	5	0
22	C	512	CLA	1	0
22	C	513	CLA	5	0
22	C	514	CLA	5	0
24	C	515	BCR	4	0
24	C	516	BCR	1	0
35	C	518	DGD	1	0
35	C	519	DGD	2	0
25	C	520	LMG	1	0
34	C	521	HTG	1	0
27	C	522	LHG	1	0
25	C	531	LMG	2	0
34	C	532	HTG	1	0
22	D	401	CLA	4	0
23	D	402	PHO	5	0
22	D	403	CLA	2	0
22	D	404	CLA	1	0
24	D	405	BCR	1	0
26	D	406	PL9	5	0
27	D	409	LHG	7	0
27	D	410	LHG	3	0
27	D	411	LHG	8	0
25	D	412	LMG	5	0
34	D	414	HTG	2	0
34	D	415	HTG	8	0
29	E	101	LMT	1	0
36	E	102	HEM	1	0
37	H	101	RRX	12	0
35	H	102	DGD	4	0
25	J	101	LMG	2	0
24	K	101	BCR	2	0
27	L	101	LHG	7	0
29	T	102	LMT	1	0

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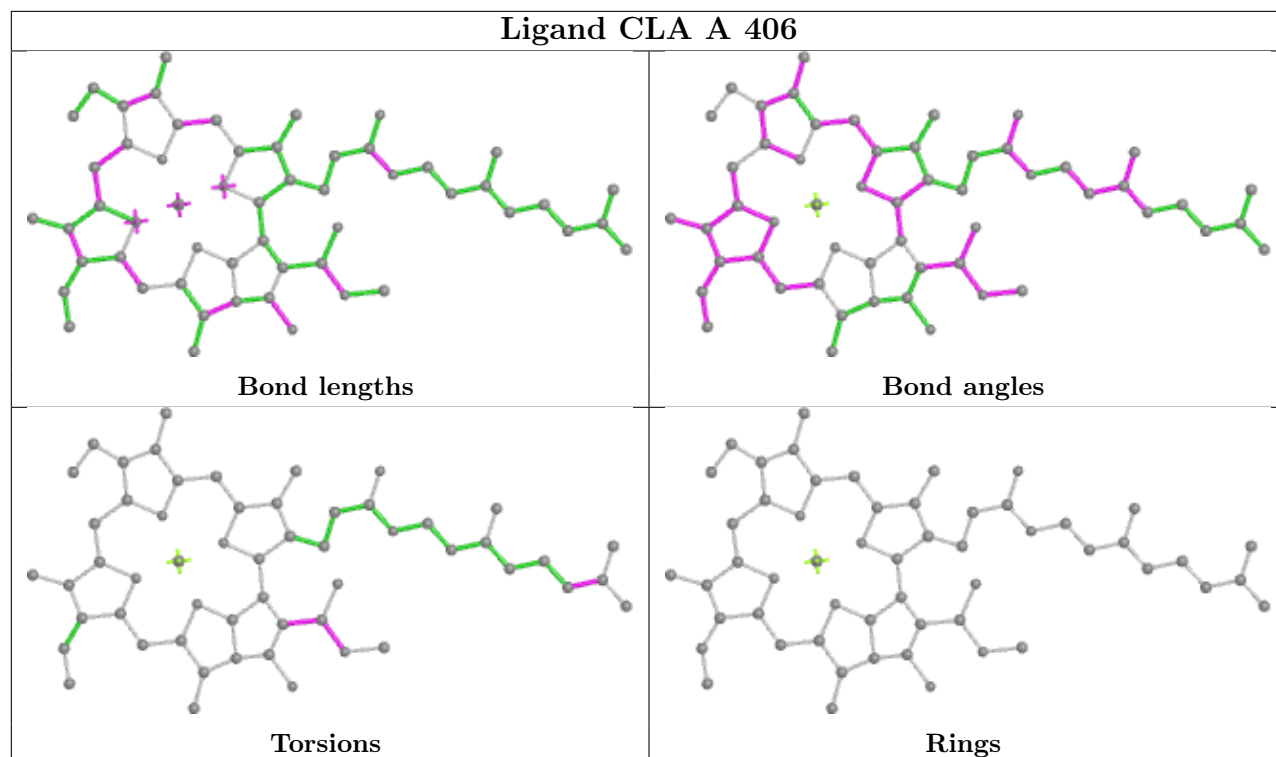
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	V	202	HEC	4	0
24	Y	101	BCR	4	0
29	Z	101	LMT	1	0

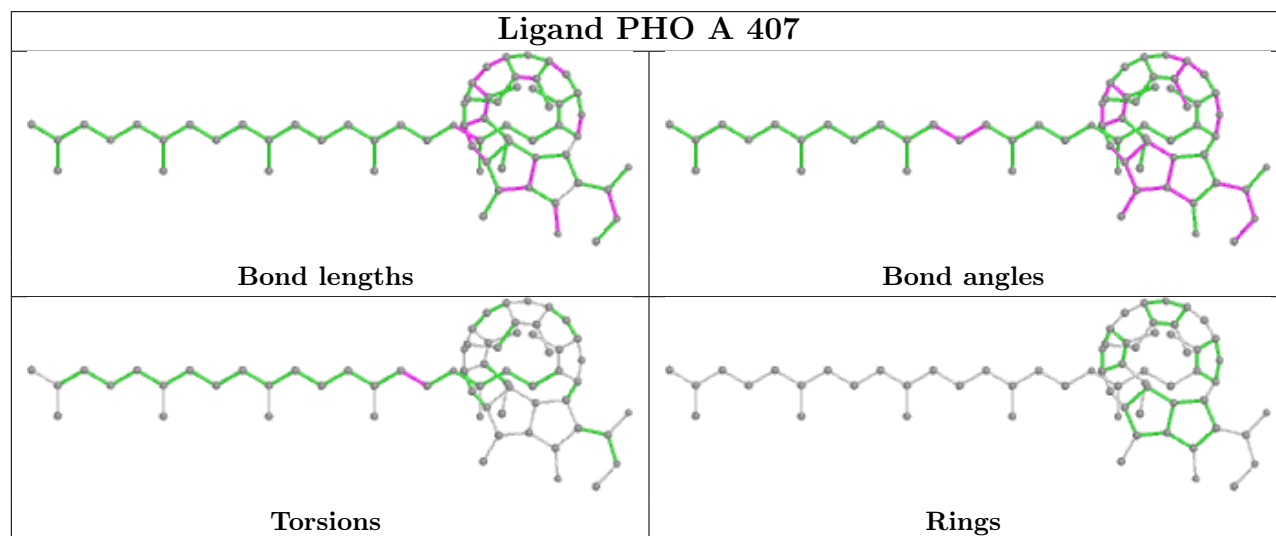
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



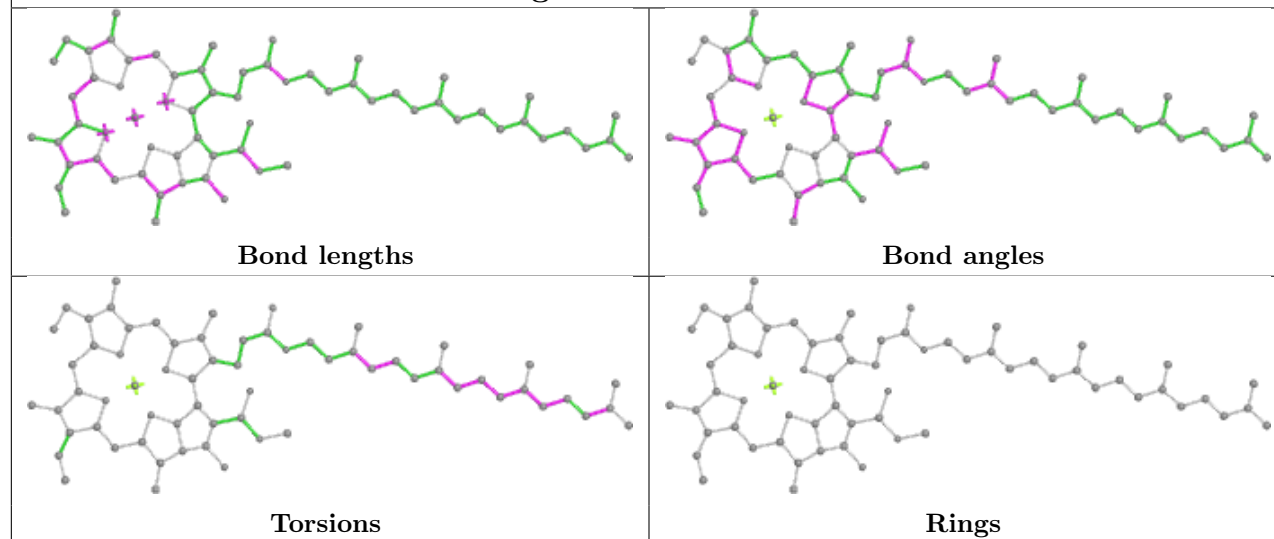
Ligand CLA A 406



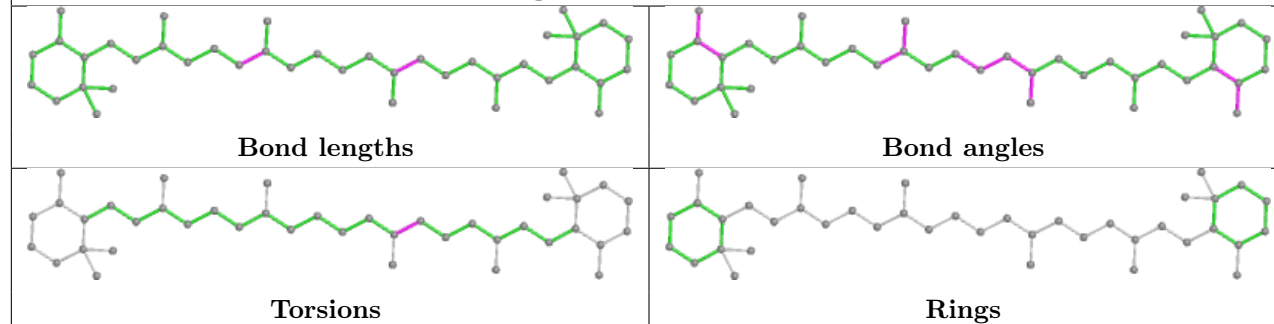
Ligand PHO A 407



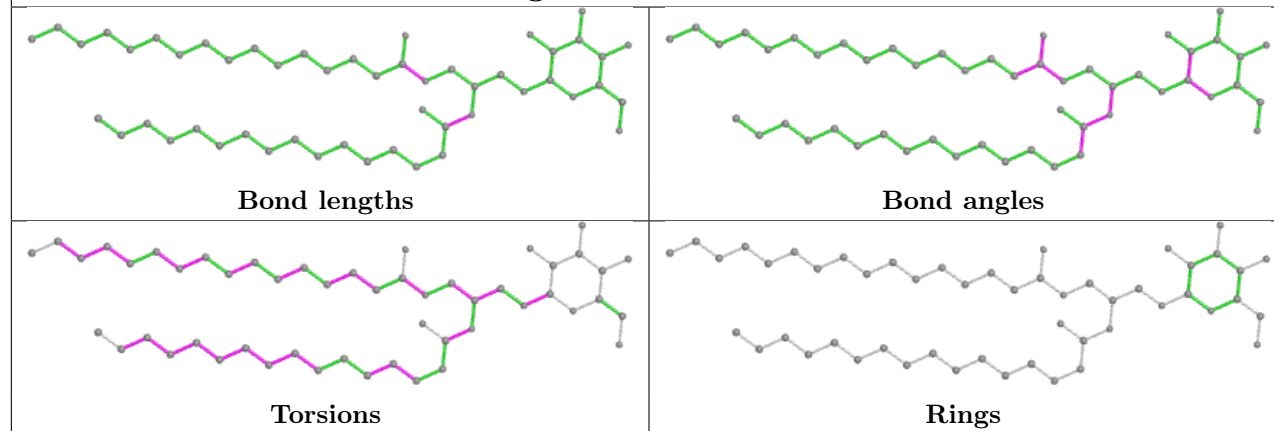
Ligand CLA A 408



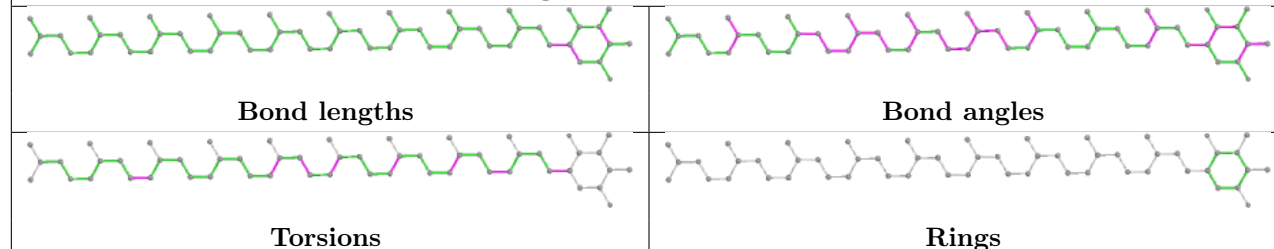
Ligand BCR A 409

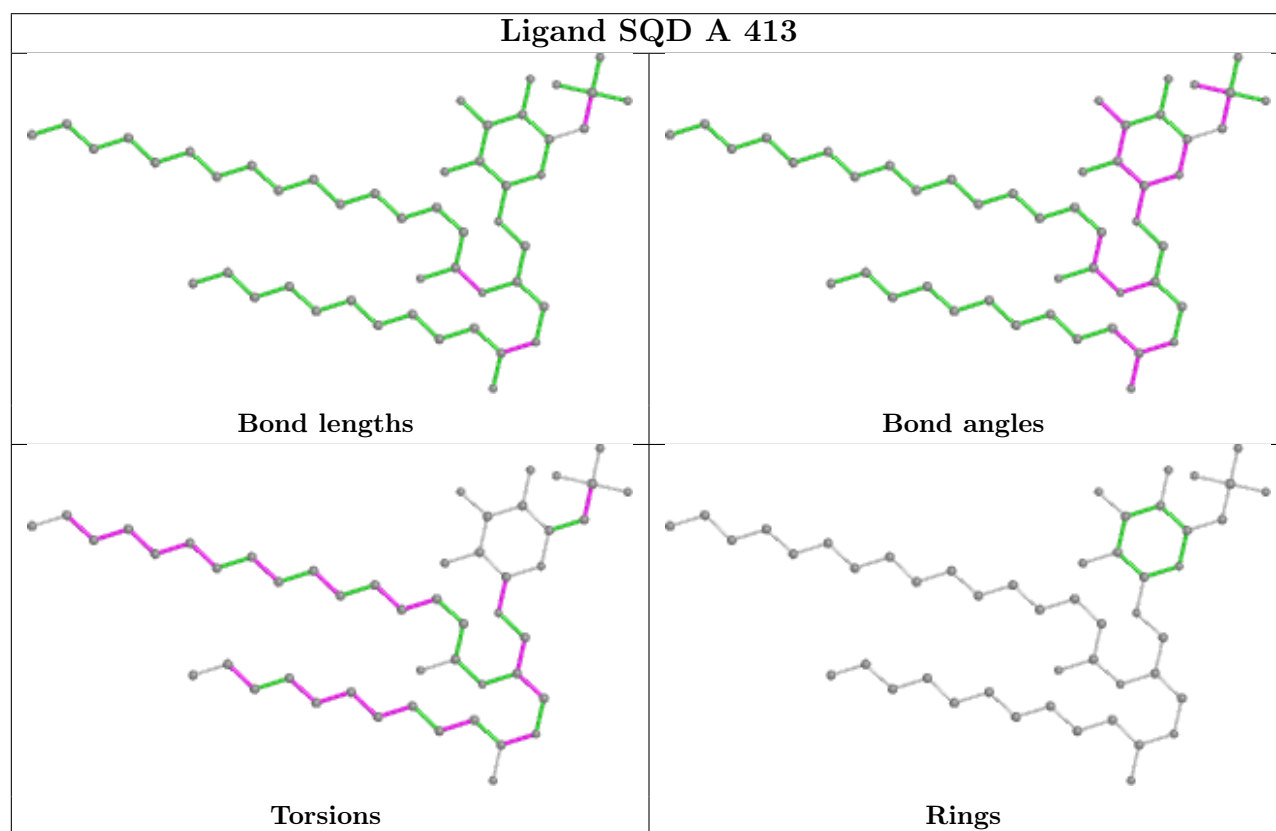
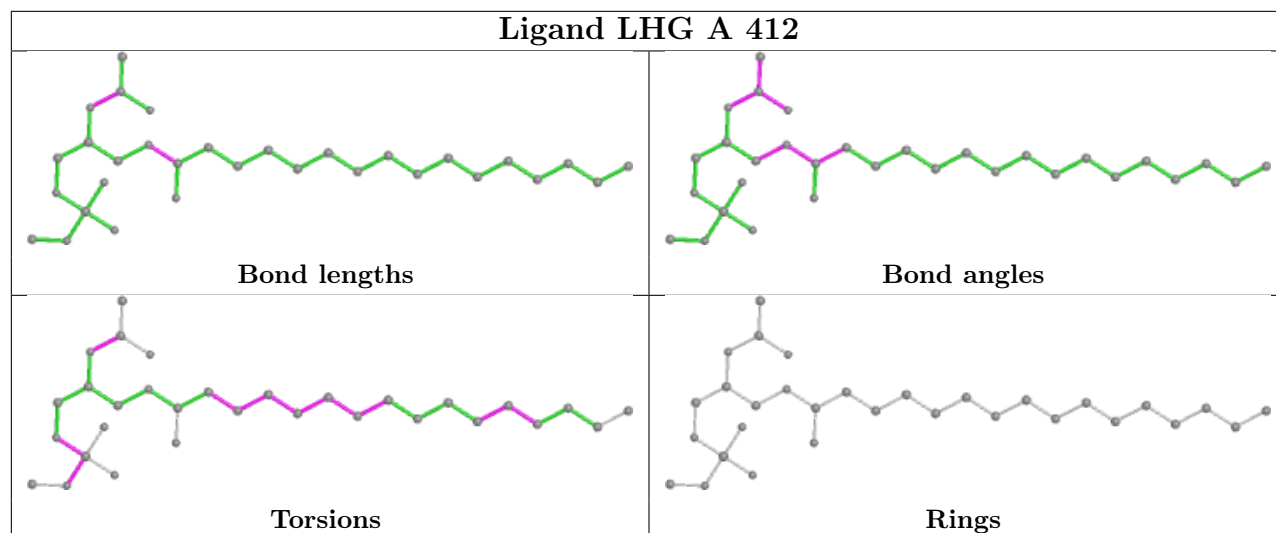


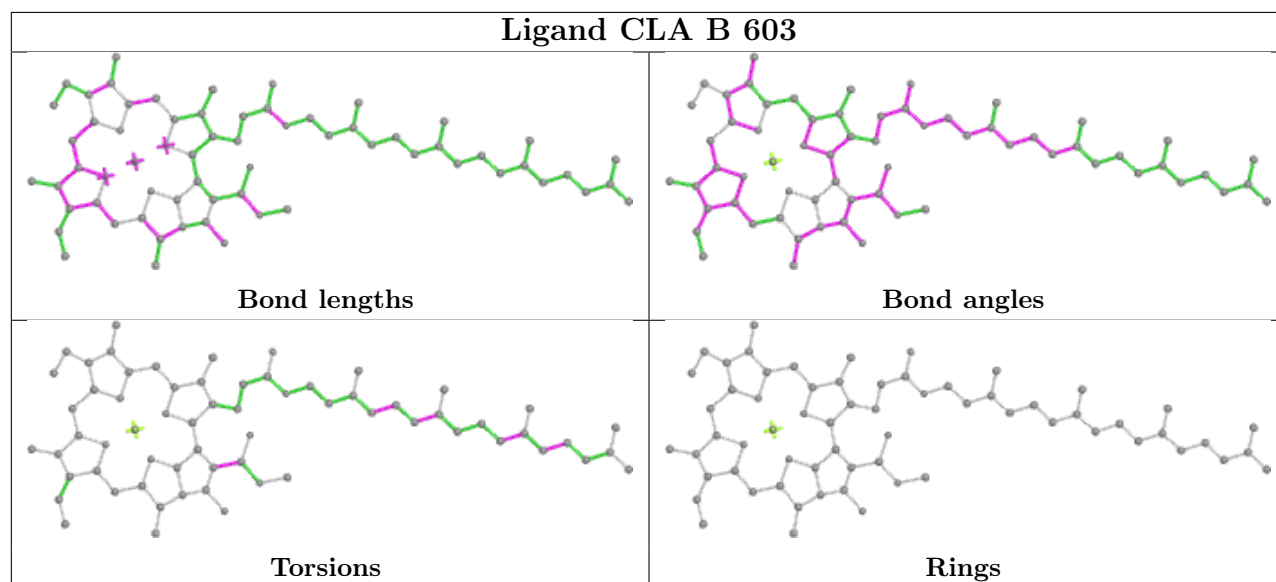
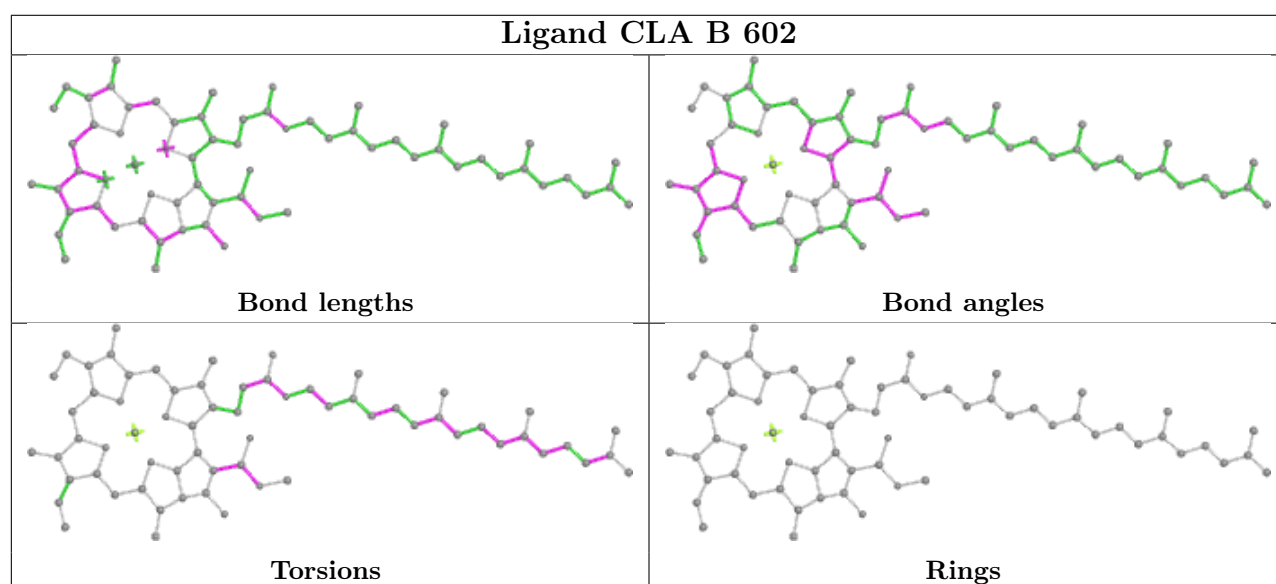
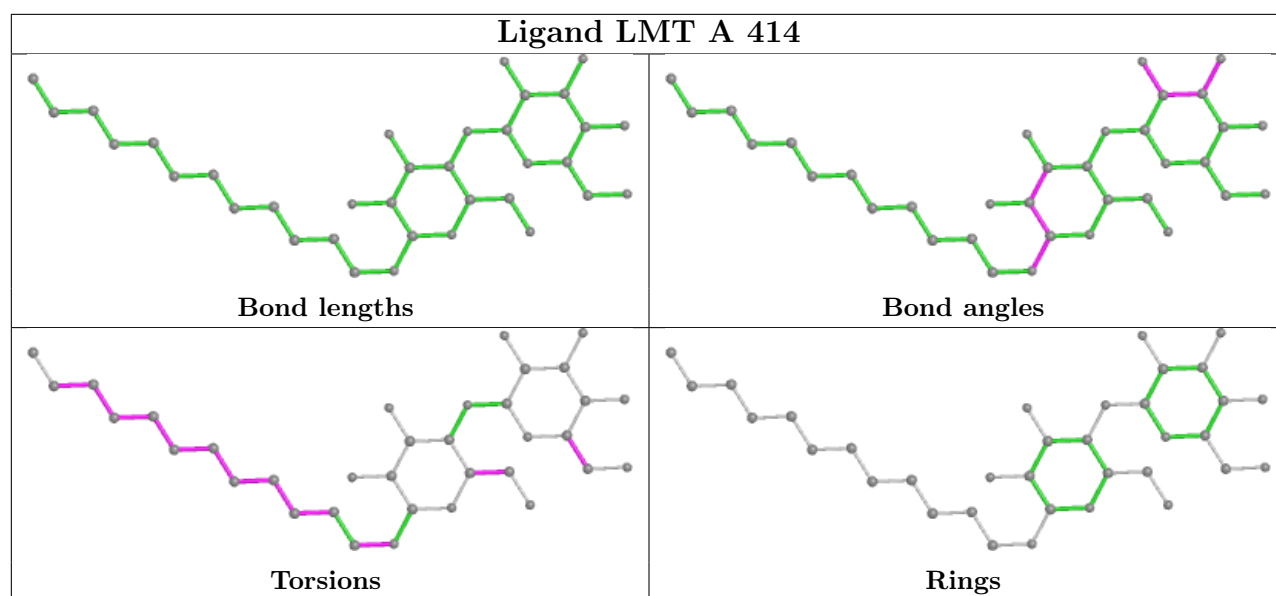
Ligand LMG A 410



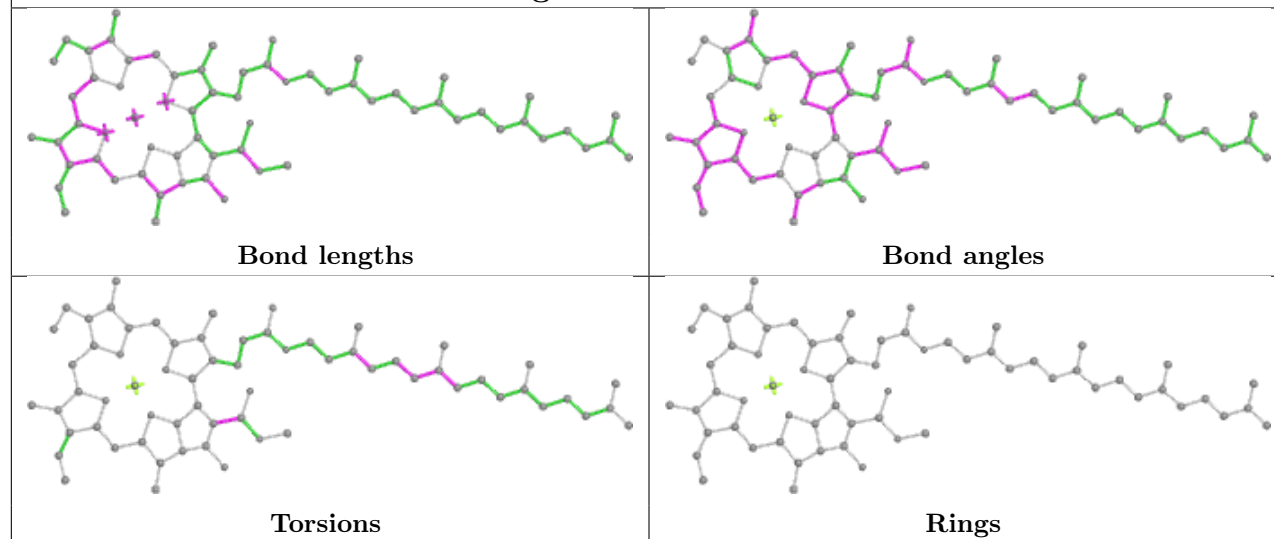
Ligand PL9 A 411



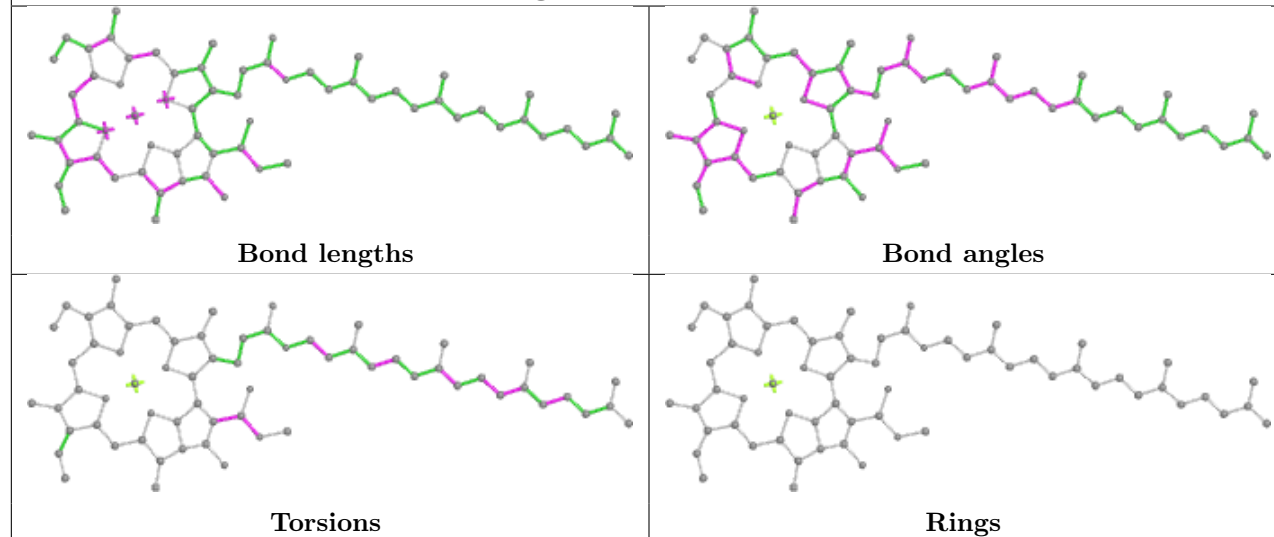




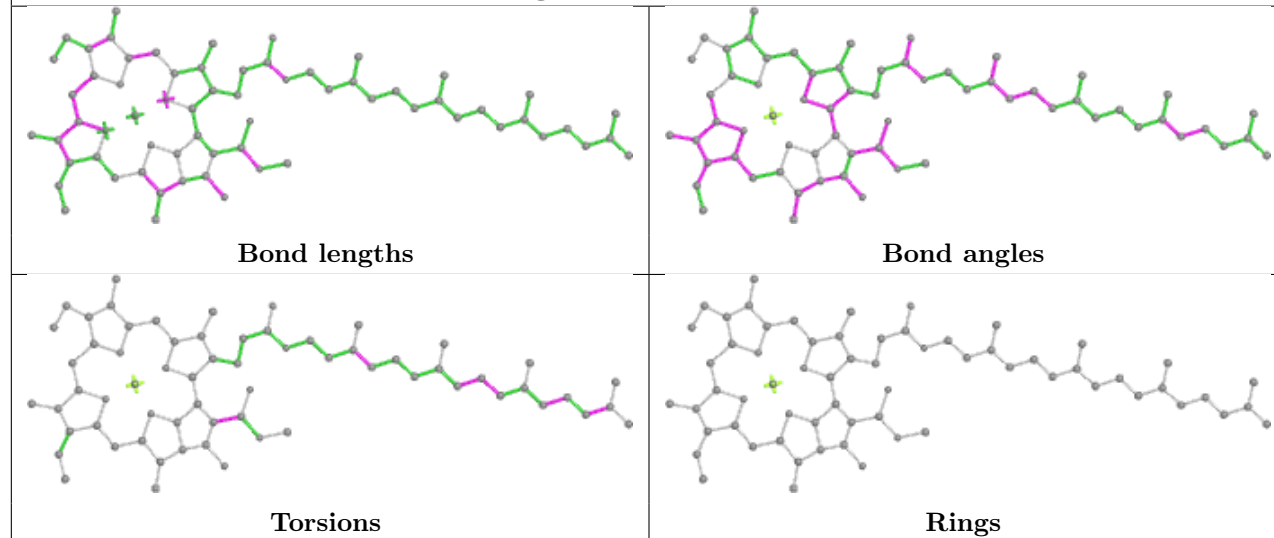
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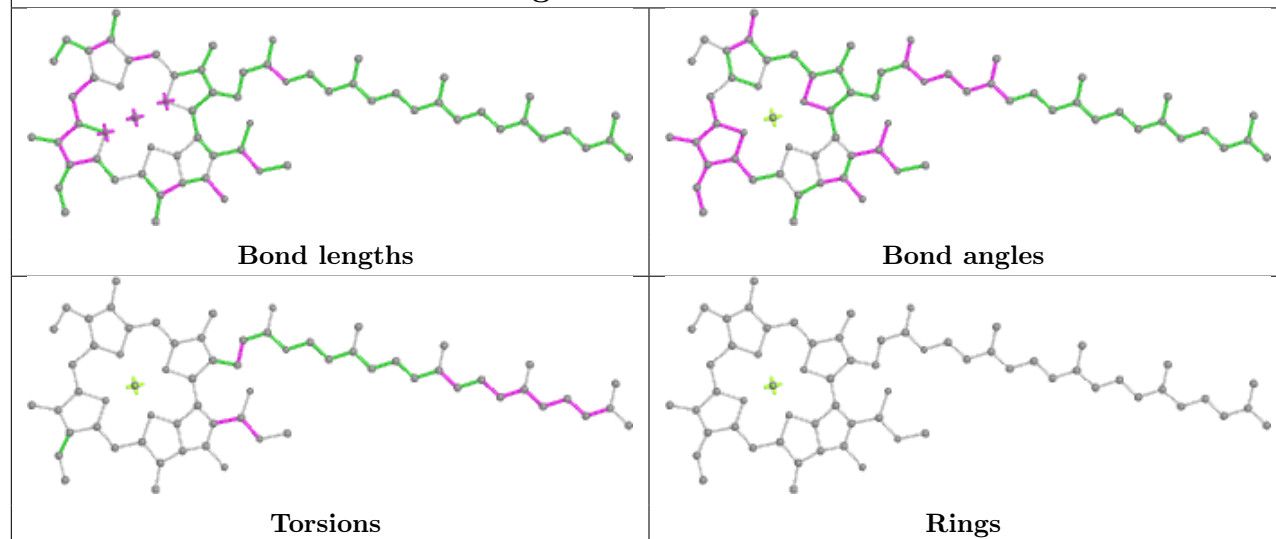
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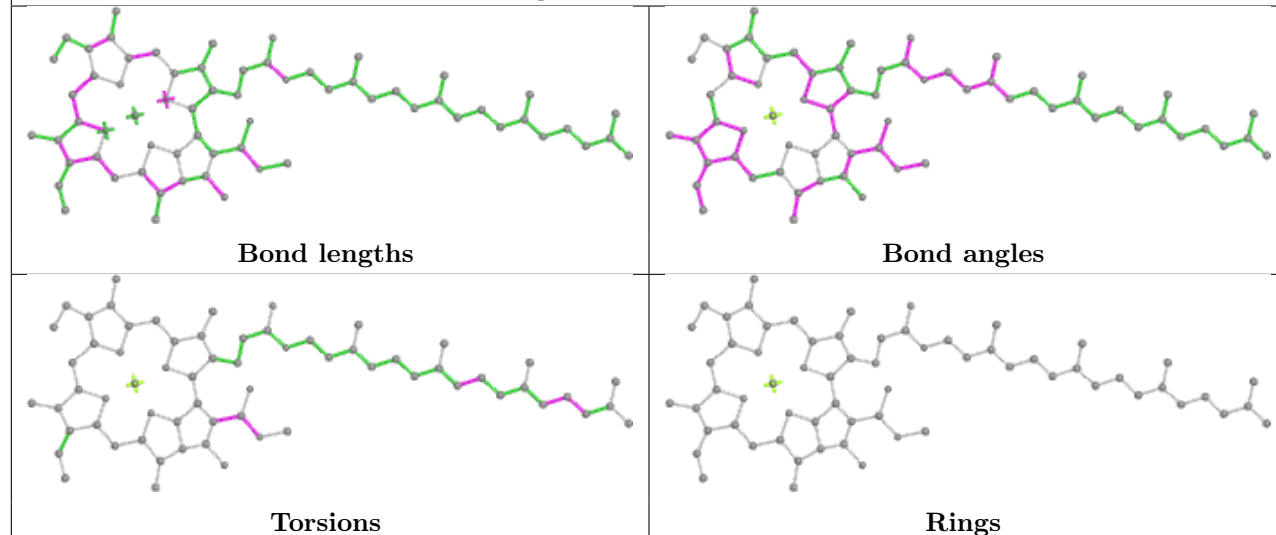
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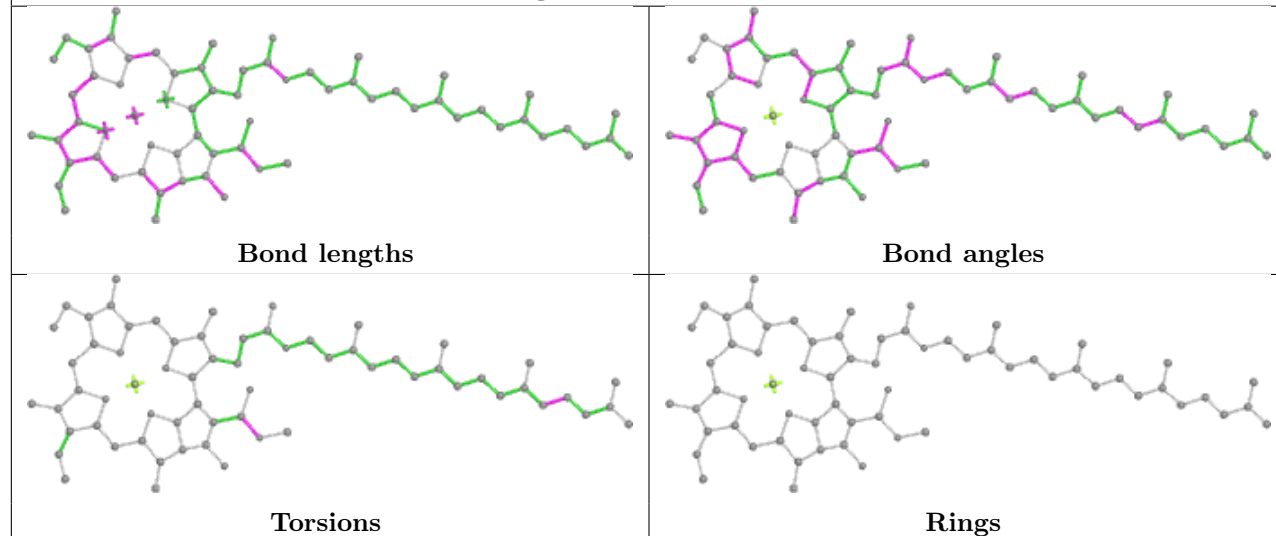
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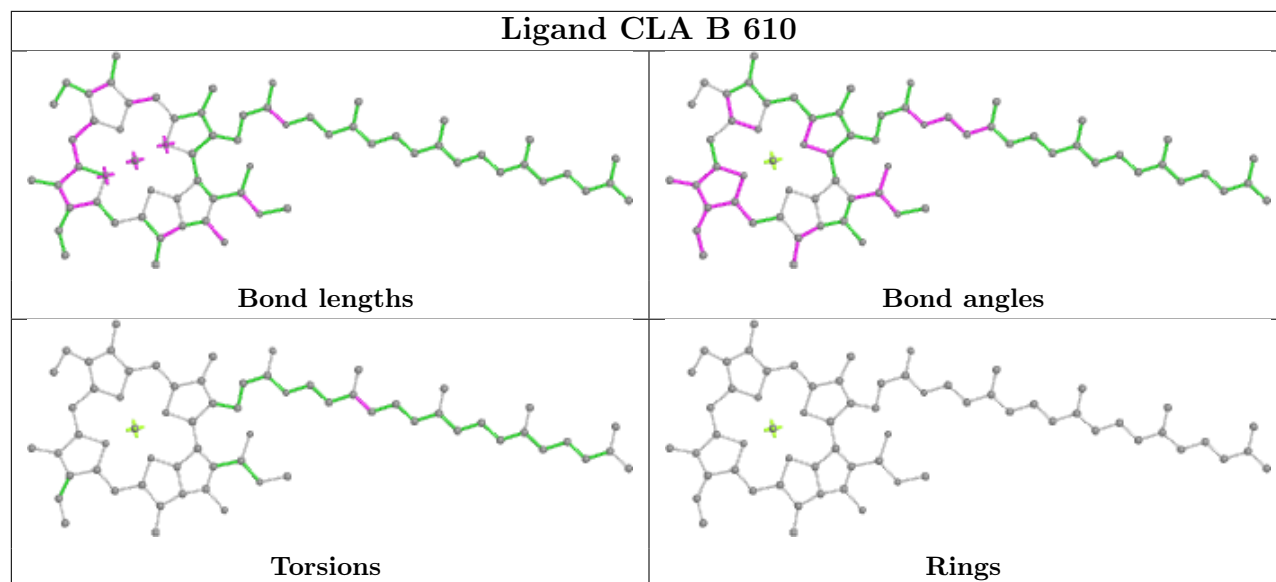
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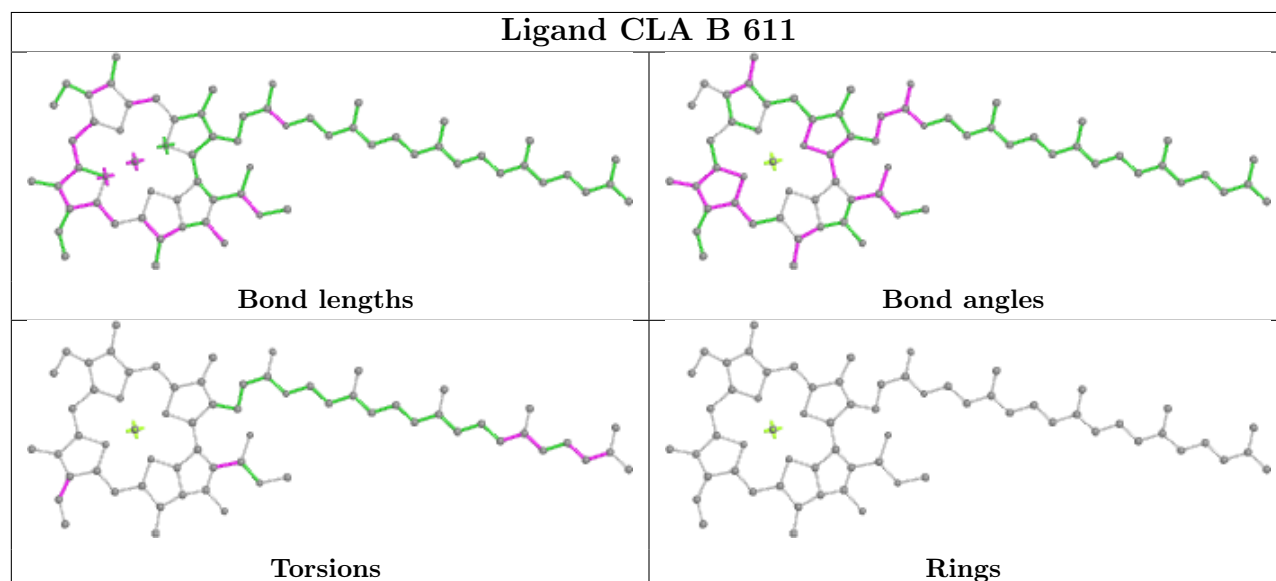
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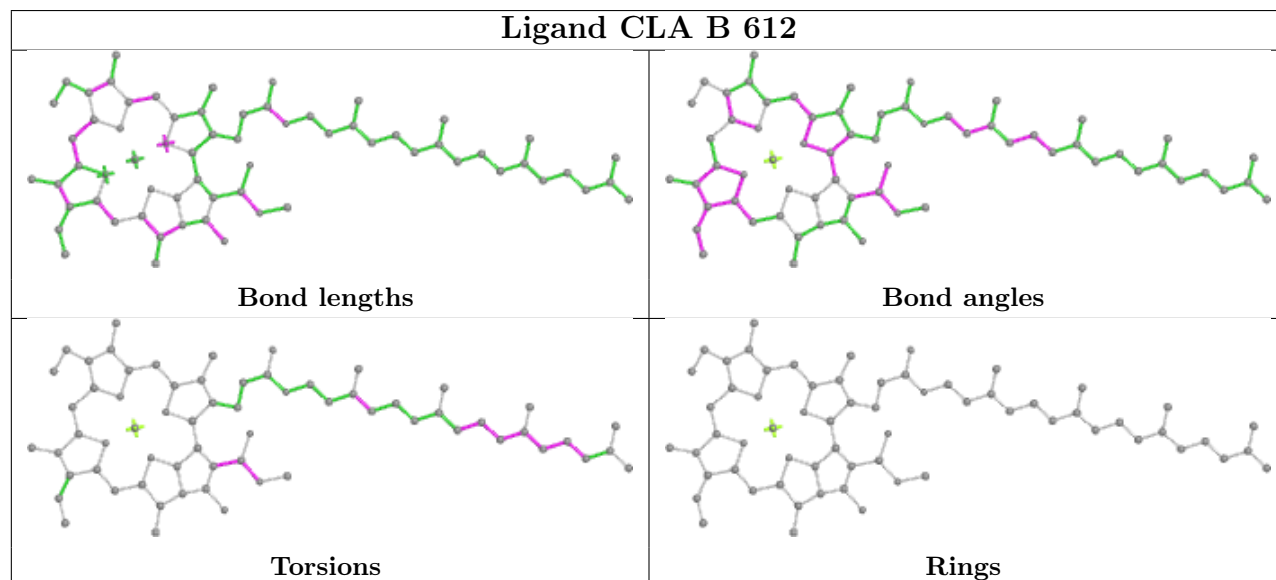
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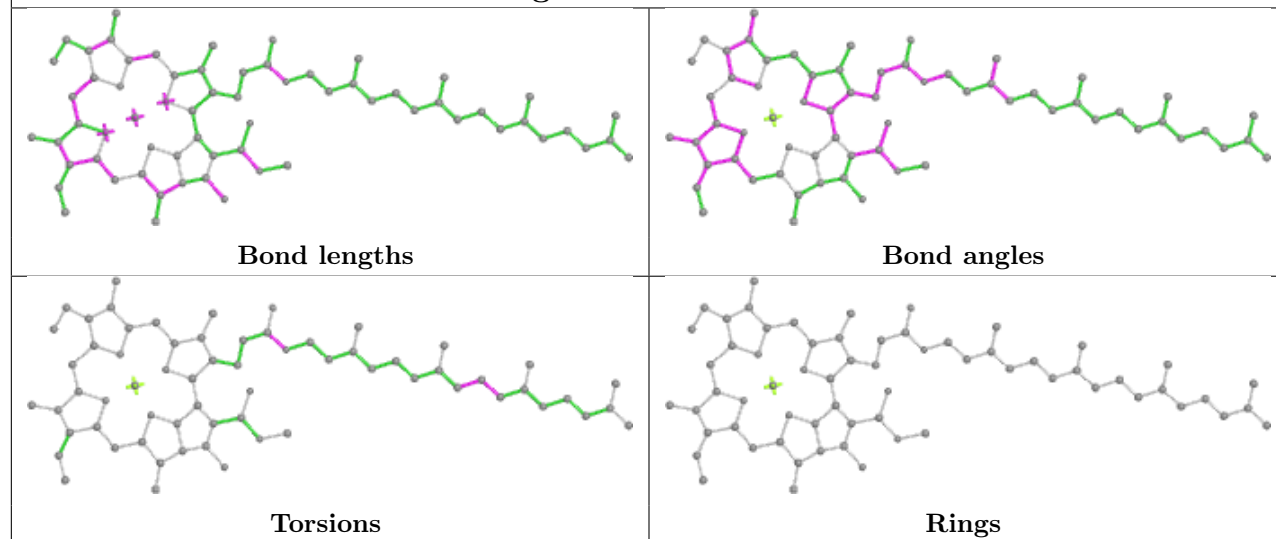
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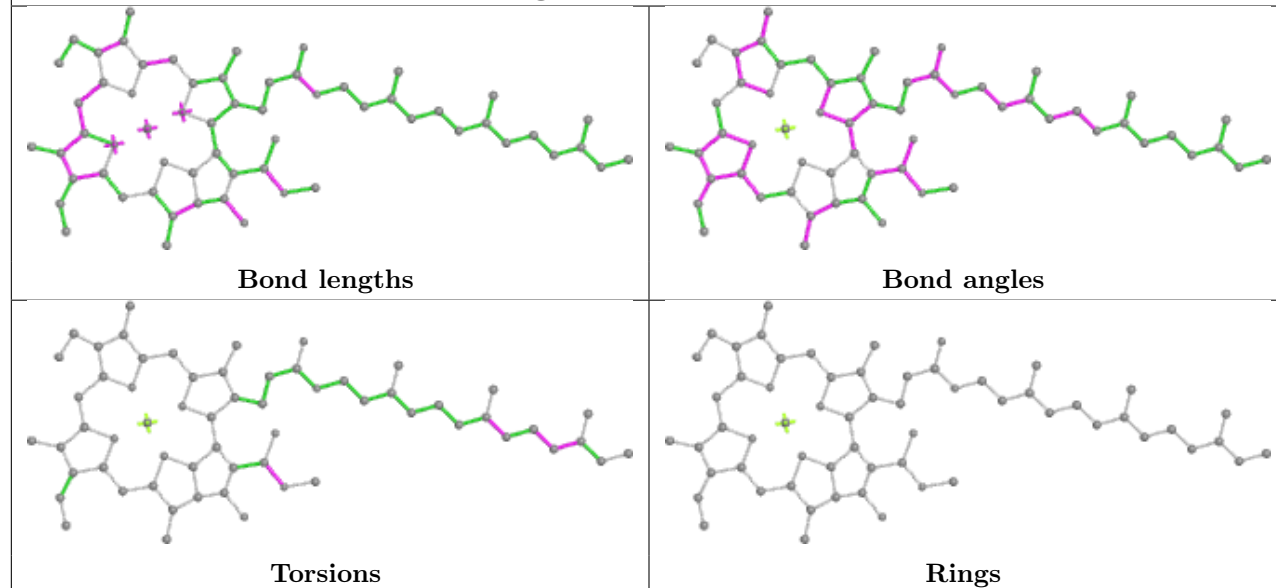
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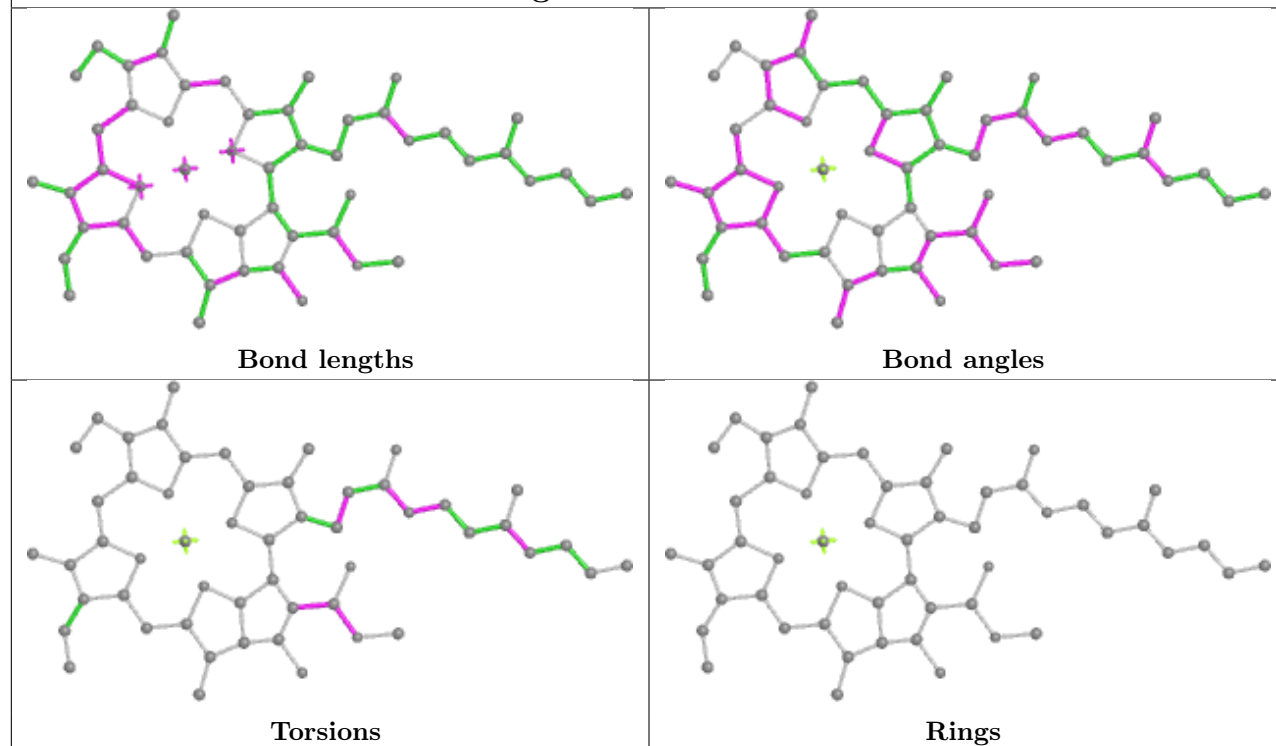
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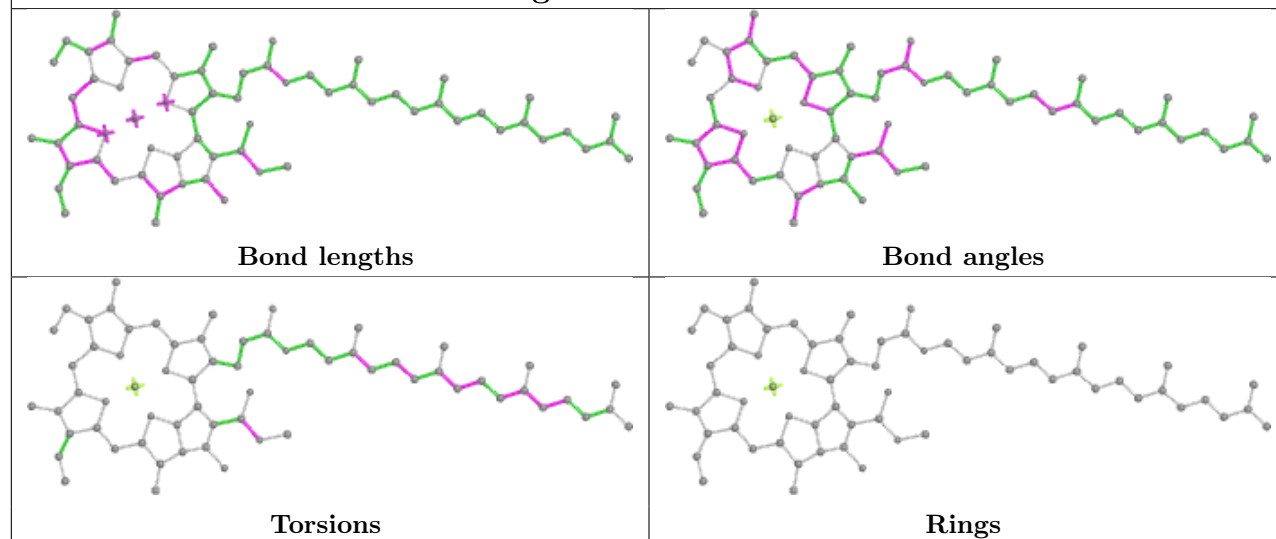
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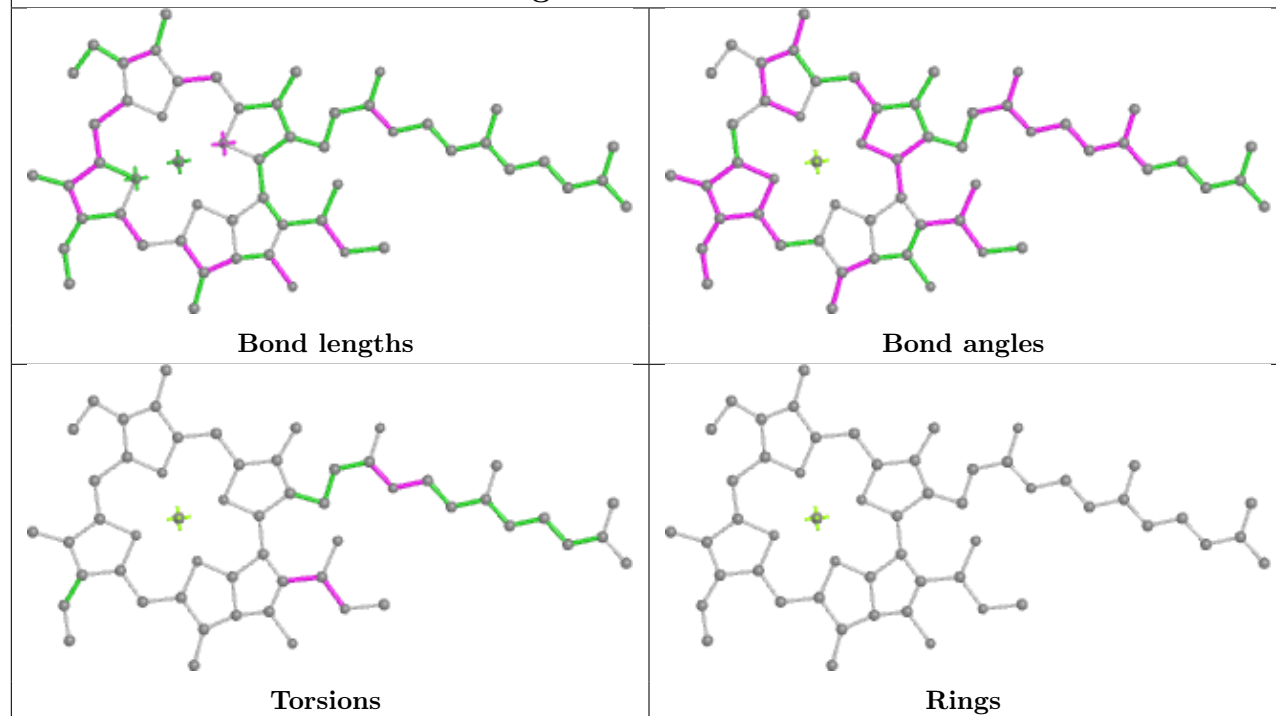
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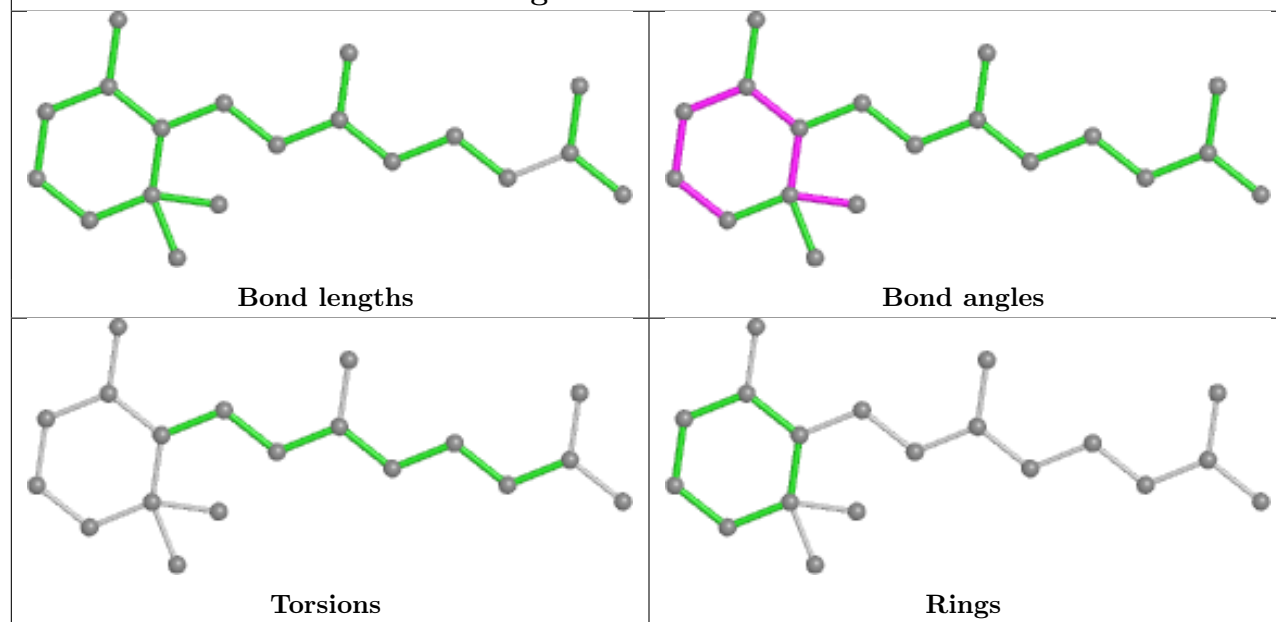
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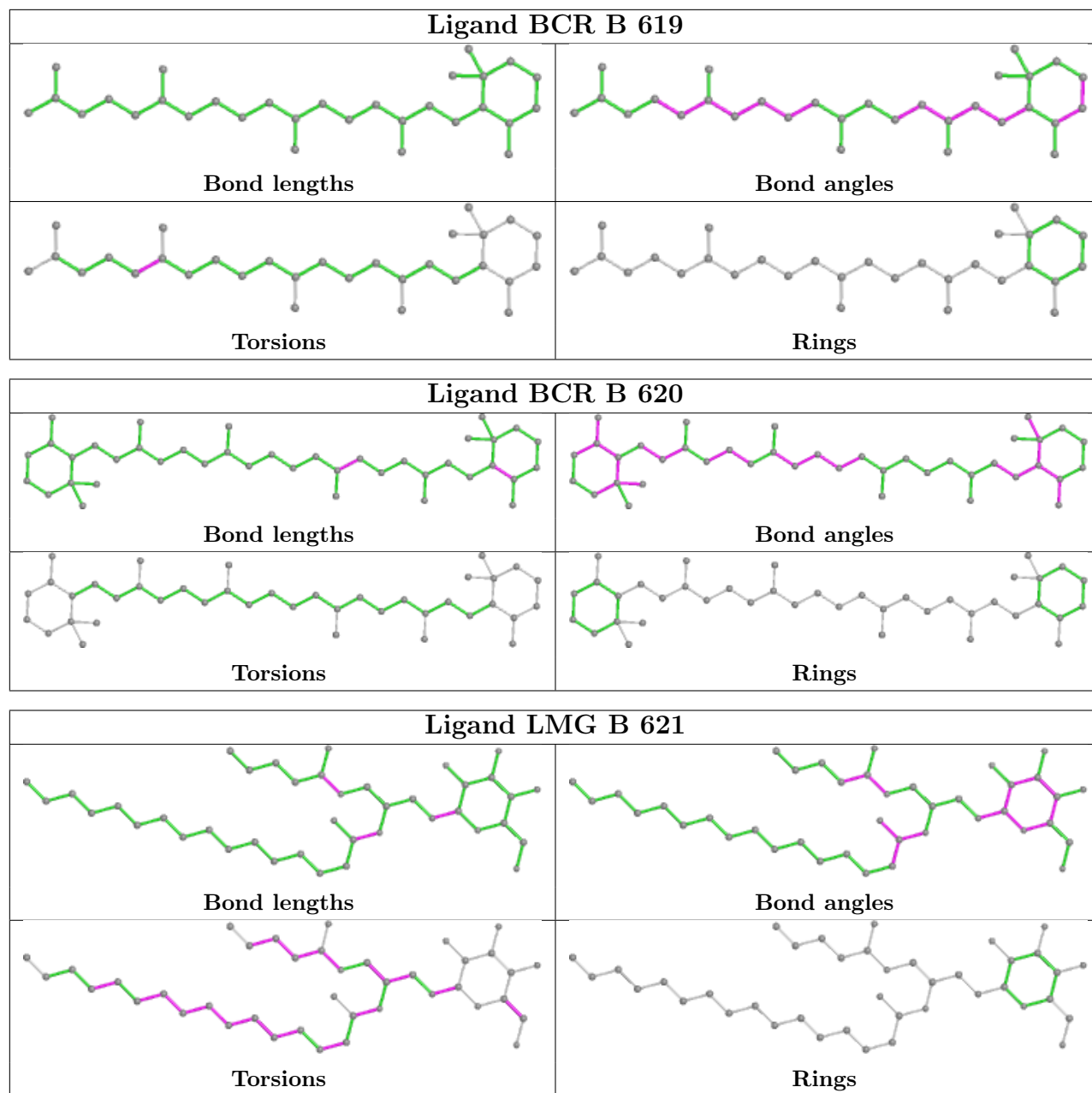


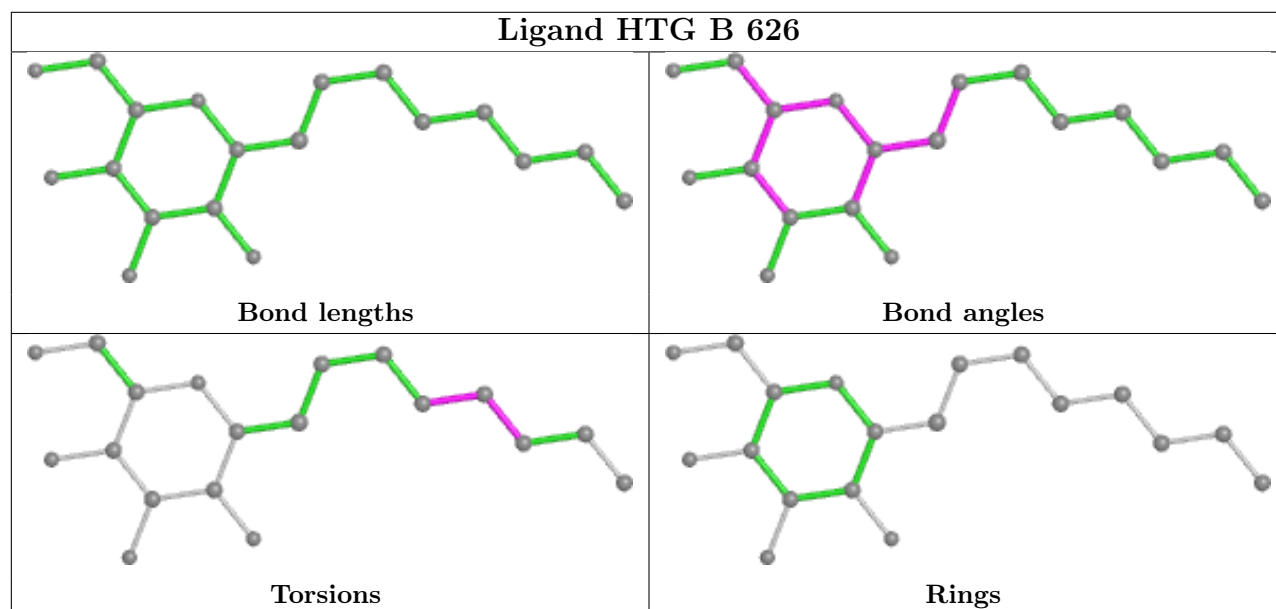
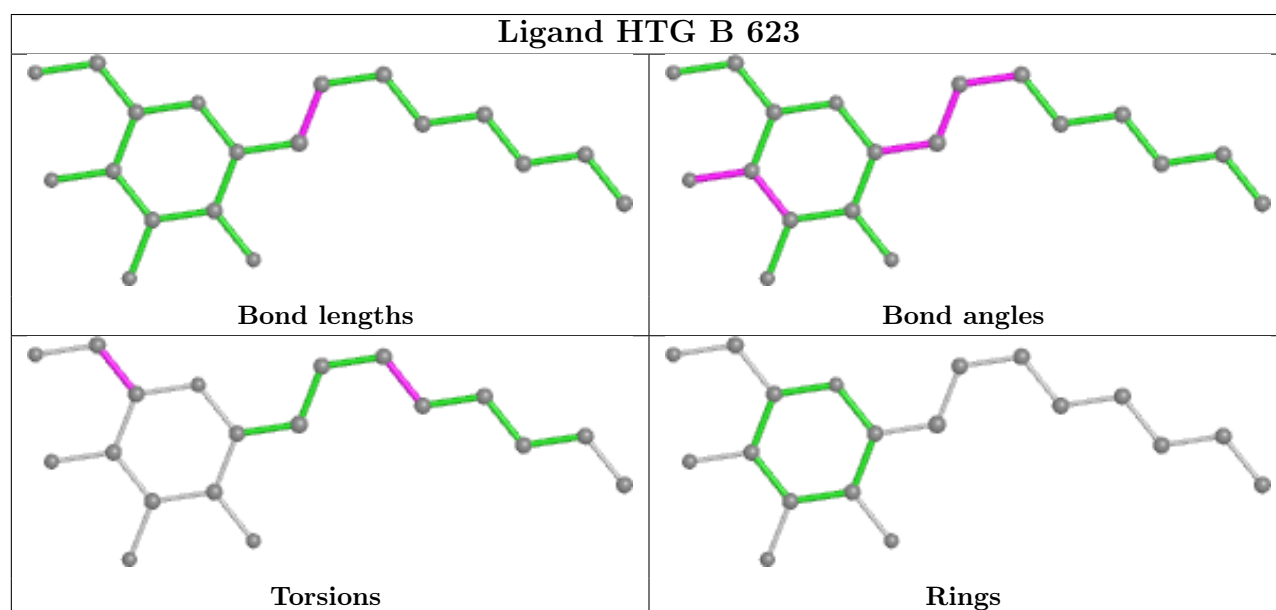
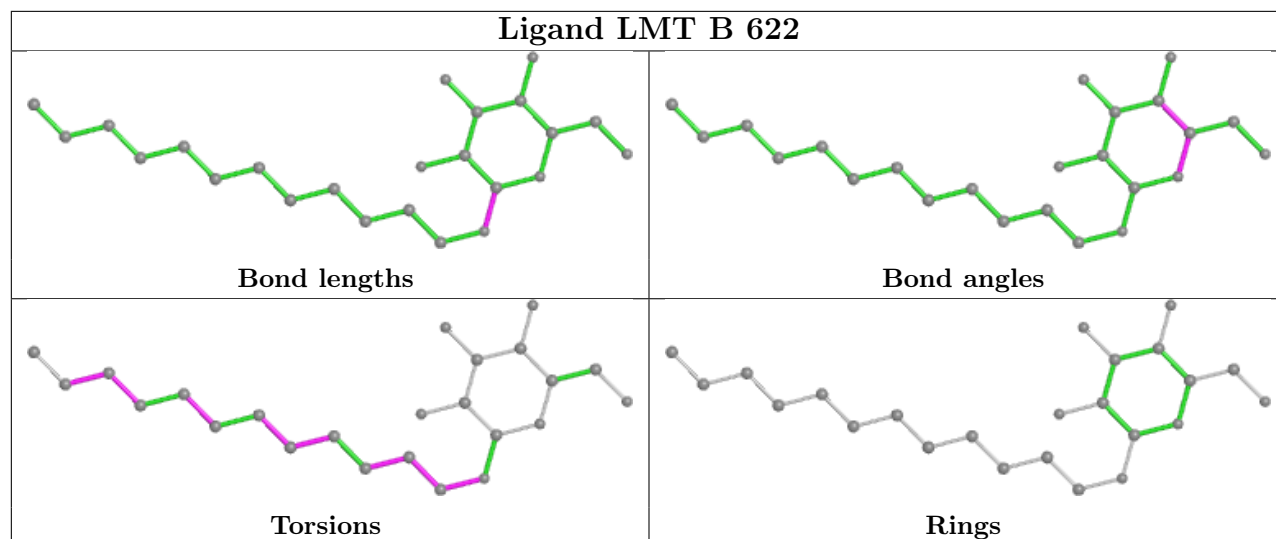
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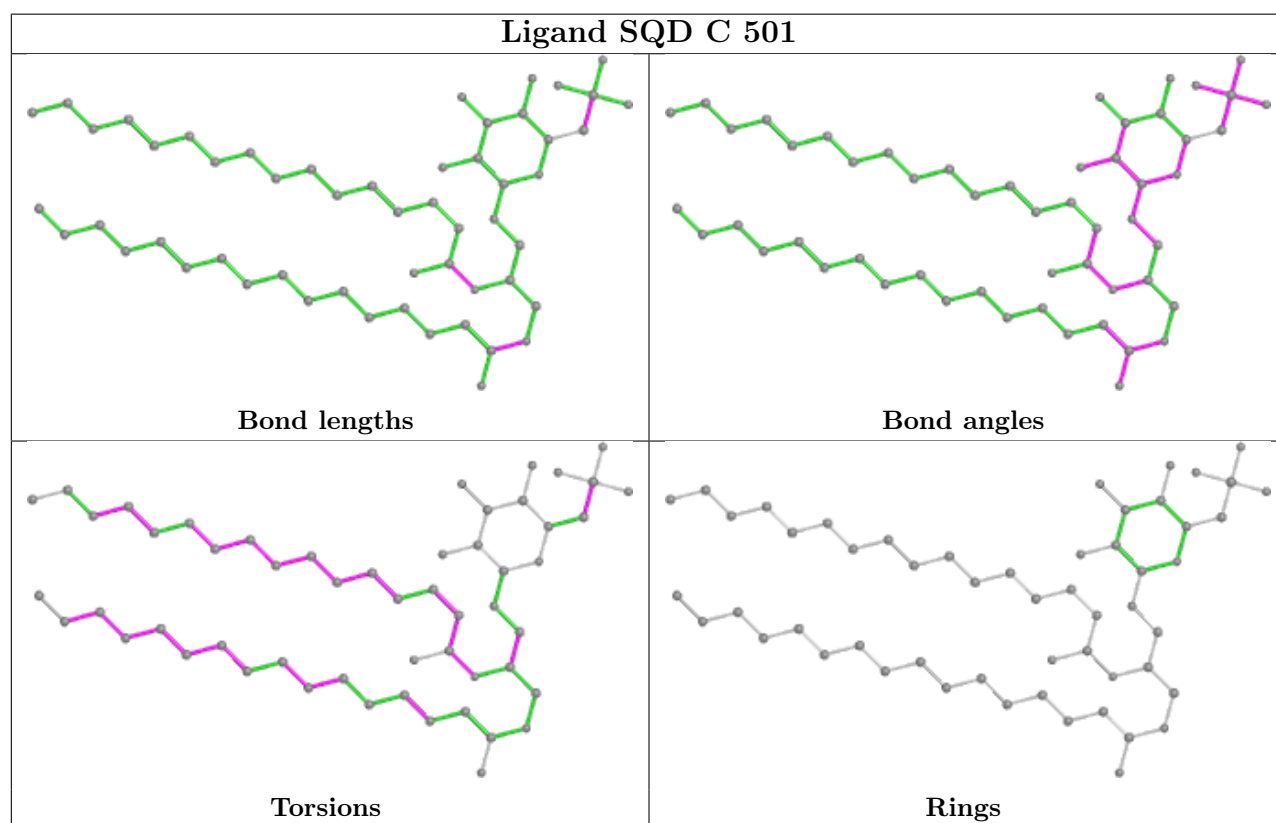
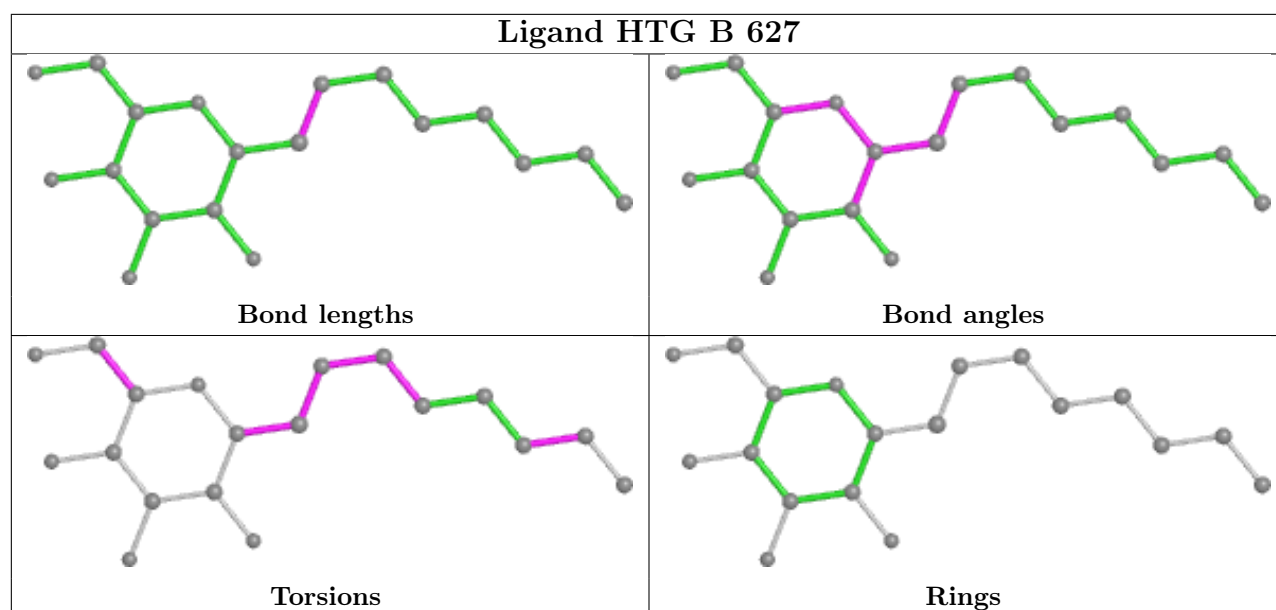


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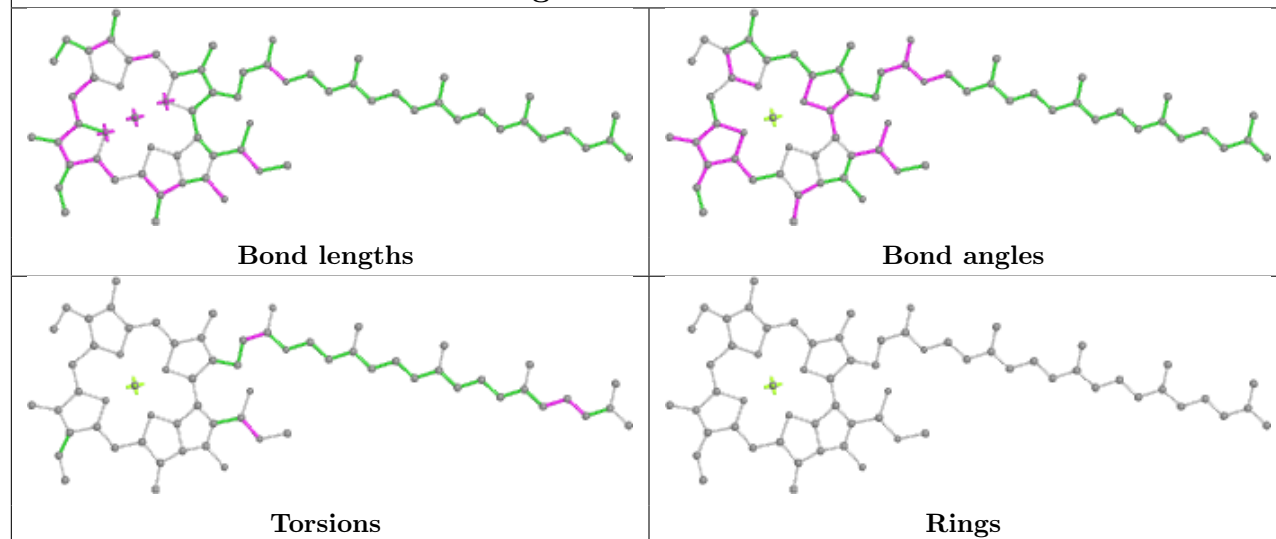




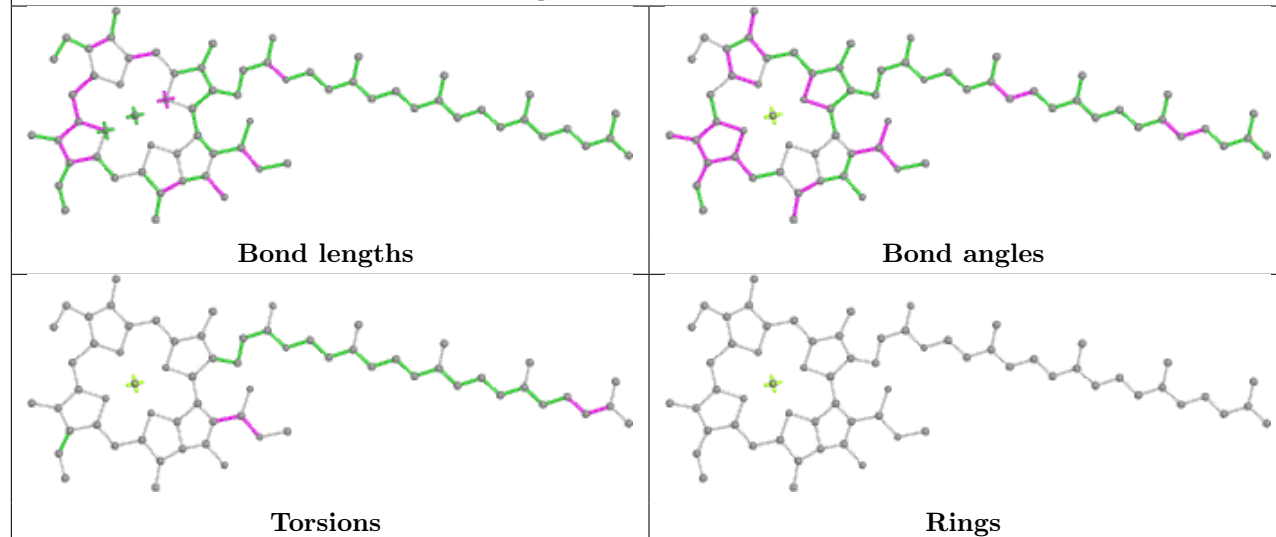




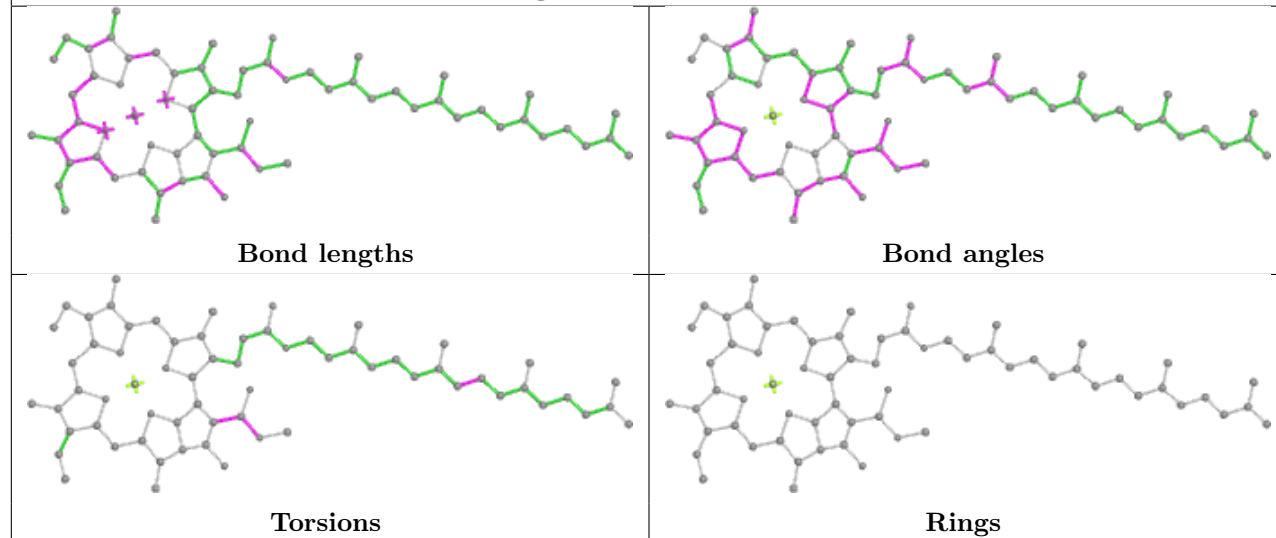
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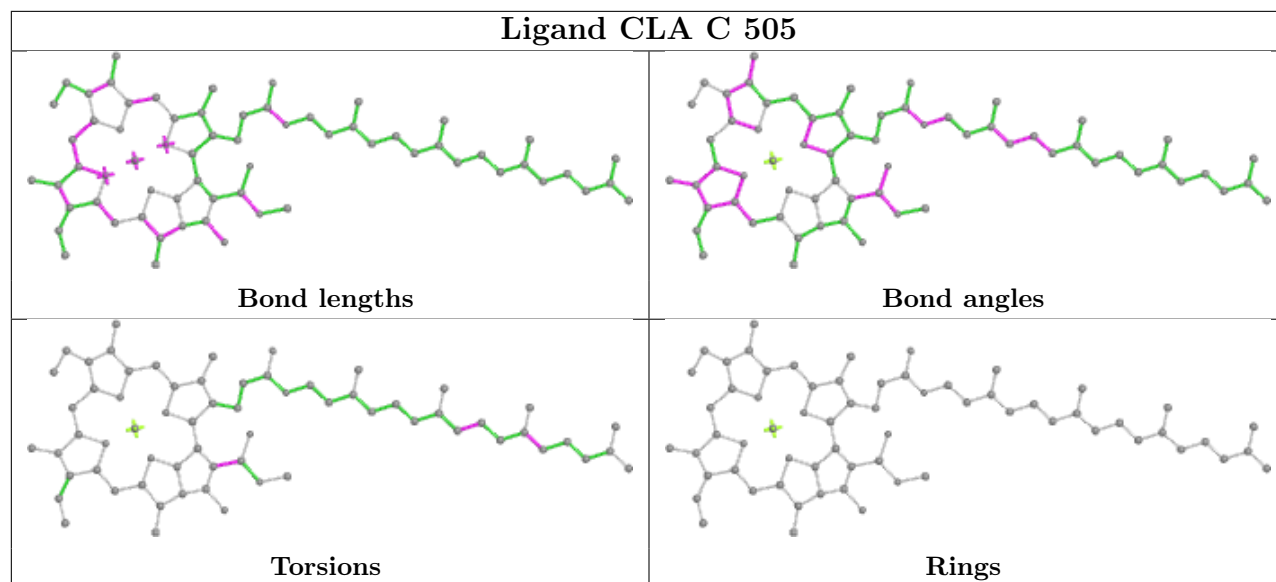
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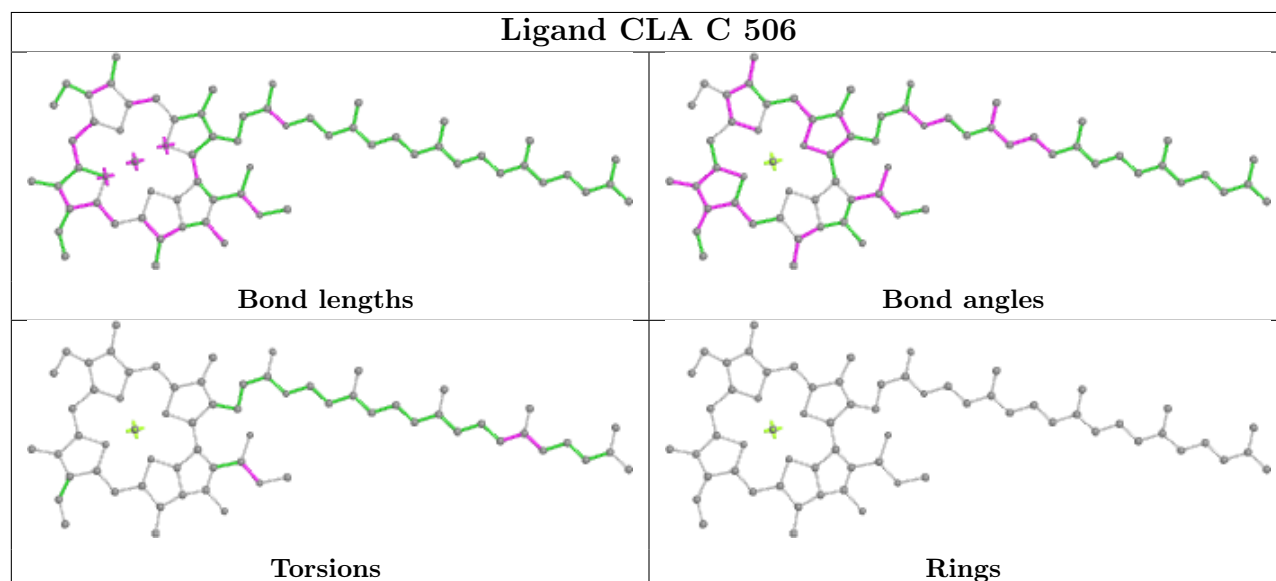
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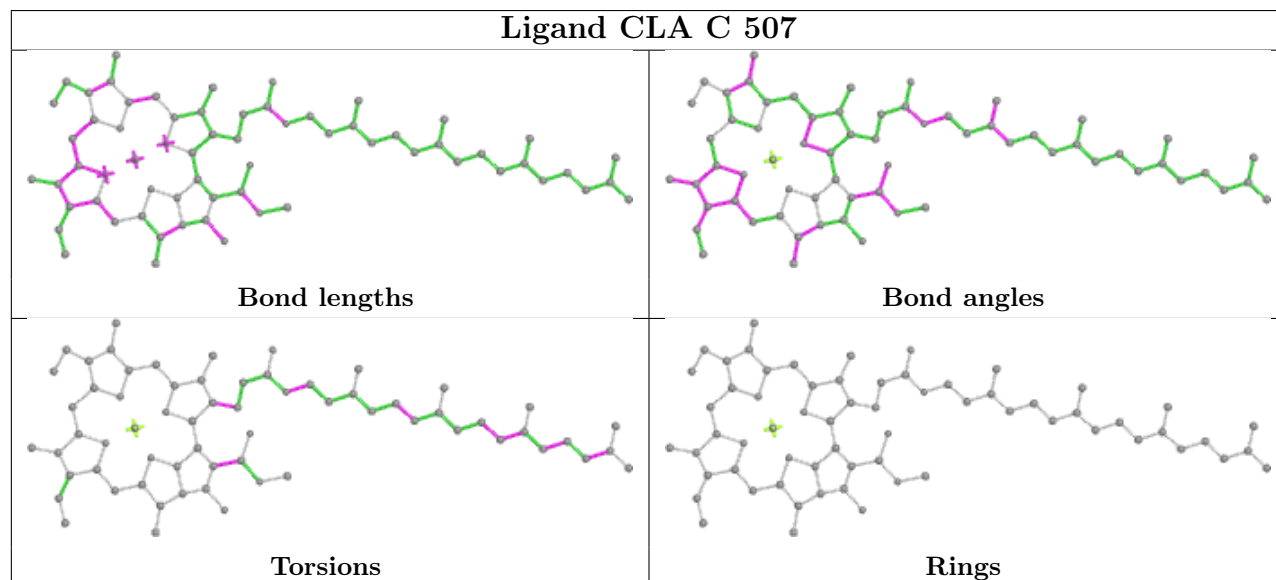
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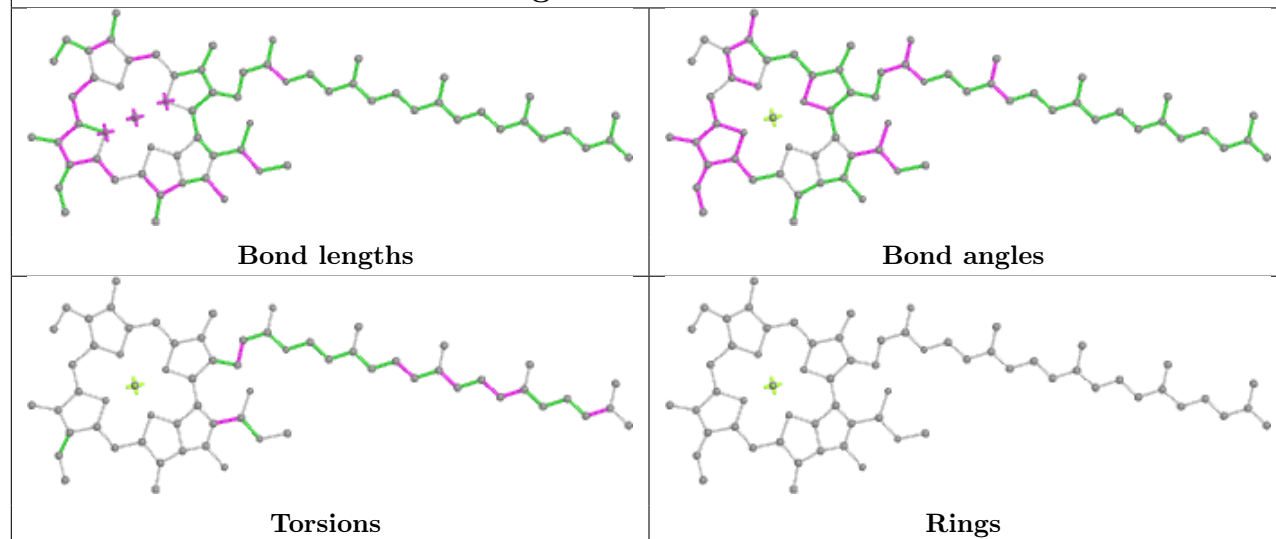
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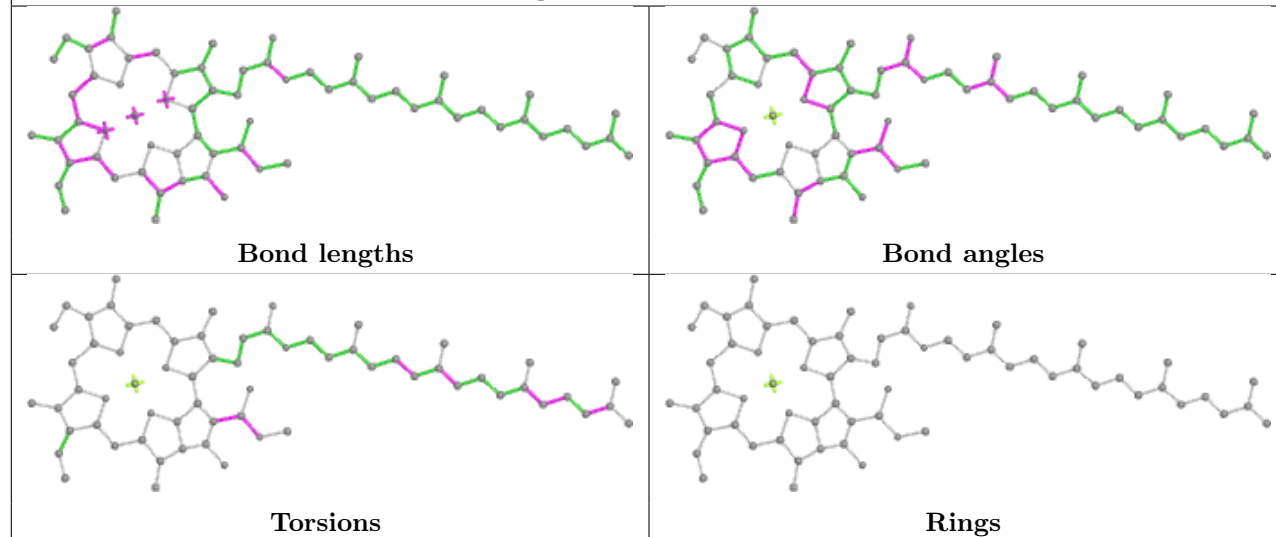
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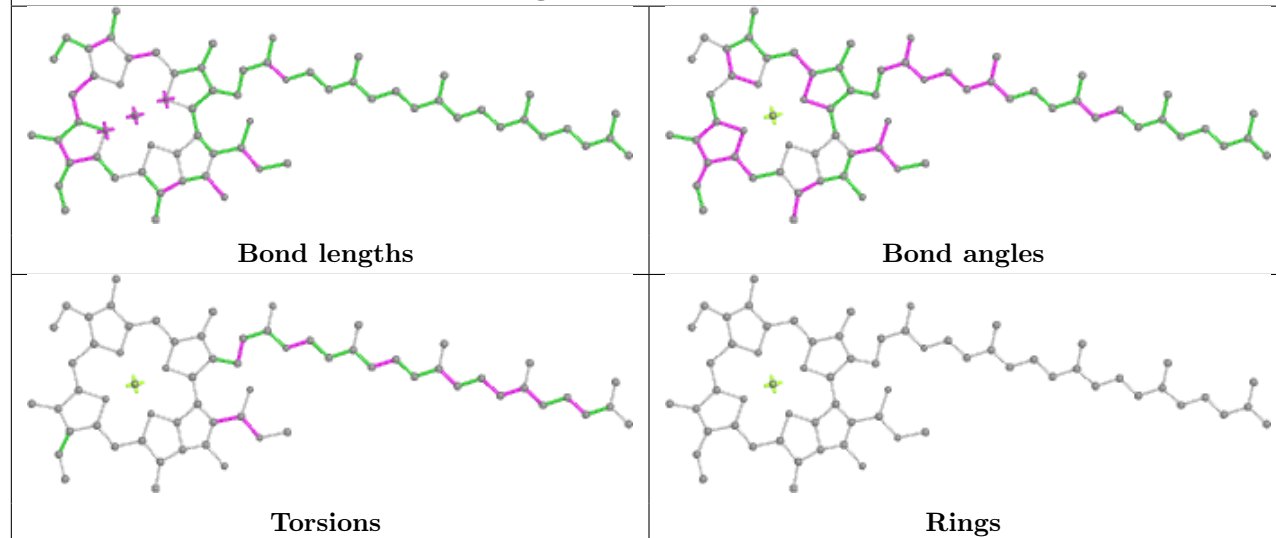
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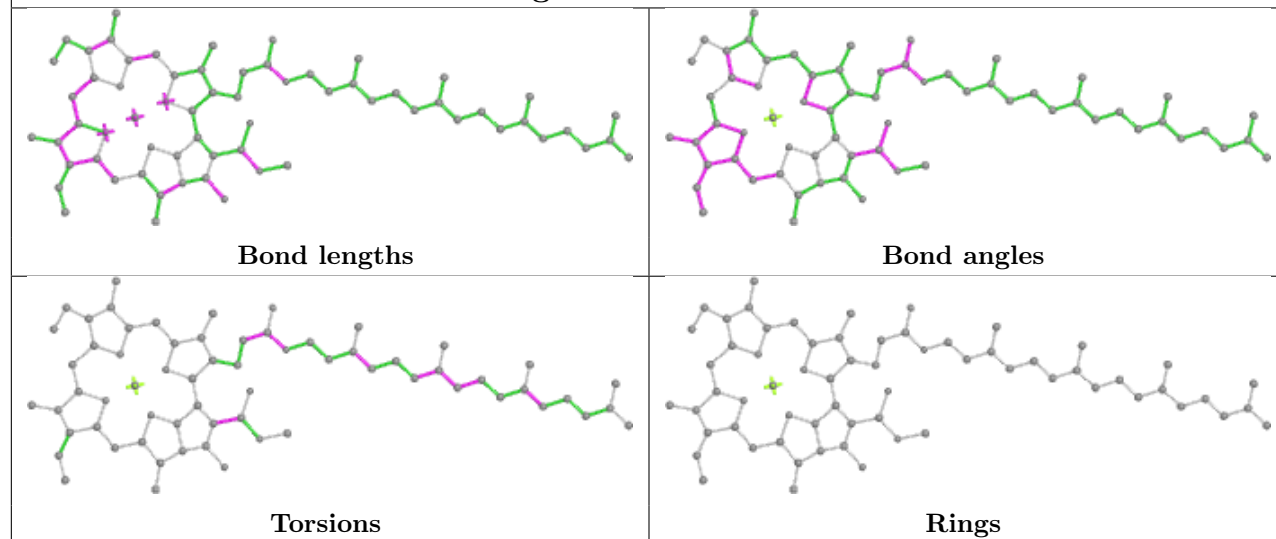
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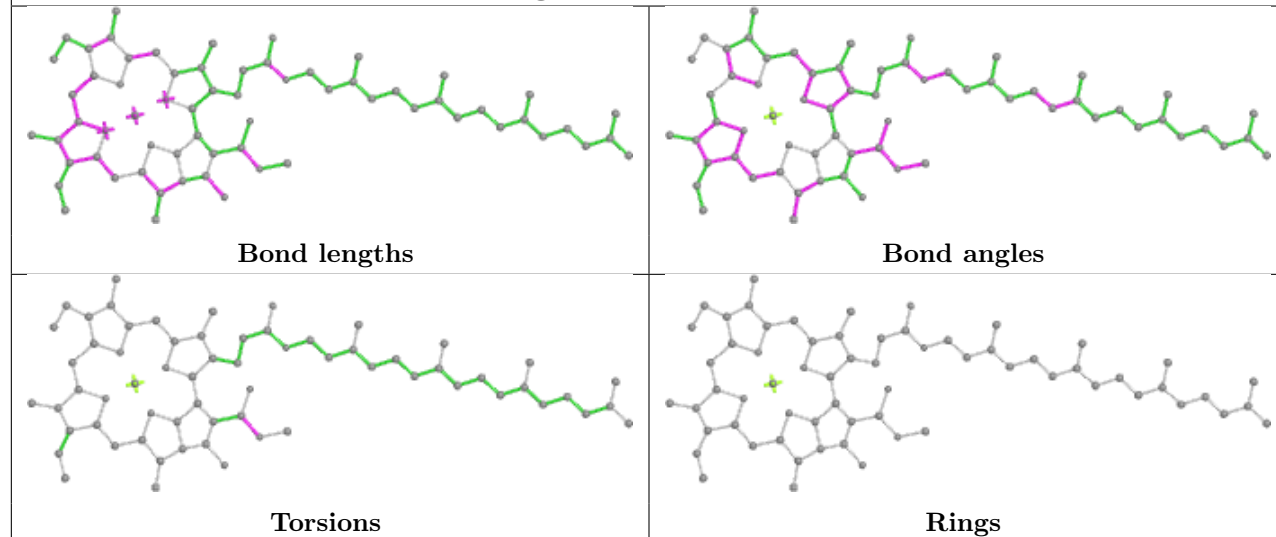
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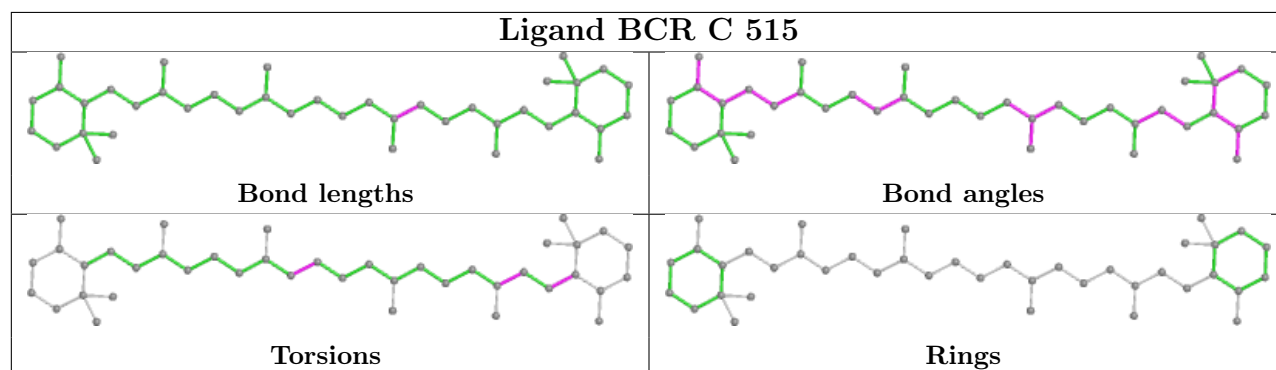
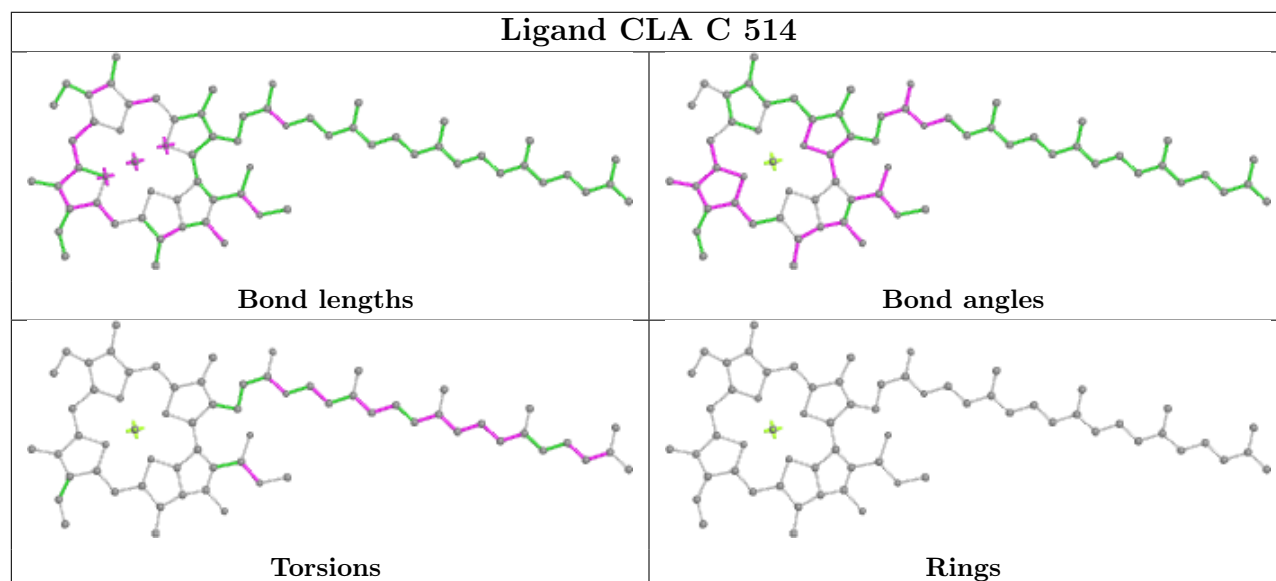
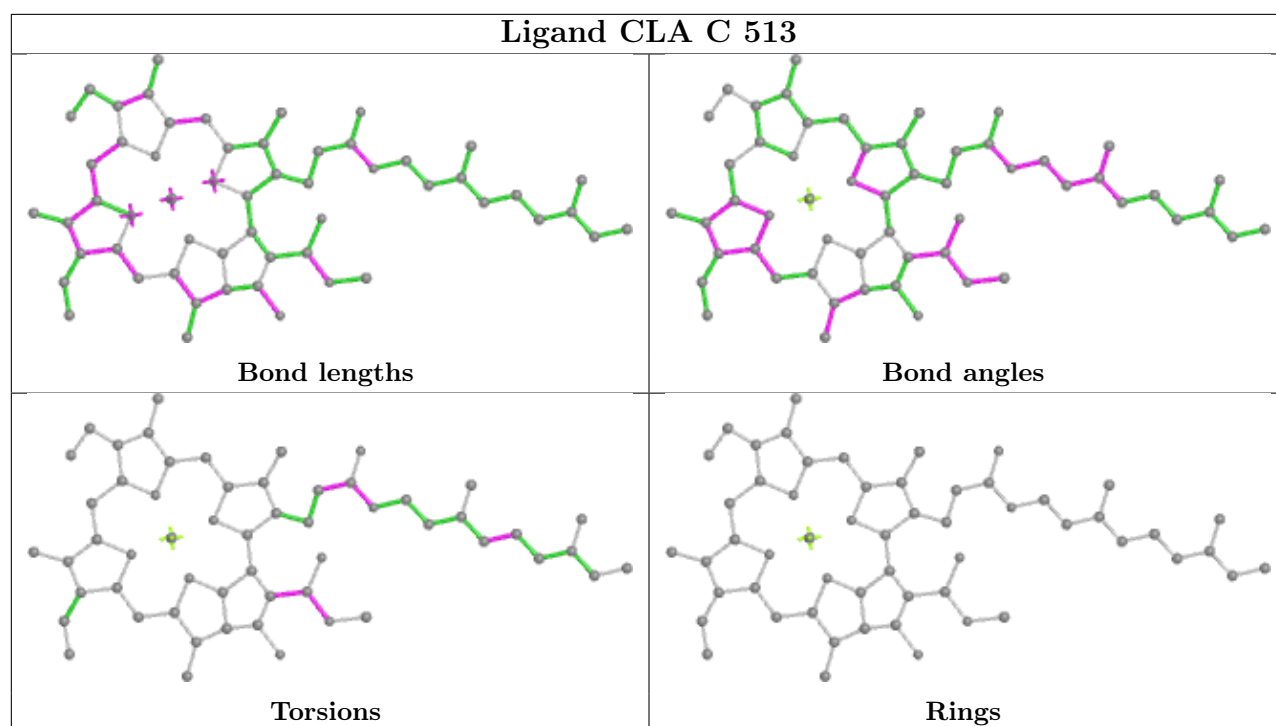


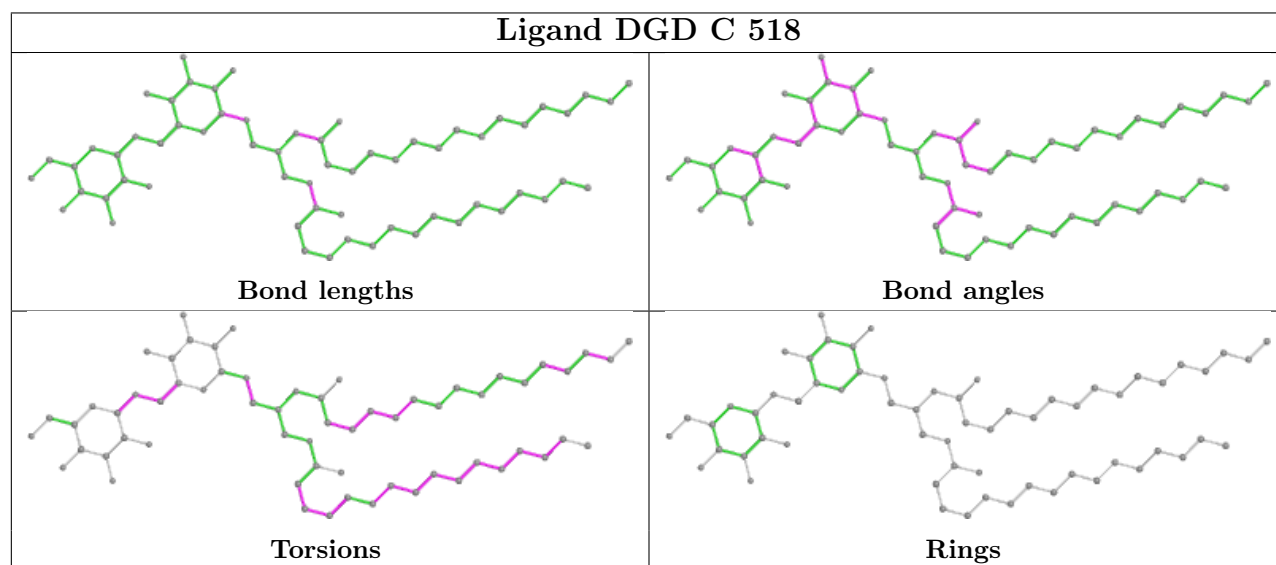
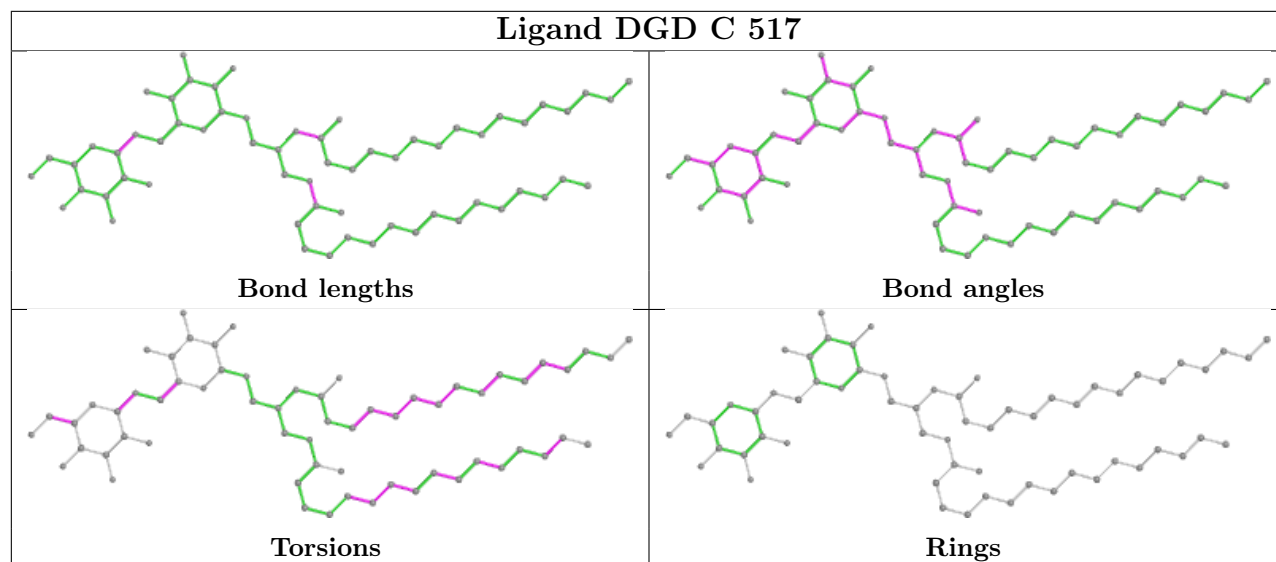
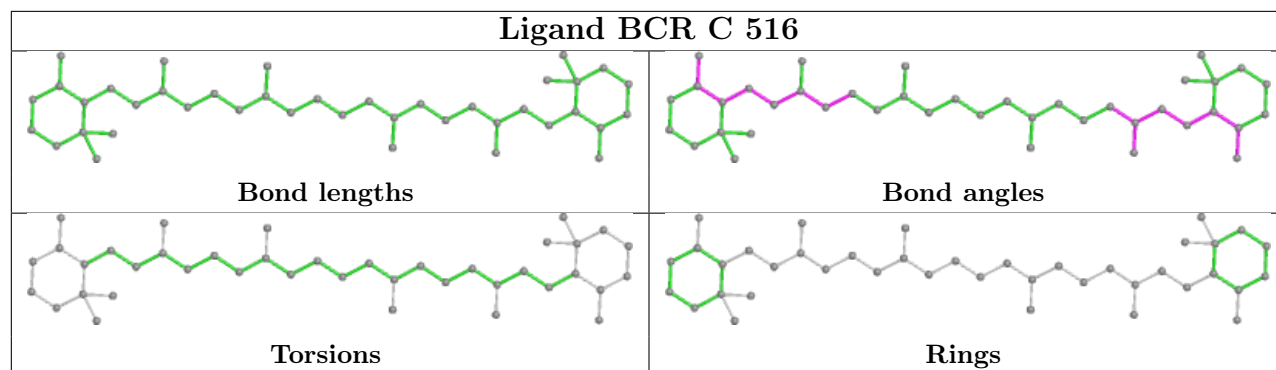
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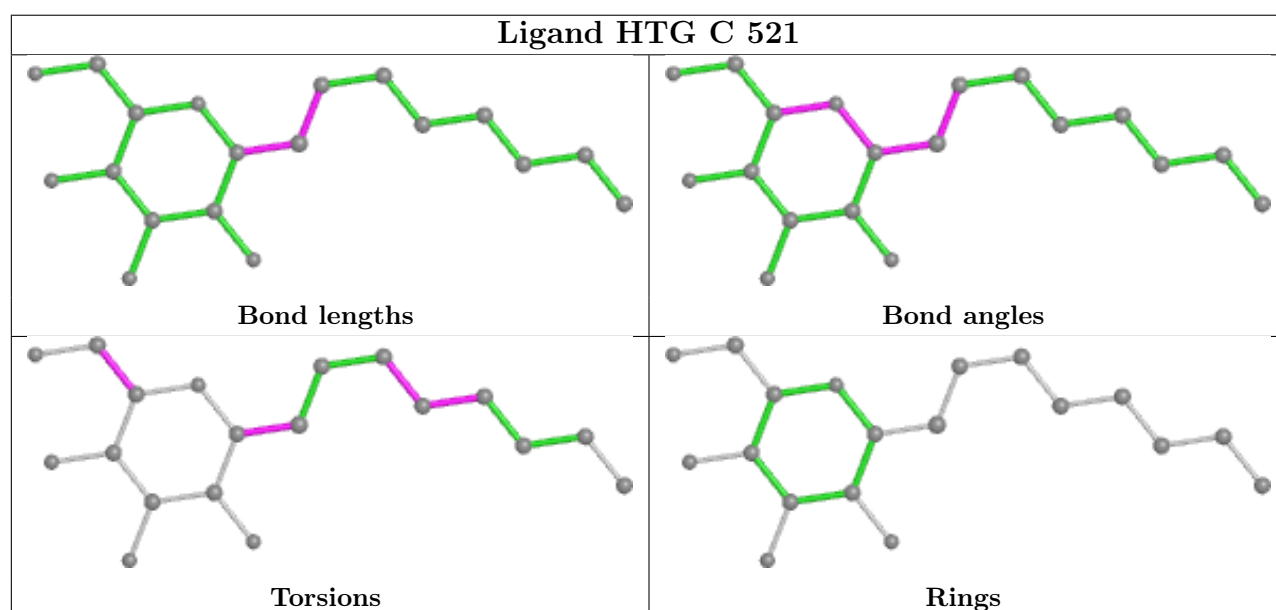
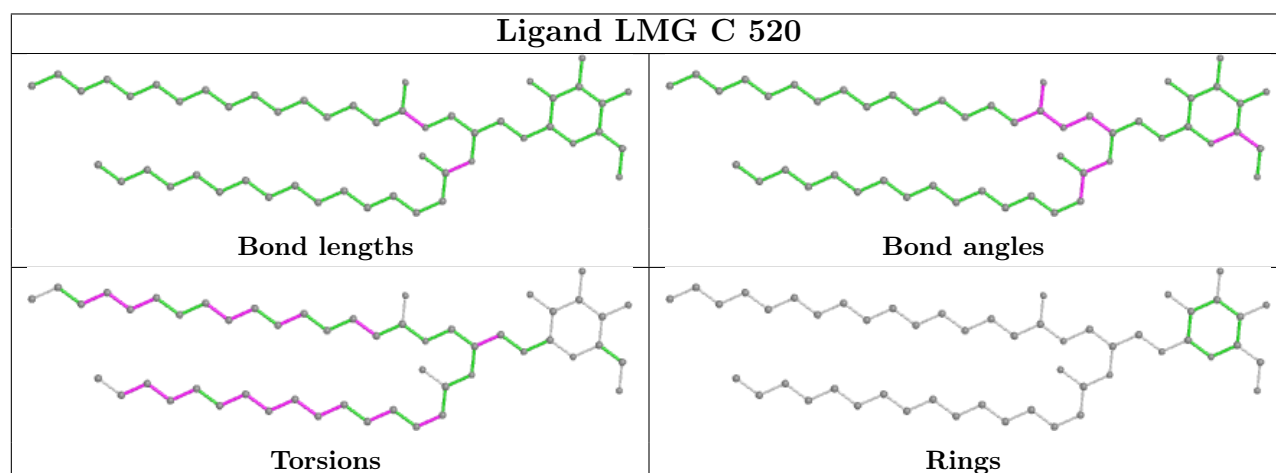
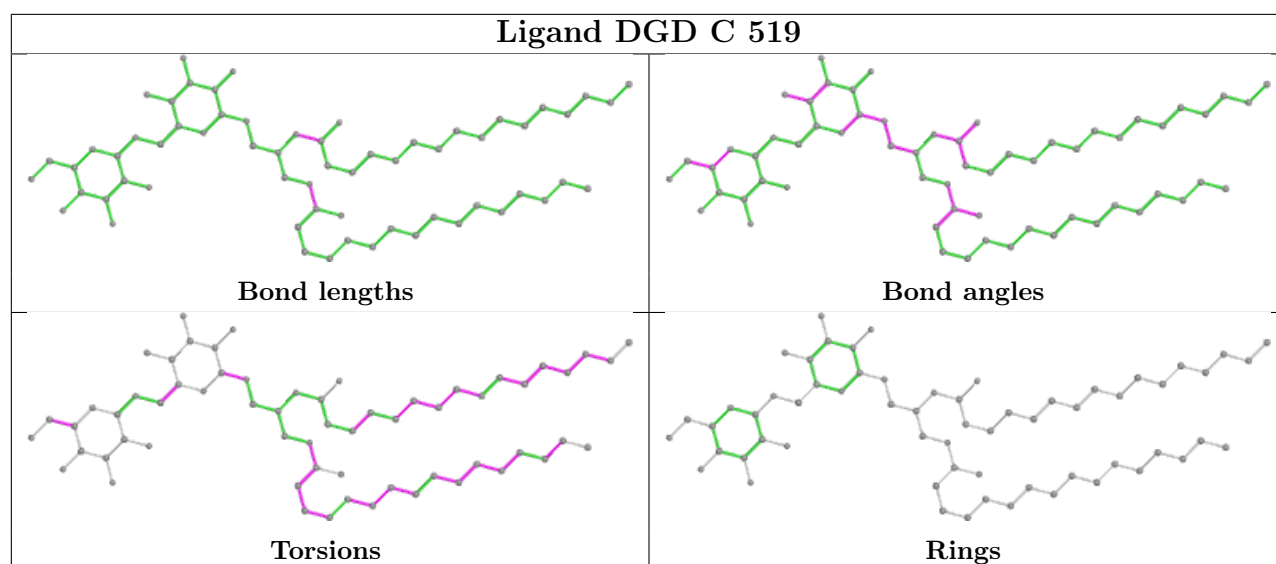


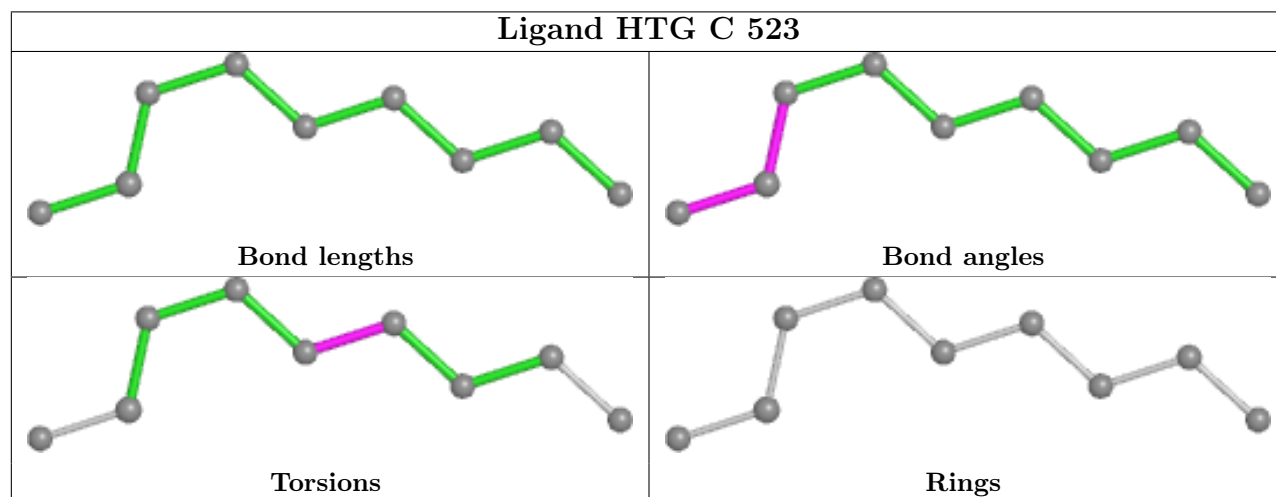
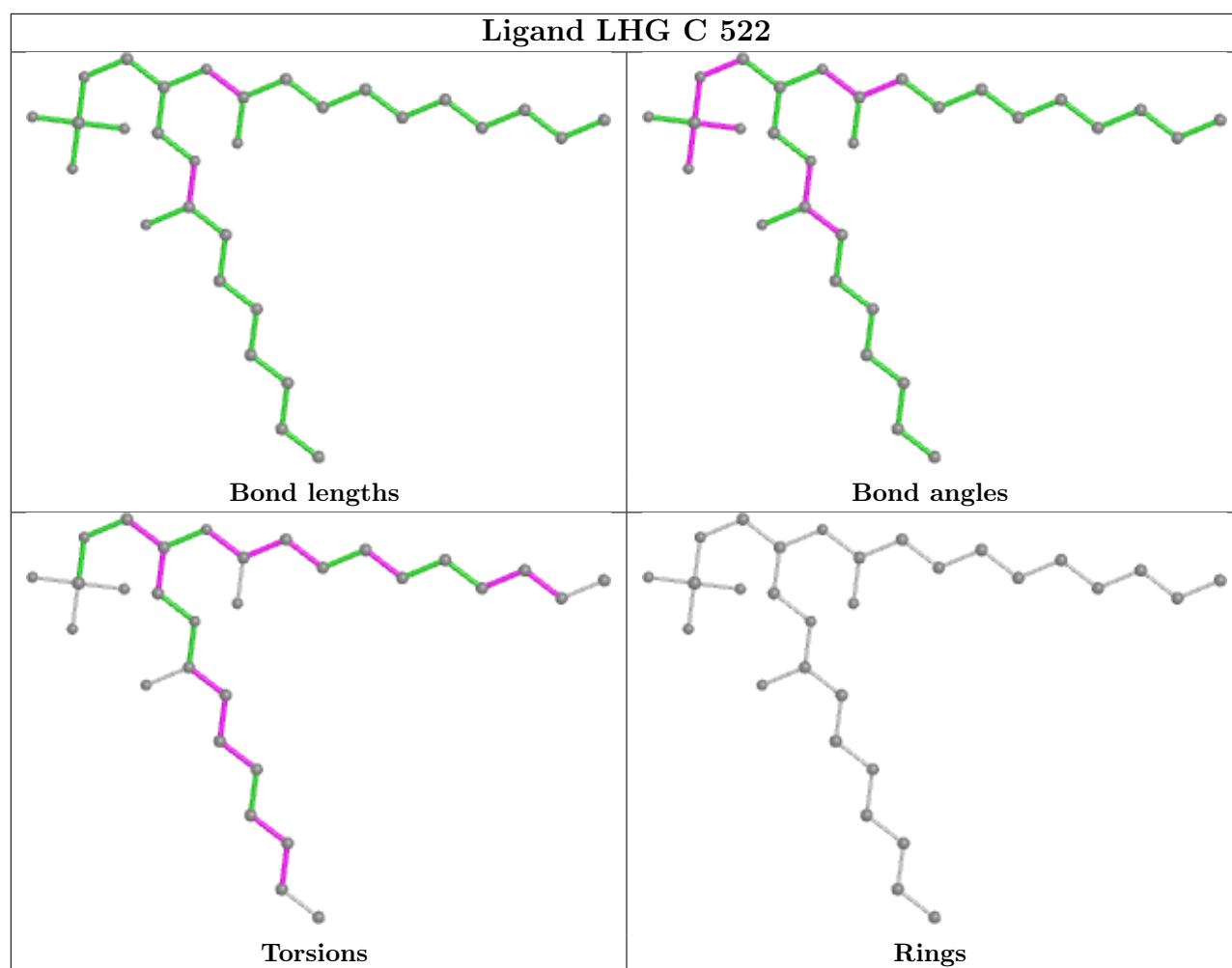
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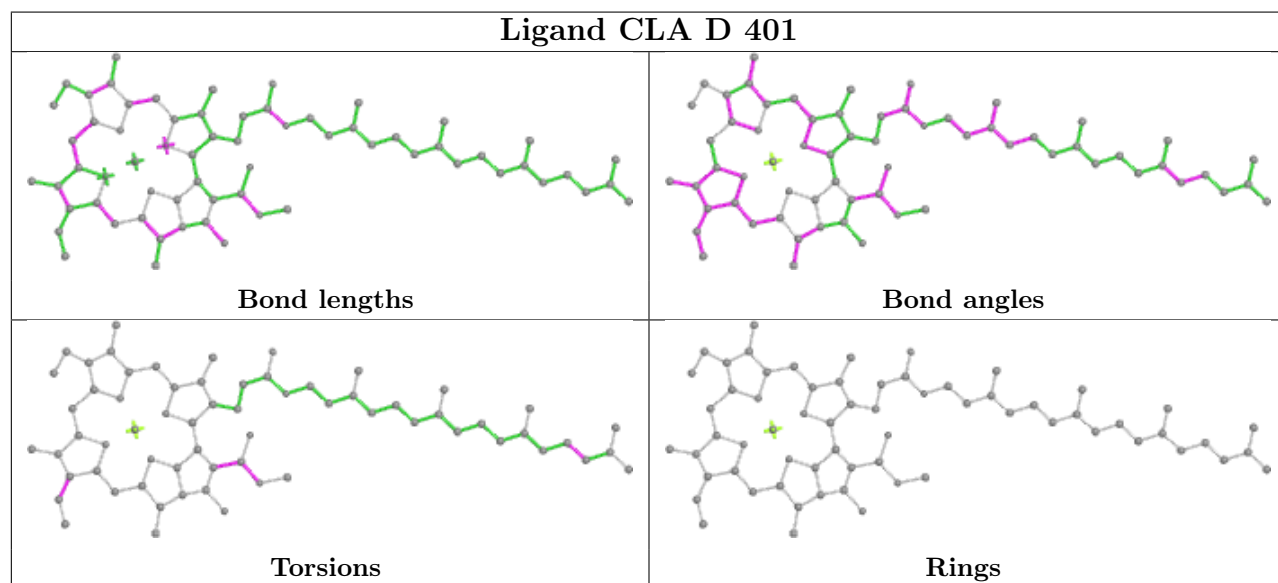
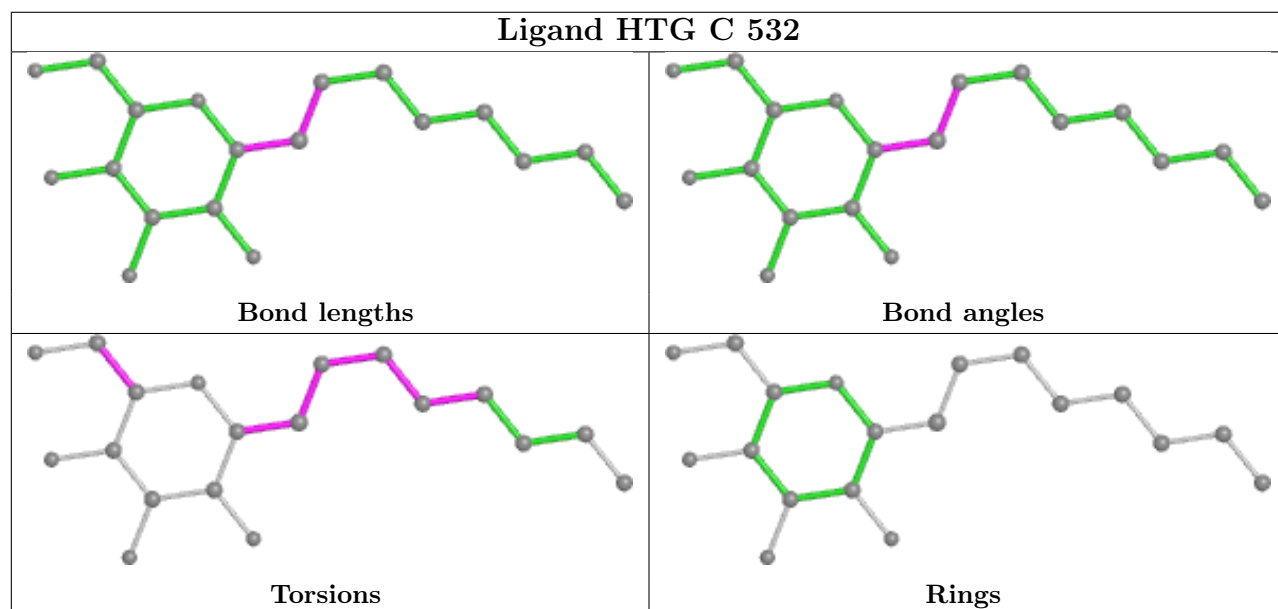
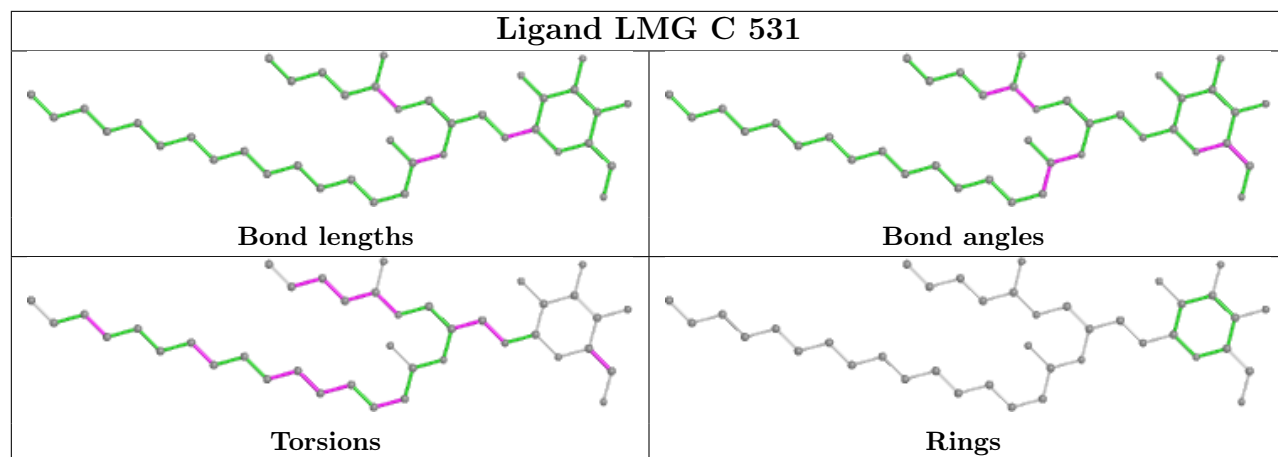


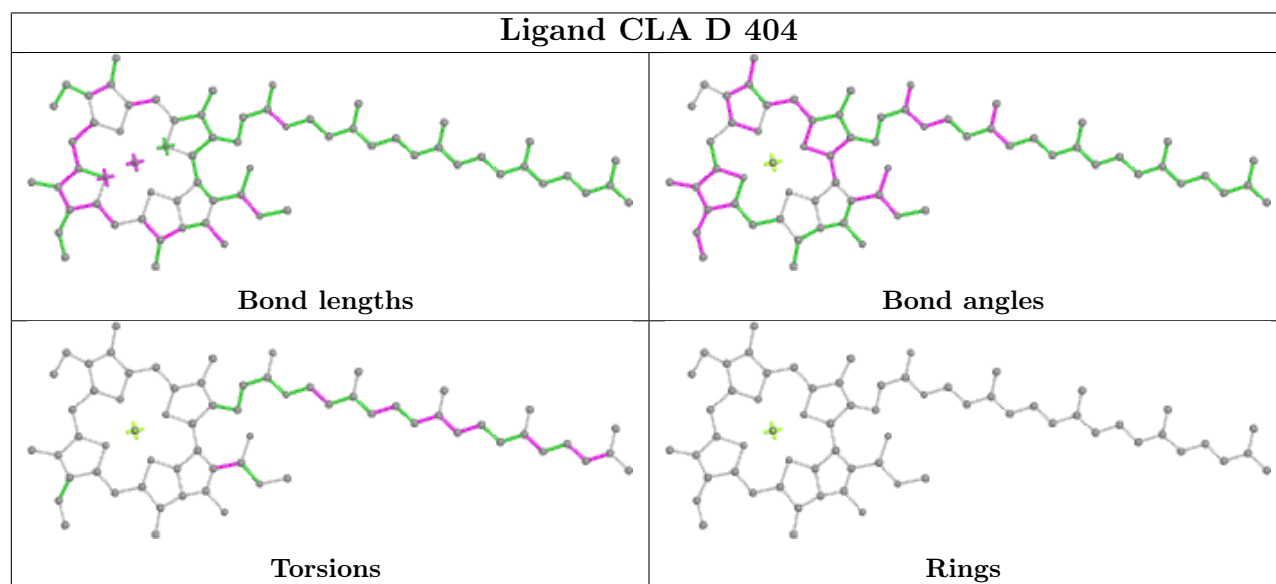
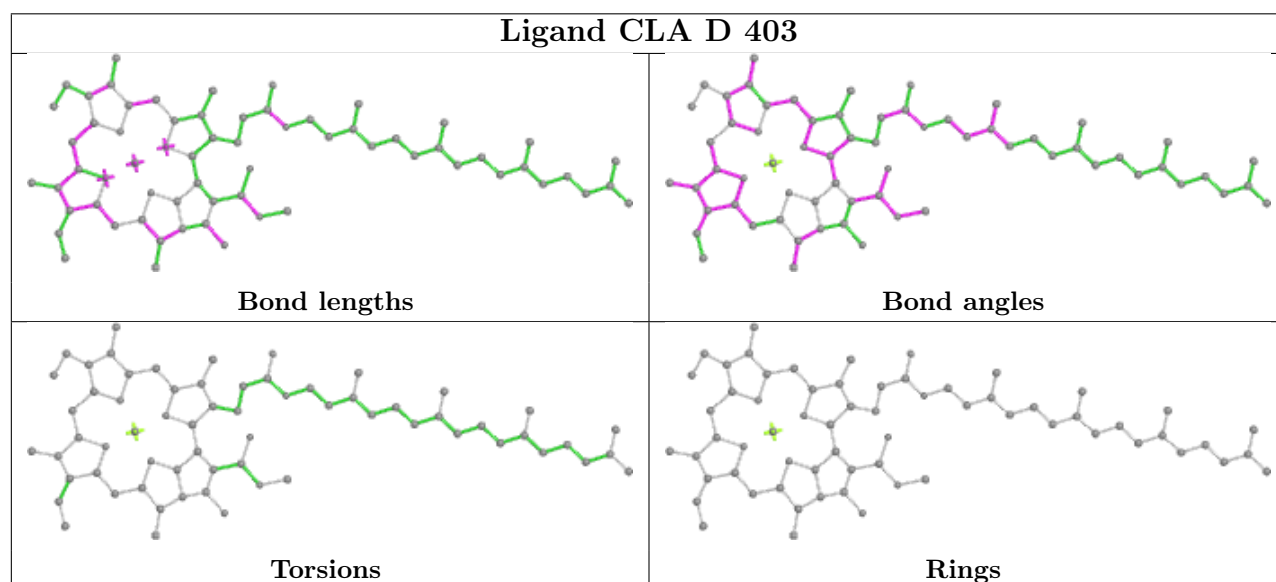
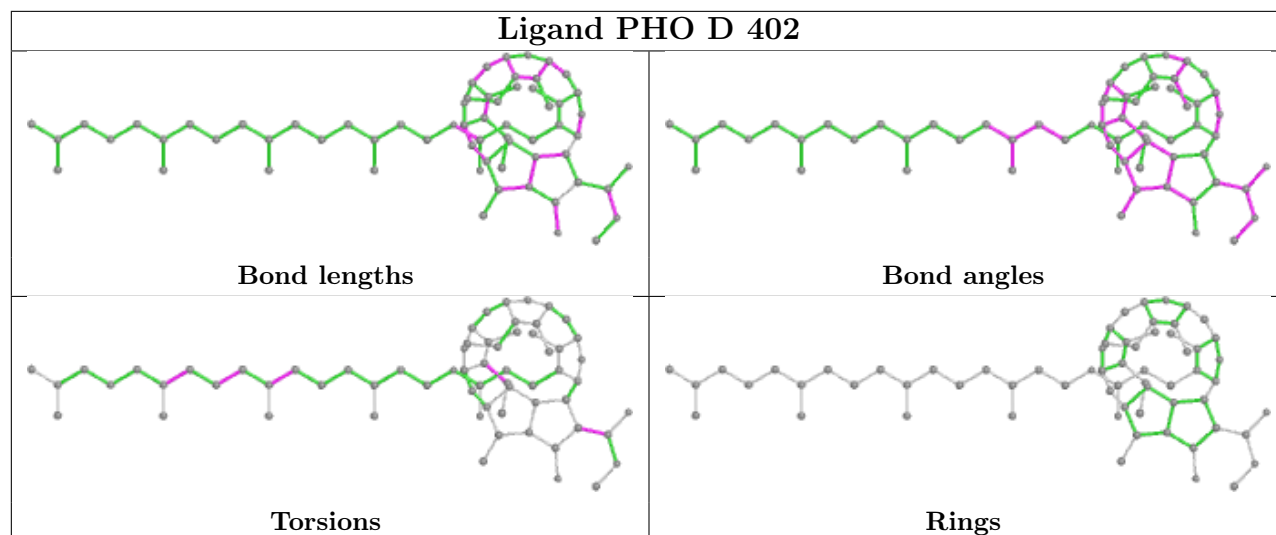


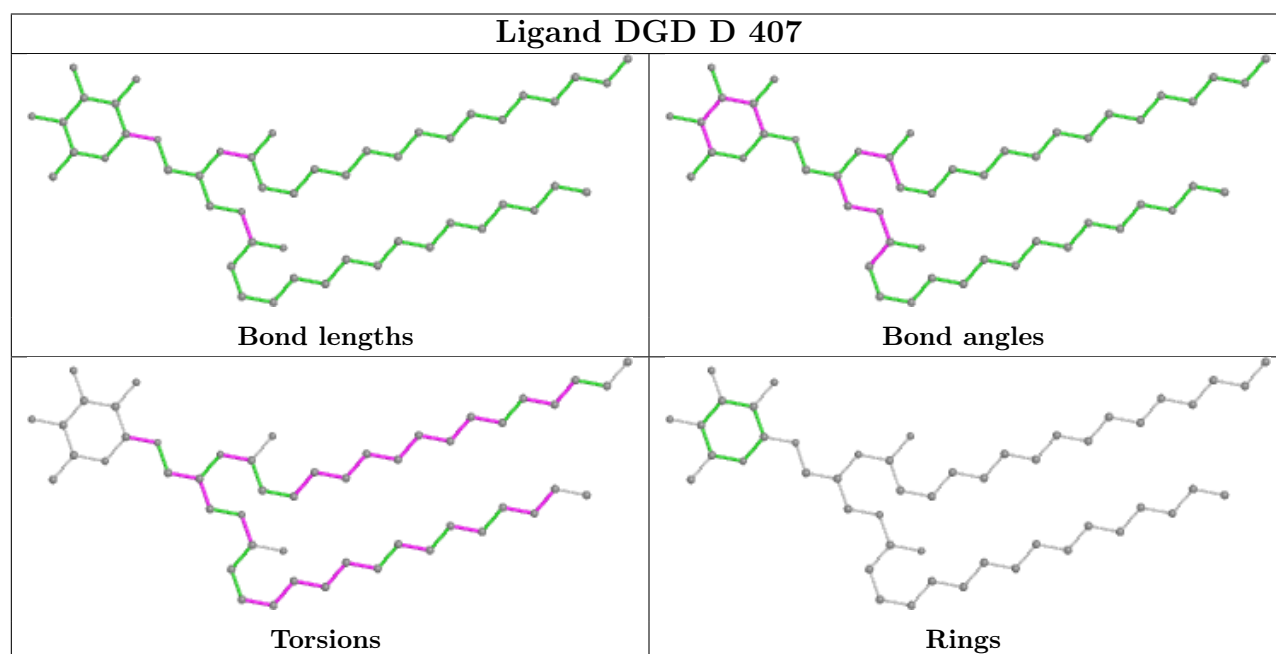
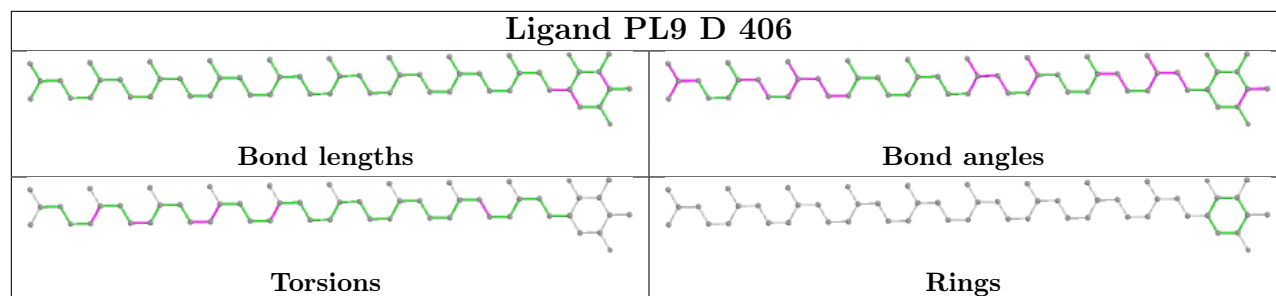
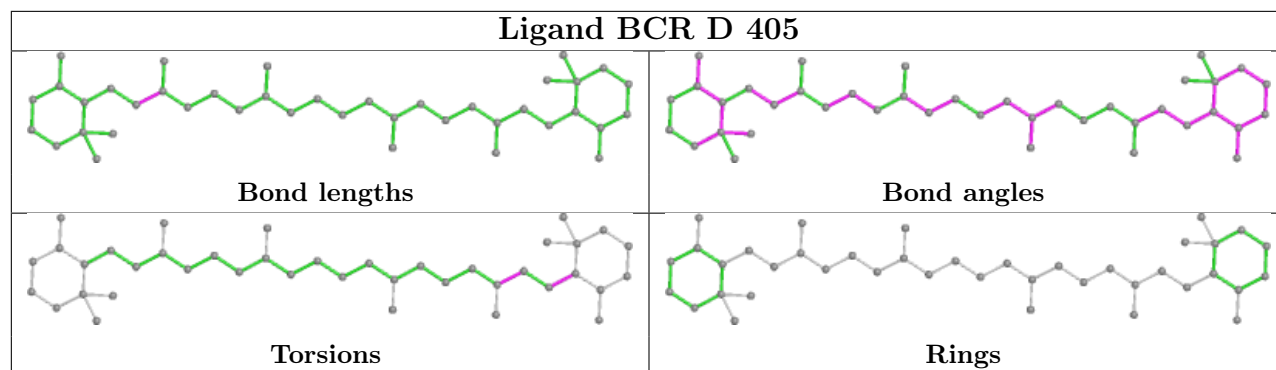


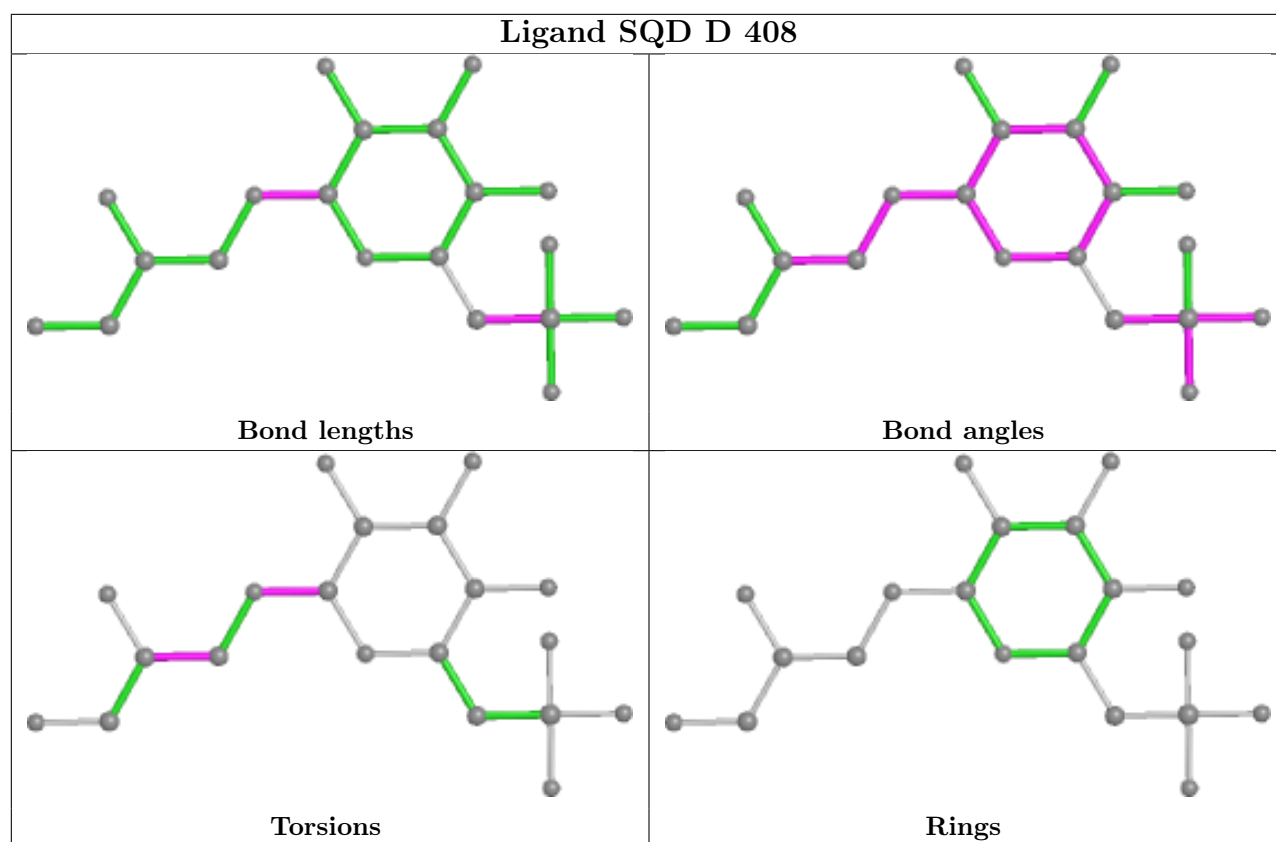


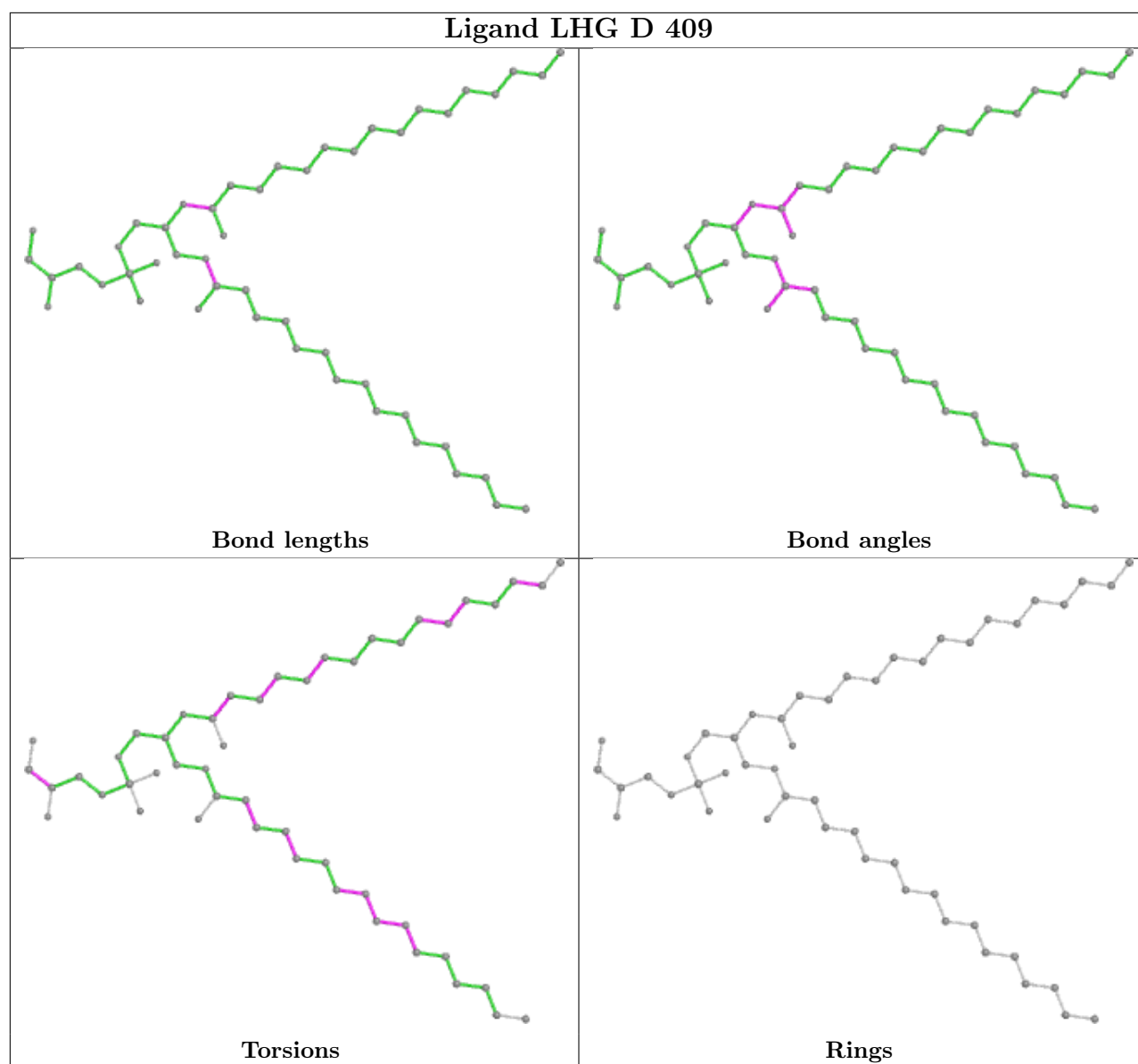


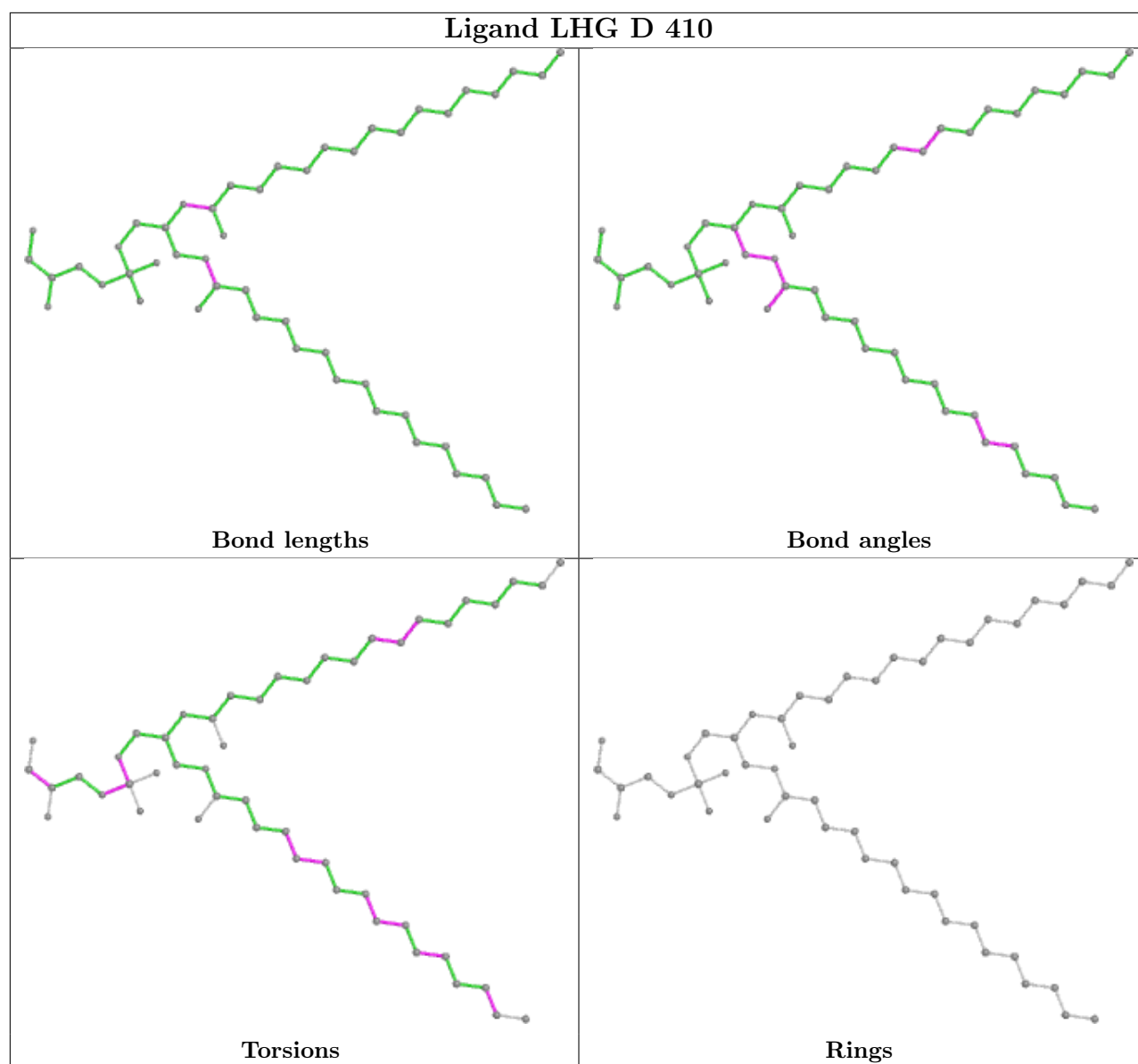


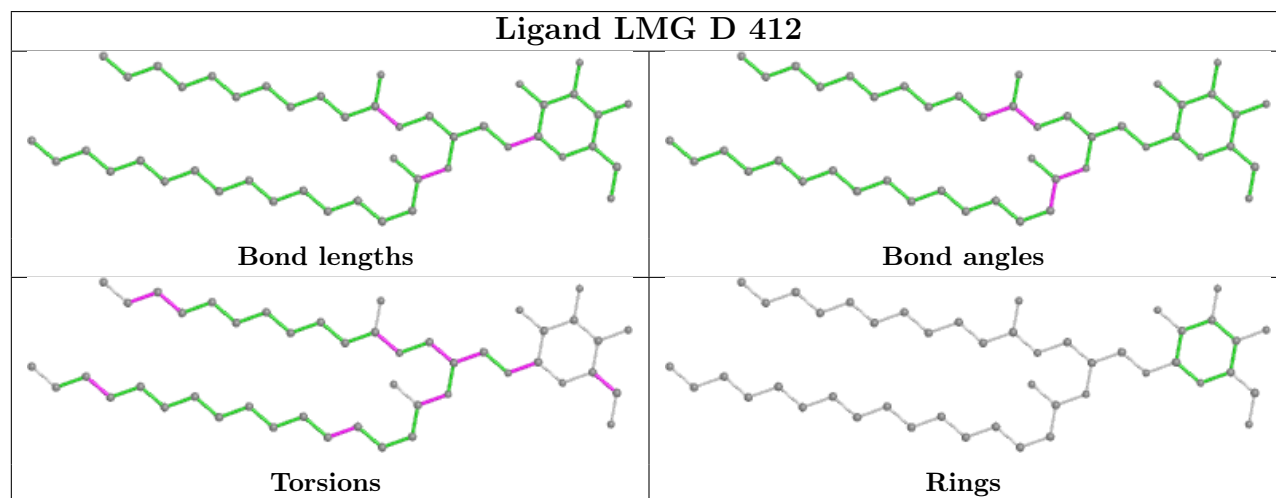
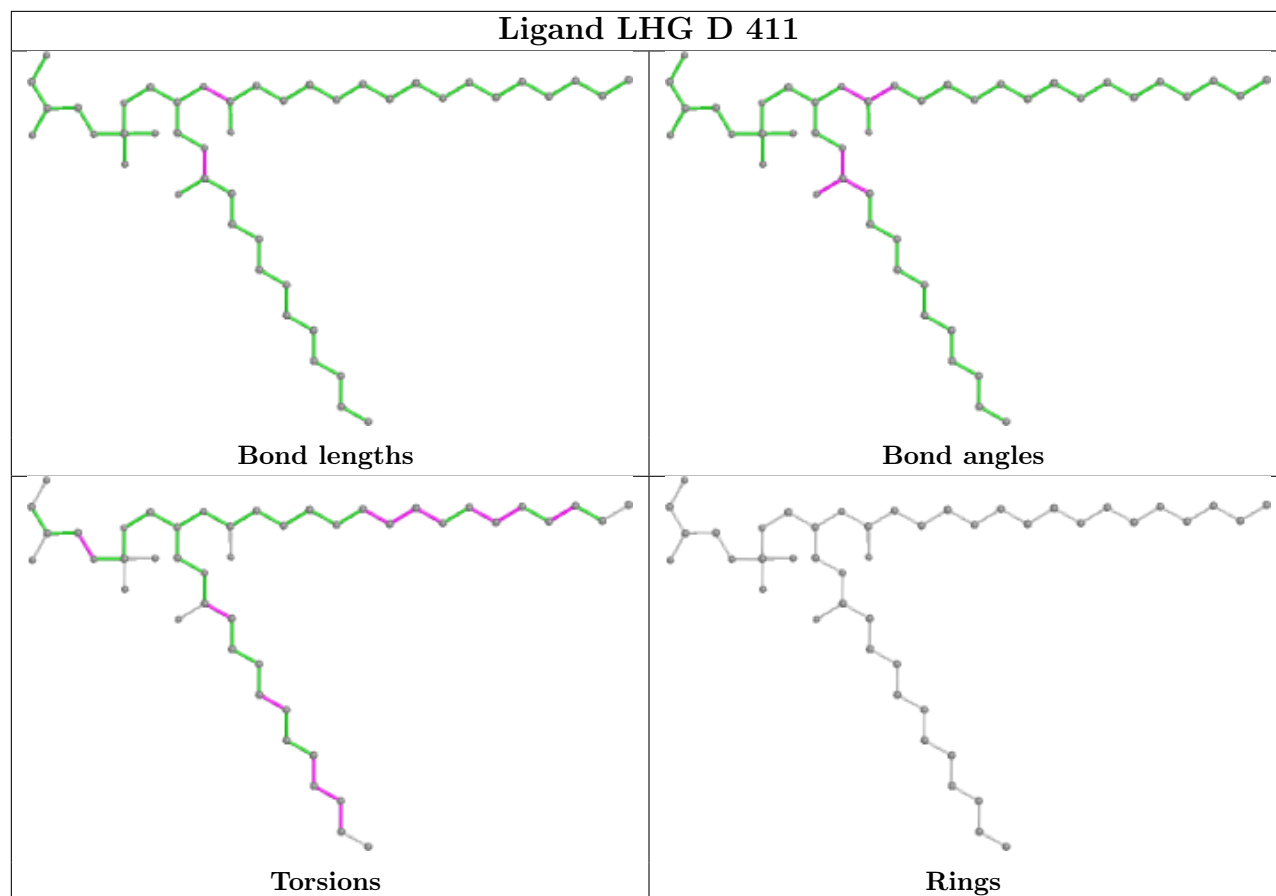


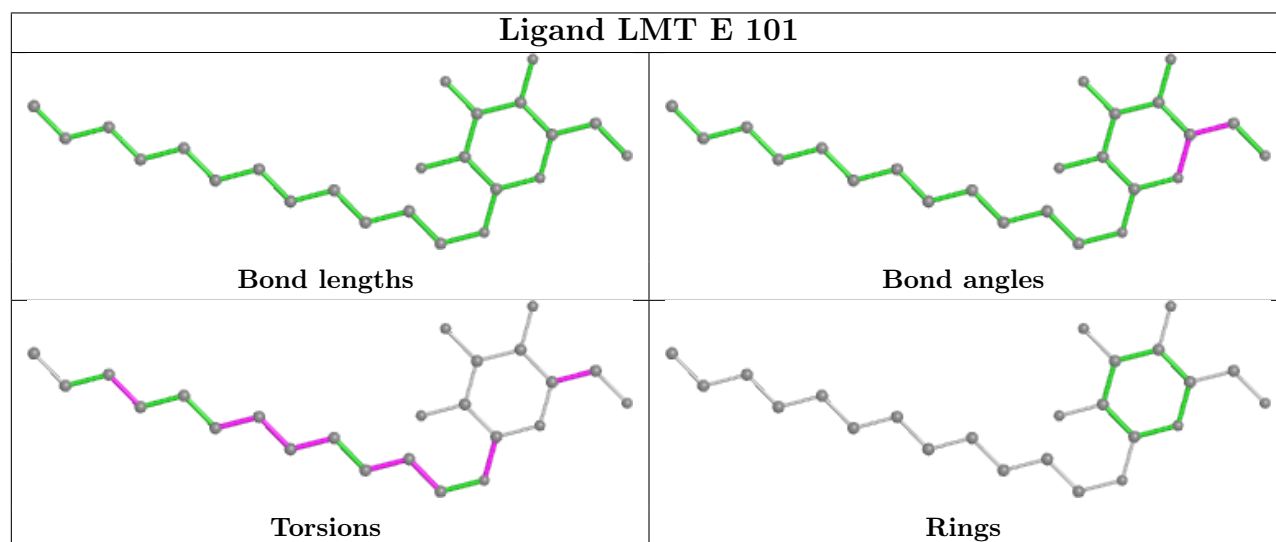
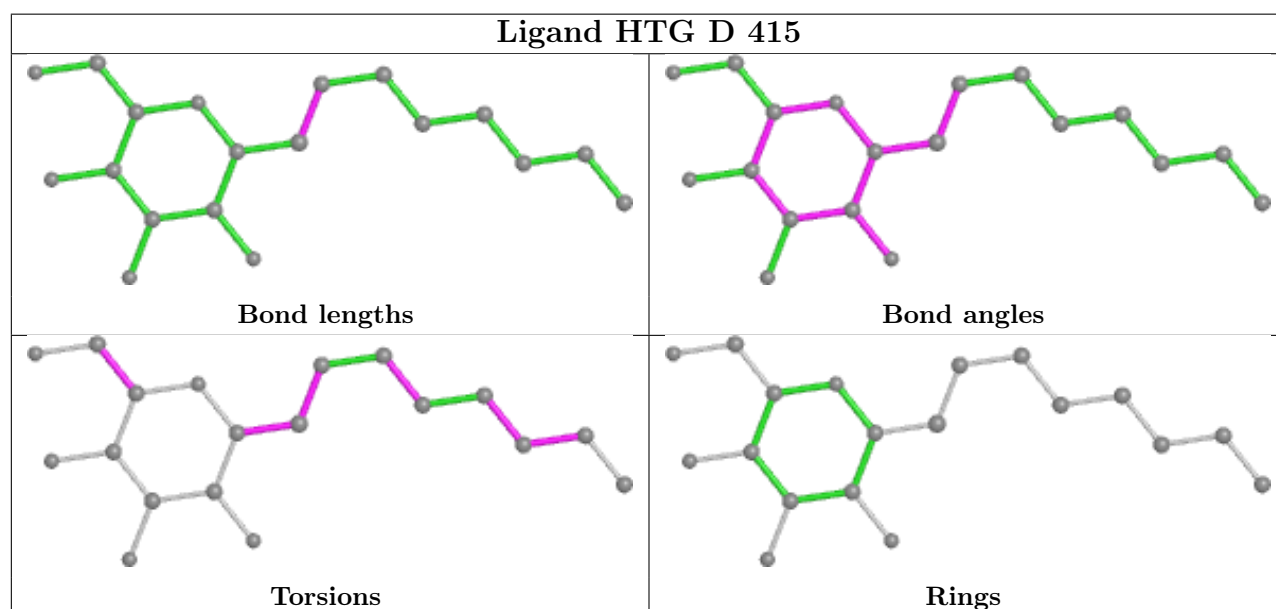
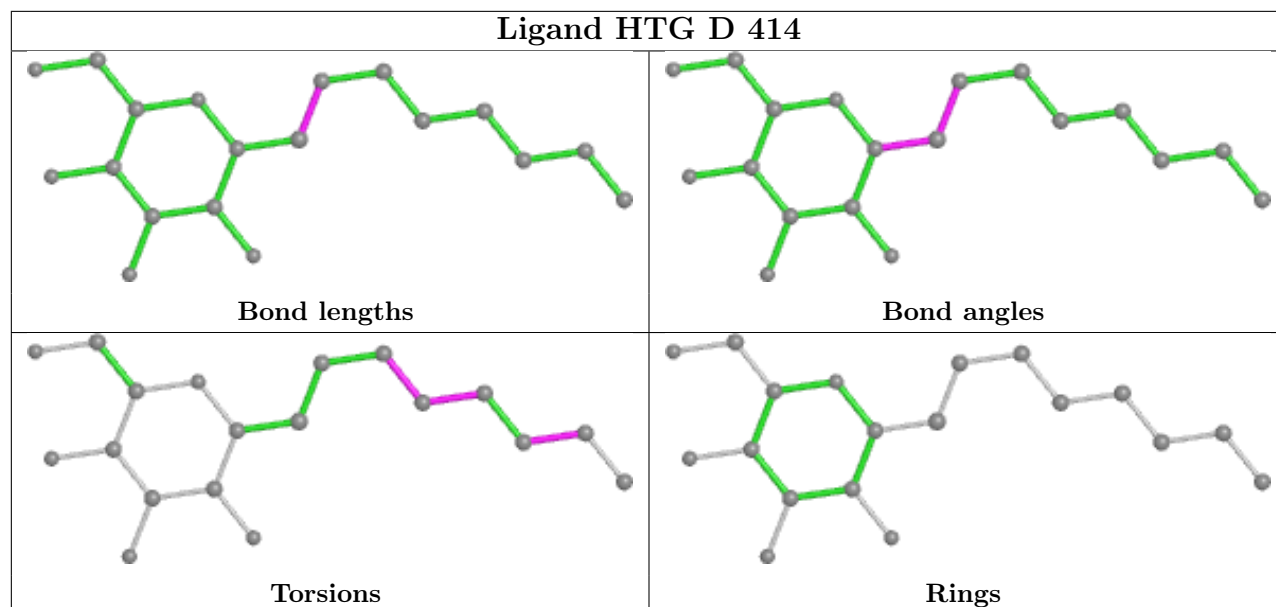


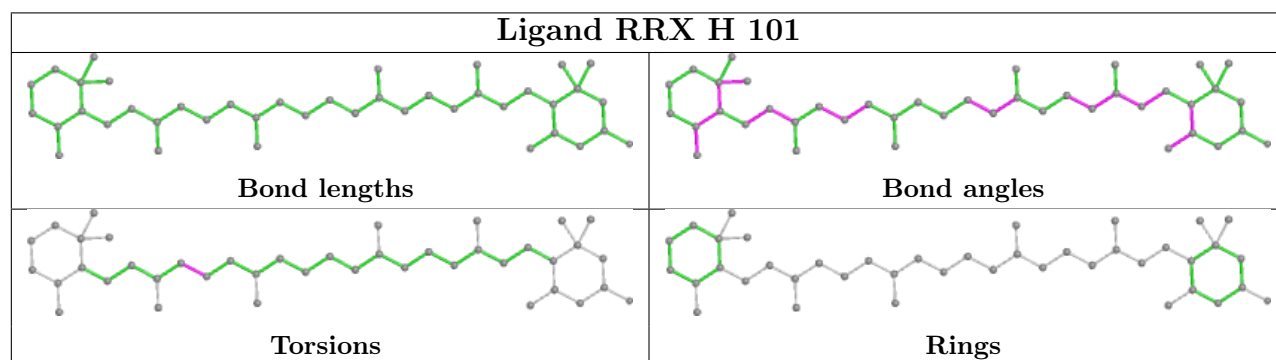
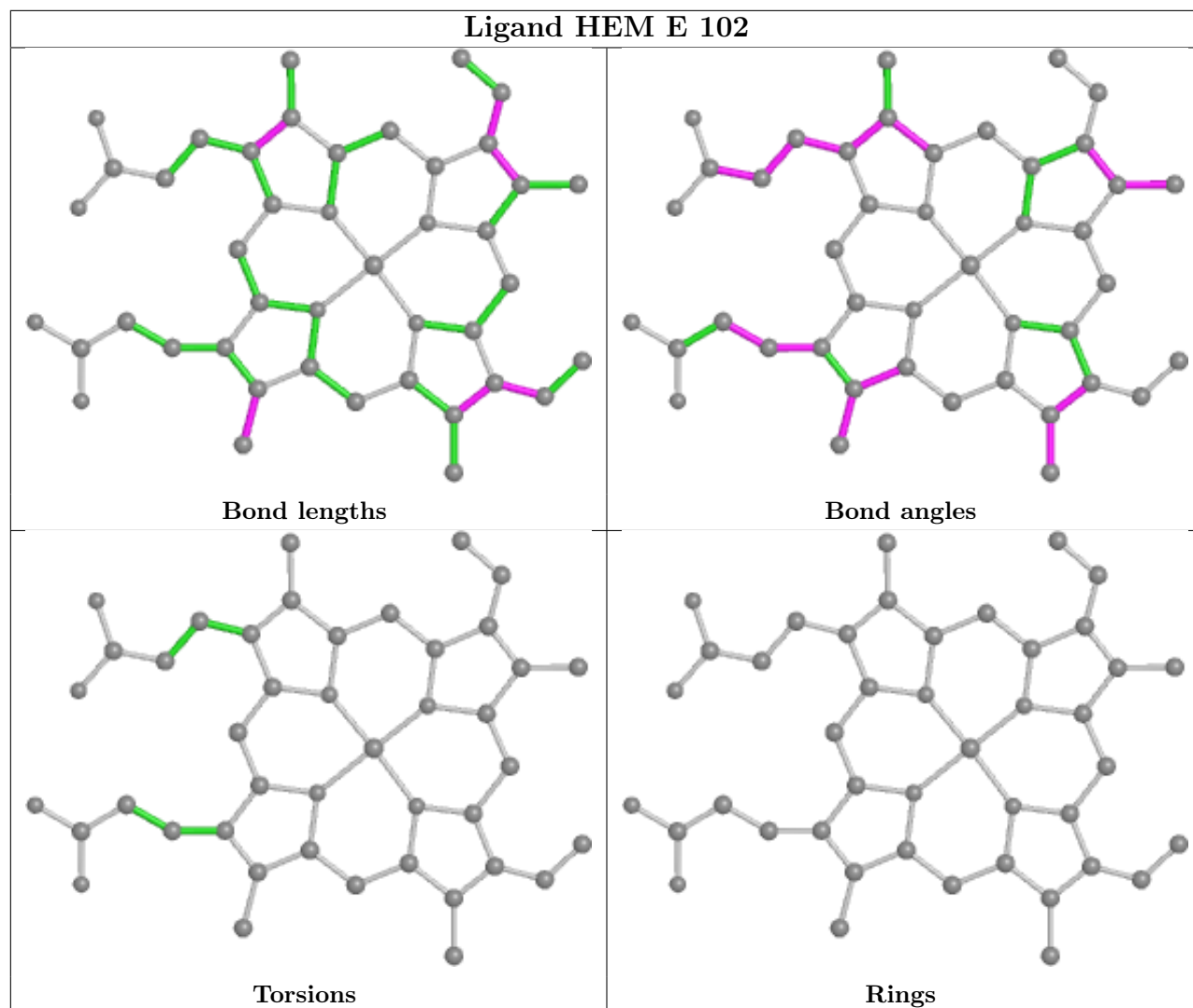


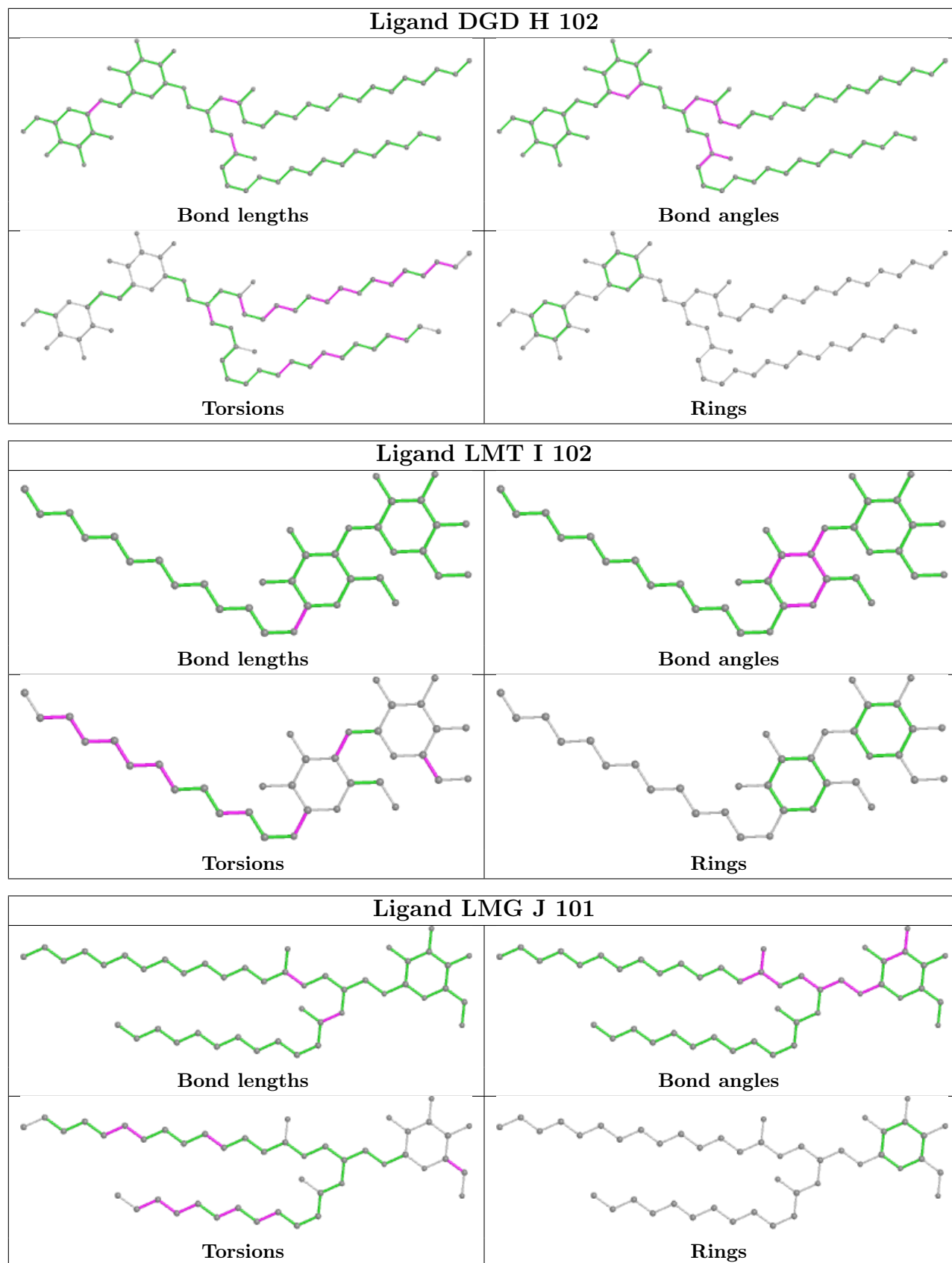


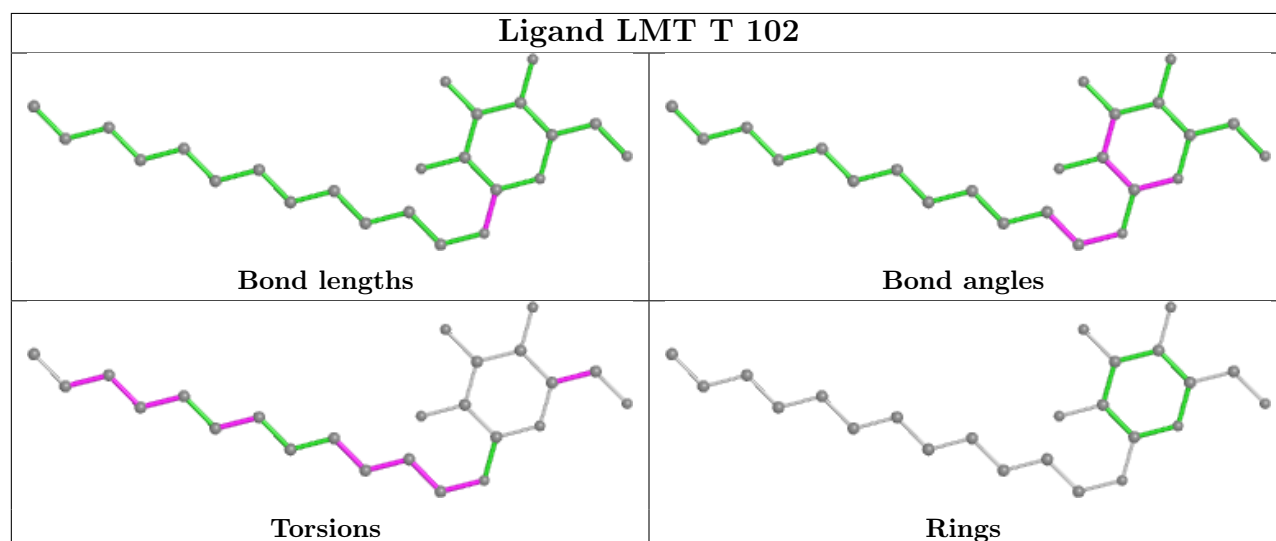
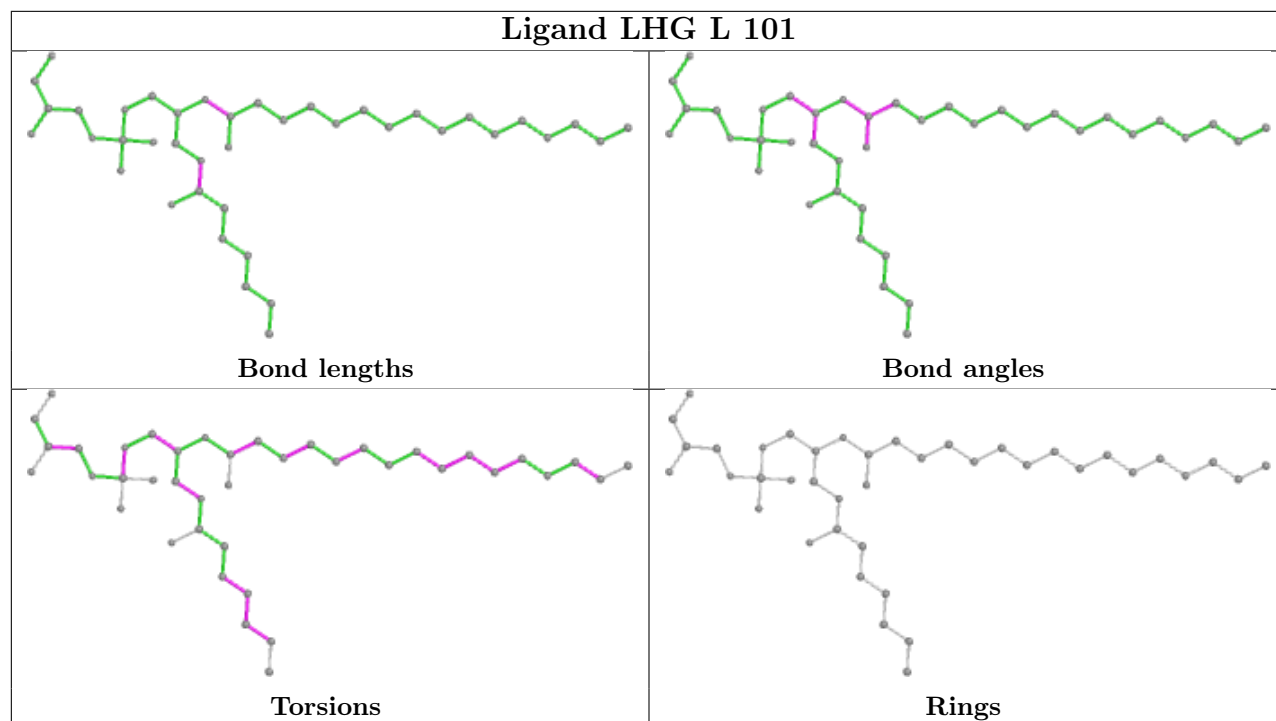
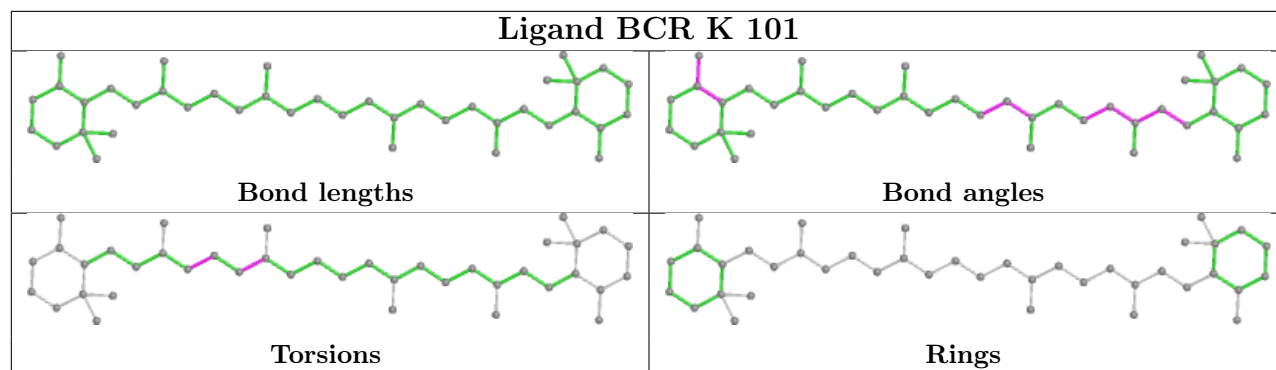


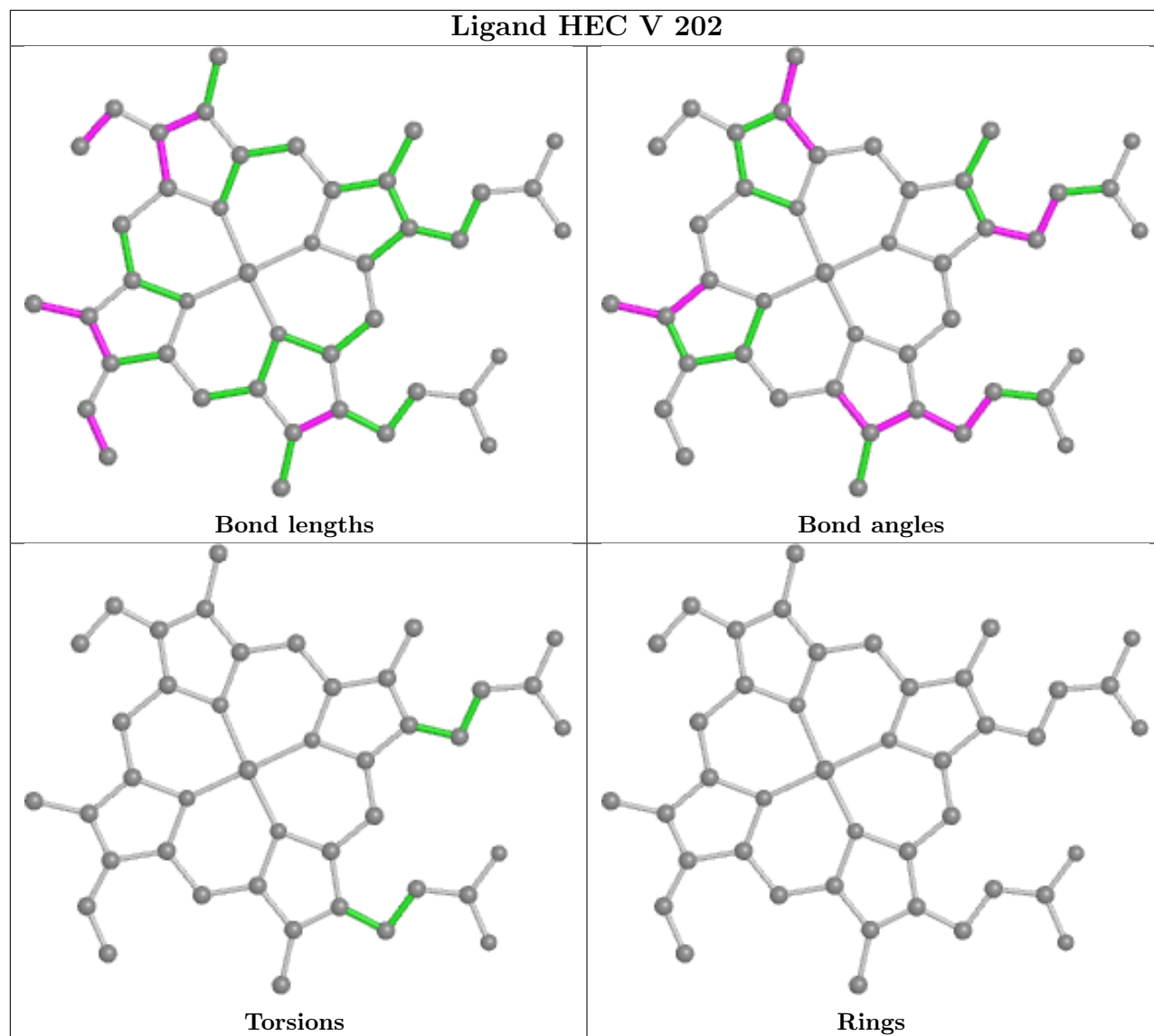


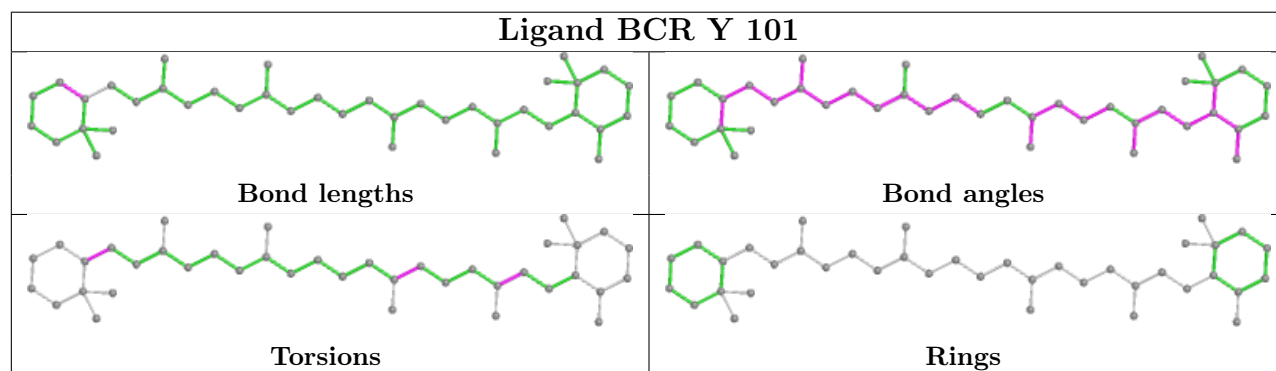
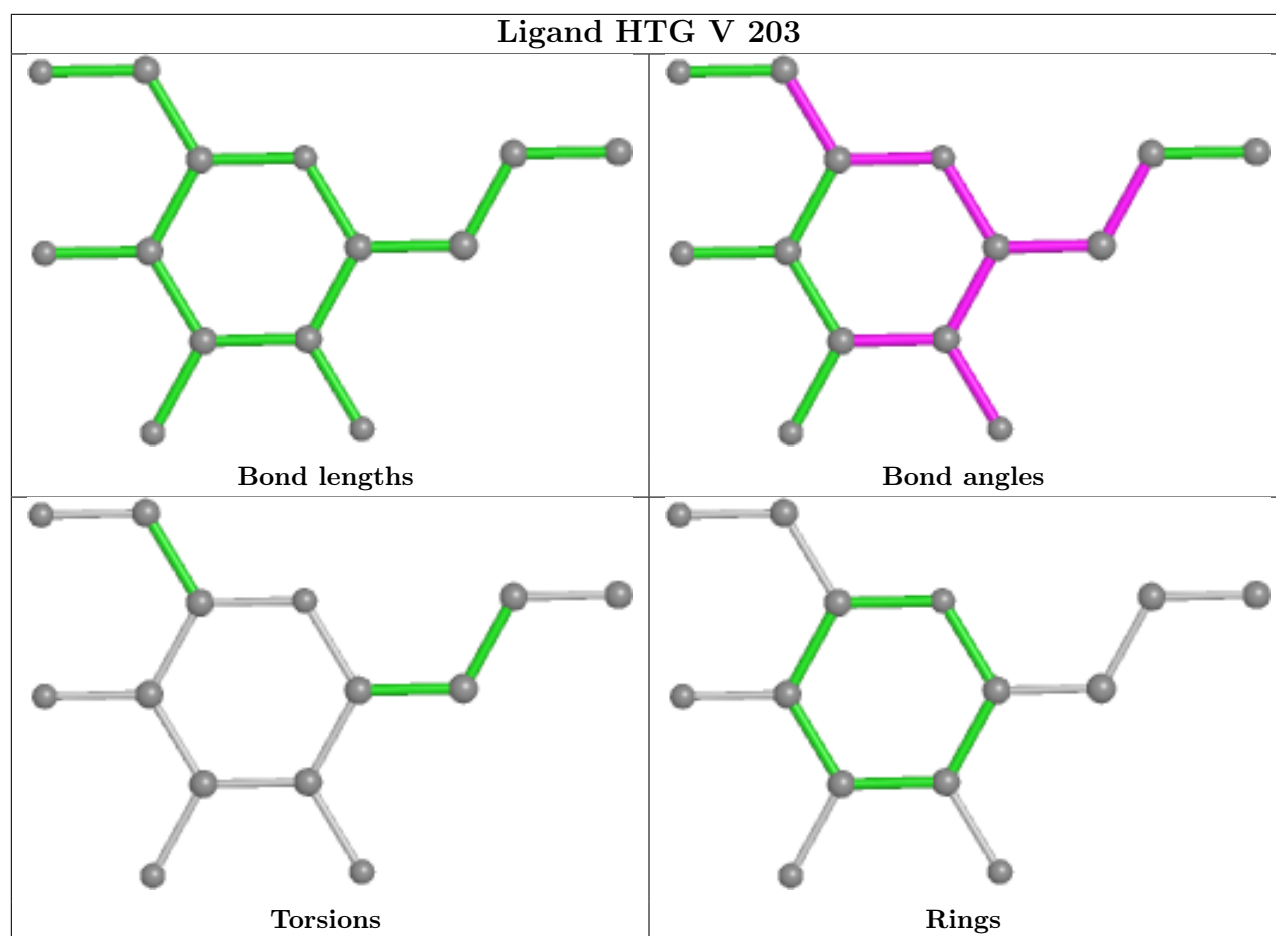


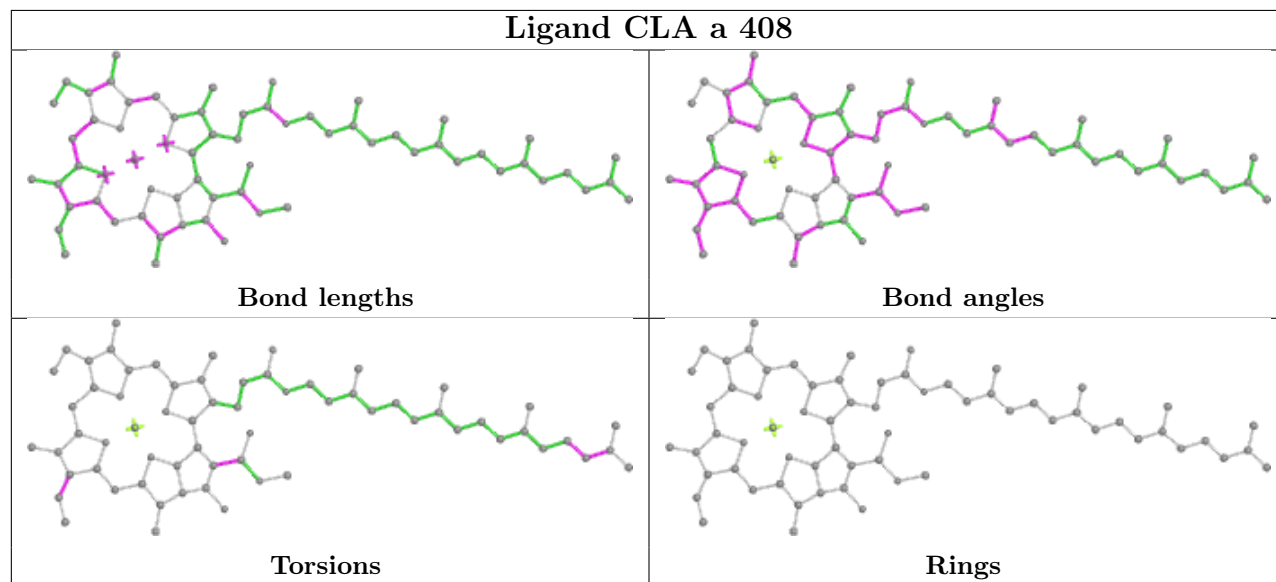
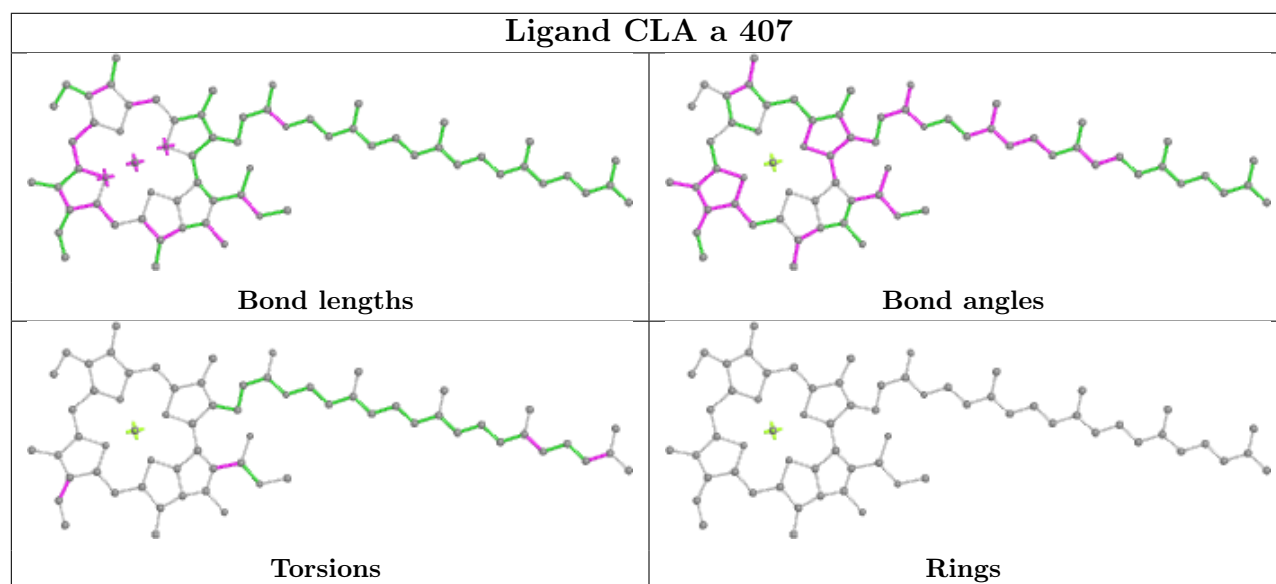
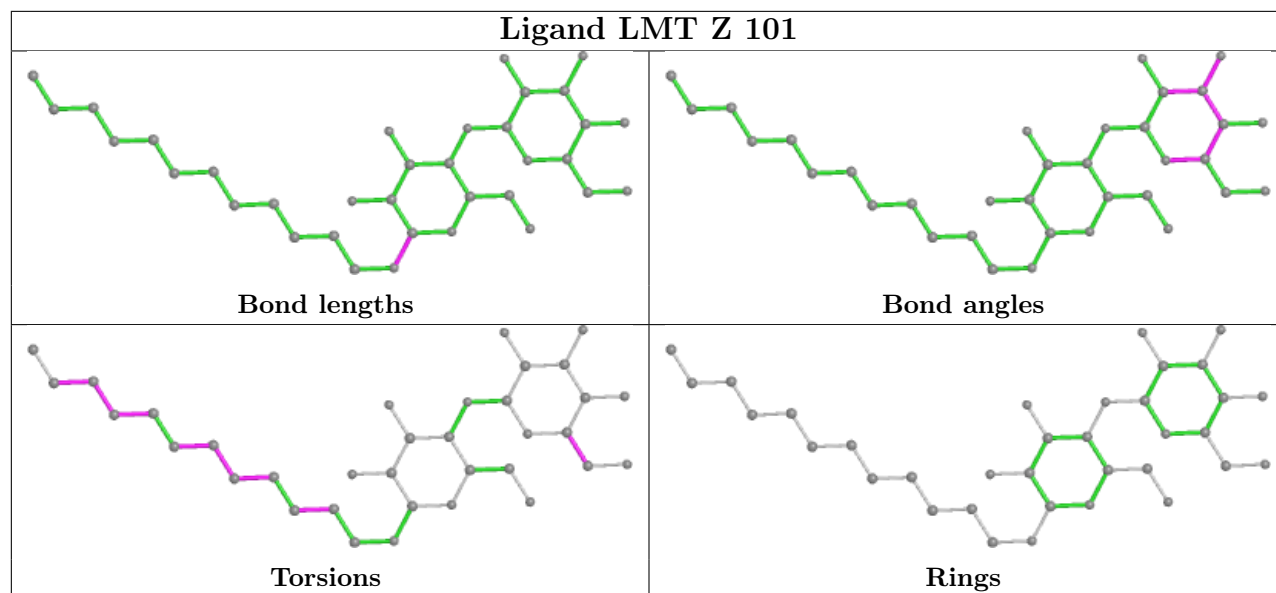




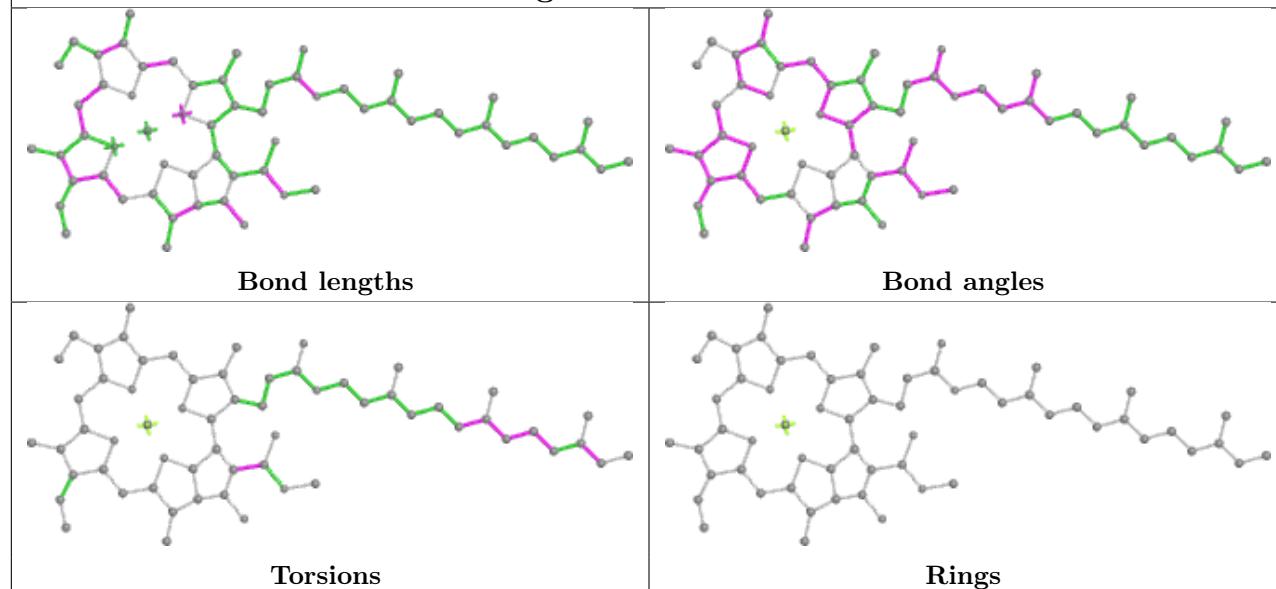




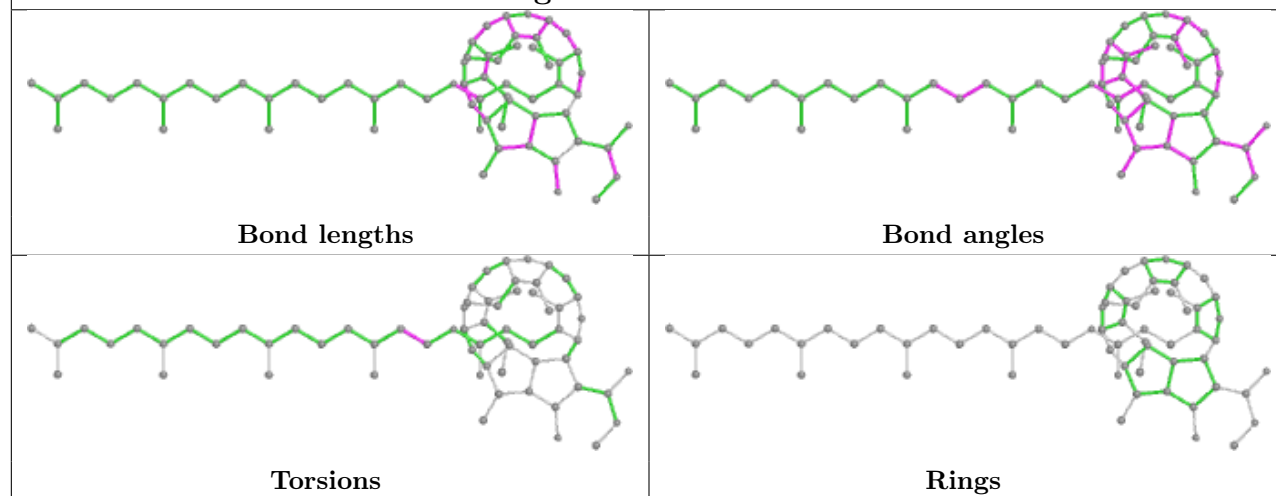




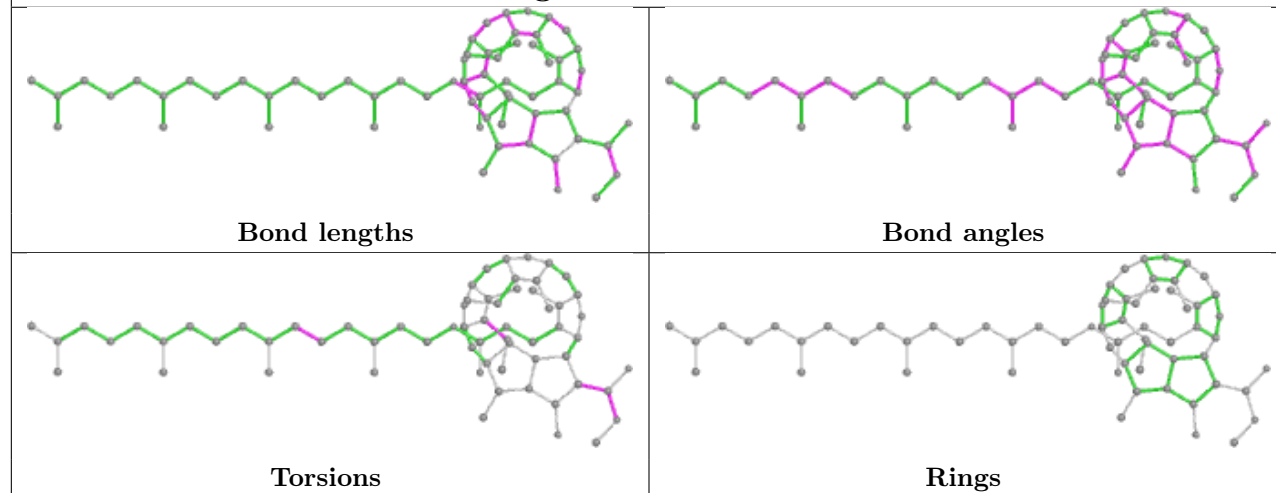
Ligand CLA a 409



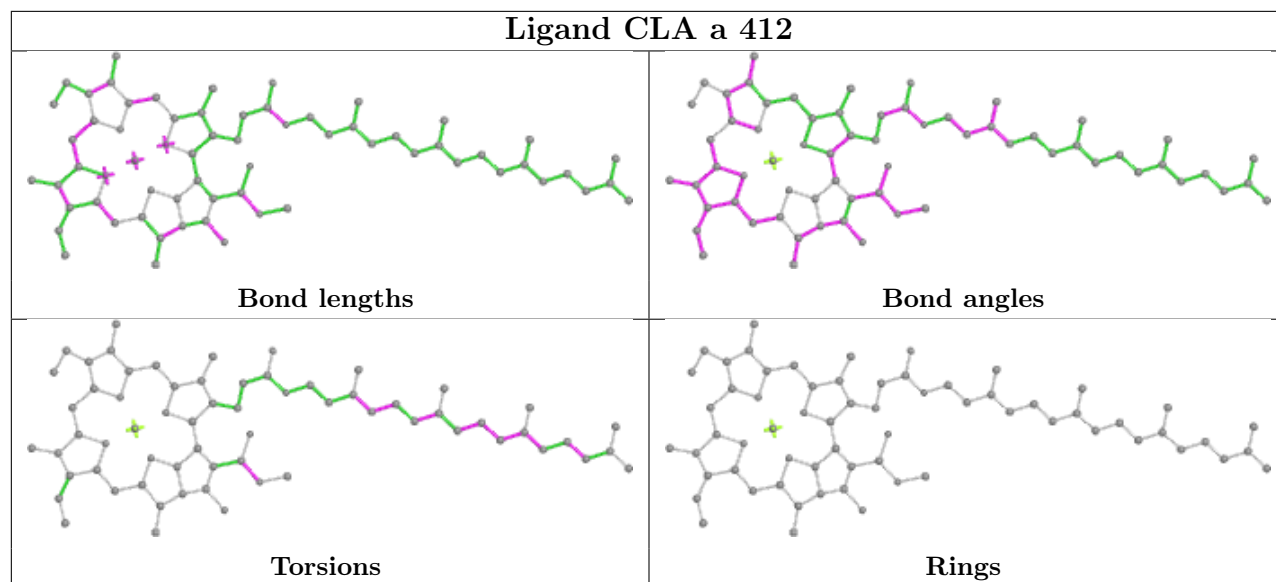
Ligand PHO a 410



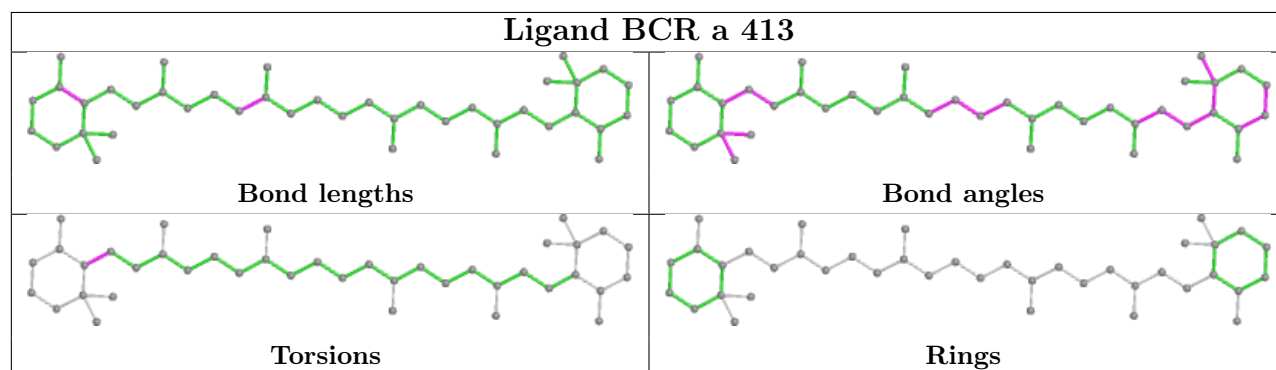
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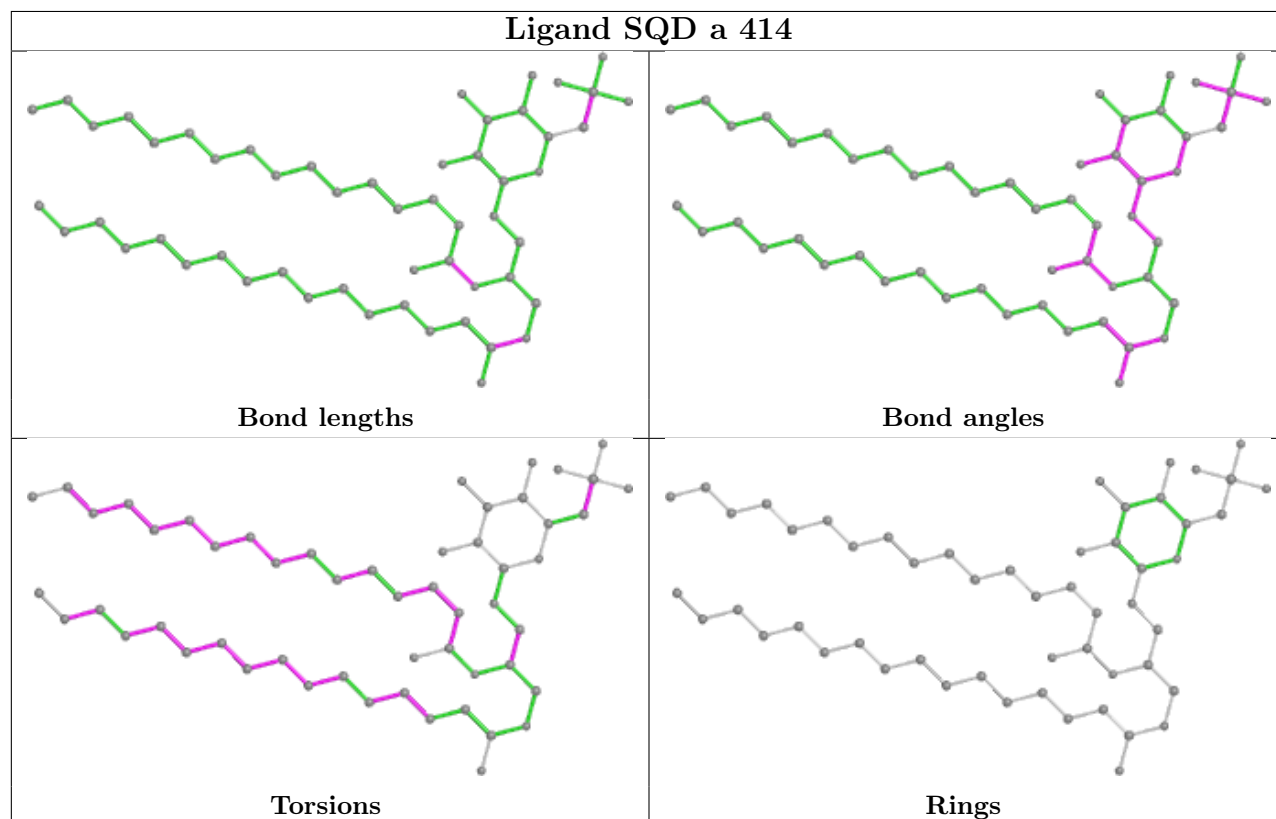
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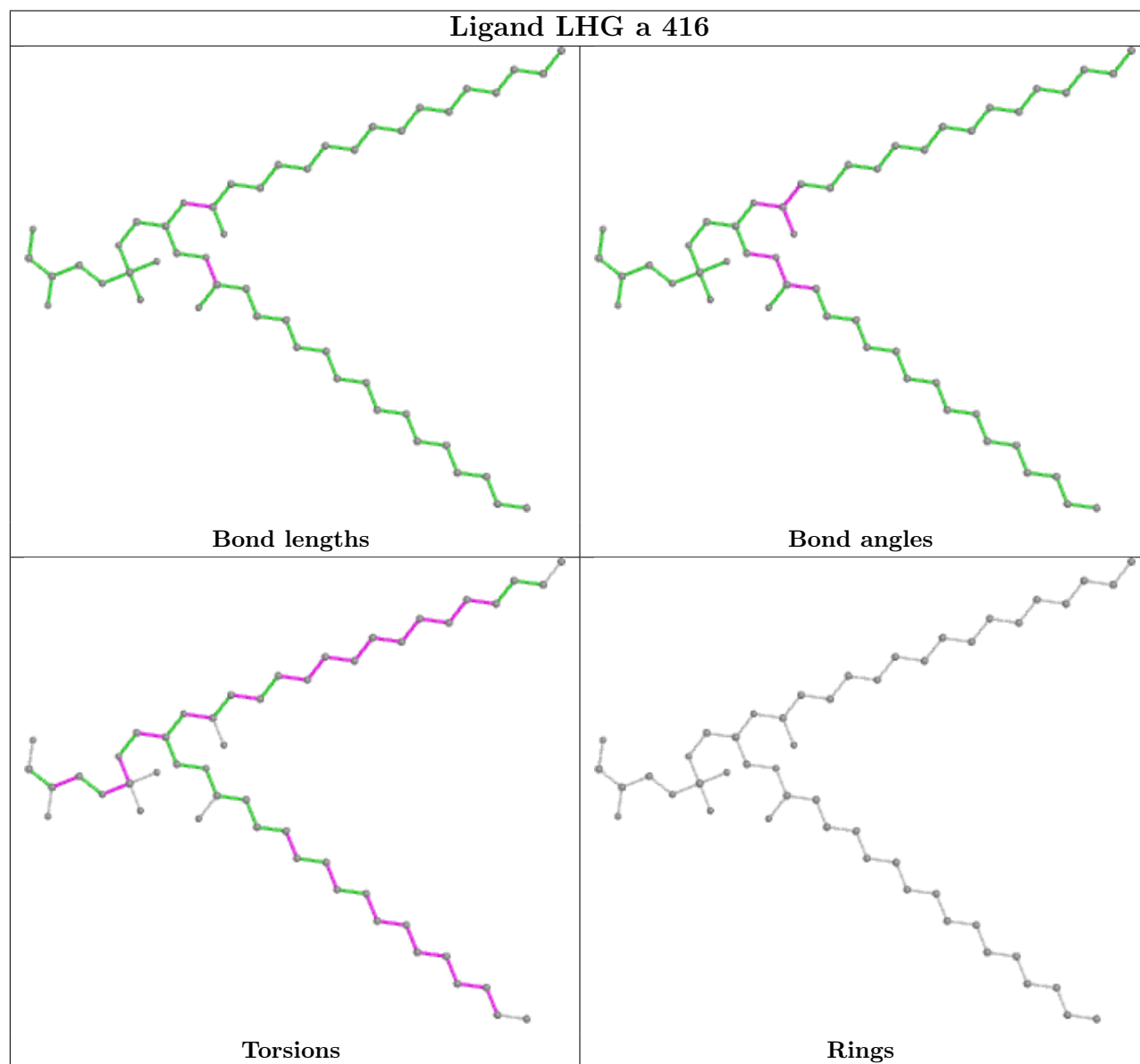
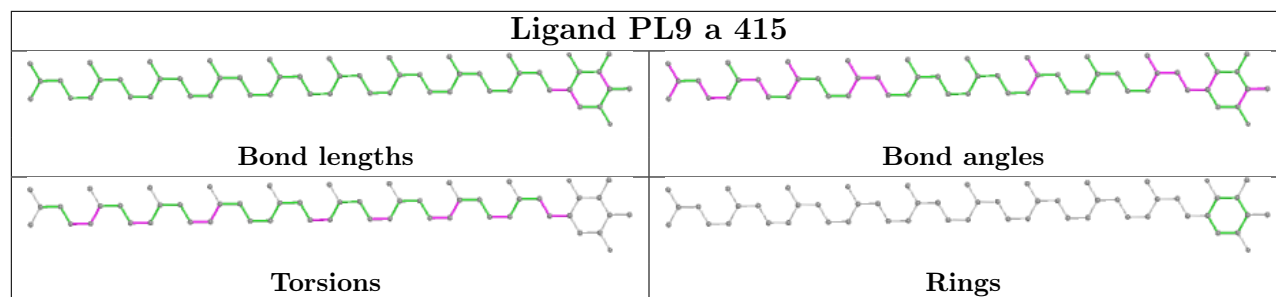


Ligand BCR a 413

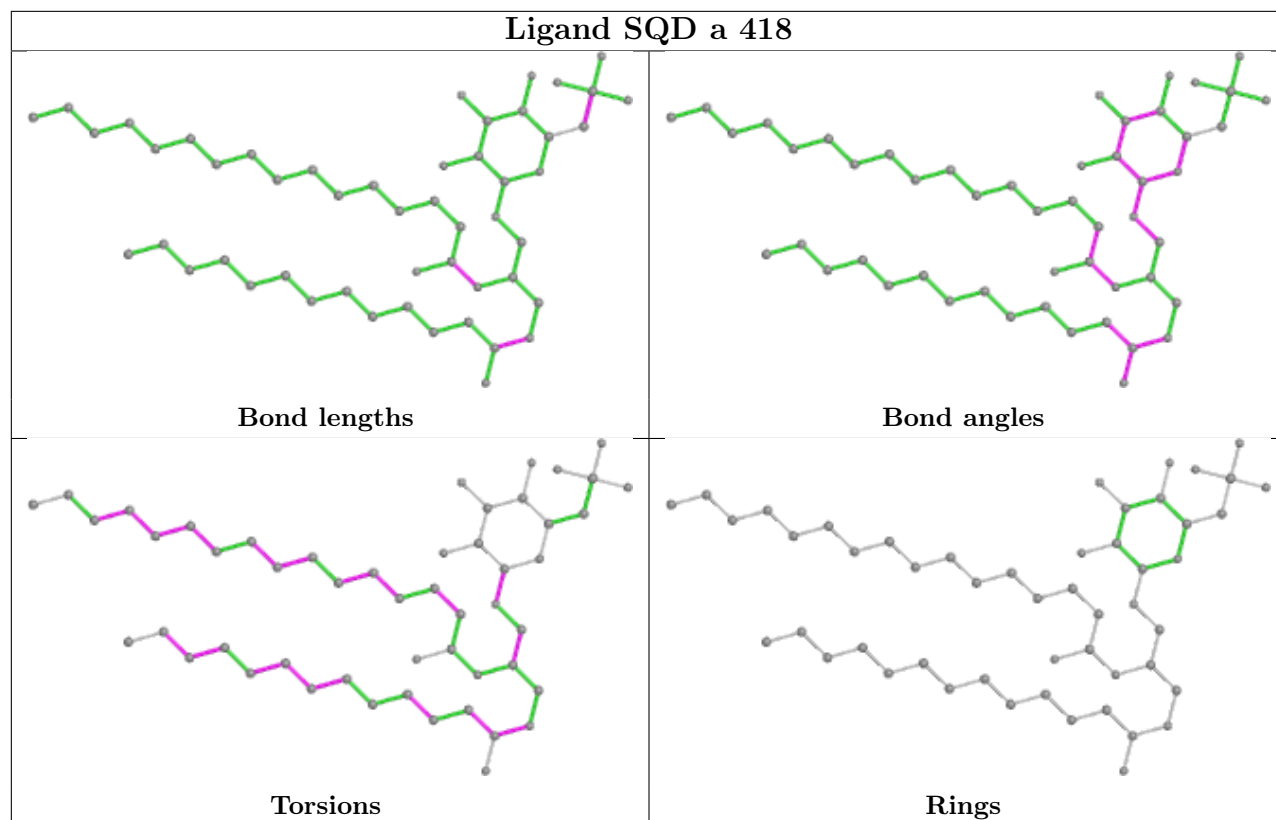


Ligand SQD a 414

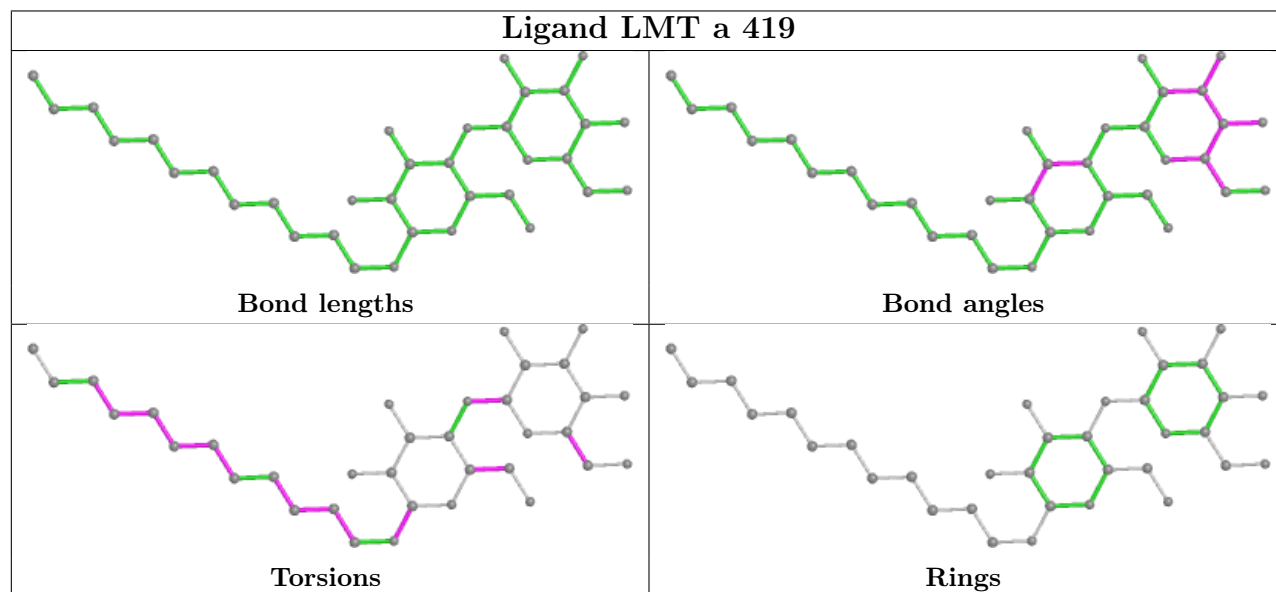




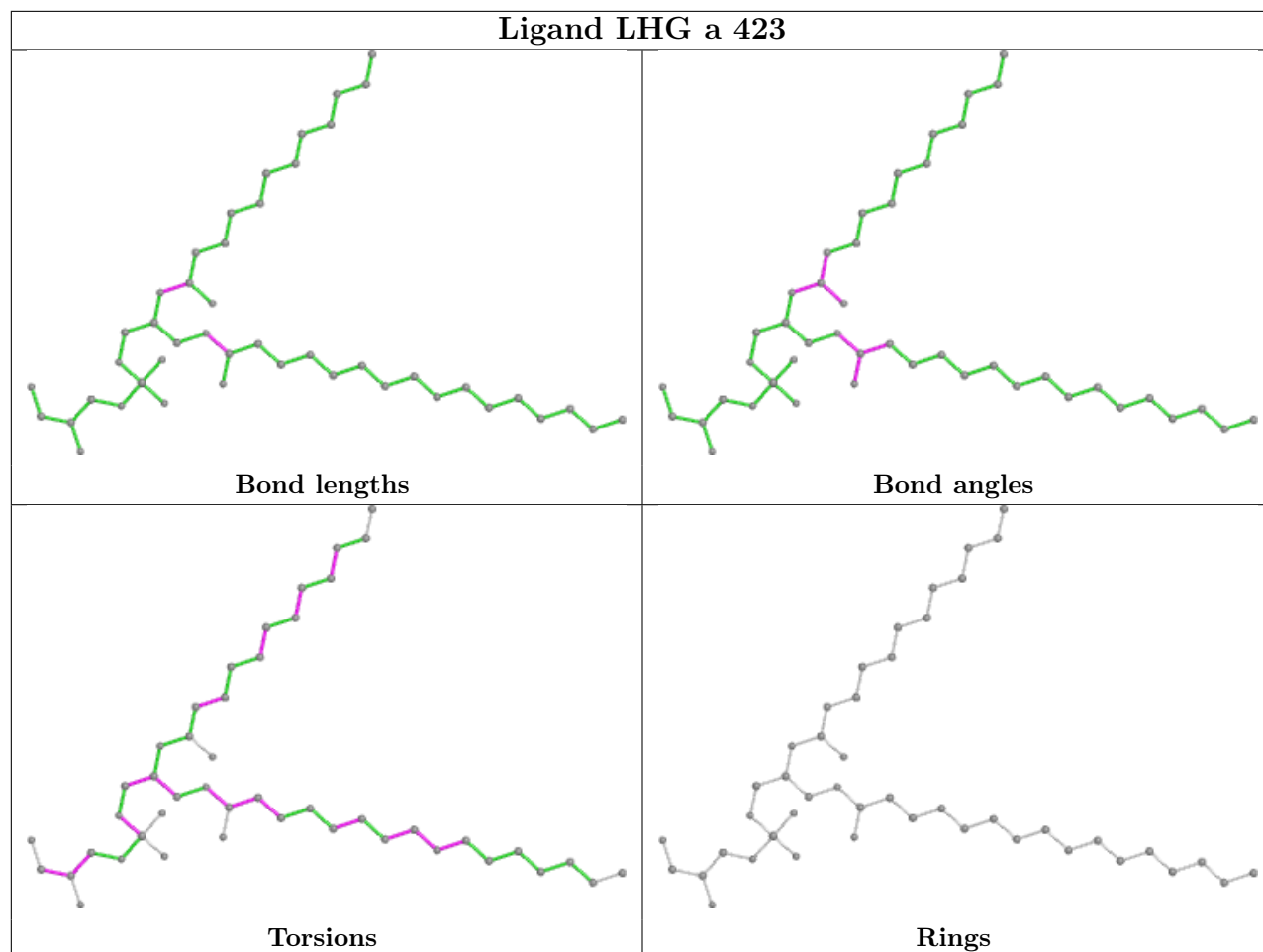
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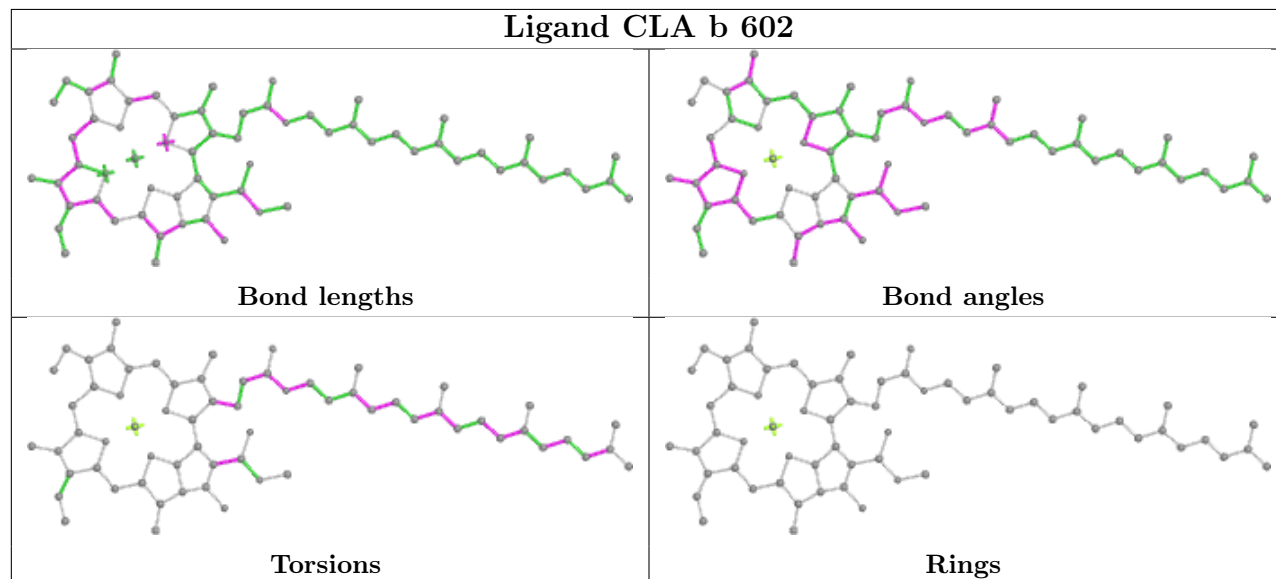
Ligand LMT a 419



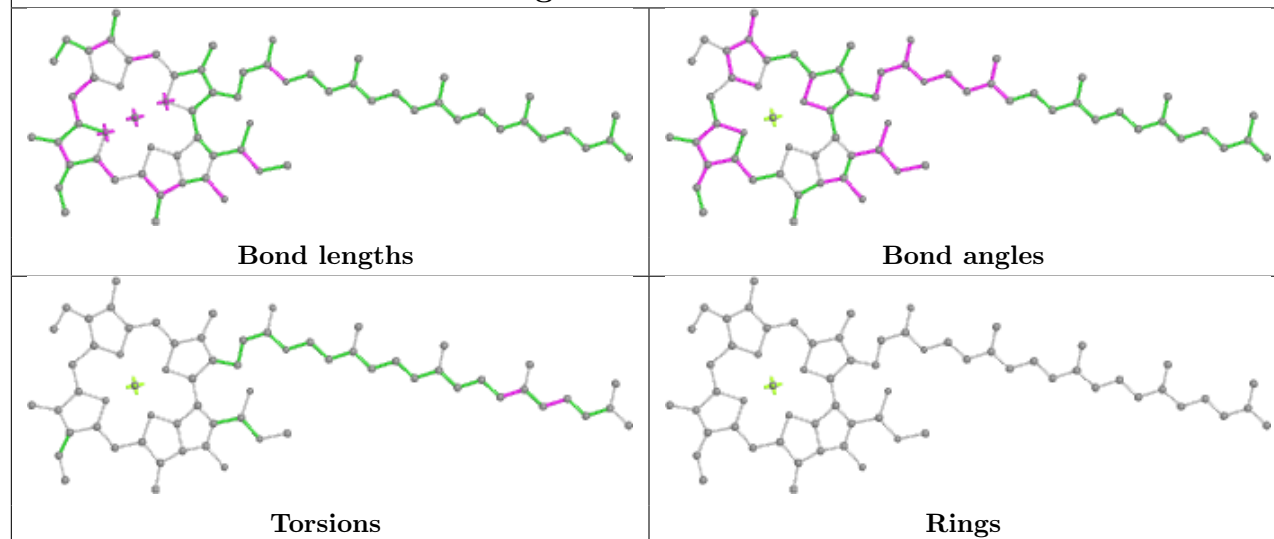
Ligand LHG a 423



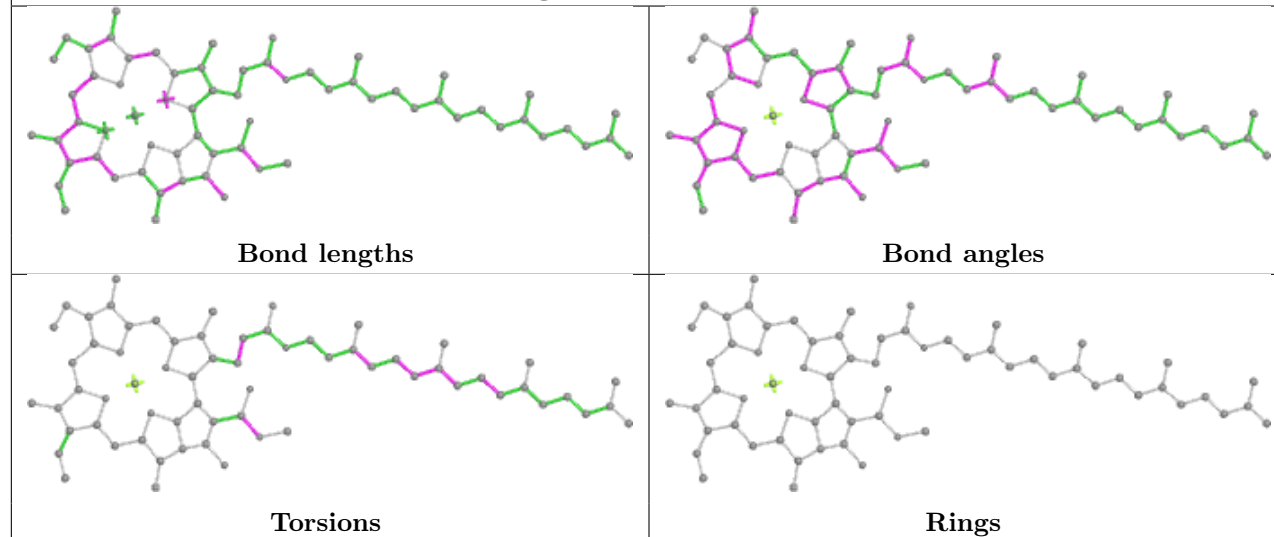
Ligand CLA b 602



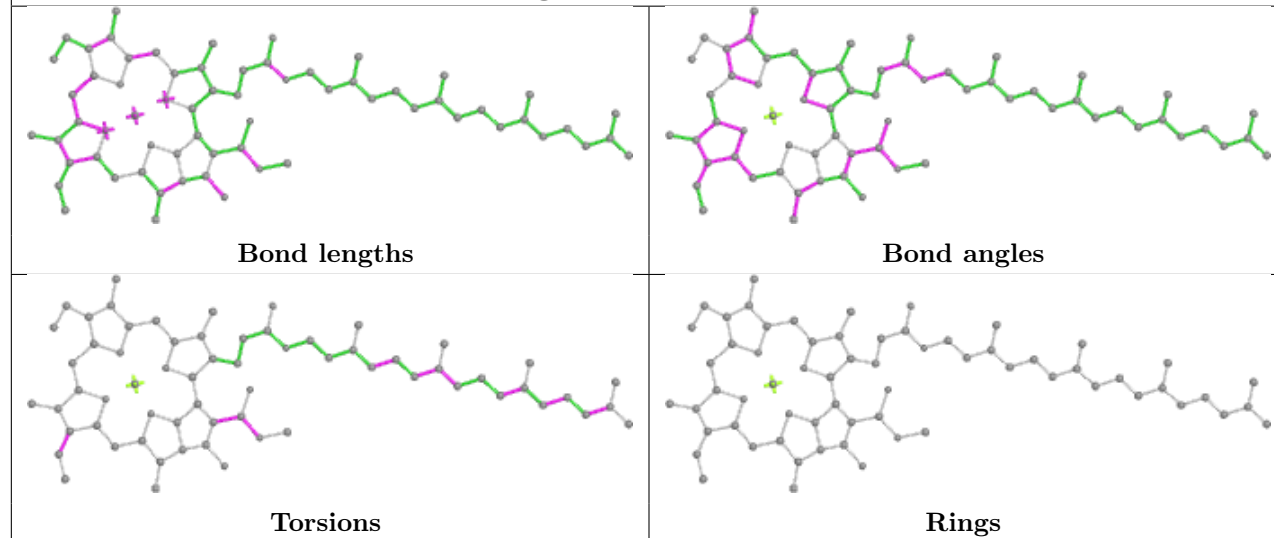
Ligand CLA b 603



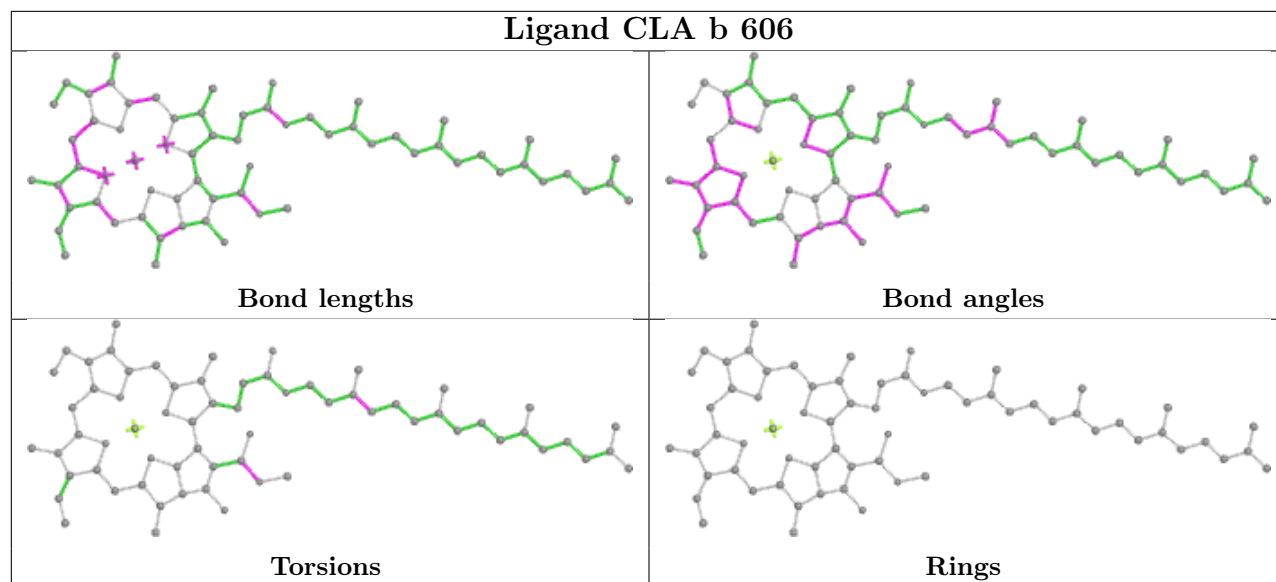
Ligand CLA b 604



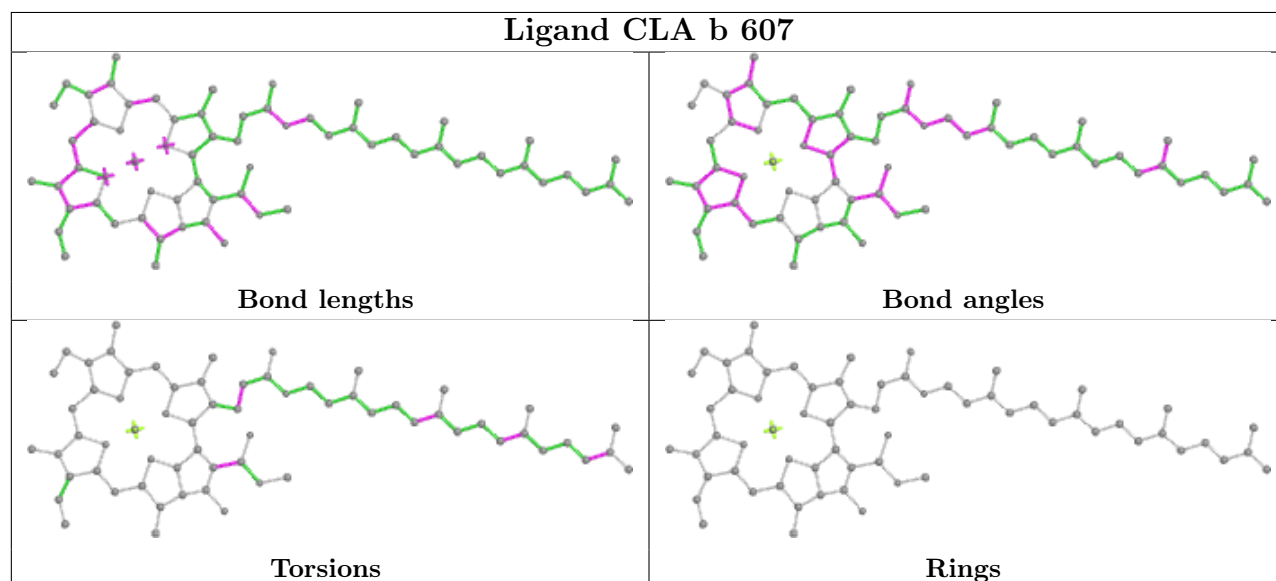
Ligand CLA b 605



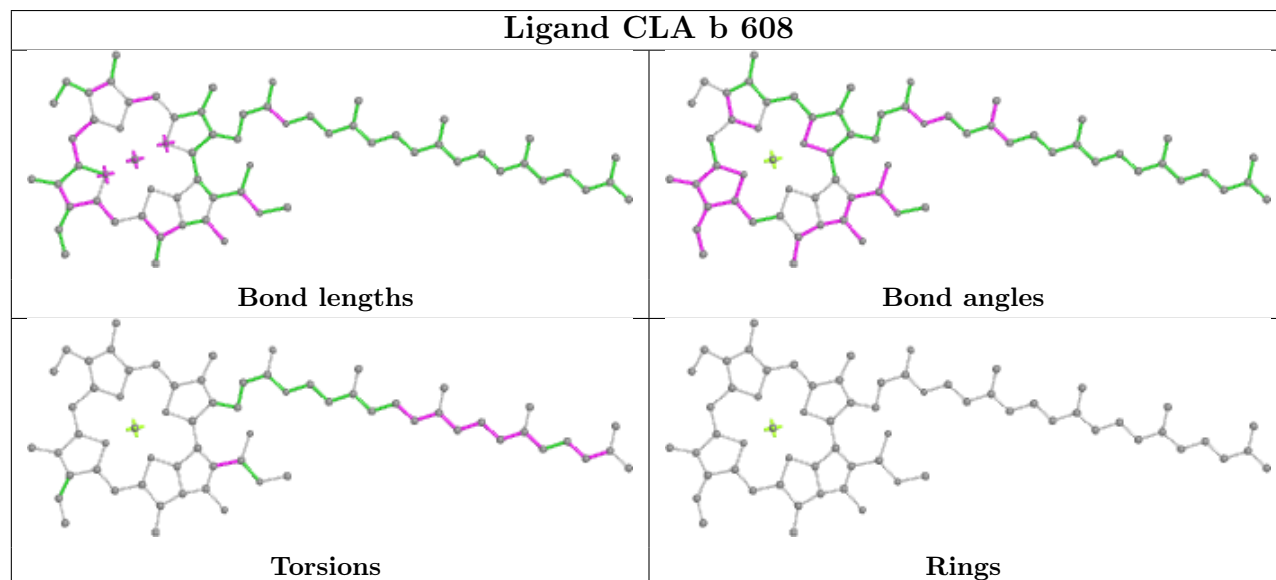
Ligand CLA b 606



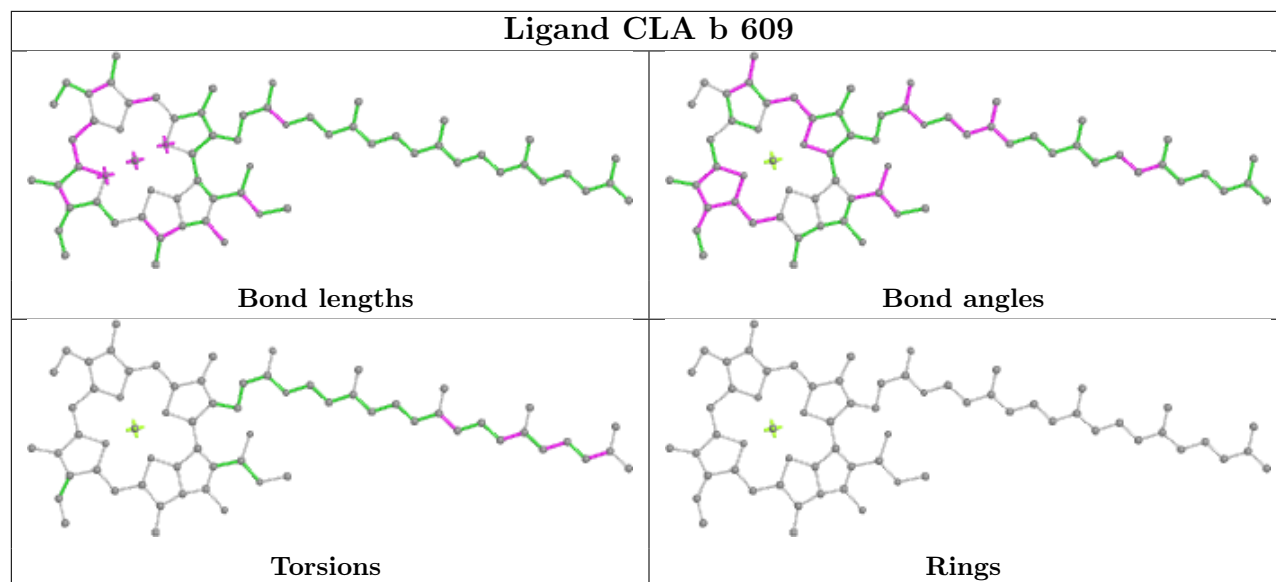
Ligand CLA b 607



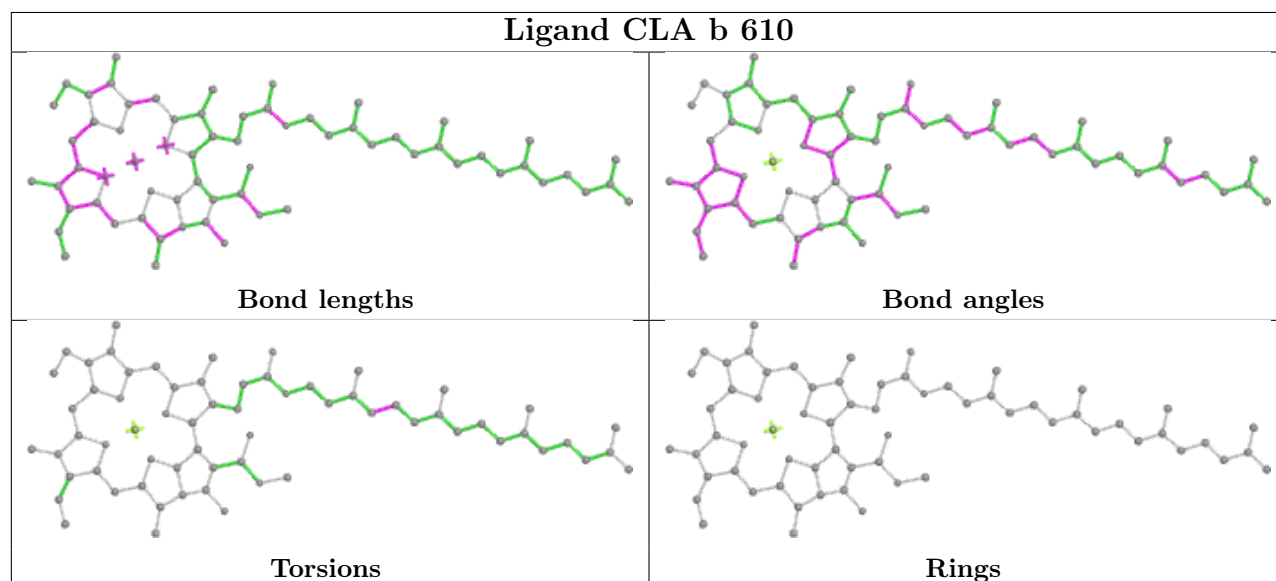
Ligand CLA b 608



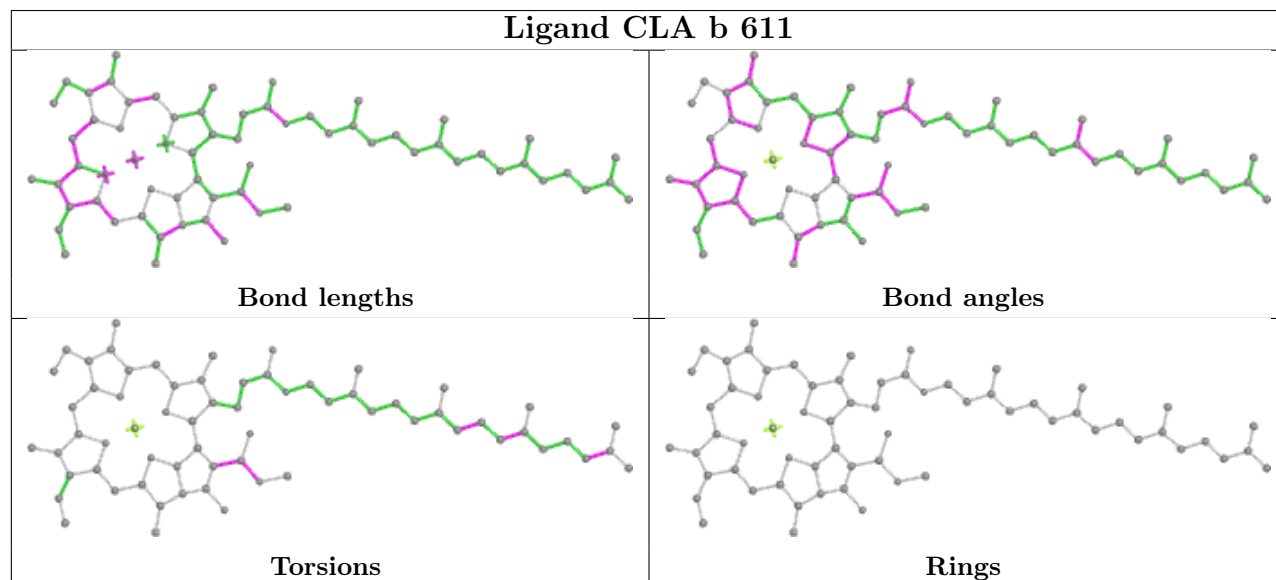
Ligand CLA b 609



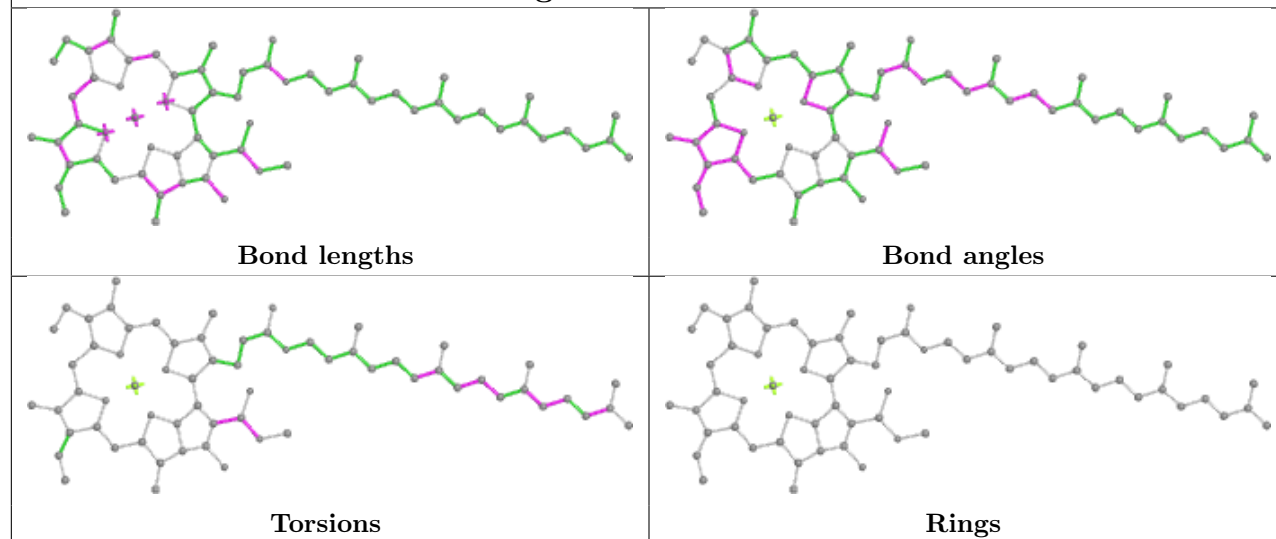
Ligand CLA b 610



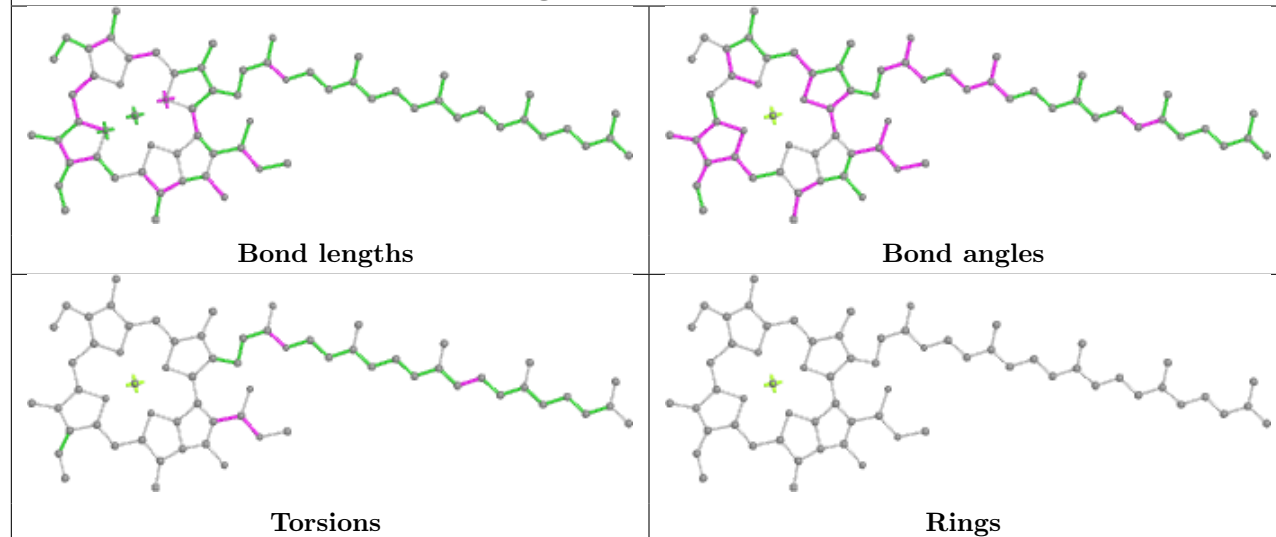
Ligand CLA b 611



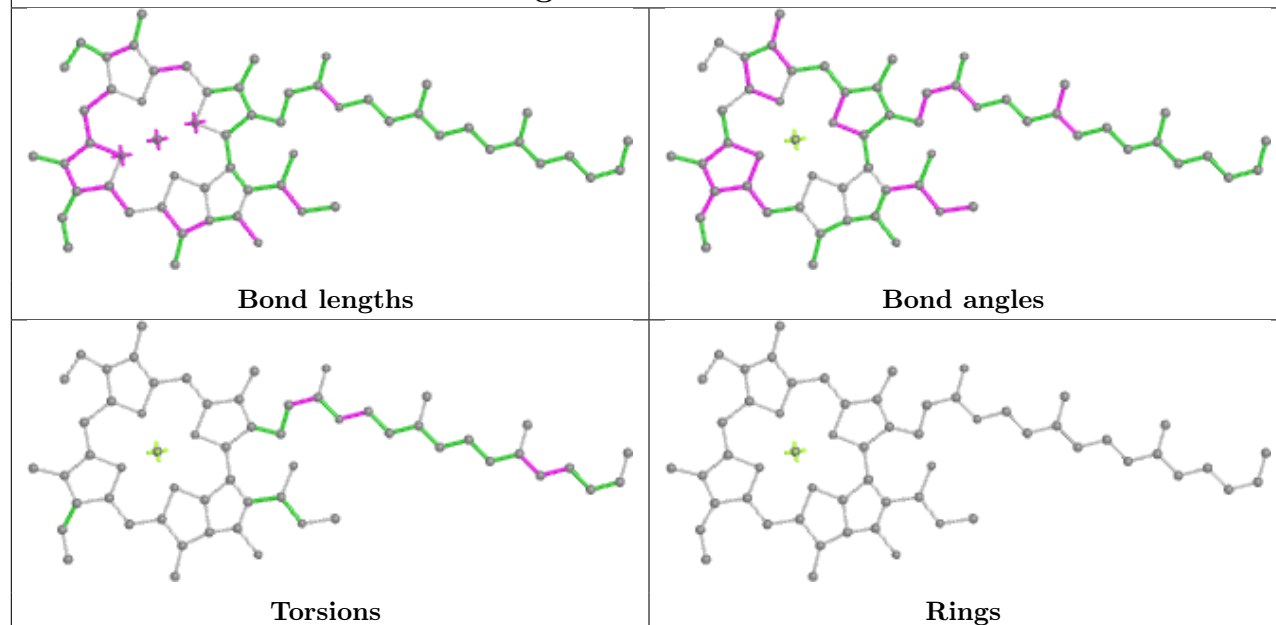
Ligand CLA b 612



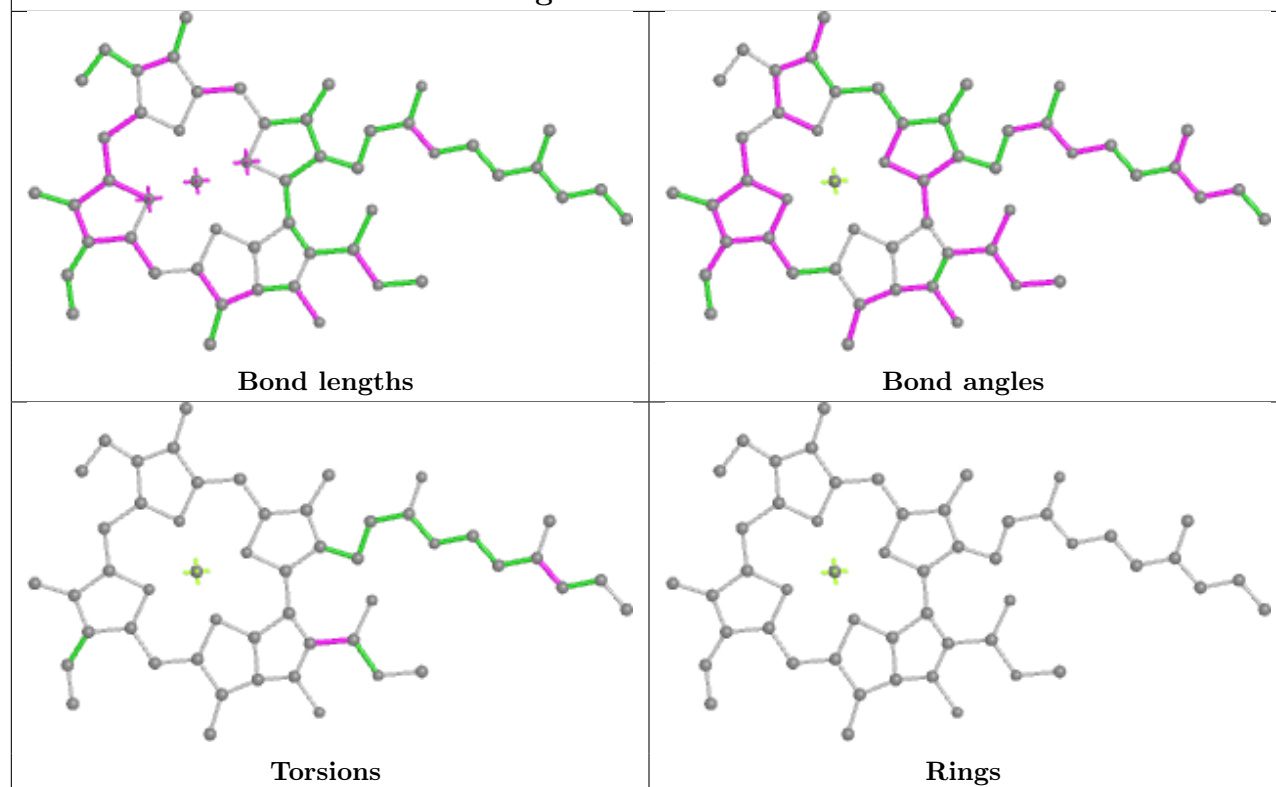
Ligand CLA b 613



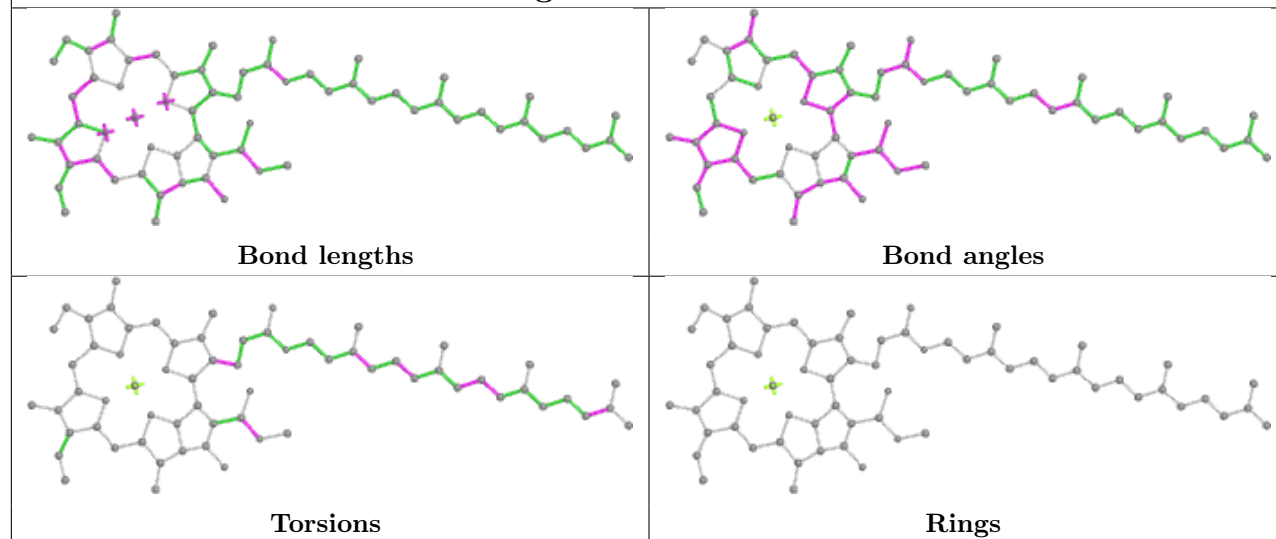
Ligand CLA b 614



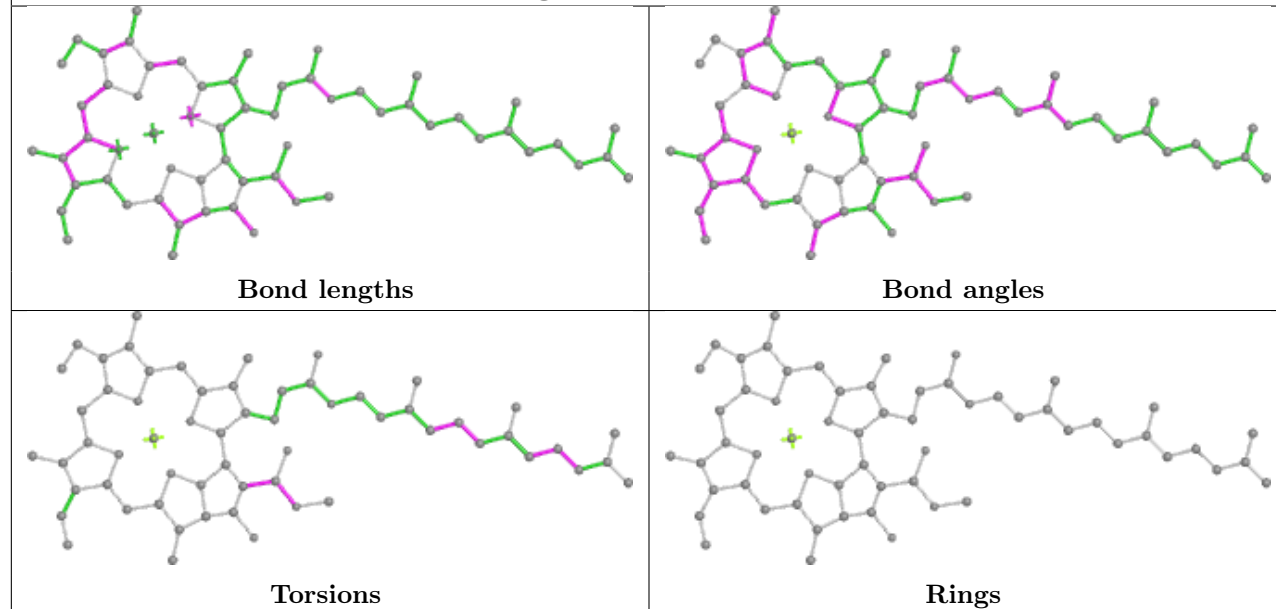
Ligand CLA b 615



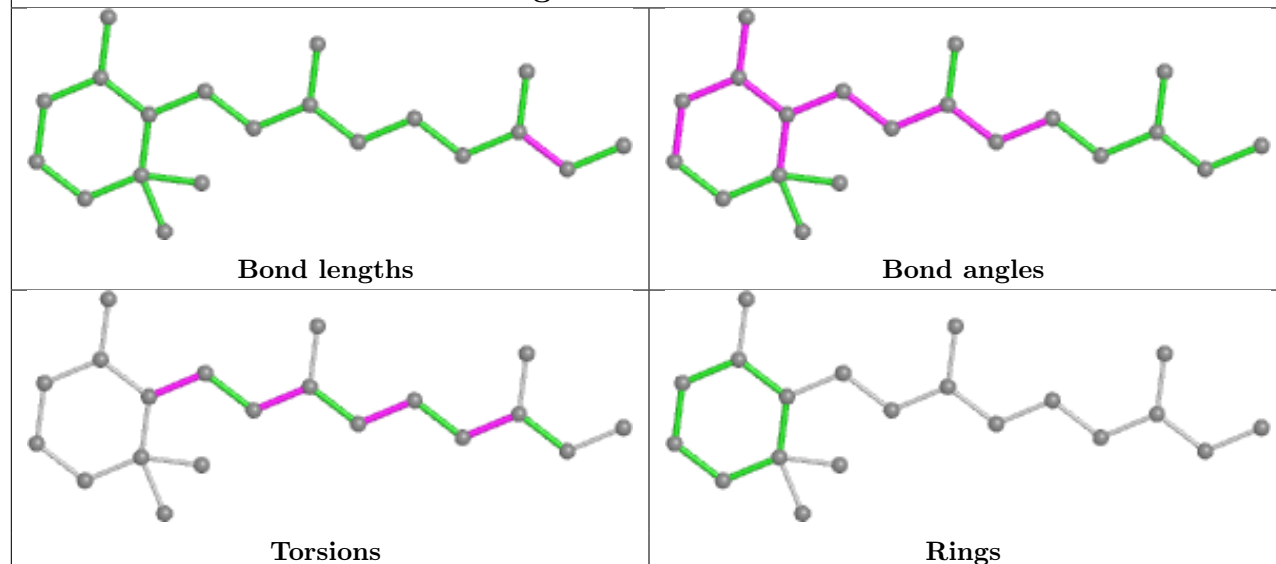
Ligand CLA b 616



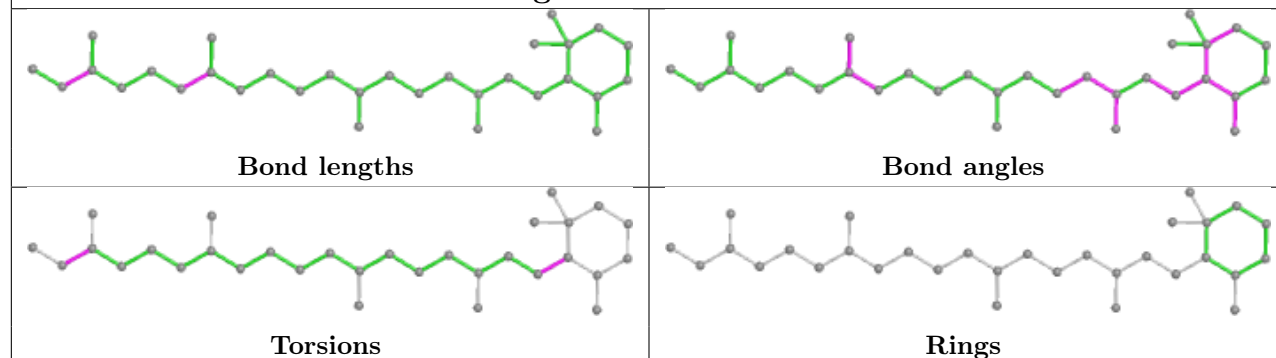
Ligand CLA b 617



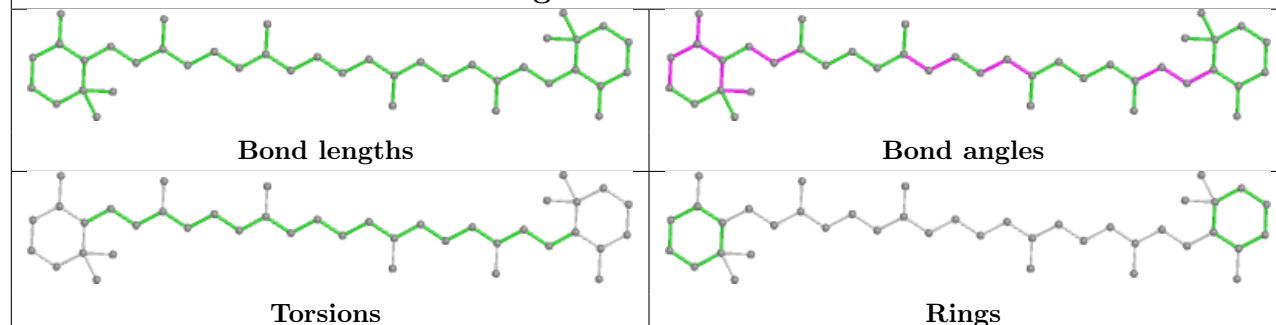
Ligand BCR b 618

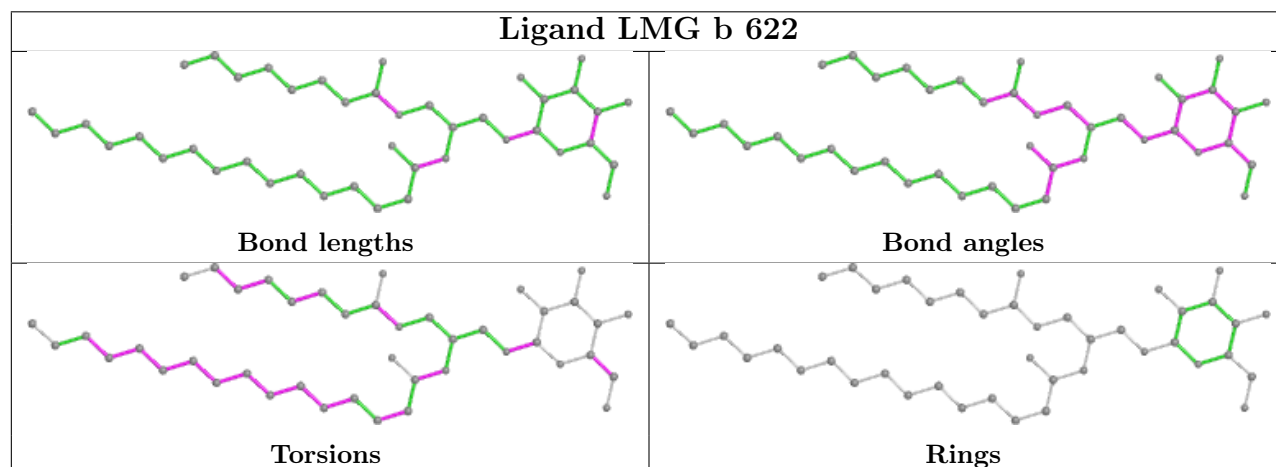
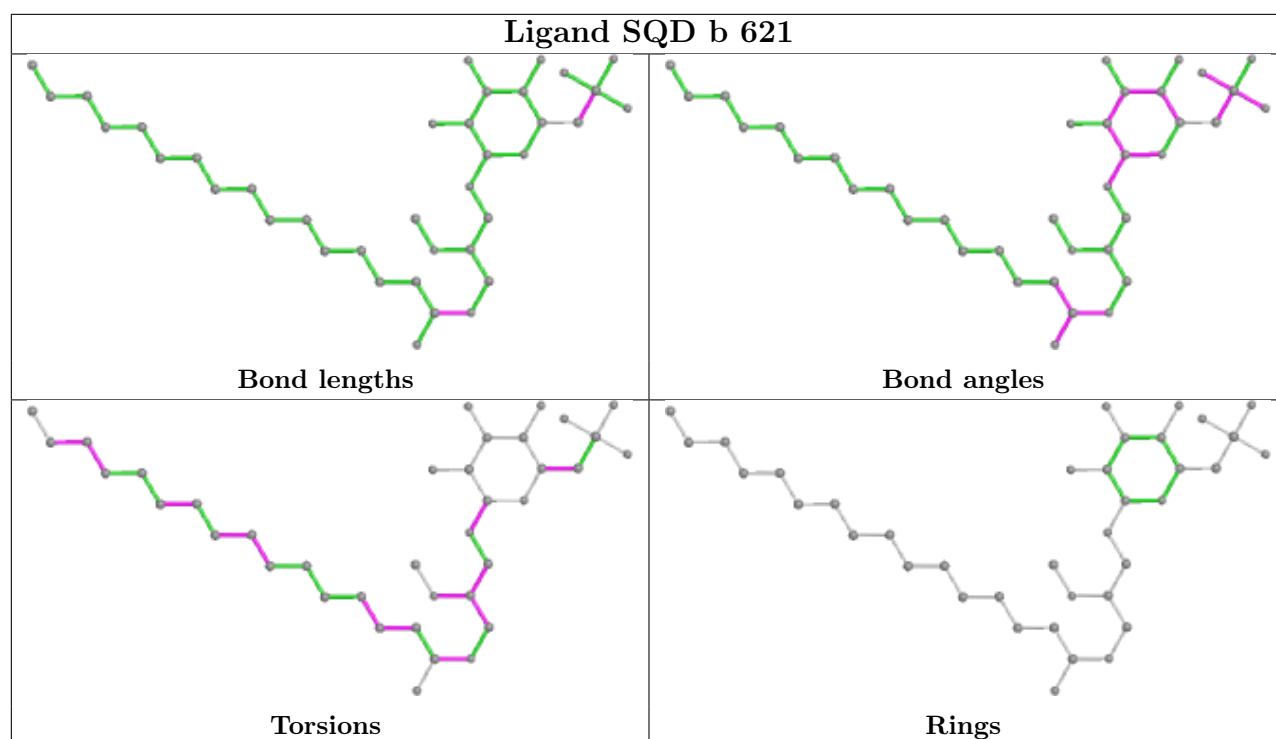


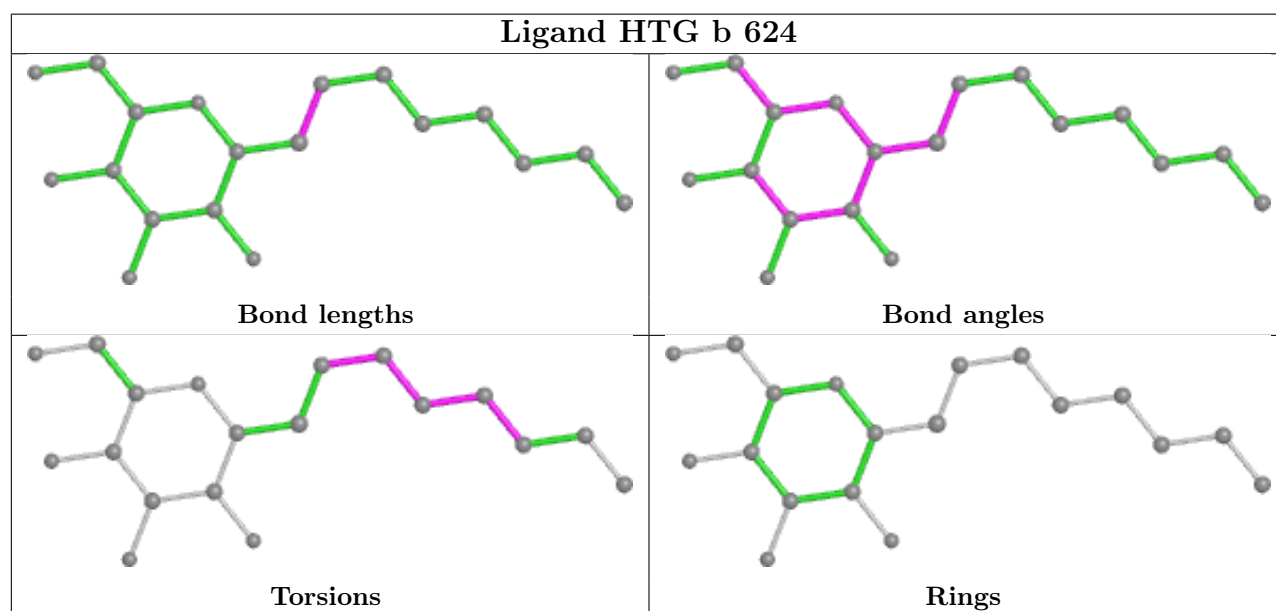
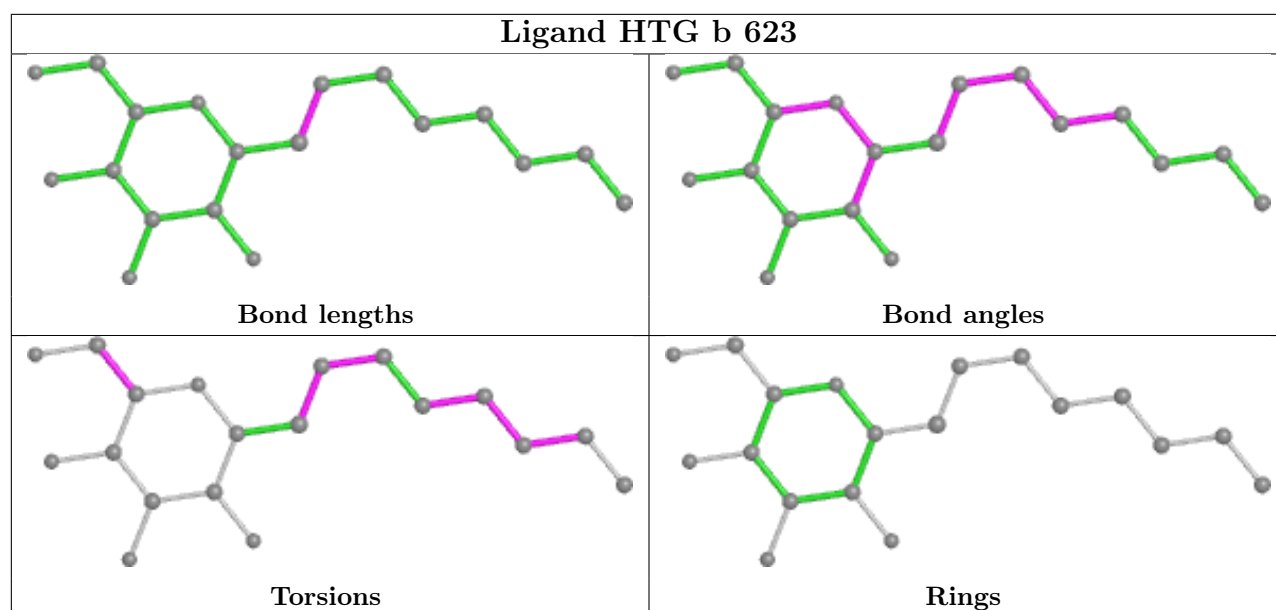
Ligand BCR b 619

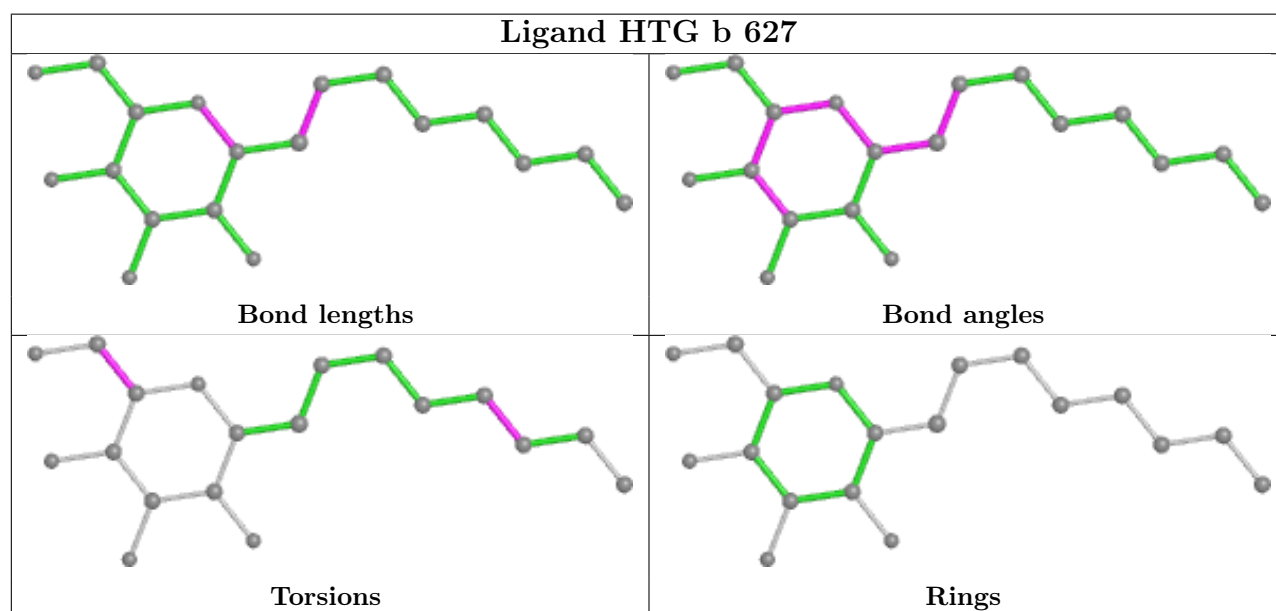
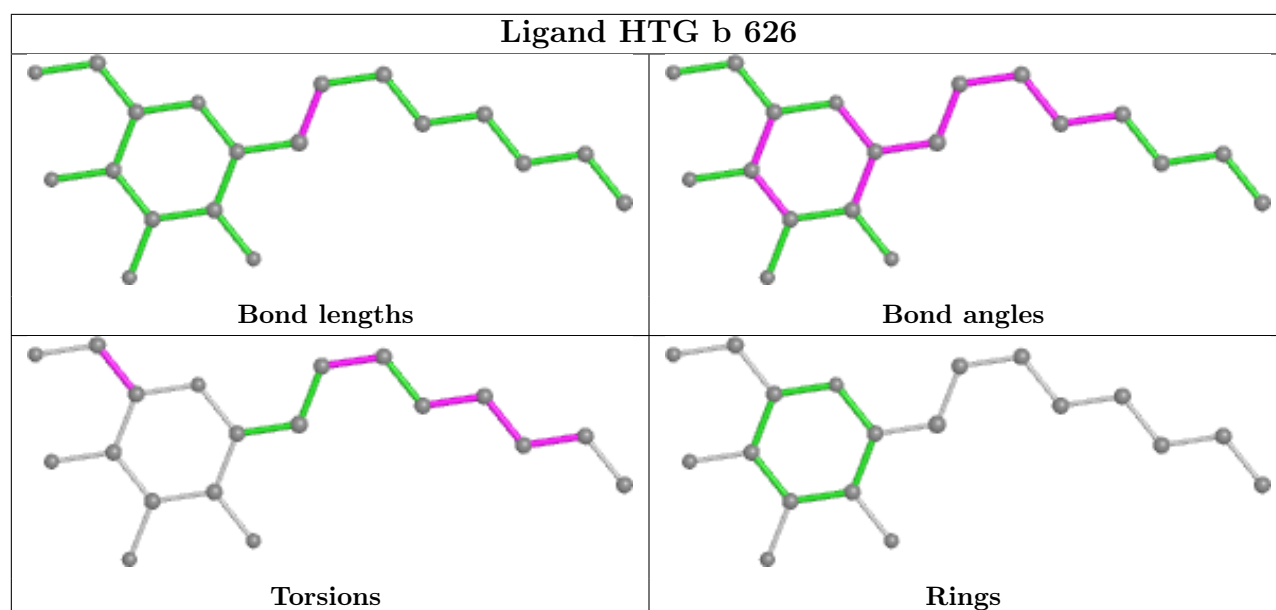


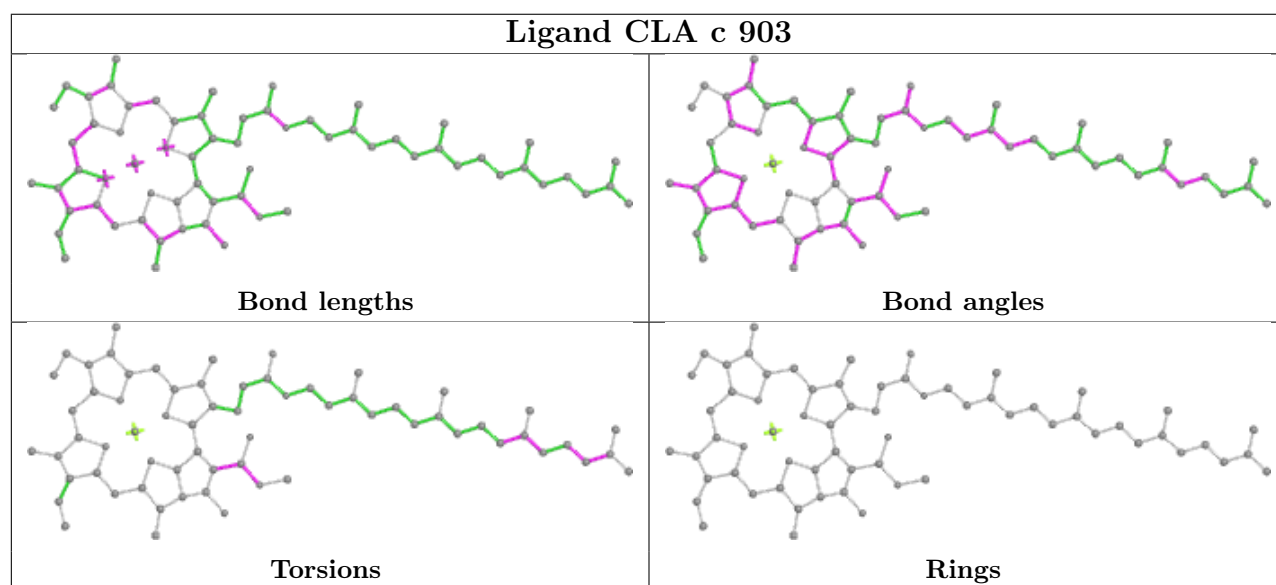
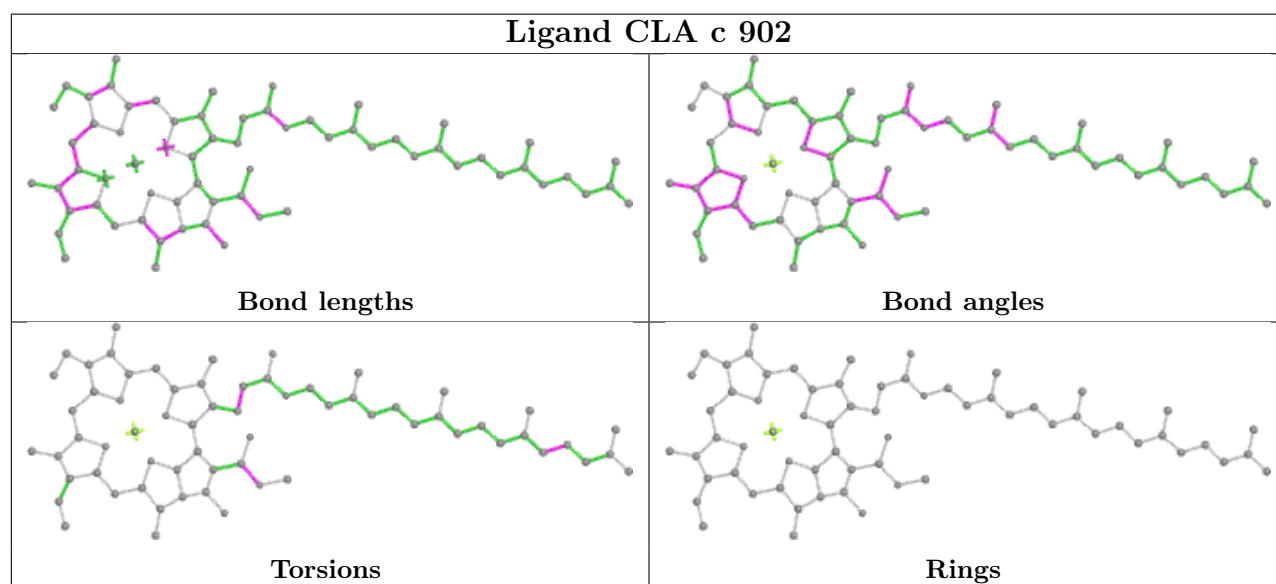
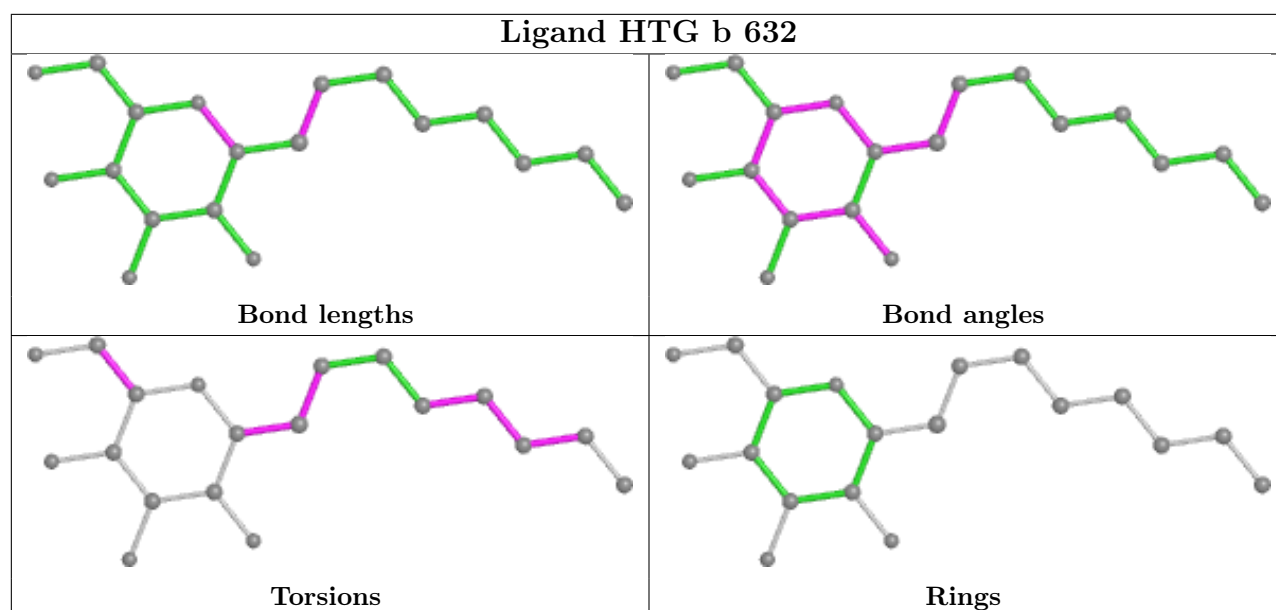
Ligand BCR b 620



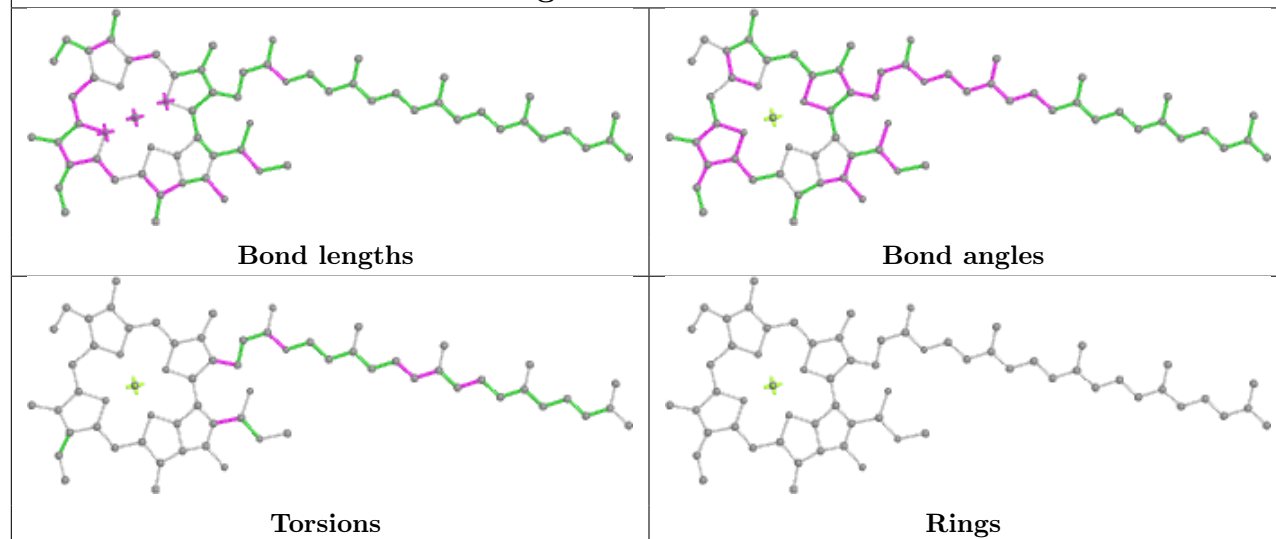




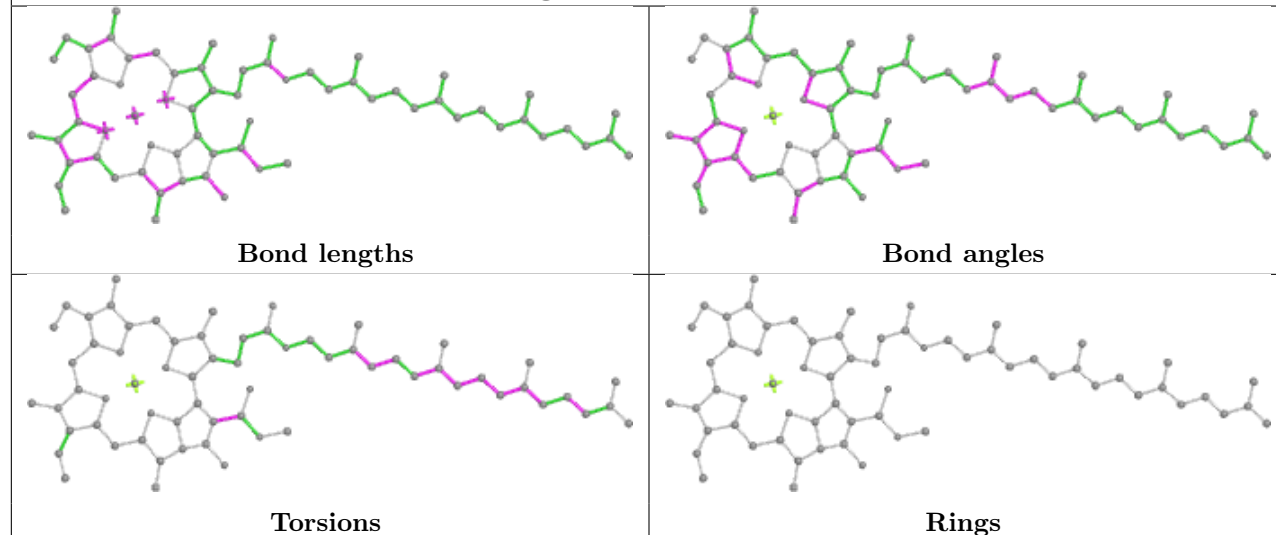




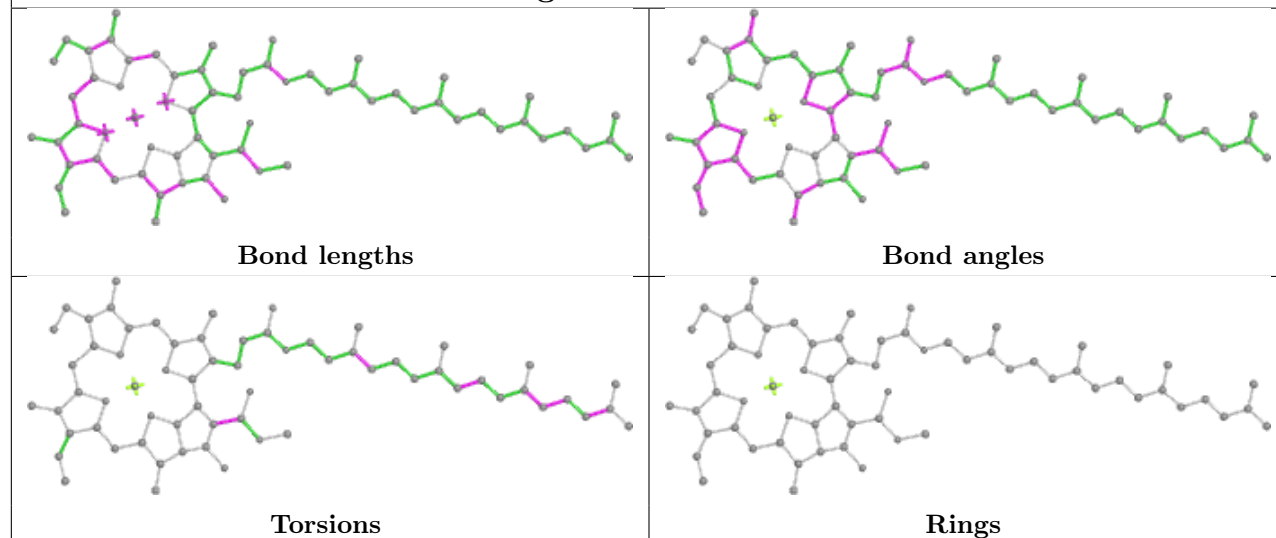
Ligand CLA c 904



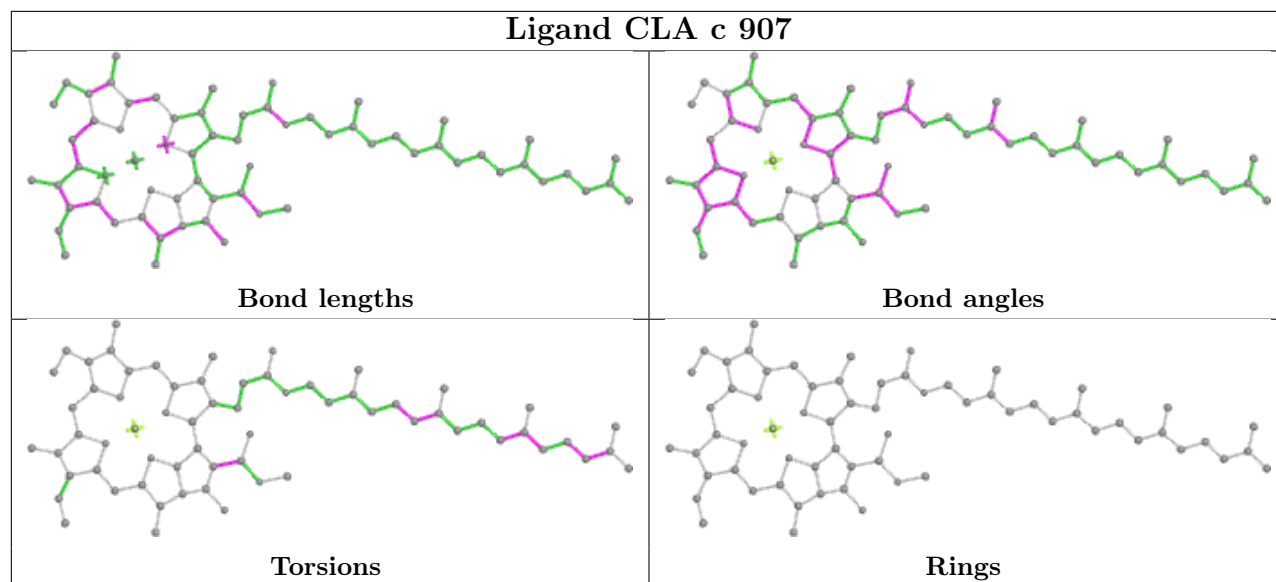
Ligand CLA c 905



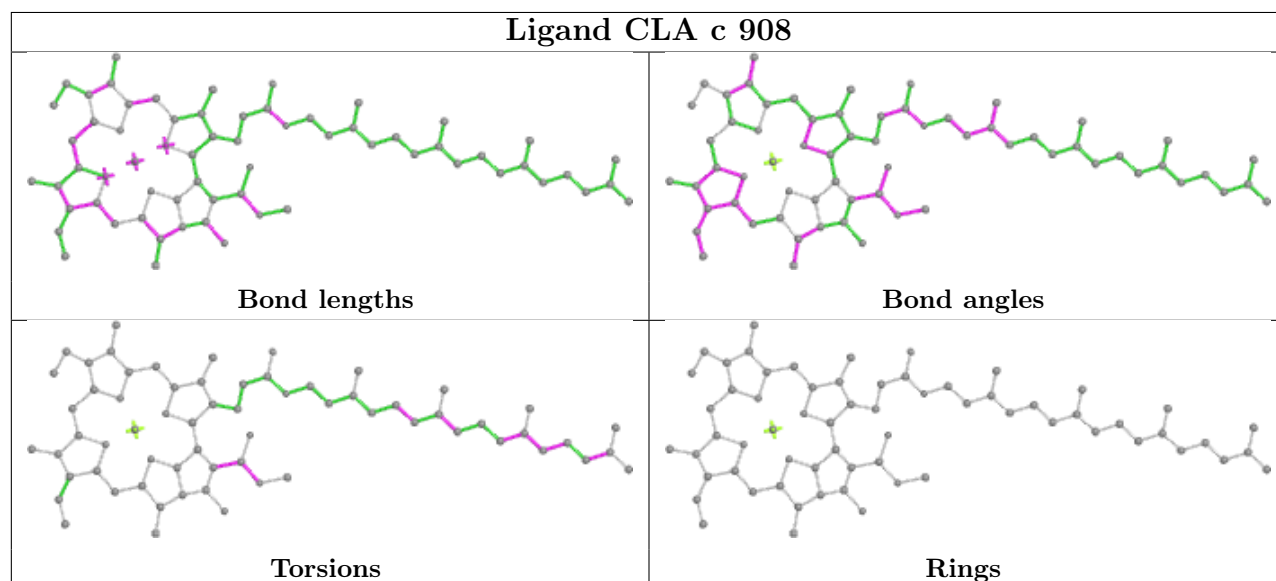
Ligand CLA c 906



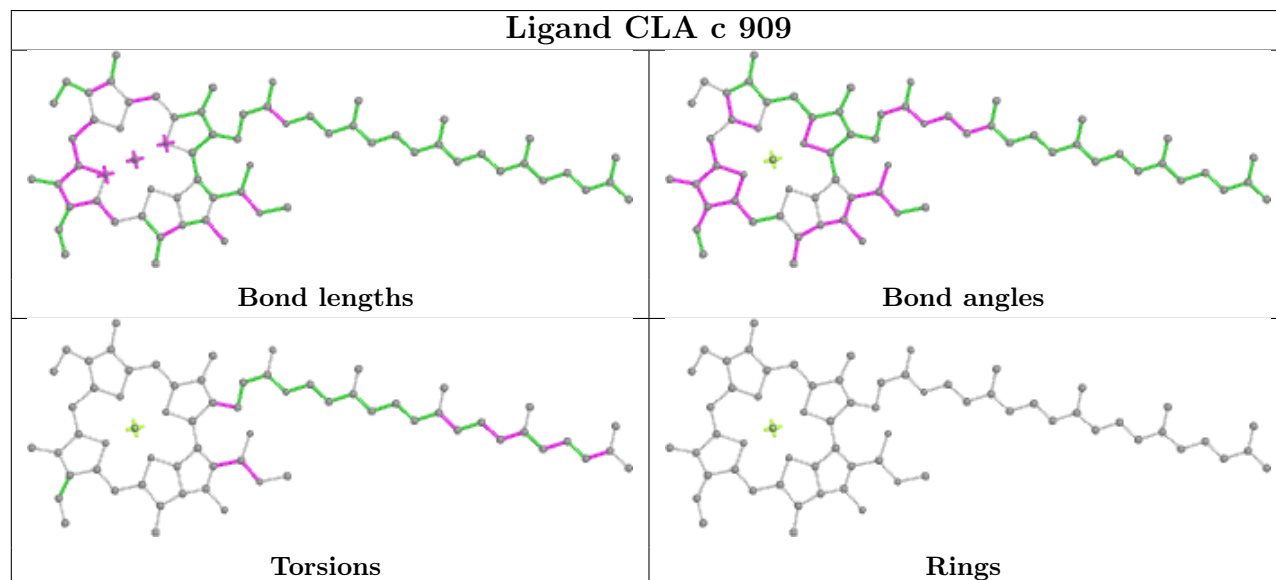
Ligand CLA c 907



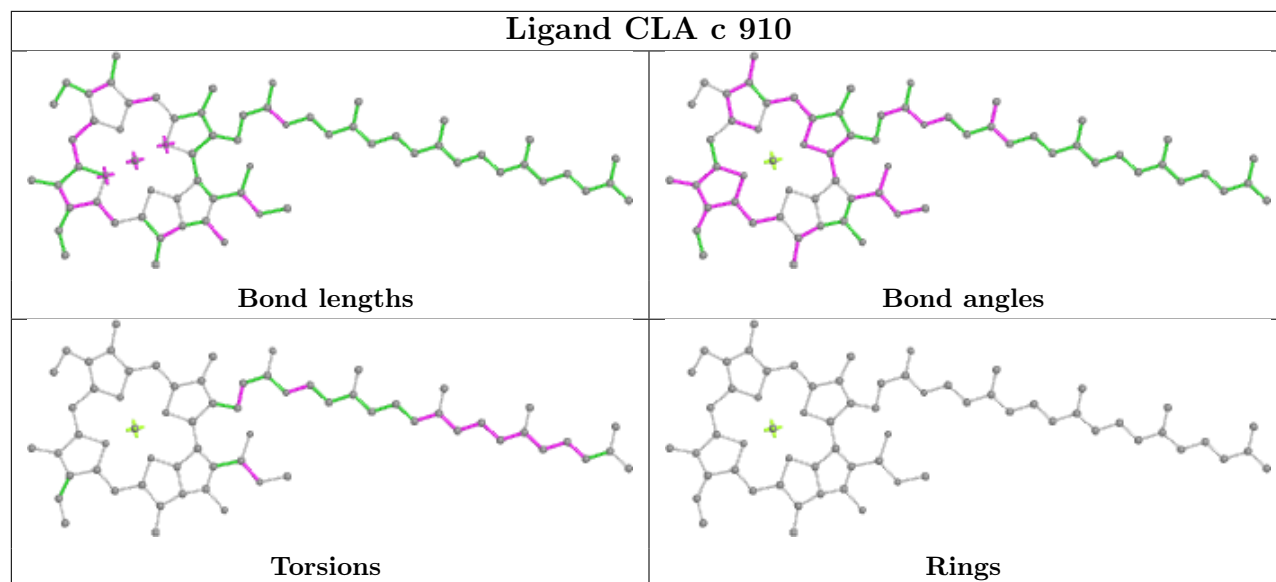
Ligand CLA c 908



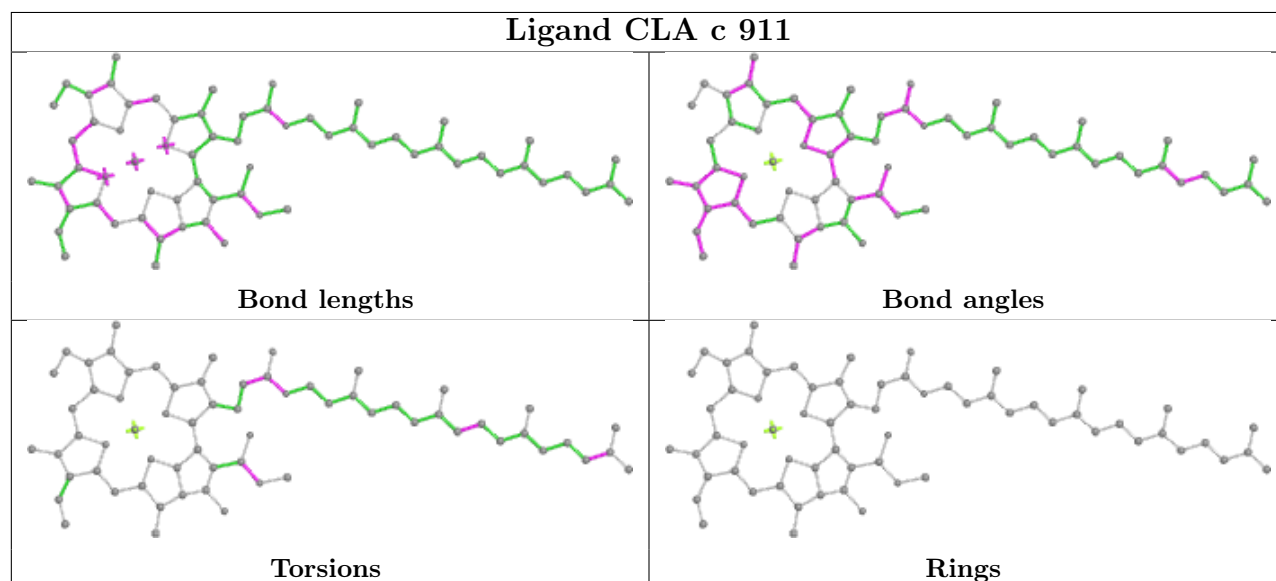
Ligand CLA c 909



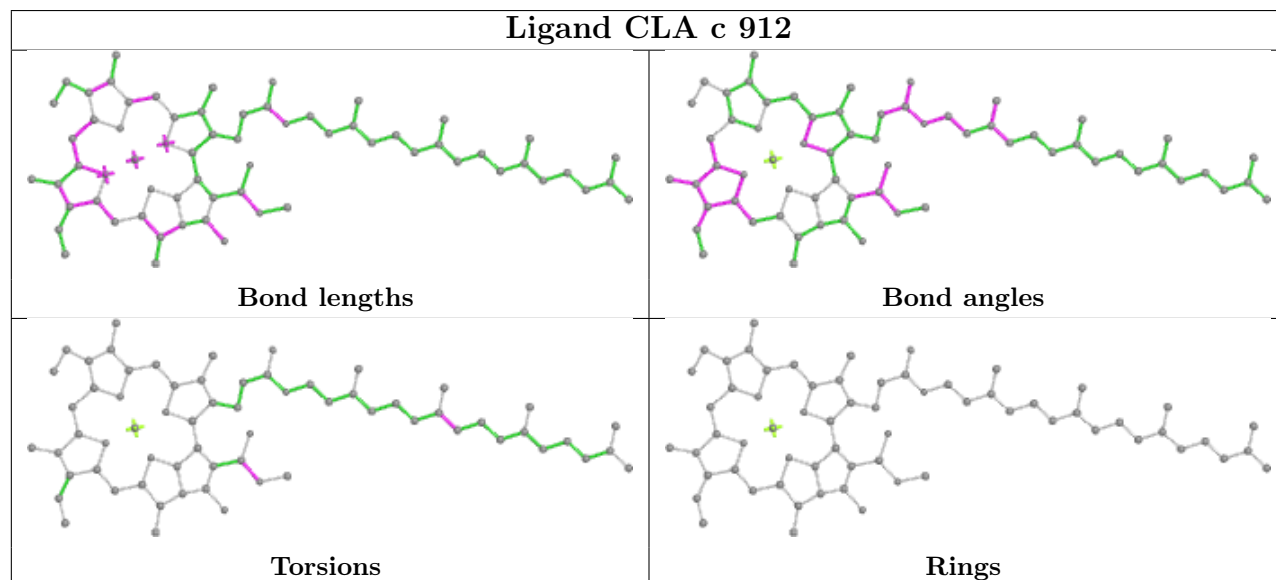
Ligand CLA c 910



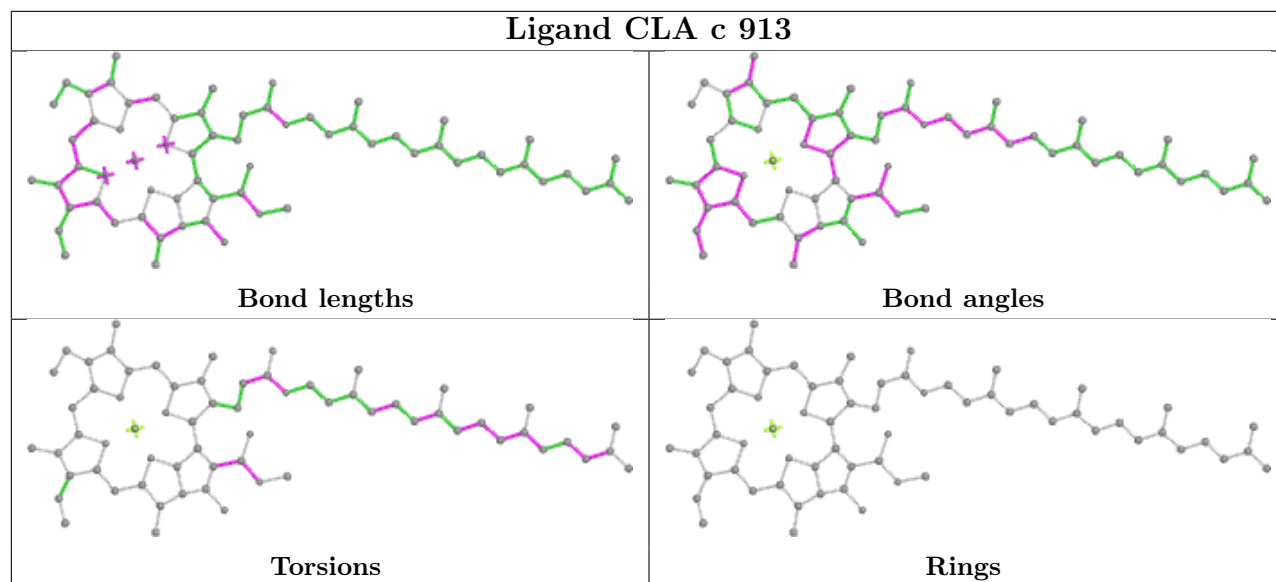
Ligand CLA c 911



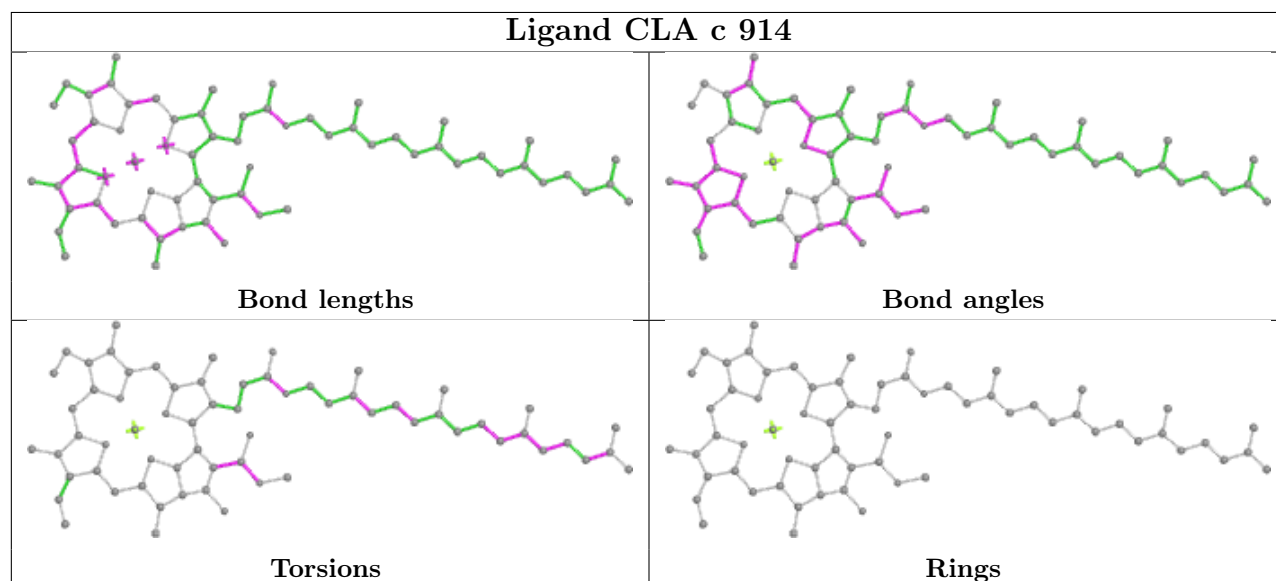
Ligand CLA c 912



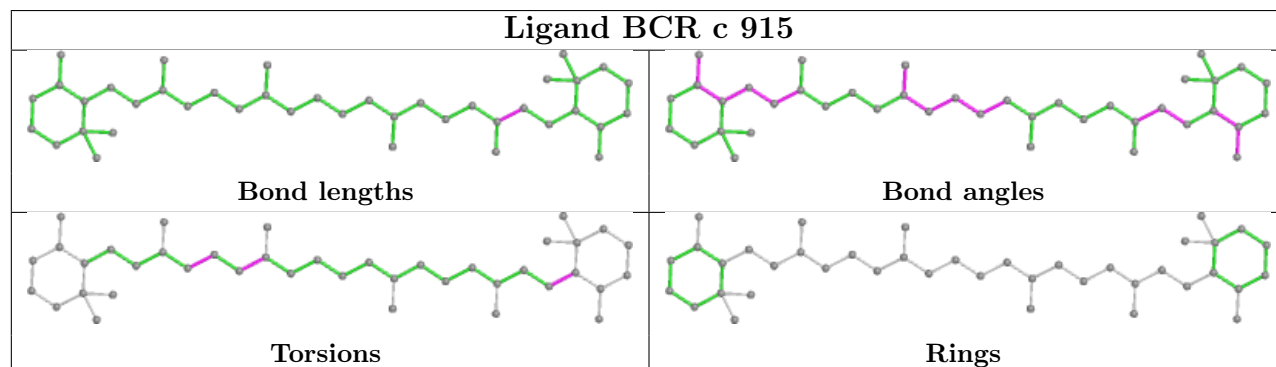
Ligand CLA c 913

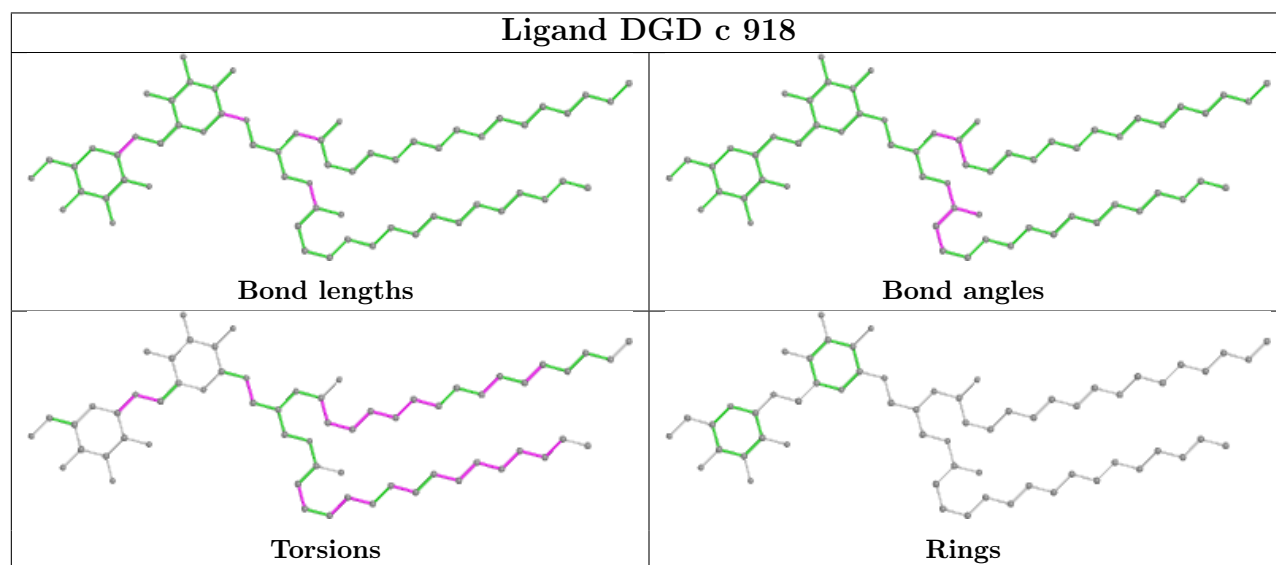
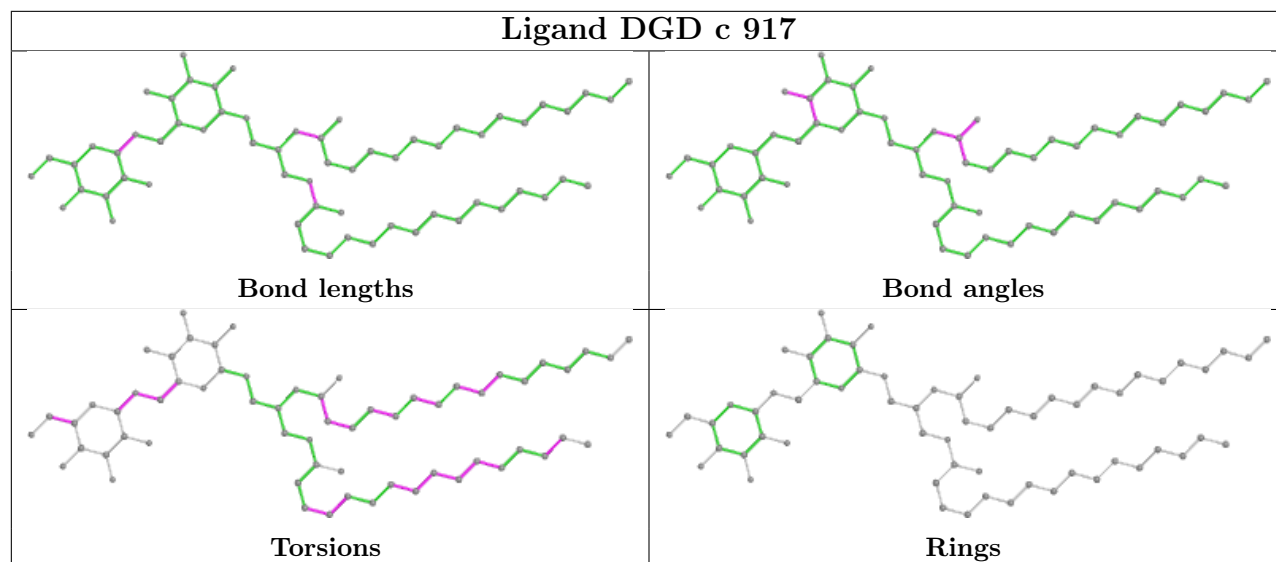
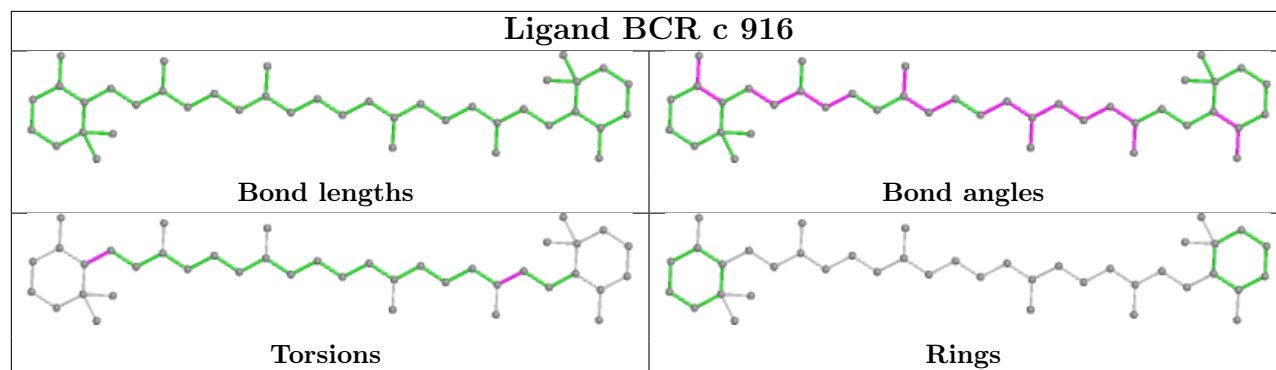


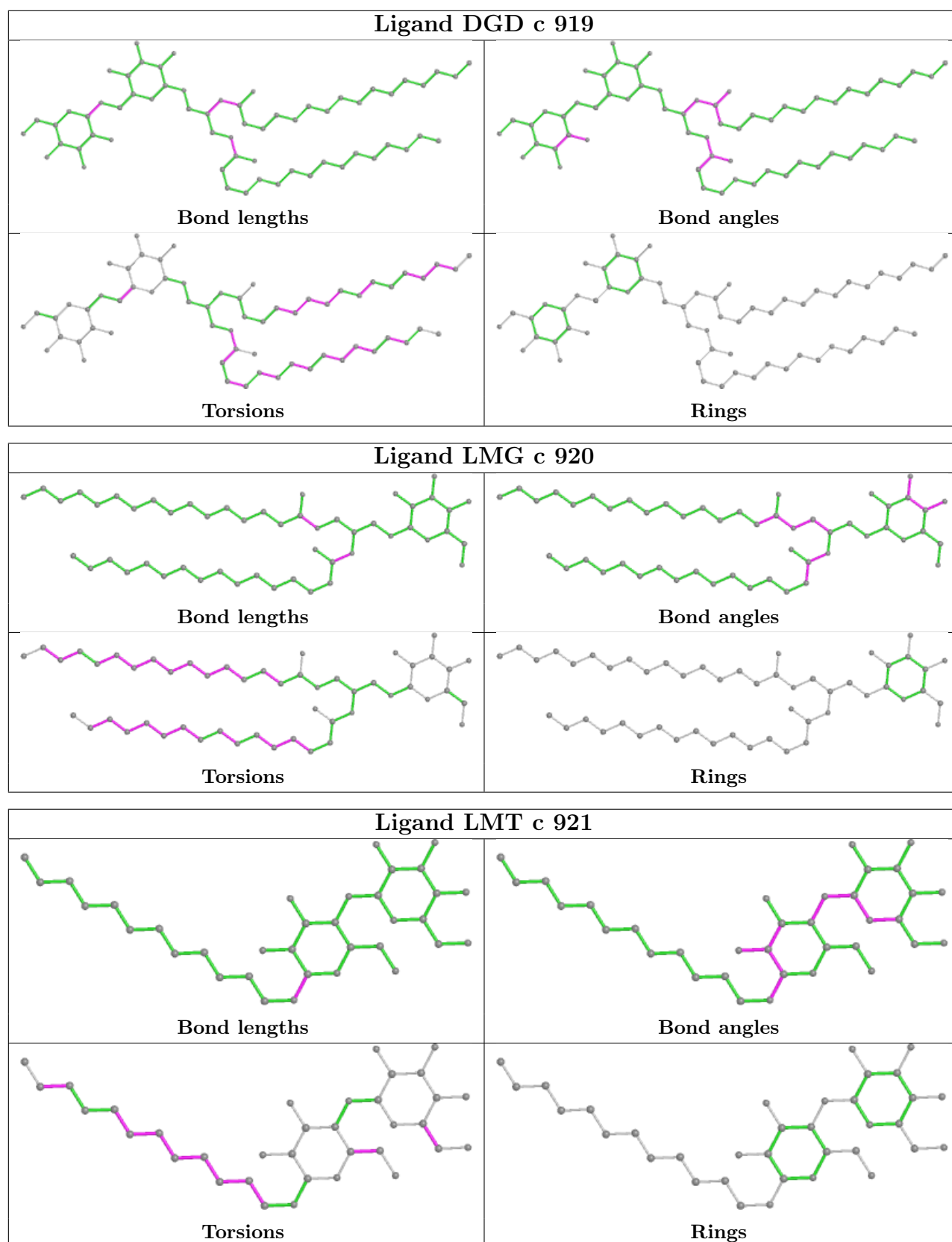
Ligand CLA c 914

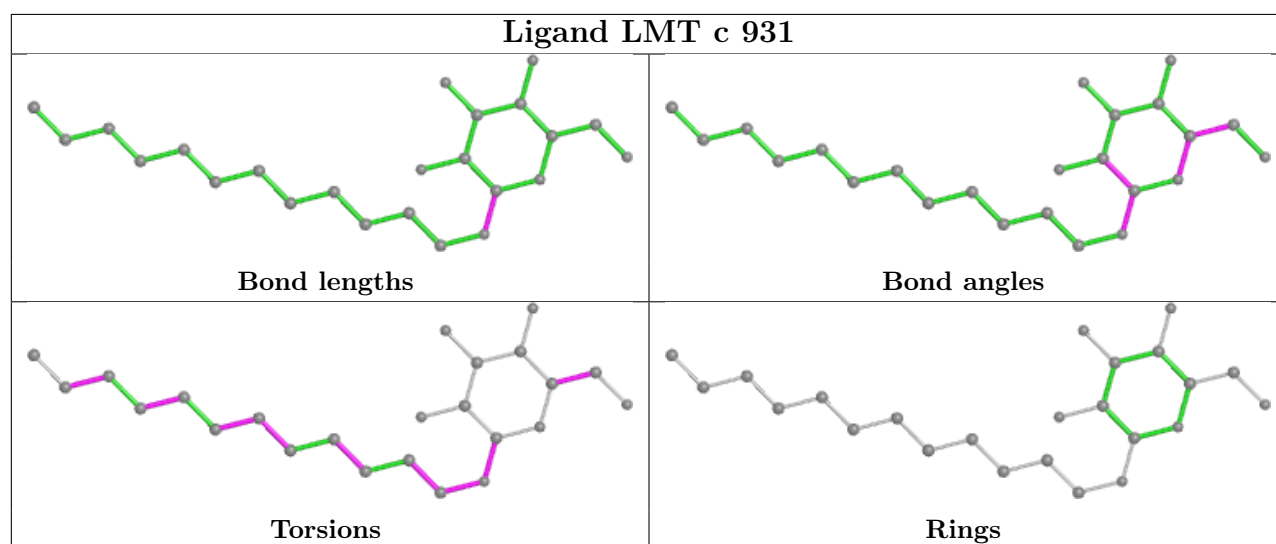
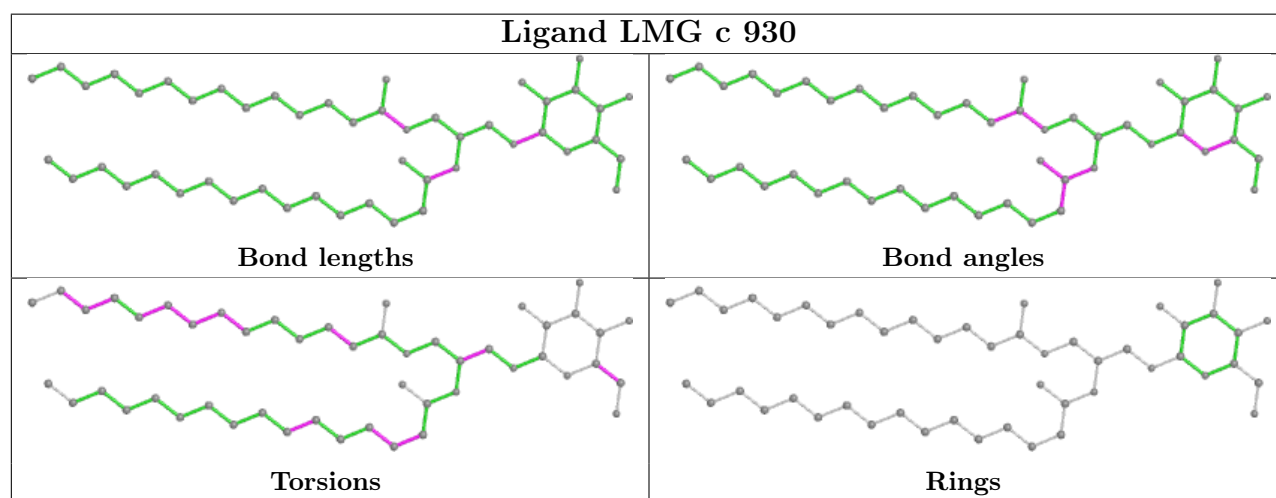
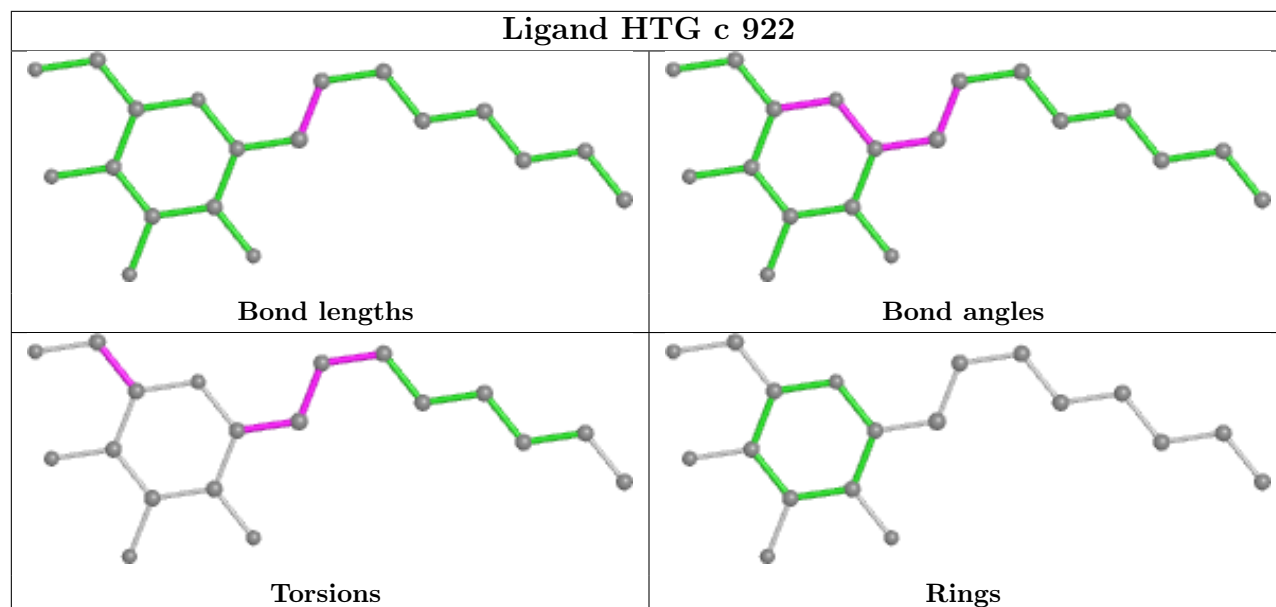


Ligand BCR c 915

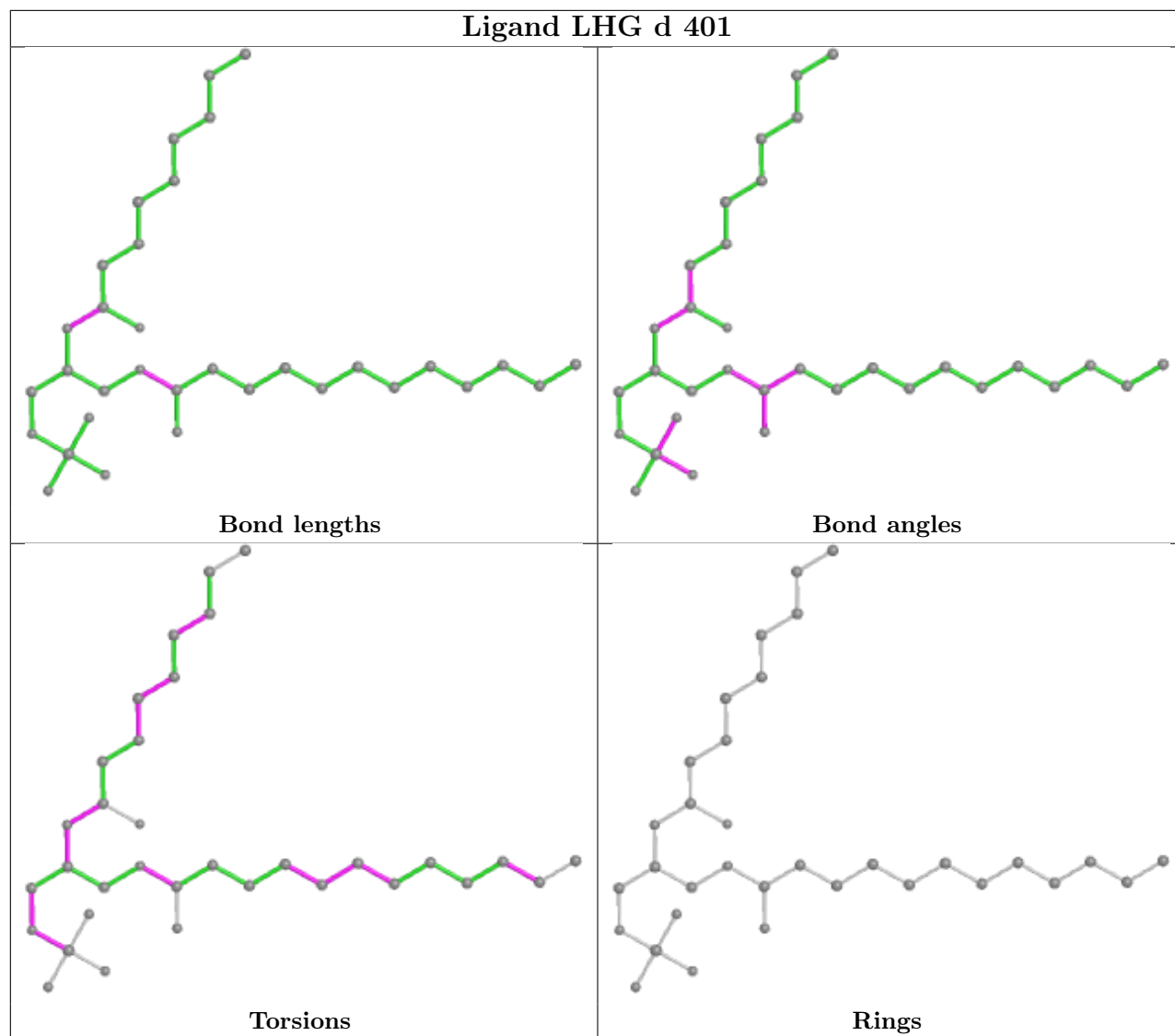




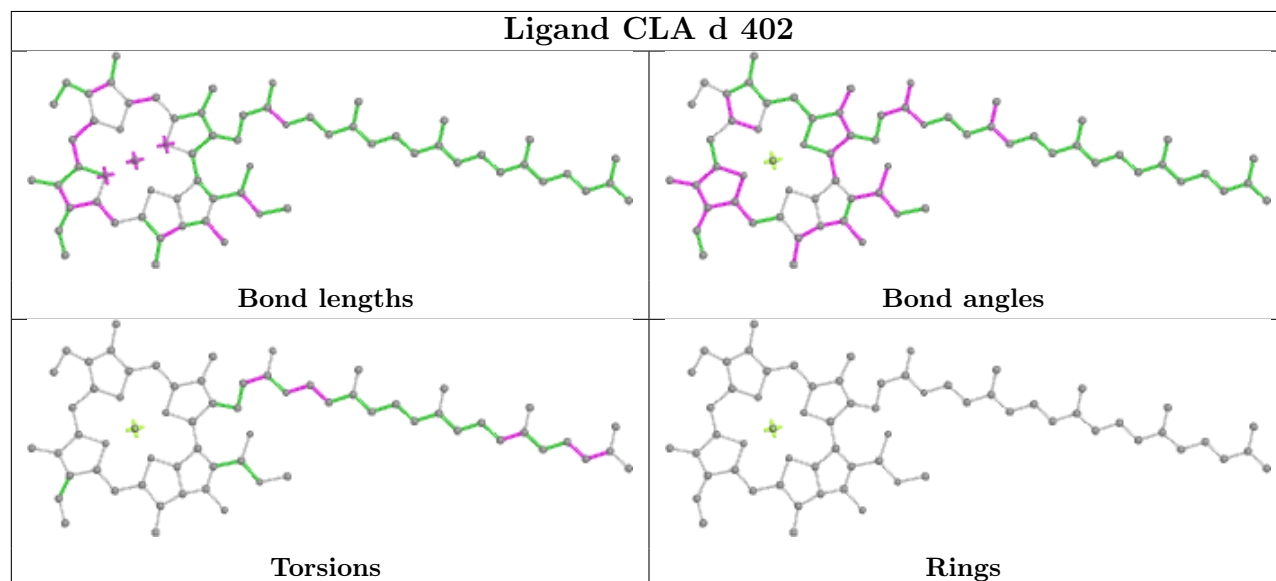


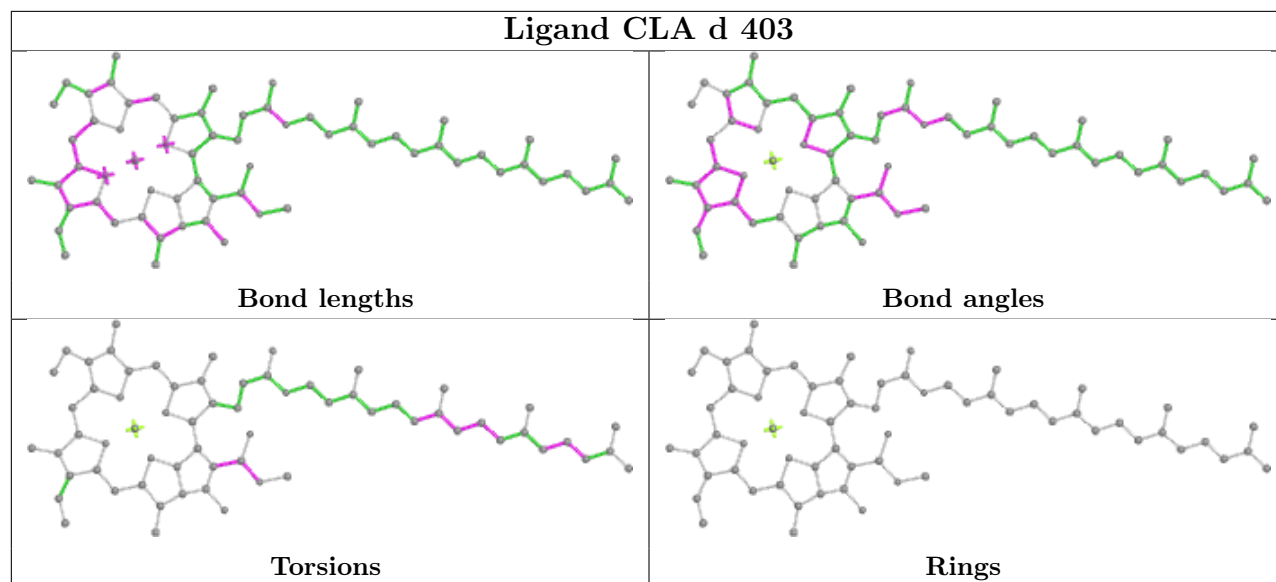
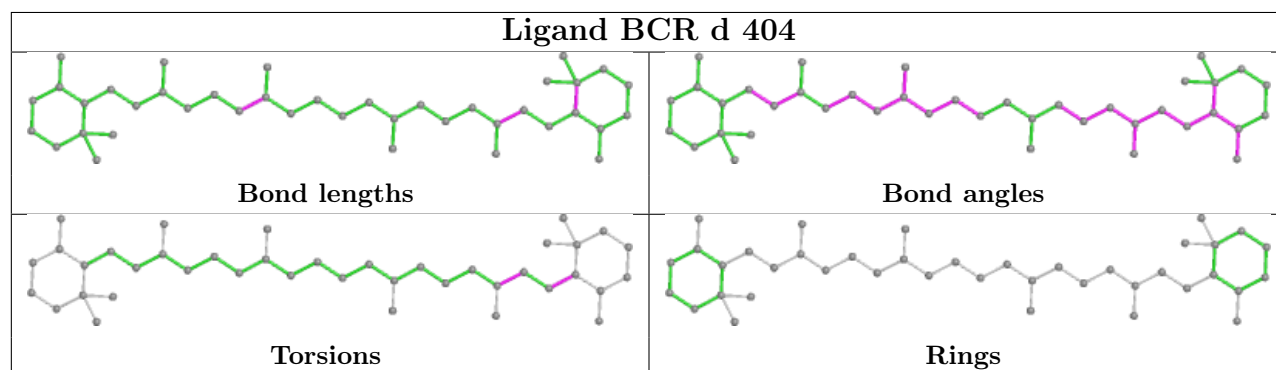
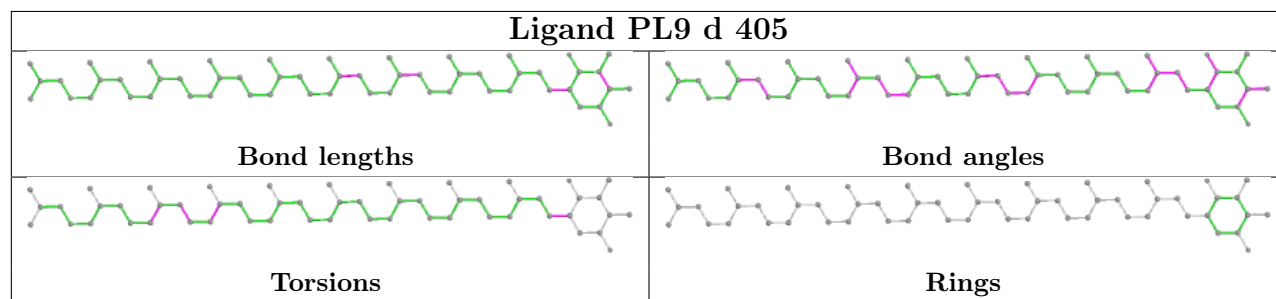


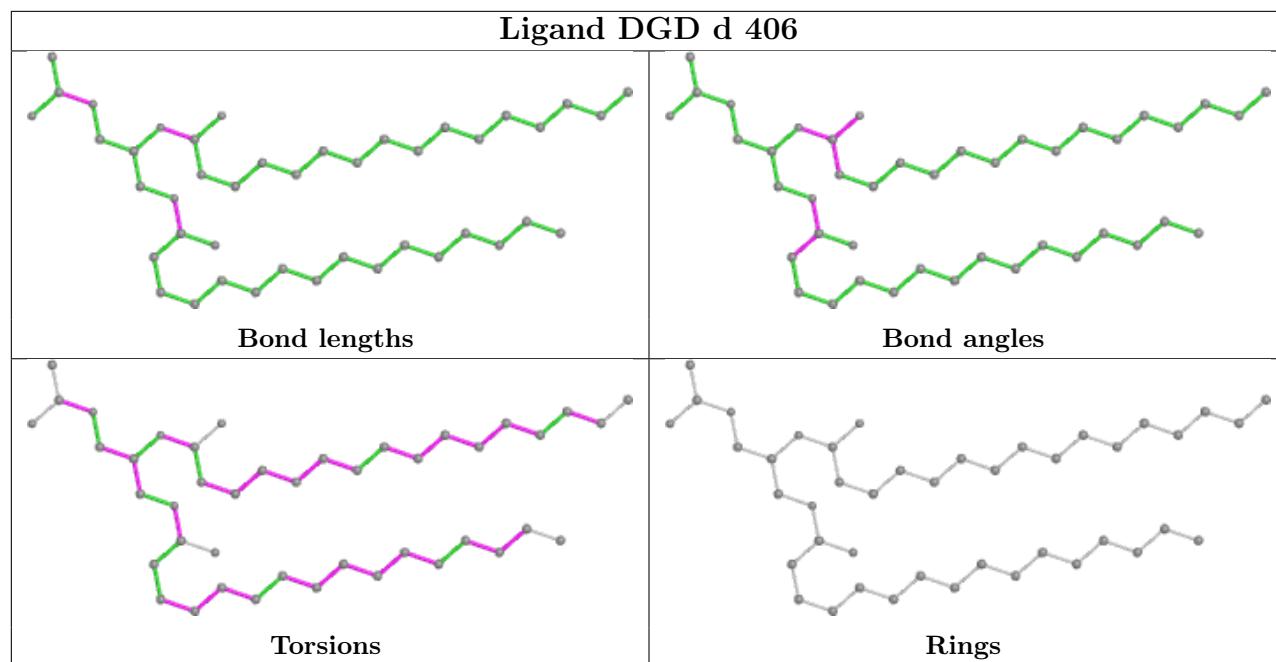
Ligand LHG d 401

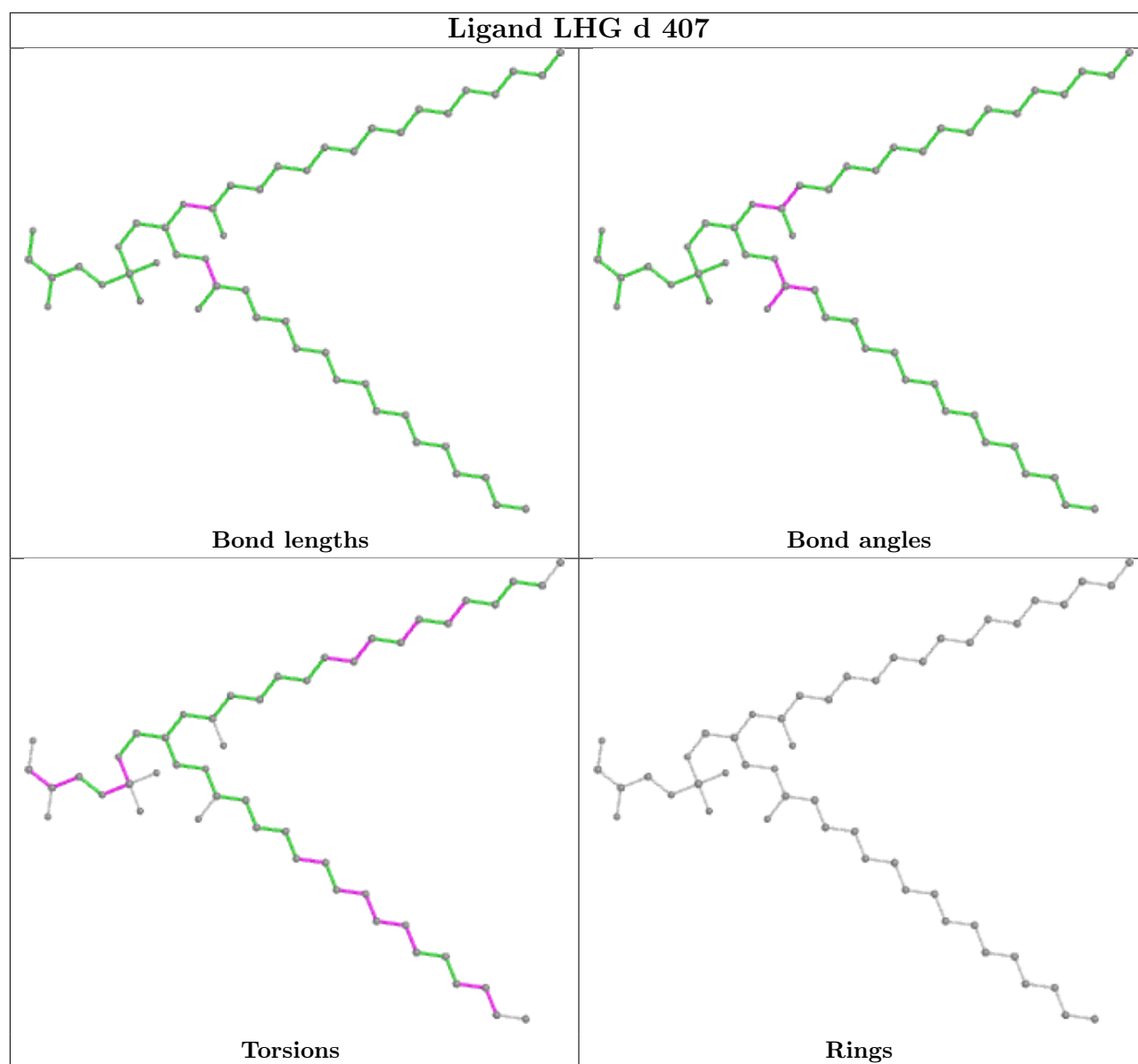


Ligand CLA d 402

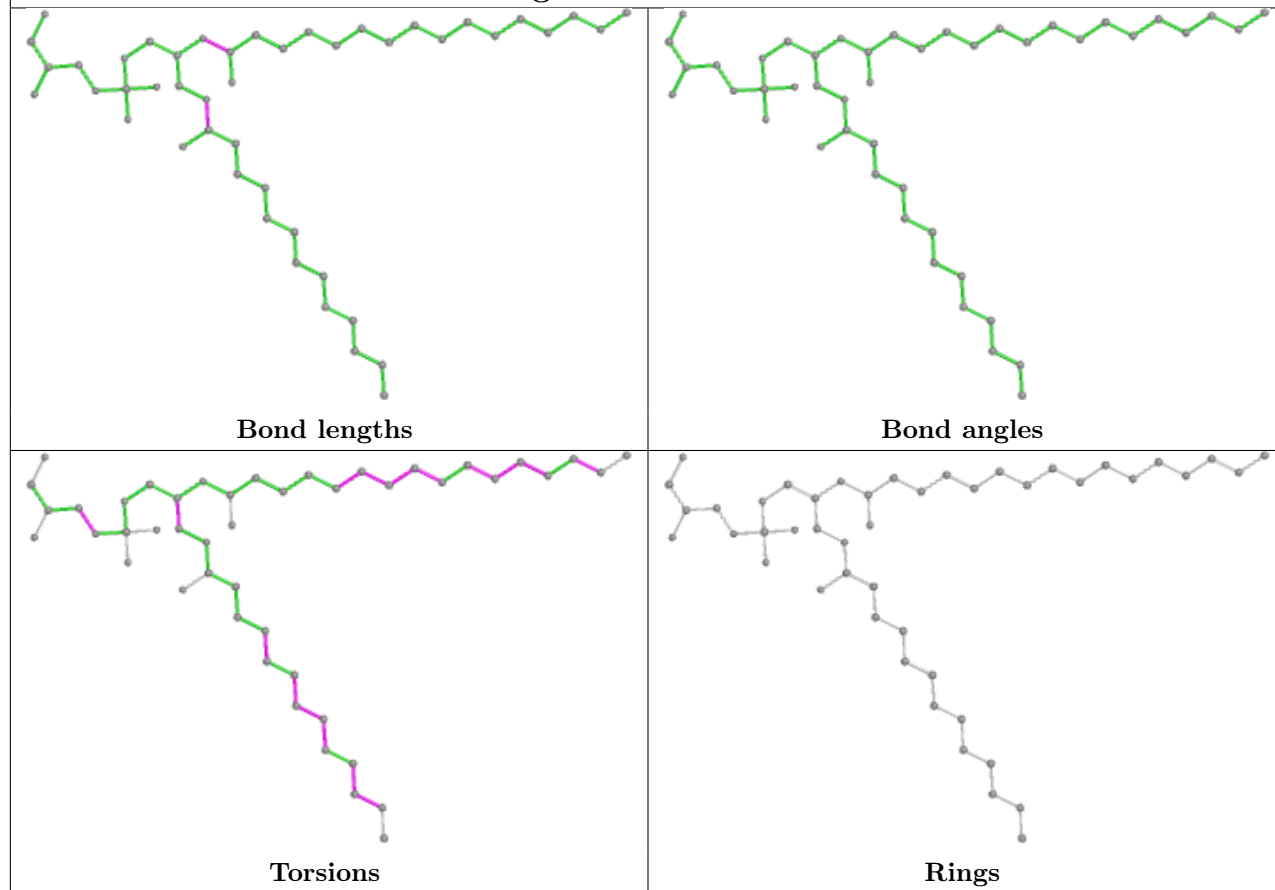


Ligand CLA d 403**Ligand BCR d 404****Ligand PL9 d 405**

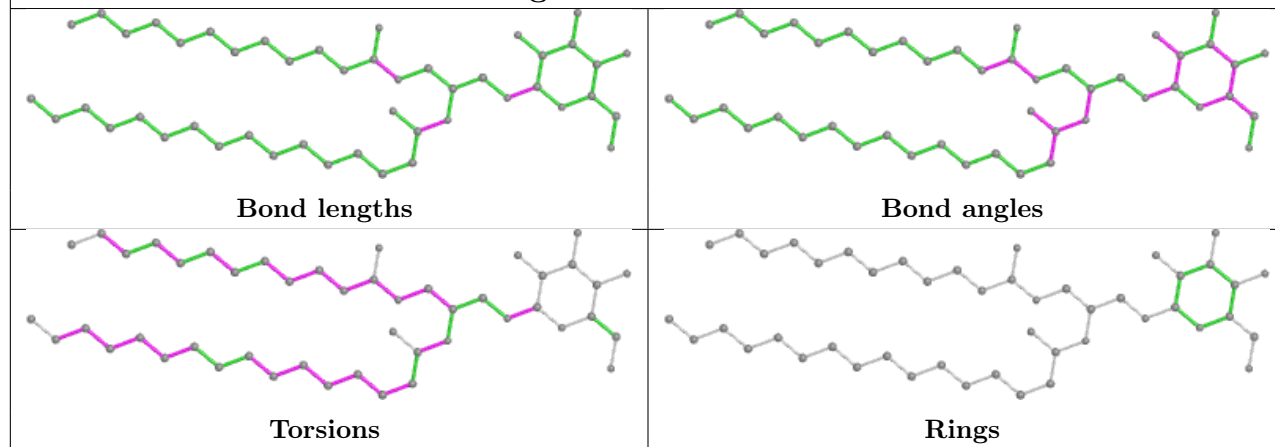




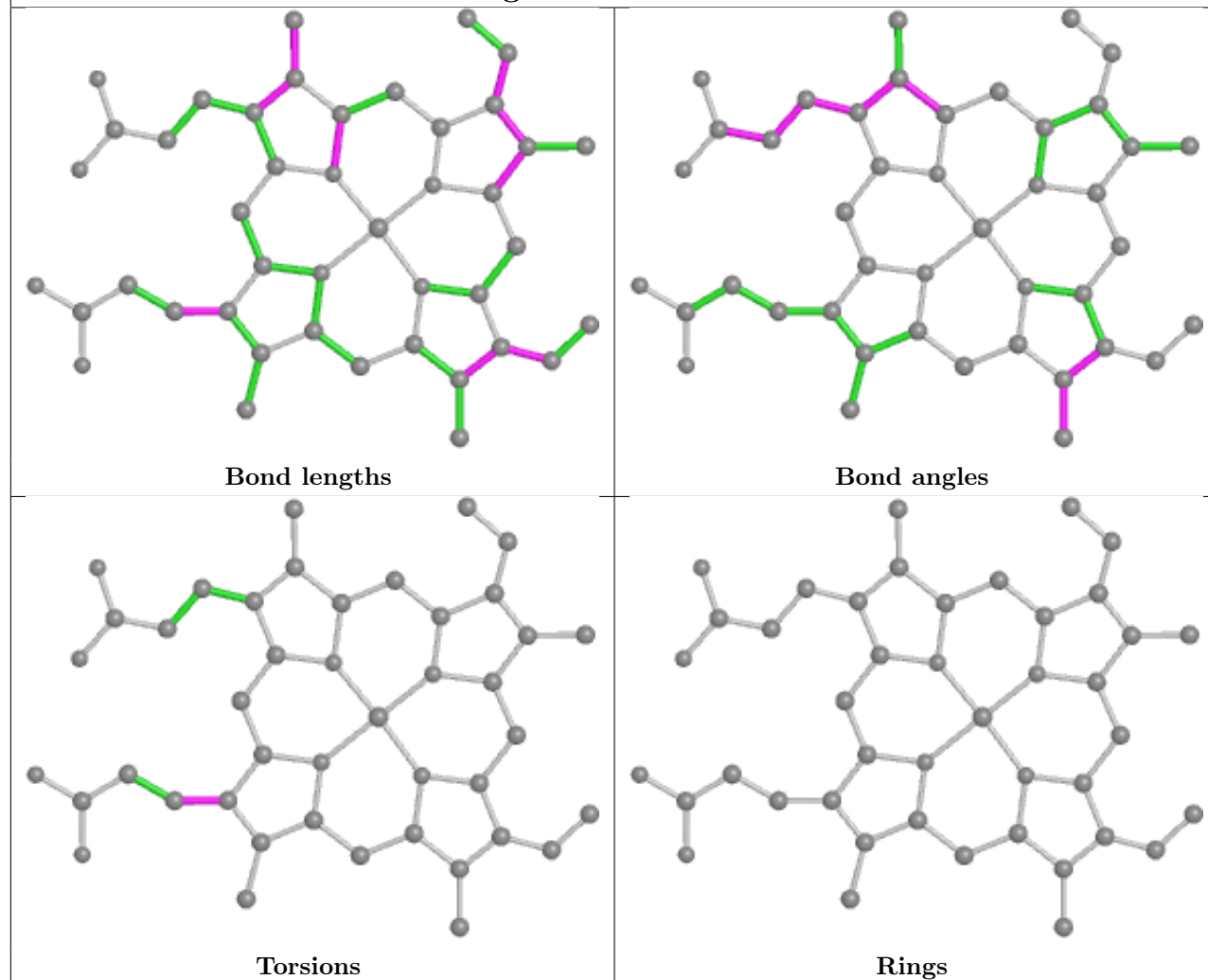
Ligand LHG d 408



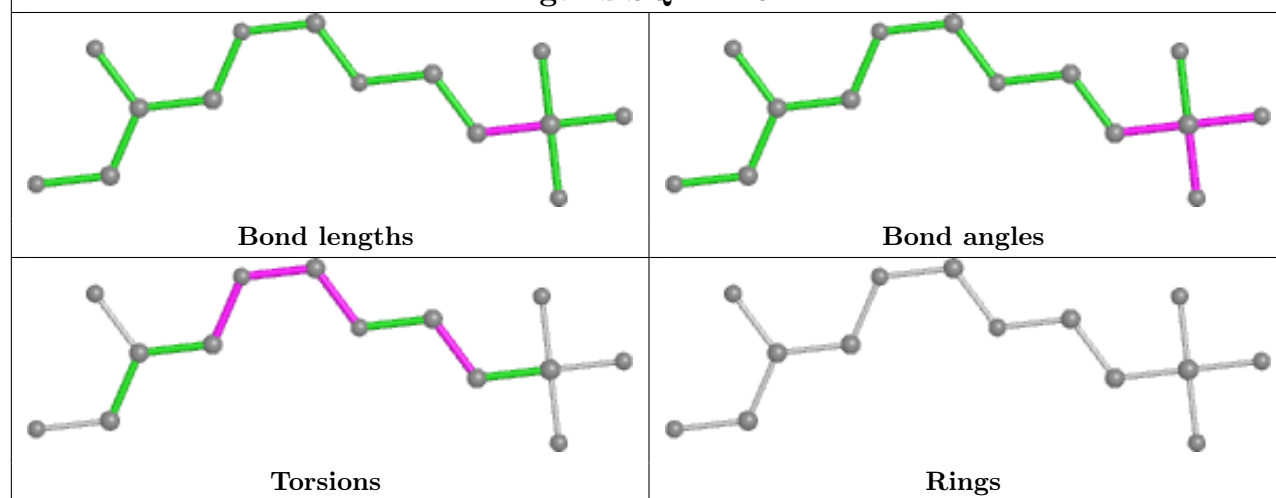
Ligand LMG d 409



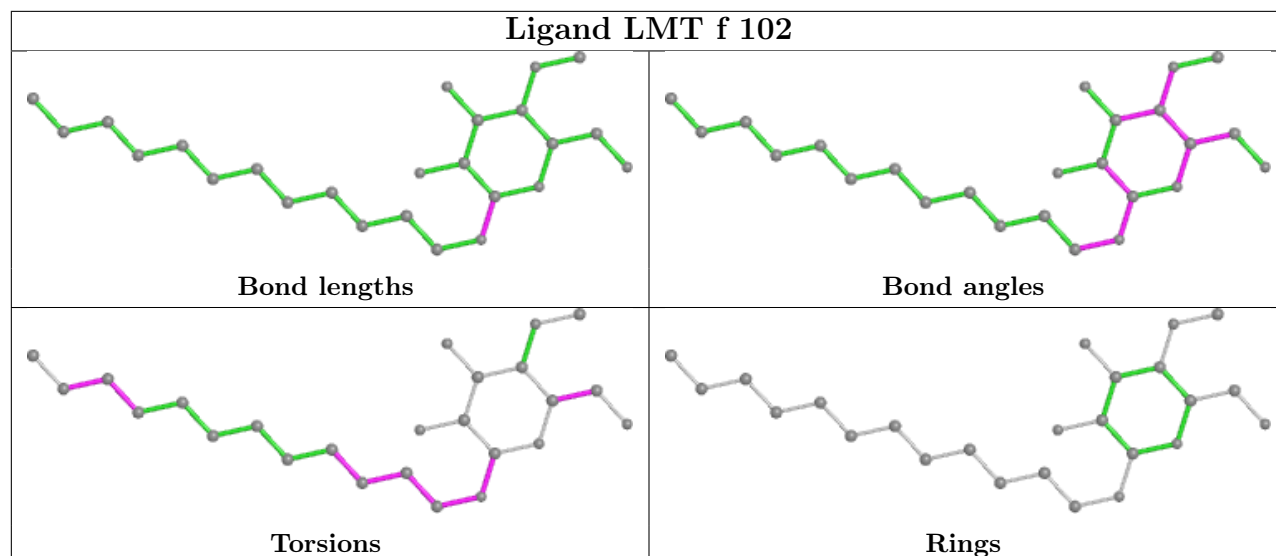
Ligand HEM e 101



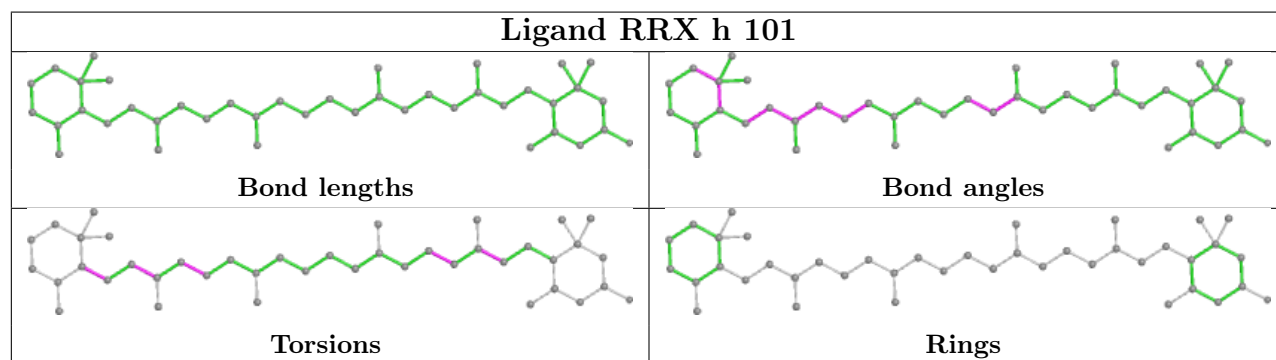
Ligand SQD f 101



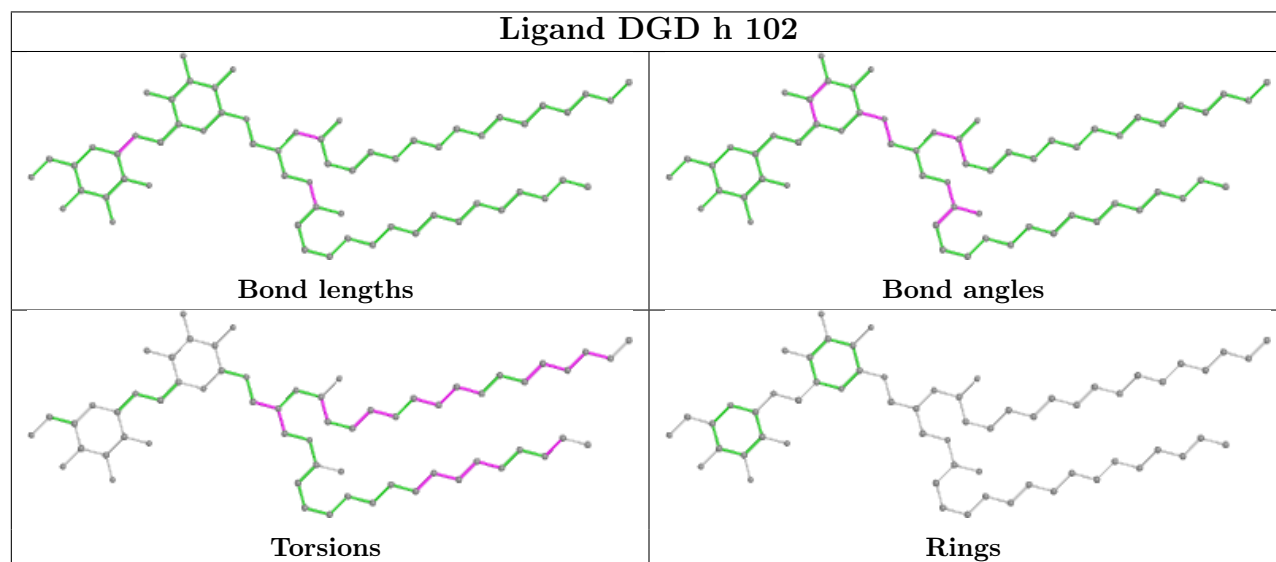
Ligand LMT f 102

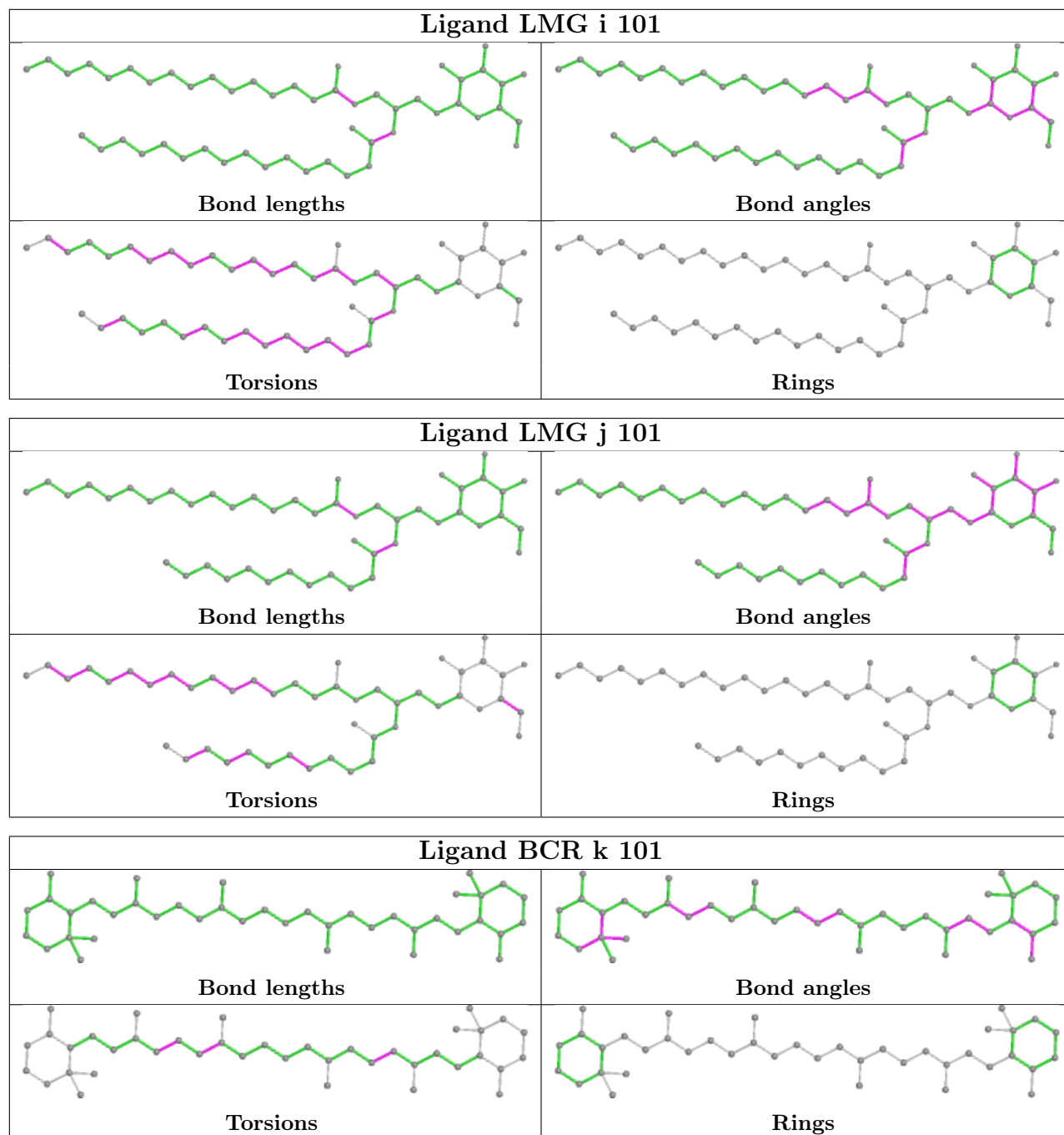


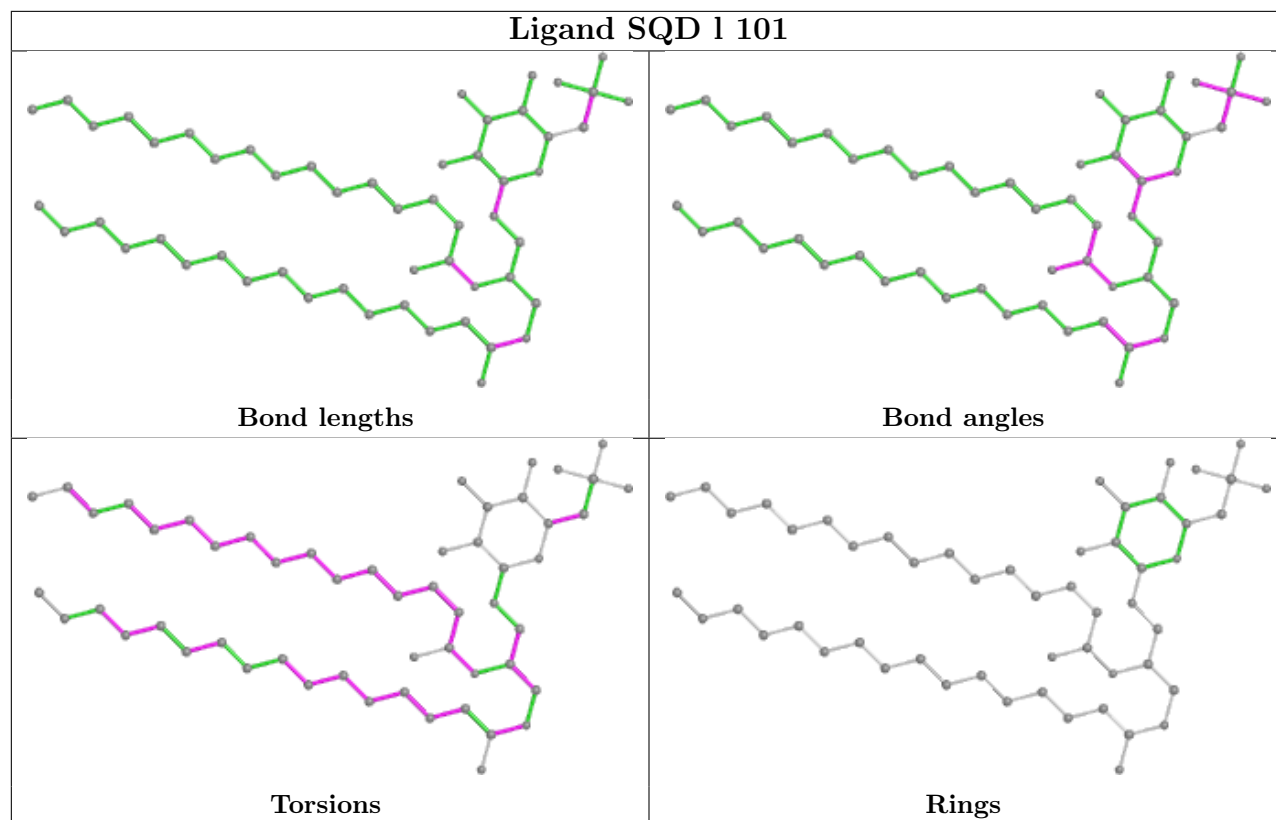
Ligand RRX h 101



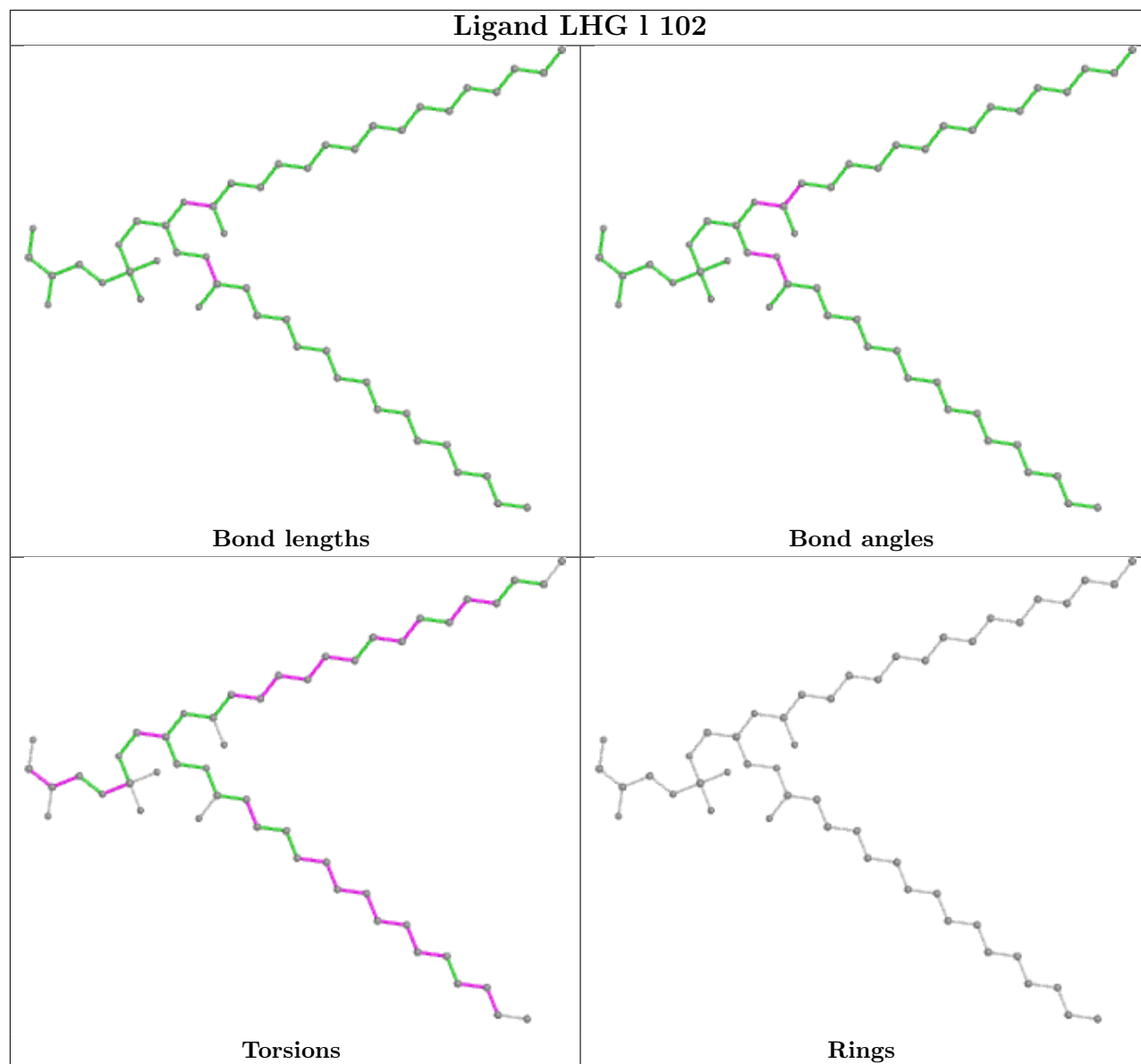
Ligand DGD h 102



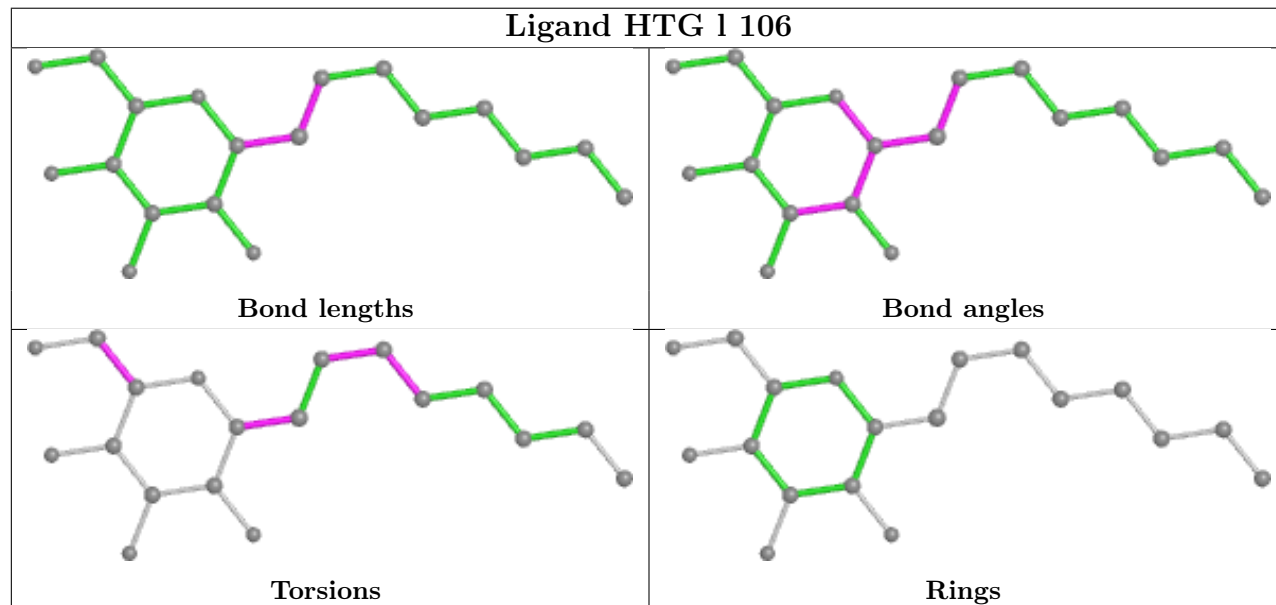




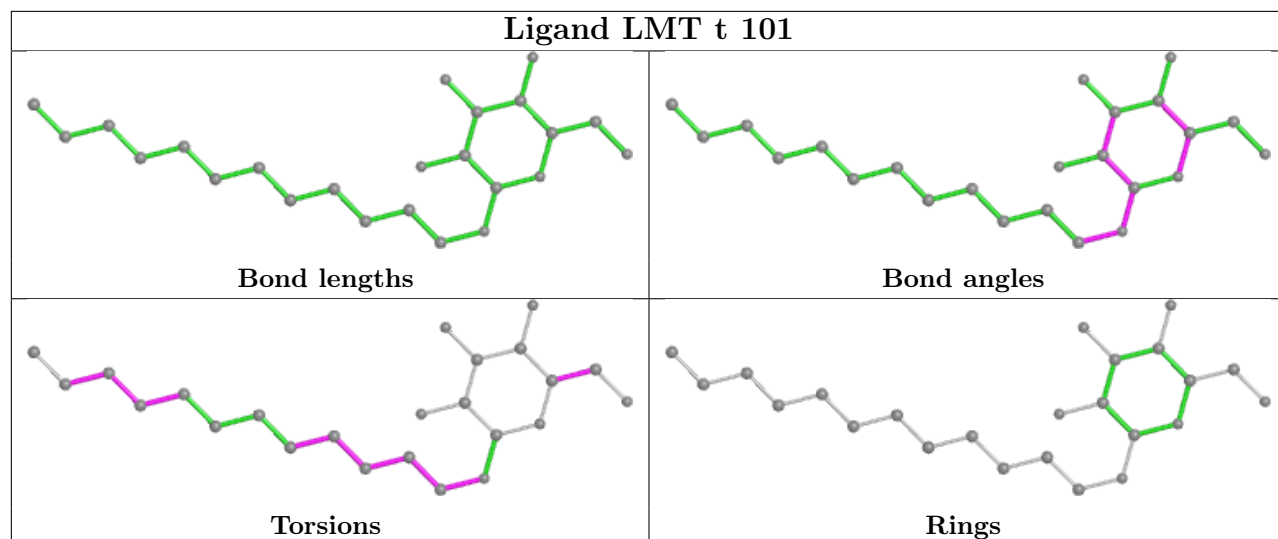
Ligand LHG 1 102



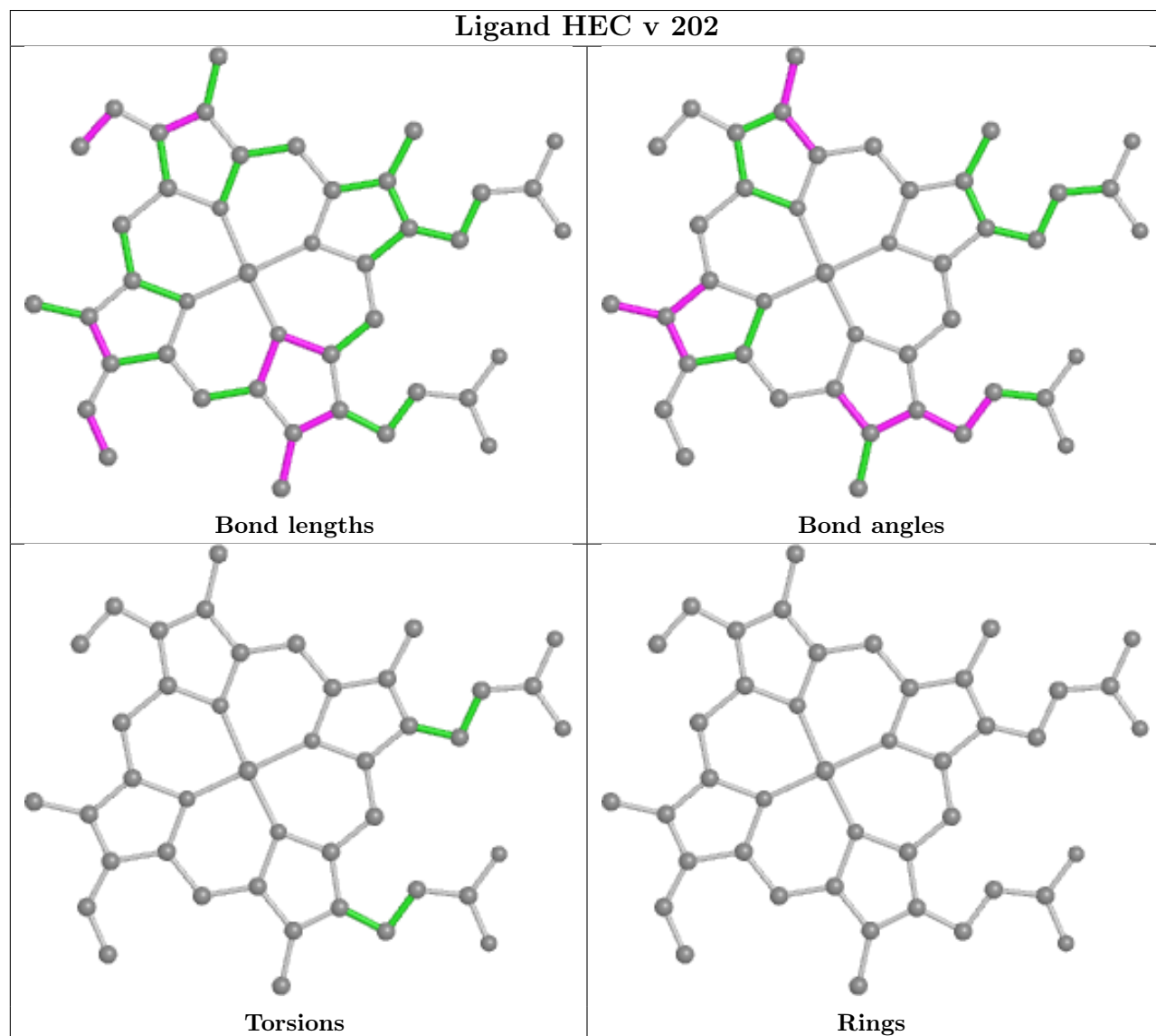
Ligand HTG 1 106

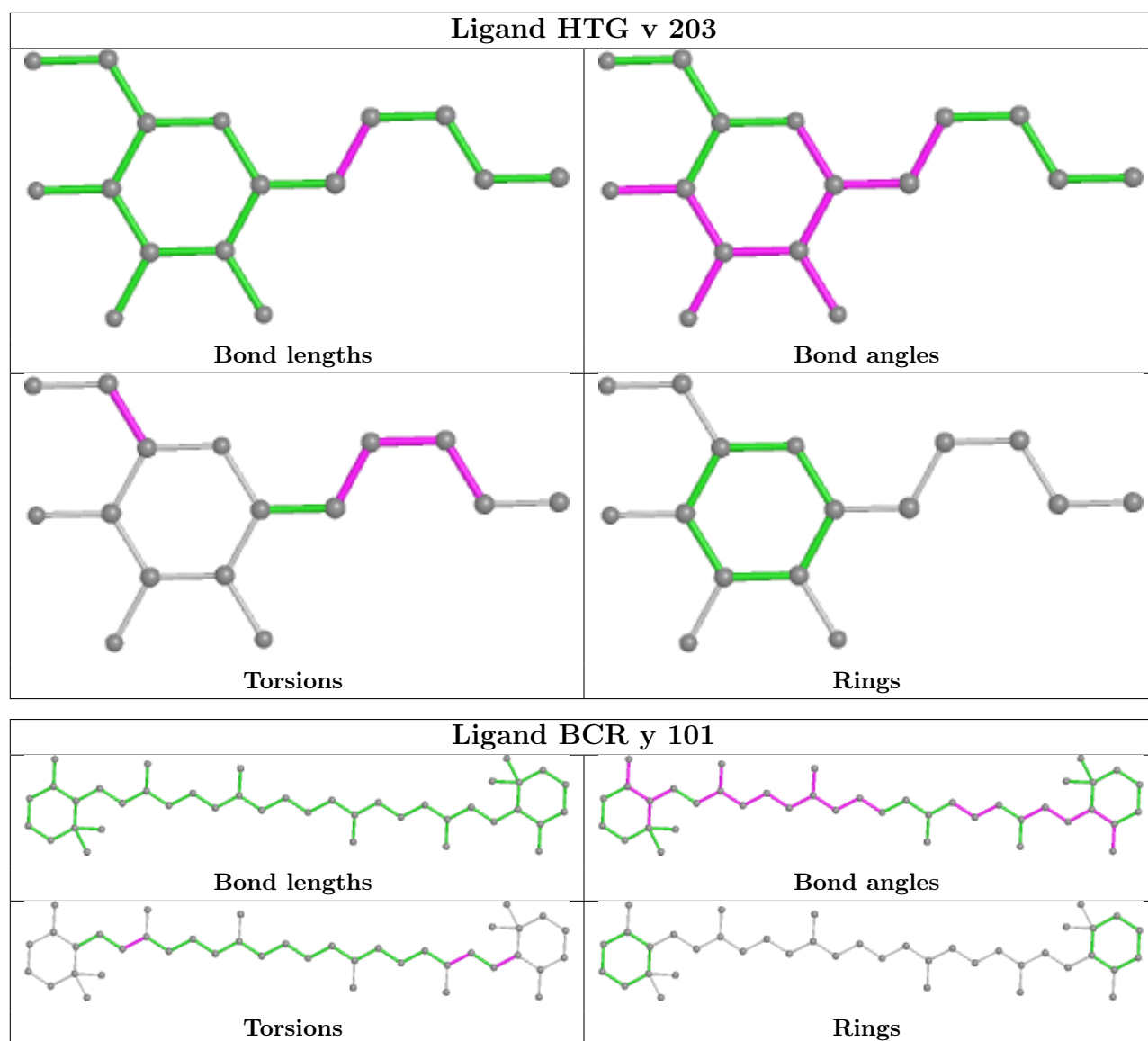


Ligand LMT t 101



Ligand HEC v 202





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/334 (100%)	-0.34	14 (4%) 36 34	21, 28, 66, 87	0
1	a	334/334 (100%)	-0.01	34 (10%) 7 6	22, 30, 96, 135	0
2	B	505/505 (100%)	-0.21	36 (7%) 16 15	22, 33, 67, 109	0
2	b	483/505 (95%)	-0.35	22 (4%) 32 31	24, 35, 57, 124	0
3	C	451/455 (99%)	-0.32	12 (2%) 54 52	24, 37, 55, 106	0
3	c	455/455 (100%)	-0.34	2 (0%) 92 91	27, 41, 57, 89	0
4	D	342/342 (100%)	-0.52	5 (1%) 73 72	21, 29, 51, 86	0
4	d	341/342 (99%)	-0.25	14 (4%) 37 35	22, 32, 59, 85	0
5	E	79/80 (98%)	0.53	10 (12%) 3 3	30, 53, 77, 89	0
5	e	79/80 (98%)	0.80	12 (15%) 2 1	35, 54, 91, 96	0
6	F	33/33 (100%)	-0.39	4 (12%) 4 3	32, 38, 68, 87	0
6	f	31/33 (93%)	-0.18	1 (3%) 47 45	34, 42, 62, 95	0
7	H	63/63 (100%)	-0.33	1 (1%) 72 70	32, 42, 52, 104	0
7	h	62/63 (98%)	0.27	8 (12%) 3 3	34, 48, 62, 74	0
8	I	34/36 (94%)	-0.50	1 (2%) 51 49	33, 42, 60, 78	0
8	i	35/36 (97%)	-0.64	0 100 100	34, 43, 71, 95	0
9	J	36/40 (90%)	-0.52	2 (5%) 24 23	29, 46, 73, 82	0
9	j	40/40 (100%)	0.08	6 (15%) 2 2	34, 47, 81, 92	0
10	K	37/37 (100%)	-0.43	0 100 100	36, 44, 55, 70	0
10	k	37/37 (100%)	-0.19	1 (2%) 54 52	39, 47, 68, 81	0
11	L	35/35 (100%)	-0.14	7 (20%) 1 1	23, 32, 66, 78	0
11	l	35/35 (100%)	-0.15	4 (11%) 5 4	25, 35, 75, 92	0
12	O	243/243 (100%)	-0.27	8 (3%) 46 44	23, 39, 69, 104	0
12	o	243/243 (100%)	-0.29	15 (6%) 20 19	24, 42, 71, 102	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	T	29/30 (96%)	-0.60	0 100 100	26, 32, 59, 89	0
13	t	29/30 (96%)	-0.51	2 (6%) 17 15	27, 34, 66, 98	0
14	U	97/97 (100%)	-0.19	0 100 100	26, 36, 58, 89	0
14	u	97/97 (100%)	-0.66	0 100 100	28, 37, 51, 76	0
15	V	137/137 (100%)	-0.63	0 100 100	25, 34, 50, 70	0
15	v	137/137 (100%)	-0.22	3 (2%) 62 59	29, 44, 61, 84	0
16	Y	29/29 (100%)	0.45	4 (13%) 3 2	40, 54, 69, 81	0
16	y	29/29 (100%)	0.52	4 (13%) 3 2	51, 62, 70, 74	0
17	X	37/37 (100%)	0.21	4 (10%) 6 4	41, 50, 72, 83	0
17	x	36/37 (97%)	0.94	8 (22%) 0 0	41, 54, 88, 89	0
18	Z	62/62 (100%)	0.41	13 (20%) 1 0	42, 54, 88, 106	0
18	z	61/62 (98%)	0.90	13 (21%) 1 0	49, 64, 98, 102	0
All	All	5147/5190 (99%)	-0.23	270 (5%) 27 26	21, 37, 70, 135	0

All (270) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	z	3	ILE	7.2
2	B	486	LEU	6.5
1	a	235	TYR	6.4
1	a	228	THR	6.3
2	B	488	PRO	6.2
17	x	2	THR	6.2
1	a	229	GLU	6.1
1	A	230	THR	5.9
18	z	4	LEU	5.8
3	C	24	THR	5.8
1	A	246	TYR	5.7
1	a	230	THR	5.7
2	b	484	PRO	5.6
18	z	2	THR	5.5
1	a	260	PHE	5.4
2	b	483	ASP	5.4
2	B	2	GLY	5.3
7	H	64	ALA	5.2
2	B	485	GLU	5.1
1	a	227	THR	5.0
1	a	225	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
1	a	11	ALA	5.0
18	Z	33	TRP	5.0
2	B	484	PRO	4.9
2	B	496	TYR	4.9
2	B	479	PHE	4.8
1	A	245	THR	4.8
18	Z	32	ASP	4.7
18	z	60	PHE	4.6
12	o	36	GLN	4.6
2	B	495	PHE	4.5
2	b	480	SER	4.5
12	o	132	ASN	4.5
18	z	1	MET	4.5
1	A	11	ALA	4.4
18	z	5	PHE	4.4
2	B	503	THR	4.3
2	b	482	ILE	4.3
1	a	245	THR	4.3
1	a	256	GLY	4.3
2	B	483	ASP	4.2
18	z	61	VAL	4.2
12	o	134	THR	4.1
12	o	246	ALA	4.1
6	F	15	ILE	4.1
1	a	224	ILE	4.1
2	B	487	SER	4.1
2	b	293	ALA	4.0
4	d	27	PHE	4.0
12	o	38	TYR	4.0
9	j	1	MET	3.9
1	a	242	GLU	3.9
15	v	16	GLY	3.9
1	a	246	TYR	3.9
3	c	143	TYR	3.9
1	a	259	ILE	3.8
2	B	506	ARG	3.8
18	z	6	GLN	3.8
18	Z	3	ILE	3.8
2	b	481	GLY	3.7
6	F	16	PHE	3.7
1	a	237	TYR	3.7
5	E	21	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
11	L	5	PRO	3.7
2	B	501	ASP	3.7
13	t	29	ILE	3.6
5	E	83	LEU	3.6
1	a	262	TYR	3.6
9	j	4	GLU	3.6
17	x	37	VAL	3.6
1	a	226	GLU	3.6
7	h	22	ALA	3.6
12	o	133	VAL	3.6
2	B	293	ALA	3.5
16	y	22	LEU	3.5
1	a	263	ALA	3.5
9	J	5	GLY	3.4
1	a	231	GLU	3.4
18	Z	36	SER	3.4
13	t	30	THR	3.4
1	a	236	GLY	3.3
2	b	126	PRO	3.3
11	L	9	PRO	3.3
18	Z	30	PRO	3.3
2	b	295	GLY	3.3
5	e	72	ALA	3.3
3	C	257	PHE	3.3
1	A	228	THR	3.3
6	F	13	TYR	3.3
17	x	34	ILE	3.3
1	A	249	VAL	3.3
12	o	35	SER	3.3
1	a	261	GLN	3.2
1	a	250	ALA	3.2
11	l	9	PRO	3.2
10	k	18	PHE	3.2
6	F	14	PRO	3.2
11	L	7	ARG	3.2
2	B	489	GLU	3.2
2	B	161[A]	LEU	3.2
5	E	25	ILE	3.1
5	e	10	PHE	3.1
1	a	232	SER	3.1
1	A	229	GLU	3.1
2	B	504	THR	3.1

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Mol	Chain	Res	Type	RSRZ
17	x	3	ILE	3.1
5	e	21	VAL	3.1
1	a	240	GLY	3.1
4	D	240	ALA	3.1
5	e	20	TRP	3.1
2	B	295	GLY	3.1
4	D	12	ARG	3.0
4	d	238	THR	3.0
5	E	79	PHE	3.0
2	B	480	SER	3.0
2	B	494	GLY	3.0
2	b	129	GLY	3.0
4	d	237	PRO	3.0
2	b	218	LEU	3.0
4	d	240	ALA	3.0
18	Z	34	ASP	3.0
3	C	145	SER	3.0
3	C	434	ALA	3.0
11	L	8	GLN	2.9
1	A	225	ARG	2.9
1	a	233	ALA	2.9
12	o	32	ILE	2.9
1	A	12	ASN	2.9
5	e	79	PHE	2.9
2	B	502	VAL	2.9
18	Z	31	GLN	2.9
2	b	294	SER	2.9
5	E	17	VAL	2.9
18	Z	29	SER	2.9
4	d	12	ARG	2.9
17	x	29	ILE	2.8
5	E	10	PHE	2.8
17	X	38	GLN	2.8
4	d	236	ASN	2.8
9	j	3	SER	2.8
7	h	23	PRO	2.8
4	D	238	THR	2.8
1	a	252	HIS	2.8
3	C	25	ASN	2.8
1	a	255	PHE	2.7
12	O	133	VAL	2.7
18	Z	38	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	127	ARG	2.7
5	E	20	TRP	2.7
9	j	2	MET	2.7
12	O	135	SER	2.7
1	A	235	TYR	2.7
4	d	25	ASP	2.7
2	B	505	ARG	2.7
5	e	19	TYR	2.7
3	C	433	LEU	2.7
4	d	287	VAL	2.7
9	j	5	GLY	2.7
2	B	85	GLY	2.6
2	B	162	PHE	2.6
4	d	158	LEU	2.6
18	Z	7	LEU	2.6
17	x	36	LYS	2.6
1	a	264	SER	2.6
16	Y	46	LEU	2.6
17	x	32	SER	2.6
7	h	2	ALA	2.6
3	C	255	THR	2.6
11	L	3	PRO	2.6
17	x	30	ALA	2.6
12	O	130	GLN	2.6
7	h	58	VAL	2.6
4	d	17	ILE	2.6
12	o	25	THR	2.5
16	y	20	ALA	2.5
18	Z	35	ARG	2.5
5	e	25	ILE	2.5
11	l	3	PRO	2.5
12	O	60	ARG	2.5
5	E	74	GLN	2.5
1	a	257	ARG	2.5
18	Z	39	LEU	2.5
4	d	159	ILE	2.5
12	O	27	ARG	2.5
17	X	37	VAL	2.4
2	B	490	GLN	2.4
5	e	71	GLU	2.4
1	a	241	GLN	2.4
17	X	34	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
18	z	7	LEU	2.4
11	l	4	ASN	2.4
12	o	33	ASP	2.4
2	B	481	GLY	2.4
7	h	57	GLY	2.4
16	Y	18	VAL	2.4
17	X	2	THR	2.4
12	o	37	THR	2.4
2	b	291	SER	2.4
18	z	8	ALA	2.3
3	c	200	THR	2.3
2	b	251	VAL	2.3
1	A	236	GLY	2.3
3	C	261	ARG	2.3
5	E	78	THR	2.3
2	B	250	PHE	2.3
11	L	10	VAL	2.3
2	B	246	PHE	2.3
5	E	82	GLN	2.3
4	D	237	PRO	2.3
16	Y	19	ILE	2.3
16	y	37	PHE	2.3
3	C	23	ALA	2.3
3	C	256	PRO	2.2
1	A	243	GLU	2.2
3	C	144	SER	2.2
4	d	234	ALA	2.2
2	b	250	PHE	2.2
18	z	33	TRP	2.2
2	B	290	ALA	2.2
2	b	2	GLY	2.2
7	h	24	GLY	2.2
1	a	14	TRP	2.2
4	d	150	ILE	2.2
12	O	132	ASN	2.2
2	b	298	LEU	2.2
1	a	238	LYS	2.2
12	O	131	PRO	2.2
12	o	245	PRO	2.2
12	o	135	SER	2.2
1	a	234	ASN	2.2
2	b	456	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
12	o	34	SER	2.2
15	v	15	GLU	2.2
2	B	248	ALA	2.1
18	Z	26	ALA	2.1
6	f	15	ILE	2.1
7	h	63	LYS	2.1
7	h	56	ASP	2.1
18	z	9	LEU	2.1
2	B	244	ALA	2.1
2	B	251	VAL	2.1
1	A	247	ASN	2.1
12	O	136	ILE	2.1
2	b	125	ASP	2.1
12	o	24	ASP	2.1
1	a	249	VAL	2.1
2	B	249	ALA	2.1
2	B	459	ALA	2.1
5	e	17	VAL	2.1
5	e	59	GLU	2.1
11	L	4	ASN	2.1
9	J	6	GLY	2.1
16	y	41	VAL	2.1
9	j	6	GLY	2.1
2	B	126	PRO	2.1
5	e	61	ARG	2.1
16	Y	43	ARG	2.1
1	A	266	ASN	2.1
3	C	201	ASN	2.1
4	d	228	GLY	2.1
15	v	14	SER	2.1
4	D	11	GLU	2.0
2	b	292	LEU	2.0
2	b	246	PHE	2.0
2	B	292	LEU	2.0
5	e	14	ILE	2.0
11	l	8	GLN	2.0
2	b	478	VAL	2.0
18	z	38	GLN	2.0
8	I	34	ARG	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
13	FME	T	1	10/11	0.95	0.19	38,42,72,75	0
8	FME	I	1	10/11	0.95	0.14	33,37,40,41	0
8	FME	i	1	10/11	0.97	0.11	36,41,45,48	0
13	FME	t	1	10/11	0.97	0.09	33,38,80,91	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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
31	DMS	O	305	4/4	0.54	0.23	68,70,79,99	0
31	DMS	c	942	4/4	0.55	0.23	101,103,111,117	0
30	UNL	I	105	16/-	0.56	0.36	70,82,88,90	0
29	LMT	f	102	25/35	0.57	0.45	61,93,105,108	0
30	UNL	i	105	10/-	0.58	0.33	67,78,86,87	0
34	HTG	B	627	19/19	0.59	0.32	51,104,113,116	0
34	HTG	b	627	19/19	0.60	0.25	50,92,108,109	0
34	HTG	b	632	19/19	0.61	0.27	56,74,91,92	0
25	LMG	b	622	43/55	0.63	0.28	48,78,88,98	0
31	DMS	d	414	4/4	0.64	0.37	102,112,113,120	0
30	UNL	u	201	11/-	0.65	0.27	47,53,69,69	0
35	DGD	d	406	43/66	0.66	0.32	58,85,139,146	0
31	DMS	a	401	4/4	0.66	0.29	75,84,85,104	0
30	UNL	a	417	10/-	0.66	0.41	75,80,84,87	0
34	HTG	D	414	19/19	0.66	0.31	63,103,114,115	0
25	LMG	B	621	40/55	0.67	0.24	47,82,108,112	0
31	DMS	C	537	4/4	0.68	0.37	88,103,104,113	0
34	HTG	D	415	19/19	0.68	0.28	39,69,80,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	UNL	t	102	16/-	0.68	0.32	59,71,78,80	0
34	HTG	C	532	19/19	0.69	0.27	69,98,111,112	0
30	UNL	i	104	16/-	0.69	0.34	67,76,87,89	0
25	LMG	D	412	46/55	0.69	0.25	41,68,138,142	0
29	LMT	c	931	24/35	0.69	0.26	50,84,95,98	0
29	LMT	T	102	24/35	0.70	0.23	42,80,98,101	0
31	DMS	c	936	4/4	0.70	0.26	106,116,116,124	0
28	SQD	l	101	54/54	0.70	0.25	53,82,119,123	0
29	LMT	A	414	35/35	0.71	0.35	59,86,109,114	0
29	LMT	Z	101	35/35	0.71	0.36	40,105,123,128	0
35	DGD	D	407	50/66	0.71	0.29	60,87,120,123	0
27	LHG	a	416	49/49	0.71	0.28	60,84,100,108	0
31	DMS	c	937	4/4	0.72	0.17	80,90,91,100	0
25	LMG	C	531	40/55	0.72	0.24	37,81,103,107	0
30	UNL	a	420	6/-	0.73	0.35	56,59,60,60	0
25	LMG	c	930	49/55	0.73	0.20	44,78,96,106	0
30	UNL	I	103	13/-	0.73	0.23	53,57,77,82	0
29	LMT	a	419	35/35	0.73	0.27	46,69,93,100	0
30	UNL	T	101	13/-	0.74	0.34	63,71,77,79	0
27	LHG	A	412	31/49	0.74	0.27	66,83,107,117	0
31	DMS	B	634	4/4	0.74	0.25	57,68,73,95	0
31	DMS	B	639	4/4	0.74	0.41	72,87,90,102	0
30	UNL	Z	102	9/-	0.75	0.30	57,71,79,81	0
26	PL9	a	415	55/55	0.76	0.28	64,84,106,111	0
34	HTG	c	922	19/19	0.76	0.29	70,93,109,112	0
29	LMT	t	101	24/35	0.76	0.19	50,71,109,119	0
31	DMS	C	534	4/4	0.76	0.33	105,111,112,121	0
34	HTG	b	624	19/19	0.78	0.28	69,97,109,110	0
37	RRX	h	101	41/41	0.78	0.21	40,49,75,82	0
26	PL9	A	411	55/55	0.78	0.23	61,73,87,92	0
30	UNL	c	932	10/-	0.79	0.23	56,74,80,83	0
31	DMS	b	636	4/4	0.79	0.25	88,95,109,113	0
31	DMS	L	102	4/4	0.80	0.22	79,80,91,100	0
29	LMT	E	101	24/35	0.80	0.27	61,82,97,113	0
31	DMS	b	637	4/4	0.80	0.18	90,97,101,112	0
31	DMS	l	105	4/4	0.80	0.19	100,103,110,115	0
22	CLA	b	602	65/65	0.81	0.31	49,67,89,98	0
27	LHG	d	401	33/49	0.81	0.16	62,94,138,142	0
29	LMT	I	102	35/35	0.81	0.30	76,88,100,102	0
30	UNL	j	103	16/-	0.81	0.17	59,67,71,74	0
27	LHG	C	522	30/49	0.82	0.16	55,79,127,134	0
30	UNL	U	201	14/-	0.82	0.25	44,57,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	B	618	19/40	0.82	0.18	50,59,74,77	0
25	LMG	A	410	51/55	0.83	0.19	47,62,83,91	0
31	DMS	C	536	4/4	0.83	0.22	77,80,94,95	0
31	DMS	V	211	4/4	0.83	0.23	77,84,85,85	0
34	HTG	l	106	19/19	0.83	0.18	63,97,108,109	0
31	DMS	H	103	4/4	0.83	0.25	63,67,69,74	0
30	UNL	i	103	16/-	0.83	0.20	53,64,79,82	0
31	DMS	v	207	4/4	0.83	0.17	84,93,97,117	0
29	LMT	B	622	24/35	0.84	0.16	57,67,73,78	0
30	UNL	b	628	11/-	0.84	0.32	58,63,78,79	0
29	LMT	c	921	35/35	0.84	0.36	74,90,99,103	0
28	SQD	b	621	38/54	0.84	0.17	58,90,110,112	0
34	HTG	B	626	19/19	0.84	0.20	42,69,81,87	0
34	HTG	v	203	16/19	0.84	0.16	52,69,81,97	0
28	SQD	A	413	49/54	0.84	0.20	46,65,91,95	0
37	RRX	H	101	41/41	0.85	0.16	32,42,58,62	0
25	LMG	c	920	51/55	0.85	0.18	37,61,87,91	0
31	DMS	C	540	4/4	0.85	0.33	82,83,91,97	0
25	LMG	d	409	47/55	0.85	0.18	49,76,113,114	0
30	UNL	I	104	16/-	0.86	0.27	60,71,84,86	0
24	BCR	b	618	20/40	0.86	0.25	57,65,70,71	0
30	UNL	B	624	7/-	0.86	0.17	30,45,51,56	0
31	DMS	O	307	4/4	0.86	0.26	84,97,98,104	0
35	DGD	h	102	62/66	0.86	0.20	28,42,53,58	0
31	DMS	t	105	4/4	0.86	0.18	89,93,101,108	0
31	DMS	B	632	4/4	0.86	0.20	49,57,67,69	0
31	DMS	l	103	4/4	0.87	0.20	91,95,97,99	0
31	DMS	U	203	4/4	0.87	0.24	62,73,74,76	0
25	LMG	C	520	51/55	0.87	0.19	34,60,90,92	0
31	DMS	c	938	4/4	0.87	0.31	86,91,98,103	0
28	SQD	a	418	51/54	0.87	0.15	47,70,91,97	0
31	DMS	t	104	4/4	0.87	0.15	101,101,104,111	0
31	DMS	v	210	4/4	0.87	0.24	63,71,80,91	0
31	DMS	b	638	4/4	0.88	0.24	49,52,54,70	0
31	DMS	a	425	4/4	0.88	0.15	39,47,51,62	0
25	LMG	i	101	51/55	0.88	0.16	45,57,80,81	0
30	UNL	b	625	16/-	0.88	0.13	43,52,64,67	0
30	UNL	D	413	16/-	0.88	0.23	38,46,52,58	0
31	DMS	u	204	4/4	0.88	0.33	50,68,69,75	0
30	UNL	A	415	5/-	0.88	0.35	68,72,73,75	0
31	DMS	u	205	4/4	0.88	0.33	64,67,73,83	0
34	HTG	C	521	19/19	0.88	0.22	55,80,93,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	DMS	f	103	4/4	0.88	0.28	87,89,90,100	0
31	DMS	V	204	4/4	0.88	0.24	66,73,76,76	0
28	SQD	f	101	14/54	0.88	0.22	77,89,96,96	0
28	SQD	D	408	20/54	0.89	0.30	65,97,105,108	0
30	UNL	J	103	16/-	0.89	0.20	44,57,77,77	0
30	UNL	X	101	16/-	0.89	0.13	35,53,62,64	0
30	UNL	x	101	15/-	0.89	0.13	43,50,56,58	0
31	DMS	C	529	4/4	0.89	0.32	72,78,78,86	0
31	DMS	l	104	4/4	0.89	0.16	79,80,86,87	0
31	DMS	c	927	4/4	0.89	0.23	87,89,91,97	0
27	LHG	l	102	49/49	0.89	0.18	38,61,91,95	0
31	DMS	c	929	4/4	0.89	0.32	69,73,76,78	0
31	DMS	u	203	4/4	0.89	0.17	56,68,72,84	0
31	DMS	O	314	4/4	0.89	0.26	78,80,86,91	0
31	DMS	a	421	4/4	0.90	0.26	85,87,87,94	0
31	DMS	c	935	4/4	0.90	0.33	71,78,81,84	0
31	DMS	D	417	4/4	0.90	0.19	72,72,77,86	0
31	DMS	O	308	4/4	0.90	0.19	64,72,73,80	0
31	DMS	V	210	4/4	0.90	0.13	70,73,78,88	0
31	DMS	b	635	4/4	0.90	0.17	62,69,76,86	0
34	HTG	b	626	19/19	0.90	0.13	47,69,86,90	0
31	DMS	v	205	4/4	0.90	0.26	70,72,78,80	0
31	DMS	O	313	4/4	0.90	0.25	89,100,100,107	0
31	DMS	B	631	4/4	0.90	0.27	78,80,84,87	0
27	LHG	a	423	45/49	0.90	0.15	39,58,72,74	0
31	DMS	o	303	4/4	0.90	0.21	60,77,80,83	0
31	DMS	c	943	4/4	0.91	0.16	77,82,87,92	0
35	DGD	H	102	62/66	0.91	0.19	28,37,46,50	0
34	HTG	V	203	14/19	0.91	0.23	48,52,79,84	0
31	DMS	C	535	4/4	0.91	0.38	70,79,83,86	0
31	DMS	V	212	4/4	0.91	0.18	51,54,55,72	0
31	DMS	V	207	4/4	0.91	0.15	64,71,71,76	0
34	HTG	C	523	9/19	0.91	0.22	63,69,81,86	0
24	BCR	y	101	40/40	0.91	0.12	32,41,51,53	0
28	SQD	a	414	54/54	0.91	0.14	36,69,81,87	0
31	DMS	d	415	4/4	0.91	0.15	60,63,67,79	0
31	DMS	C	533	4/4	0.91	0.22	79,84,85,89	0
27	LHG	D	409	49/49	0.91	0.19	38,56,85,97	0
24	BCR	b	619	31/40	0.92	0.15	47,54,63,67	0
31	DMS	A	420	4/4	0.92	0.15	37,39,39,57	0
31	DMS	v	211	4/4	0.92	0.18	65,77,82,90	0
31	DMS	o	308	4/4	0.92	0.26	76,77,82,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	BCR	B	619	30/40	0.92	0.14	44,51,61,63	0
31	DMS	o	305	4/4	0.92	0.36	78,82,86,87	0
22	CLA	B	602	65/65	0.92	0.17	39,56,101,107	0
35	DGD	C	518	62/66	0.92	0.17	29,40,89,109	0
22	CLA	C	514	65/65	0.92	0.15	44,55,83,86	0
30	UNL	i	102	16/-	0.92	0.13	41,51,80,81	0
31	DMS	c	944	4/4	0.92	0.20	79,82,89,92	0
22	CLA	c	913	65/65	0.92	0.14	42,54,96,98	0
31	DMS	B	637	4/4	0.93	0.30	69,76,80,88	0
22	CLA	c	914	65/65	0.93	0.16	47,60,95,108	0
31	DMS	F	101	4/4	0.93	0.20	69,70,74,77	0
24	BCR	k	101	40/40	0.93	0.11	36,45,51,52	0
31	DMS	b	634	4/4	0.93	0.25	68,76,79,86	0
31	DMS	c	940	4/4	0.93	0.30	74,74,75,80	0
22	CLA	B	610	65/65	0.93	0.12	30,37,42,46	0
31	DMS	O	303	4/4	0.93	0.17	68,71,78,79	0
22	CLA	c	912	65/65	0.93	0.10	35,45,50,53	0
31	DMS	U	202	4/4	0.93	0.15	42,49,58,67	0
22	CLA	B	615	53/65	0.93	0.11	31,36,71,84	0
31	DMS	I	101	4/4	0.93	0.23	64,69,74,76	0
24	BCR	c	915	40/40	0.93	0.12	43,59,68,69	0
22	CLA	B	603	65/65	0.93	0.14	27,36,43,47	0
30	UNL	O	301	16/-	0.93	0.13	39,47,73,74	0
22	CLA	b	607	65/65	0.93	0.11	29,37,58,65	0
24	BCR	C	515	40/40	0.94	0.10	37,50,58,59	0
26	PL9	D	406	55/55	0.94	0.12	21,30,37,51	0
31	DMS	d	412	4/4	0.94	0.18	58,59,66,66	0
31	DMS	C	538	4/4	0.94	0.36	79,86,86,87	0
22	CLA	c	904	65/65	0.94	0.21	32,44,50,54	0
30	UNL	d	410	16/-	0.94	0.16	40,49,57,60	0
31	DMS	O	304	4/4	0.94	0.38	74,80,84,88	0
31	DMS	C	539	4/4	0.94	0.24	88,90,93,95	0
22	CLA	c	903	65/65	0.94	0.21	27,34,54,65	0
28	SQD	C	501	54/54	0.94	0.13	32,64,83,89	0
22	CLA	B	607	65/65	0.94	0.10	28,34,56,65	0
22	CLA	b	617	60/65	0.94	0.11	32,41,75,80	0
31	DMS	B	636	4/4	0.94	0.23	60,62,67,69	0
31	DMS	B	630	4/4	0.94	0.15	63,67,68,75	0
31	DMS	B	642	4/4	0.94	0.20	65,66,75,82	0
22	CLA	b	610	65/65	0.94	0.10	32,41,45,54	0
31	DMS	o	304	4/4	0.94	0.17	70,70,70,74	0
27	LHG	L	101	40/49	0.94	0.12	37,53,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	DMS	c	928	4/4	0.94	0.17	73,74,74,80	0
27	LHG	d	408	46/49	0.94	0.15	29,41,93,97	0
31	DMS	b	631	4/4	0.94	0.17	68,72,79,80	0
25	LMG	j	101	47/55	0.94	0.11	33,43,69,74	0
31	DMS	v	204	4/4	0.94	0.13	87,88,90,91	0
31	DMS	B	638	4/4	0.94	0.16	81,82,86,93	0
22	CLA	b	616	65/65	0.94	0.10	30,37,53,57	0
22	CLA	b	603	65/65	0.94	0.14	29,36,46,49	0
31	DMS	v	208	4/4	0.94	0.13	88,90,91,94	0
22	CLA	C	507	65/65	0.94	0.12	37,45,85,88	0
24	BCR	b	620	40/40	0.95	0.12	33,39,48,49	0
25	LMG	J	101	45/55	0.95	0.13	28,36,71,79	0
22	CLA	C	502	65/65	0.95	0.13	33,39,52,62	0
31	DMS	c	939	4/4	0.95	0.31	88,92,95,102	0
24	BCR	d	404	40/40	0.95	0.10	27,38,63,66	0
31	DMS	I	106	4/4	0.95	0.29	64,74,78,80	0
31	DMS	o	302	4/4	0.95	0.17	59,64,71,75	0
34	HTG	B	623	19/19	0.95	0.10	41,47,64,66	0
22	CLA	B	608	65/65	0.95	0.12	24,29,64,79	0
22	CLA	D	404	65/65	0.95	0.11	30,37,94,104	0
22	CLA	b	608	65/65	0.95	0.10	27,31,73,74	0
24	BCR	B	620	40/40	0.95	0.10	30,37,49,50	0
24	BCR	C	516	40/40	0.95	0.10	32,39,47,54	0
22	CLA	C	513	56/65	0.95	0.10	37,48,62,65	0
22	CLA	d	403	65/65	0.95	0.11	35,40,85,90	0
22	CLA	c	906	65/65	0.95	0.10	30,40,50,54	0
30	UNL	B	625	16/-	0.95	0.09	40,47,59,59	0
34	HTG	b	623	19/19	0.95	0.10	42,46,54,63	0
22	CLA	B	604	65/65	0.95	0.15	26,30,40,47	0
31	DMS	O	309	4/4	0.95	0.25	61,70,70,74	0
35	DGD	C	519	62/66	0.95	0.15	23,36,76,85	0
31	DMS	t	103	4/4	0.95	0.13	89,102,103,103	0
22	CLA	c	908	65/65	0.95	0.10	34,39,53,61	0
31	DMS	V	209	4/4	0.95	0.32	76,87,89,93	0
31	DMS	C	528	4/4	0.95	0.28	88,89,90,90	0
31	DMS	B	635	4/4	0.95	0.18	61,63,66,73	0
33	CA	B	601	1/1	0.95	0.04	64,64,64,64	0
31	DMS	C	530	4/4	0.95	0.32	71,79,82,83	0
35	DGD	C	517	62/66	0.95	0.13	24,35,80,88	0
22	CLA	c	907	65/65	0.95	0.12	39,47,102,108	0
22	CLA	C	510	65/65	0.95	0.16	31,36,59,64	0
35	DGD	c	918	62/66	0.95	0.15	34,42,98,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	DMS	B	641	4/4	0.95	0.10	46,49,61,66	0
22	CLA	b	615	52/65	0.95	0.10	36,42,71,76	0
24	BCR	D	405	40/40	0.95	0.12	26,35,62,66	0
31	DMS	A	416	4/4	0.95	0.12	60,67,69,72	0
22	CLA	C	512	65/65	0.95	0.09	31,39,48,51	0
31	DMS	O	311	4/4	0.95	0.13	48,56,59,61	0
31	DMS	i	106	4/4	0.95	0.22	72,76,79,89	0
31	DMS	V	205	4/4	0.95	0.16	64,66,67,71	0
22	CLA	C	505	65/65	0.96	0.17	28,34,58,60	0
31	DMS	c	941	4/4	0.96	0.24	73,79,87,88	0
22	CLA	C	508	65/65	0.96	0.10	32,42,55,59	0
31	DMS	c	933	4/4	0.96	0.10	57,64,66,70	0
22	CLA	C	504	65/65	0.96	0.13	29,37,42,51	0
22	CLA	b	611	65/65	0.96	0.11	28,35,40,43	0
26	PL9	d	405	55/55	0.96	0.11	23,32,39,43	0
31	DMS	V	201	4/4	0.96	0.19	46,48,54,58	0
22	CLA	C	506	65/65	0.96	0.14	30,37,50,54	0
22	CLA	c	910	65/65	0.96	0.15	28,38,58,64	0
33	CA	O	302	1/1	0.96	0.04	59,59,59,59	0
36	HEM	E	102	43/43	0.96	0.15	48,56,62,65	0
22	CLA	c	909	65/65	0.96	0.14	31,37,80,97	0
32	BCT	a	422	4/4	0.96	0.07	51,52,56,57	0
31	DMS	b	630	4/4	0.96	0.15	56,63,63,64	0
35	DGD	c	917	62/66	0.96	0.14	26,42,81,94	0
31	DMS	B	629	4/4	0.96	0.16	48,52,58,65	0
27	LHG	D	411	45/49	0.96	0.13	31,39,90,94	0
22	CLA	C	509	65/65	0.96	0.14	29,35,81,102	0
22	CLA	b	613	65/65	0.96	0.14	26,32,37,40	0
22	CLA	B	611	65/65	0.96	0.17	26,33,41,46	0
22	CLA	c	902	65/65	0.96	0.11	34,39,50,51	0
24	BCR	c	916	40/40	0.96	0.10	33,42,48,49	0
27	LHG	d	407	49/49	0.96	0.11	28,36,56,63	0
22	CLA	B	612	65/65	0.96	0.13	23,29,55,60	0
35	DGD	c	919	62/66	0.96	0.12	29,40,73,79	0
22	CLA	c	905	65/65	0.96	0.18	30,35,62,66	0
22	CLA	b	612	65/65	0.96	0.12	27,31,72,83	0
23	PHO	a	411	64/64	0.96	0.14	26,33,40,48	0
22	CLA	a	412	65/65	0.96	0.11	27,32,102,116	0
31	DMS	B	640	4/4	0.96	0.30	47,53,57,63	0
31	DMS	C	527	4/4	0.96	0.17	74,80,80,81	0
24	BCR	Y	101	39/40	0.96	0.09	34,40,48,50	0
31	DMS	u	202	4/4	0.96	0.15	47,53,55,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	C	503	65/65	0.96	0.17	28,32,47,56	0
31	DMS	V	206	4/4	0.96	0.09	45,48,51,62	0
22	CLA	b	609	65/65	0.96	0.14	27,34,42,45	0
31	DMS	o	306	4/4	0.96	0.21	66,71,74,83	0
31	DMS	a	424	4/4	0.96	0.15	38,47,50,65	0
24	BCR	K	101	40/40	0.96	0.10	31,39,43,43	0
22	CLA	B	613	65/65	0.96	0.15	24,30,37,40	0
31	DMS	A	417	4/4	0.96	0.15	76,82,83,85	0
22	CLA	B	617	55/65	0.96	0.08	28,35,72,76	0
24	BCR	a	413	40/40	0.96	0.09	26,31,38,39	0
22	CLA	A	405	65/65	0.97	0.11	18,23,36,54	0
22	CLA	b	606	65/65	0.97	0.14	24,28,40,40	0
38	MG	k	102	1/1	0.97	0.05	48,48,48,48	0
31	DMS	A	419	4/4	0.97	0.21	58,60,70,72	0
22	CLA	B	609	65/65	0.97	0.17	25,30,38,39	0
31	DMS	v	209	4/4	0.97	0.25	72,74,76,81	0
22	CLA	b	605	65/65	0.97	0.17	23,29,63,65	0
31	DMS	O	310	4/4	0.97	0.14	66,68,68,73	0
22	CLA	D	403	65/65	0.97	0.12	18,24,45,52	0
31	DMS	v	201	4/4	0.97	0.13	42,48,50,51	0
23	PHO	a	410	64/64	0.97	0.13	21,28,32,36	0
31	DMS	b	633	4/4	0.97	0.09	68,68,70,78	0
31	DMS	b	629	4/4	0.97	0.14	29,31,36,45	0
31	DMS	V	208	4/4	0.97	0.10	73,74,77,78	0
31	DMS	O	312	4/4	0.97	0.18	37,51,56,59	0
22	CLA	B	616	65/65	0.97	0.11	30,36,50,57	0
22	CLA	c	911	65/65	0.97	0.20	29,38,46,52	0
31	DMS	c	925	4/4	0.97	0.13	51,58,60,61	0
31	DMS	v	206	4/4	0.97	0.21	69,72,72,77	0
22	CLA	b	614	59/65	0.97	0.14	26,32,76,82	0
23	PHO	D	402	64/64	0.97	0.14	25,29,35,39	0
22	CLA	b	604	65/65	0.97	0.16	26,32,45,50	0
23	PHO	A	407	64/64	0.97	0.13	20,25,30,32	0
22	CLA	C	511	65/65	0.97	0.20	31,36,41,46	0
22	CLA	B	605	65/65	0.97	0.18	24,28,60,66	0
38	MG	K	102	1/1	0.97	0.06	51,51,51,51	0
22	CLA	a	409	61/65	0.97	0.15	25,29,80,87	0
31	DMS	c	926	4/4	0.97	0.17	63,64,67,68	0
27	LHG	D	410	49/49	0.97	0.12	29,36,51,61	0
22	CLA	A	408	65/65	0.97	0.11	19,29,99,110	0
24	BCR	A	409	40/40	0.97	0.12	25,30,37,38	0
22	CLA	B	614	61/65	0.97	0.14	25,31,70,83	0

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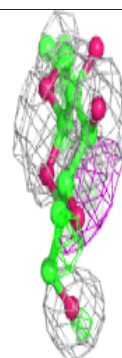
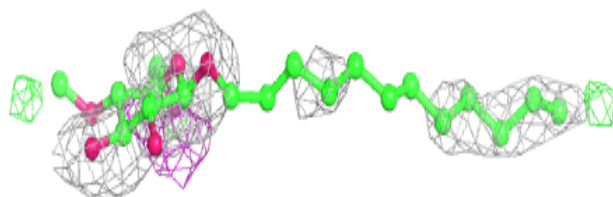
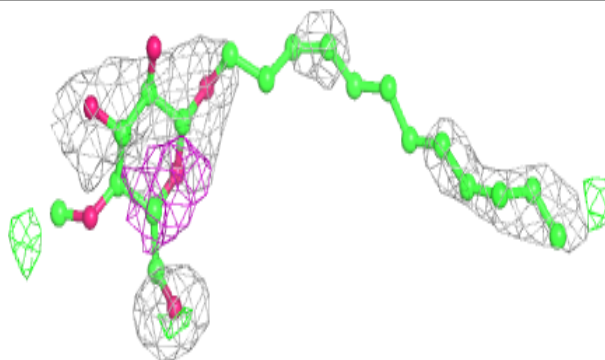
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
22	CLA	B	606	65/65	0.97	0.14	24,30,42,46	0
39	HEC	V	202	43/43	0.98	0.09	23,29,36,40	0
31	DMS	d	413	4/4	0.98	0.19	67,69,73,80	0
22	CLA	a	408	65/65	0.98	0.10	20,26,35,41	0
22	CLA	D	401	65/65	0.98	0.09	19,23,31,36	0
39	HEC	v	202	43/43	0.98	0.08	33,37,42,46	0
31	DMS	O	306	4/4	0.98	0.19	69,69,70,81	0
31	DMS	B	633	4/4	0.98	0.16	65,71,71,73	0
32	BCT	A	421[A]	4/4	0.98	0.08	34,36,39,39	4
22	CLA	d	402	65/65	0.98	0.13	21,27,42,50	0
32	BCT	A	421[B]	4/4	0.98	0.08	27,29,30,34	4
31	DMS	c	924	4/4	0.98	0.14	37,42,47,49	0
31	DMS	D	416	4/4	0.98	0.18	55,59,60,69	0
22	CLA	a	407	65/65	0.98	0.13	23,26,45,61	0
36	HEM	e	101	43/43	0.98	0.17	43,55,85,93	0
22	CLA	A	406	55/65	0.98	0.12	21,27,49,60	0
31	DMS	c	934	4/4	0.98	0.24	64,73,74,77	0
31	DMS	d	411	4/4	0.98	0.13	60,62,64,64	0
21	CL	A	403	1/1	0.99	0.09	29,29,29,29	0
31	DMS	a	402	4/4	0.99	0.10	30,32,34,34	0
21	CL	a	405	1/1	0.99	0.07	31,31,31,31	0
33	CA	o	301	1/1	0.99	0.02	55,55,55,55	0
31	DMS	B	628	4/4	0.99	0.14	27,29,32,38	0
31	DMS	C	525	4/4	0.99	0.06	34,35,38,40	0
20	FE2	a	404	1/1	0.99	0.07	42,42,42,42	0
33	CA	b	601	1/1	0.99	0.03	59,59,59,59	0
31	DMS	c	923	4/4	0.99	0.15	37,40,42,43	0
31	DMS	C	526	4/4	0.99	0.08	48,48,50,51	0
31	DMS	D	418	4/4	0.99	0.11	35,39,42,43	0
33	CA	c	901	1/1	0.99	0.03	48,48,48,48	0
38	MG	j	102	1/1	0.99	0.11	40,40,40,40	0
21	CL	A	404	1/1	0.99	0.12	28,28,28,28	0
19	OEX	A	401	10/10	0.99	0.12	25,27,31,32	0
38	MG	J	102	1/1	0.99	0.07	30,30,30,30	0
31	DMS	o	307	4/4	0.99	0.30	48,56,62,64	0
31	DMS	A	418	4/4	0.99	0.10	29,30,31,31	0
31	DMS	C	524	4/4	0.99	0.07	38,42,43,43	0
21	CL	a	406	1/1	0.99	0.13	32,32,32,32	0
20	FE2	A	402	1/1	1.00	0.07	39,39,39,39	0
19	OEX	a	403	10/10	1.00	0.09	29,31,32,33	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.

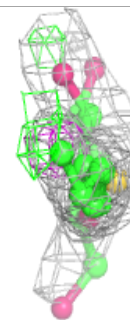
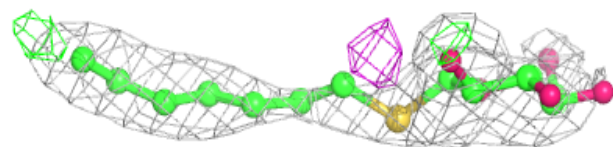
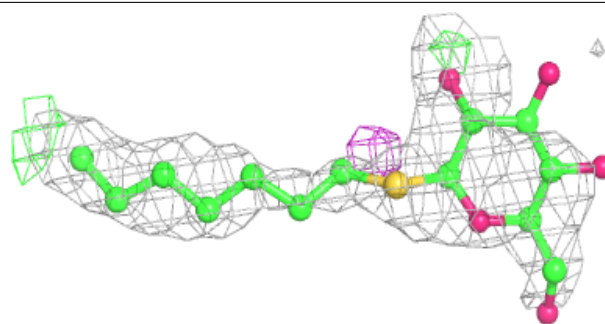
Electron density around LMT f 102:

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



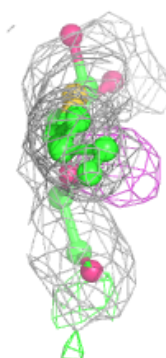
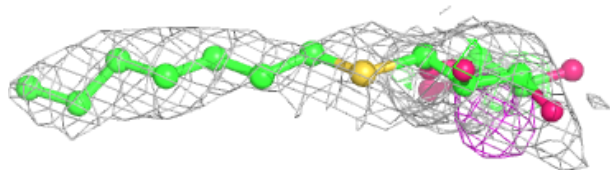
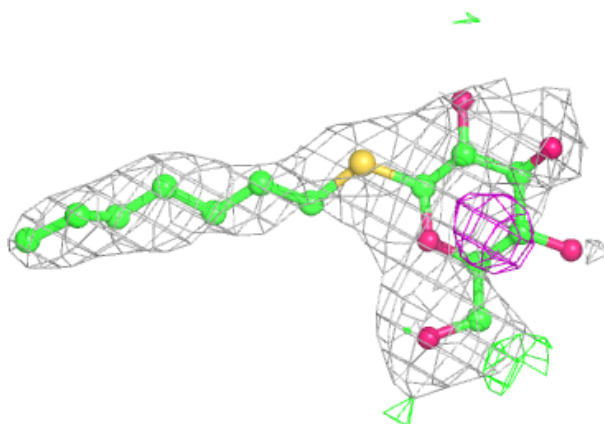
Electron density around HTG B 627:

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

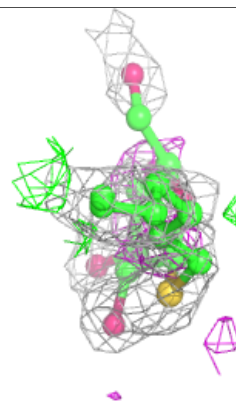
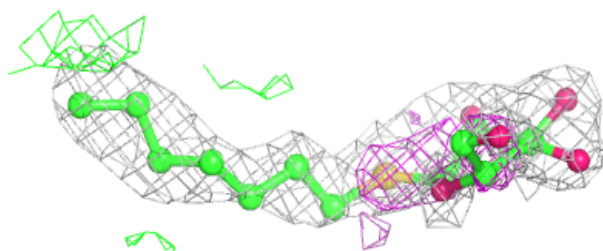
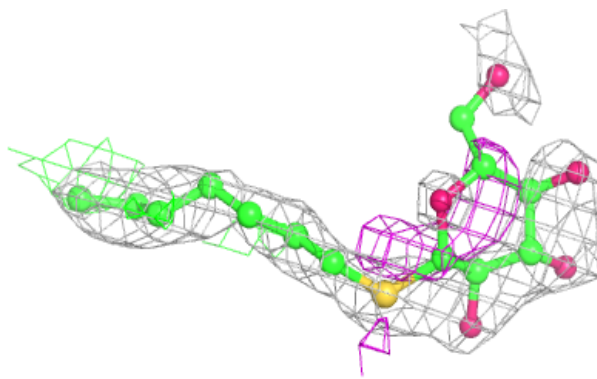


Electron density around HTG b 627:

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

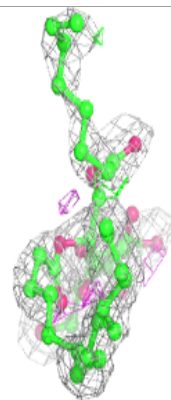
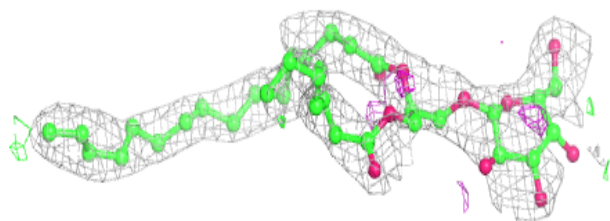
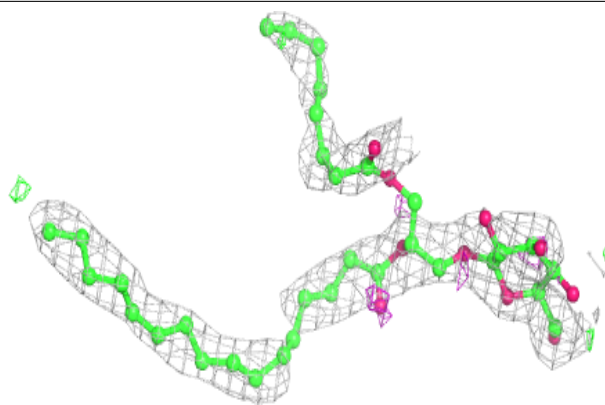
**Electron density around HTG b 632:**

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

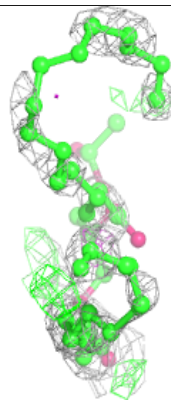
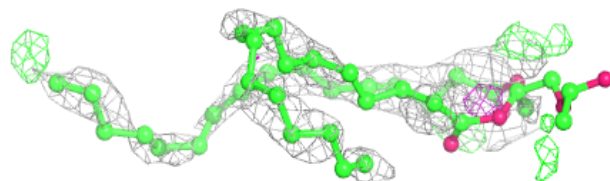
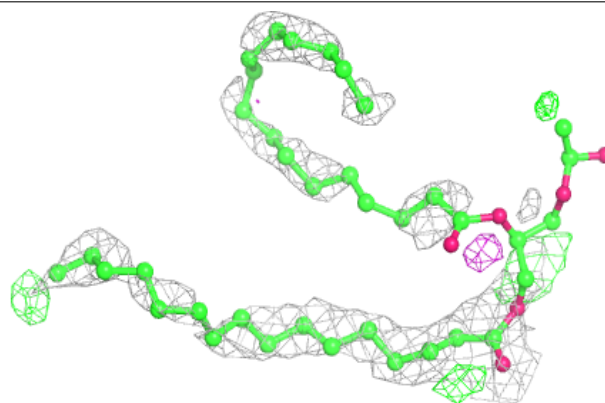


Electron density around LMG b 622:

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

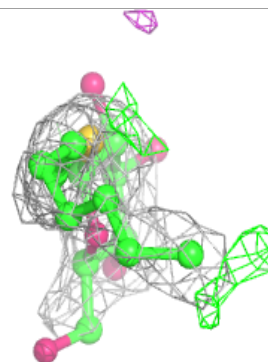
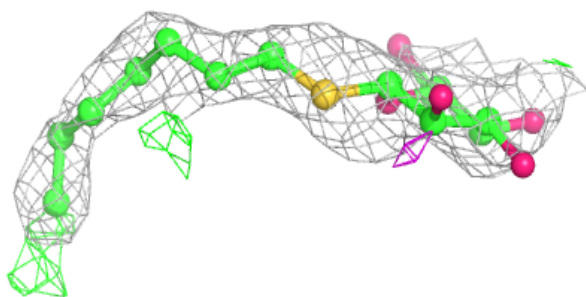
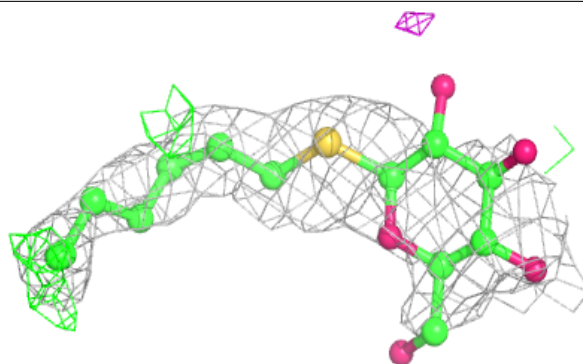
**Electron density around DGD d 406:**

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

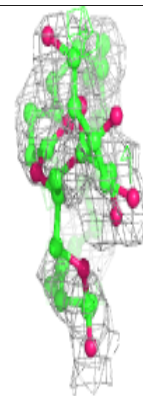
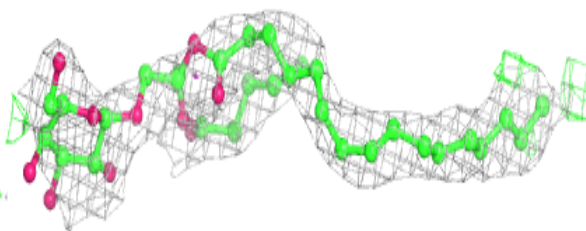
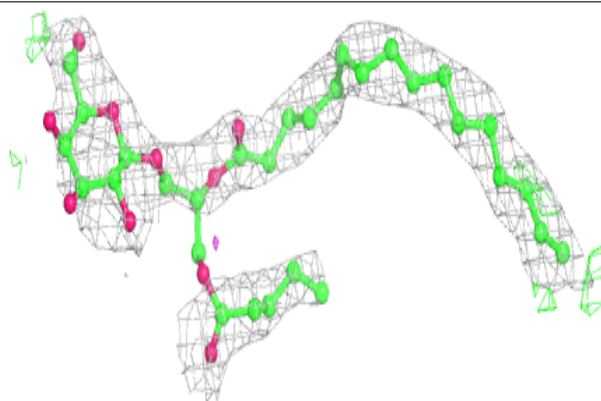


Electron density around HTG D 414:

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

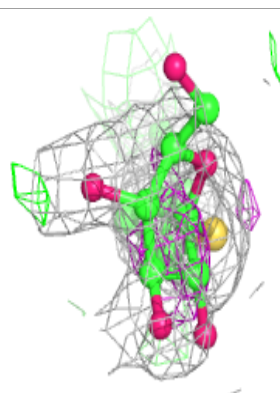
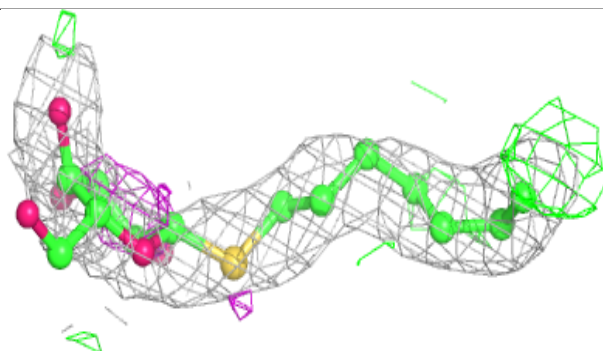
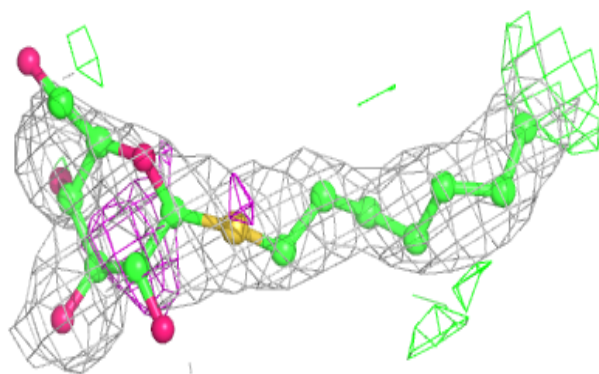
**Electron density around LMG B 621:**

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

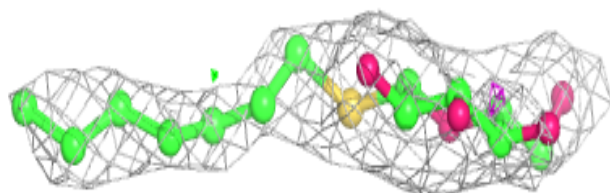
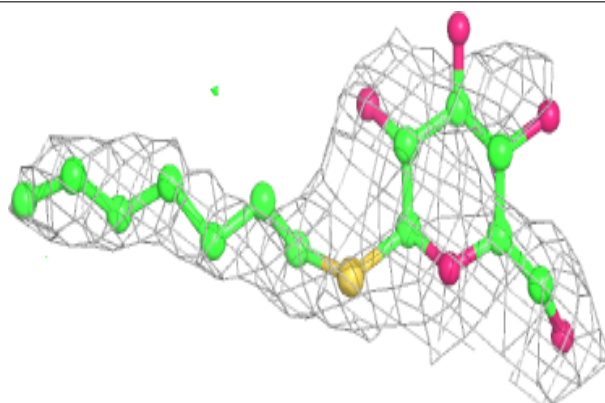


Electron density around HTG D 415:

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

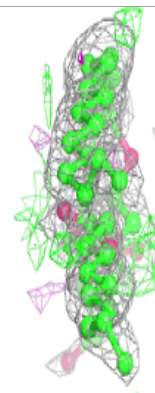
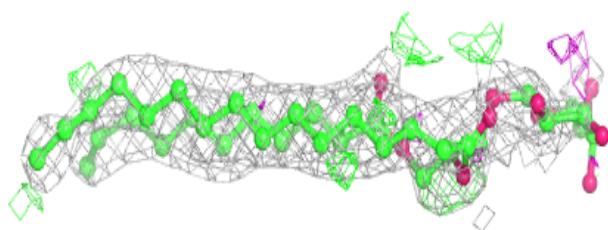
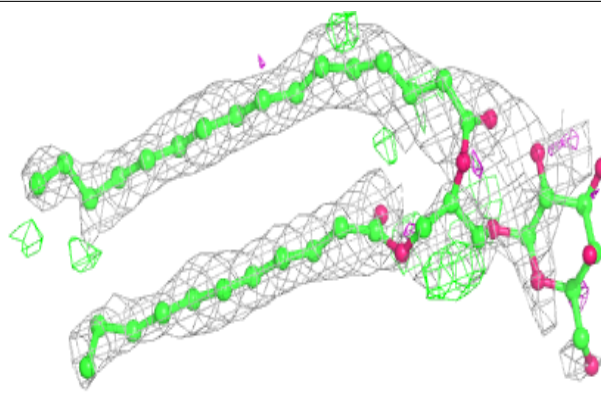
**Electron density around HTG C 532:**

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

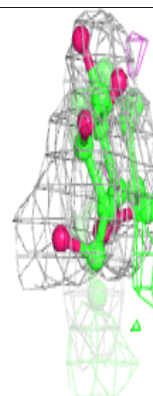
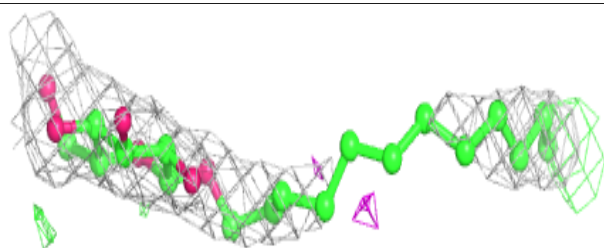
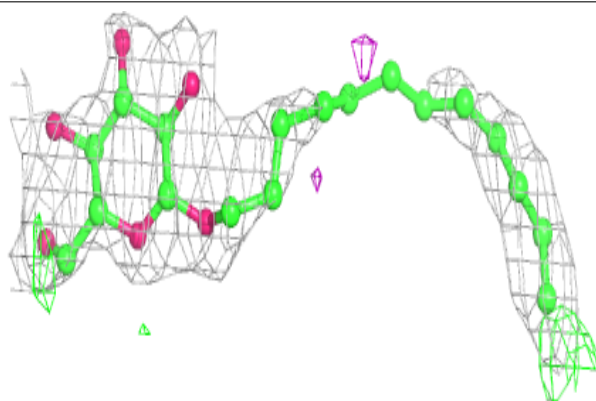


Electron density around LMG D 412:

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

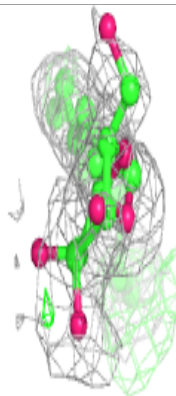
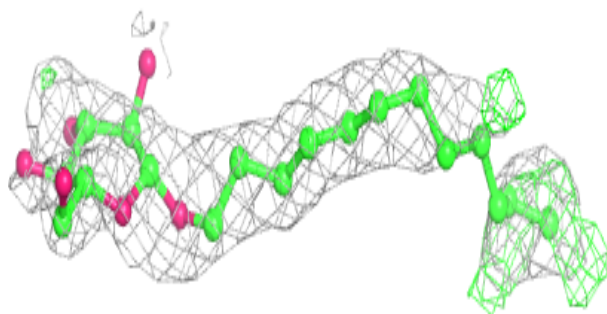
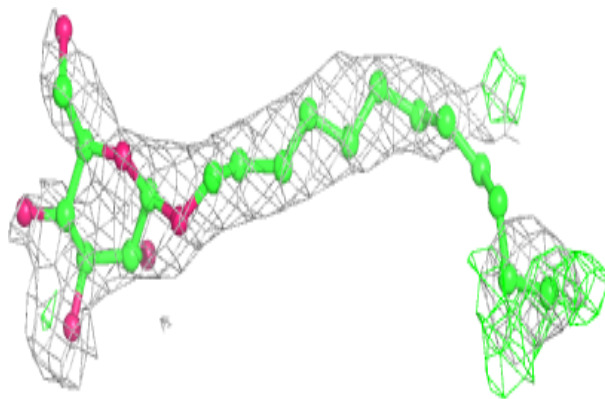
**Electron density around LMT c 931:**

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

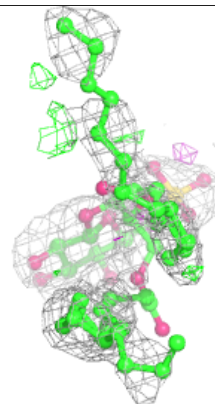
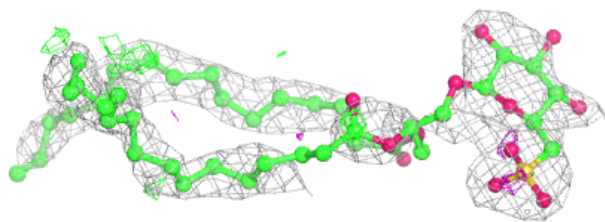
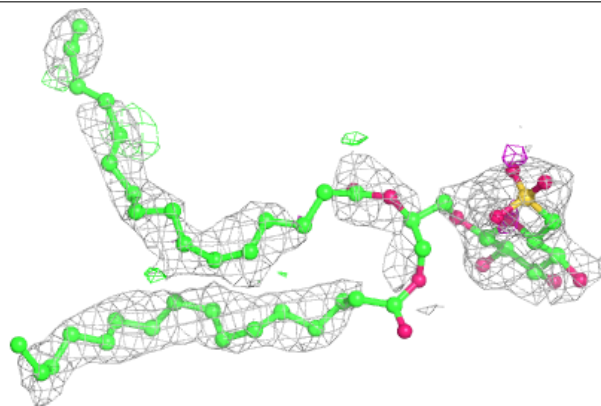


Electron density around LMT T 102:

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

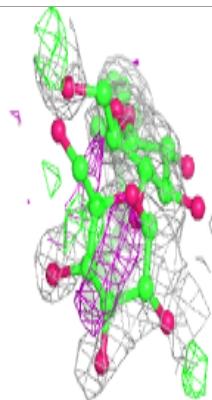
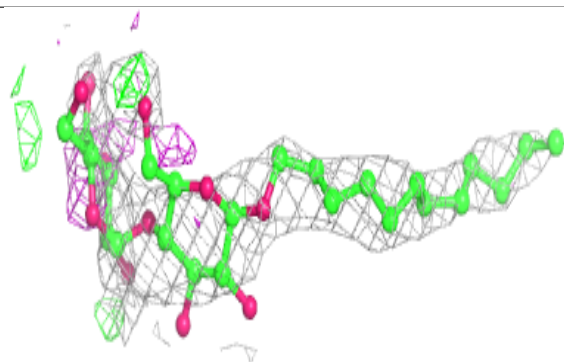
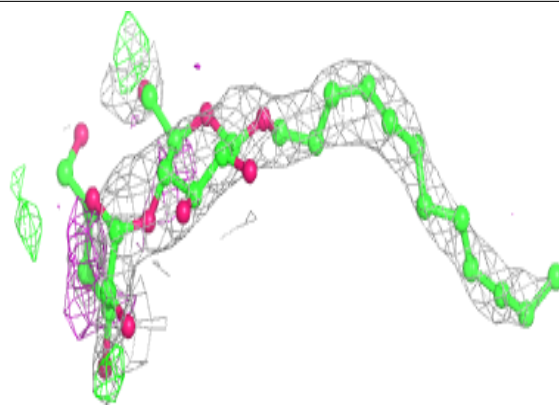
**Electron density around SQD I 101:**

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

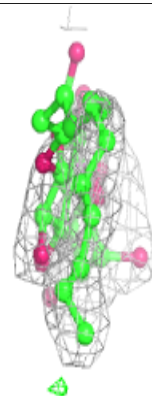
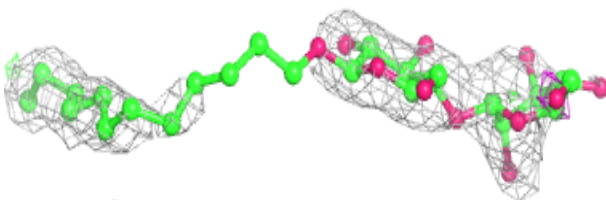
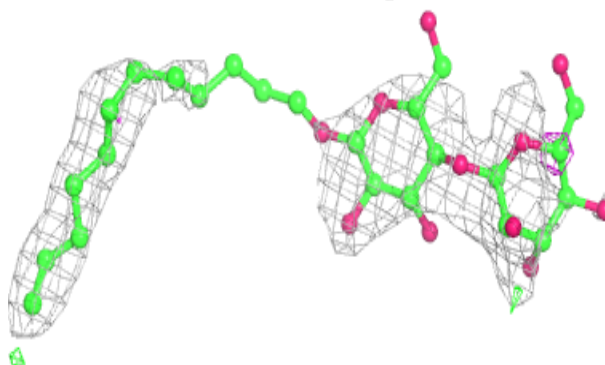


Electron density around LMT A 414:

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

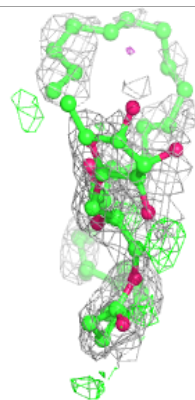
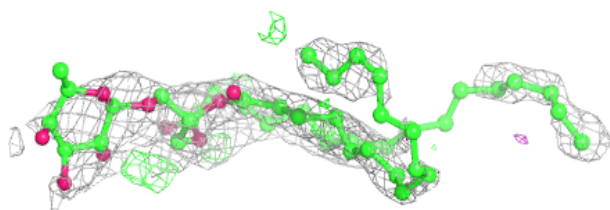
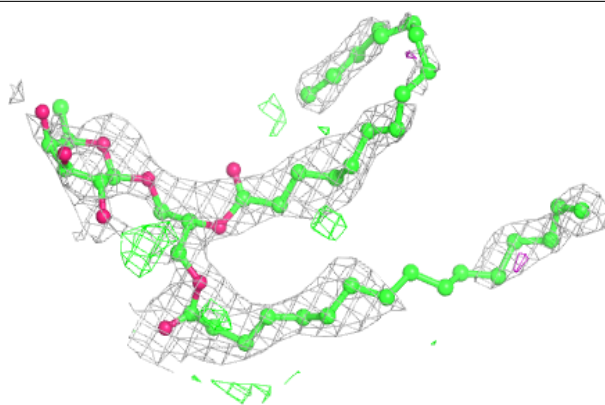
**Electron density around LMT Z 101:**

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

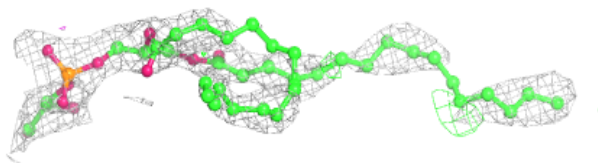
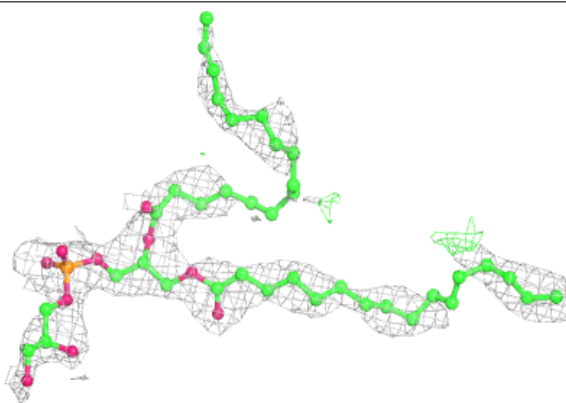


Electron density around DGD D 407:

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

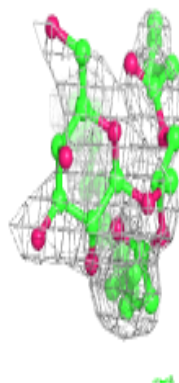
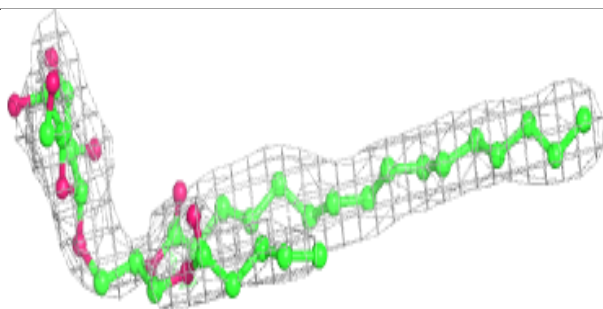
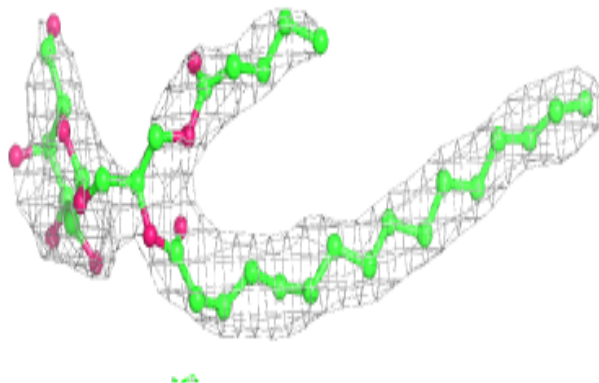
**Electron density around LHG a 416:**

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

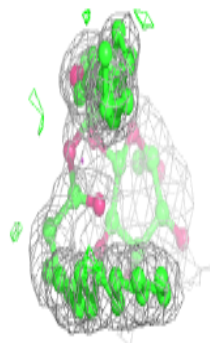
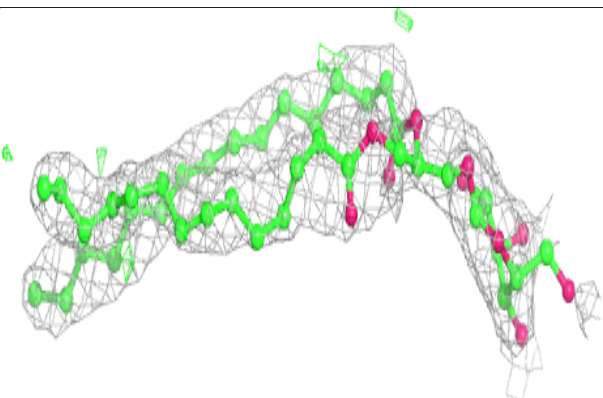
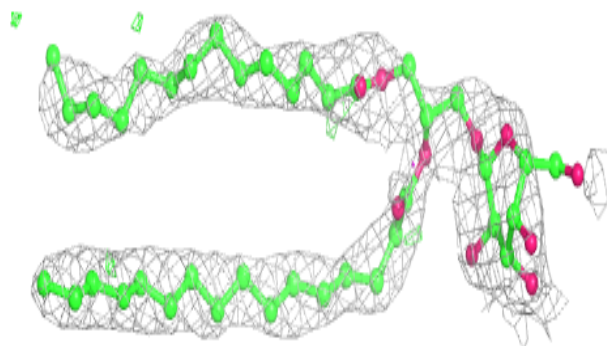


Electron density around LMG C 531:

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

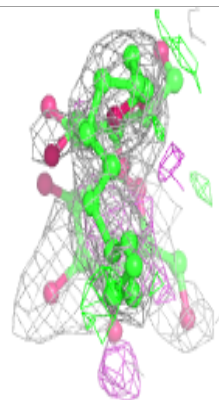
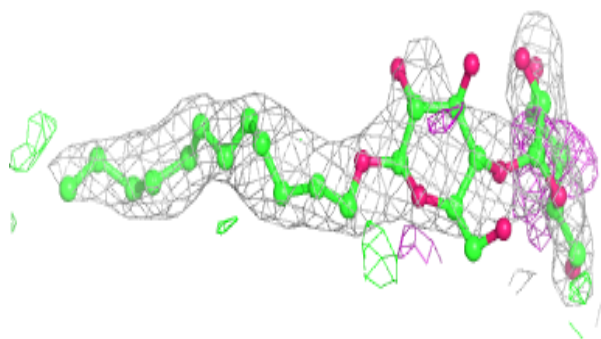
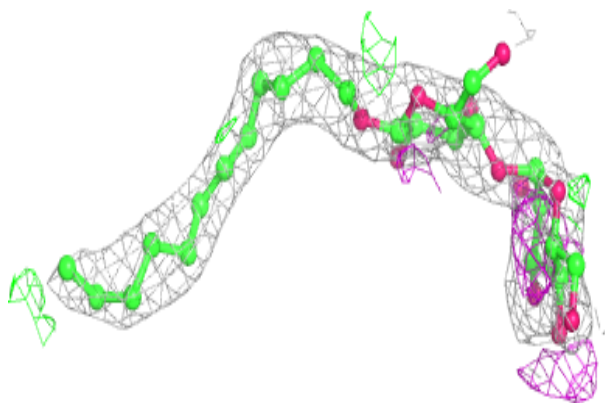
**Electron density around LMG c 930:**

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

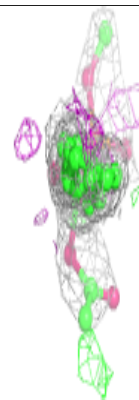
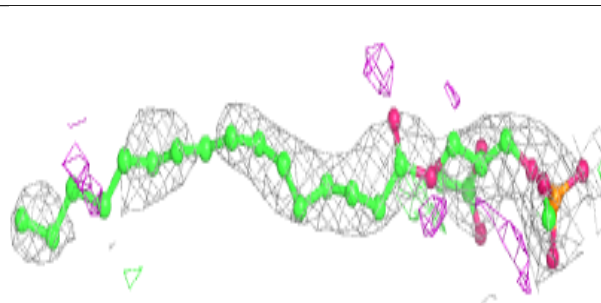
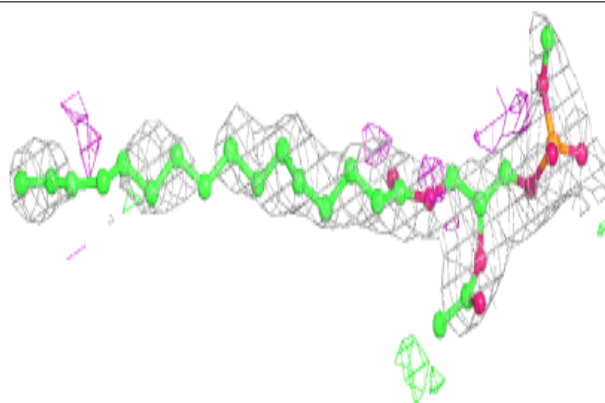


Electron density around LMT a 419:

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

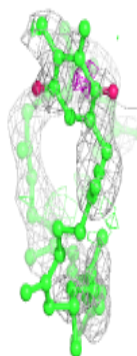
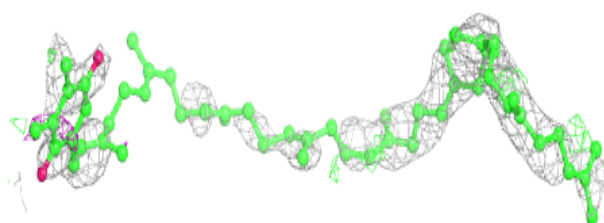
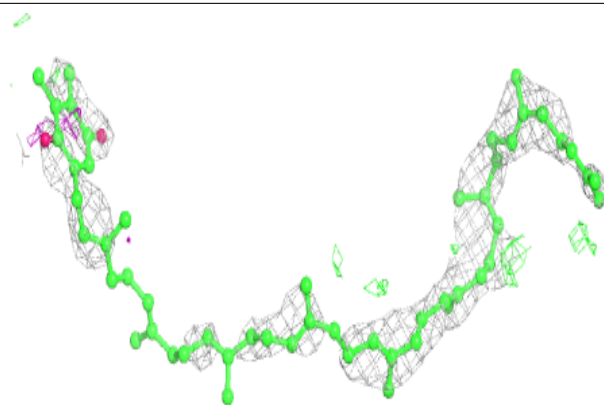
**Electron density around LHG A 412:**

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

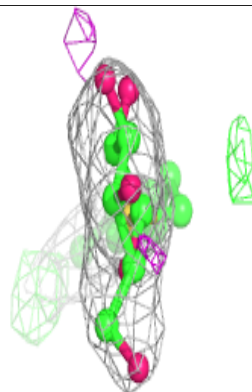
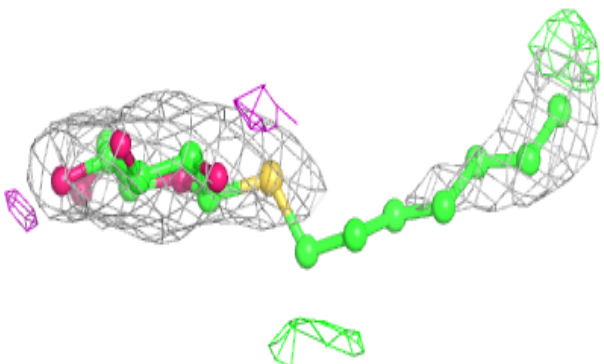
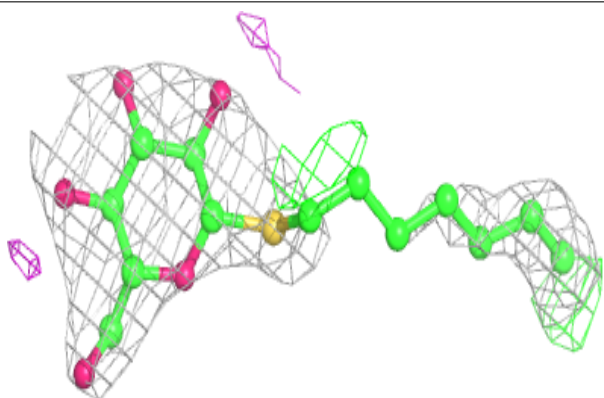


Electron density around PL9 a 415:

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

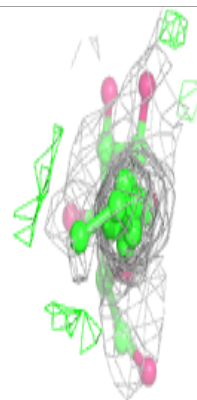
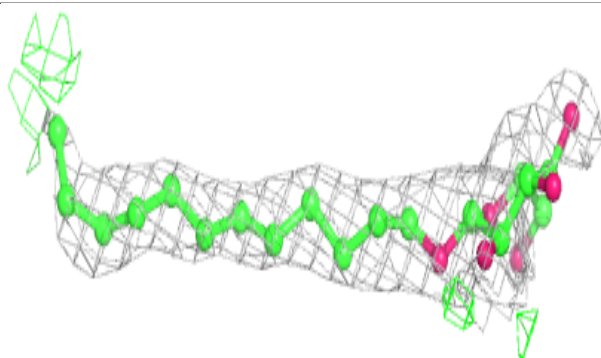
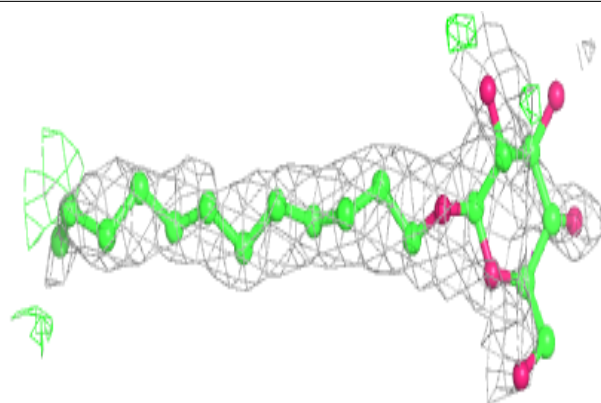
**Electron density around HTG c 922:**

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

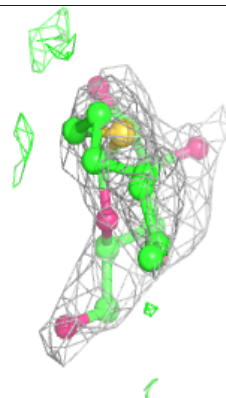
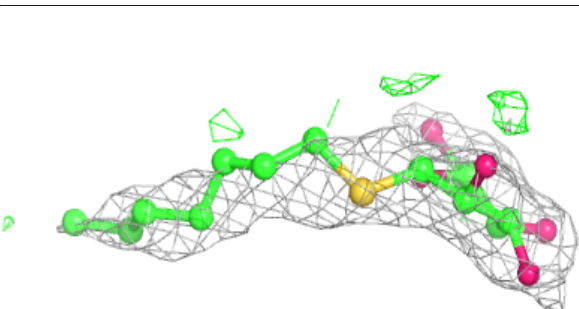
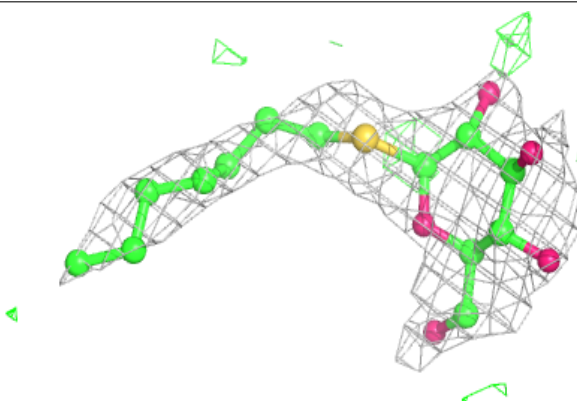


Electron density around LMT t 101:

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

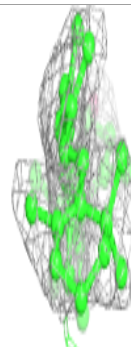
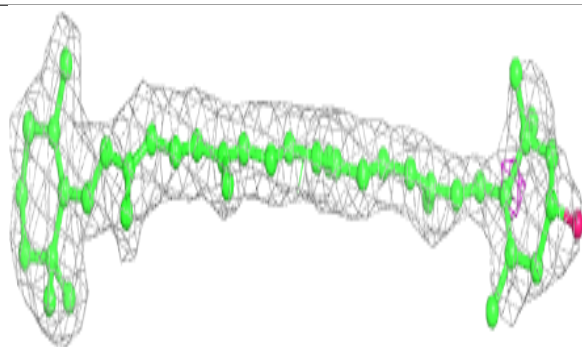
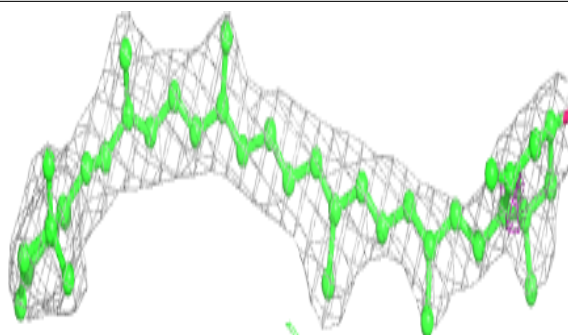
**Electron density around HTG b 624:**

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

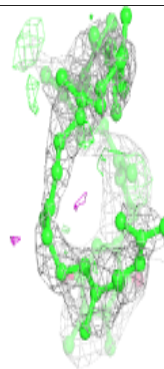
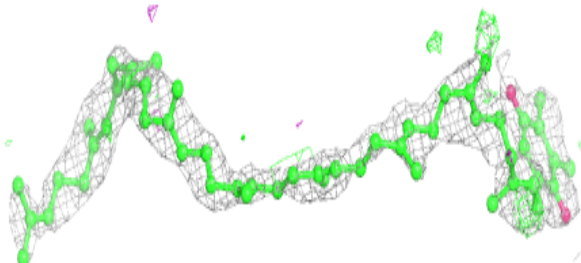
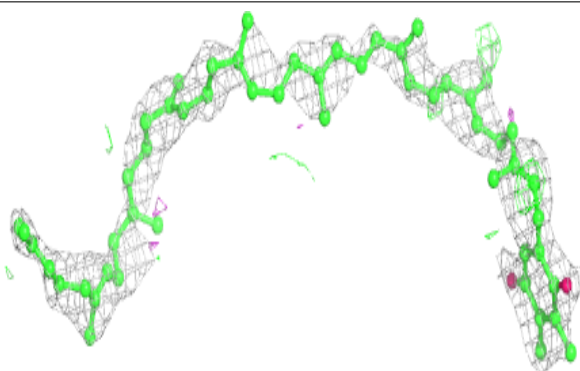


Electron density around RRX h 101:

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

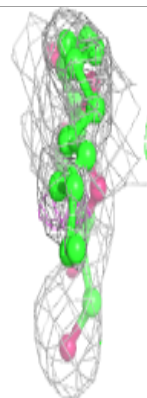
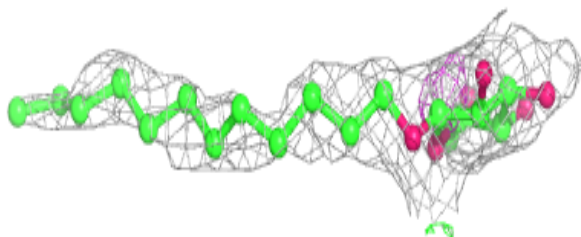
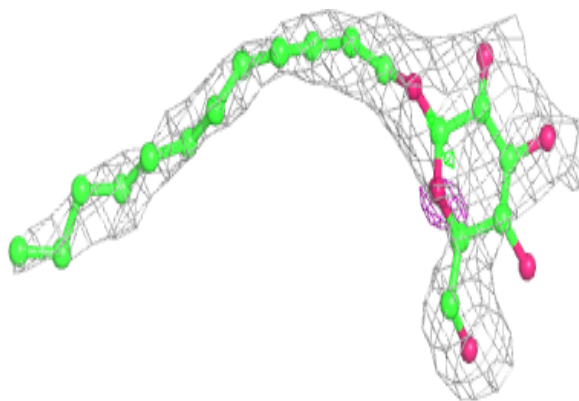
**Electron density around PL9 A 411:**

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

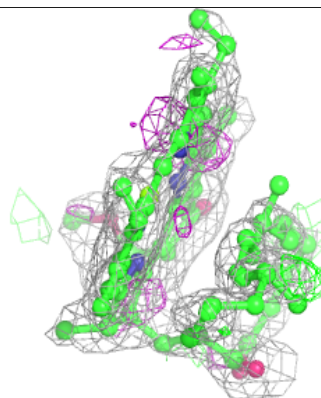
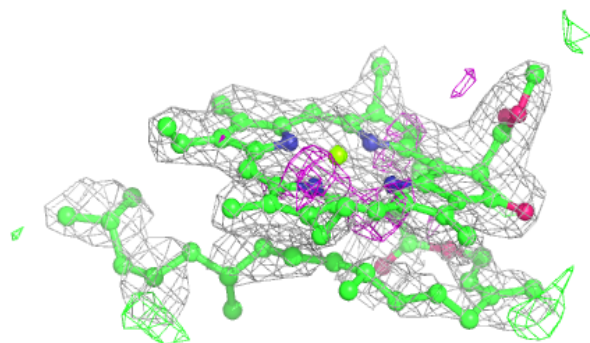
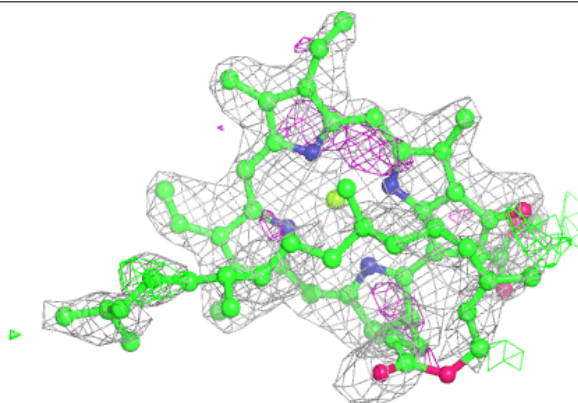


Electron density around LMT E 101:

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

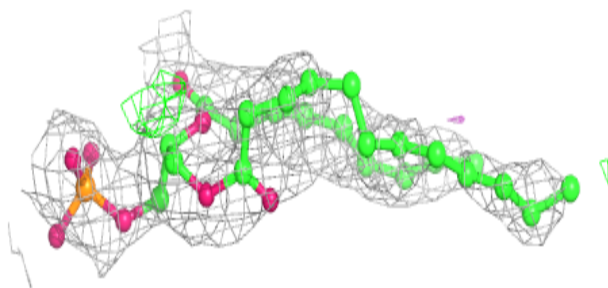
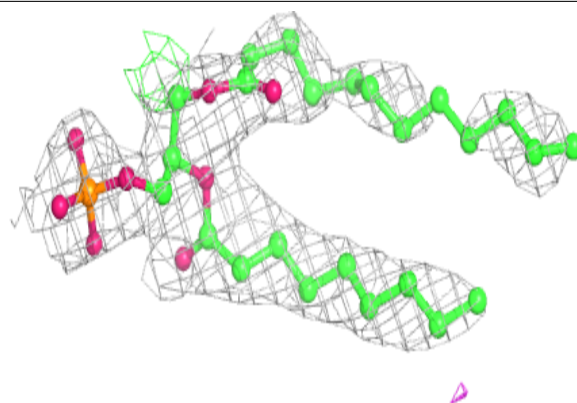
**Electron density around CLA b 602:**

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

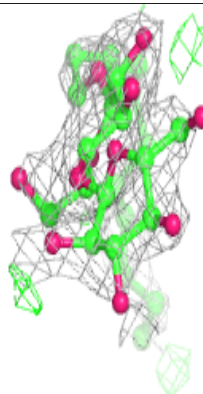
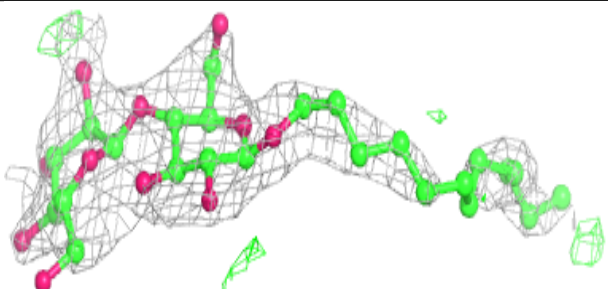
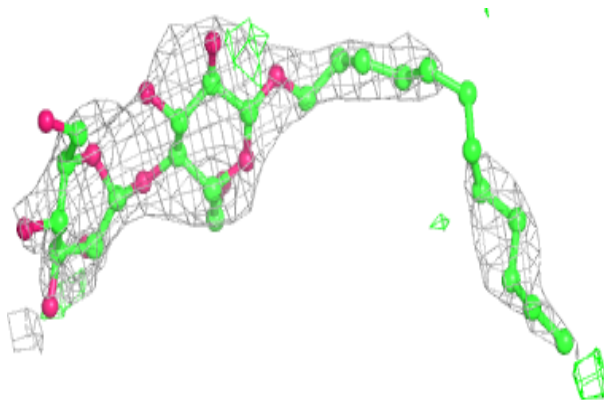


Electron density around LHG d 401:

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

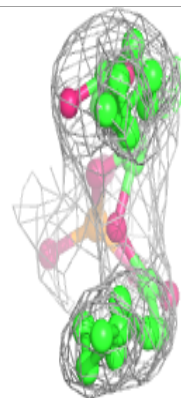
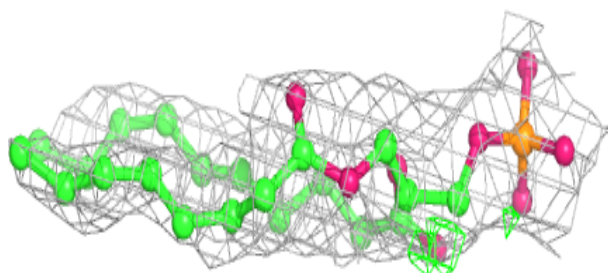
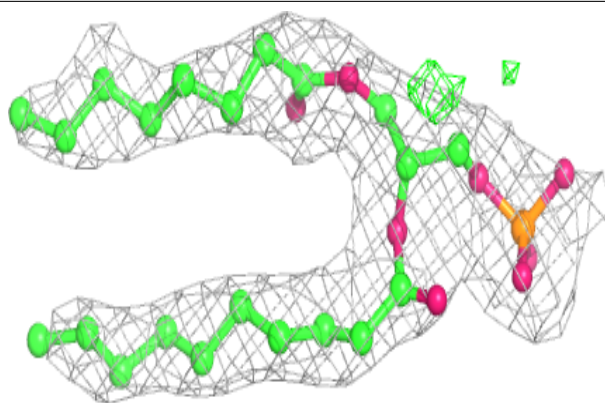
**Electron density around LMT I 102:**

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

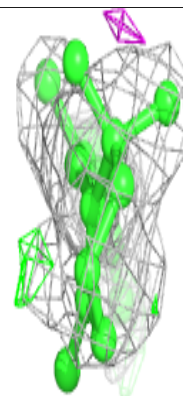
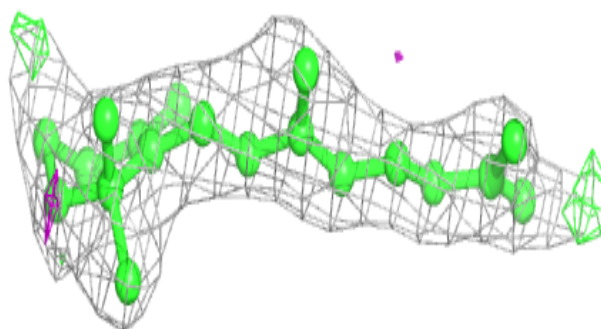
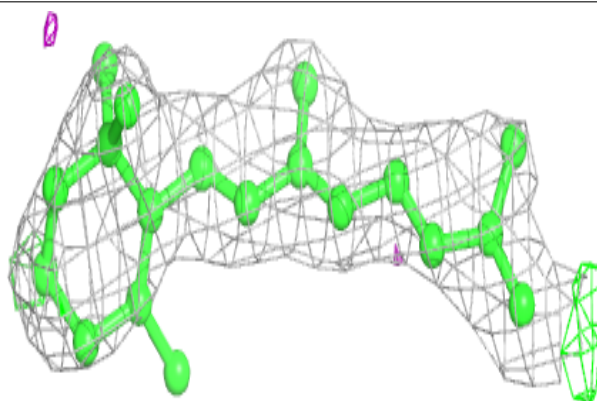


Electron density around LHG C 522:

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

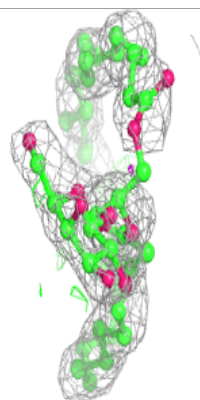
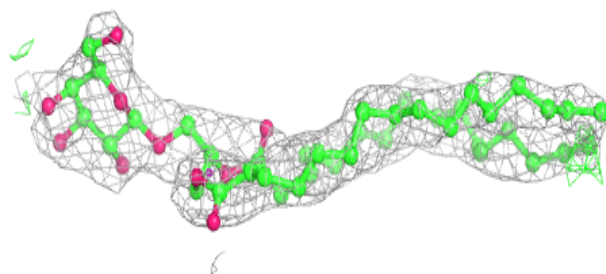
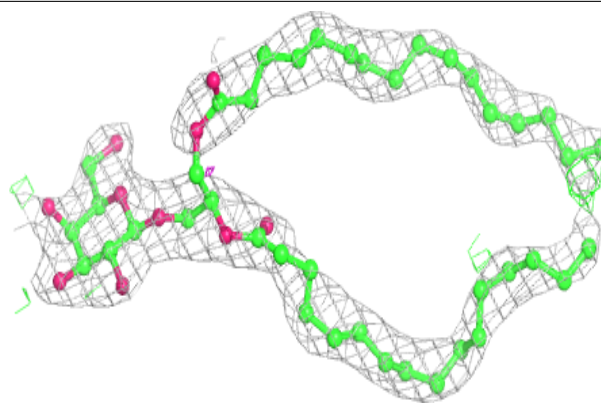
**Electron density around BCR B 618:**

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

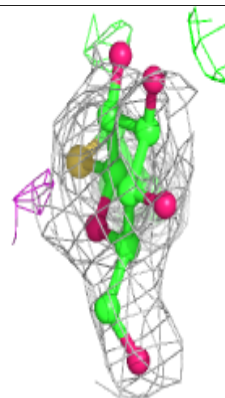
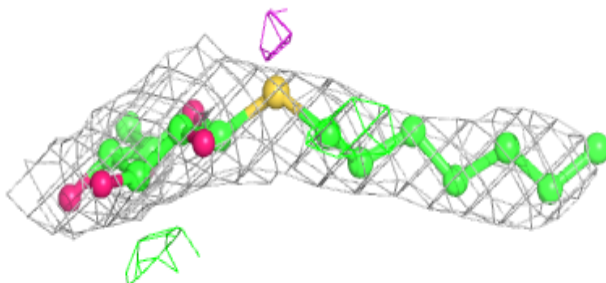
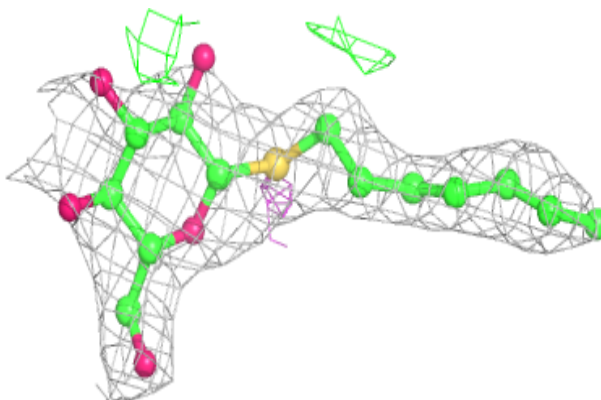


Electron density around LMG A 410:

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

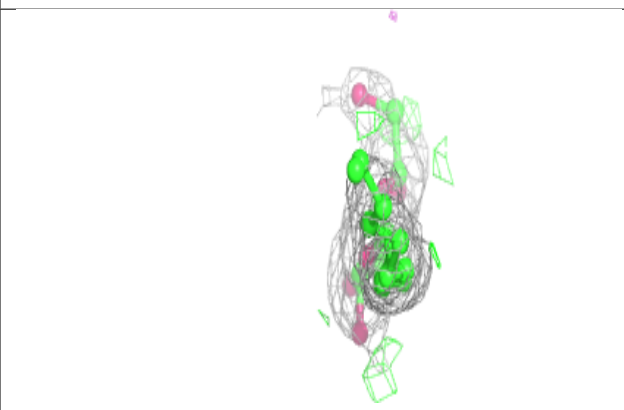
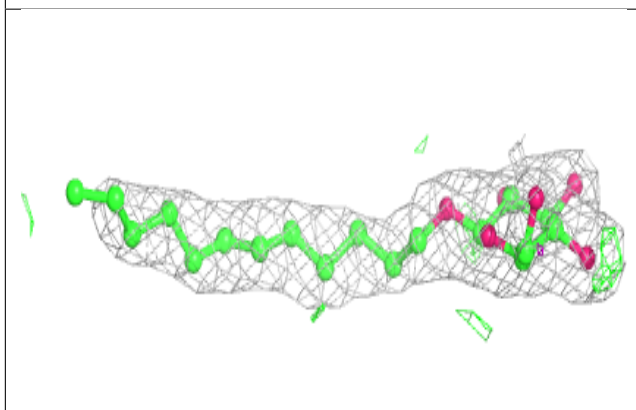
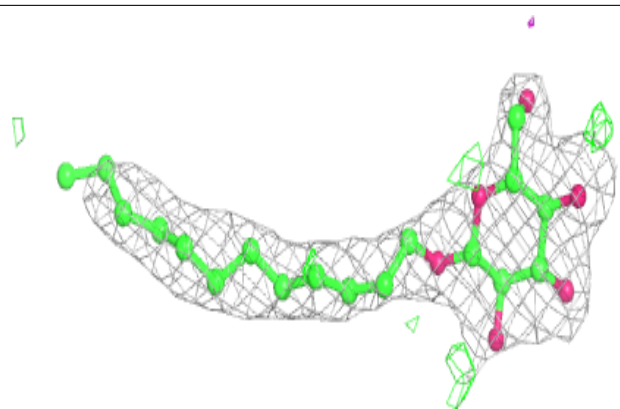
**Electron density around HTG 1 106:**

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

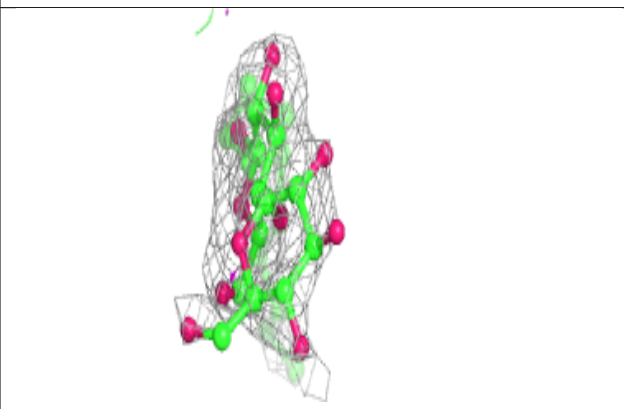
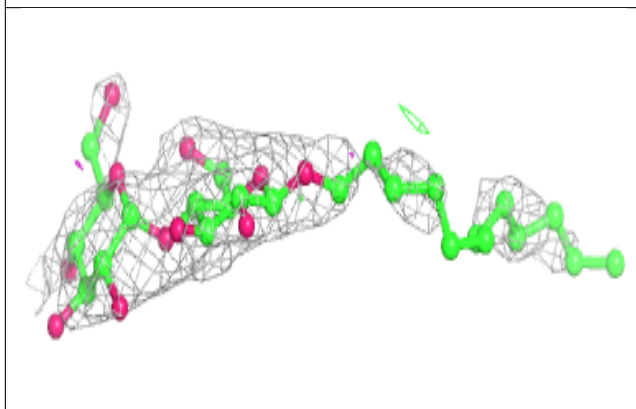
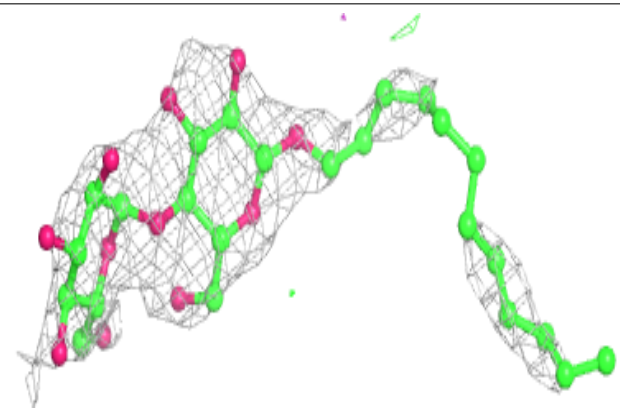


Electron density around LMT B 622:

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

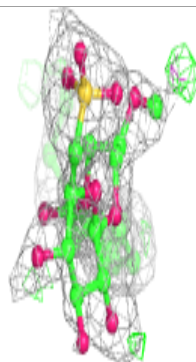
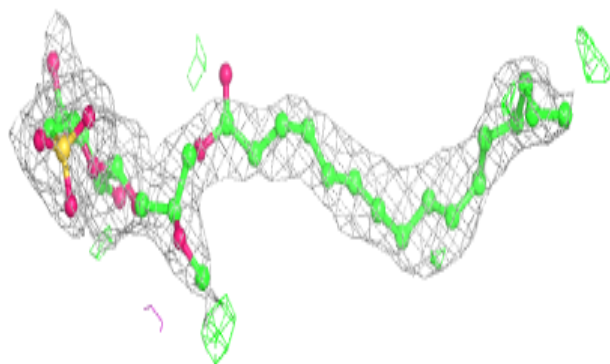
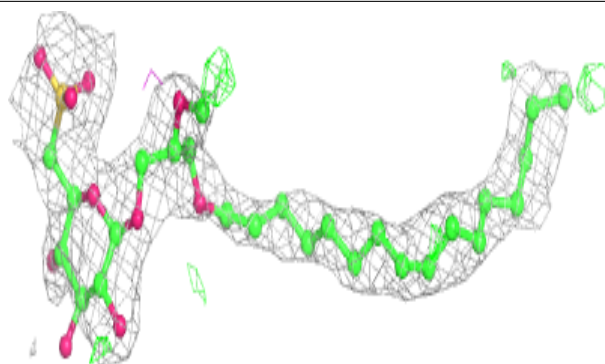
**Electron density around LMT c 921:**

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

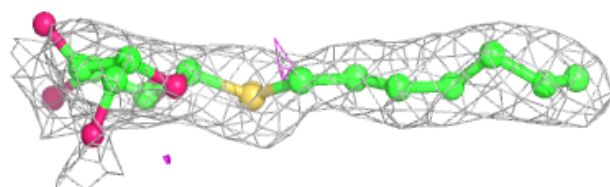
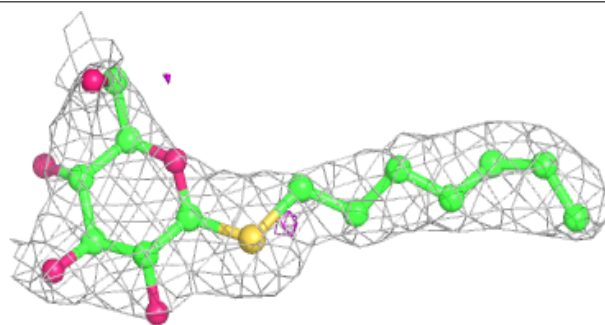


Electron density around SQD b 621:

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

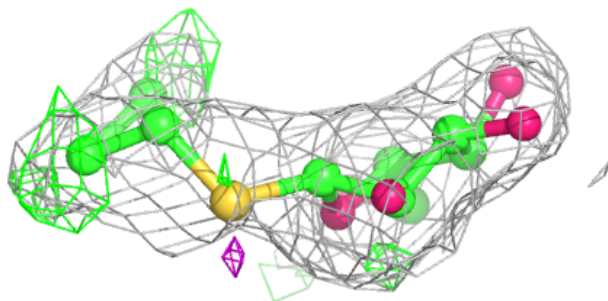
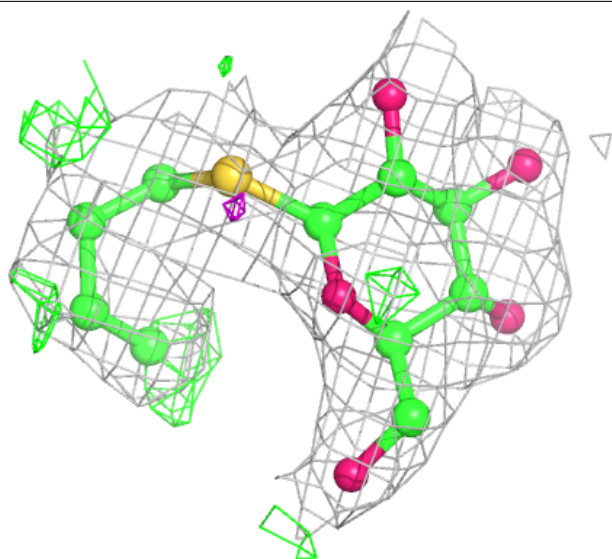
**Electron density around HTG B 626:**

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



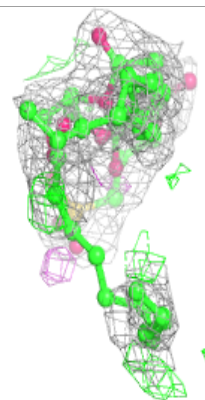
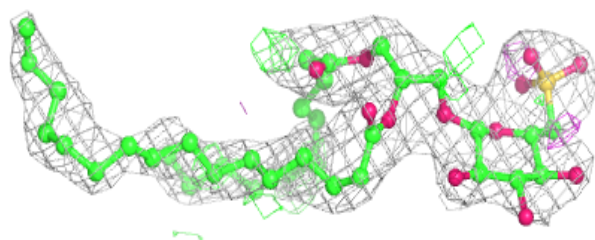
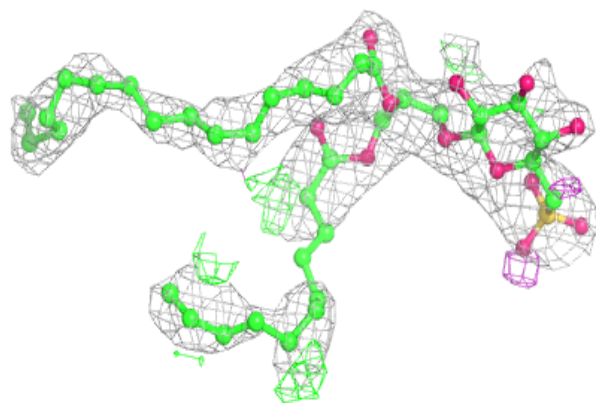
Electron density around HTG v 203:

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

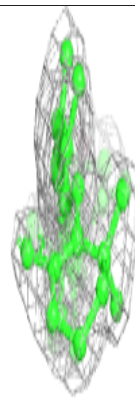
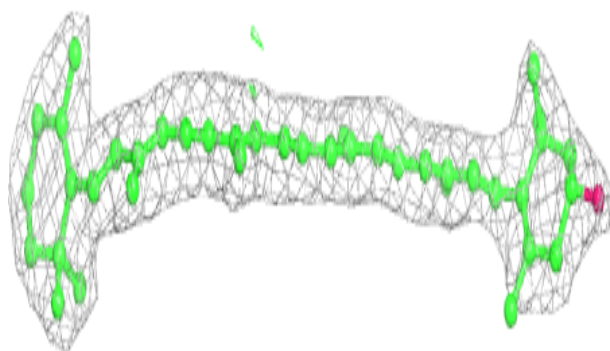
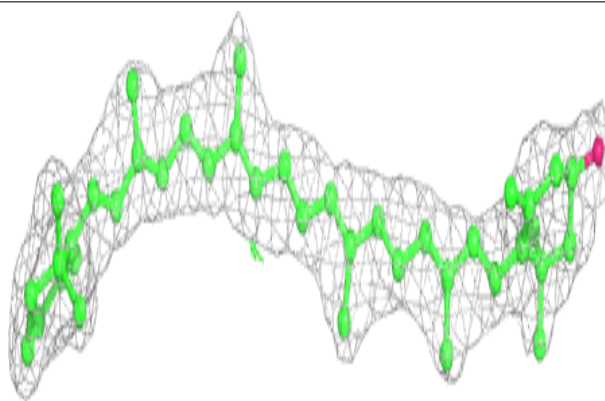


Electron density around SQD A 413:

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

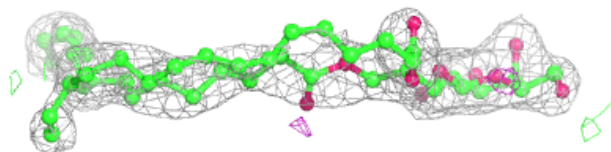
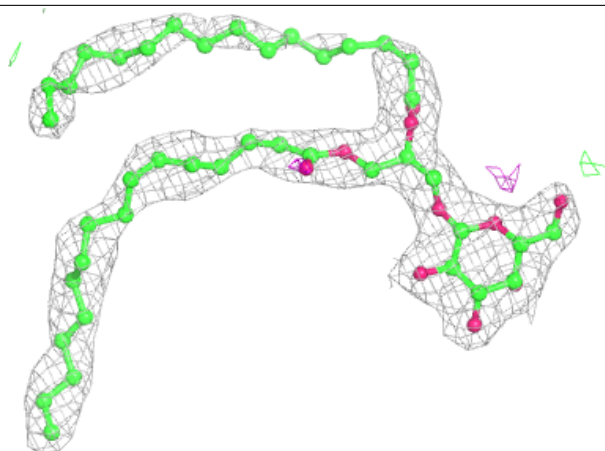
**Electron density around RRX H 101:**

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

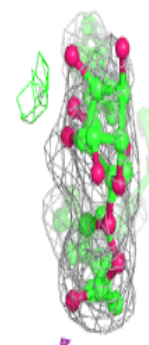
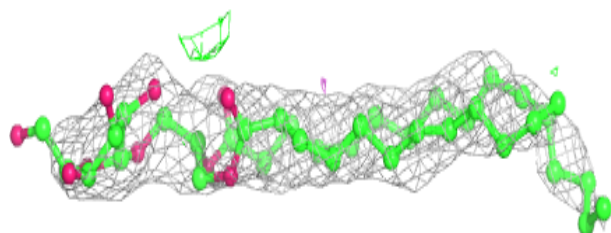
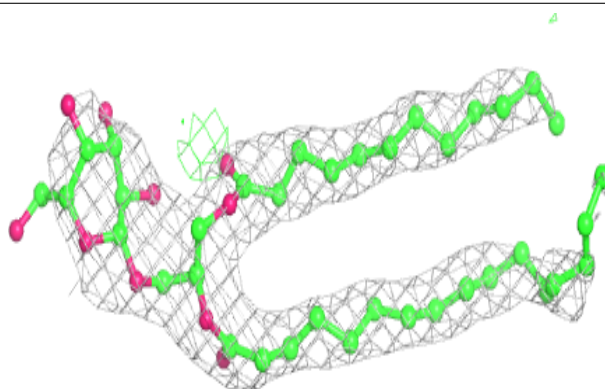


Electron density around LMG c 920:

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

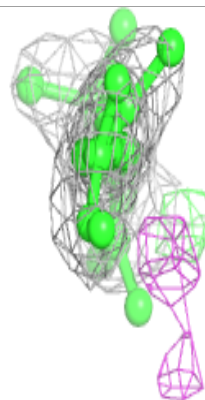
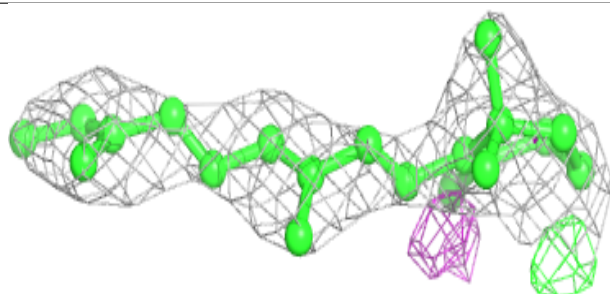
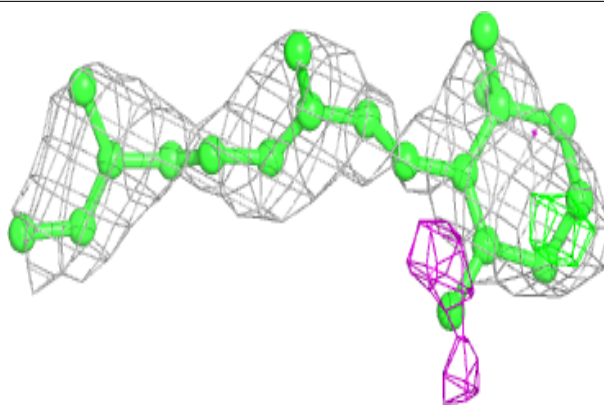
**Electron density around LMG d 409:**

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

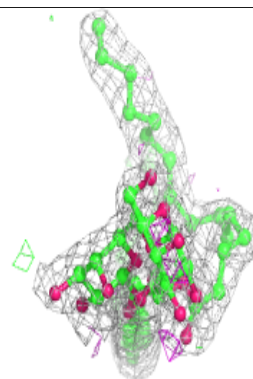
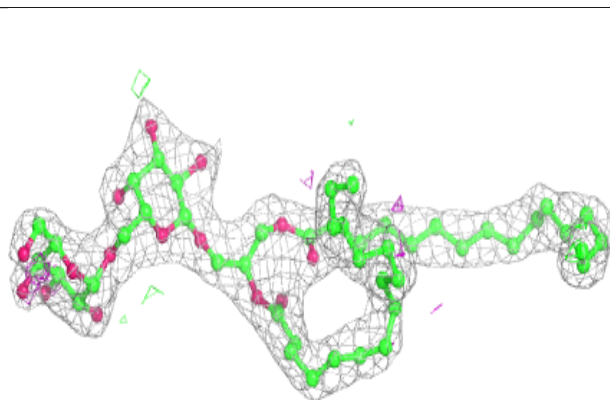
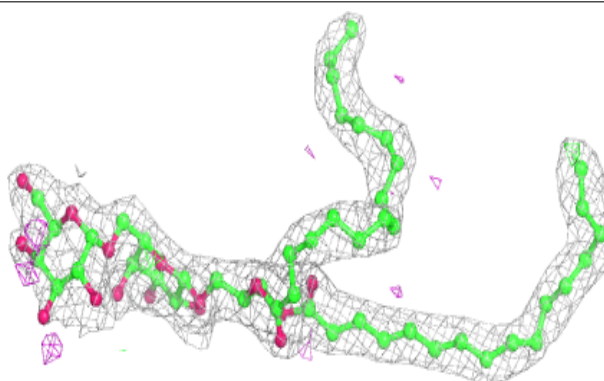


Electron density around BCR b 618:

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

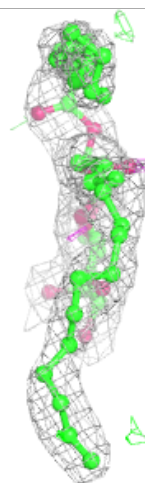
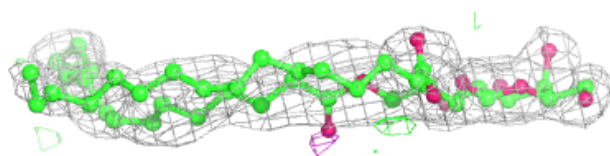
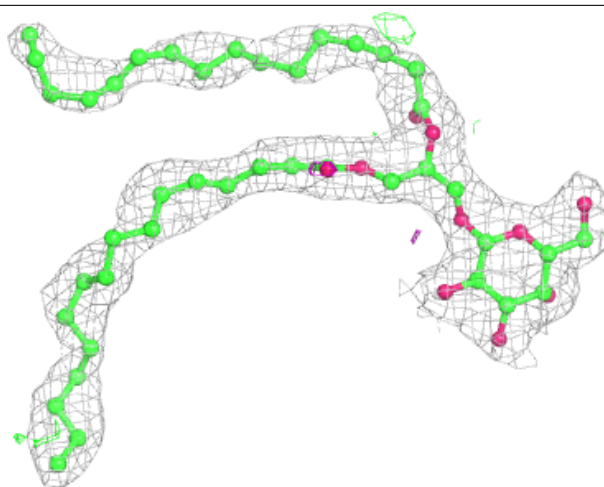
**Electron density around DGD h 102:**

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



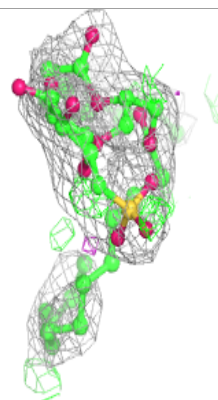
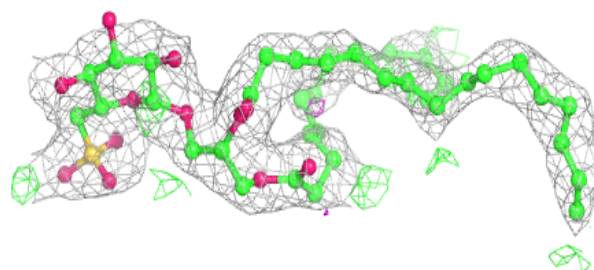
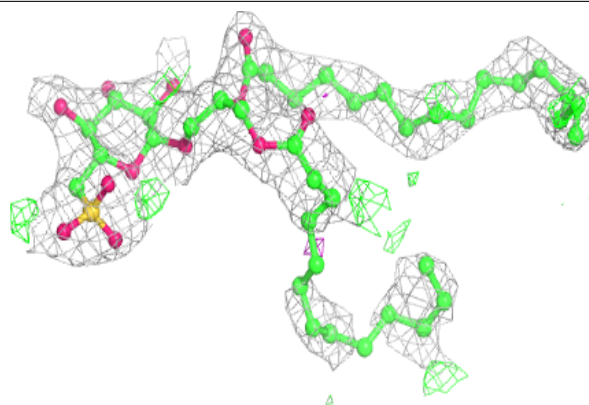
Electron density around LMG C 520:

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

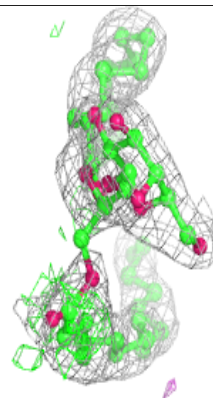
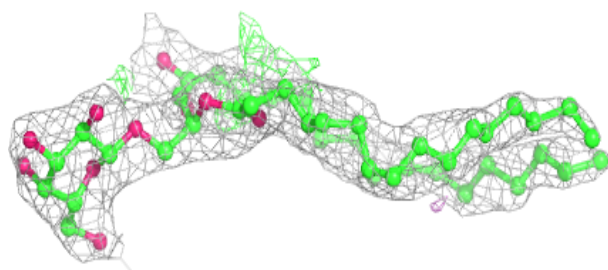
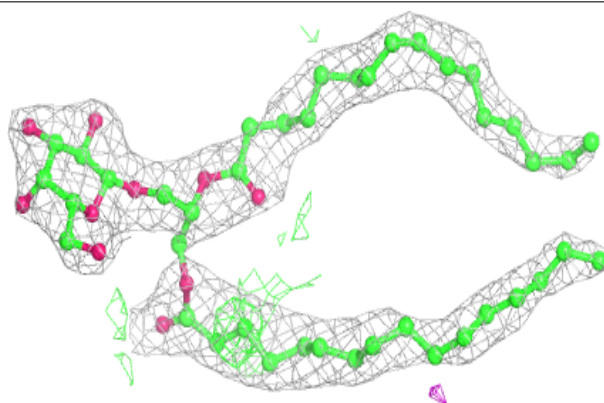


Electron density around SQD a 418:

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

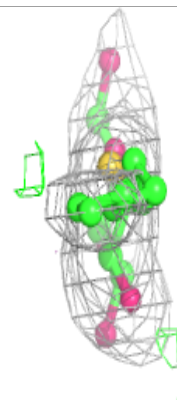
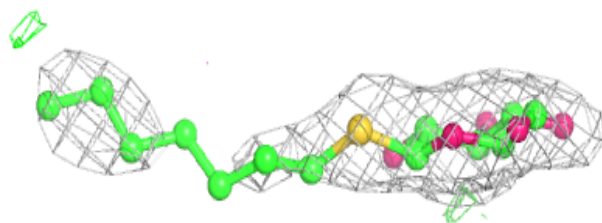
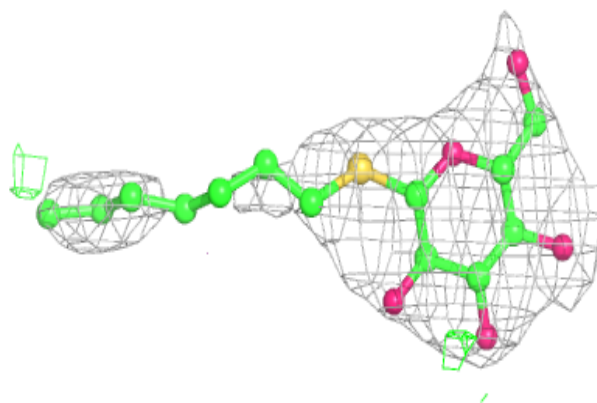
**Electron density around LMG i 101:**

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

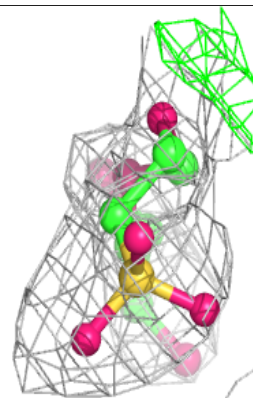
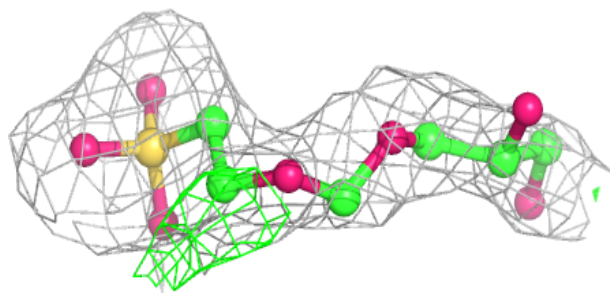
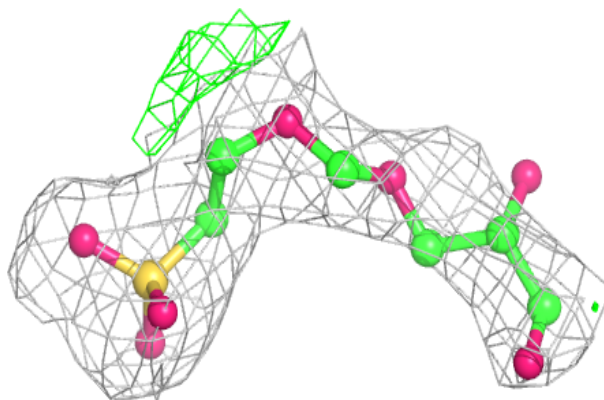


Electron density around HTG C 521:

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

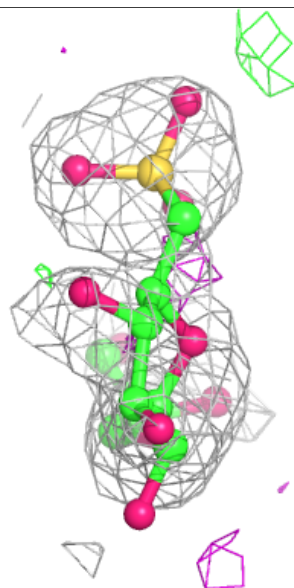
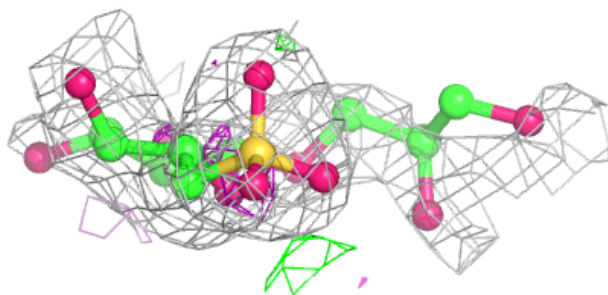
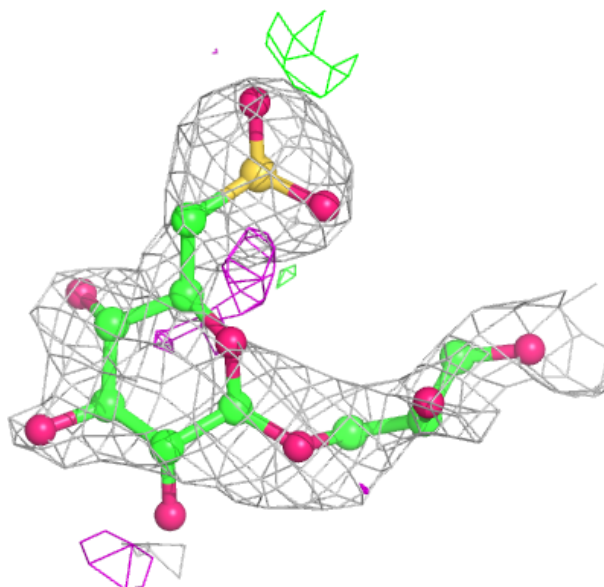
**Electron density around SQD f 101:**

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



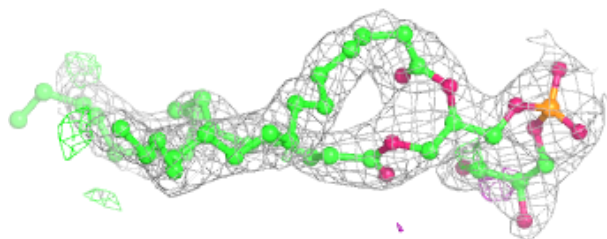
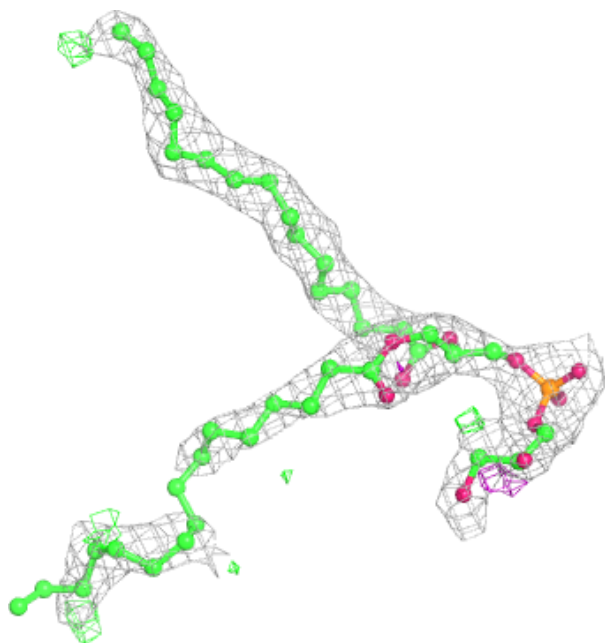
Electron density around SQD D 408:

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



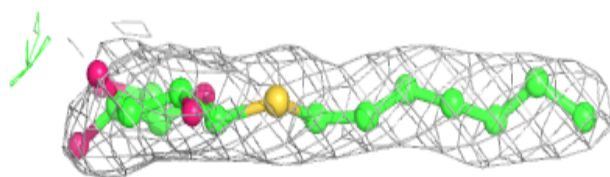
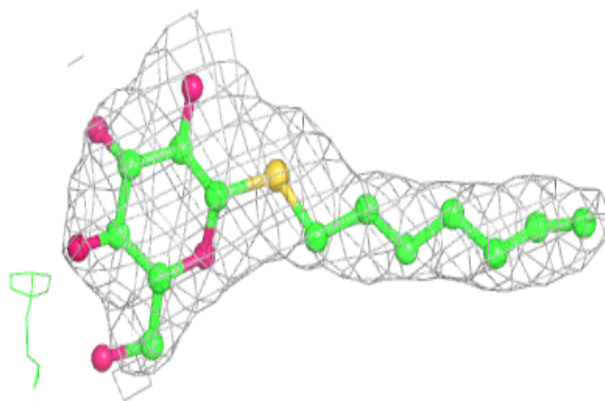
Electron density around LHG 1 102:

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

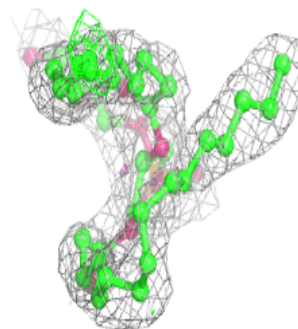
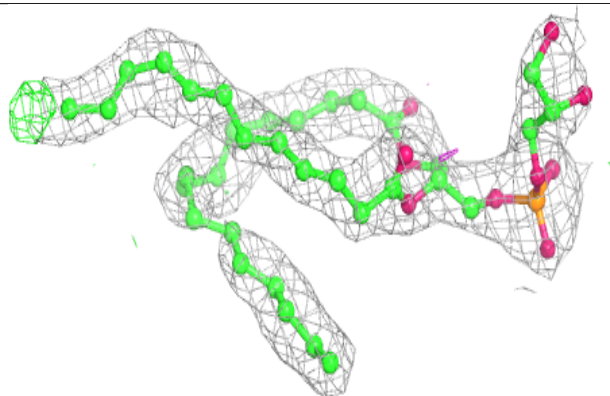
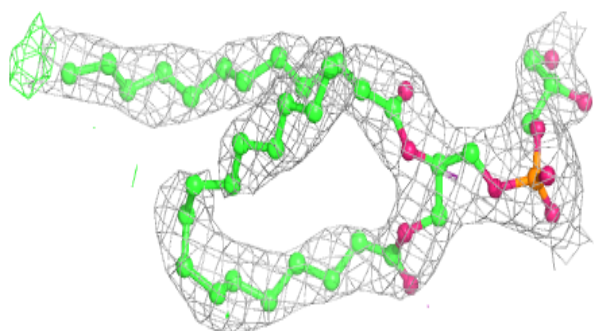


Electron density around HTG b 626:

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

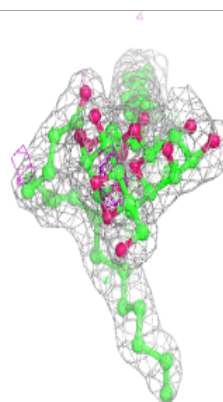
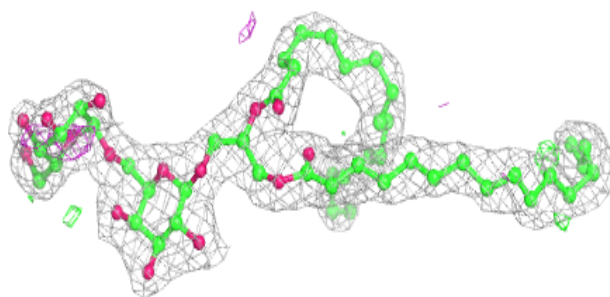
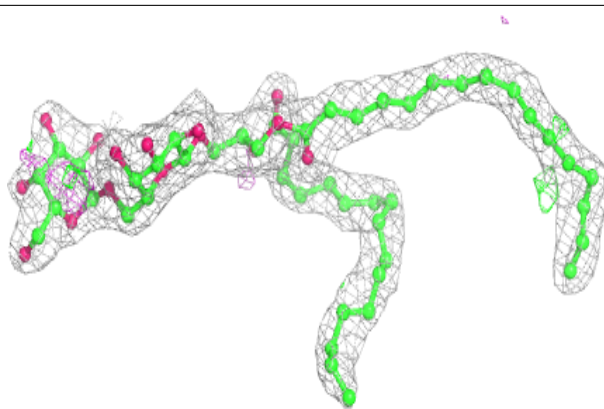
**Electron density around LHG a 423:**

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



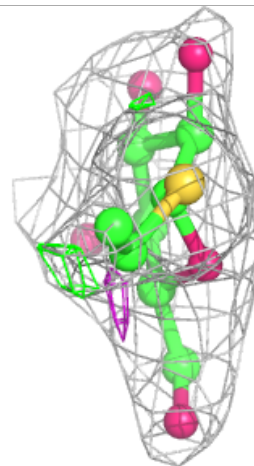
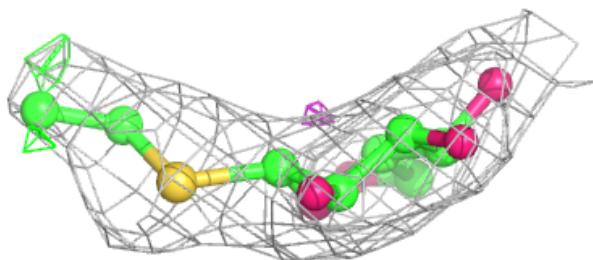
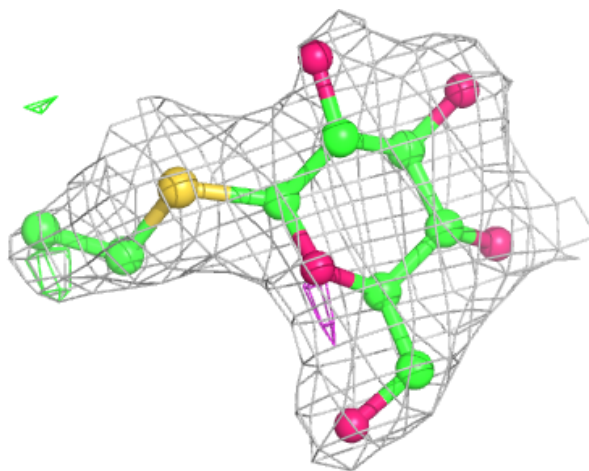
Electron density around DGD H 102:

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



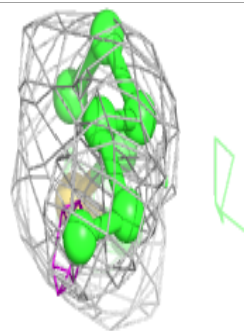
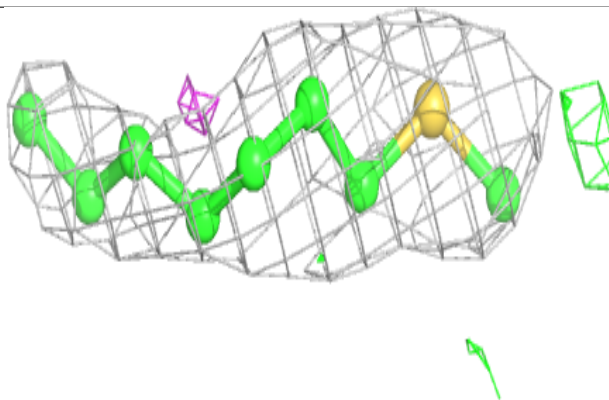
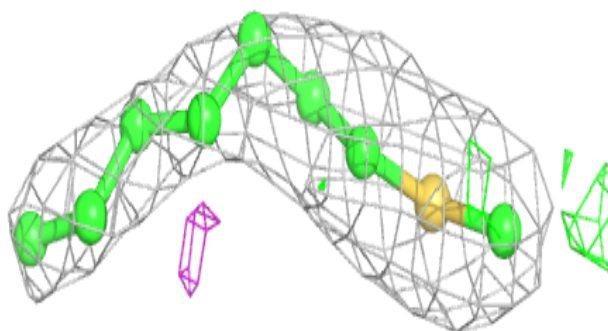
Electron density around HTG V 203:

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

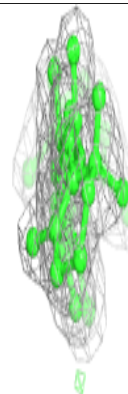
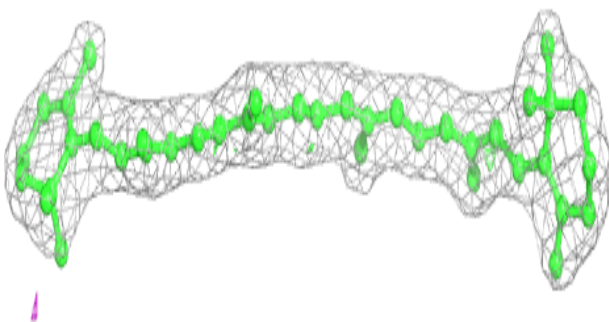
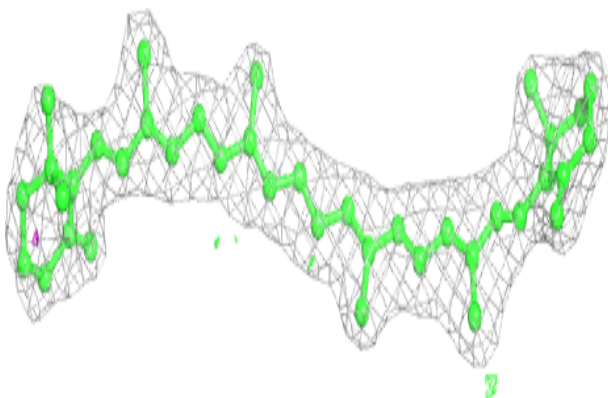


Electron density around HTG C 523:

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

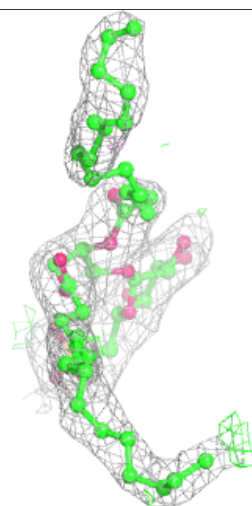
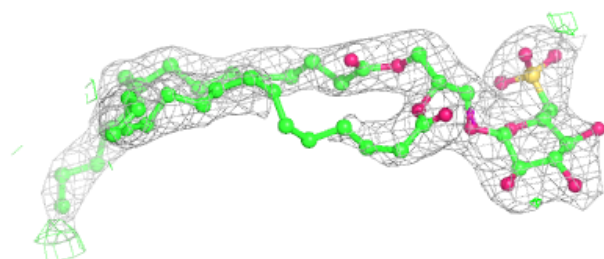
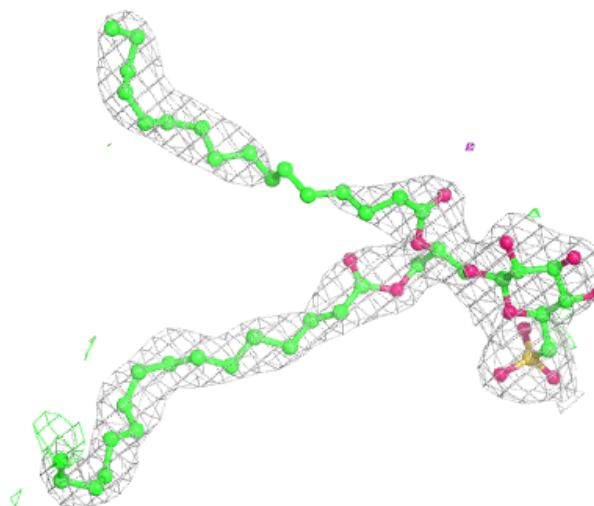
**Electron density around BCR y 101:**

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



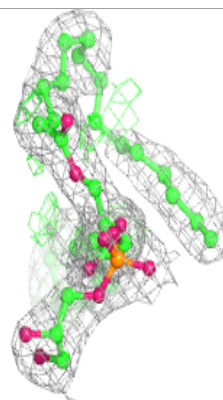
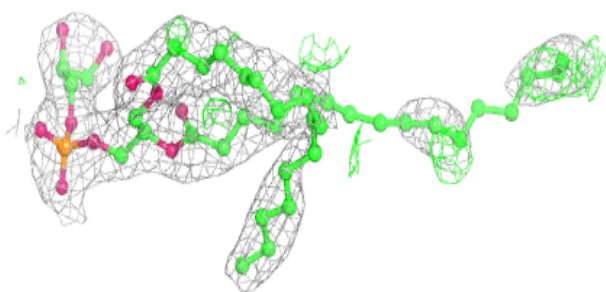
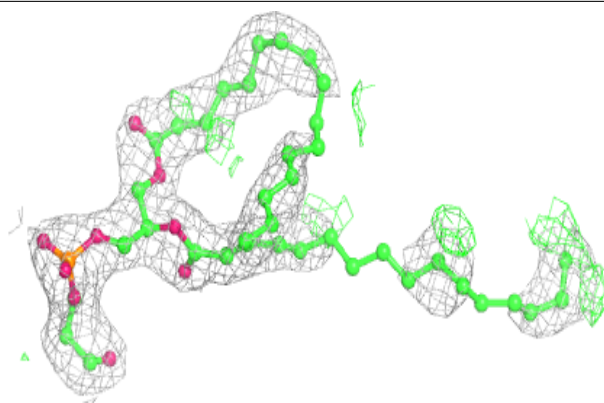
Electron density around SQD a 414:

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

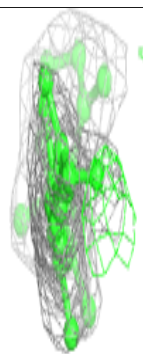
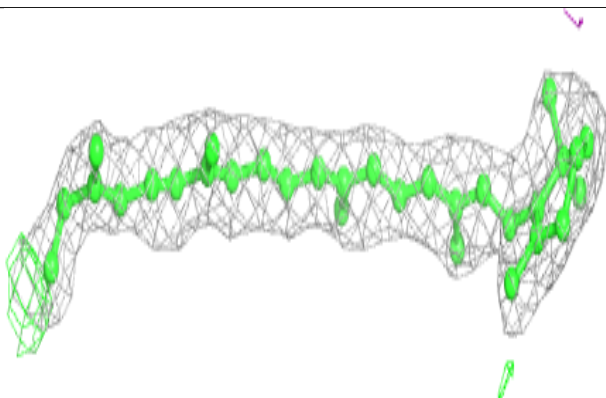
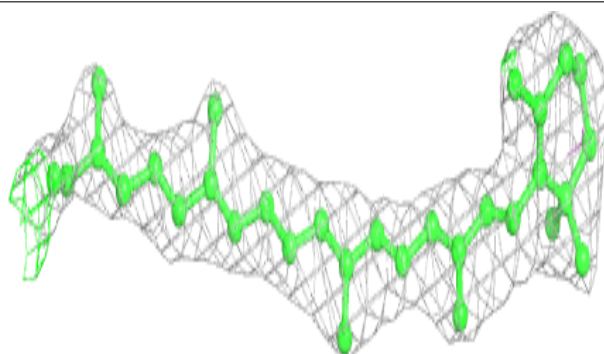


Electron density around LHG D 409:

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

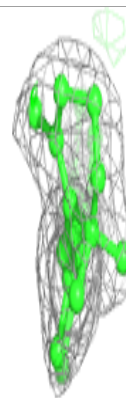
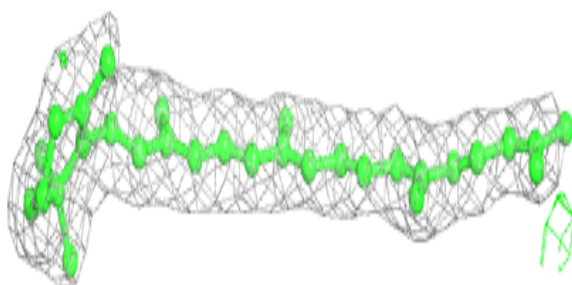
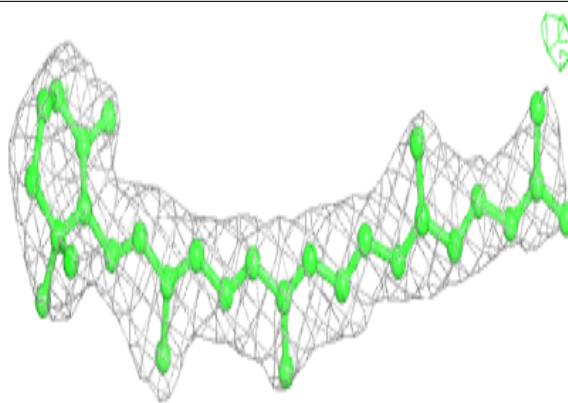
**Electron density around BCR b 619:**

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

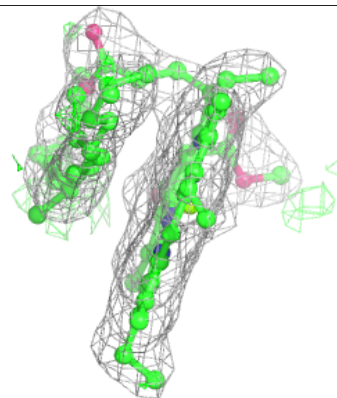
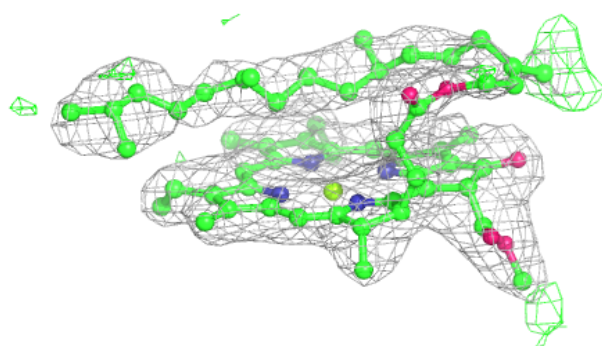
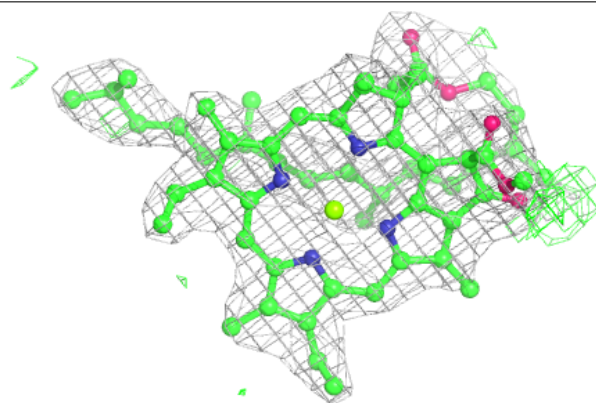


Electron density around BCR B 619:

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

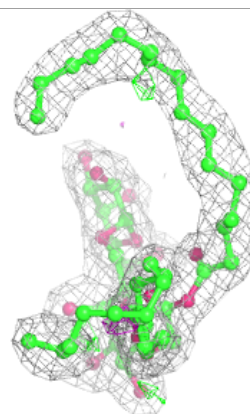
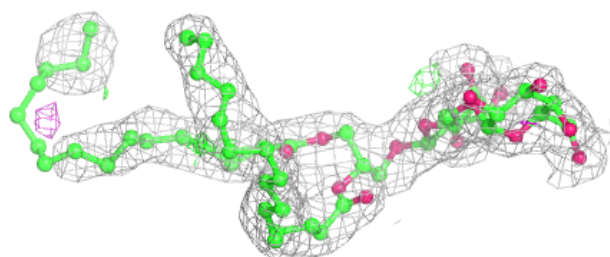
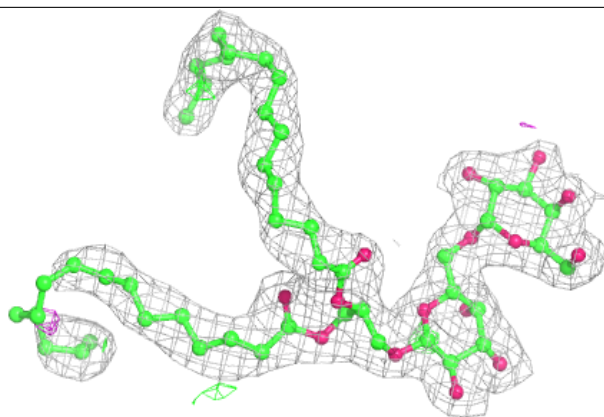
**Electron density around CLA B 602:**

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

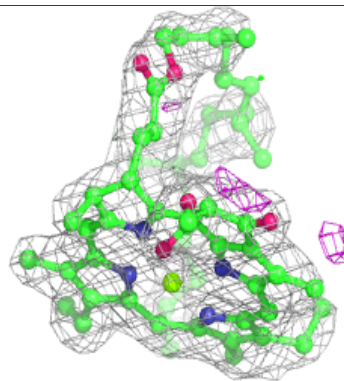
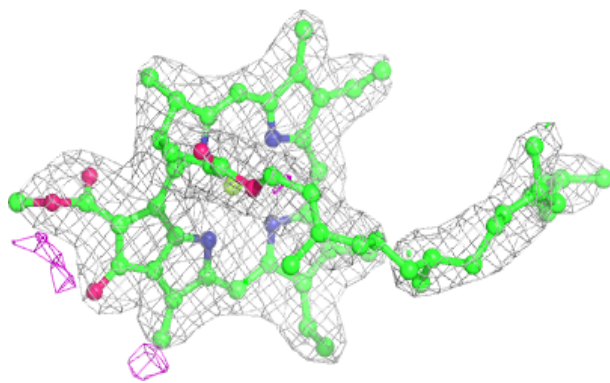
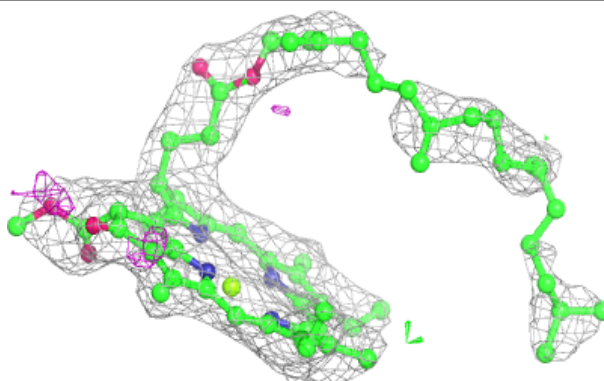


Electron density around DGD C 518:

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

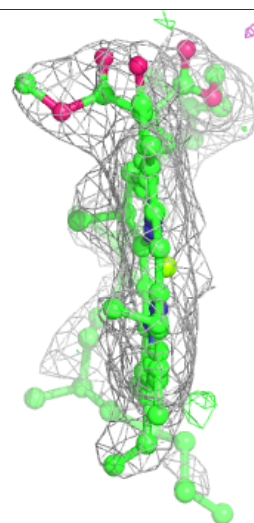
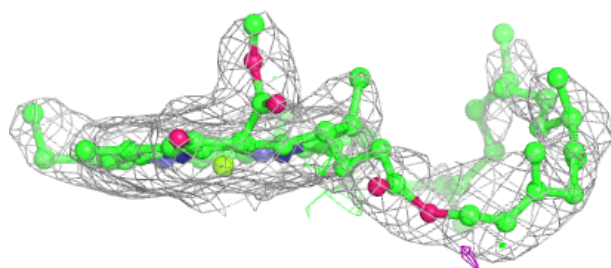
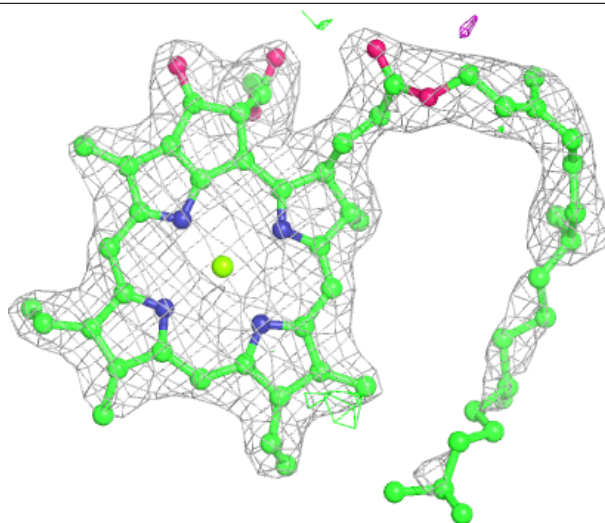
**Electron density around CLA C 514:**

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



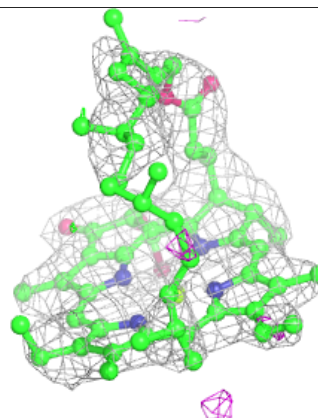
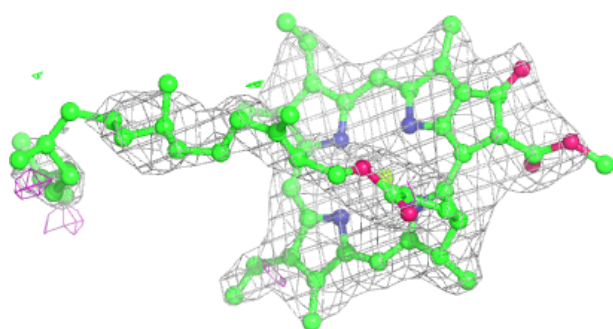
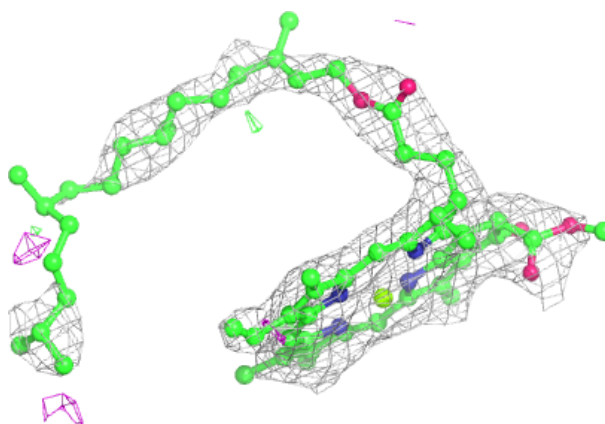
Electron density around CLA c 913:

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

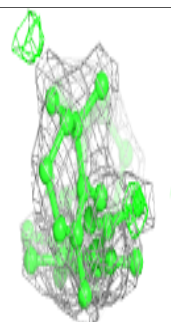
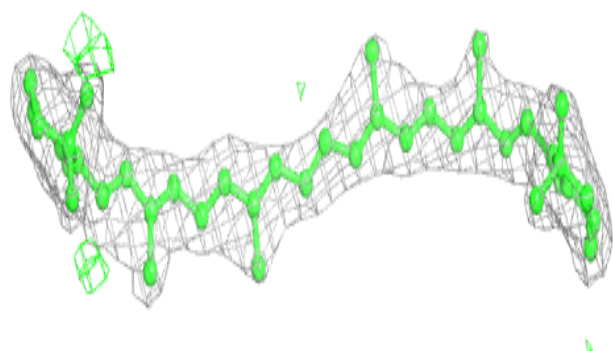
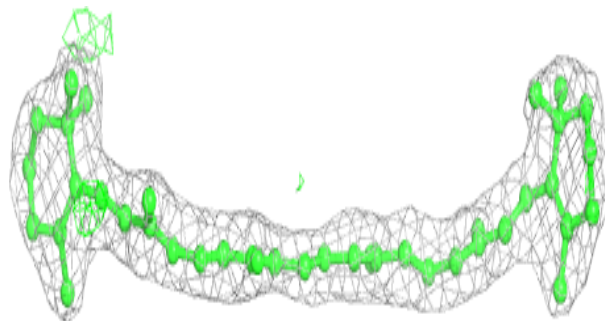


Electron density around CLA c 914:

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

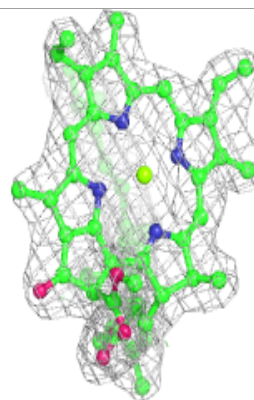
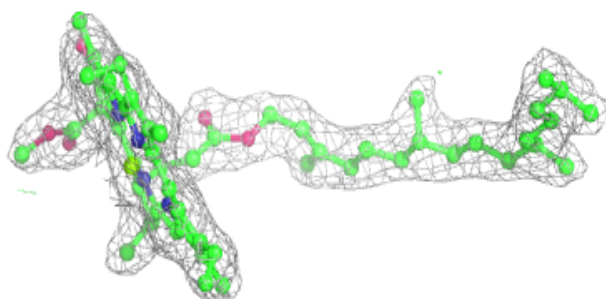
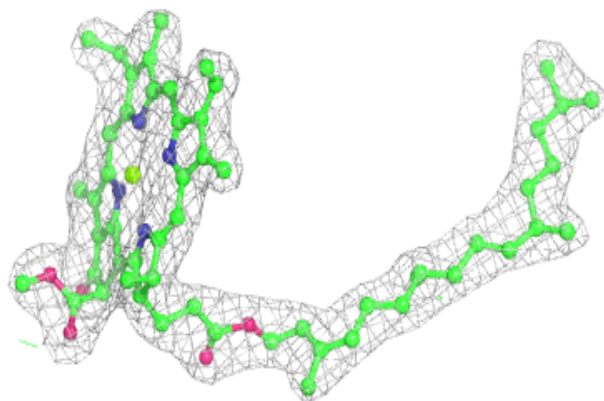
**Electron density around BCR k 101:**

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

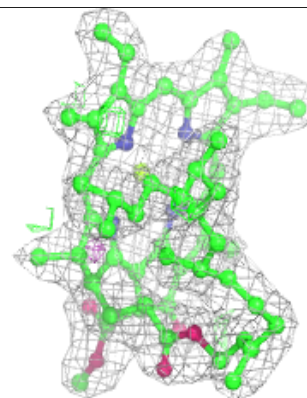
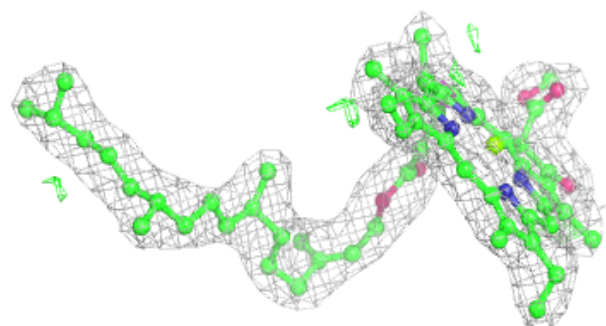
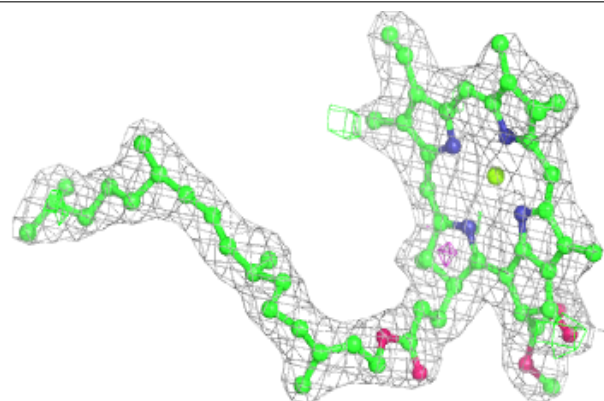


Electron density around CLA B 610:

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

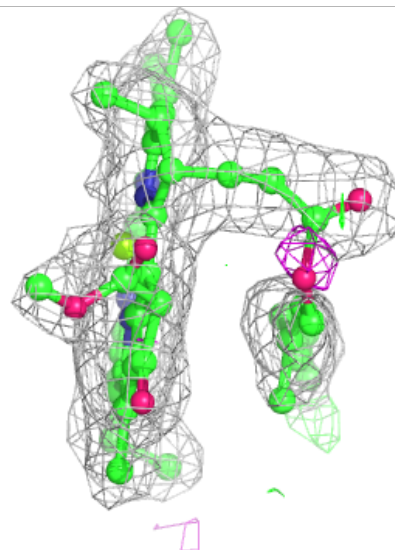
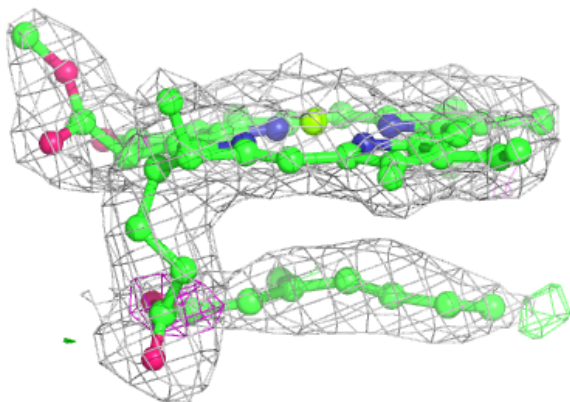
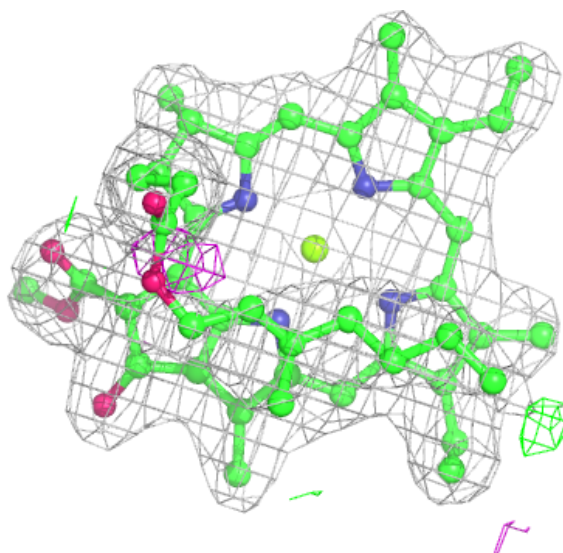
**Electron density around CLA c 912:**

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



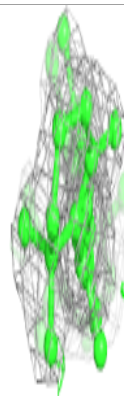
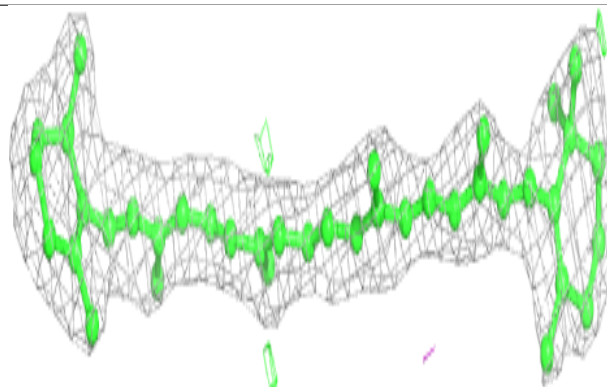
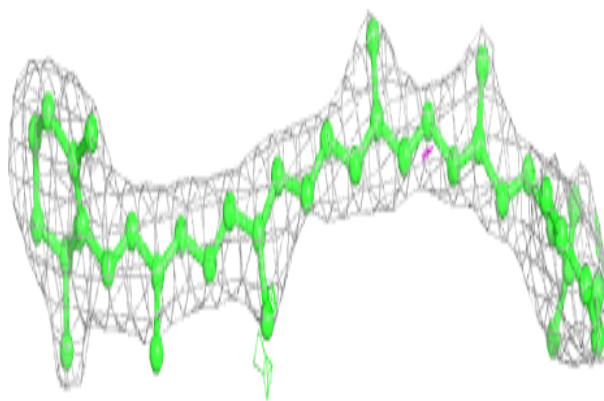
Electron density around CLA B 615:

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

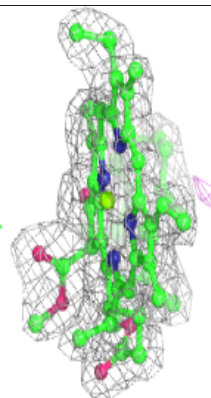
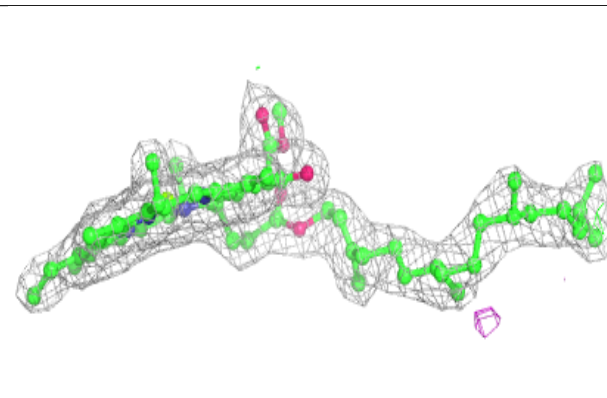
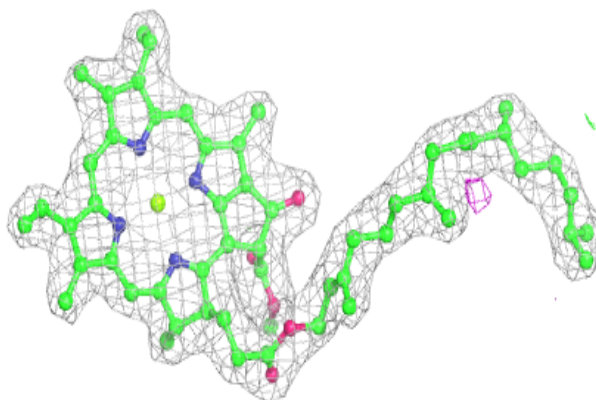


Electron density around BCR c 915:

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

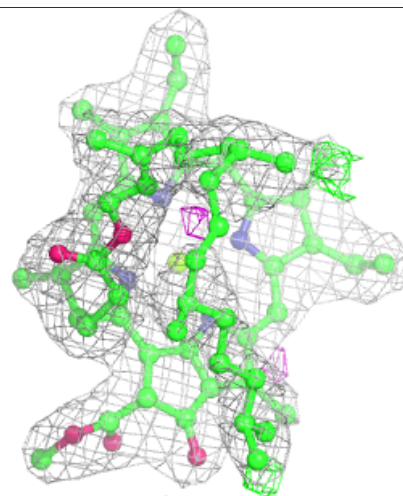
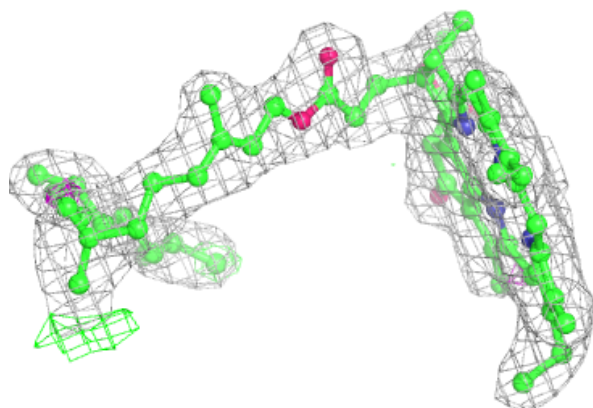
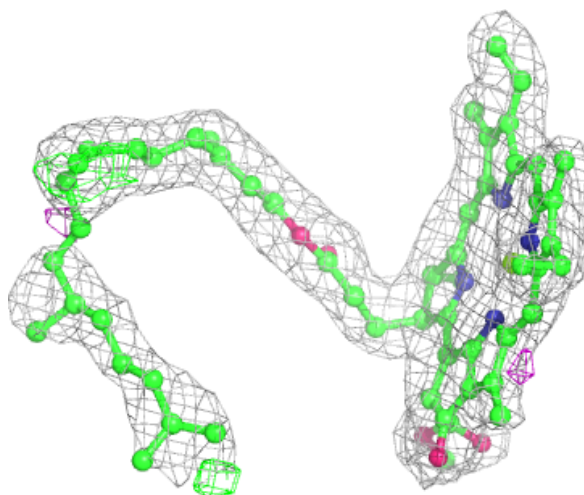
**Electron density around CLA B 603:**

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



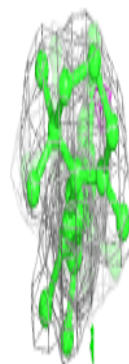
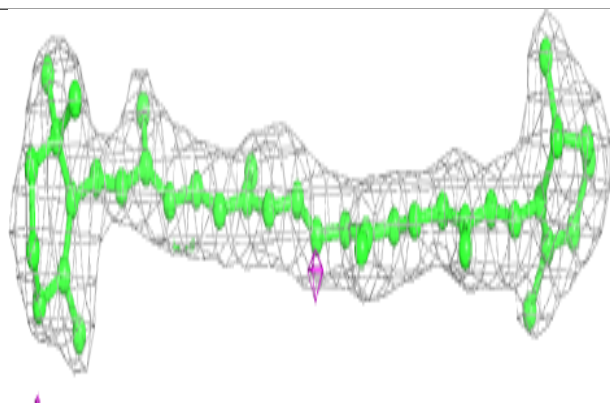
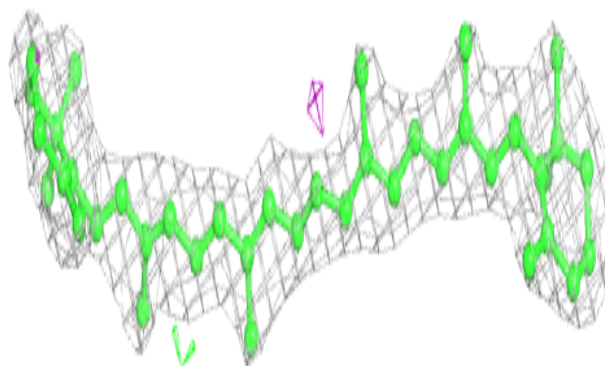
Electron density around CLA b 607:

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

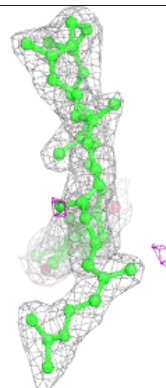
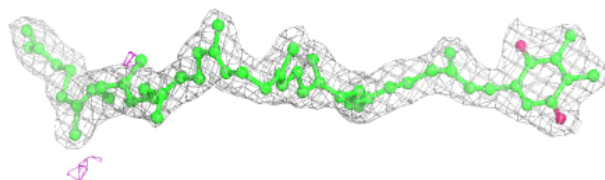
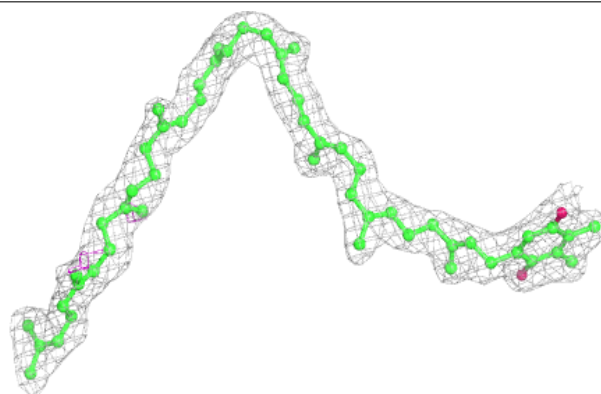


Electron density around BCR C 515:

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

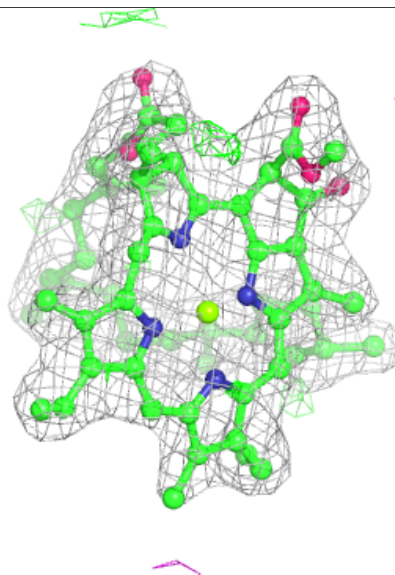
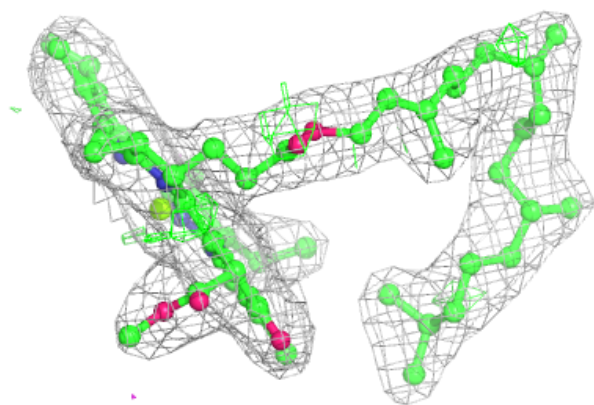
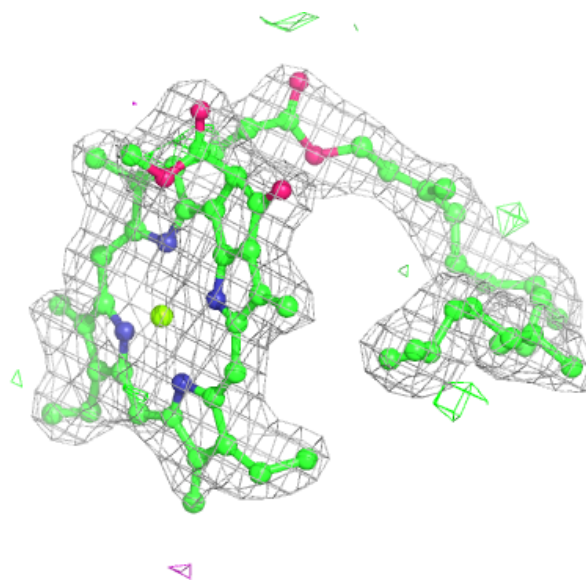
**Electron density around PL9 D 406:**

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



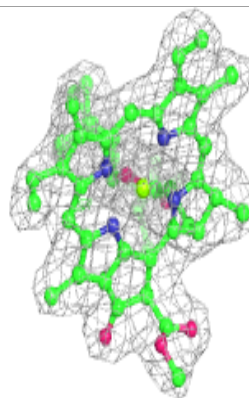
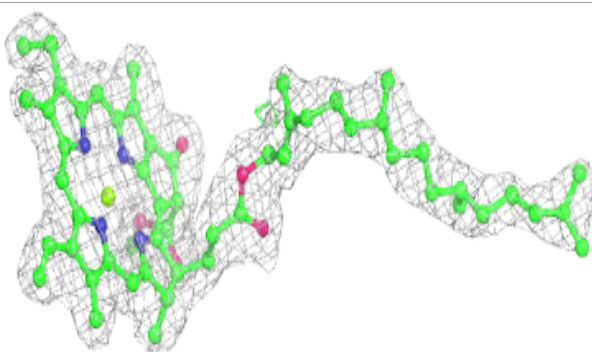
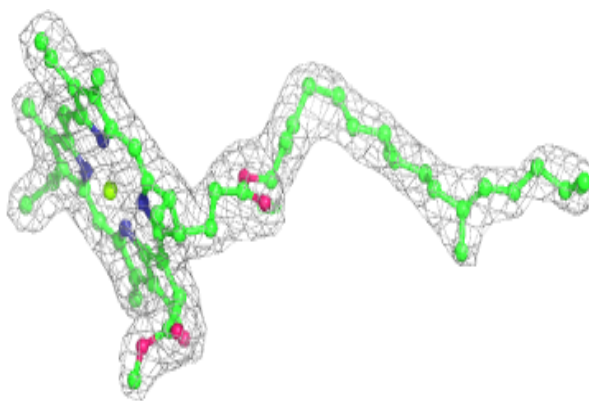
Electron density around CLA c 904:

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



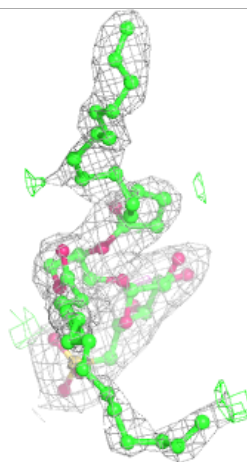
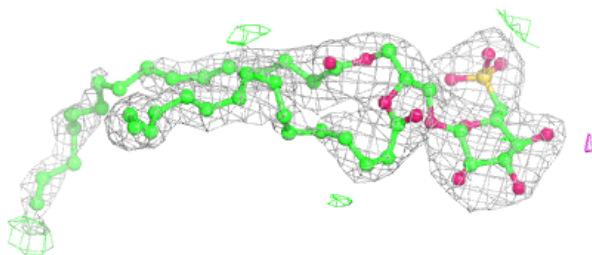
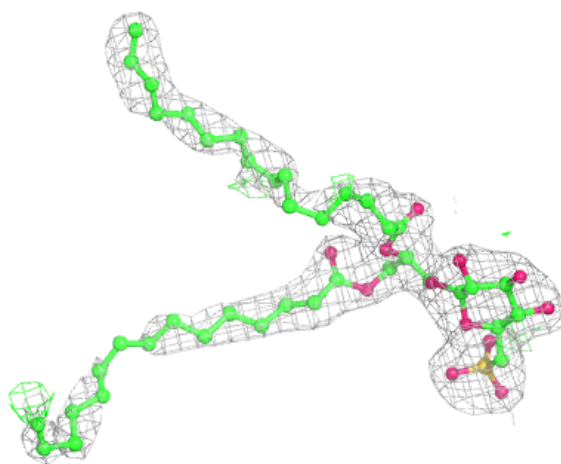
Electron density around CLA c 903:

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



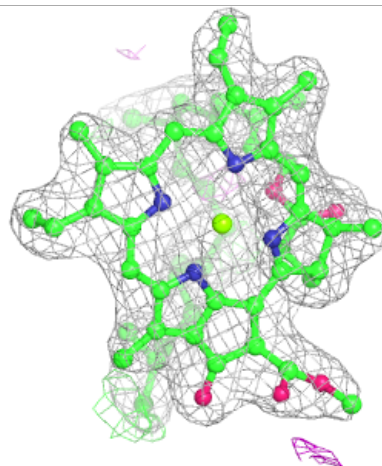
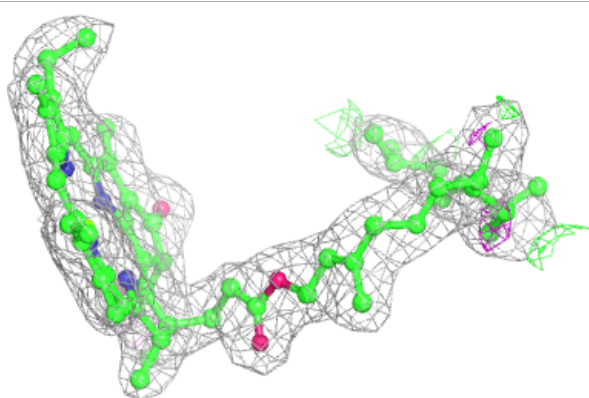
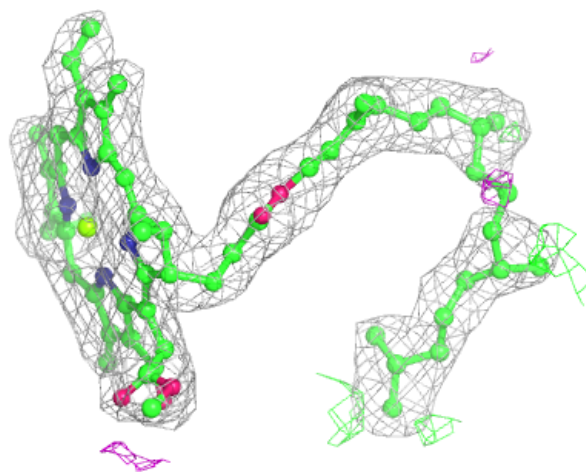
Electron density around SQD C 501:

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



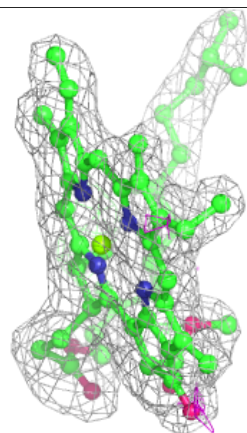
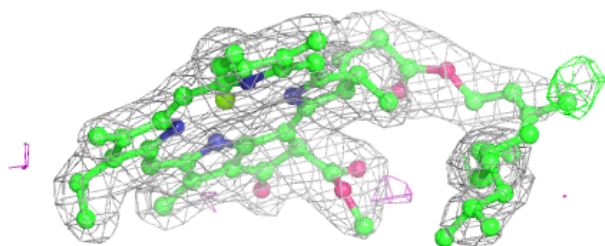
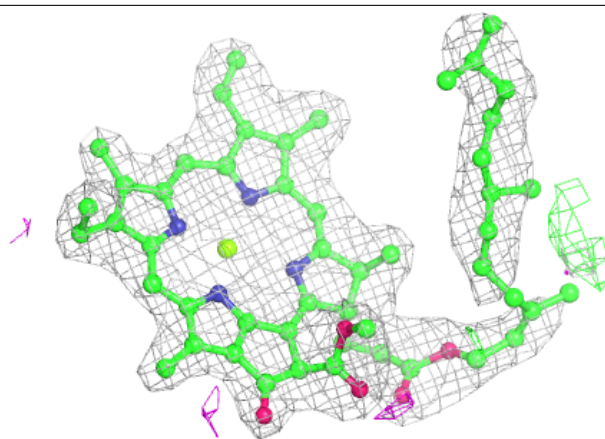
Electron density around CLA B 607:

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

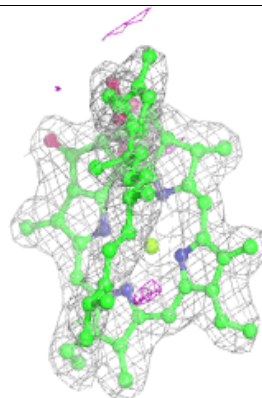
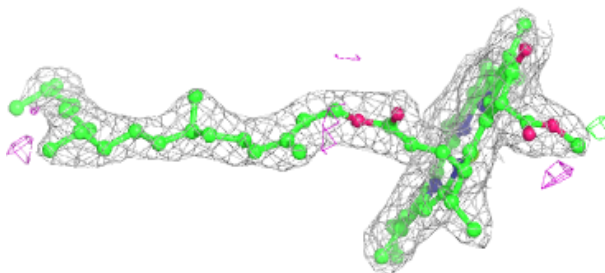
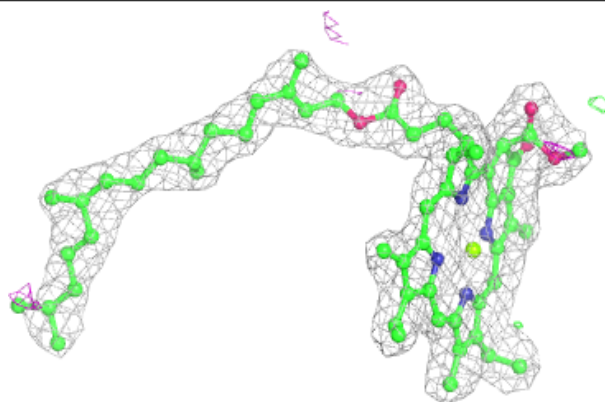


Electron density around CLA b 617:

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

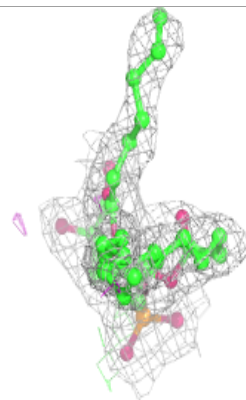
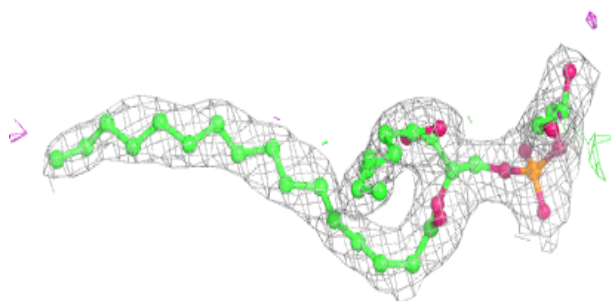
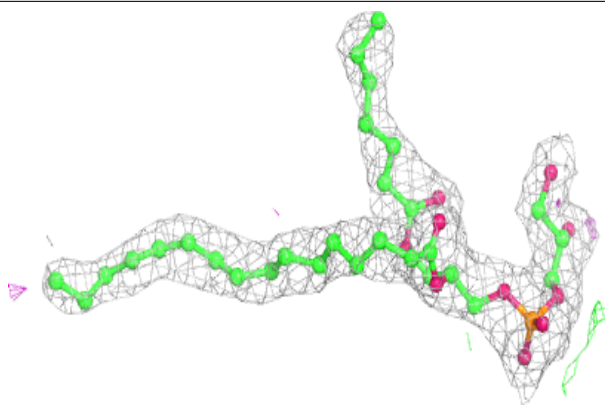
**Electron density around CLA b 610:**

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

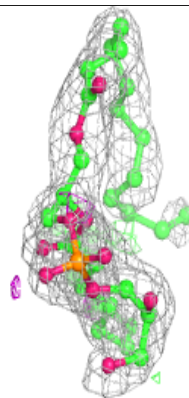
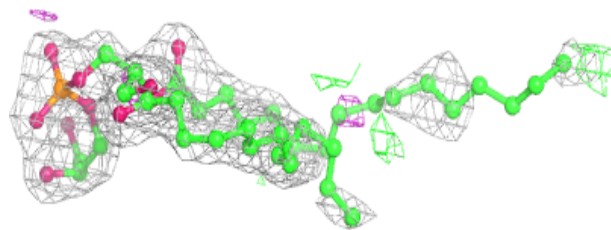
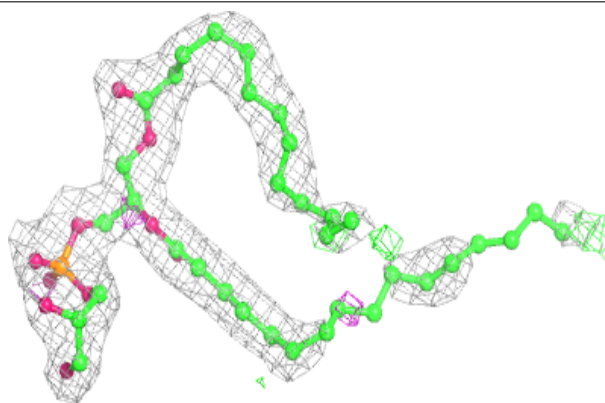


Electron density around LHG L 101:

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

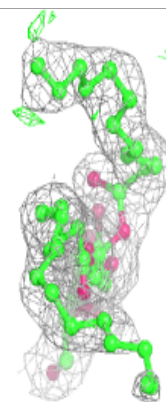
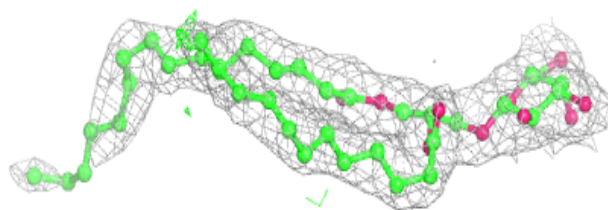
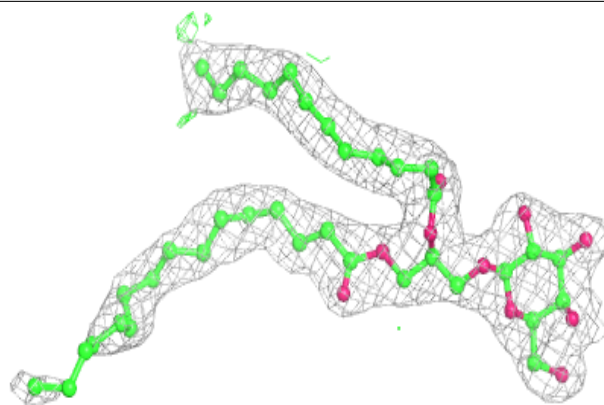
**Electron density around LHG d 408:**

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



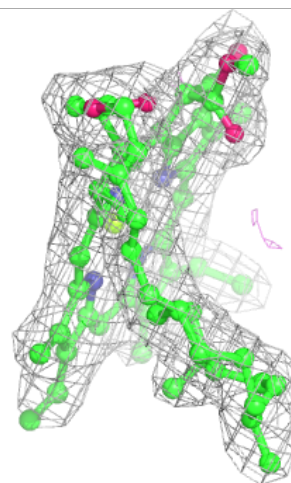
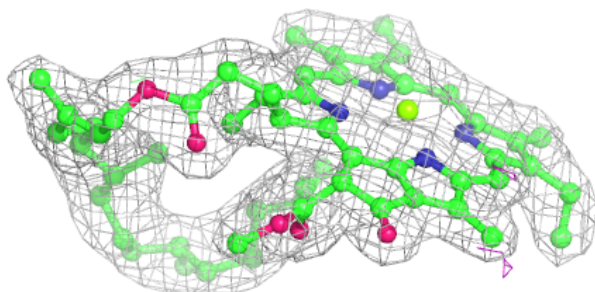
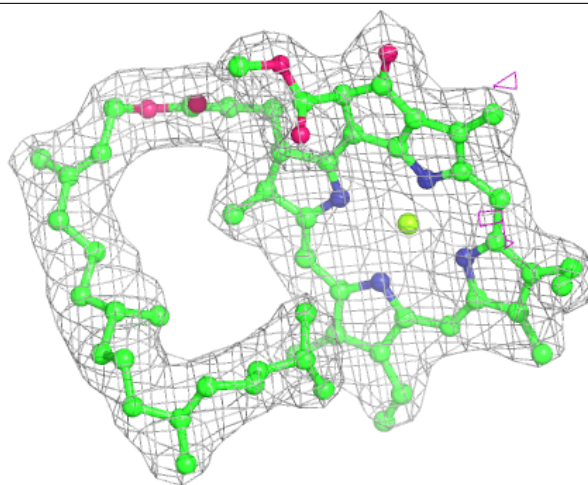
Electron density around LMG j 101:

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



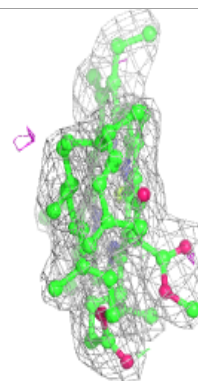
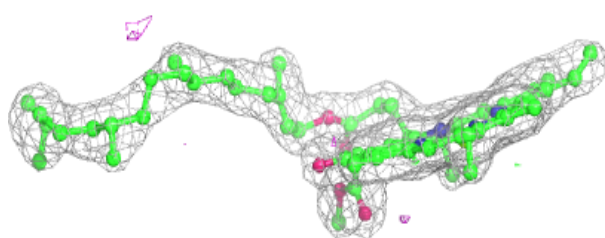
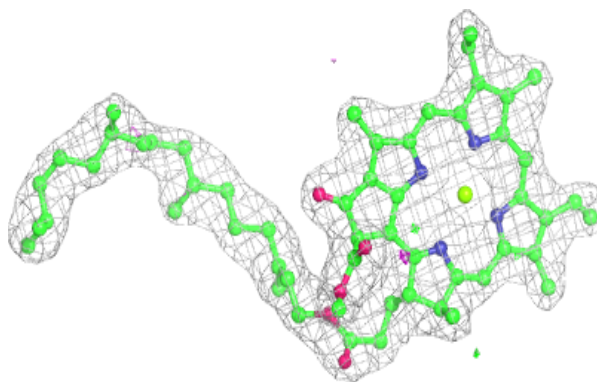
Electron density around CLA b 616:

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

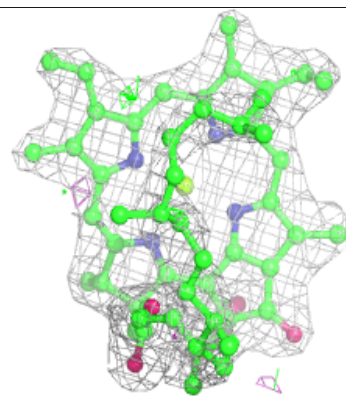
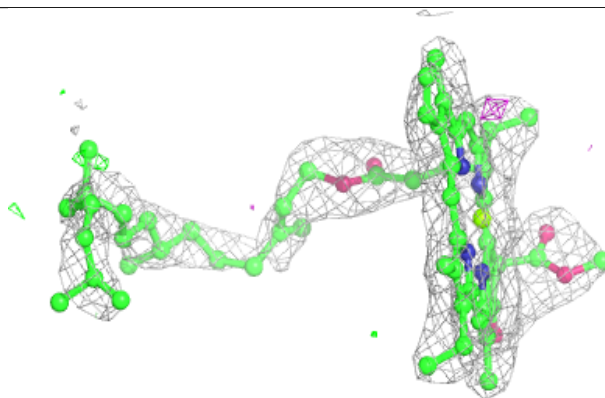
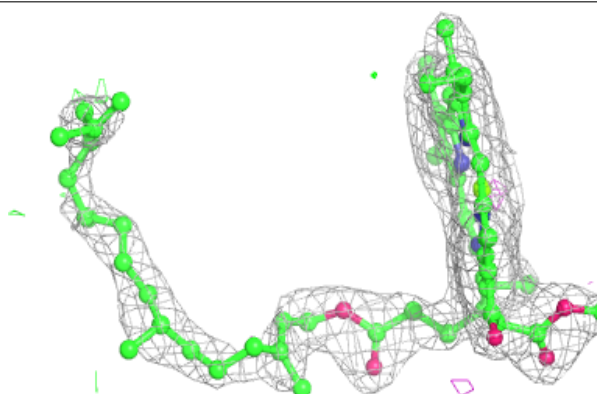


Electron density around CLA b 603:

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

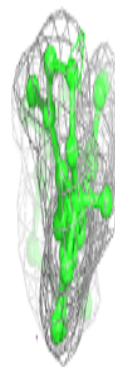
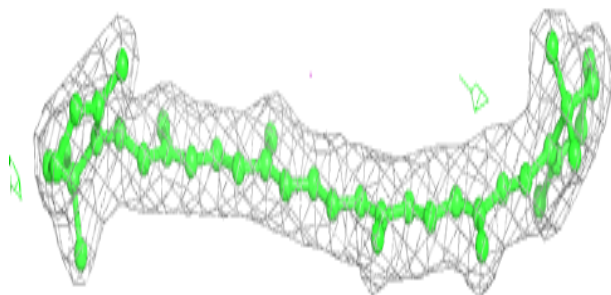
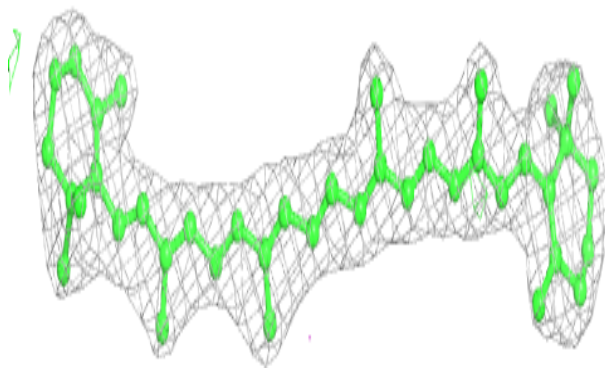
**Electron density around CLA C 507:**

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

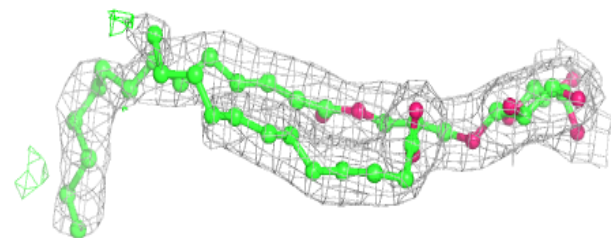
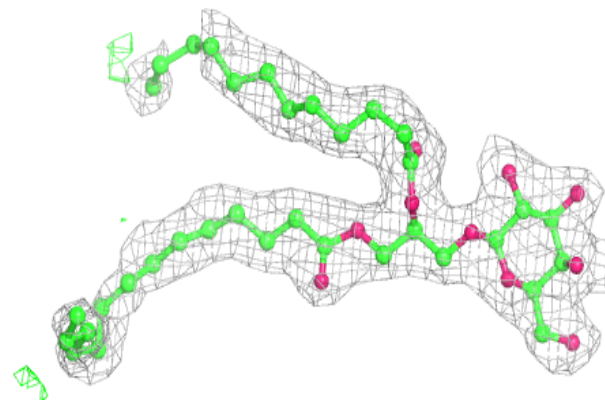


Electron density around BCR b 620:

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

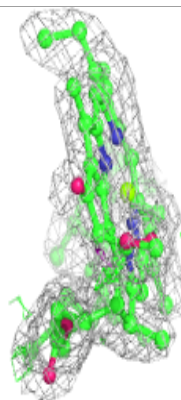
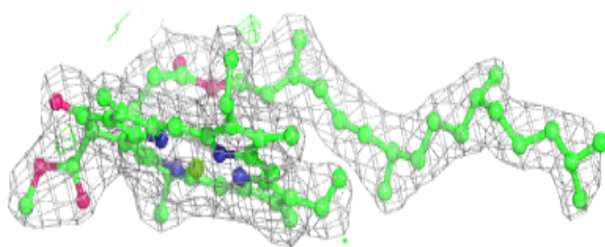
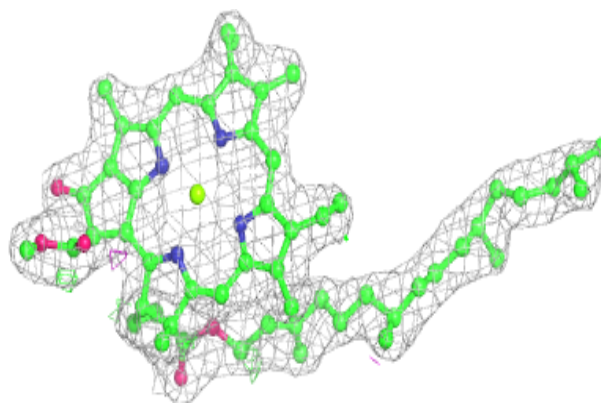
**Electron density around LMG J 101:**

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

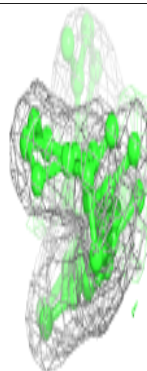
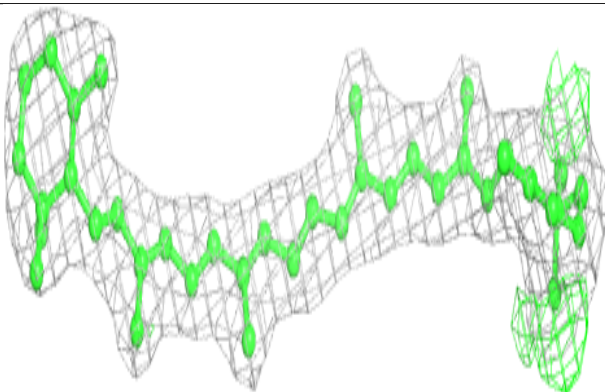
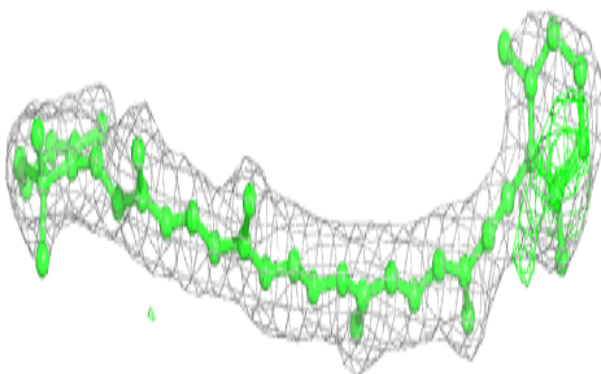


Electron density around CLA C 502:

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

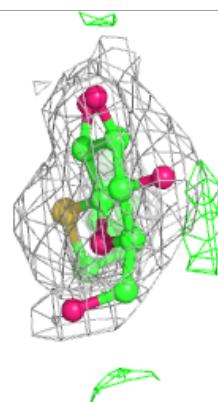
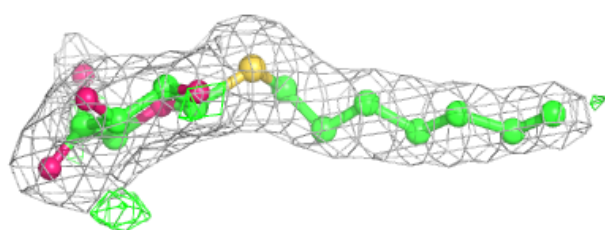
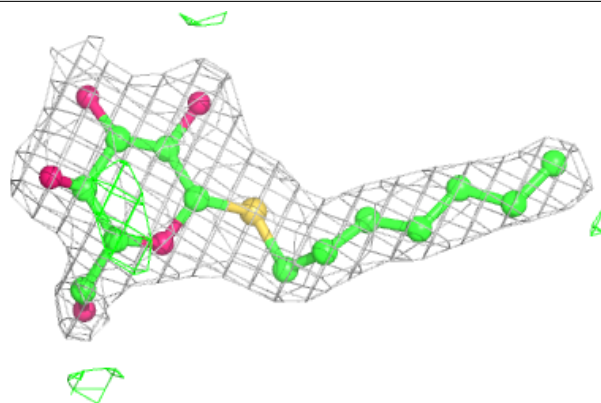
**Electron density around BCR d 404:**

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

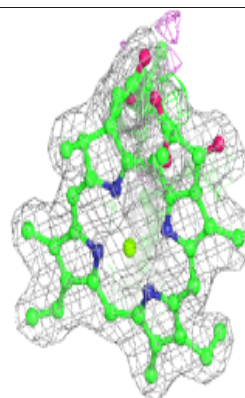
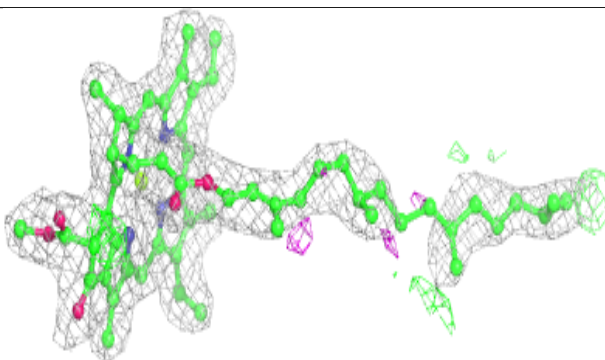
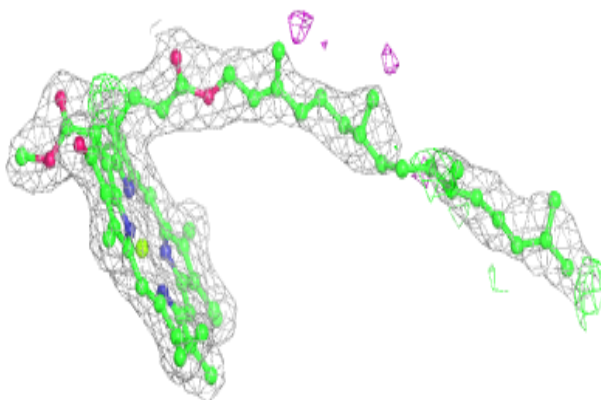


Electron density around HTG B 623:

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

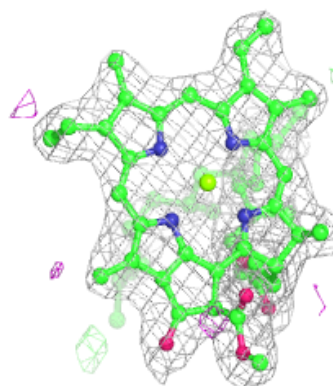
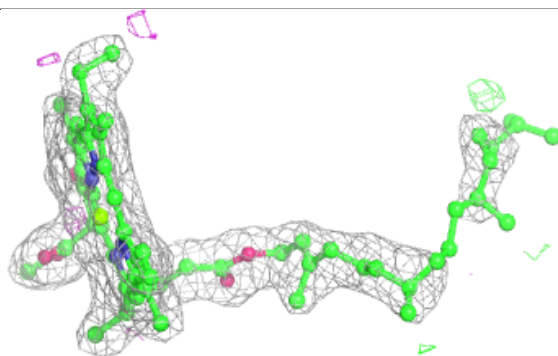
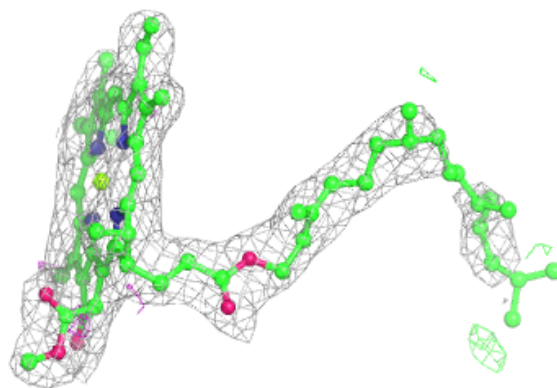
**Electron density around CLA B 608:**

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

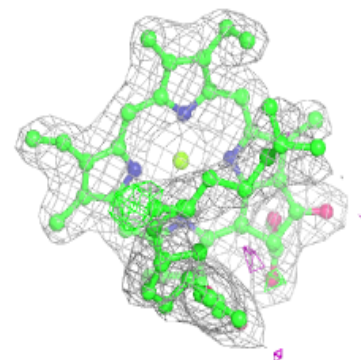
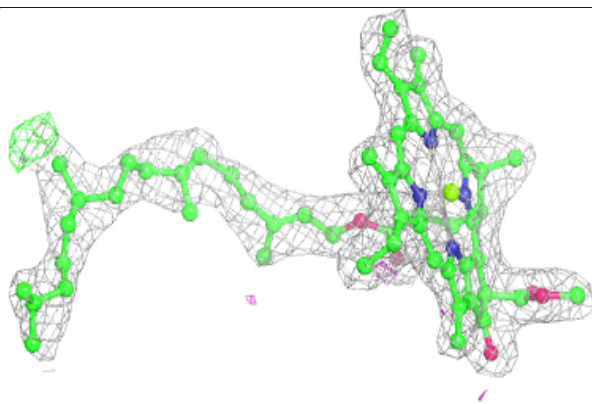
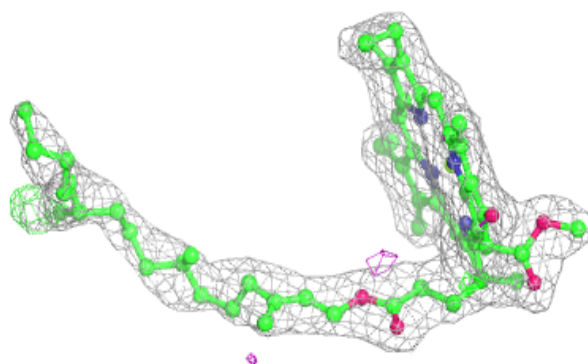


Electron density around CLA D 404:

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

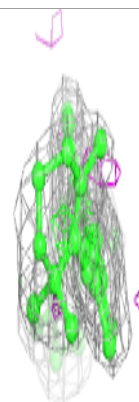
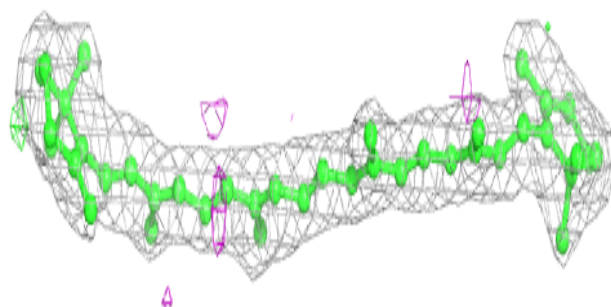
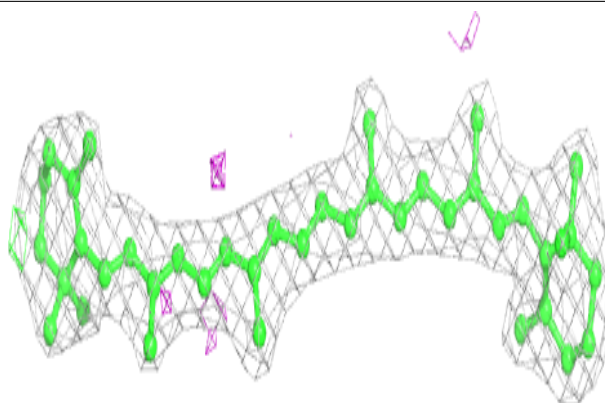
**Electron density around CLA b 608:**

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

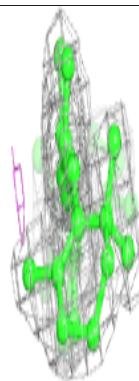
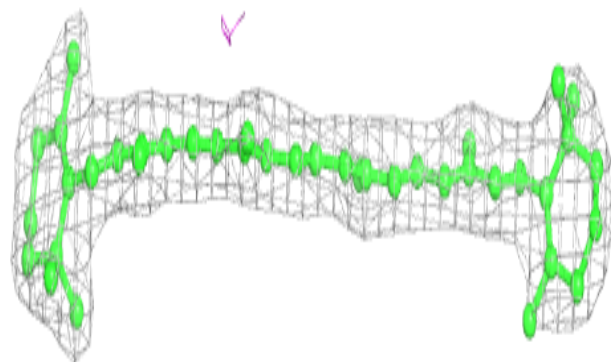
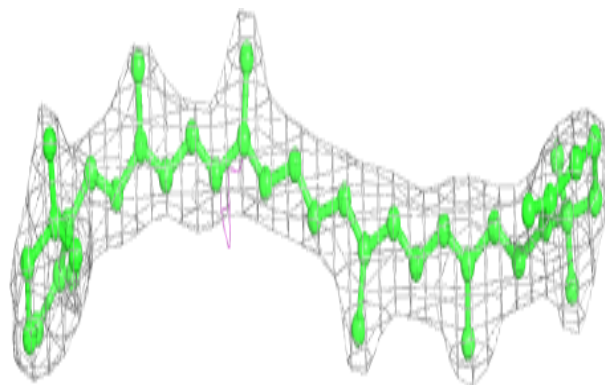


Electron density around BCR B 620:

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

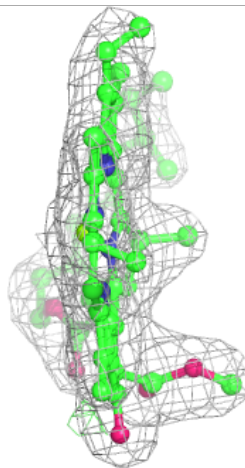
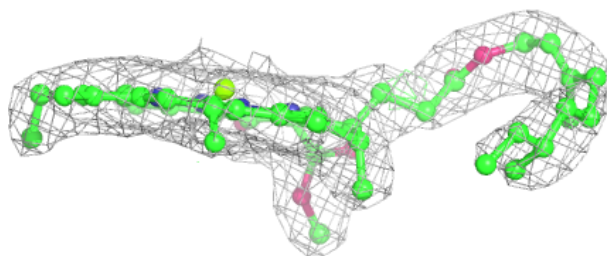
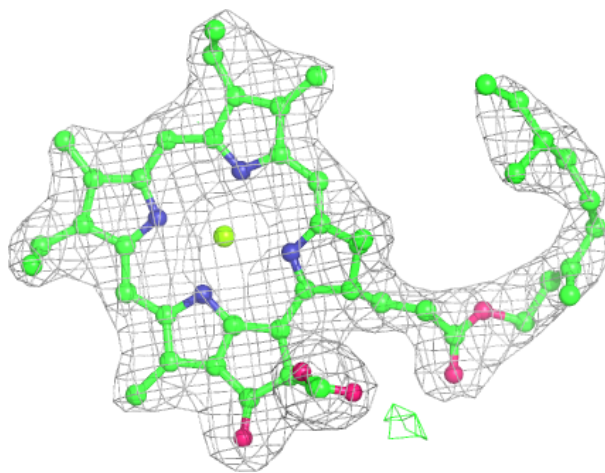
**Electron density around BCR C 516:**

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



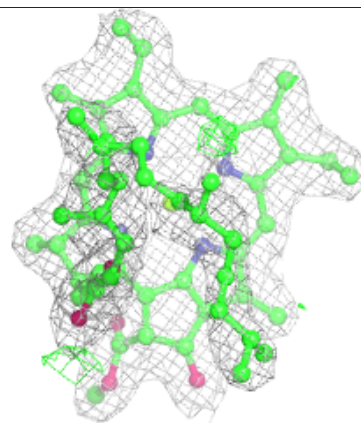
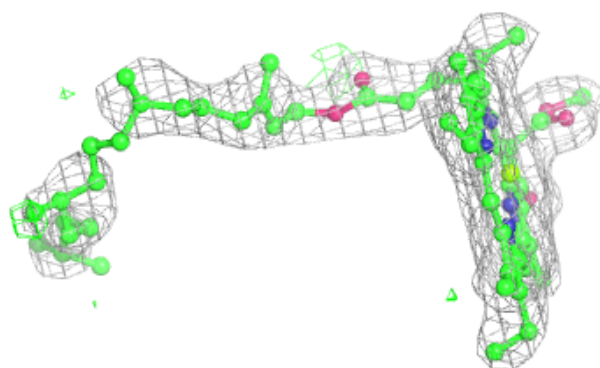
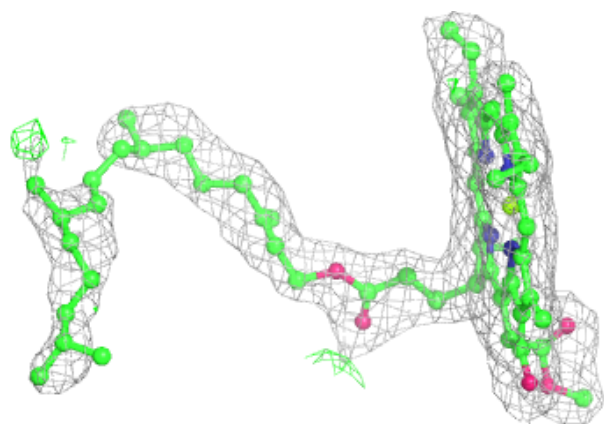
Electron density around CLA C 513:

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

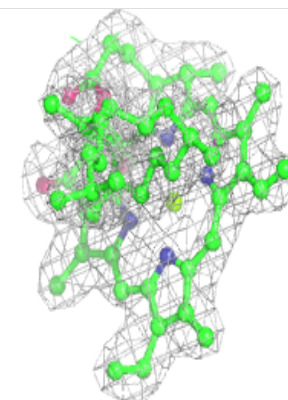
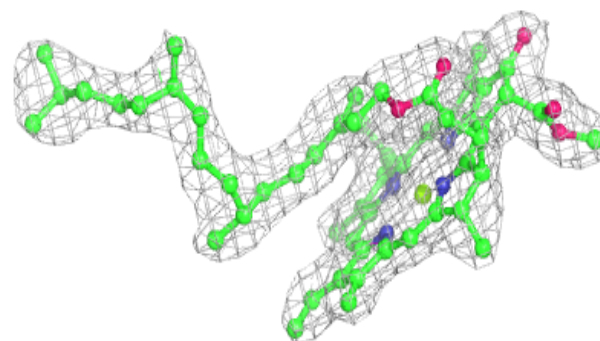
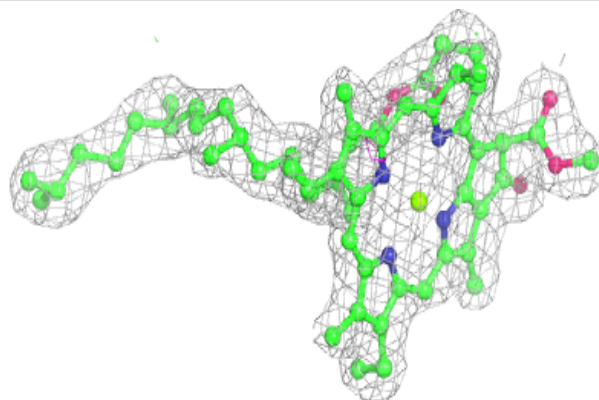


Electron density around CLA d 403:

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

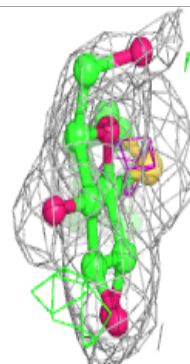
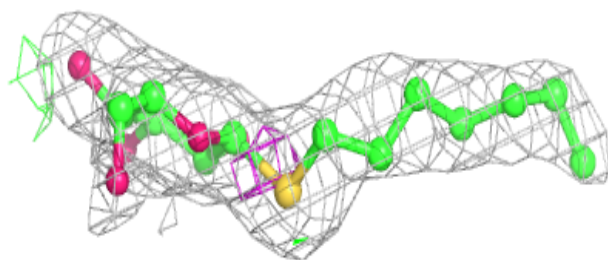
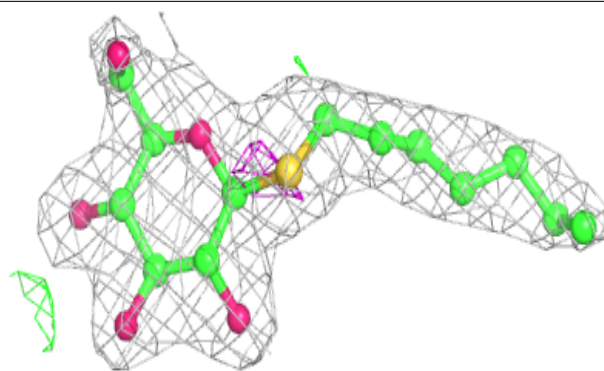
**Electron density around CLA c 906:**

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

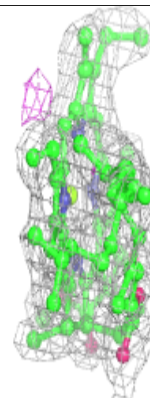
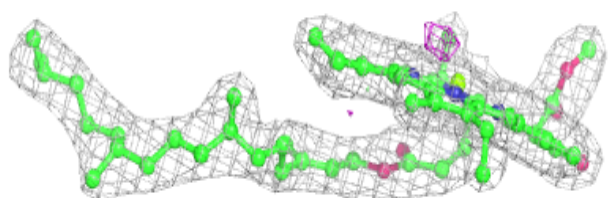
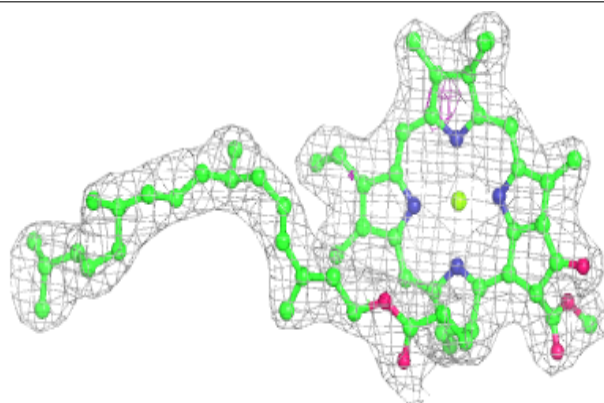


Electron density around HTG b 623:

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

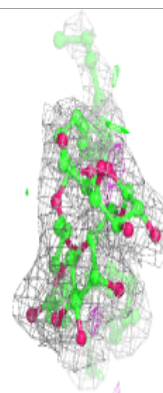
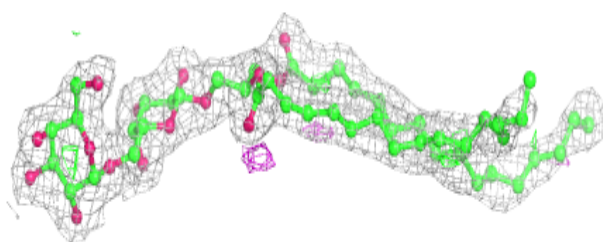
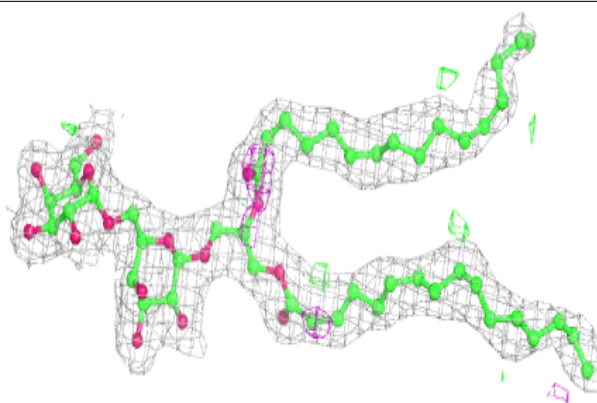
**Electron density around CLA B 604:**

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



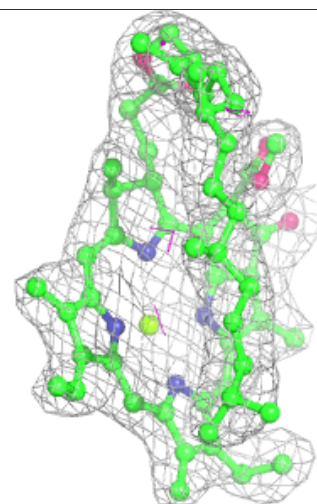
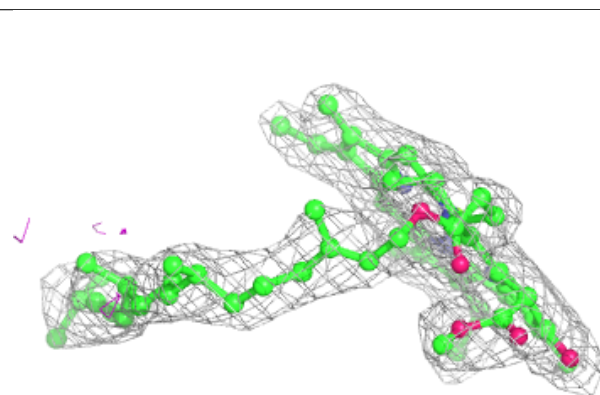
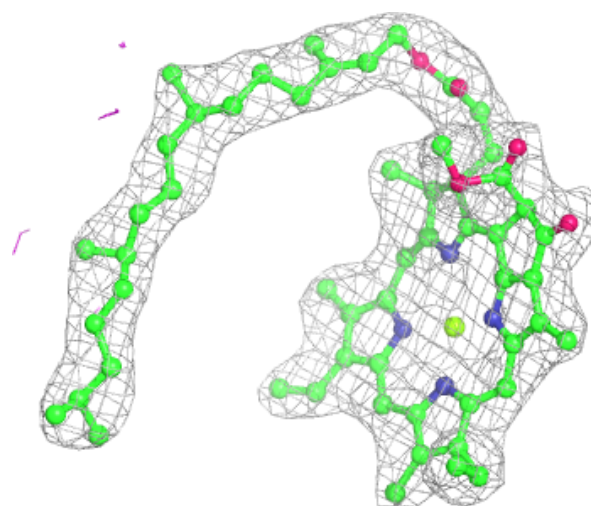
Electron density around DGD C 519:

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



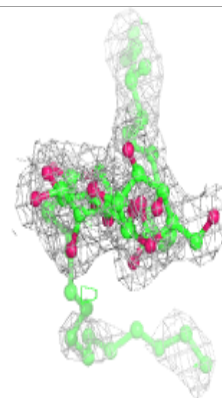
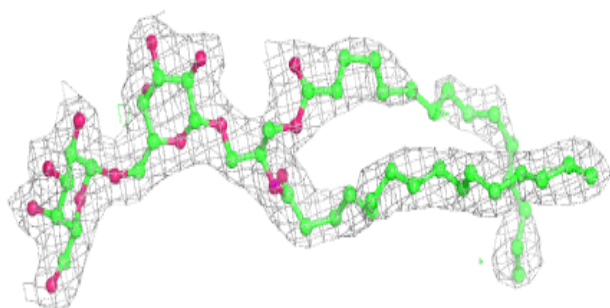
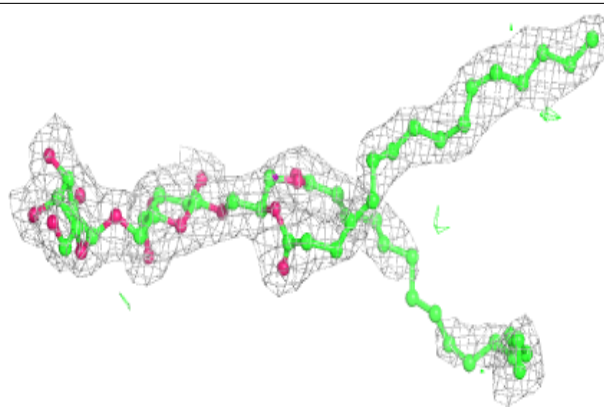
Electron density around CLA c 908:

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

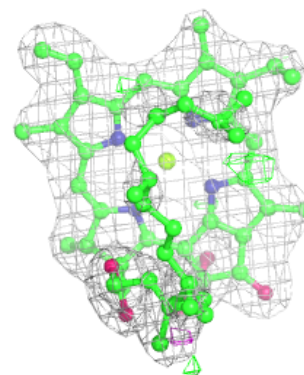
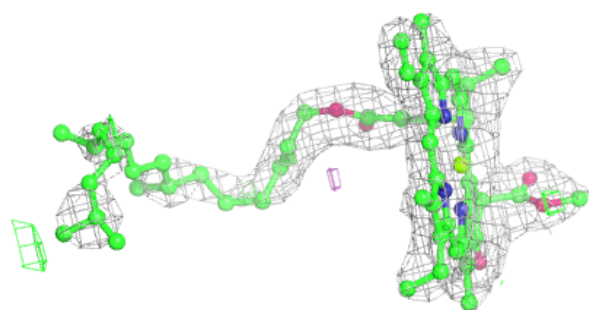
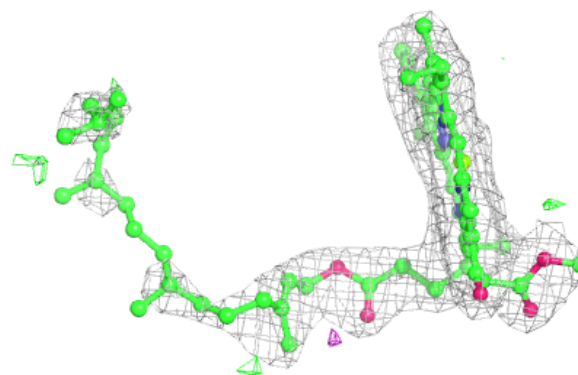


Electron density around DGD C 517:

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

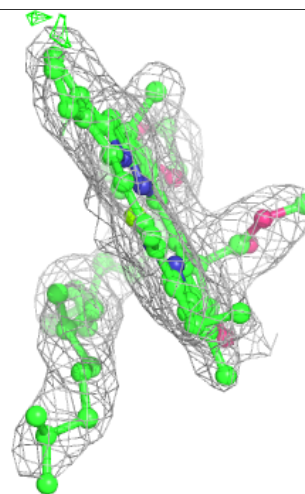
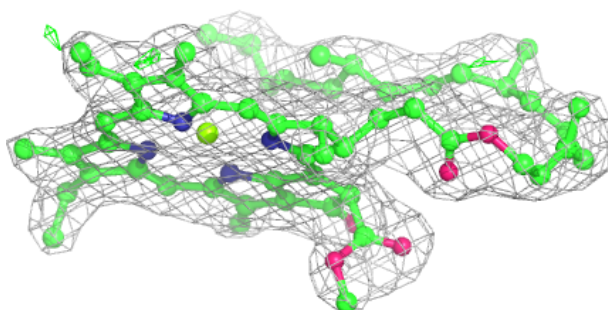
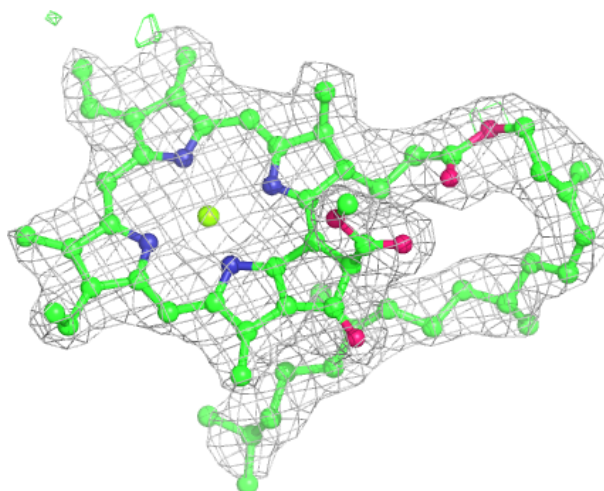
**Electron density around CLA c 907:**

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



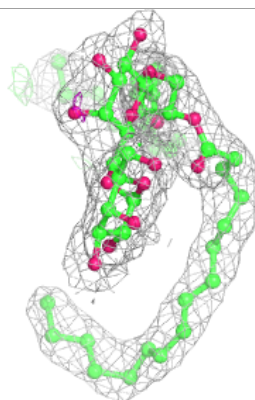
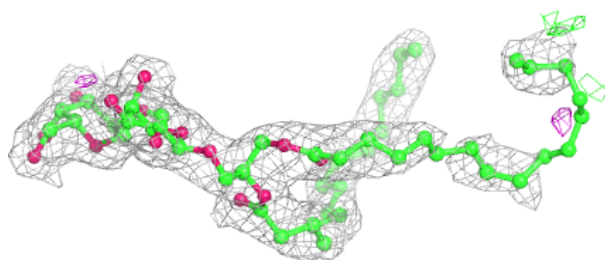
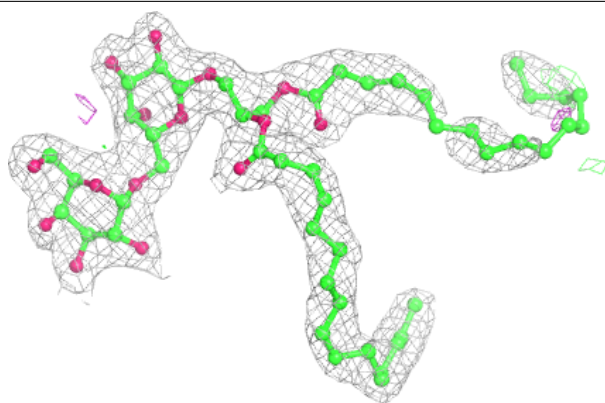
Electron density around CLA C 510:

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

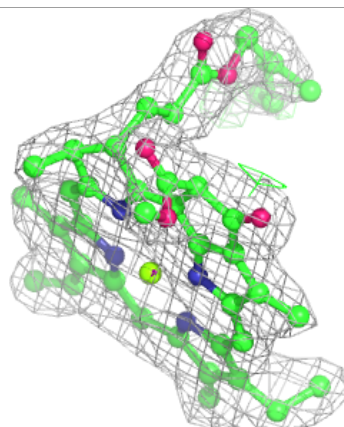
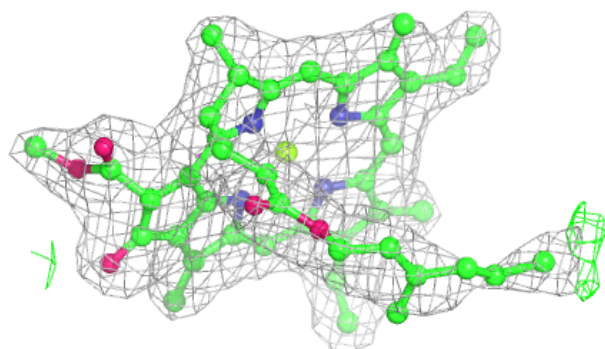
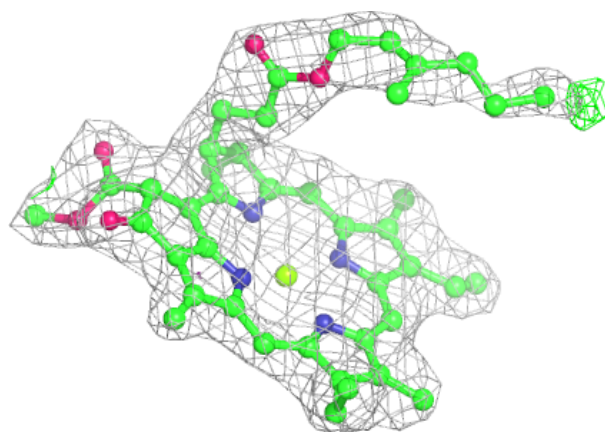


Electron density around DGD c 918:

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

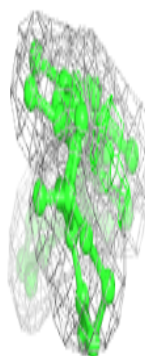
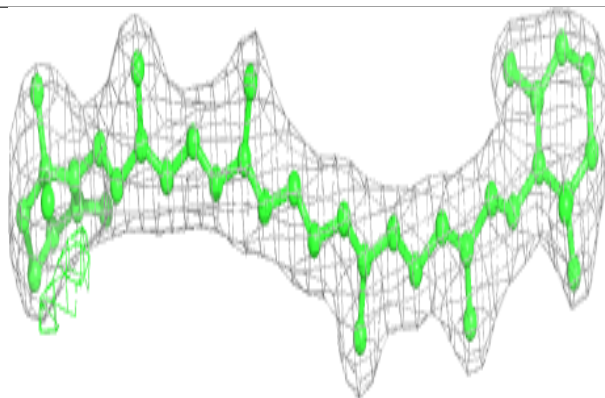
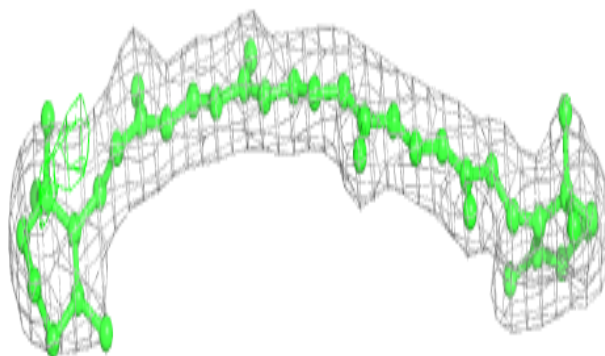
**Electron density around CLA b 615:**

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

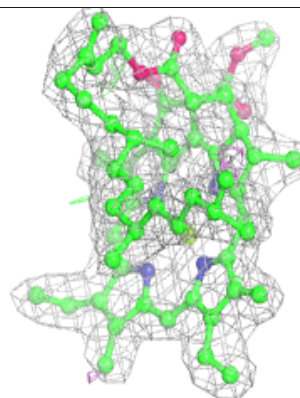
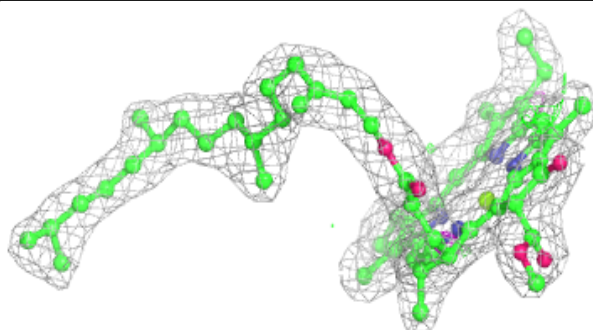
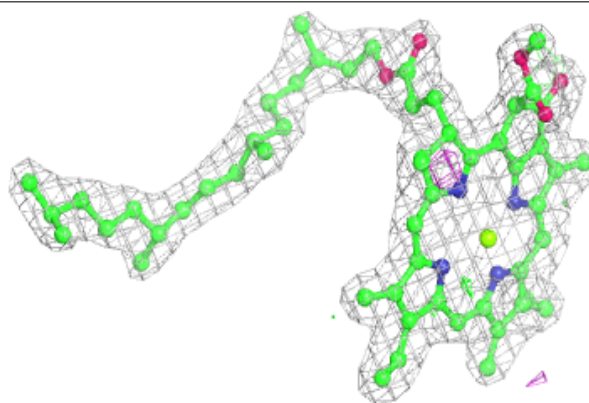


Electron density around BCR D 405:

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

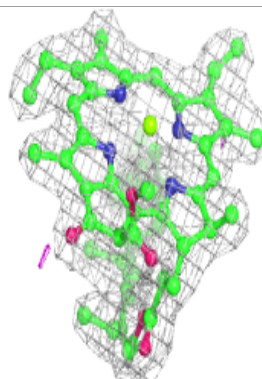
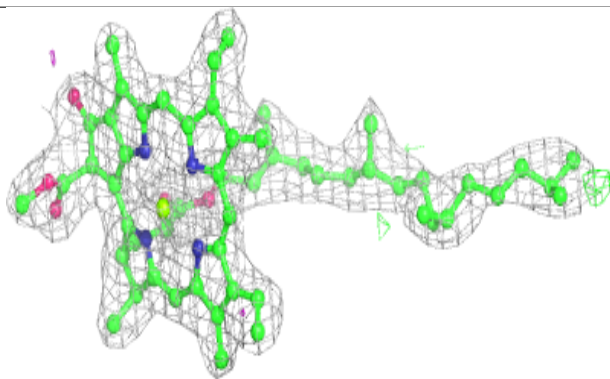
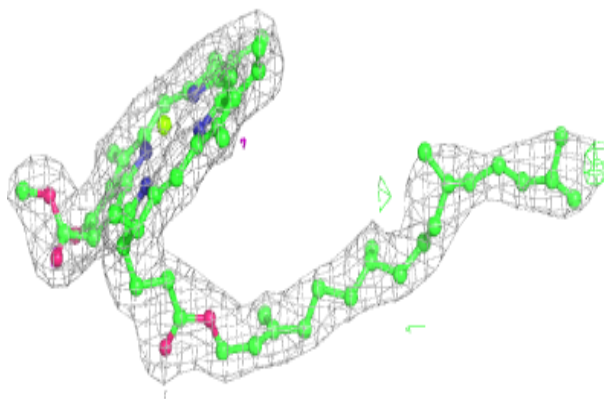
**Electron density around CLA C 512:**

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



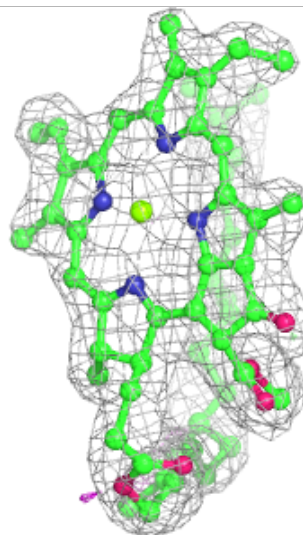
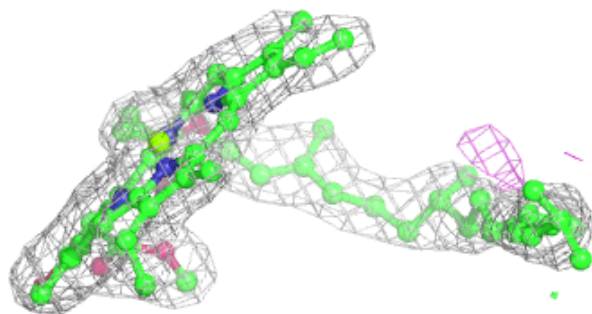
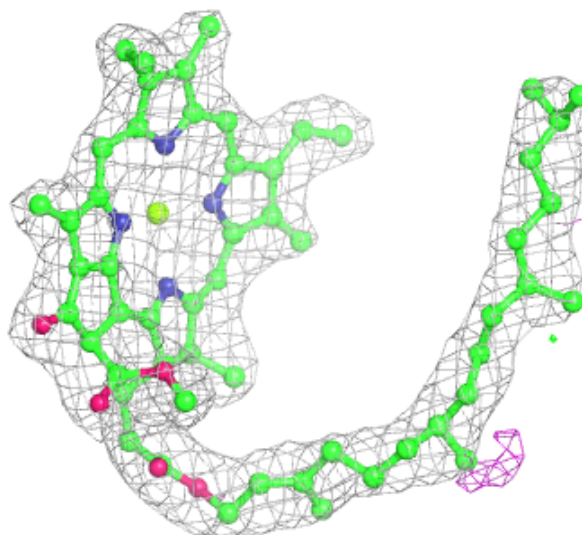
Electron density around CLA C 505:

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



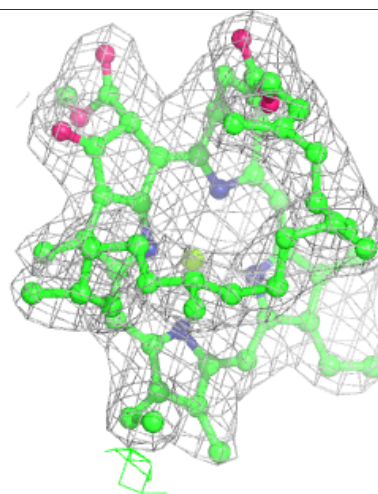
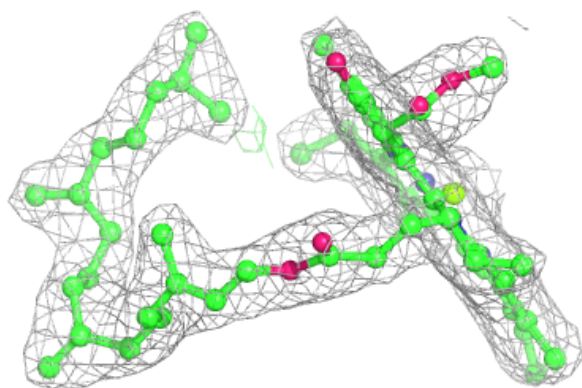
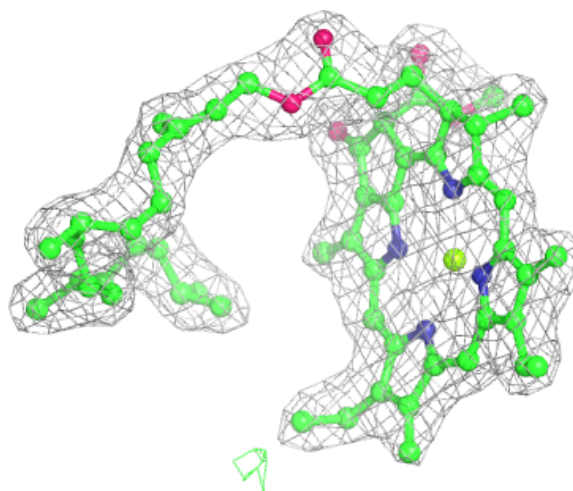
Electron density around CLA C 508:

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



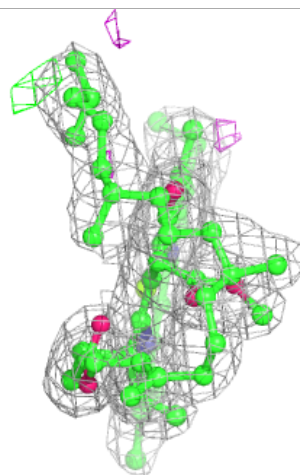
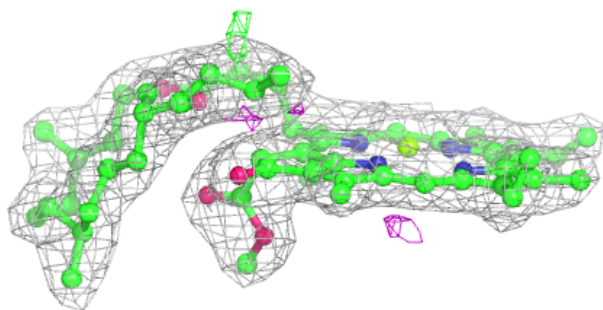
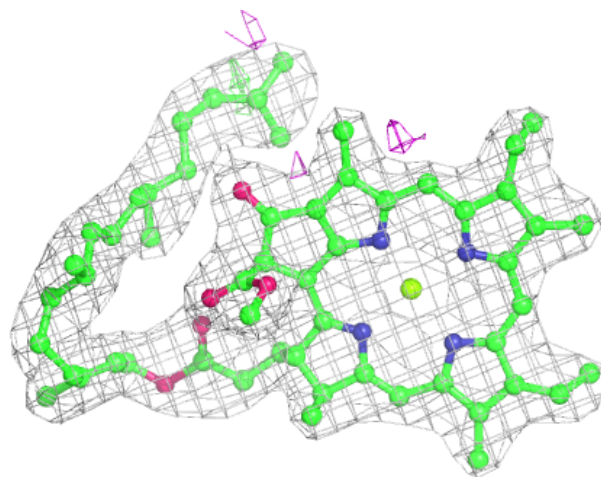
Electron density around CLA C 504:

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



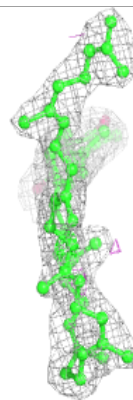
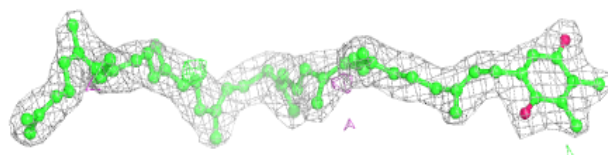
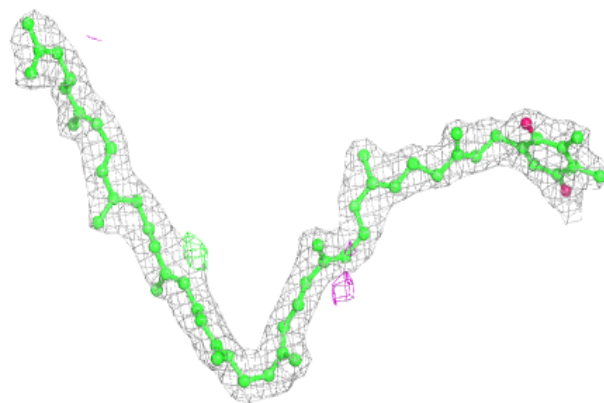
Electron density around CLA b 611:

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

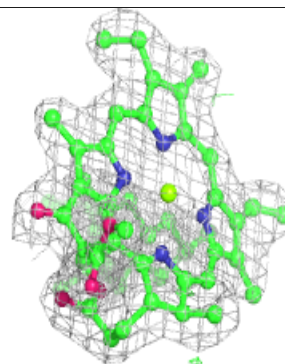
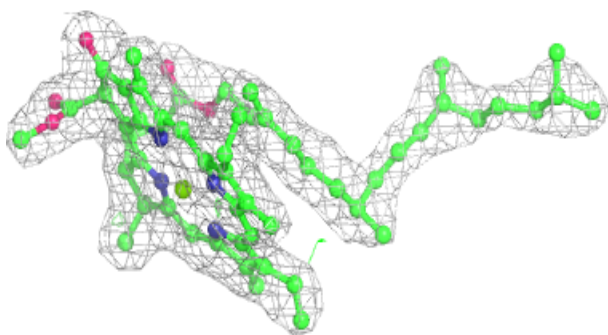
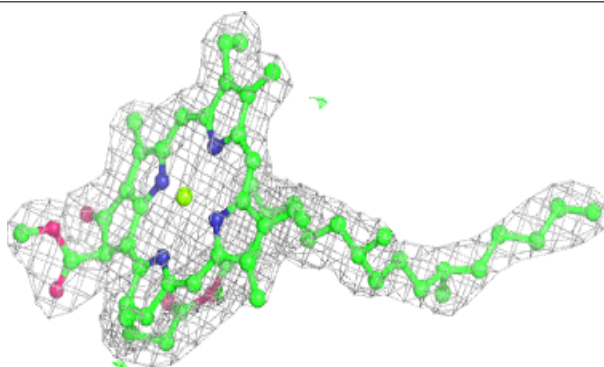


Electron density around PL9 d 405:

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

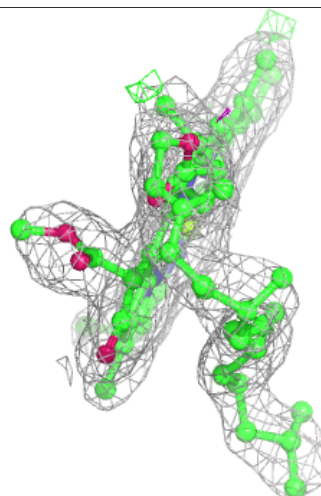
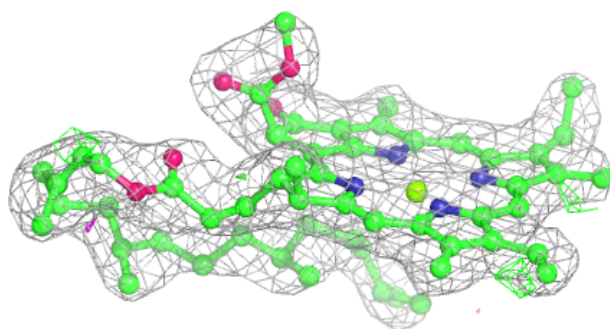
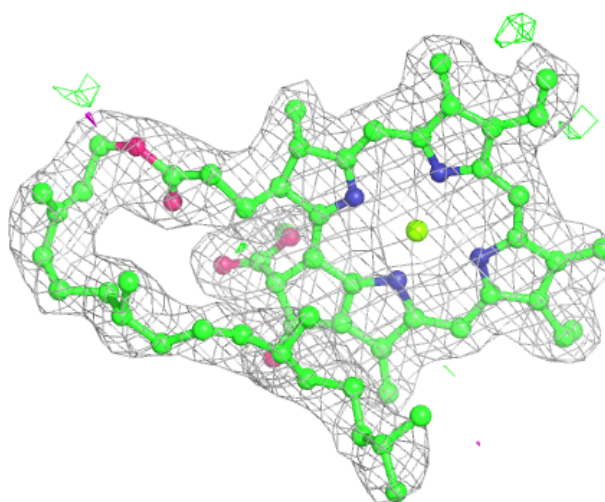
**Electron density around CLA C 506:**

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



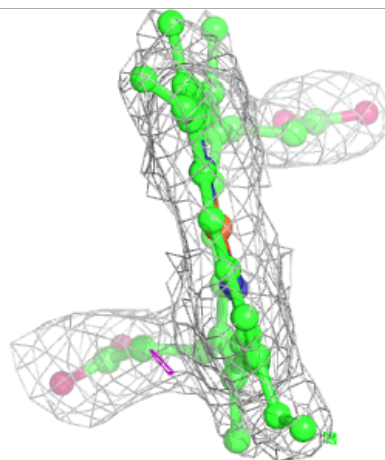
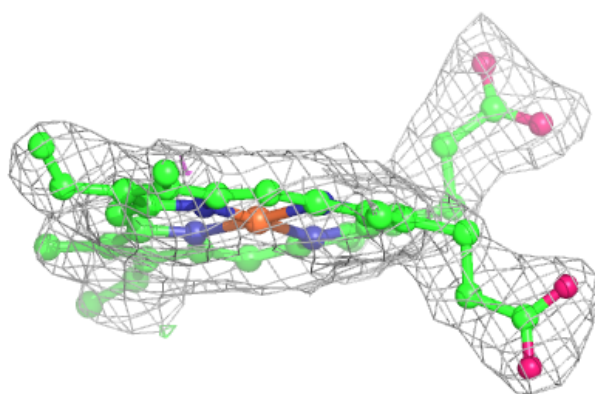
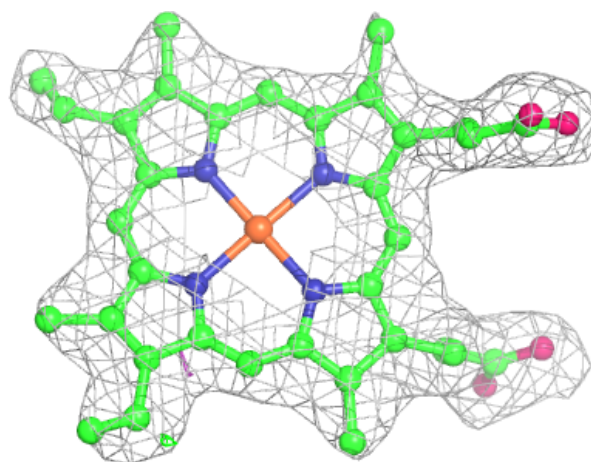
Electron density around CLA c 910:

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



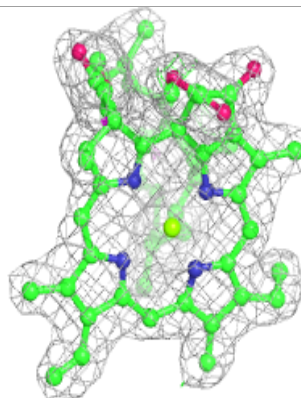
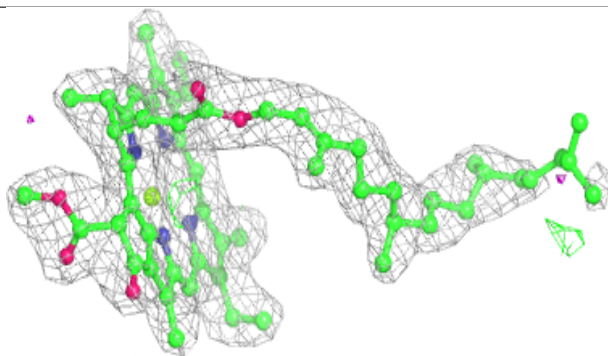
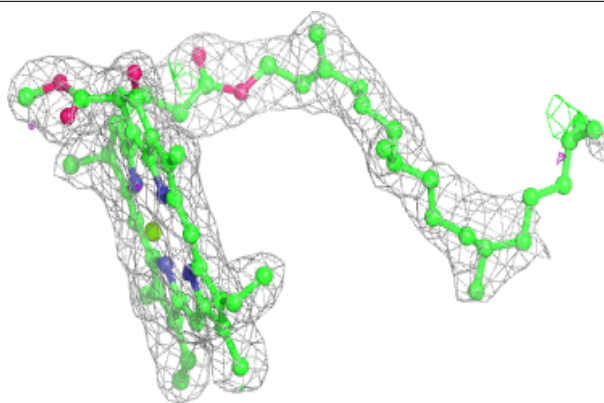
Electron density around HEM E 102:

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

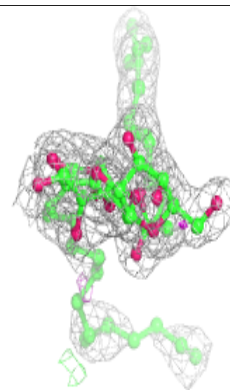
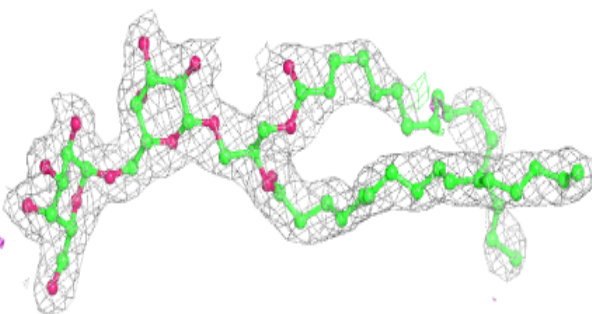
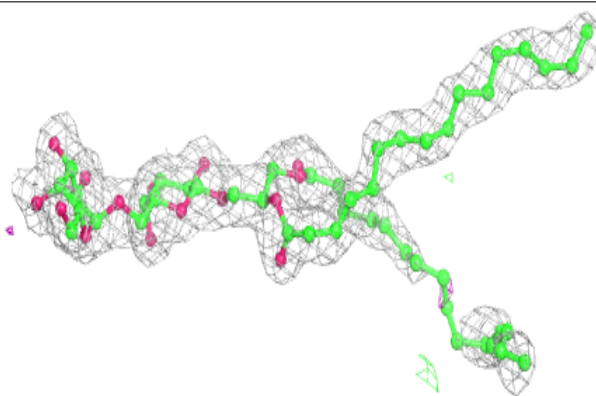


Electron density around CLA c 909:

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

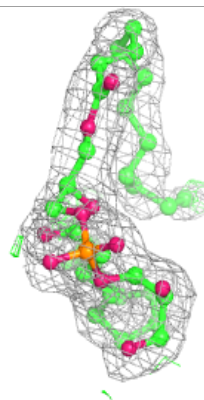
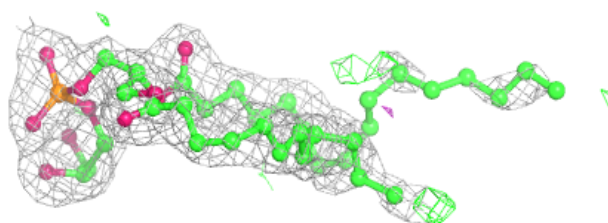
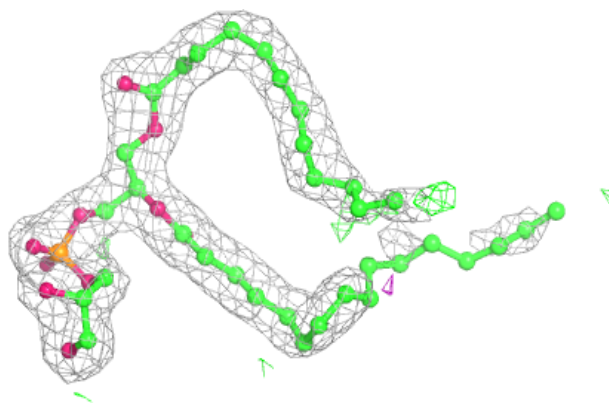
**Electron density around DGD c 917:**

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

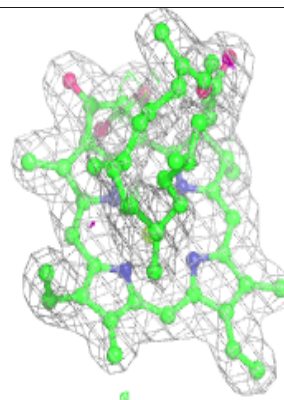
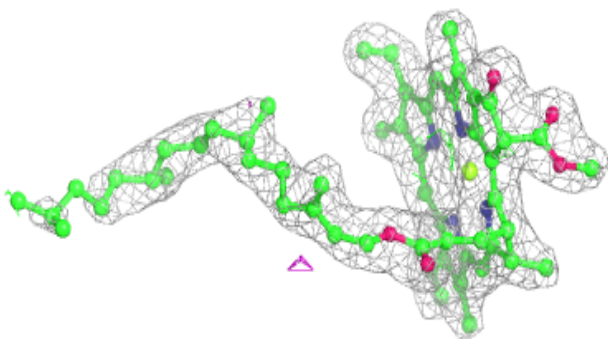
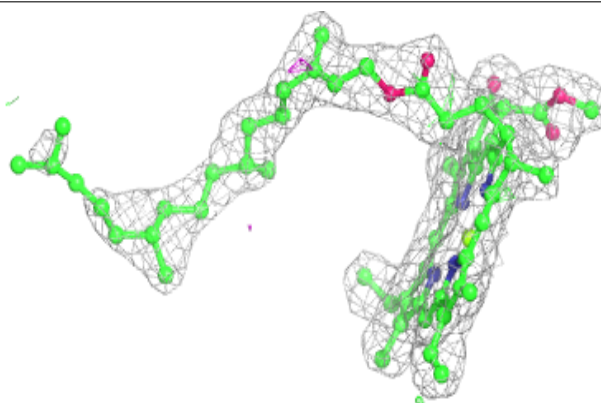


Electron density around LHG D 411:

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

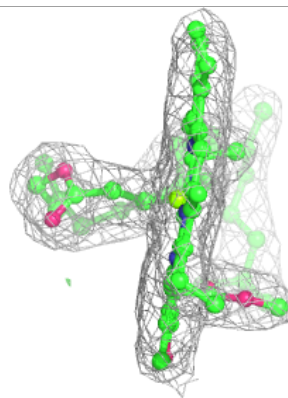
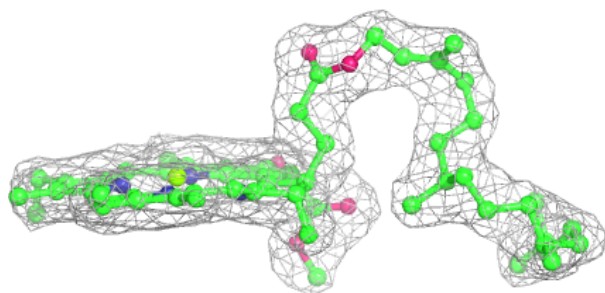
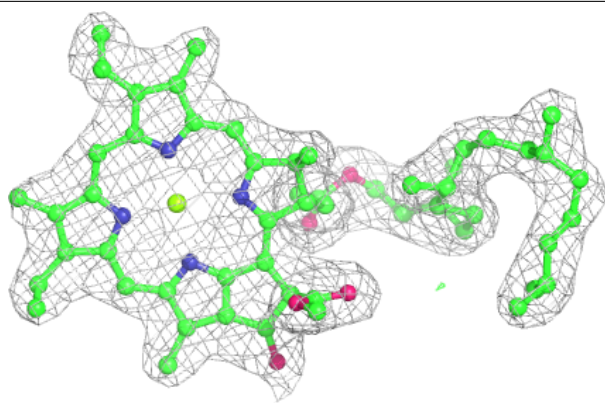
**Electron density around CLA C 509:**

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

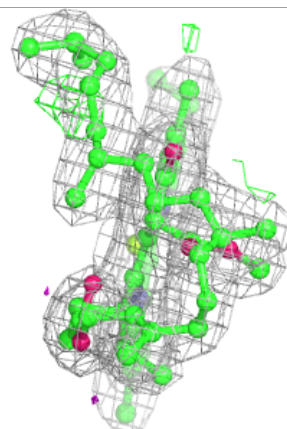
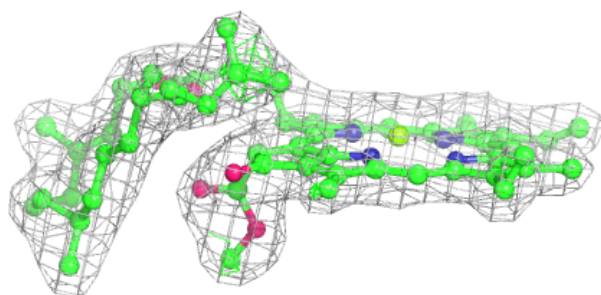
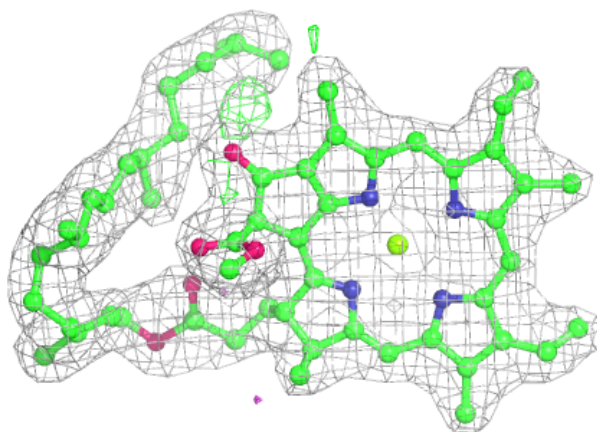


Electron density around CLA b 613:

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

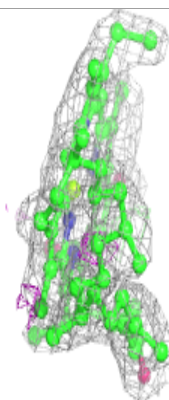
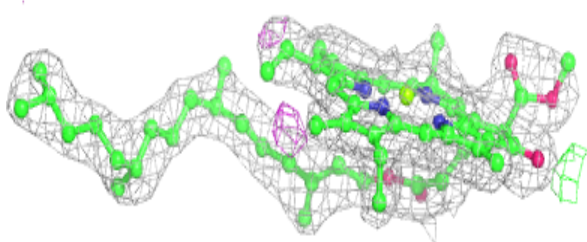
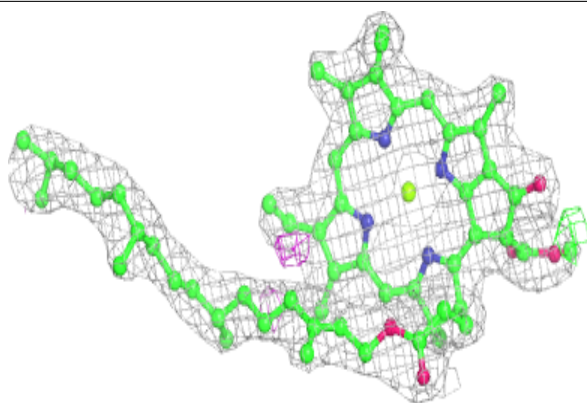
**Electron density around CLA B 611:**

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

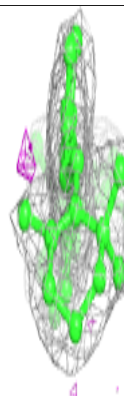
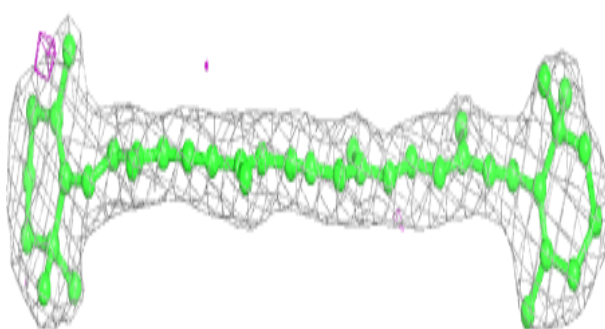
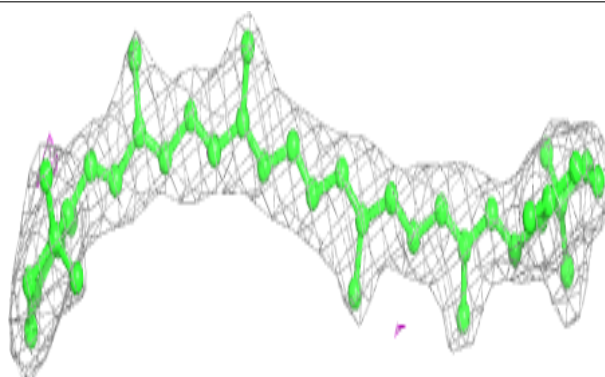


Electron density around CLA c 902:

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

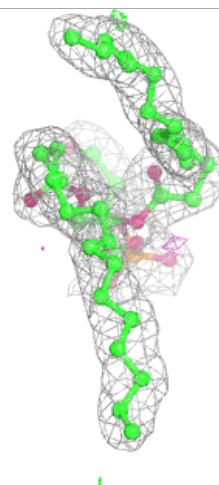
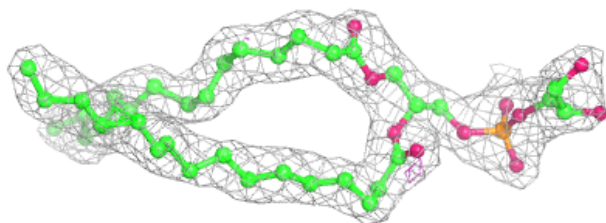
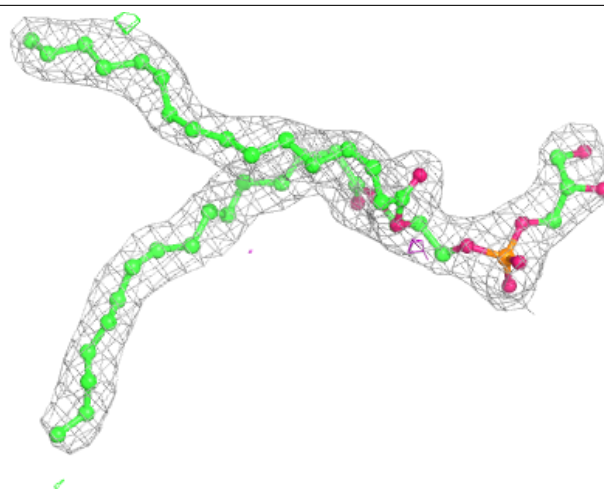
**Electron density around BCR c 916:**

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



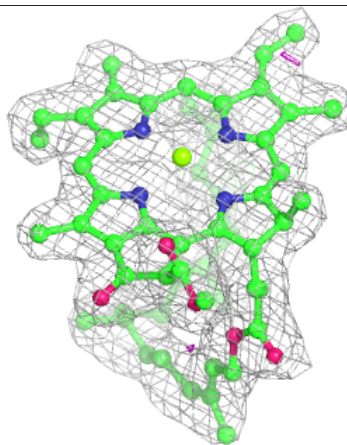
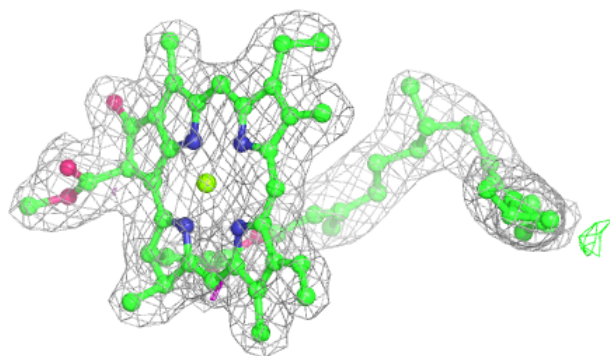
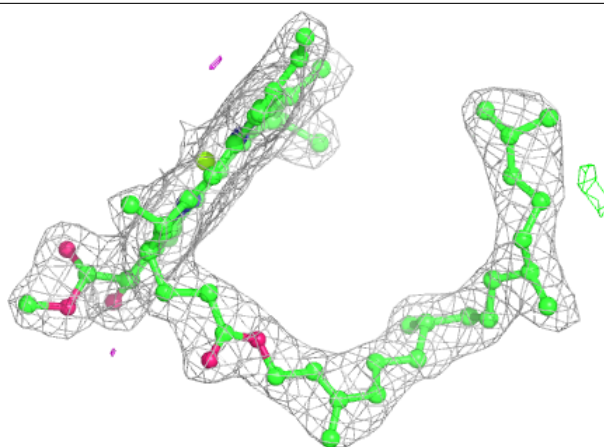
Electron density around LHG d 407:

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

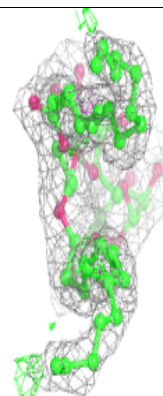
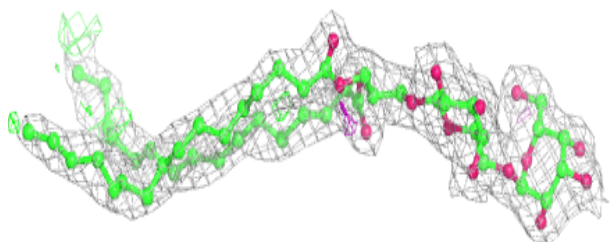
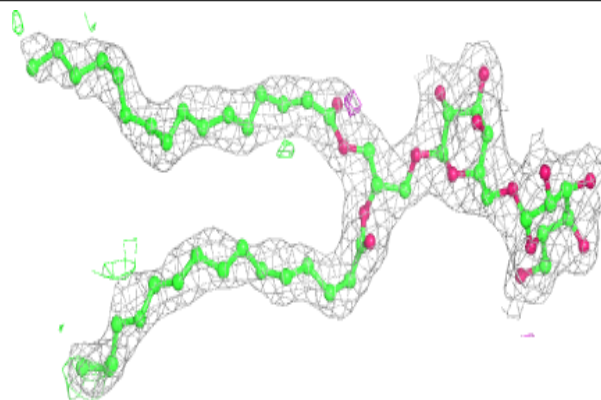


Electron density around CLA B 612:

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

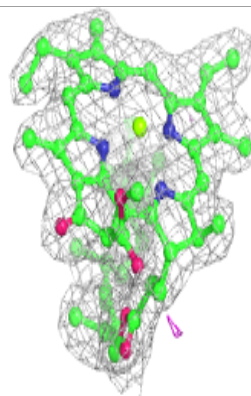
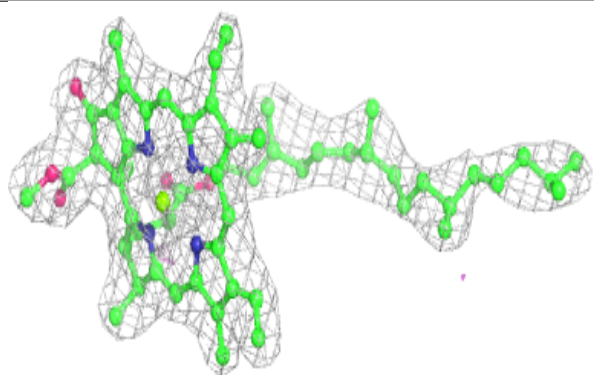
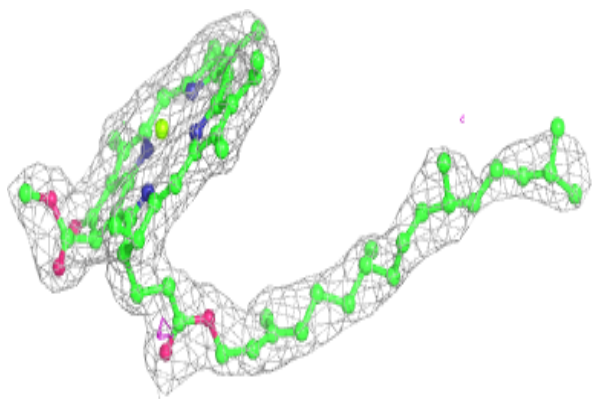
**Electron density around DGD c 919:**

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



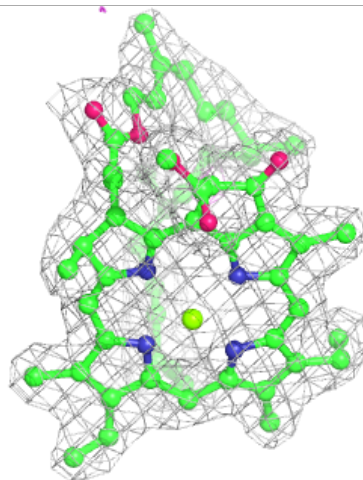
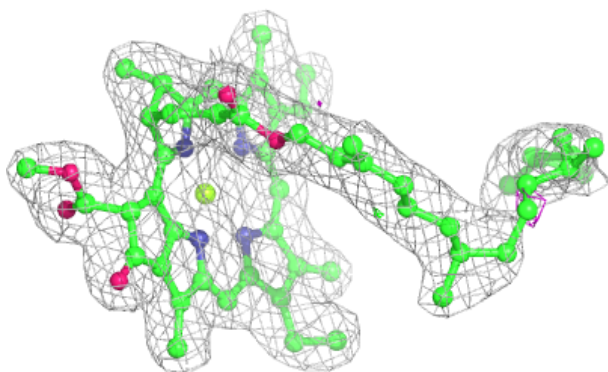
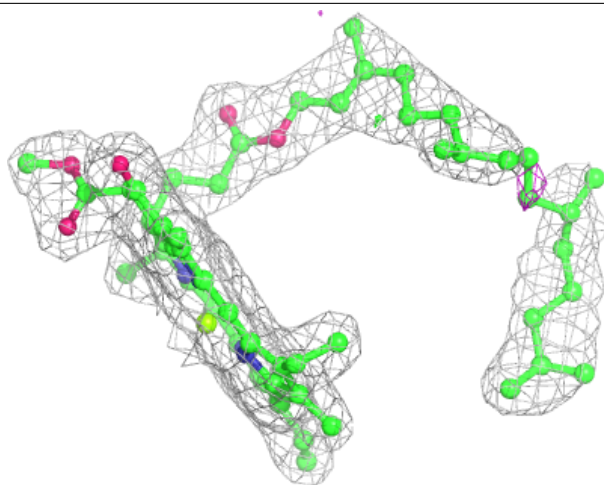
Electron density around CLA c 905:

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



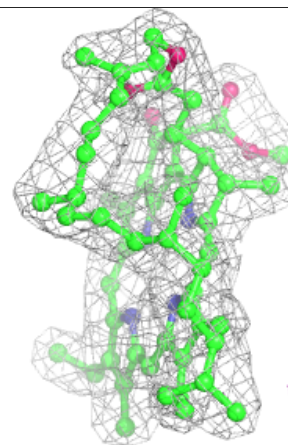
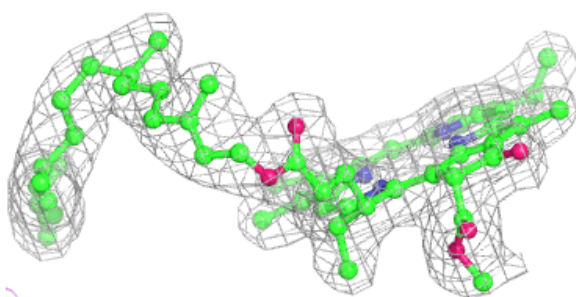
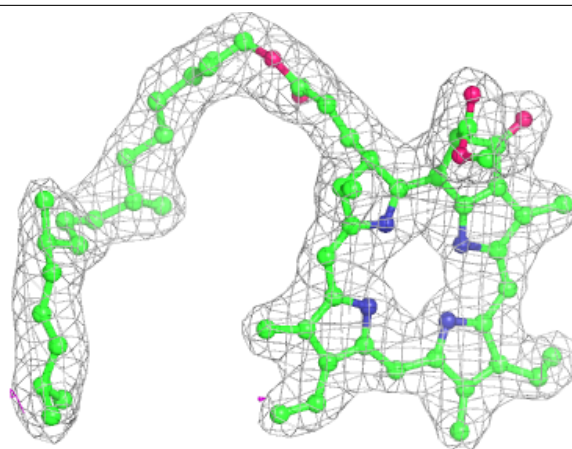
Electron density around CLA b 612:

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

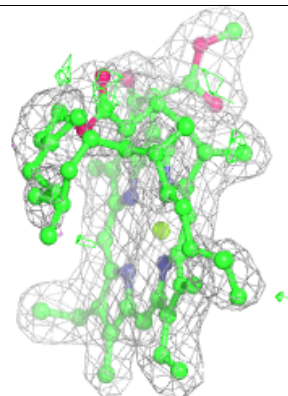
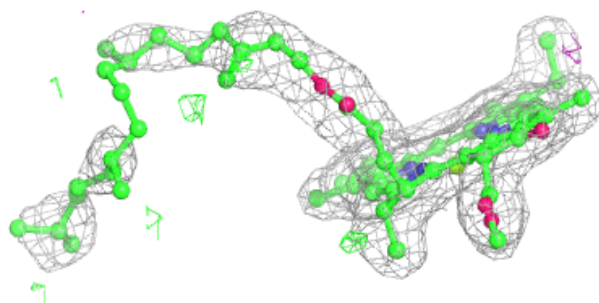
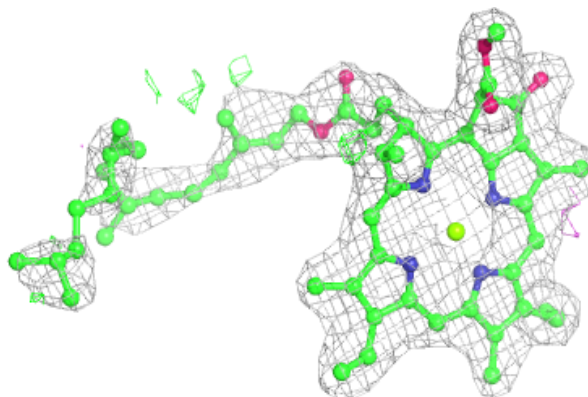


Electron density around PHO a 411:

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

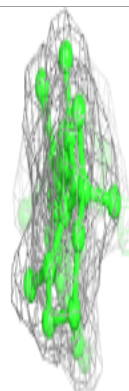
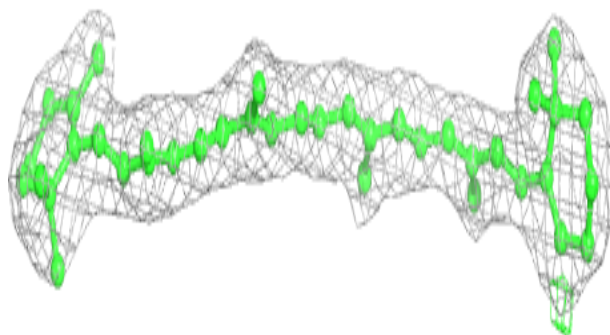
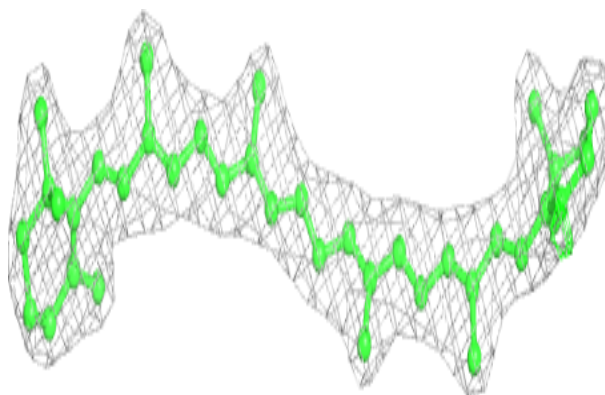
**Electron density around CLA a 412:**

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

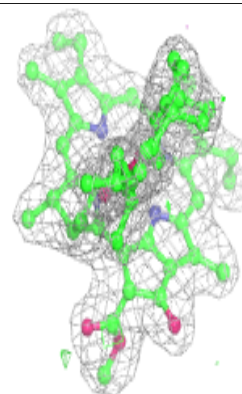
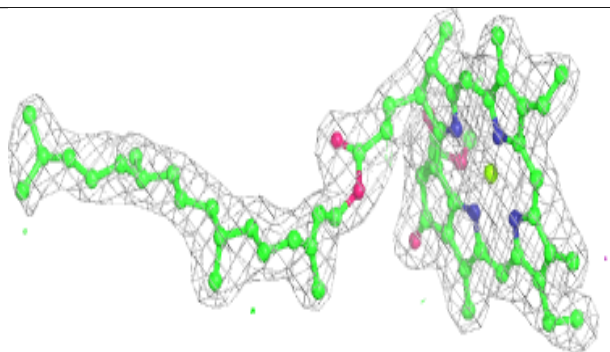
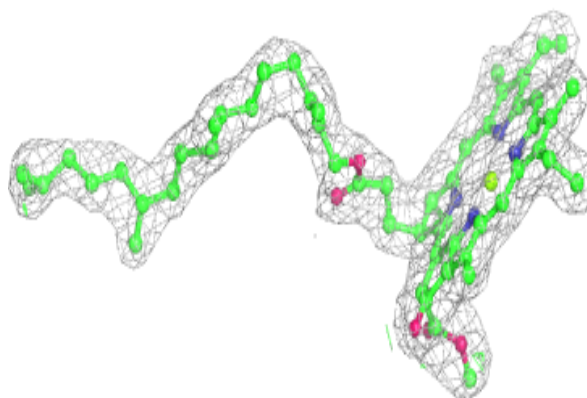


Electron density around BCR Y 101:

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

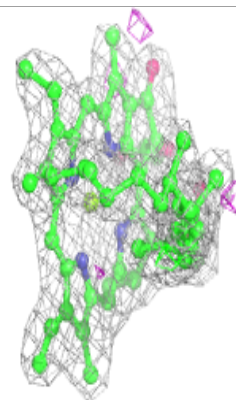
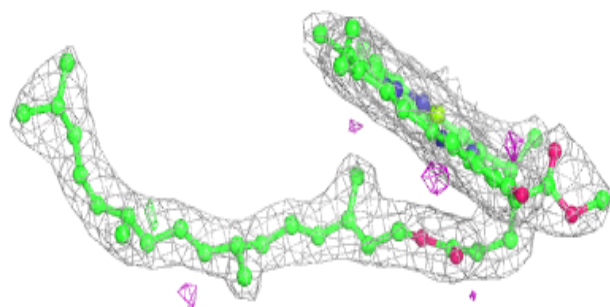
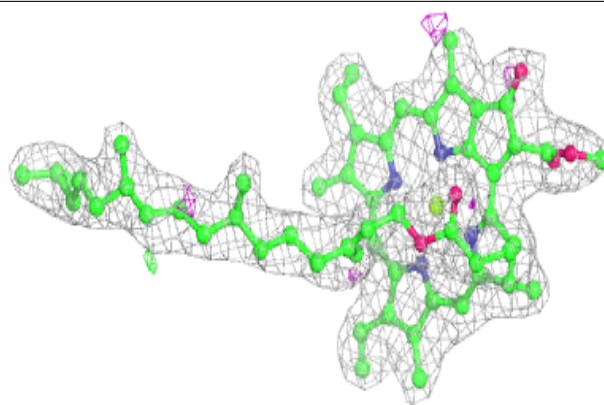
**Electron density around CLA C 503:**

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

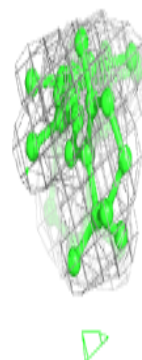
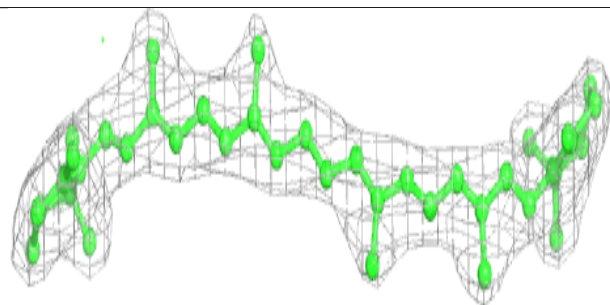
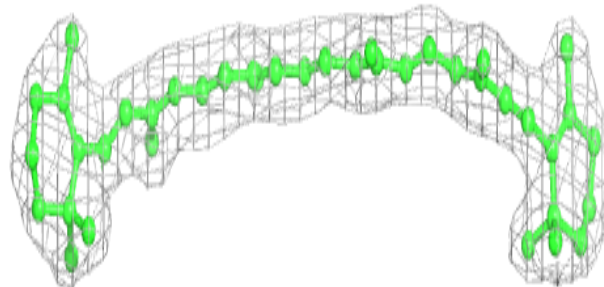


Electron density around CLA b 609:

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

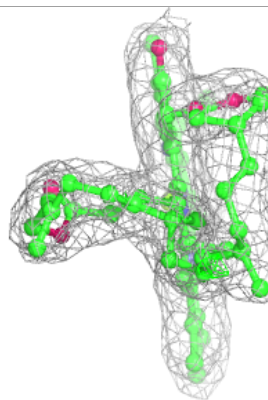
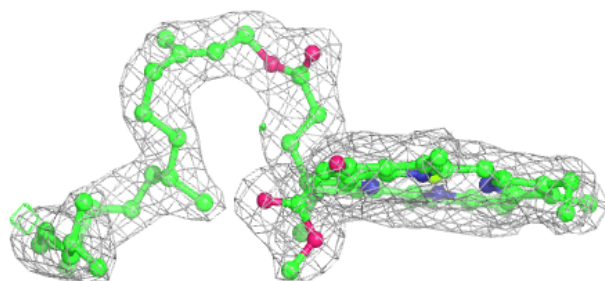
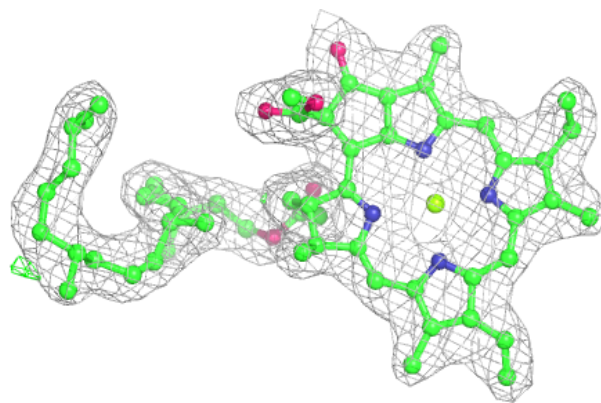
**Electron density around BCR K 101:**

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



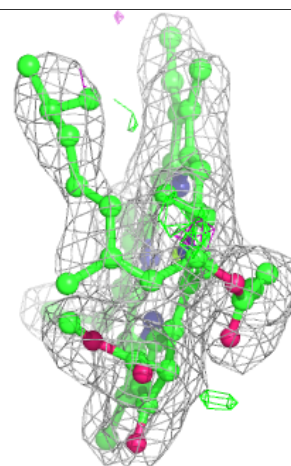
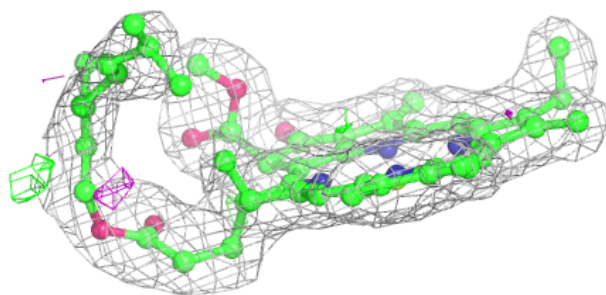
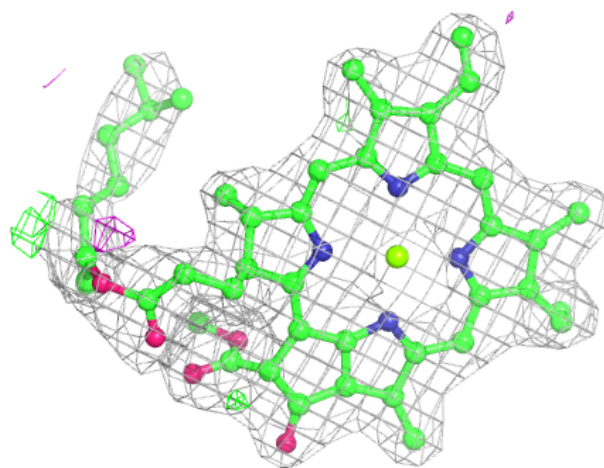
Electron density around CLA B 613:

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



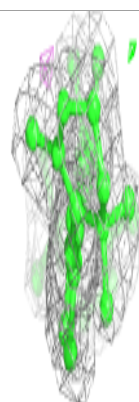
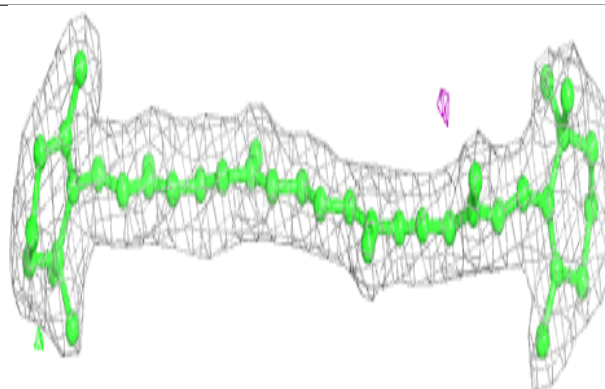
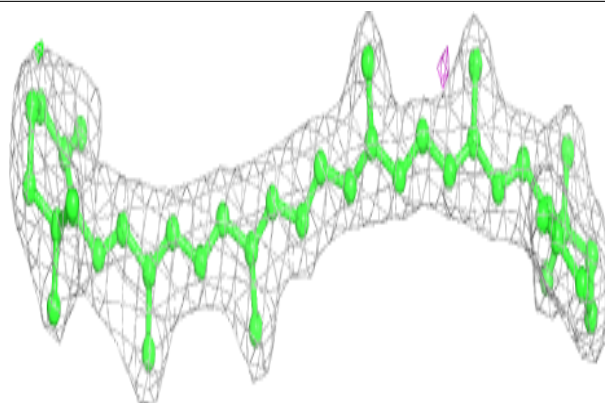
Electron density around CLA B 617:

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

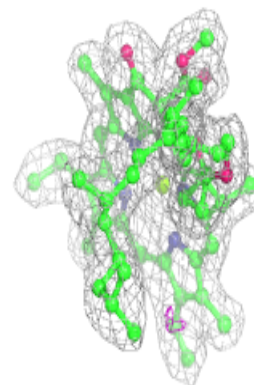
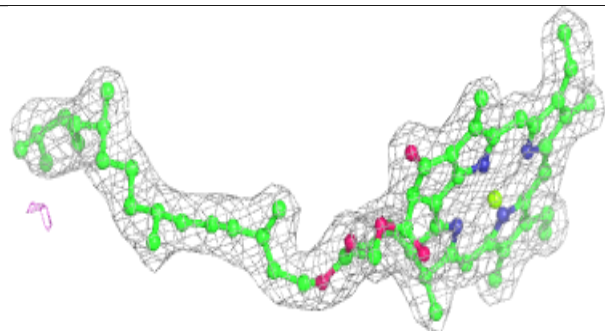
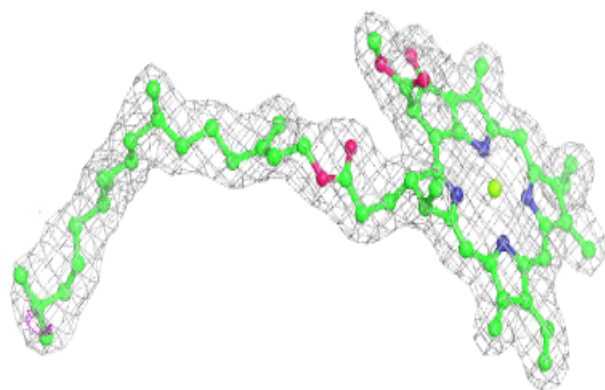


Electron density around BCR a 413:

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

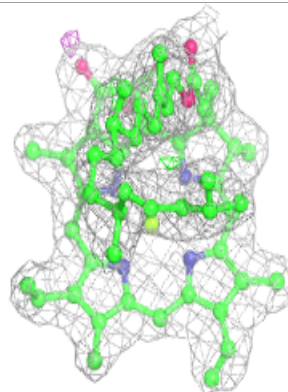
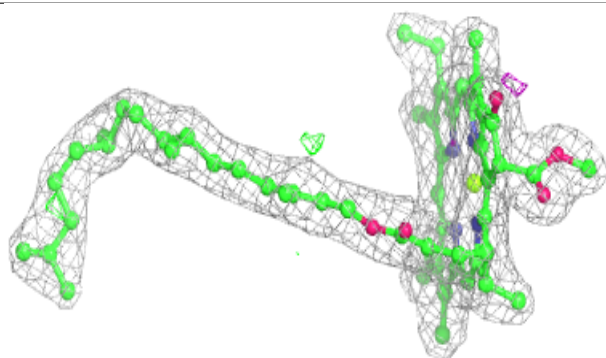
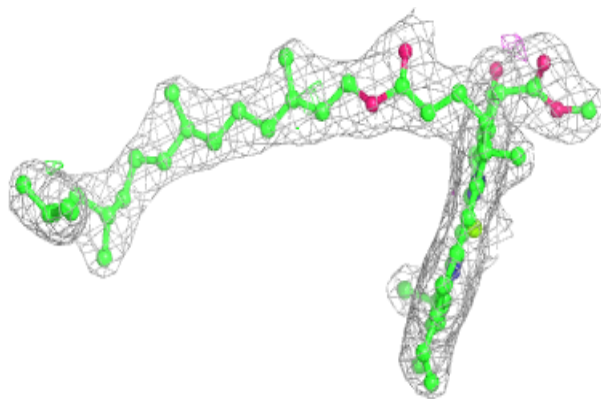
**Electron density around CLA A 405:**

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

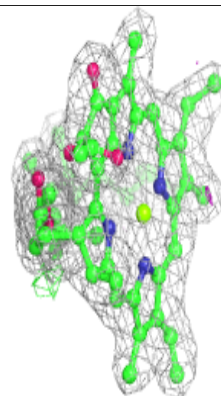
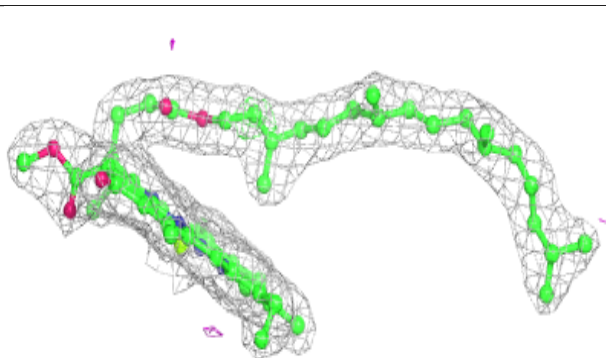
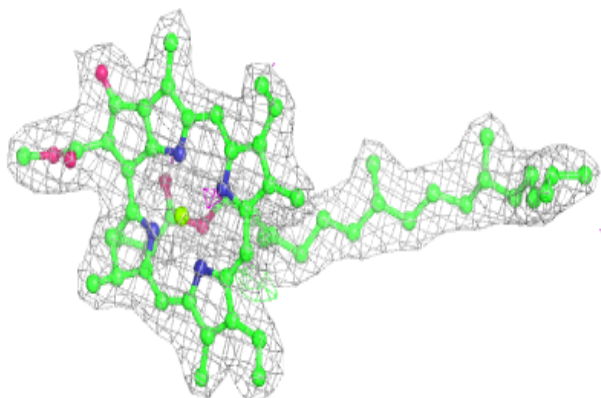


Electron density around CLA b 606:

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

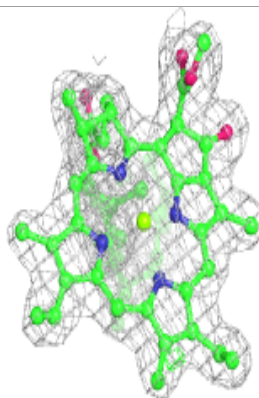
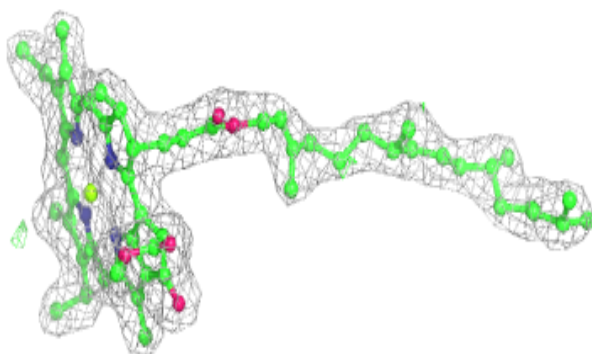
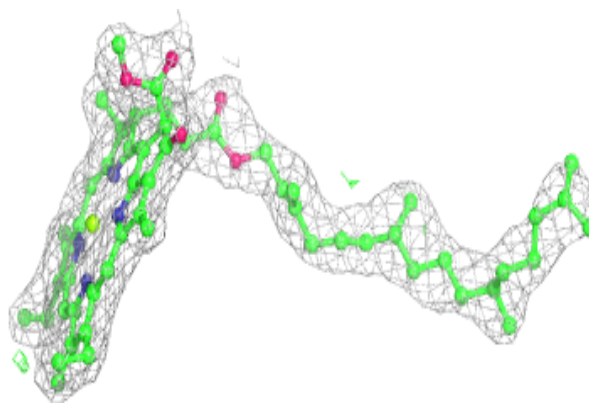
**Electron density around CLA B 609:**

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

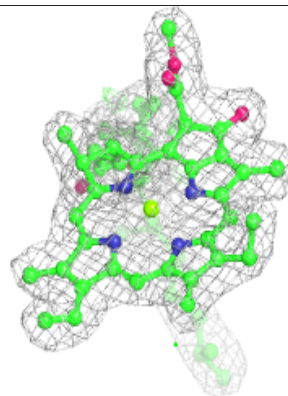
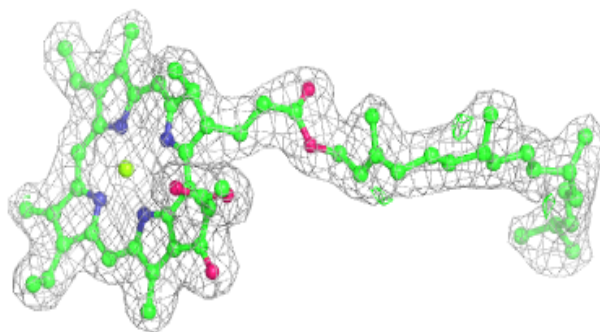
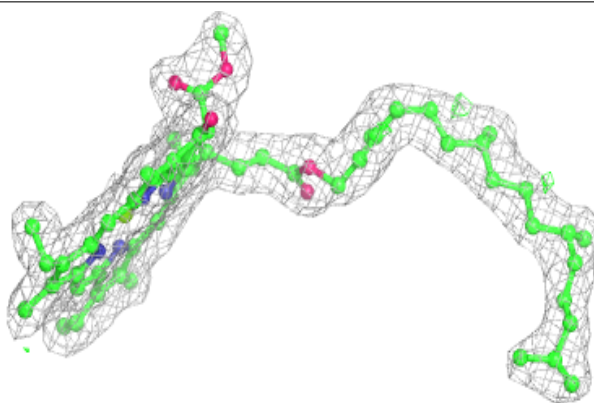


Electron density around CLA b 605:

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

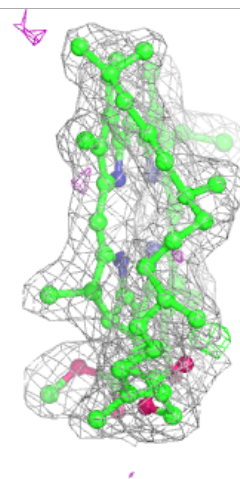
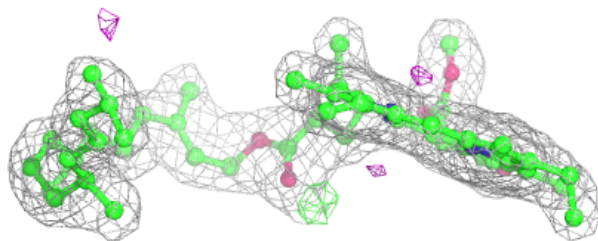
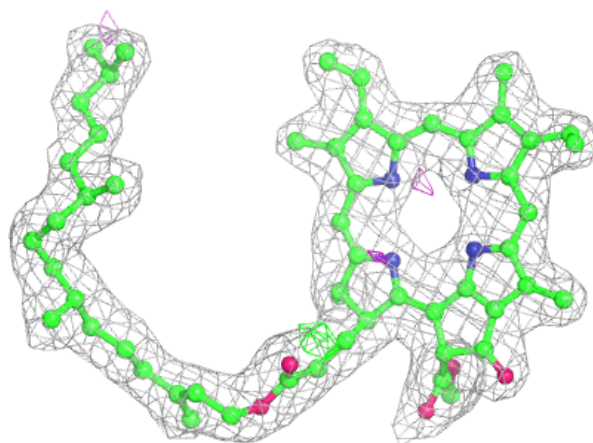
**Electron density around CLA D 403:**

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



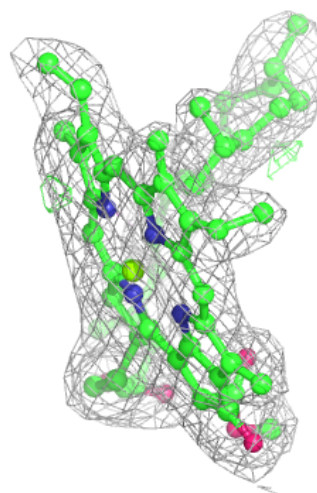
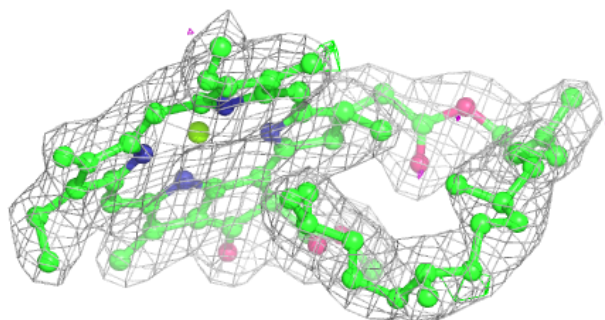
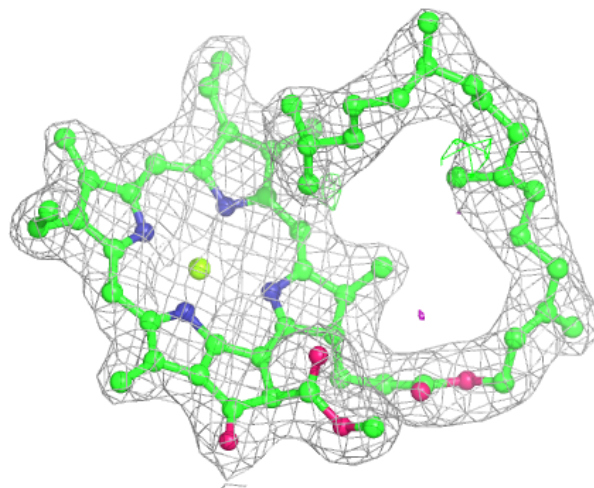
Electron density around PHO a 410:

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



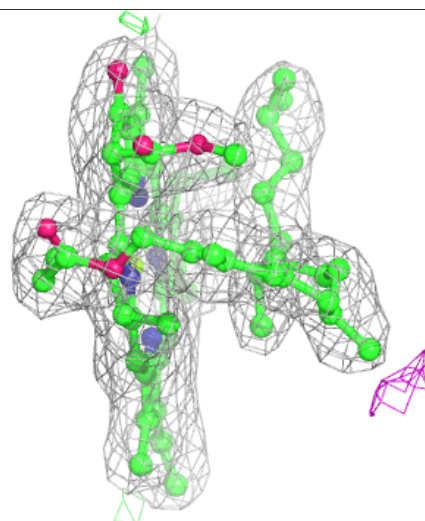
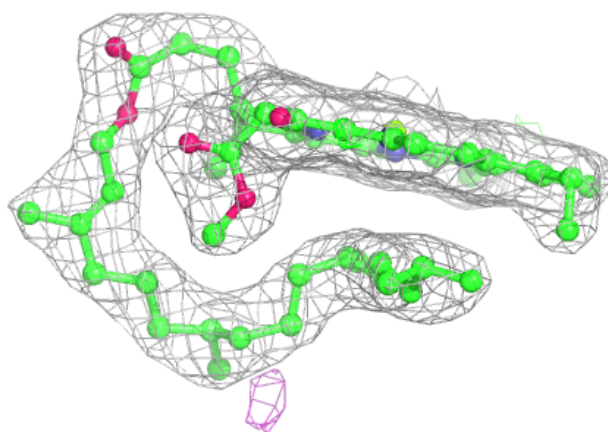
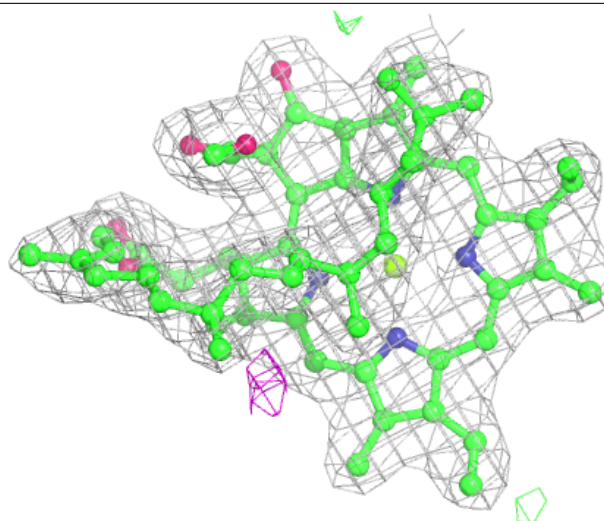
Electron density around CLA B 616:

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



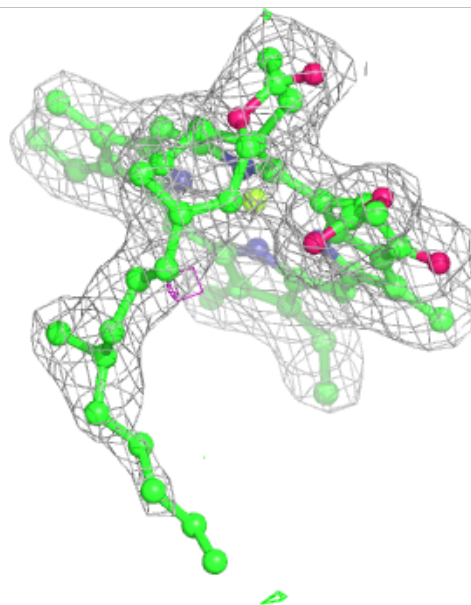
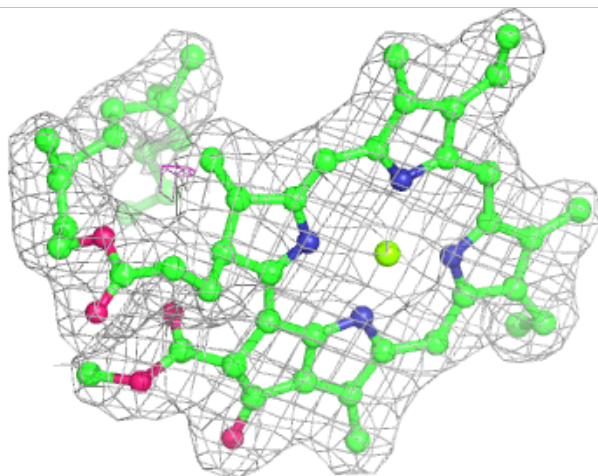
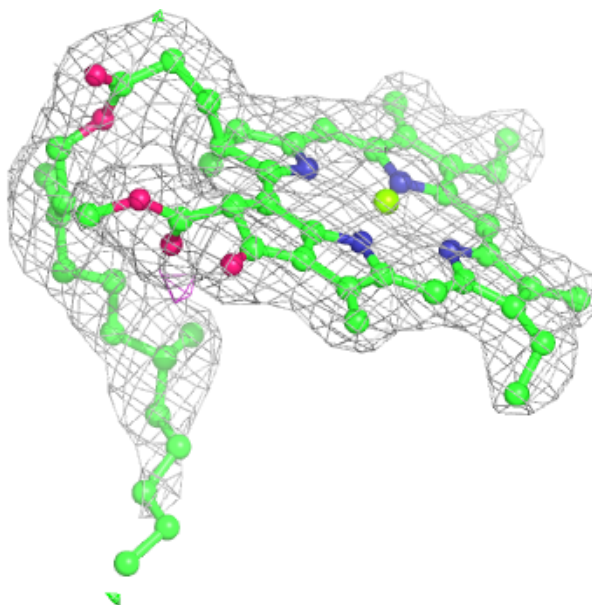
Electron density around CLA c 911:

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



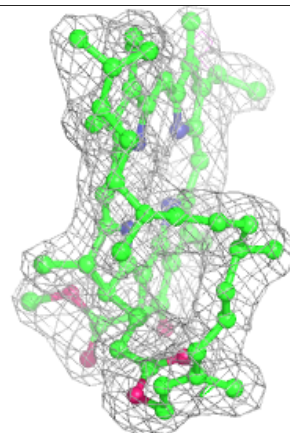
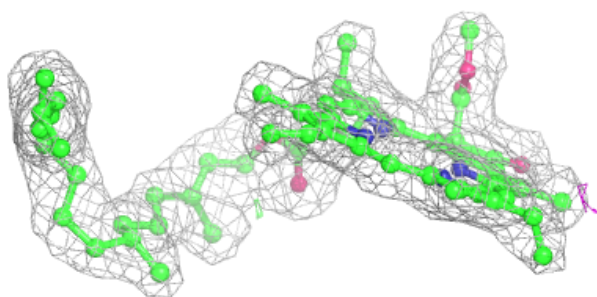
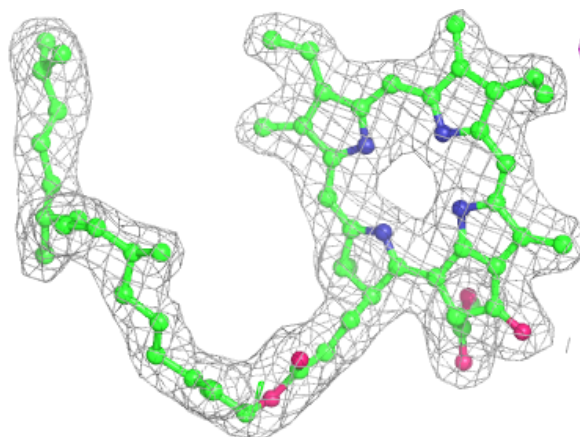
Electron density around CLA b 614:

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

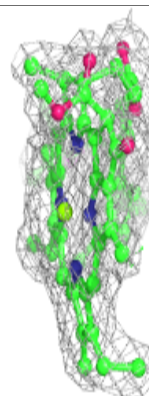
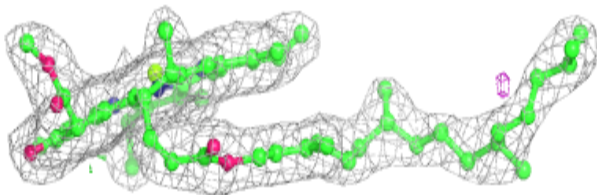
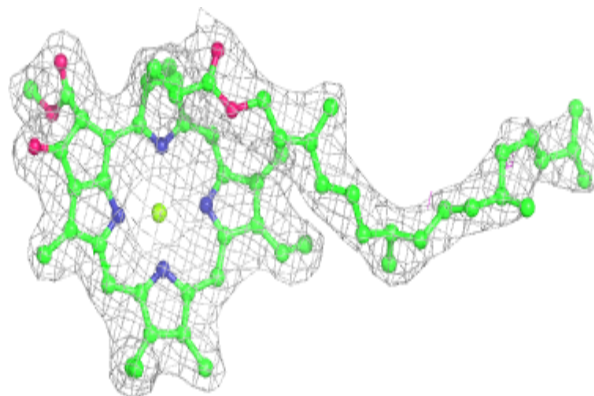


Electron density around PHO D 402:

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

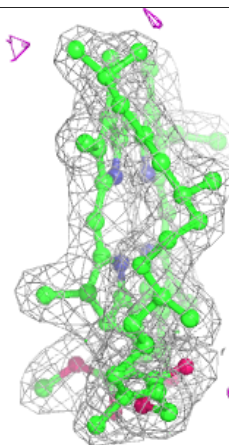
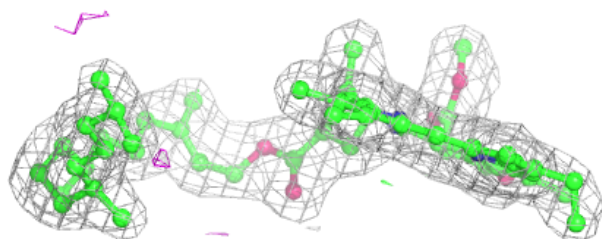
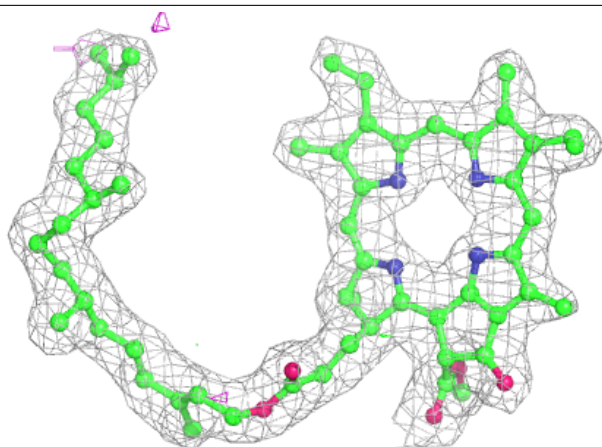
**Electron density around CLA b 604:**

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



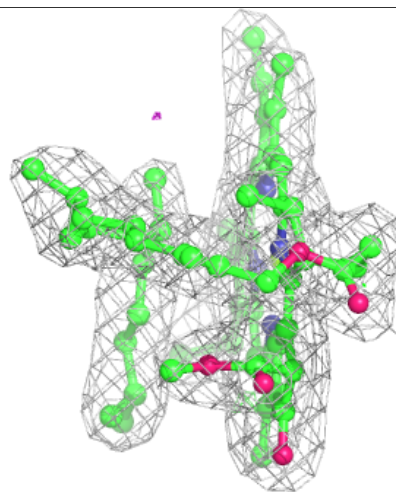
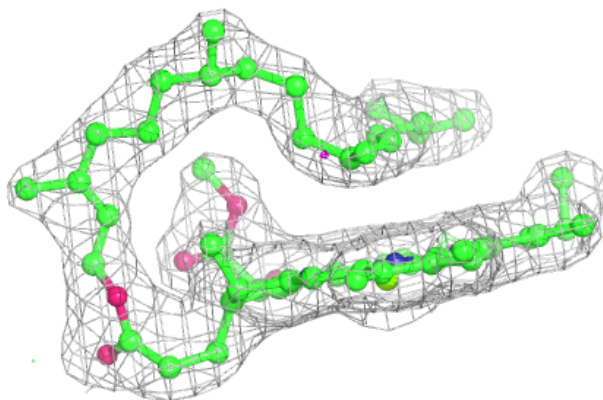
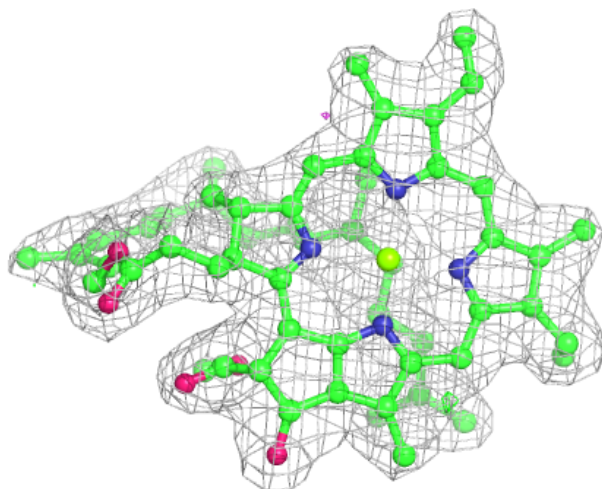
Electron density around PHO A 407:

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



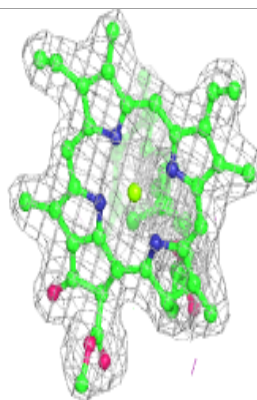
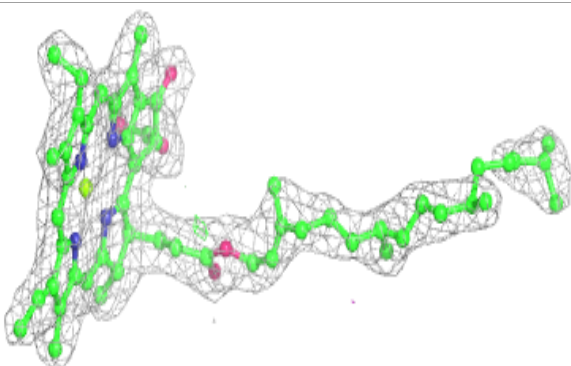
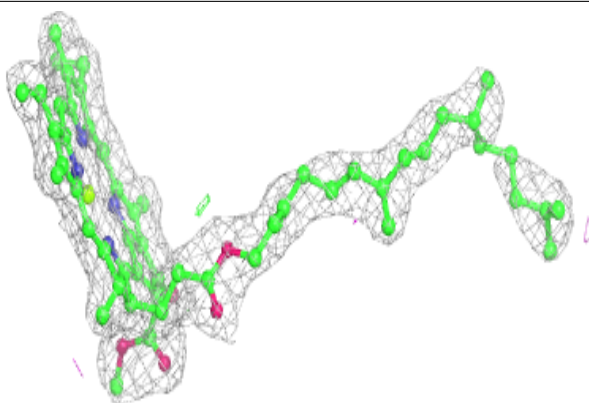
Electron density around CLA C 511:

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

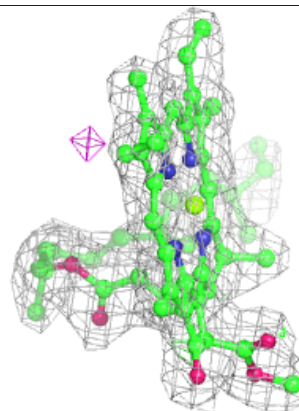
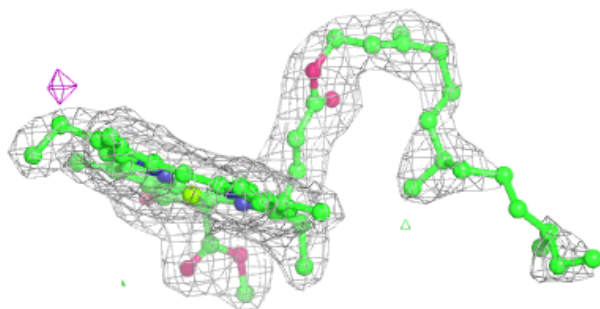
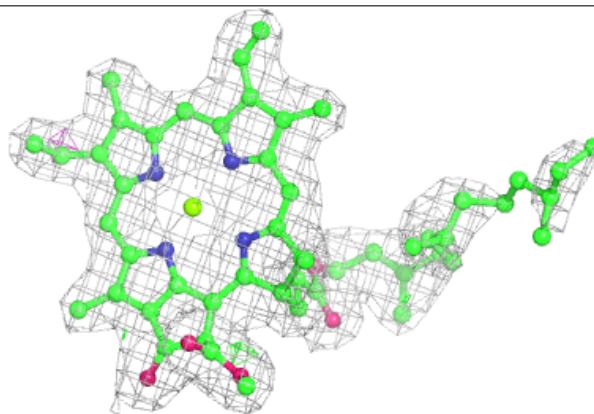


Electron density around CLA B 605:

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

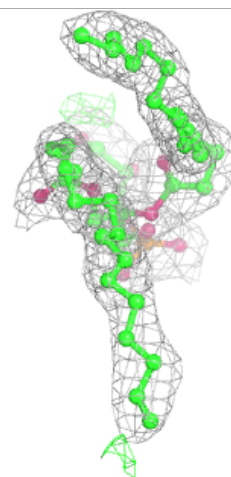
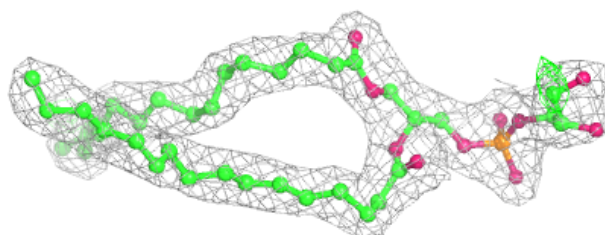
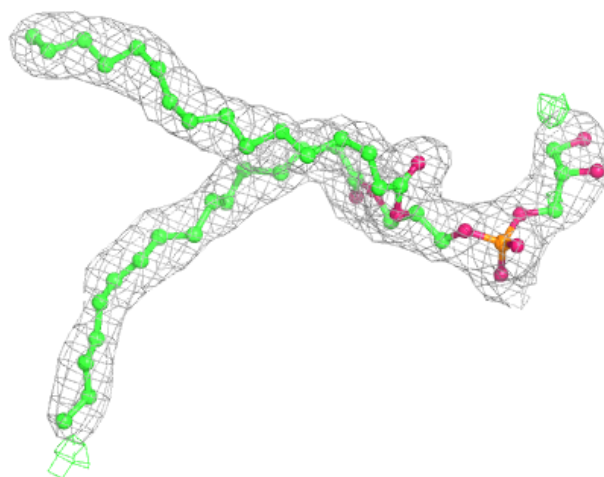
**Electron density around CLA a 409:**

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



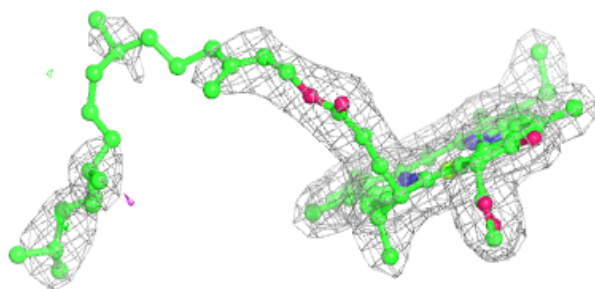
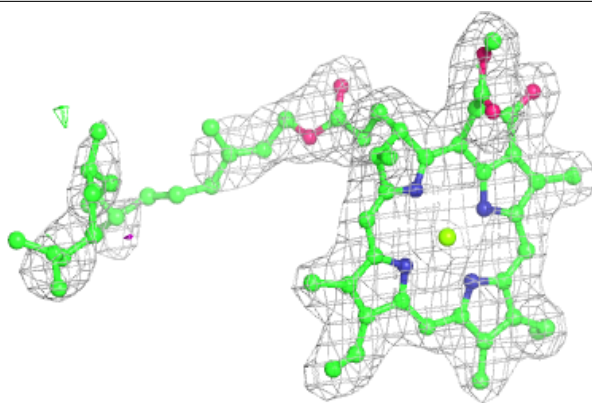
Electron density around LHG D 410:

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

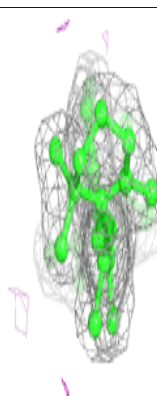
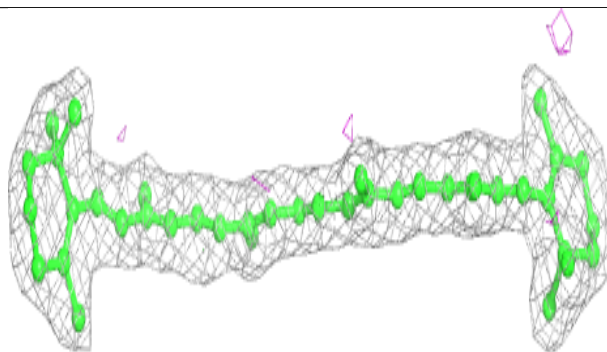
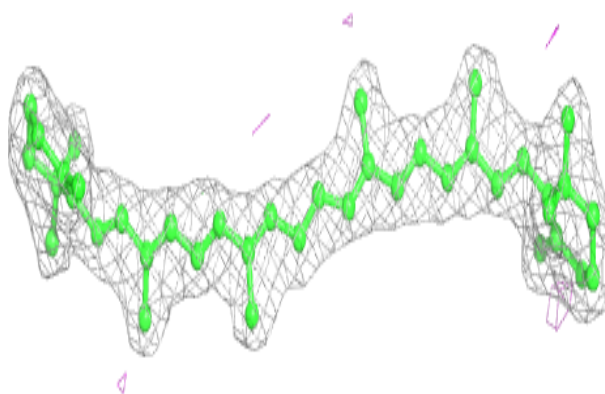


Electron density around CLA A 408:

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

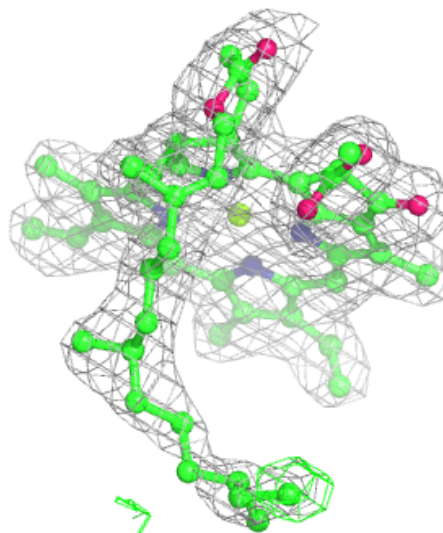
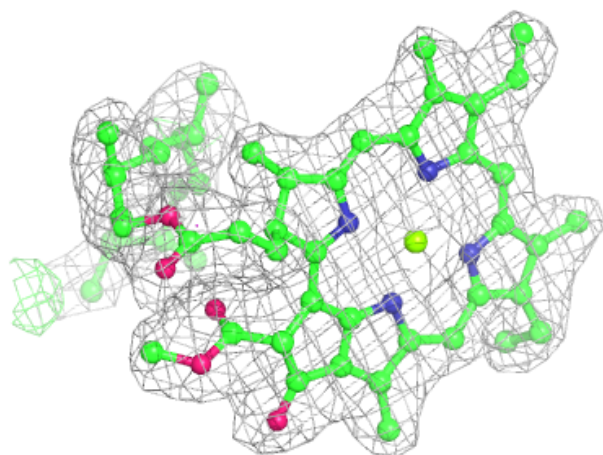
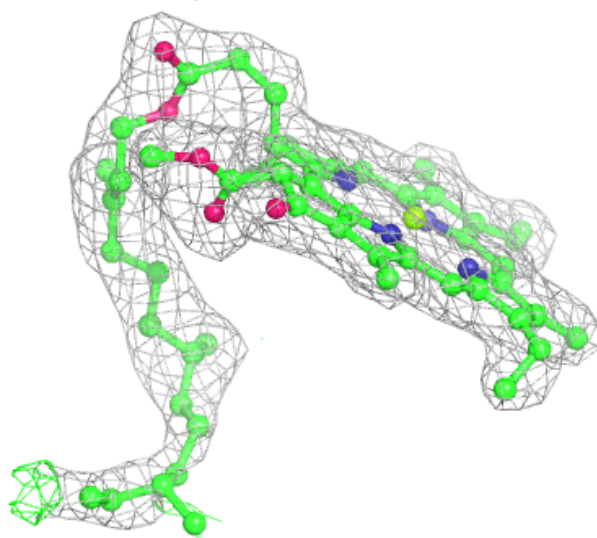
**Electron density around BCR A 409:**

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



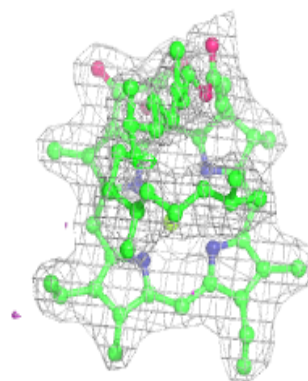
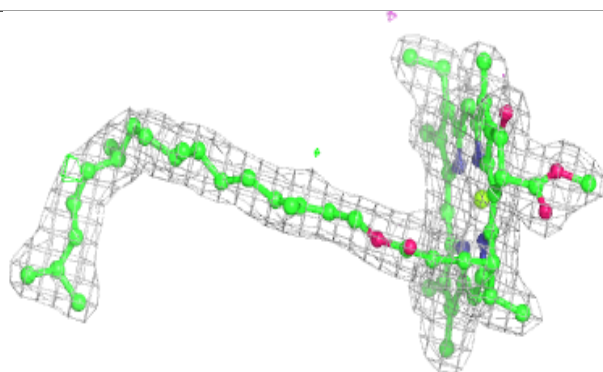
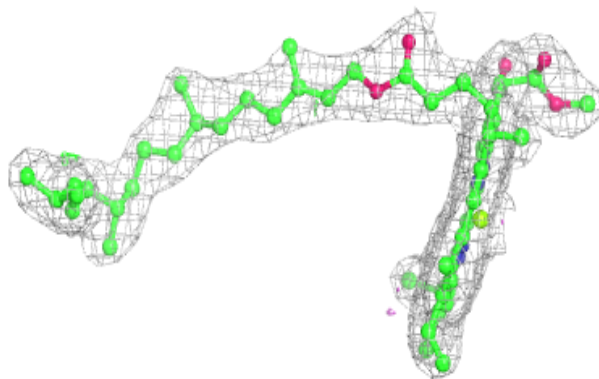
Electron density around CLA B 614:

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



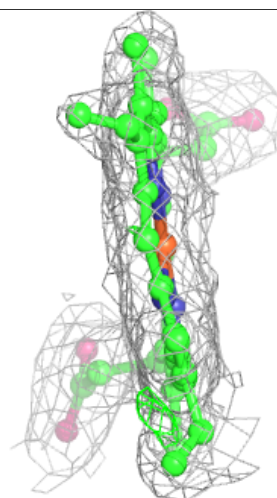
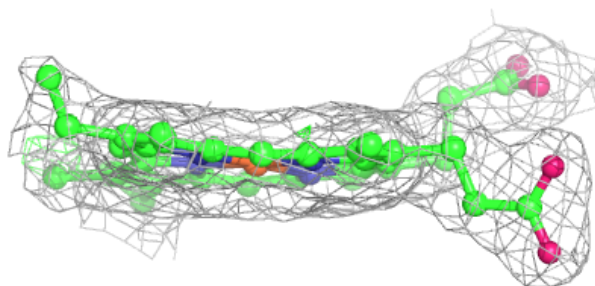
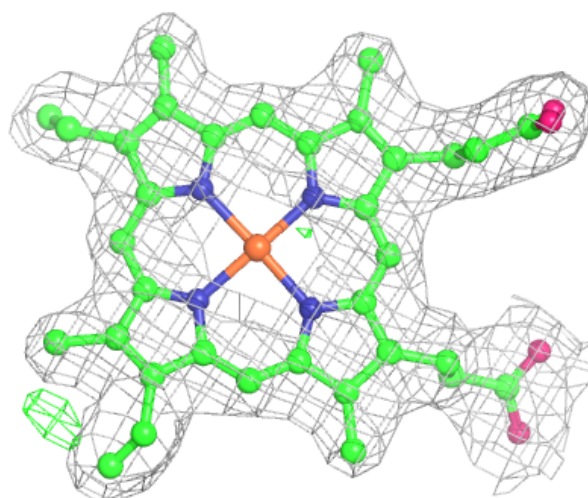
Electron density around CLA B 606:

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



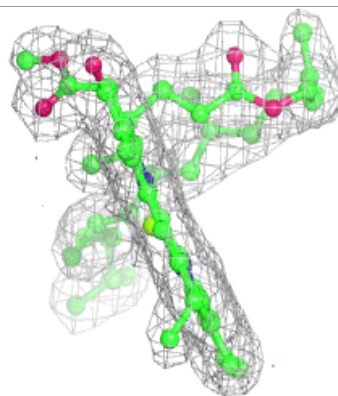
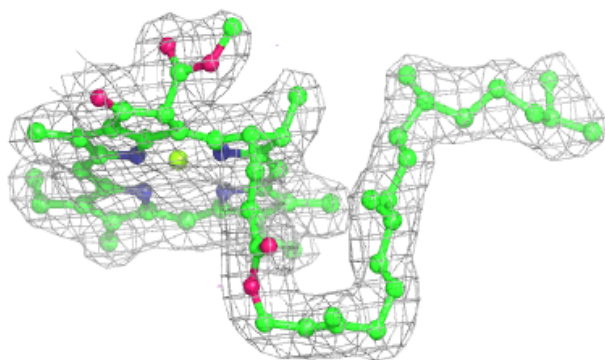
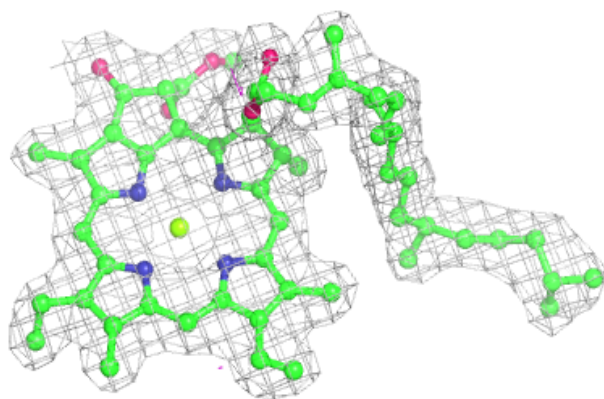
Electron density around HEC V 202:

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

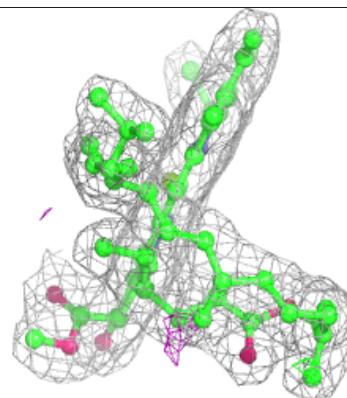
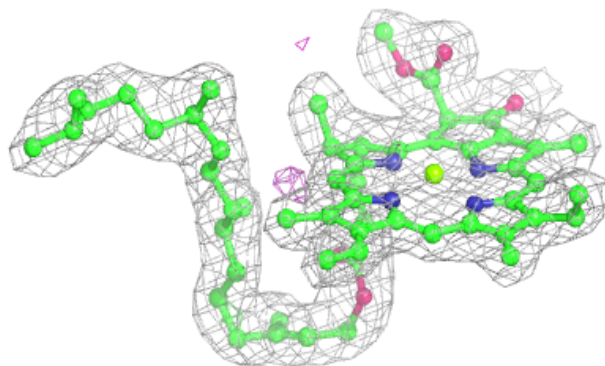
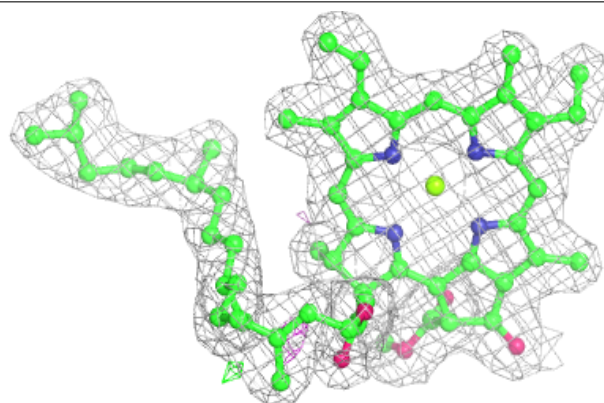


Electron density around CLA a 408:

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

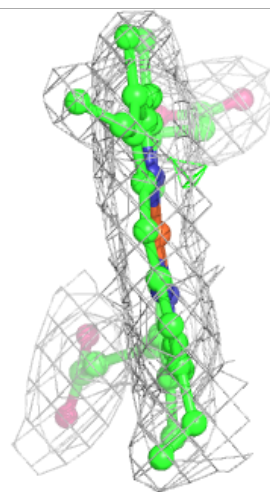
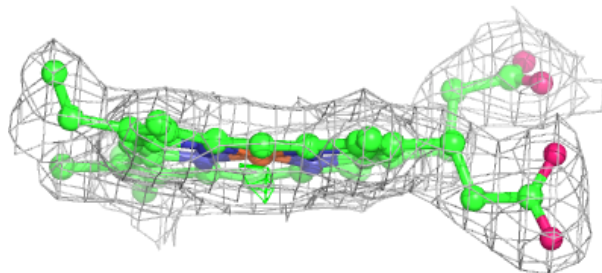
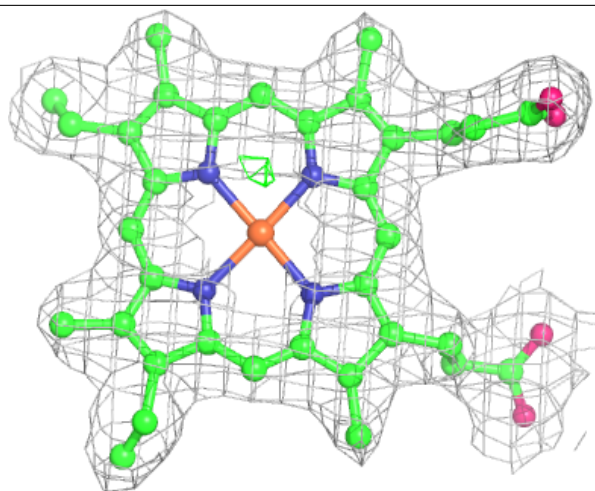
**Electron density around CLA D 401:**

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



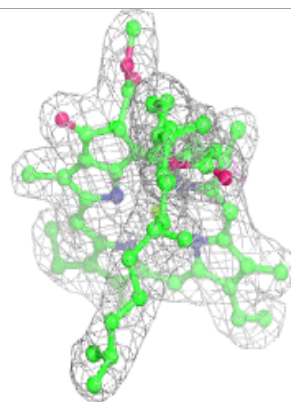
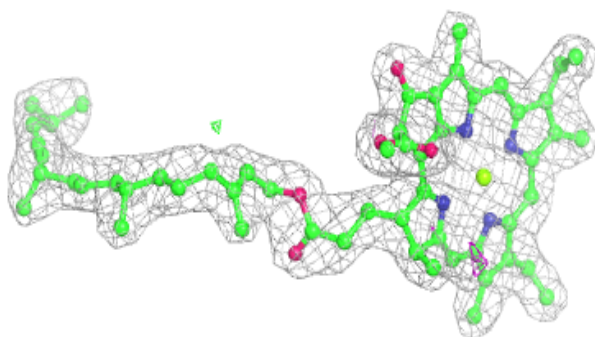
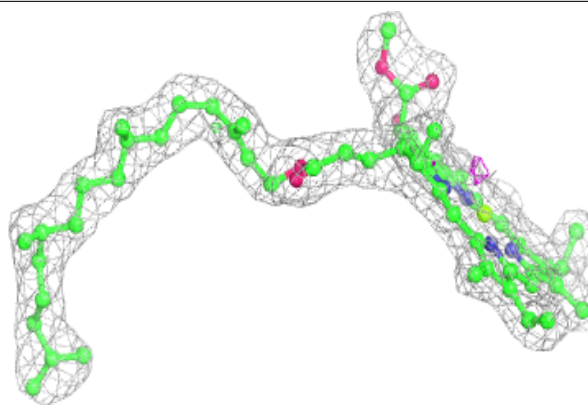
Electron density around HEC v 202:

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

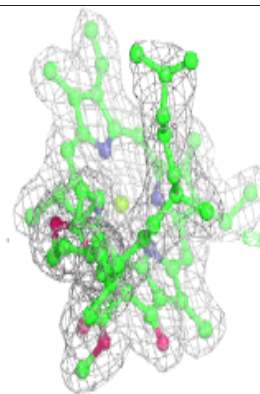
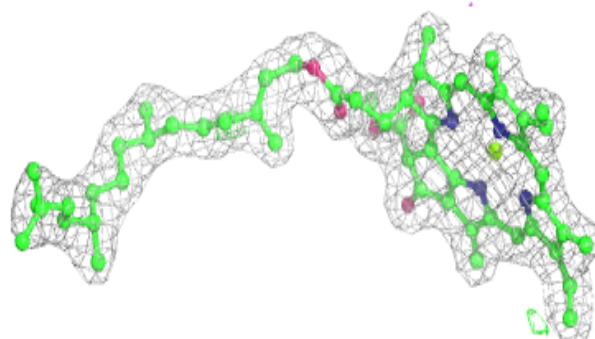
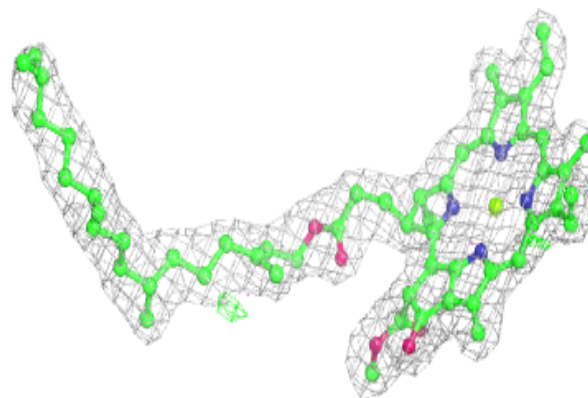


Electron density around CLA d 402:

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

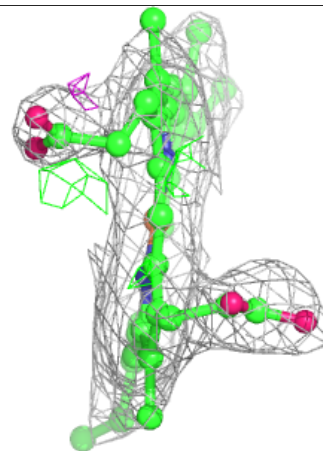
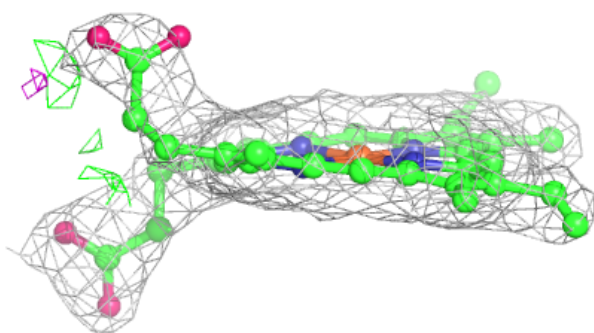
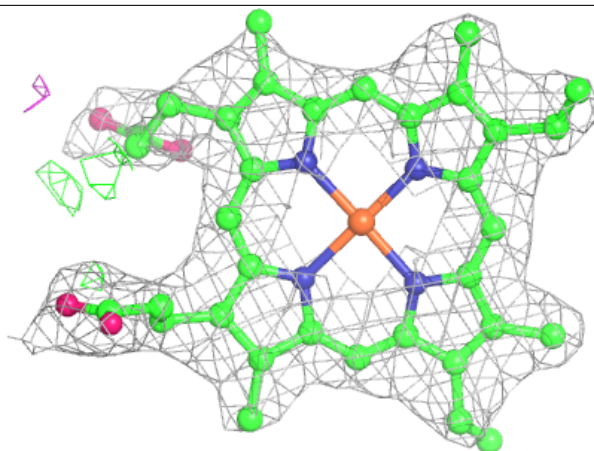
**Electron density around CLA a 407:**

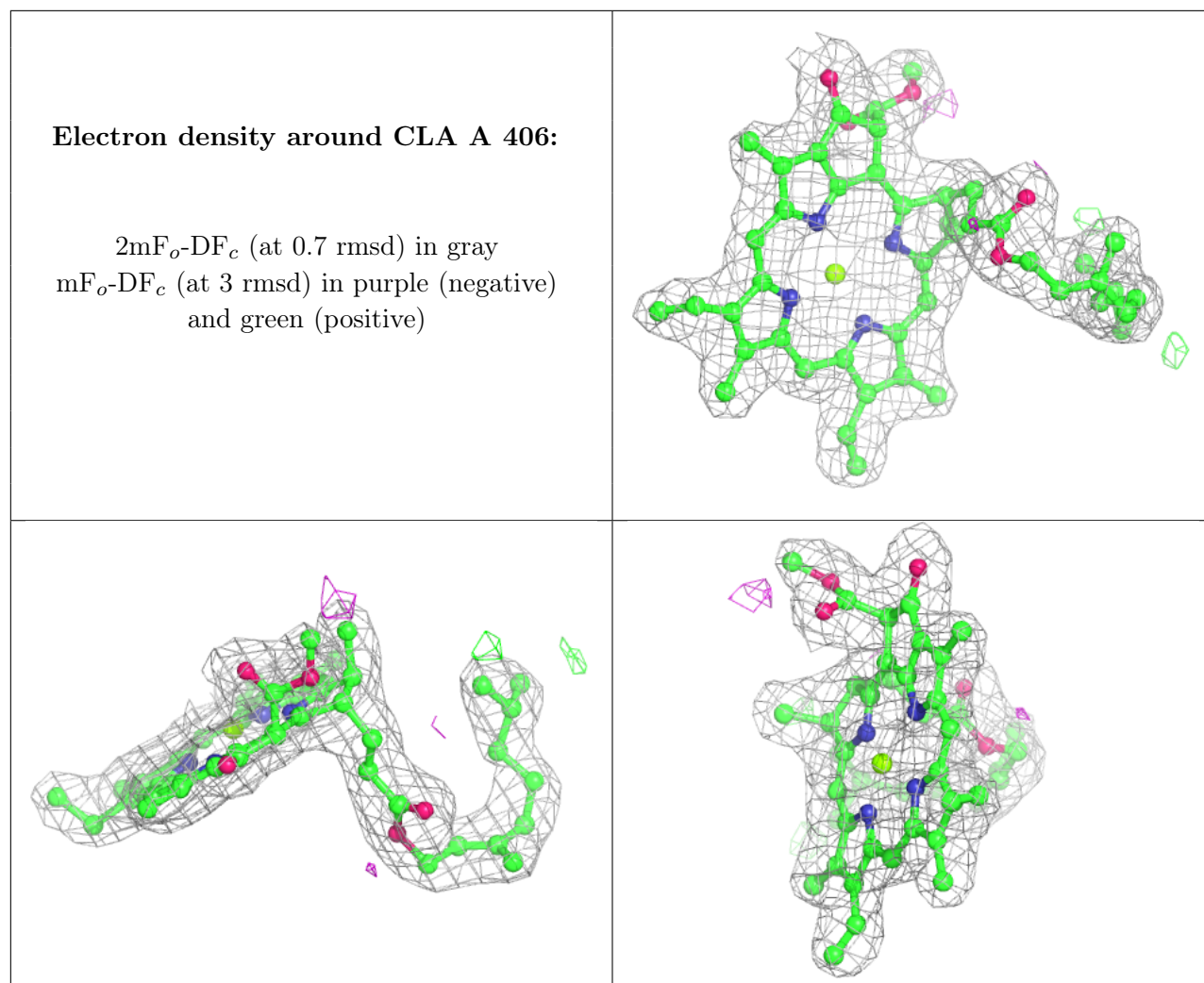
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM e 101:

$2mF_o - DF_c$ (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.