



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:22 AM JST

PDB ID : 5B66 / pdb_00005b66
Title : Crystal structure analysis of Photosystem II complex
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.
Deposited on : 2016-05-25
Resolution : 1.85 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

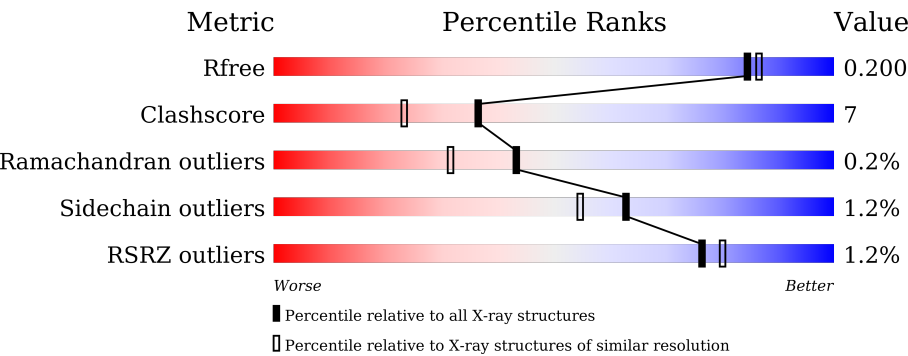
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



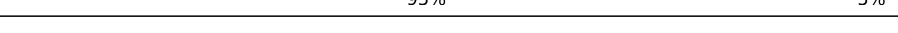
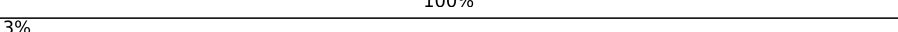
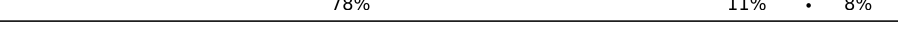
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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

Mol	Chain	Length	Quality of chain
1	A	344	0% 87% 10% .
1	a	344	88% 9% .
2	B	505	2% 89% 10%
2	b	505	3% 90% 8% ..
3	C	455	91% 8% .
3	c	455	90% 10%

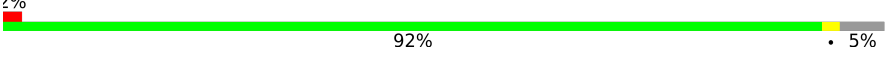
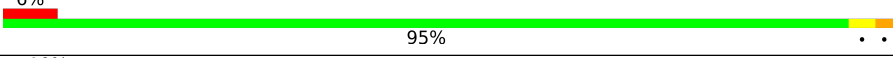
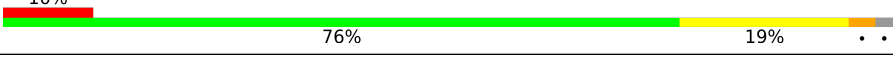
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Mol	Chain	Length	Quality of chain
4	D	342	 90% 9% .
4	d	342	 91% 9%
5	E	83	 77% 16% . 6%
5	e	83	 80% 13% . 6%
6	F	44	 64% 11% 25%
6	f	44	 59% 14% 27%
7	H	65	 91% 6% . .
7	h	65	 88% 6% . 5%
8	I	38	 82% 8% . 8%
8	i	38	 79% 13% . 5%
9	J	40	 80% 8% . 10%
9	j	40	 95% 5%
10	K	37	 89% 11%
10	k	37	 81% 16% .
11	L	37	 95% 5%
11	l	37	 100%
12	M	36	 78% 11% . 8%
12	m	36	 86% 8% 6%
13	O	244	 89% 10%
13	o	244	 88% 11%
14	T	32	 81% . 6% 9%
14	t	32	 81% 9% . 6%
15	U	104	 82% 12% 7%
15	u	104	 87% 7% 7%
16	V	137	 96% .

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	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
26	UNL	U	901	-	-	X	-
28	DMS	B	635	-	-	X	-
28	DMS	B	642	-	-	X	-
28	DMS	B	644	-	-	X	-
28	DMS	C	531	-	-	X	-
28	DMS	C	532	-	-	X	-
28	DMS	D	414	-	-	X	-
28	DMS	U	903[B]	-	-	X	-
28	DMS	b	631	-	-	X	-
28	DMS	b	639	-	-	X	-
28	DMS	c	530	-	-	X	-
28	DMS	c	536	-	-	X	-
28	DMS	d	414	-	-	X	-
28	DMS	i	104	-	-	X	-
28	DMS	o	302	-	-	X	-
28	DMS	o	303	-	-	X	-
28	DMS	o	306	-	-	X	-
28	DMS	v	206	-	-	X	-
31	BCT	A	421	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 54996 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	3	0
			2626	1721	430	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2622	1719	431	457	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- 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	11	0
			4012	2632	668	699	13			
2	b	495	Total	C	N	O	S	0	4	0
			3884	2550	650	671	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	1	0
			3483	2280	582	608	13			
3	c	455	Total	C	N	O	S	0	1	0
			3523	2305	591	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- 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	1	0
			2728	1808	446	462	12			
4	d	342	Total	C	N	O	S	0	0	0
			2722	1803	445	462	12			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	78	Total	C	N	O	0	1	0
			632	413	101	118			
5	e	78	Total	C	N	O	0	2	0
			636	419	99	118			

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	1	0
			508	339	81	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
			284	194	45	44	1			
8	i	36	Total	C	N	O	S	0	1	0
			300	203	49	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
			272	183	41	47	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			
10	k	37	Total	C	N	O	0	0	0
			285	199	42	44			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			302	203	48	51			
11	l	37	Total	C	N	O	0	1	0
			296	200	45	51			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			259	175	37	46	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	6	0
			1870	1172	309	384	5			
13	o	243	Total	C	N	O	S	0	2	0
			1838	1153	305	376	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	29	Total	C	N	O	S	0	1	0
			257	181	35	39	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	0	0
			770	489	129	152				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	3	0
			1080	685	181	210	4			
16	v	137	Total	C	N	O	S	0	0	0
			1052	666	174	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			212	139	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			213	140	37	33	3			

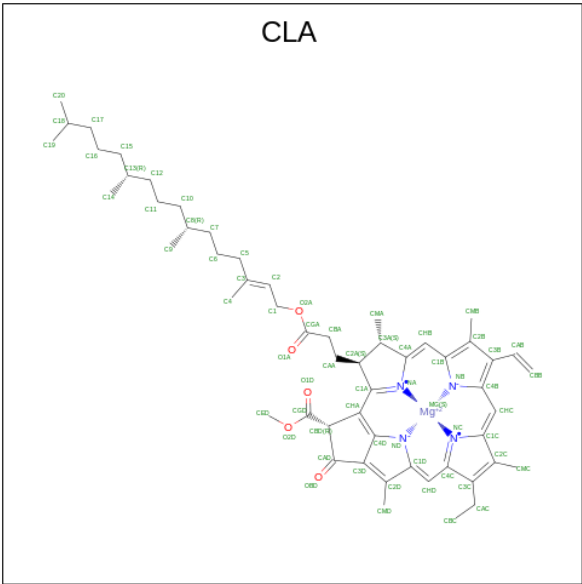
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	0	0
			274	183	44	47				
18	x	35	Total	C	N	O		0	0	0
			252	171	38	43				

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			450	308	67	73	2			
19	z	61	Total	C	N	O	S	0	0	0
			433	297	66	69	1			

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			59	49	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	C	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	a	1	Total 47	C 37	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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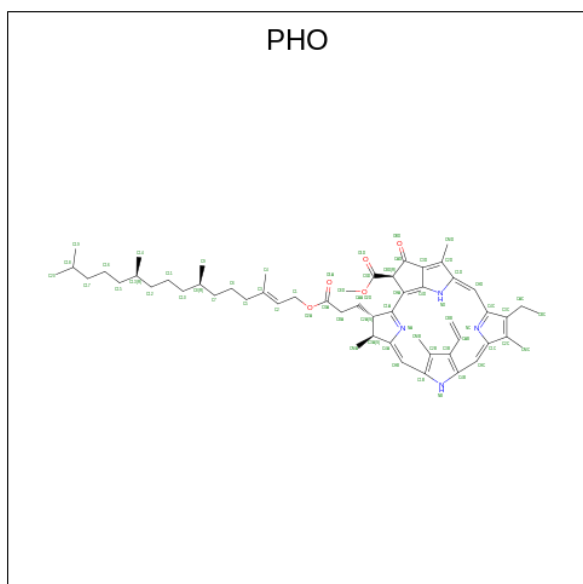
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 60	C 50	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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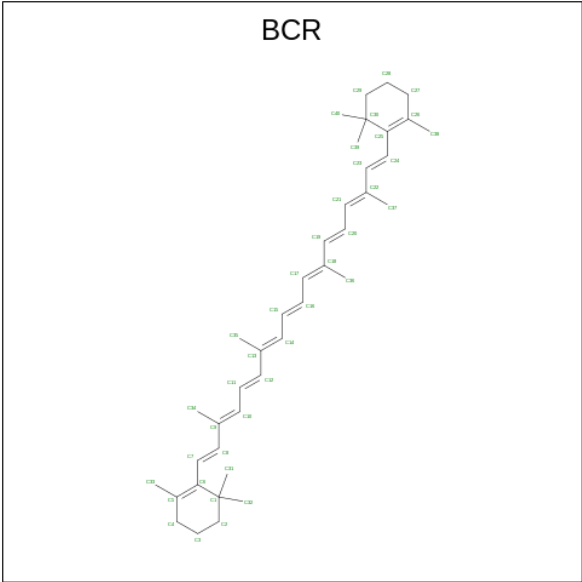
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 21 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



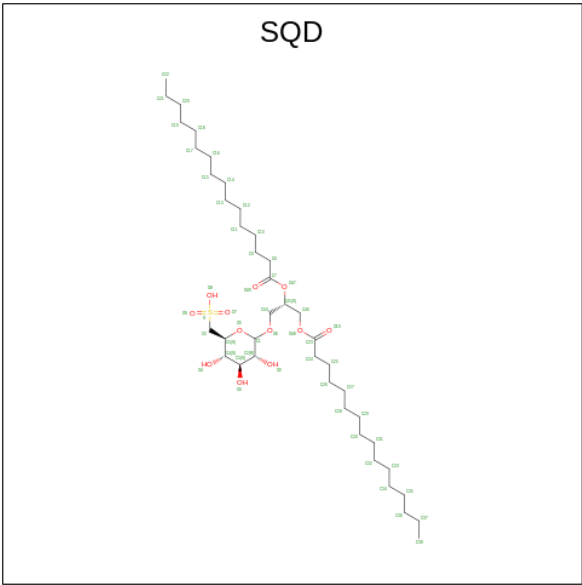
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	C	1	Total C 40 40	0	0
22	D	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	T	1	Total C 40 40	0	0
22	a	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0
22	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	c	1	Total C 40 40	0	0
22	d	1	Total C 40 40	0	0
22	j	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	k	1	Total C 40 40	0	0
22	t	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



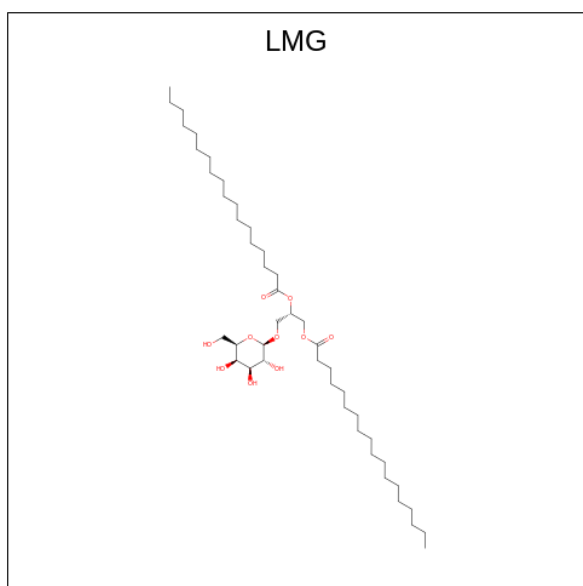
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O S 54 41 12 1	0	0
23	A	1	Total C O S 54 41 12 1	0	0
23	F	1	Total C O S 35 23 11 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0
23	a	1	Total C O S 54 41 12 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	b	1	Total	C	O	S	0	0
			54	41	12	1		
23	f	1	Total	C	O	S	0	0
			40	27	12	1		
23	l	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	O		0	0
			51	41	10			
24	B	1	Total	C	O		0	0
			51	41	10			
24	C	1	Total	C	O		0	0
			51	41	10			
24	C	1	Total	C	O		0	0
			45	35	10			
24	J	1	Total	C	O		0	0
			45	35	10			
24	a	1	Total	C	O		0	0
			51	41	10			
24	b	1	Total	C	O		0	0
			49	39	10			
24	c	1	Total	C	O		0	0
			51	41	10			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	c	1	Total	C	O	0	0
			51	41	10		
24	j	1	Total	C	O	0	0
			45	35	10		

- Molecule 25 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 26 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

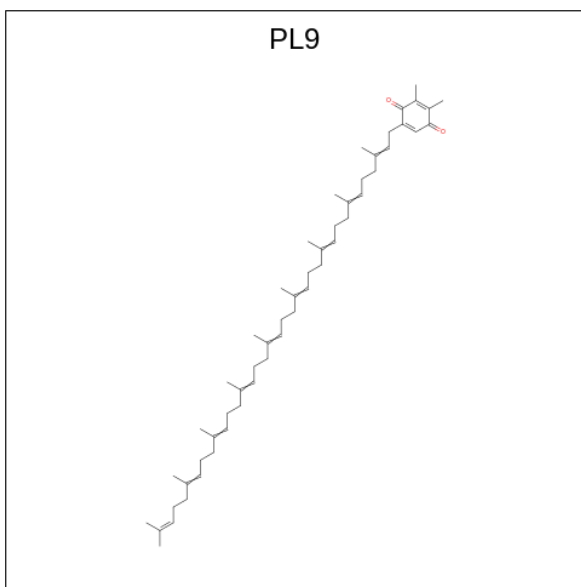
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	2	Total	C	O	0	0
			40	35	5		
26	B	6	Total	C		0	0
			84	84			
26	C	1	Total	C	O	0	0
			34	29	5		
26	D	2	Total	C	O	0	0
			53	48	5		
26	E	1	Total	C		0	0
			15	15			
26	H	2	Total	C		0	0
			10	10			
26	I	5	Total	C		0	0
			61	61			
26	J	4	Total	C		0	0
			33	33			
26	L	1	Total	C		0	0
			14	14			
26	M	1	Total	C		0	0
			12	12			
26	T	1	Total	C		0	0
			13	13			
26	U	1	Total	C		0	0
			14	14			
26	X	1	Total	C		0	0
			16	16			

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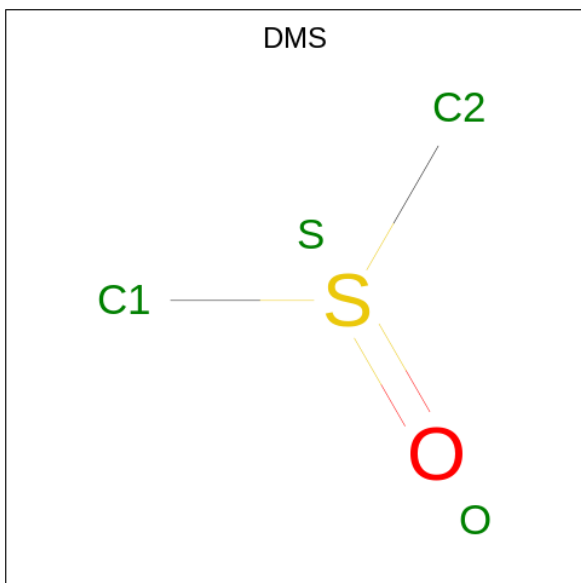
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	Z	1	Total C 4 4	0	0
26	a	3	Total C O 45 40 5	0	0
26	b	7	Total C 68 68	0	0
26	c	3	Total C O 48 43 5	0	0
26	d	3	Total C O 68 63 5	0	0
26	e	1	Total C 7 7	0	0
26	h	1	Total C 16 16	0	0
26	i	3	Total C 38 38	0	0
26	j	2	Total C 22 22	0	0
26	t	1	Total C 16 16	0	0
26	x	1	Total C 9 9	0	0
26	z	1	Total C 6 6	0	0

- Molecule 27 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



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

- Molecule 28 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	A	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	B	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 8	C 4	O 2	S 2	0	1
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	C	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	D	1	Total 4	C 2	O 1	S 1	0	0
28	F	1	Total 4	C 2	O 1	S 1	0	0
28	H	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	O	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 4	C 2	O 1	S 1	0	0
28	U	1	Total 8	C 4	O 2	S 2	0	1

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	c	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	d	1	Total 4	C 2	O 1	S 1	0	0
28	h	1	Total 4	C 2	O 1	S 1	0	0
28	i	1	Total 4	C 2	O 1	S 1	0	0
28	j	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	o	1	Total 4	C 2	O 1	S 1	0	0
28	u	1	Total 4	C 2	O 1	S 1	0	0

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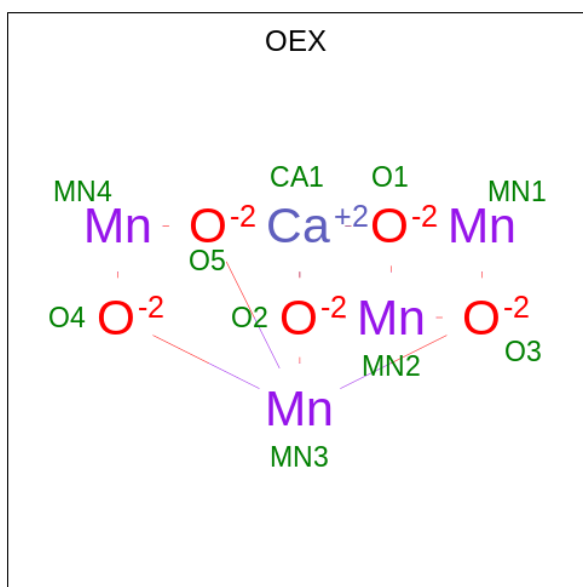
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	u	1	Total C O S 4 2 1 1	0	0
28	u	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4 2 1 1	0	0
28	v	1	Total C O S 4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

- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

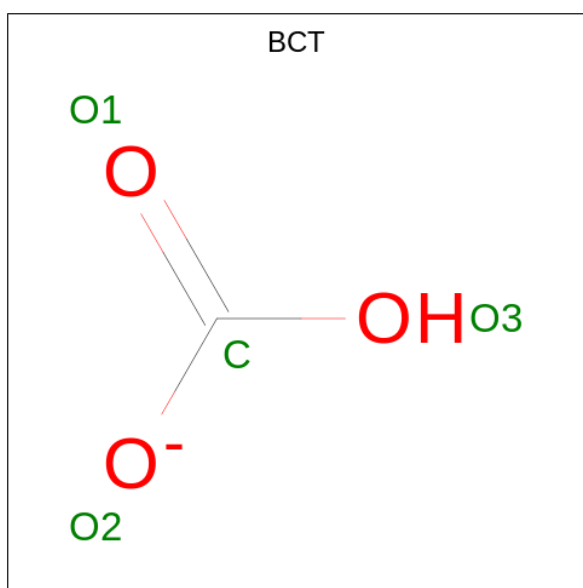
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total Fe 1 1	0	0
29	a	1	Total Fe 1 1	0	0

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn₄O₅).



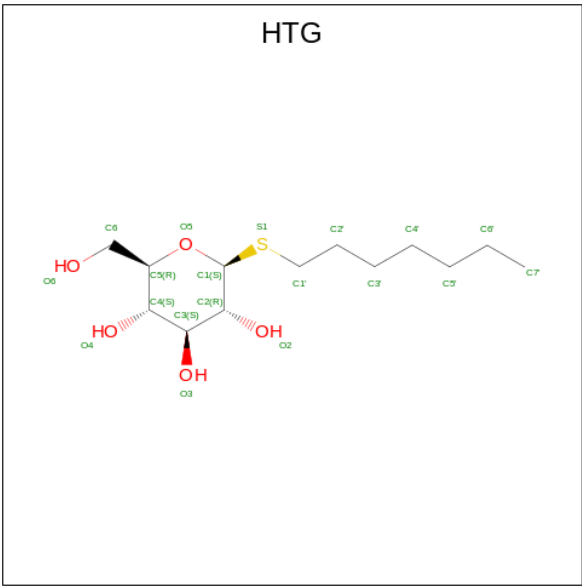
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			4	1	3		
31	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	B	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	C	1	Total	C	O	S	0	0
			19	13	5	1		
32	D	1	Total	C	O	S	0	0
			19	13	5	1		
32	O	1	Total	C	O	S	0	0
			19	13	5	1		
32	V	1	Total	C	O	S	0	0
			13	7	5	1		
32	b	1	Total	C	O	S	0	0
			19	13	5	1		

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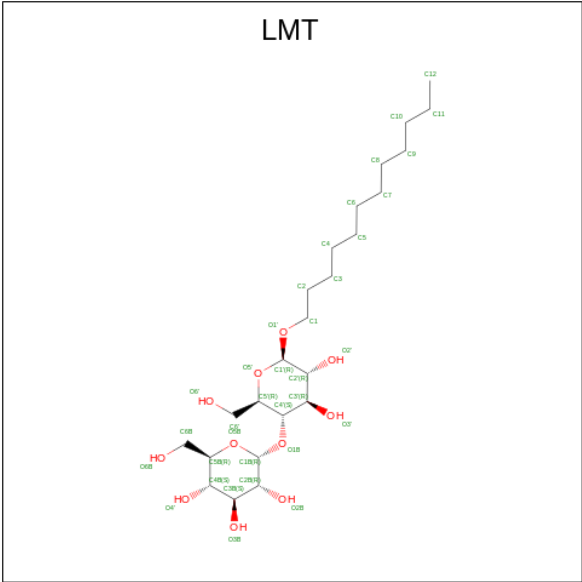
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	b	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	c	1	Total C O S 19 13 5 1	0	0
32	d	1	Total C O S 19 13 5 1	0	0
32	u	1	Total C S 8 7 1	0	0
32	v	1	Total C O S 14 8 5 1	0	0

- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 34 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



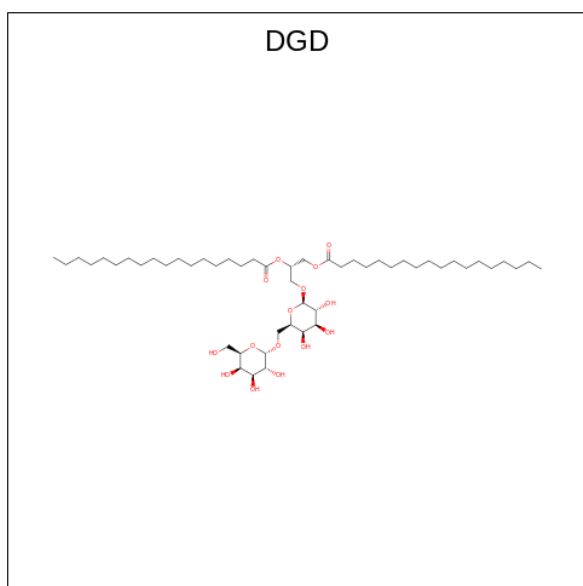
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			24	18	6		
34	B	1	Total	C	O	0	0
			16	14	2		
34	E	1	Total	C	O	0	0
			24	18	6		
34	I	1	Total	C	O	0	0
			35	24	11		
34	J	1	Total	C	O	0	0
			24	18	6		
34	M	1	Total	C	O	0	0
			35	24	11		
34	T	1	Total	C	O	0	0
			24	18	6		
34	Z	1	Total	C	O	0	0
			35	24	11		
34	a	1	Total	C	O	0	0
			35	24	11		
34	b	1	Total	C	O	0	0
			32	21	11		
34	b	1	Total	C	O	0	0
			25	19	6		
34	c	1	Total	C	O	0	0
			35	24	11		
34	f	1	Total	C	O	0	0
			24	18	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	m	1	Total	C	O	0	0
			35	24	11		
34	m	1	Total	C	O	0	0
			35	24	11		
34	z	1	Total	C	O	0	0
			35	24	11		

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



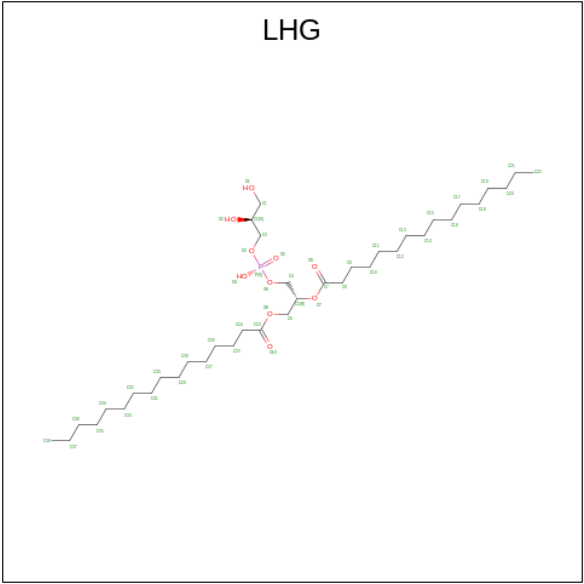
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	C	1	Total	C	O	0	0
			62	47	15		
35	C	1	Total	C	O	0	0
			55	40	15		
35	C	1	Total	C	O	0	0
			62	47	15		
35	D	1	Total	C	O	0	0
			51	41	10		
35	H	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			62	47	15		
35	c	1	Total	C	O	0	0
			57	42	15		
35	c	1	Total	C	O	0	0
			62	47	15		

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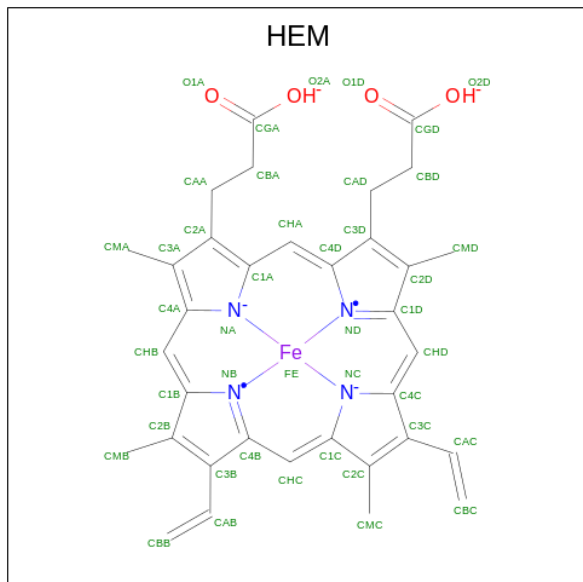
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	d	1	Total	C	O	0	0
			51	41	10		
35	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 36 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



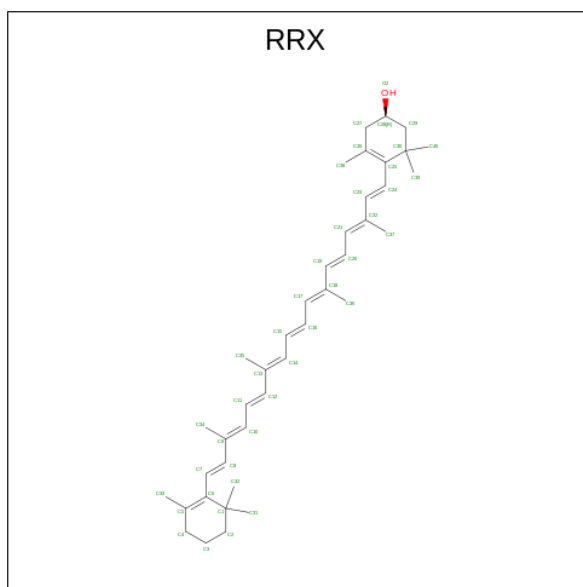
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	D	1	Total	C	O	P	0	0
			49	38	10	1		
36	E	1	Total	C	O	P	0	0
			48	37	10	1		
36	L	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	d	1	Total	C	O	P	0	0
			49	38	10	1		
36	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).

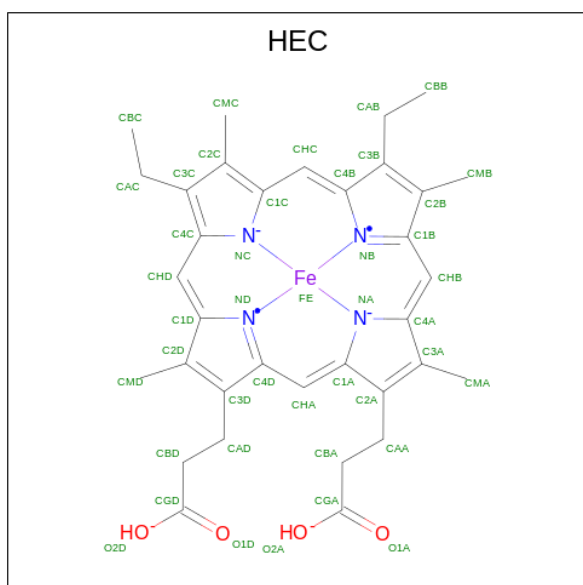


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	B	447	Total 473	O 473	0	25
41	C	317	Total 324	O 324	0	7
41	D	175	Total 180	O 180	0	5
41	E	62	Total 66	O 66	0	4
41	F	8	Total 8	O 8	0	0
41	H	62	Total 65	O 65	0	3
41	I	16	Total 16	O 16	0	0
41	J	23	Total 23	O 23	0	0
41	K	12	Total 12	O 12	0	0
41	L	19	Total 21	O 21	0	2
41	M	12	Total 12	O 12	0	0
41	O	263	Total 273	O 273	0	10
41	T	19	Total 20	O 20	0	1
41	U	133	Total 136	O 136	0	3
41	V	177	Total 183	O 183	0	6
41	Y	7	Total 7	O 7	0	0
41	X	22	Total 22	O 22	0	0
41	Z	5	Total 5	O 5	0	0
41	a	182	Total 185	O 185	0	3
41	b	451	Total 465	O 465	0	14
41	c	362	Total 374	O 374	0	12

Continued on next page...

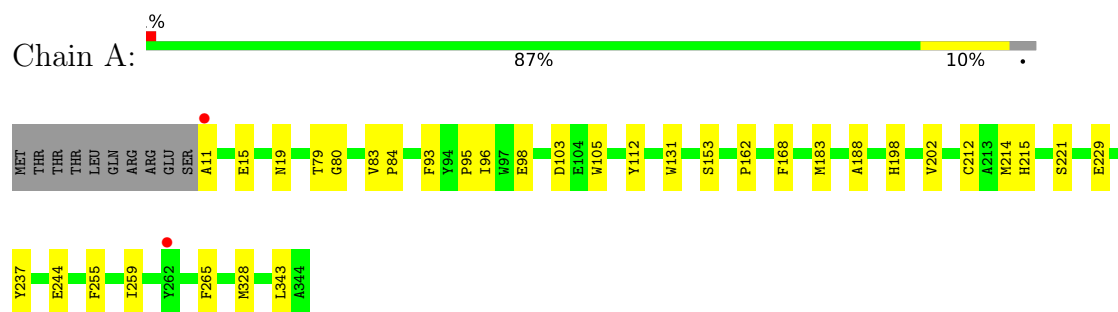
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	d	176	Total 182	O 182	0	6
41	e	48	Total 49	O 49	0	1
41	f	15	Total 16	O 16	0	1
41	h	68	Total 70	O 70	0	2
41	i	19	Total 21	O 21	0	2
41	j	23	Total 24	O 24	0	1
41	k	11	Total 12	O 12	0	1
41	l	22	Total 24	O 24	0	2
41	m	23	Total 24	O 24	0	1
41	o	214	Total 230	O 230	0	15
41	t	19	Total 20	O 20	0	1
41	u	146	Total 150	O 150	0	4
41	v	144	Total 147	O 147	0	3
41	y	7	Total 7	O 7	0	0
41	x	25	Total 26	O 26	0	1
41	z	12	Total 12	O 12	0	0

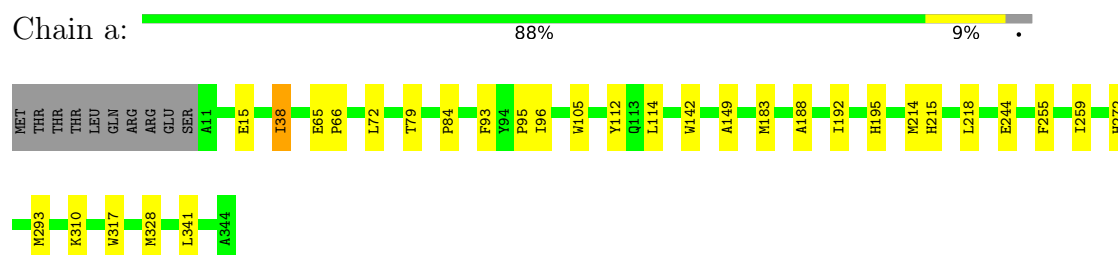
3 Residue-property plots [i](#)

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

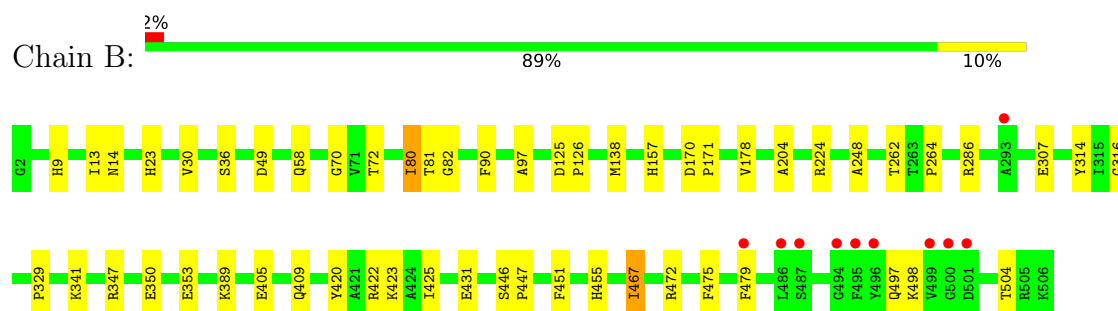
- Molecule 1: Photosystem II protein D1



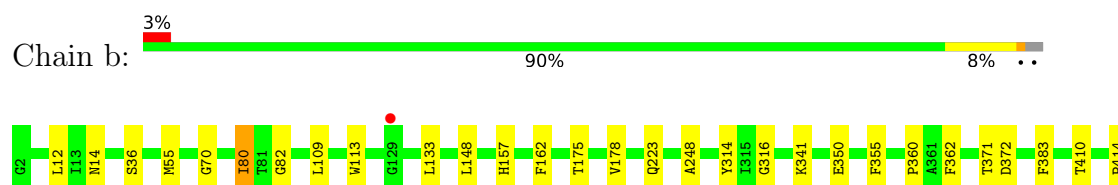
- Molecule 1: Photosystem II protein D1

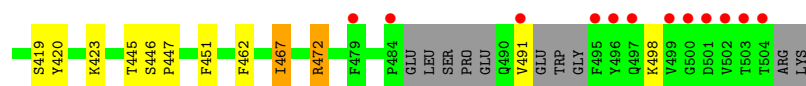


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 8% .



• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 90% 10% .



• Molecule 4: Photosystem II D2 protein

Chain D: 90% 9% .



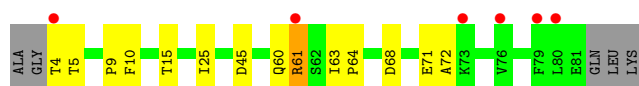
• Molecule 4: Photosystem II D2 protein

Chain d: 91% 9% .

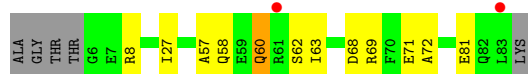
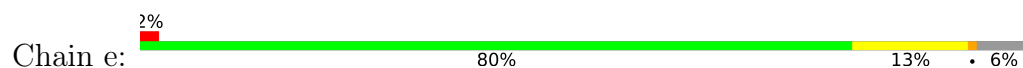


• Molecule 5: Cytochrome b559 subunit alpha

Chain E: 7% 77% 16% 6% .



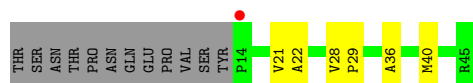
- Molecule 5: Cytochrome b559 subunit alpha



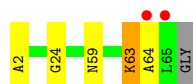
- Molecule 6: Cytochrome b559 subunit beta



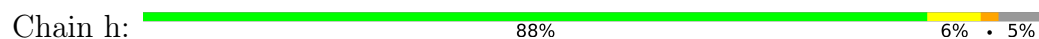
- Molecule 6: Cytochrome b559 subunit beta



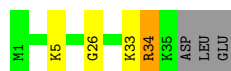
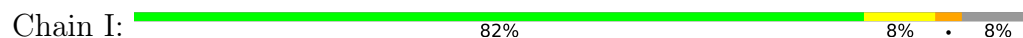
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

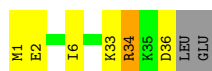


- Molecule 8: Photosystem II reaction center protein I



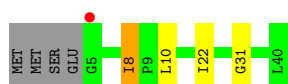
- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 13% • 5%

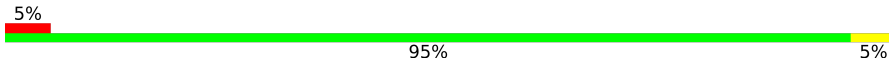


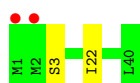
- Molecule 9: Photosystem II reaction center protein J

Chain J:  80% 8% • 10%



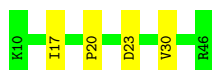
- Molecule 9: Photosystem II reaction center protein J

Chain j:  95% 5% • 5%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  89% 11%

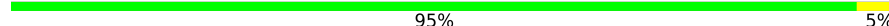


- Molecule 10: Photosystem II reaction center protein K

Chain k:  81% 16% •

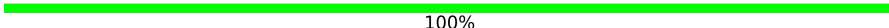


- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%



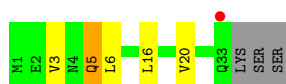
- Molecule 11: Photosystem II reaction center protein L

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 11% • 8%



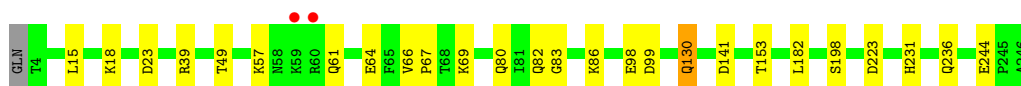
- Molecule 12: Photosystem II reaction center protein M

Chain m: 86% 8% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 89% 10%



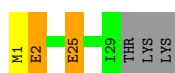
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 88% 11%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 6% 9%



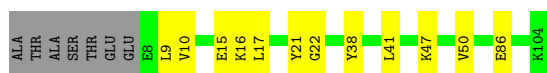
- Molecule 14: Photosystem II reaction center protein T

Chain t: 81% 9% 6%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 82% 12% 7%



- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 87% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V: 96% .



- Molecule 16: Cytochrome c-550

Chain v: 91% 9% .



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 73% 23% .



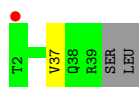
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 83% 13% .



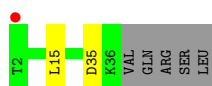
- Molecule 18: Photosystem II reaction center protein X

Chain X: 92% 5% .



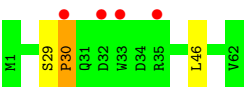
- Molecule 18: Photosystem II reaction center protein X

Chain x: 82% 5% 12% .

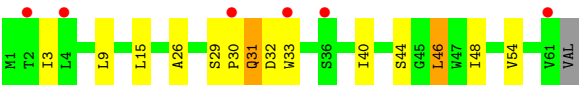
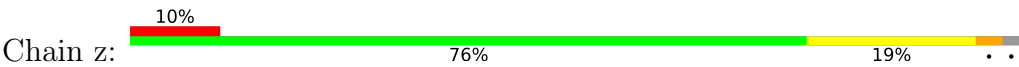


- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 95% . .



● Molecule 19: 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	121.47Å 228.18Å 286.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 1.85 19.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-1.85) 99.9 (19.99-1.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.162 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	33616 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	54996	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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: HEM, DMS, FME, HEC, BCT, HTG, DGD, BCR, FE2, CL, OEX, RRX, LMG, LMT, CLA, MG, UNL, LHG, SQD, PHO, PL9, CA

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	1.19	3/2717 (0.1%)	0.98	2/3707 (0.1%)
1	a	1.15	3/2718 (0.1%)	1.02	3/3707 (0.1%)
2	B	1.10	4/4181 (0.1%)	0.96	1/5700 (0.0%)
2	b	1.13	1/4029 (0.0%)	0.96	1/5490 (0.0%)
3	C	1.06	2/3599 (0.1%)	0.95	1/4901 (0.0%)
3	c	1.03	1/3640 (0.0%)	0.96	1/4956 (0.0%)
4	D	1.17	3/2826 (0.1%)	0.99	6/3850 (0.2%)
4	d	1.15	3/2817 (0.1%)	0.94	0/3839
5	E	0.89	0/654	0.96	0/896
5	e	0.85	0/661	0.99	2/904 (0.2%)
6	F	0.93	0/278	0.82	0/379
6	f	0.98	0/265	0.93	0/360
7	H	0.95	0/524	0.94	0/715
7	h	0.97	0/517	0.91	0/704
8	I	0.86	0/281	0.93	1/380 (0.3%)
8	i	0.80	0/300	0.90	0/405
9	J	0.89	0/257	0.88	0/349
9	j	0.88	0/278	1.00	0/378
10	K	0.89	0/303	0.95	0/416
10	k	0.85	0/295	0.91	0/407
11	L	0.98	1/312 (0.3%)	0.95	0/425
11	l	1.02	0/306	1.00	0/418
12	M	0.87	0/265	1.02	0/362
12	m	0.84	0/270	0.97	0/369
13	O	0.95	0/1919	0.98	0/2607
13	o	0.91	0/1875	0.98	0/2548
14	T	0.92	0/259	1.11	4/352 (1.1%)
14	t	0.95	0/257	0.98	0/349
15	U	0.99	0/777	0.91	0/1055
15	u	0.94	0/781	0.91	0/1059
16	V	1.05	0/1110	0.99	0/1506

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.94	0/1073	0.94	1/1461 (0.1%)
17	Y	0.72	0/213	0.96	0/285
17	y	0.63	0/214	0.97	0/286
18	X	0.75	0/277	1.07	0/375
18	x	0.77	0/255	0.92	0/345
19	Z	0.78	0/461	0.95	0/632
19	z	0.68	0/444	1.03	0/611
All	All	1.05	21/42208 (0.0%)	0.97	23/57488 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
13	o	0	1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	LEU	C-N	11.57	1.49	1.33
2	b	414	PRO	CA-C	6.43	1.58	1.52
4	D	87	HIS	CG-CD2	6.31	1.42	1.35
4	d	330	ALA	C-O	-6.04	1.18	1.24
4	d	117	HIS	ND1-CE1	5.87	1.38	1.32
2	B	9	HIS	ND1-CE1	5.84	1.38	1.32
1	a	38	ILE	CA-CB	5.72	1.57	1.54
4	D	87	HIS	ND1-CE1	5.50	1.38	1.32
1	a	149	ALA	CA-C	5.50	1.58	1.52
2	B	9	HIS	CG-CD2	5.46	1.41	1.35
2	B	23	HIS	CG-CD2	5.37	1.41	1.35
1	A	198	HIS	ND1-CE1	5.32	1.37	1.32
3	C	444	HIS	CG-CD2	5.20	1.41	1.35
2	B	97	ALA	N-CA	5.20	1.52	1.46
3	C	91	HIS	CG-CD2	5.14	1.41	1.35
1	a	195	HIS	CG-CD2	5.13	1.41	1.35
11	L	34	TYR	N-CA	5.07	1.52	1.46
1	A	80	GLY	N-CA	5.06	1.52	1.45
4	D	197	HIS	CE1-NE2	5.06	1.37	1.32
3	c	365	TRP	CD2-CE2	5.03	1.50	1.41
4	d	248	THR	CA-C	5.03	1.59	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	139	ARG	CA-C-N	-7.16	114.42	121.65
4	D	139	ARG	C-N-CA	-7.16	114.42	121.65
14	T	25[A]	GLU	CA-C-N	-6.25	113.94	120.38
14	T	25[A]	GLU	C-N-CA	-6.25	113.94	120.38
14	T	25[B]	GLU	CA-C-N	-6.25	113.94	120.38
14	T	25[B]	GLU	C-N-CA	-6.25	113.94	120.38
4	D	170	ALA	CA-C-N	-6.17	113.59	119.76
4	D	170	ALA	C-N-CA	-6.17	113.59	119.76
1	a	142	TRP	N-CA-C	6.04	120.35	112.92
1	A	83	VAL	N-CA-C	5.87	113.68	108.63
1	a	65	GLU	CA-C-N	-5.81	113.71	119.99
1	a	65	GLU	C-N-CA	-5.81	113.71	119.99
5	e	63	ILE	N-CA-C	5.80	114.42	109.02
1	A	131	TRP	CA-CB-CG	-5.26	103.61	113.60
4	D	94	GLY	CA-C-N	5.18	125.26	119.87
4	D	94	GLY	C-N-CA	5.18	125.26	119.87
2	b	175	THR	CB-CA-C	-5.17	102.57	111.45
3	C	421	SER	N-CA-C	5.15	115.52	109.60
8	I	34	ARG	N-CA-C	5.10	117.05	109.25
2	B	23	HIS	N-CA-C	5.06	116.79	111.28
3	c	408	GLY	N-CA-C	-5.04	105.31	112.37
5	e	58	GLN	N-CA-C	5.02	116.75	111.28
16	v	105	ARG	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	o	60	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2626	0	2515	26	0
1	a	2622	0	2529	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4012	0	3860	58	0
2	b	3884	0	3743	50	0
3	C	3483	0	3397	33	0
3	c	3523	0	3439	39	0
4	D	2728	0	2636	35	0
4	d	2722	0	2623	27	0
5	E	632	0	605	16	0
5	e	636	0	612	9	0
6	F	269	0	277	4	0
6	f	257	0	269	4	0
7	H	508	0	524	6	0
7	h	501	0	526	4	0
8	I	284	0	303	6	0
8	i	300	0	320	2	0
9	J	251	0	257	3	0
9	j	272	0	271	2	0
10	K	293	0	305	4	0
10	k	285	0	290	4	0
11	L	302	0	316	1	0
11	l	296	0	305	0	0
12	M	259	0	281	32	0
12	m	264	0	283	26	0
13	O	1870	0	1836	29	0
13	o	1838	0	1789	30	0
14	T	257	0	260	1	0
14	t	258	0	261	3	0
15	U	766	0	758	21	0
15	u	770	0	769	6	0
16	V	1080	0	1097	9	0
16	v	1052	0	1040	14	0
17	Y	212	0	237	4	0
17	y	213	0	239	4	0
18	X	274	0	297	1	0
18	x	252	0	277	2	0
19	Z	450	0	455	1	0
19	z	433	0	422	7	0
20	A	189	0	202	8	0
20	B	1040	0	1152	22	0
20	C	830	0	900	25	0
20	D	195	0	216	4	0
20	a	172	0	166	5	0
20	b	1040	0	1152	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	c	840	0	923	29	0
20	d	195	0	216	4	0
21	A	64	0	74	1	0
21	D	64	0	74	1	0
21	a	128	0	148	2	0
22	A	40	0	56	5	0
22	B	120	0	168	6	0
22	C	80	0	112	3	0
22	D	40	0	56	3	0
22	K	80	0	112	3	0
22	T	40	0	56	4	0
22	a	40	0	56	1	0
22	b	120	0	168	5	0
22	c	40	0	56	1	0
22	d	40	0	56	3	0
22	j	40	0	56	5	0
22	k	80	0	112	6	0
22	t	40	0	56	4	0
23	A	108	0	156	5	0
23	F	35	0	40	1	0
23	a	108	0	156	9	0
23	b	54	0	78	3	0
23	f	40	0	47	2	0
23	l	54	0	78	2	0
24	A	51	0	72	4	0
24	B	51	0	72	0	0
24	C	96	0	132	5	0
24	J	45	0	60	0	0
24	a	51	0	72	4	0
24	b	49	0	68	2	0
24	c	102	0	144	0	0
24	j	45	0	60	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	40	0	0	0	0
26	B	84	0	0	3	0
26	C	34	0	0	0	0
26	D	53	0	0	0	0
26	E	15	0	0	0	0
26	H	10	0	0	0	0
26	I	61	0	0	0	0
26	J	33	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	14	0	0	0	0
26	M	12	0	0	0	0
26	T	13	0	0	0	0
26	U	14	0	0	3	0
26	X	16	0	0	0	0
26	Z	4	0	0	0	0
26	a	45	0	0	1	0
26	b	68	0	0	2	0
26	c	48	0	0	0	0
26	d	68	0	0	0	0
26	e	7	0	0	0	0
26	h	16	0	0	0	0
26	i	38	0	0	0	0
26	j	22	0	0	0	0
26	t	16	0	0	0	0
26	x	9	0	0	0	0
26	z	6	0	0	0	0
27	A	55	0	80	11	0
27	D	55	0	80	0	0
27	a	55	0	80	10	0
27	d	55	0	80	0	0
28	A	20	0	30	8	0
28	B	48	0	72	24	0
28	C	40	0	60	15	0
28	D	16	0	24	12	0
28	F	4	0	6	3	0
28	H	4	0	6	0	0
28	O	36	0	54	7	0
28	U	16	0	24	16	0
28	V	24	0	36	5	0
28	b	44	0	66	27	0
28	c	40	0	60	16	0
28	d	12	0	18	8	0
28	h	4	0	6	0	0
28	i	4	0	6	4	0
28	j	4	0	6	0	0
28	o	28	0	42	22	0
28	u	12	0	18	3	0
28	v	32	0	48	4	0
29	A	1	0	0	0	0
29	a	1	0	0	0	0
30	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	10	0	0	0	0
31	A	4	0	0	5	0
31	a	4	0	0	0	0
32	B	95	0	130	17	0
32	C	76	0	104	2	0
32	D	19	0	26	3	0
32	O	19	0	26	0	0
32	V	13	0	11	0	0
32	b	76	0	104	6	0
32	c	38	0	52	1	0
32	d	19	0	26	0	0
32	u	8	0	15	0	0
32	v	14	0	13	1	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	V	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	64	0	95	4	0
34	E	24	0	35	0	0
34	I	35	0	46	2	0
34	J	24	0	35	1	0
34	M	35	0	46	0	0
34	T	24	0	35	0	0
34	Z	35	0	46	0	0
34	a	35	0	46	10	0
34	b	57	0	72	3	0
34	c	35	0	46	2	0
34	f	24	0	35	0	0
34	m	70	0	92	1	0
34	z	35	0	46	5	0
35	C	179	0	232	0	0
35	D	51	0	71	5	0
35	H	62	0	82	2	0
35	c	181	0	236	3	0
35	d	51	0	71	2	0
35	h	62	0	82	1	0
36	D	147	0	222	19	0
36	E	48	0	71	6	0
36	L	49	0	74	0	0
36	d	147	0	222	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	l	49	0	74	1	0
37	E	43	0	30	1	0
37	e	43	0	30	3	0
38	H	41	0	56	0	0
38	x	41	0	56	3	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	182	0	0	3	0
41	B	473	0	0	18	0
41	C	324	0	0	9	0
41	D	180	0	0	1	0
41	E	66	0	0	1	0
41	F	8	0	0	0	0
41	H	65	0	0	2	0
41	I	16	0	0	1	0
41	J	23	0	0	0	0
41	K	12	0	0	0	0
41	L	21	0	0	0	0
41	M	12	0	0	1	0
41	O	273	0	0	10	0
41	T	20	0	0	0	0
41	U	136	0	0	4	0
41	V	183	0	0	4	0
41	X	22	0	0	1	0
41	Y	7	0	0	0	0
41	Z	5	0	0	0	0
41	a	185	0	0	6	0
41	b	465	0	0	8	0
41	c	374	0	0	4	0
41	d	182	0	0	5	0
41	e	49	0	0	0	0
41	f	16	0	0	0	0
41	h	70	0	0	1	0
41	i	21	0	0	2	0
41	j	24	0	0	0	0
41	k	12	0	0	0	0
41	l	24	0	0	1	0
41	m	24	0	0	0	0
41	o	230	0	0	10	0
41	t	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	u	150	0	0	0	0
41	v	147	0	0	2	0
41	x	26	0	0	1	0
41	y	7	0	0	1	0
41	z	12	0	0	1	0
All	All	54996	0	51554	741	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (741) 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)
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:CD2	1.18	1.58
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD22	1.43	1.45
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD11	1.55	1.32
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CD2	2.06	1.19
3:c:362:ARG:HD3	28:c:530:DMS:H11	1.21	1.19
32:B:621:HTG:H5	34:a:418:LMT:O2'	1.42	1.18
2:B:347[B]:ARG:NH1	41:B:1031[B]:HOH:O	1.81	1.14
2:b:350:GLU:HG3	28:b:639:DMS:H12	1.29	1.13
15:U:22:GLY:HA2	28:U:903[B]:DMS:H13	1.30	1.12
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD21	1.80	1.12
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:HD13	1.30	1.12
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:CD1	1.79	1.12
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:HD21	1.14	1.11
1:A:214:MET:HG2	27:A:411:PL9:H102	1.10	1.10
36:D:409:LHG:H382	36:D:409:LHG:H132	1.25	1.09
36:D:409:LHG:H382	36:D:409:LHG:C13	1.81	1.09
5:E:61:ARG:NH2	41:E:201:HOH:O	1.83	1.08
5:e:57:ALA:HB3	5:e:60[A]:GLN:HE22	1.15	1.06
20:c:510:CLA:H41	36:d:408:LHG:H383	1.37	1.05
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CD2	1.88	1.02
15:U:86:GLU:HG2	26:U:901:UNL:C16	1.88	1.02
4:d:233:ARG:HG2	4:d:233:ARG:HH11	1.23	1.02
2:B:178:VAL:H	28:B:642:DMS:H22	1.25	1.02
36:D:409:LHG:H342	36:D:409:LHG:H302	1.36	1.02
15:U:22:GLY:HA2	28:U:903[B]:DMS:C1	1.90	1.02
13:o:115:ARG:HH11	28:o:302:DMS:H11	1.20	1.01
36:d:408:LHG:H132	36:d:408:LHG:C37	1.91	1.00
28:o:302:DMS:H12	41:o:600:HOH:O	1.58	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:362:ARG:HH11	28:c:530:DMS:H12	1.27	1.00
13:O:141:ASP:HB2	28:O:310:DMS:H11	1.43	0.99
15:U:17:LEU:HD23	28:U:903[B]:DMS:H11	1.44	0.99
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD1	2.37	0.98
34:a:418:LMT:H6E	41:a:540:HOH:O	1.63	0.98
1:a:214:MET:HG2	27:a:415:PL9:H102	1.40	0.97
16:V:5:PRO:HD3	28:V:206:DMS:H21	1.50	0.93
2:b:350:GLU:HG3	28:b:639:DMS:C1	1.98	0.93
41:B:980:HOH:O	28:D:414:DMS:H21	1.67	0.93
16:v:90:GLU:HB2	28:v:206:DMS:C1	1.98	0.93
3:C:364:PRO:HA	28:C:531:DMS:H23	1.48	0.93
2:B:405:GLU:HG2	41:B:1060:HOH:O	1.68	0.93
36:D:409:LHG:H132	36:D:409:LHG:C38	1.99	0.93
31:A:421:BCT:O1	4:D:264[A]:LYS:NZ	2.03	0.92
13:O:130[A]:GLN:H	13:O:130[A]:GLN:HE21	1.17	0.91
28:c:536:DMS:H11	16:v:47:LYS:NZ	1.86	0.90
16:v:90:GLU:HB2	28:v:206:DMS:H11	1.52	0.90
3:c:362:ARG:NH1	28:c:530:DMS:H12	1.87	0.89
1:A:214:MET:CG	27:A:411:PL9:H102	2.02	0.89
1:A:214:MET:HG2	27:A:411:PL9:C10	1.99	0.89
20:c:510:CLA:H41	36:d:408:LHG:C38	2.04	0.88
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:HD21	1.54	0.88
20:C:510:CLA:H41	36:D:409:LHG:H381	1.56	0.88
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:CD1	2.03	0.87
28:c:536:DMS:H11	16:v:47:LYS:HZ3	1.39	0.87
28:c:530:DMS:H13	41:o:417:HOH:O	1.72	0.87
32:B:621:HTG:H5	34:a:418:LMT:H2O2	1.36	0.87
12:M:16[B]:LEU:CG	12:m:16[B]:LEU:HD21	2.04	0.86
3:c:362:ARG:HD3	28:c:530:DMS:C1	2.05	0.86
4:D:140:PRO:HD2	28:D:414:DMS:H22	1.57	0.86
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CD1	2.53	0.86
1:a:66:PRO:HG2	28:o:302:DMS:H13	1.57	0.85
20:C:504:CLA:H201	36:D:409:LHG:H352	1.58	0.85
5:e:57:ALA:HB3	5:e:60[A]:GLN:NE2	1.92	0.84
13:o:115:ARG:HH11	28:o:302:DMS:C1	1.90	0.84
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD13	2.07	0.84
22:b:621:BCR:H331	22:b:621:BCR:C8	2.08	0.83
15:U:9:LEU:HA	28:U:904:DMS:S	2.19	0.83
2:B:389:LYS:HE3	41:B:987:HOH:O	1.79	0.83
31:A:421:BCT:C	4:D:264[A]:LYS:NZ	2.42	0.82
41:C:745:HOH:O	8:I:33:LYS:HE2	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:214:MET:HG2	27:a:415:PL9:C10	2.09	0.82
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:HD11	0.83	0.82
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.60	0.81
36:E:103:LHG:H271	36:E:103:LHG:H321	1.61	0.81
20:d:404:CLA:HBB1	20:d:404:CLA:HMB3	1.63	0.80
36:d:408:LHG:H132	36:d:408:LHG:H372	1.62	0.80
13:o:180:GLU:O	28:o:303:DMS:H21	1.81	0.79
36:d:408:LHG:H372	36:d:408:LHG:H332	1.65	0.79
13:O:49[A]:THR:HG22	41:O:613:HOH:O	1.82	0.79
3:c:362:ARG:HH11	28:c:530:DMS:C1	1.95	0.78
36:D:409:LHG:H302	36:D:409:LHG:C34	2.14	0.78
41:a:511:HOH:O	4:d:139:ARG:HD2	1.82	0.78
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:CG	2.14	0.78
20:A:401:CLA:HBB1	20:A:401:CLA:HMB3	1.65	0.77
31:A:421:BCT:C	4:D:264[A]:LYS:HZ3	1.97	0.77
13:o:74[B]:GLU:OE1	41:o:401:HOH:O	2.00	0.77
20:C:508:CLA:HBC2	36:D:409:LHG:H371	1.65	0.77
1:a:72:LEU:HD11	34:a:418:LMT:H52	1.65	0.77
13:O:64:GLU:HG3	41:O:595:HOH:O	1.83	0.77
2:b:350:GLU:H	28:b:639:DMS:C1	1.99	0.76
3:C:367:GLU:HB2	28:C:531:DMS:H21	1.66	0.76
2:B:423:LYS:HG3	32:B:622:HTG:H1'2	1.66	0.76
12:M:16[B]:LEU:CG	12:m:16[B]:LEU:CD2	2.63	0.76
36:D:409:LHG:H342	36:D:409:LHG:C30	2.16	0.75
2:b:472:ARG:HG2	28:d:414:DMS:H12	1.67	0.75
13:O:231:HIS:HD2	41:O:568:HOH:O	1.70	0.75
10:k:21:LEU:HB2	17:y:24:MET:HE3	1.66	0.75
15:U:22:GLY:CA	28:U:903[B]:DMS:H13	2.12	0.75
28:o:306:DMS:H23	41:o:607:HOH:O	1.86	0.74
28:B:642:DMS:H23	41:B:755:HOH:O	1.86	0.74
2:b:423:LYS:HE2	41:o:444:HOH:O	1.86	0.74
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.86	0.74
23:a:409:SQD:H381	9:j:22:ILE:HD11	1.70	0.73
35:D:406:DGD:HD4	5:E:45:ASP:HB3	1.71	0.73
28:o:307:DMS:H21	41:o:515:HOH:O	1.87	0.73
36:D:409:LHG:H382	36:D:409:LHG:H131	1.69	0.73
4:D:12:ARG:HG3	4:D:13:GLY:N	2.04	0.72
15:U:17:LEU:HD23	28:U:903[B]:DMS:C1	2.19	0.72
2:B:178:VAL:H	28:B:642:DMS:C2	2.00	0.72
15:U:17:LEU:CD2	28:U:903[B]:DMS:H11	2.19	0.72
32:B:621:HTG:H1	34:a:418:LMT:H11	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:621:BCR:H331	22:b:621:BCR:HC8	1.70	0.71
28:b:631:DMS:H12	41:d:537:HOH:O	1.89	0.71
28:i:104:DMS:H22	41:i:206:HOH:O	1.91	0.71
2:b:350:GLU:H	28:b:639:DMS:H11	1.55	0.71
4:d:233:ARG:HG2	4:d:233:ARG:NH1	1.98	0.71
4:D:144:ILE:CD1	28:D:414:DMS:O	2.39	0.71
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD2	2.54	0.71
12:M:16[A]:LEU:HD23	23:b:622:SQD:H381	1.72	0.70
5:E:61:ARG:HG3	28:V:208:DMS:H21	1.72	0.70
2:b:410:THR:H	28:b:640:DMS:H23	1.57	0.70
13:O:57:LYS:HD2	41:b:755:HOH:O	1.92	0.70
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CG	2.22	0.70
2:b:360:PRO:HA	28:b:631:DMS:H11	1.74	0.69
28:A:418:DMS:H12	5:E:63:ILE:HD11	1.72	0.69
3:c:362:ARG:CD	28:c:530:DMS:H11	2.13	0.69
2:B:423:LYS:CG	32:B:622:HTG:H1'2	2.23	0.69
13:O:130[A]:GLN:H	13:O:130[A]:GLN:NE2	1.90	0.69
7:h:63:LYS:HG3	41:h:257:HOH:O	1.93	0.69
13:O:198:SER:OG	28:O:306:DMS:H23	1.93	0.69
28:C:532:DMS:H22	16:V:47:LYS:HE3	1.74	0.69
2:B:82:GLY:O	28:o:308:DMS:S	2.50	0.68
36:d:408:LHG:H132	36:d:408:LHG:H371	1.74	0.68
31:A:421:BCT:O3	4:D:264[A]:LYS:NZ	2.27	0.68
4:D:12:ARG:HG3	4:D:13:GLY:H	1.56	0.68
28:c:536:DMS:C1	16:v:47:LYS:NZ	2.57	0.68
13:O:49[A]:THR:HG23	41:O:437:HOH:O	1.93	0.68
28:C:527:DMS:H23	41:C:797:HOH:O	1.93	0.67
28:C:532:DMS:H21	41:C:603:HOH:O	1.93	0.67
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.74	0.67
20:C:508:CLA:CBC	36:D:409:LHG:H371	2.25	0.67
20:c:508:CLA:HBC2	36:d:408:LHG:H361	1.77	0.67
7:H:59:ASN:HD22	7:H:64:ALA:HB3	1.60	0.67
2:B:409:GLN:HE21	28:B:644:DMS:C1	2.08	0.66
20:c:513:CLA:HBB1	20:c:513:CLA:HMB3	1.77	0.66
13:O:15:LEU:HD23	13:O:18:LYS:HD2	1.76	0.66
13:o:115:ARG:HD3	28:o:302:DMS:H11	1.76	0.66
15:U:17:LEU:CD2	28:U:903[B]:DMS:C1	2.74	0.66
28:B:641:DMS:H11	41:B:931:HOH:O	1.95	0.65
2:B:341:LYS:NZ	32:B:622:HTG:S1	2.62	0.65
2:B:472:ARG:HG2	28:D:414:DMS:C1	2.26	0.65
2:b:371:THR:OG1	28:b:638:DMS:H13	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:GLU:OE1	2:B:431[A]:GLU:OE1	2.14	0.65
16:v:90:GLU:CB	28:v:206:DMS:C1	2.73	0.65
20:B:601:CLA:HED2	20:B:601:CLA:H43	1.79	0.65
20:B:602:CLA:H42	41:B:1029:HOH:O	1.97	0.65
3:C:367:GLU:HB2	28:C:531:DMS:C2	2.26	0.64
28:b:631:DMS:H13	41:d:541:HOH:O	1.95	0.64
36:D:409:LHG:H152	36:D:409:LHG:H362	1.80	0.64
5:E:15:THR:HB	9:J:8:ILE:O	1.97	0.64
28:d:413:DMS:H11	41:d:586[A]:HOH:O	1.98	0.64
20:B:606:CLA:C14	20:B:611:CLA:HED2	2.28	0.63
23:a:401:SQD:H442	41:a:667:HOH:O	1.96	0.63
13:O:130[A]:GLN:HG3	28:O:310:DMS:H12	1.79	0.63
22:T:101:BCR:H321	22:T:101:BCR:HC8	1.80	0.63
28:o:307:DMS:H22	41:o:488:HOH:O	1.97	0.63
5:E:10:PHE:H	36:E:103:LHG:HC32	1.64	0.63
3:C:117:VAL:CG1	24:C:524:LMG:H202	2.28	0.63
28:A:418:DMS:H23	5:E:63:ILE:HD12	1.81	0.63
4:d:342:PRO:HA	28:d:413:DMS:H12	1.81	0.63
15:U:10:VAL:H	28:U:904:DMS:H21	1.64	0.62
4:d:123:ILE:HD11	35:h:101:DGD:HAW2	1.80	0.62
32:v:210:HTG:H1'1	41:v:439:HOH:O	1.98	0.62
20:B:616:CLA:HBB1	20:B:616:CLA:HMB3	1.81	0.62
3:C:364:PRO:O	28:C:531:DMS:H12	1.98	0.62
28:c:536:DMS:C1	16:v:47:LYS:HZ1	2.13	0.62
22:t:101:BCR:HC8	22:t:101:BCR:H311	1.81	0.62
3:c:201:ASN:HB2	41:c:844:HOH:O	1.99	0.62
13:o:115:ARG:NH1	28:o:302:DMS:H11	2.04	0.62
1:A:98[A]:GLU:OE2	41:A:501:HOH:O	2.11	0.62
22:B:618:BCR:H331	22:B:618:BCR:C8	2.29	0.62
13:o:231:HIS:HD2	28:o:306:DMS:O	1.83	0.62
1:A:265:PHE:HE2	27:A:411:PL9:H122	1.64	0.61
36:D:409:LHG:C34	36:D:409:LHG:C30	2.75	0.61
34:a:418:LMT:C6'	41:a:540:HOH:O	2.36	0.61
20:B:601:CLA:H201	26:B:628:UNL:C15	2.31	0.61
2:b:248:ALA:HA	20:b:605:CLA:H42	1.81	0.61
2:b:341:LYS:NZ	32:b:625:HTG:S1	2.66	0.61
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CG	2.77	0.61
28:F:102:DMS:C1	16:V:27:LEU:HD21	2.31	0.60
13:O:49[B]:THR:HG23	13:O:236:GLN:HB2	1.81	0.60
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.36	0.60
1:a:66:PRO:CG	28:o:302:DMS:H13	2.29	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:d:404:CLA:HBB1	20:d:404:CLA:CMB	2.31	0.60
24:A:407:LMG:C25	24:A:407:LMG:H422	2.31	0.60
15:U:86:GLU:H	26:U:901:UNL:C16	2.15	0.60
2:b:341:LYS:NZ	32:b:625:HTG:O2	2.21	0.60
28:F:102:DMS:H12	16:V:27:LEU:HD21	1.84	0.60
15:u:56:GLU:N	28:u:203:DMS:O	2.23	0.60
20:C:506:CLA:H92	34:I:101:LMT:H111	1.84	0.60
28:b:634:DMS:H23	41:b:1015:HOH:O	2.02	0.60
13:O:231:HIS:CD2	41:O:568:HOH:O	2.50	0.59
41:a:511:HOH:O	4:d:139:ARG:CD	2.45	0.59
15:U:22:GLY:HA2	28:U:903[B]:DMS:H12	1.83	0.59
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.59
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.84	0.59
28:V:204:DMS:H21	41:V:474:HOH:O	2.02	0.59
2:b:341:LYS:HZ1	32:b:625:HTG:C2	2.14	0.59
37:E:104:HEM:HMC2	6:F:31:ILE:HG13	1.84	0.59
13:o:115:ARG:CD	28:o:302:DMS:H11	2.32	0.59
27:A:411:PL9:H162	36:E:103:LHG:H322	1.84	0.59
34:B:626:LMT:H5'	34:a:418:LMT:O6'	2.03	0.59
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.85	0.59
32:B:621:HTG:H1'1	28:B:643:DMS:H22	1.83	0.59
20:C:504:CLA:C20	36:D:409:LHG:H352	2.30	0.59
2:b:350:GLU:N	28:b:639:DMS:C1	2.64	0.59
19:z:44:SER:O	19:z:48:ILE:HG13	2.03	0.59
3:C:117:VAL:HG12	24:C:524:LMG:H202	1.84	0.58
4:D:144:ILE:HD11	28:D:414:DMS:O	2.01	0.58
7:H:59:ASN:HD22	7:H:64:ALA:CB	2.16	0.58
20:B:611:CLA:H151	20:B:611:CLA:H203	1.84	0.58
5:E:9:PRO:HA	36:E:103:LHG:HC32	1.84	0.58
20:B:605:CLA:H43	20:B:606:CLA:H2	1.85	0.58
20:b:617:CLA:H2	20:b:618:CLA:HBB2	1.86	0.58
13:o:42:ARG:O	13:o:241:ALA:HA	2.03	0.58
2:b:472:ARG:CG	28:d:414:DMS:H12	2.32	0.58
27:A:411:PL9:H502	4:D:39:PRO:HG3	1.86	0.57
23:A:406:SQD:C12	23:A:406:SQD:H162	2.34	0.57
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.87	0.57
20:c:501:CLA:H192	20:c:506:CLA:C1B	2.35	0.57
1:A:103:ASP:OD2	28:A:415:DMS:H22	2.05	0.57
16:V:106[A]:ASN:OD1	41:V:301:HOH:O	2.17	0.57
2:B:224[B]:ARG:NH2	41:B:702:HOH:O	2.37	0.57
16:v:91:VAL:HG13	28:v:206:DMS:H12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:B:635:DMS:H11	41:B:902:HOH:O	2.03	0.57
3:c:182:PHE:HA	32:c:520:HTG:H61	1.85	0.57
12:M:16[A]:LEU:CD2	23:b:622:SQD:H381	2.34	0.56
34:b:628:LMT:H6E	4:d:19:ASP:OD2	2.05	0.56
22:B:619:BCR:H331	22:B:619:BCR:C8	2.34	0.56
34:J:103:LMT:H123	26:J:107:UNL:C3	2.35	0.56
1:a:183:MET:HA	20:a:403:CLA:HMD1	1.86	0.56
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.40	0.56
35:c:516:DGD:HAT2	35:c:517:DGD:HBH2	1.86	0.56
20:B:601:CLA:C20	26:B:628:UNL:C15	2.83	0.56
34:z:102:LMT:H6'2	34:z:102:LMT:H2B	1.87	0.56
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CG	2.80	0.56
15:u:50:VAL:O	28:u:202:DMS:H23	2.04	0.56
20:b:609:CLA:H2	24:b:623:LMG:H152	1.87	0.56
36:d:408:LHG:H132	36:d:408:LHG:C38	2.36	0.56
24:C:519:LMG:H221	10:K:30:VAL:HG11	1.87	0.56
13:o:179:GLU:HG2	41:o:420:HOH:O	2.06	0.56
28:C:531:DMS:H22	41:C:878:HOH:O	2.06	0.55
23:F:101:SQD:H461	41:X:201:HOH:O	2.07	0.55
3:c:409:GLY:HA2	28:c:536:DMS:S	2.46	0.55
1:a:38:ILE:HG12	23:a:401:SQD:H142	1.87	0.55
22:C:515:BCR:H331	22:C:515:BCR:C8	2.36	0.55
2:b:355:PHE:HB2	28:b:638:DMS:H11	1.88	0.55
2:B:409:GLN:HE21	28:B:644:DMS:H12	1.71	0.55
20:b:611:CLA:NC	38:x:101:RRX:H56	2.21	0.55
2:B:13:ILE:O	28:B:645:DMS:H11	2.06	0.55
28:B:641:DMS:H13	41:B:1079:HOH:O	2.07	0.55
24:C:519:LMG:H242	9:J:22:ILE:HD13	1.88	0.55
22:D:405:BCR:H313	35:D:406:DGD:HAW2	1.88	0.55
5:e:57:ALA:CB	5:e:60[A]:GLN:HE22	2.05	0.55
41:l:211[B]:HOH:O	12:m:4:ASN:ND2	2.39	0.55
3:C:279:LEU:HD12	3:C:282:MET:CE	2.37	0.54
13:o:183:ALA:HB3	28:o:303:DMS:H22	1.88	0.54
13:O:39:ARG:HH11	13:O:82:GLN:HE21	1.54	0.54
28:A:418:DMS:H12	5:E:63:ILE:CD1	2.37	0.54
15:U:10:VAL:H	28:U:904:DMS:C2	2.20	0.54
22:b:621:BCR:HC8	22:b:621:BCR:C33	2.38	0.54
7:H:2:ALA:N	41:H:201:HOH:O	2.41	0.54
22:d:405:BCR:H331	22:d:405:BCR:C8	2.38	0.54
2:B:171:PRO:HB3	7:H:63:LYS:HA	1.90	0.54
28:C:532:DMS:H22	16:V:47:LYS:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.89	0.54
3:c:452:ALA:O	28:i:104:DMS:H13	2.08	0.54
20:a:404:CLA:HBB1	20:a:404:CLA:HMB1	1.89	0.54
3:c:127:PHE:CE1	34:z:102:LMT:H21	2.43	0.54
3:C:409:GLY:HA2	28:C:532:DMS:S	2.48	0.54
23:A:406:SQD:H162	23:A:406:SQD:H122	1.90	0.53
20:c:509:CLA:HMB1	20:c:509:CLA:HBB1	1.90	0.53
41:C:745:HOH:O	8:I:33:LYS:CE	2.47	0.53
7:H:59:ASN:ND2	7:H:64:ALA:HB3	2.23	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.53
27:A:411:PL9:H151	36:E:103:LHG:H331	1.90	0.53
28:C:532:DMS:C2	41:C:603:HOH:O	2.55	0.53
11:L:9:PRO:HA	34:m:102:LMT:H6D	1.90	0.53
28:U:903[A]:DMS:H23	41:U:1017:HOH:O	2.08	0.53
20:b:616:CLA:H161	20:b:616:CLA:H111	1.89	0.53
5:e:60[B]:GLN:NE2	5:e:62:SER:O	2.40	0.53
1:a:215:HIS:HA	27:a:415:PL9:O1	2.08	0.53
4:d:272:LEU:C	4:d:272:LEU:HD23	2.33	0.53
1:A:237:TYR:CZ	4:D:264[B]:LYS:HG3	2.44	0.53
15:U:47:LYS:NZ	41:U:1002:HOH:O	2.42	0.53
20:B:604:CLA:C4D	20:B:606:CLA:H43	2.38	0.53
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.44	0.53
19:z:3:ILE:HA	41:z:201:HOH:O	2.08	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.43	0.53
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.91	0.53
3:C:150:ASP:OD2	41:C:601:HOH:O	2.19	0.53
2:B:36[A]:SER:OG	22:B:618:BCR:H362	2.08	0.52
28:B:635:DMS:H22	28:D:413:DMS:C1	2.40	0.52
20:b:607:CLA:HHC	20:b:607:CLA:HBB1	1.91	0.52
1:A:183:MET:HA	20:A:401:CLA:HMD1	1.91	0.52
28:b:631:DMS:H11	41:b:764:HOH:O	2.10	0.52
28:b:639:DMS:H12	41:b:1051:HOH:O	2.10	0.52
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.43	0.52
3:C:371:GLY:HA3	41:C:622:HOH:O	2.10	0.52
20:c:513:CLA:HBB1	20:c:513:CLA:CMB	2.39	0.52
13:o:129:THR:HA	13:o:141:ASP:O	2.08	0.52
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.90	0.52
28:i:104:DMS:C2	41:i:206:HOH:O	2.55	0.52
31:A:421:BCT:C	4:D:264[A]:LYS:HZ1	2.12	0.52
3:C:318:LEU:C	3:C:318:LEU:HD23	2.34	0.52
4:D:13:GLY:HA3	32:D:417:HTG:H62	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:618:CLA:H203	20:b:618:CLA:H143	1.91	0.52
13:o:231:HIS:HE1	41:o:498:HOH:O	1.93	0.52
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.40	0.52
2:B:14[B]:ASN:HA	28:B:645:DMS:H21	1.91	0.52
20:c:506:CLA:HMC2	20:c:507:CLA:H102	1.92	0.52
26:B:647:UNL:C13	23:a:401:SQD:H302	2.40	0.52
20:c:508:CLA:CBC	36:d:408:LHG:H361	2.39	0.52
2:B:472:ARG:HG2	28:D:414:DMS:H12	1.92	0.51
3:c:126:GLY:O	3:c:130:VAL:HG23	2.10	0.51
20:c:502:CLA:H61	20:c:512:CLA:H42	1.91	0.51
15:U:50:VAL:O	28:U:902:DMS:H23	2.11	0.51
3:c:179:ALA:O	3:c:184:GLY:HA2	2.11	0.51
22:T:101:BCR:H382	22:T:101:BCR:H23C	1.92	0.51
20:C:504:CLA:H202	36:D:409:LHG:H361	1.92	0.51
15:U:21:TYR:O	28:U:903[B]:DMS:H13	2.11	0.51
23:l:101:SQD:H192	22:t:101:BCR:H351	1.93	0.51
4:D:99:GLY:O	35:D:406:DGD:HA21	2.10	0.51
2:b:472:ARG:CG	28:d:414:DMS:C1	2.89	0.51
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.93	0.51
17:y:18:VAL:N	41:y:101:HOH:O	2.44	0.51
16:V:5:PRO:CD	28:V:206:DMS:H21	2.34	0.51
27:a:415:PL9:H502	4:d:39:PRO:HG3	1.93	0.51
2:b:410:THR:H	28:b:640:DMS:C2	2.22	0.51
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
2:B:409:GLN:NE2	28:B:644:DMS:H13	2.26	0.51
3:c:38:GLY:HA3	20:c:511:CLA:HMD2	1.93	0.50
13:o:114:GLU:OE2	28:o:306:DMS:H12	2.11	0.50
22:d:405:BCR:H313	35:d:416:DGD:HAT2	1.94	0.50
23:A:412:SQD:H442	41:A:661:HOH:O	2.11	0.50
2:B:423:LYS:HE2	41:B:886:HOH:O	2.10	0.50
2:b:372:ASP:O	28:b:638:DMS:H12	2.12	0.50
1:A:215:HIS:HA	27:A:411:PL9:O1	2.11	0.50
20:a:403:CLA:HBB1	20:a:403:CLA:HMB1	1.94	0.50
4:d:236:ASN:O	4:d:239:GLN:HG2	2.12	0.50
7:h:12:ARG:HB3	7:h:13:PRO:HD3	1.94	0.50
24:a:410:LMG:C25	24:a:410:LMG:C43	2.90	0.50
4:D:304:ARG:HH12	34:b:627:LMT:H6'1	1.76	0.50
4:D:12:ARG:CG	4:D:13:GLY:H	2.18	0.50
2:b:148[B]:LEU:HD23	20:b:606:CLA:H202	1.93	0.50
20:b:607:CLA:C14	20:b:612:CLA:HED2	2.42	0.50
20:c:504:CLA:H191	36:d:408:LHG:H362	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:406:SQD:H142	36:D:409:LHG:H161	1.94	0.49
2:B:409:GLN:HE21	28:B:644:DMS:H13	1.77	0.49
3:C:279:LEU:HA	3:C:282:MET:HE3	1.94	0.49
15:U:16:LYS:NZ	41:U:1004:HOH:O	2.45	0.49
2:b:350:GLU:CG	28:b:639:DMS:C1	2.84	0.49
28:B:635:DMS:H22	28:D:413:DMS:H11	1.94	0.49
20:C:506:CLA:HMC2	20:C:507:CLA:H102	1.93	0.49
2:B:224[B]:ARG:HH11	34:B:625:LMT:H2'	1.76	0.49
17:Y:18:VAL:O	17:Y:22:LEU:HD12	2.12	0.49
35:c:517:DGD:HBf1	36:d:408:LHG:H223	1.95	0.49
12:M:5:GLN:H	12:M:5:GLN:HE21	1.60	0.49
17:Y:38:LEU:O	17:Y:42:ARG:HD3	2.13	0.49
2:b:341:LYS:NZ	32:b:625:HTG:C2	2.75	0.49
2:B:350:GLU:HG3	28:B:637:DMS:O	2.12	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.49
15:u:97:ARG:NH1	28:u:202:DMS:O	2.38	0.49
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.94	0.49
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.78	0.49
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.95	0.49
20:C:510:CLA:H41	36:D:409:LHG:C38	2.35	0.49
5:E:10:PHE:H	36:E:103:LHG:C3	2.24	0.49
4:D:272:LEU:C	4:D:272:LEU:HD23	2.38	0.49
2:B:178:VAL:N	28:B:642:DMS:H22	2.10	0.49
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.95	0.48
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.94	0.48
16:v:122:GLU:HG3	16:v:126:LEU:HD12	1.95	0.48
1:A:229:GLU:HG2	41:A:577:HOH:O	2.13	0.48
22:d:405:BCR:HC22	35:d:416:DGD:HA82	1.95	0.48
2:B:409:GLN:NE2	28:B:644:DMS:C1	2.76	0.48
22:D:405:BCR:C8	22:D:405:BCR:H331	2.44	0.48
28:o:307:DMS:C2	41:o:488:HOH:O	2.57	0.48
21:A:403:PHO:NC	21:A:403:PHO:ND	2.62	0.48
24:A:407:LMG:H231	24:A:407:LMG:H201	1.56	0.48
20:c:508:CLA:HMB3	20:c:508:CLA:HBB1	1.96	0.48
23:A:412:SQD:H272	2:b:109:LEU:HD13	1.96	0.48
20:C:510:CLA:H52	36:D:409:LHG:H372	1.95	0.48
4:D:13:GLY:HA3	32:D:417:HTG:C6	2.43	0.48
1:A:215:HIS:ND1	27:A:411:PL9:O1	2.39	0.48
2:B:90:PHE:H	32:B:632:HTG:H62	1.78	0.48
4:D:209:LEU:HD23	4:D:209:LEU:C	2.39	0.48
7:h:3[B]:ARG:HG2	7:h:3[B]:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:y:44:GLY:HA2	19:z:30:PRO:HD3	1.95	0.48
27:A:411:PL9:H403	6:F:22:ALA:HB2	1.96	0.48
32:B:621:HTG:H2'2	34:a:418:LMT:H21	1.96	0.48
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.95	0.48
2:b:162:PHE:O	20:b:608:CLA:HHD	2.14	0.48
2:b:472:ARG:HG3	28:d:414:DMS:C1	2.44	0.48
20:b:615:CLA:H18	36:d:406:LHG:H202	1.96	0.48
23:b:622:SQD:H311	23:b:622:SQD:H342	1.39	0.48
20:c:506:CLA:H51	34:c:523:LMT:H102	1.96	0.48
19:z:15:LEU:HD22	19:z:46:LEU:HD23	1.94	0.48
3:C:60:ILE:HG22	20:C:503:CLA:HHD	1.95	0.48
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.96	0.48
20:A:401:CLA:CBD	20:D:402:CLA:HAC2	2.44	0.47
3:C:104:GLU:HB2	28:C:527:DMS:H22	1.95	0.47
22:j:102:BCR:H321	22:j:102:BCR:HC8	1.96	0.47
13:o:231:HIS:CD2	28:o:306:DMS:O	2.66	0.47
20:B:614:CLA:HBB1	20:B:614:CLA:HMB1	1.95	0.47
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CD1	2.33	0.47
13:O:244:GLU:HG2	28:O:307:DMS:C1	2.43	0.47
14:t:25:GLU:OE1	14:t:25:GLU:HA	2.13	0.47
36:d:408:LHG:H372	36:d:408:LHG:C33	2.41	0.47
2:B:248:ALA:HA	20:B:604:CLA:H42	1.96	0.47
23:a:409:SQD:H272	36:d:408:LHG:H142	1.97	0.47
20:B:605:CLA:H93	20:B:606:CLA:HAB	1.96	0.47
20:C:502:CLA:H193	32:C:520:HTG:H3'1	1.95	0.47
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.47
1:a:341:LEU:HD13	28:c:536:DMS:H12	1.97	0.47
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.96	0.47
28:c:536:DMS:H13	16:v:47:LYS:HZ1	1.77	0.47
20:C:509:CLA:CMB	20:C:509:CLA:HBB1	2.45	0.47
20:C:509:CLA:HBB1	20:C:509:CLA:HMB3	1.95	0.47
20:C:513:CLA:C4B	22:C:514:BCR:H383	2.43	0.47
20:b:609:CLA:C1D	24:b:623:LMG:H111	2.45	0.47
28:A:416:DMS:H13	8:I:5:LYS:HZ3	1.78	0.47
20:b:603:CLA:H91	38:x:101:RRX:H25	1.97	0.47
3:c:443:TRP:CE2	20:c:508:CLA:HMD2	2.50	0.47
7:h:38:PHE:HB2	38:x:101:RRX:C10	2.44	0.47
18:x:15:LEU:HD23	41:x:214:HOH:O	2.14	0.47
1:a:310:LYS:NZ	41:a:505:HOH:O	2.46	0.47
2:b:467:ILE:HG12	4:d:126:MET:HE1	1.97	0.47
13:o:54:GLU:HA	28:o:306:DMS:H22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:14:ASN:HA	28:b:632:DMS:H11	1.96	0.47
2:b:350:GLU:N	28:b:639:DMS:H13	2.29	0.47
20:c:504:CLA:C19	36:d:408:LHG:H362	2.45	0.47
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.50	0.46
22:A:405:BCR:H382	22:A:405:BCR:H23C	1.97	0.46
13:O:39:ARG:HH11	13:O:82:GLN:NE2	2.13	0.46
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.97	0.46
28:A:416:DMS:H13	8:I:5:LYS:NZ	2.30	0.46
20:b:604:CLA:CMB	20:b:604:CLA:HBB1	2.46	0.46
36:d:408:LHG:H161	36:d:408:LHG:H331	1.97	0.46
2:B:157:HIS:C	2:B:157:HIS:CD2	2.94	0.46
22:T:101:BCR:H382	22:T:101:BCR:C23	2.45	0.46
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.97	0.46
28:A:416:DMS:H22	28:A:417:DMS:H22	1.96	0.46
20:B:611:CLA:CBB	20:B:611:CLA:HHC	2.44	0.46
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.46
13:O:49[B]:THR:CG2	13:O:236:GLN:HB2	2.46	0.46
23:a:401:SQD:H382	26:a:402:UNL:C16	2.46	0.46
20:c:512:CLA:C1B	22:k:102:BCR:H401	2.46	0.46
2:B:30:VAL:HG12	20:B:606:CLA:HHD	1.98	0.46
2:B:286:ARG:HG2	2:B:286:ARG:HH11	1.80	0.46
13:o:158:ASP:HB2	13:o:159:PRO:CD	2.46	0.46
32:B:621:HTG:C5	34:a:418:LMT:H2O2	2.19	0.46
20:A:401:CLA:CAD	20:D:402:CLA:HAC2	2.46	0.46
28:B:642:DMS:C2	41:B:755:HOH:O	2.53	0.46
4:d:52:THR:O	4:d:66:SER:HA	2.16	0.46
26:U:901:UNL:C15	41:U:1118:HOH:O	2.63	0.46
13:o:115:ARG:HD3	28:o:302:DMS:C1	2.45	0.46
2:B:420:TYR:CD1	32:B:622:HTG:H1'1	2.50	0.46
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.51	0.46
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.97	0.46
22:k:101:BCR:H331	22:k:101:BCR:C8	2.46	0.46
13:O:223:ASP:OD2	28:O:305:DMS:H12	2.16	0.46
1:a:218:LEU:HD12	27:a:415:PL9:C3	2.46	0.46
2:b:157:HIS:C	2:b:157:HIS:CD2	2.93	0.46
28:b:634:DMS:H22	28:b:640:DMS:H11	1.98	0.46
2:b:36:SER:OG	22:b:620:BCR:H362	2.17	0.45
2:b:462:PHE:CE1	20:b:615:CLA:HMB3	2.51	0.45
20:b:612:CLA:HHC	20:b:612:CLA:HBB1	1.97	0.45
15:U:10:VAL:HG11	15:U:15:GLU:OE1	2.16	0.45
28:b:631:DMS:C1	41:b:764:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:84:PRO:HA	1:a:112:TYR:CG	2.52	0.45
27:a:415:PL9:H403	6:f:22:ALA:HB2	1.98	0.45
37:e:102:HEM:HMC1	37:e:102:HEM:HBC2	1.99	0.45
2:B:138:MET:HE3	20:B:616:CLA:CHD	2.46	0.45
4:D:103:ARG:O	4:D:107:LEU:HG	2.17	0.45
1:a:214:MET:CG	27:a:415:PL9:H102	2.29	0.45
23:a:409:SQD:H252	36:d:408:LHG:H142	1.97	0.45
3:c:318:LEU:C	3:c:318:LEU:HD23	2.41	0.45
16:v:45:ILE:C	16:v:45:ILE:HD12	2.41	0.45
22:A:405:BCR:H24C	22:A:405:BCR:H371	1.78	0.45
2:B:204:ALA:CB	20:B:603:CLA:HAB	2.47	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.45
4:D:246:MET:HB2	4:D:264[B]:LYS:HE2	1.99	0.45
8:I:26:GLY:HA3	34:I:101:LMT:H6'1	1.99	0.45
21:a:406:PHO:HBC2	21:a:406:PHO:HHD	1.99	0.45
2:b:55:MET:CE	2:b:80:ILE:HG12	2.47	0.45
3:c:60:ILE:HG22	20:c:503:CLA:HHD	1.99	0.45
34:B:626:LMT:H123	14:t:8:PHE:HA	1.99	0.45
13:O:86:LYS:HD3	41:O:449:HOH:O	2.17	0.45
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.99	0.45
24:C:519:LMG:H221	10:K:30:VAL:CG1	2.46	0.45
22:A:405:BCR:H401	28:A:415:DMS:H12	1.98	0.45
34:a:418:LMT:H6'1	4:d:304:ARG:HH12	1.82	0.45
28:b:631:DMS:C1	41:d:541:HOH:O	2.59	0.45
20:c:504:CLA:H42	35:c:516:DGD:HB31	1.99	0.45
22:K:101:BCR:HC7	22:K:101:BCR:H331	1.67	0.44
20:A:402:CLA:HAB	20:A:402:CLA:HHC	1.82	0.44
32:B:631:HTG:C6	41:B:829:HOH:O	2.64	0.44
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.53	0.44
22:c:514:BCR:H11C	22:c:514:BCR:H341	1.87	0.44
22:j:102:BCR:H311	22:j:102:BCR:C8	2.47	0.44
13:o:181:GLU:HA	28:o:303:DMS:H11	1.99	0.44
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:HD22	0.48	0.44
19:z:31:GLN:O	19:z:33:TRP:N	2.51	0.44
22:A:405:BCR:H382	22:A:405:BCR:C23	2.48	0.44
2:B:497:GLN:HB2	2:B:504:THR:HB	2.00	0.44
4:D:140:PRO:CD	28:D:414:DMS:H22	2.37	0.44
19:z:26:ALA:HB3	19:z:40:ILE:HD11	2.00	0.44
1:A:15:GLU:HG3	41:I:201:HOH:O	2.16	0.44
20:d:403:CLA:H203	20:d:403:CLA:H162	1.70	0.44
23:f:101:SQD:O10	23:f:101:SQD:H262	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:180:GLU:CD	13:o:180:GLU:H	2.26	0.44
20:B:606:CLA:H62	20:B:606:CLA:H41	1.79	0.44
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.53	0.44
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.98	0.44
20:b:610:CLA:H161	20:b:610:CLA:H141	1.85	0.44
20:b:611:CLA:CBB	20:b:611:CLA:HHC	2.48	0.44
28:b:635:DMS:C2	41:b:731:HOH:O	2.66	0.44
15:U:22:GLY:HA2	28:U:903[A]:DMS:H21	1.99	0.44
36:d:408:LHG:H122	36:d:408:LHG:H381	1.99	0.44
5:e:60[A]:GLN:HE21	5:e:60[A]:GLN:HB3	1.49	0.44
8:i:2:GLU:O	8:i:6:ILE:HG12	2.18	0.44
22:j:102:BCR:H382	22:j:102:BCR:H23C	2.00	0.44
13:o:60:ARG:O	13:o:61:GLN:CB	2.65	0.44
28:B:642:DMS:H12	41:B:719:HOH:O	2.17	0.44
3:C:276:LEU:HD23	20:C:509:CLA:HED1	2.00	0.44
4:D:304:ARG:HH22	34:b:627:LMT:H4B	1.82	0.44
12:M:5:GLN:HE21	12:M:5:GLN:N	2.14	0.44
1:a:15:GLU:HB2	34:c:523:LMT:H6'1	1.99	0.44
27:a:415:PL9:H172	27:a:415:PL9:H13	1.47	0.44
20:b:612:CLA:C15	20:b:612:CLA:H203	2.48	0.44
36:d:408:LHG:H132	36:d:408:LHG:H381	1.99	0.44
20:A:401:CLA:HBB1	20:A:401:CLA:CMB	2.40	0.43
28:C:527:DMS:C2	41:C:797:HOH:O	2.61	0.43
35:H:102:DGD:HAW2	35:H:102:DGD:HAN2	1.89	0.43
20:b:618:CLA:H61	20:b:618:CLA:H41	1.78	0.43
24:A:407:LMG:H292	3:C:216:SER:HA	2.00	0.43
20:b:606:CLA:H43	20:b:607:CLA:H2	2.00	0.43
24:A:407:LMG:H321	3:C:217:PRO:HD3	2.01	0.43
3:C:31:SER:CB	3:C:41:ARG:HG2	2.48	0.43
4:D:26:ARG:HA	5:E:5:THR:HB	1.99	0.43
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.01	0.43
4:D:244:TYR:OH	4:D:264[A]:LYS:NZ	2.46	0.43
4:d:85:MET:CE	4:d:96:GLU:HG2	2.48	0.43
28:d:413:DMS:C1	41:d:586[A]:HOH:O	2.61	0.43
6:f:21:VAL:HG21	23:f:101:SQD:H241	2.00	0.43
3:C:95:LEU:HD21	20:C:501:CLA:OBD	2.18	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.43
21:D:403:PHO:HBC2	21:D:403:PHO:HHD	2.00	0.43
2:b:472:ARG:HG2	28:d:414:DMS:C1	2.44	0.43
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.01	0.43
3:C:221:GLU:O	3:C:226:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:D:417:HTG:H61	41:D:591:HOH:O	2.18	0.43
13:O:39:ARG:HB2	13:O:83:GLY:O	2.19	0.43
3:C:220:GLY:O	28:C:530:DMS:H21	2.18	0.43
3:C:409:GLY:HA2	28:C:532:DMS:C1	2.49	0.43
3:C:443:TRP:CE2	20:C:508:CLA:HMD2	2.54	0.43
22:a:408:BCR:H20C	22:a:408:BCR:H361	1.89	0.43
41:c:937:HOH:O	15:u:51:LYS:HD2	2.17	0.43
16:V:45:ILE:HG12	41:V:469:HOH:O	2.18	0.43
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.01	0.43
2:B:49:ASP:OD1	13:o:57:LYS:NZ	2.51	0.43
20:B:611:CLA:HHC	20:B:611:CLA:HBB1	2.00	0.43
21:a:405:PHO:NC	21:a:405:PHO:ND	2.66	0.43
20:b:605:CLA:CMD	20:b:608:CLA:HMB1	2.49	0.43
20:b:606:CLA:H201	26:b:630:UNL:C16	2.49	0.43
36:d:406:LHG:O9	36:l:102:LHG:HC81	2.19	0.43
37:e:102:HEM:HBC2	37:e:102:HEM:CMC	2.49	0.43
15:u:51:LYS:HB2	15:u:51:LYS:HE3	1.66	0.43
41:B:732:HOH:O	13:o:57:LYS:HD2	2.19	0.42
20:a:403:CLA:HBB1	20:a:403:CLA:CMB	2.49	0.42
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.54	0.42
22:B:619:BCR:C23	22:B:619:BCR:H383	2.49	0.42
23:a:409:SQD:H302	20:c:508:CLA:H93	2.01	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42
2:B:467:ILE:HG13	4:D:126:MET:HE1	2.01	0.42
2:B:479:PHE:HA	41:B:980:HOH:O	2.19	0.42
32:B:622:HTG:H6'2	32:B:622:HTG:H3'2	1.28	0.42
22:T:101:BCR:C23	22:T:101:BCR:C38	2.97	0.42
3:c:48:LYS:HG2	3:c:133:ALA:O	2.18	0.42
3:c:472:LEU:HD11	4:d:255:GLN:HG3	2.01	0.42
4:d:24:ARG:NH2	18:x:35:ASP:O	2.52	0.42
28:F:102:DMS:H11	16:V:27:LEU:HD21	2.01	0.42
23:a:409:SQD:H192	36:d:408:LHG:H212	2.00	0.42
24:a:410:LMG:H391	3:c:281:MET:HG3	1.99	0.42
20:b:607:CLA:HHC	20:b:607:CLA:CBB	2.49	0.42
3:c:443:TRP:CD2	20:c:508:CLA:HMD2	2.54	0.42
2:B:341:LYS:NZ	32:B:622:HTG:O2	2.37	0.42
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.08	0.42
13:O:244:GLU:HG2	28:O:307:DMS:H13	2.02	0.42
2:b:82:GLY:O	28:b:641:DMS:O	2.38	0.42
2:b:350:GLU:H	28:b:639:DMS:H13	1.78	0.42
22:k:102:BCR:H11C	22:k:102:BCR:H341	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:137:THR:C	13:o:139:SER:H	2.27	0.42
20:B:601:CLA:H41	20:B:601:CLA:H62	1.46	0.42
22:B:618:BCR:H382	22:t:101:BCR:H11C	2.01	0.42
1:a:218:LEU:HD12	27:a:415:PL9:C4	2.49	0.42
24:a:410:LMG:H232	20:c:505:CLA:H92	2.02	0.42
2:b:498:LYS:HA	4:d:24:ARG:HA	2.00	0.42
22:b:621:BCR:H361	22:b:621:BCR:H20C	1.80	0.42
3:C:279:LEU:HD22	20:C:509:CLA:HED2	2.01	0.42
3:C:381:LYS:NZ	13:O:99:ASP:OD1	2.45	0.42
1:a:215:HIS:ND1	27:a:415:PL9:O1	2.41	0.42
2:b:133:LEU:HD12	28:b:632:DMS:H22	2.02	0.42
28:b:641:DMS:H22	41:b:706:HOH:O	2.19	0.42
3:c:31:SER:CB	3:c:41:ARG:HG2	2.50	0.42
3:c:286:ALA:HB2	20:c:502:CLA:HMD2	2.01	0.42
20:B:602:CLA:H143	20:B:602:CLA:H161	1.89	0.42
3:c:153:ASP:HA	28:c:533:DMS:H12	2.02	0.42
3:c:266:TRP:CZ3	20:c:507:CLA:HAC2	2.55	0.42
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.42
20:c:509:CLA:H192	20:c:512:CLA:HMD1	2.01	0.42
36:d:408:LHG:H141	36:d:408:LHG:H111	1.82	0.42
22:j:102:BCR:H382	22:j:102:BCR:C23	2.50	0.42
2:B:80:ILE:HD12	2:B:80:ILE:HA	1.80	0.42
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.01	0.42
2:b:80:ILE:HD12	2:b:80:ILE:HA	1.94	0.42
2:B:422:ARG:O	2:B:425:ILE:HG12	2.20	0.42
20:C:501:CLA:H42	20:C:502:CLA:HMD3	2.01	0.42
34:B:627:LMT:H12	12:M:6:LEU:HD11	2.01	0.41
20:C:501:CLA:C4D	20:C:503:CLA:H2	2.49	0.41
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.19	0.41
13:O:69:LYS:HE2	41:O:480:HOH:O	2.19	0.41
20:b:604:CLA:H111	20:b:604:CLA:H151	1.94	0.41
3:c:397:THR:HA	28:c:536:DMS:H21	2.02	0.41
4:d:23:LYS:HD3	4:d:135:LEU:HD21	2.02	0.41
5:e:68:ASP:O	5:e:72:ALA:HB2	2.20	0.41
3:C:472:LEU:HD11	4:D:255:GLN:HG3	2.01	0.41
28:D:415:DMS:H22	13:O:182:LEU:HD11	2.03	0.41
35:H:102:DGD:HE5	41:H:238:HOH:O	2.19	0.41
28:V:205:DMS:H23	41:V:343:HOH:O	2.19	0.41
2:b:12:LEU:HB2	20:b:614:CLA:HMC2	2.02	0.41
2:b:445:THR:HA	41:b:709:HOH:O	2.18	0.41
1:a:272:HIS:CD2	4:d:218:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:446:SER:HB2	2:b:447:PRO:HD2	2.01	0.41
22:j:102:BCR:C23	22:j:102:BCR:C38	2.98	0.41
13:o:66:VAL:HB	13:o:67:PRO:HD2	2.01	0.41
16:v:79:PRO:HD3	16:v:94:SER:HB3	2.02	0.41
2:B:72:THR:HB	28:B:642:DMS:H11	2.02	0.41
20:B:607:CLA:H202	32:B:632:HTG:H61	2.01	0.41
5:E:63:ILE:HG23	5:E:64:PRO:HD2	2.02	0.41
8:I:33:LYS:HB3	8:I:34:ARG:H	1.70	0.41
2:b:467:ILE:HG12	4:d:126:MET:CE	2.50	0.41
20:b:608:CLA:H93	20:b:608:CLA:H111	1.92	0.41
22:k:101:BCR:H371	22:k:101:BCR:H24C	1.85	0.41
1:a:114:LEU:C	1:a:114:LEU:HD23	2.45	0.41
2:b:451:PHE:CD2	2:b:451:PHE:C	2.98	0.41
3:c:135[A]:ARG:NH2	34:z:102:LMT:H5B	2.35	0.41
2:B:81:THR:HG21	28:B:642:DMS:S	2.60	0.41
28:B:635:DMS:H13	41:B:763:HOH:O	2.21	0.41
22:K:101:BCR:C8	22:K:101:BCR:H311	2.50	0.41
16:v:118:HIS:HE1	41:v:395:HOH:O	2.03	0.41
1:A:153:SER:HB2	20:A:401:CLA:H43	2.03	0.41
3:C:406:SER:HA	3:C:420:VAL:HG23	2.02	0.41
22:D:405:BCR:HC21	35:D:406:DGD:HAT2	2.02	0.41
28:D:415:DMS:H13	41:M:205:HOH:O	2.20	0.41
2:b:420:TYR:CE1	32:b:625:HTG:H3'1	2.56	0.41
10:k:17:ILE:HG23	10:k:18:PHE:CD2	2.56	0.41
1:A:11:ALA:HB1	1:A:15:GLU:OE1	2.20	0.41
2:B:262:THR:C	2:B:264:PRO:HD3	2.45	0.41
22:B:619:BCR:H371	22:B:619:BCR:H24C	1.82	0.41
22:C:514:BCR:H15C	22:C:514:BCR:H351	1.92	0.41
2:b:113:TRP:CD1	20:b:618:CLA:HBA2	2.56	0.41
1:A:221:SER:HB2	4:D:139:ARG:O	2.21	0.41
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.50	0.41
2:B:498:LYS:HE3	4:D:20:ASP:HA	2.02	0.41
3:C:377:LEU:HB3	13:O:80:GLN:OE1	2.21	0.41
20:C:509:CLA:H91	20:C:509:CLA:H111	1.89	0.41
20:C:513:CLA:HBC2	32:C:534:HTG:H6'2	2.03	0.41
36:D:409:LHG:H362	36:D:409:LHG:H332	1.81	0.41
24:a:410:LMG:H401	24:a:410:LMG:H371	1.69	0.41
20:b:613:CLA:H112	20:b:613:CLA:H72	1.88	0.41
22:k:101:BCR:H20C	22:k:101:BCR:H361	1.96	0.41
23:l:101:SQD:H311	23:l:101:SQD:H341	1.67	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ARG:HG2	28:D:414:DMS:H11	2.02	0.41
5:E:60:GLN:O	5:E:61:ARG:NE	2.54	0.41
20:a:403:CLA:CB2	20:d:403:CLA:HAC2	2.51	0.41
3:c:406:SER:O	3:c:418:ASN:HA	2.21	0.41
2:B:125:ASP:HA	2:B:126:PRO:HD3	1.95	0.40
2:B:347[B]:ARG:HG2	2:B:353:GLU:HA	2.04	0.40
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.56	0.40
13:O:98:GLU:HG3	41:O:418:HOH:O	2.21	0.40
3:c:156:LYS:HE3	41:c:675:HOH:O	2.20	0.40
20:c:501:CLA:H42	20:c:502:CLA:HMD3	2.03	0.40
5:e:8:ARG:NH1	9:j:3:SER:O	2.55	0.40
5:e:27:ILE:HG12	37:e:102:HEM:HMC3	2.02	0.40
1:A:202:VAL:HG11	20:A:402:CLA:C3D	2.51	0.40
32:B:622:HTG:C7'	41:O:407:HOH:O	2.69	0.40
3:C:38:GLY:O	3:C:41:ARG:HB2	2.22	0.40
20:D:401:CLA:HBC3	20:D:401:CLA:HHD	2.04	0.40
15:U:17:LEU:CD2	28:U:903[B]:DMS:H12	2.50	0.40
2:b:419:SER:CB	32:b:625:HTG:H3'2	2.51	0.40
20:b:608:CLA:H193	26:b:642:UNL:C4	2.52	0.40
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.02	0.40
22:A:405:BCR:C23	22:A:405:BCR:C38	2.98	0.40
2:B:286:ARG:HG2	2:B:286:ARG:NH1	2.37	0.40
20:D:402:CLA:H162	20:D:402:CLA:H203	1.80	0.40
28:O:308:DMS:H11	41:O:648:HOH:O	2.21	0.40
1:a:93:PHE:CD1	1:a:95:PRO:HD3	2.56	0.40
3:c:142:GLU:H	3:c:142:GLU:CD	2.30	0.40
3:c:453:ALA:O	8:i:34[B]:ARG:HG2	2.22	0.40
20:c:506:CLA:HMB1	20:c:507:CLA:NB	2.36	0.40
1:A:15:GLU:O	1:A:19[A]:ASN:CG	2.64	0.40
1:A:265:PHE:HE2	27:A:411:PL9:C12	2.32	0.40
2:B:224[B]:ARG:HG2	7:H:24:GLY:C	2.46	0.40
28:B:641:DMS:C1	41:B:931:HOH:O	2.64	0.40
3:C:38:GLY:HA3	20:C:511:CLA:HMD2	2.03	0.40
35:D:406:DGD:C4D	5:E:45:ASP:HB3	2.47	0.40
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.93	0.40
20:b:604:CLA:H111	20:b:604:CLA:H91	1.89	0.40
3:c:135[A]:ARG:CZ	34:z:102:LMT:H5B	2.51	0.40
3:c:457:LYS:NZ	41:c:614:HOH:O	2.55	0.40
20:c:501:CLA:C4D	20:c:503:CLA:H2	2.51	0.40
20:c:513:CLA:HMD3	34:z:102:LMT:H5'	2.03	0.40
6:f:36:ALA:O	6:f:40:MET:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:81:ILE:HA	13:o:100:GLY:HA3	2.03	0.40
13:o:93:LEU:O	13:o:128:SER:HA	2.21	0.40
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.04	0.40
2:B:341:LYS:HZ1	32:B:622:HTG:C2	2.30	0.40
20:B:612:CLA:HMB3	20:B:612:CLA:HBB1	2.04	0.40
20:C:507:CLA:H41	20:C:507:CLA:H61	1.84	0.40
22:K:102:BCR:H24C	22:K:102:BCR:H371	1.86	0.40
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.56	0.40
20:b:617:CLA:H2	20:b:618:CLA:CBB	2.50	0.40
22:k:102:BCR:H24C	22:k:102:BCR:H371	1.94	0.40
13:o:183:ALA:HB3	28:o:303:DMS:C2	2.52	0.40
22:t:101:BCR:H311	22:t:101:BCR:C8	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/344 (97%)	329 (98%)	5 (2%)	1 (0%)	36	25
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	25
2	B	514/505 (102%)	503 (98%)	11 (2%)	0	100	100
2	b	493/505 (98%)	485 (98%)	8 (2%)	0	100	100
3	C	450/455 (99%)	436 (97%)	13 (3%)	1 (0%)	43	31
3	c	454/455 (100%)	442 (97%)	11 (2%)	1 (0%)	43	31
4	D	341/342 (100%)	334 (98%)	6 (2%)	1 (0%)	36	25
4	d	340/342 (99%)	332 (98%)	8 (2%)	0	100	100
5	E	77/83 (93%)	75 (97%)	2 (3%)	0	100	100
5	e	78/83 (94%)	78 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	31/44 (70%)	31 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	61/65 (94%)	59 (97%)	2 (3%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
9	j	38/40 (95%)	38 (100%)	0	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	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	247/244 (101%)	235 (95%)	11 (4%)	1 (0%)	30	17
13	o	243/244 (100%)	231 (95%)	9 (4%)	3 (1%)	10	2
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
16	V	138/137 (101%)	133 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	27 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
18	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	1
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	0
All	All	5201/5350 (97%)	5069 (98%)	120 (2%)	12 (0%)	43	31

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	o	60	ARG
19	z	32	ASP
3	C	416	SER
4	D	12	ARG
13	O	61	GLN
3	c	416	SER
19	z	31	GLN
19	Z	30	PRO
13	o	34	SER
13	o	61	GLN
1	A	259	ILE
1	a	259	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	269/279 (96%)	268 (100%)	1 (0%)	84	82
1	a	270/279 (97%)	269 (100%)	1 (0%)	84	82
2	B	405/403 (100%)	401 (99%)	4 (1%)	68	60
2	b	390/403 (97%)	385 (99%)	5 (1%)	61	51
3	C	351/356 (99%)	347 (99%)	4 (1%)	65	57
3	c	356/356 (100%)	353 (99%)	3 (1%)	73	67
4	D	277/277 (100%)	274 (99%)	3 (1%)	65	57
4	d	276/277 (100%)	274 (99%)	2 (1%)	76	70
5	E	68/72 (94%)	65 (96%)	3 (4%)	25	10
5	e	68/72 (94%)	64 (94%)	4 (6%)	18	5
6	F	27/38 (71%)	27 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	53 (98%)	1 (2%)	50	38
7	h	54/54 (100%)	53 (98%)	1 (2%)	50	38
8	I	30/34 (88%)	30 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	i	32/34 (94%)	28 (88%)	4 (12%)	4	0
9	J	23/28 (82%)	21 (91%)	2 (9%)	9	2
9	j	24/28 (86%)	24 (100%)	0	100	100
10	K	30/30 (100%)	29 (97%)	1 (3%)	33	18
10	k	28/30 (93%)	26 (93%)	2 (7%)	13	3
11	L	34/35 (97%)	34 (100%)	0	100	100
11	l	33/35 (94%)	33 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	33	18
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	207/207 (100%)	204 (99%)	3 (1%)	59	49
13	o	199/207 (96%)	199 (100%)	0	100	100
14	T	26/28 (93%)	23 (88%)	3 (12%)	5	1
14	t	26/28 (93%)	25 (96%)	1 (4%)	29	14
15	U	82/89 (92%)	82 (100%)	0	100	100
15	u	83/89 (93%)	82 (99%)	1 (1%)	63	55
16	V	120/117 (103%)	119 (99%)	1 (1%)	73	67
16	v	114/117 (97%)	113 (99%)	1 (1%)	70	64
17	Y	21/23 (91%)	19 (90%)	2 (10%)	8	1
17	y	21/23 (91%)	21 (100%)	0	100	100
18	X	29/33 (88%)	29 (100%)	0	100	100
18	x	27/33 (82%)	27 (100%)	0	100	100
19	Z	44/52 (85%)	43 (98%)	1 (2%)	44	30
19	z	39/52 (75%)	37 (95%)	2 (5%)	21	7
All	All	4223/4376 (96%)	4166 (99%)	57 (1%)	63	51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
2	B	80	ILE
2	B	307[A]	GLU
2	B	307[B]	GLU
2	B	467	ILE
3	C	78	GLU

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Mol	Chain	Res	Type
3	C	255	THR
3	C	289	PHE
3	C	315	MET
4	D	90	LEU
4	D	136	VAL
4	D	149	PRO
5	E	4	THR
5	E	25	ILE
5	E	61	ARG
7	H	63	LYS
9	J	8	ILE
9	J	10	LEU
10	K	17	ILE
12	M	5	GLN
13	O	23	ASP
13	O	130[A]	GLN
13	O	130[B]	GLN
14	T	2	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
16	V	86	GLN
17	Y	27	MET
17	Y	30	ILE
19	Z	46	LEU
1	a	244	GLU
2	b	80	ILE
2	b	223	GLN
2	b	362	PHE
2	b	467	ILE
2	b	472	ARG
3	c	255	THR
3	c	289	PHE
3	c	355	THR
4	d	233	ARG
4	d	329	MET
5	e	60[A]	GLN
5	e	60[B]	GLN
5	e	71	GLU
5	e	81	GLU
7	h	63	LYS
8	i	33	LYS
8	i	34[A]	ARG

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Mol	Chain	Res	Type
8	i	34[B]	ARG
8	i	36	ASP
10	k	17	ILE
10	k	19	ASP
14	t	2	GLU
15	u	9	LEU
16	v	6	GLU
19	z	29	SER
19	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	315	ASN
2	B	53	ASN
2	B	179	GLN
2	B	409	GLN
3	C	44	ASN
4	D	186	GLN
4	D	255	GLN
7	H	59	ASN
12	M	5	GLN
13	O	82	GLN
16	V	34	GLN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	281	GLN
2	b	331	ASN
3	c	44	ASN
4	d	186	GLN
4	d	255	GLN
4	d	301	GLN
4	d	332	GLN
6	f	44	GLN
13	o	82	GLN
13	o	155	ASN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN

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Mol	Chain	Res	Type
16	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	$\# Z > 2$
14	FME	T	1	14	8,9,10	0.43	0	7,9,11	1.79	2 (28%)
8	FME	i	1	8	8,9,10	0.52	0	7,9,11	1.68	1 (14%)
14	FME	t	1	14	8,9,10	0.49	0	7,9,11	1.86	4 (57%)
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	T	1	14	-	3/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	2/7/9/11	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.88	114.93	109.73
14	T	1	FME	CE-SD-CG	2.70	109.68	100.40
14	T	1	FME	O-C-CA	-2.46	118.34	124.78
14	t	1	FME	CG-CB-CA	2.44	119.72	112.95
14	t	1	FME	CE-SD-CG	2.32	108.38	100.40
14	t	1	FME	C-CA-N	2.28	113.84	109.73
14	t	1	FME	O-C-CA	-2.24	118.90	124.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 349 ligands modelled in this entry, 14 are monoatomic and 55 are unknown - leaving 280 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	a	404	41	64,68,73	1.94	17 (26%)	77,107,113	2.44	27 (35%)
22	BCR	K	101	-	41,41,41	0.83	1 (2%)	56,56,56	1.48	13 (23%)
28	DMS	U	903[B]	-	3,3,3	2.44	1 (33%)	3,3,3	0.17	0
28	DMS	b	635	-	3,3,3	2.68	1 (33%)	3,3,3	0.75	0
23	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.71	10 (16%)
28	DMS	b	633	-	3,3,3	2.55	1 (33%)	3,3,3	1.05	0
20	CLA	b	605	2	69,73,73	2.13	20 (28%)	83,113,113	2.37	31 (37%)
23	SQD	l	101	-	53,54,54	1.08	4 (7%)	62,65,65	1.68	8 (12%)
20	CLA	c	501	3	69,73,73	2.13	17 (24%)	83,113,113	2.95	29 (34%)
28	DMS	B	641	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
32	HTG	c	521	-	19,19,19	0.96	1 (5%)	23,24,24	2.03	3 (13%)
20	CLA	b	616	2	69,73,73	2.02	15 (21%)	83,113,113	2.67	34 (40%)
28	DMS	V	207	-	3,3,3	2.58	1 (33%)	3,3,3	0.47	0
21	PHO	A	403	-	58,69,69	2.32	12 (20%)	56,99,99	3.15	13 (23%)
22	BCR	b	621	-	41,41,41	0.80	1 (2%)	56,56,56	1.47	8 (14%)
22	BCR	c	514	-	41,41,41	0.85	1 (2%)	56,56,56	1.49	7 (12%)
28	DMS	D	413	-	3,3,3	2.73	1 (33%)	3,3,3	0.66	0
32	HTG	C	534	-	19,19,19	1.08	1 (5%)	23,24,24	1.47	5 (21%)
20	CLA	C	501	3	69,73,73	2.09	19 (27%)	83,113,113	2.28	22 (26%)
20	CLA	B	611	41	69,73,73	2.26	18 (26%)	83,113,113	2.49	28 (33%)
21	PHO	D	403	-	58,69,69	2.60	12 (20%)	56,99,99	2.95	17 (30%)
32	HTG	D	417	-	19,19,19	1.05	1 (5%)	23,24,24	1.49	3 (13%)
28	DMS	o	305	-	3,3,3	2.73	1 (33%)	3,3,3	0.77	0
34	LMT	m	101	-	36,36,36	0.61	1 (2%)	47,47,47	0.96	1 (2%)
28	DMS	u	203	-	3,3,3	2.57	1 (33%)	3,3,3	0.78	0
20	CLA	a	407	1	51,55,73	2.37	17 (33%)	61,91,113	2.64	27 (44%)
28	DMS	B	634	-	3,3,3	1.94	1 (33%)	3,3,3	0.29	0
20	CLA	c	502	3	69,73,73	2.19	19 (27%)	83,113,113	2.55	30 (36%)
28	DMS	h	102	-	3,3,3	2.75	1 (33%)	3,3,3	0.56	0
24	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.17	7 (11%)
20	CLA	b	607	2	69,73,73	2.09	19 (27%)	83,113,113	2.40	23 (27%)
28	DMS	A	418	-	3,3,3	2.80	1 (33%)	3,3,3	0.73	0
36	LHG	D	407	-	48,48,48	0.86	1 (2%)	51,54,54	1.26	5 (9%)
27	PL9	d	412	-	55,55,55	1.09	3 (5%)	68,69,69	1.59	16 (23%)
32	HTG	O	302	-	19,19,19	1.29	2 (10%)	23,24,24	1.18	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	614	2	69,73,73	1.90	17 (24%)	83,113,113	2.22	24 (28%)
20	CLA	A	404	1	69,73,73	2.02	19 (27%)	83,113,113	2.75	30 (36%)
21	PHO	a	405	-	58,69,69	2.26	14 (24%)	56,99,99	2.61	14 (25%)
22	BCR	b	619	-	41,41,41	0.95	0	56,56,56	1.77	11 (19%)
28	DMS	V	209	-	3,3,3	2.61	1 (33%)	3,3,3	0.64	0
28	DMS	c	529	-	3,3,3	2.67	1 (33%)	3,3,3	0.56	0
28	DMS	i	104	-	3,3,3	2.62	1 (33%)	3,3,3	0.33	0
20	CLA	d	402	4	69,73,73	1.88	20 (28%)	83,113,113	2.02	25 (30%)
36	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.05	3 (5%)
32	HTG	C	521	-	19,19,19	0.98	2 (10%)	23,24,24	1.97	4 (17%)
28	DMS	C	530	-	3,3,3	2.61	1 (33%)	3,3,3	1.00	0
28	DMS	b	632	-	3,3,3	2.71	1 (33%)	3,3,3	0.55	0
28	DMS	v	203	-	3,3,3	2.59	1 (33%)	3,3,3	0.85	0
20	CLA	B	606	2	69,73,73	1.93	16 (23%)	83,113,113	2.49	30 (36%)
20	CLA	b	614	2	69,73,73	2.04	20 (28%)	83,113,113	2.37	28 (33%)
24	LMG	c	518	-	51,51,55	1.11	3 (5%)	59,59,63	1.31	7 (11%)
27	PL9	A	411	-	55,55,55	0.83	3 (5%)	68,69,69	1.69	18 (26%)
28	DMS	v	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.53	0
20	CLA	B	608	41	69,73,73	1.95	14 (20%)	83,113,113	2.22	23 (27%)
28	DMS	c	532	-	3,3,3	2.60	1 (33%)	3,3,3	0.47	0
31	BCT	A	421	29	2,3,3	0.47	0	2,3,3	1.14	0
32	HTG	b	624	-	19,19,19	1.15	2 (10%)	23,24,24	1.60	2 (8%)
28	DMS	A	416	-	3,3,3	2.68	1 (33%)	3,3,3	0.78	0
24	LMG	a	410	-	51,51,55	0.89	2 (3%)	59,59,63	1.08	2 (3%)
28	DMS	U	903[A]	-	3,3,3	2.56	1 (33%)	3,3,3	0.75	0
28	DMS	c	530	-	3,3,3	2.80	1 (33%)	3,3,3	1.01	0
28	DMS	v	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.81	0
22	BCR	t	101	-	41,41,41	1.04	2 (4%)	56,56,56	1.74	19 (33%)
28	DMS	B	638	-	3,3,3	2.76	1 (33%)	3,3,3	0.82	0
38	RRX	x	101	-	42,42,42	0.82	0	57,58,58	1.22	6 (10%)
22	BCR	D	405	-	41,41,41	1.03	3 (7%)	56,56,56	1.73	13 (23%)
28	DMS	o	302	-	3,3,3	2.75	1 (33%)	3,3,3	0.90	0
28	DMS	B	639	-	3,3,3	2.73	1 (33%)	3,3,3	0.63	0
24	LMG	j	101	39	45,45,55	1.00	3 (6%)	53,53,63	1.02	6 (11%)
20	CLA	C	510	3	69,73,73	2.20	20 (28%)	83,113,113	2.33	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	DGD	H	102	-	63,63,67	1.04	3 (4%)	77,77,81	1.27	8 (10%)
20	CLA	C	503	3	69,73,73	2.41	21 (30%)	83,113,113	2.20	27 (32%)
28	DMS	B	640	-	3,3,3	2.55	1 (33%)	3,3,3	0.97	0
22	BCR	C	515	-	41,41,41	0.97	0	56,56,56	1.19	6 (10%)
28	DMS	b	639	-	3,3,3	2.81	1 (33%)	3,3,3	0.57	0
32	HTG	C	522	-	19,19,19	1.06	2 (10%)	23,24,24	1.56	1 (4%)
34	LMT	B	626	-	24,24,36	0.54	0	29,29,47	1.14	3 (10%)
28	DMS	C	532	-	3,3,3	3.28	1 (33%)	3,3,3	1.29	1 (33%)
20	CLA	c	505	3	69,73,73	2.22	21 (30%)	83,113,113	2.16	23 (27%)
28	DMS	b	640	-	3,3,3	2.76	1 (33%)	3,3,3	1.38	1 (33%)
28	DMS	c	531	-	3,3,3	2.67	1 (33%)	3,3,3	0.48	0
28	DMS	d	413	-	3,3,3	2.57	1 (33%)	3,3,3	0.91	0
32	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.46	1 (4%)
22	BCR	k	102	-	41,41,41	0.79	0	56,56,56	1.29	9 (16%)
28	DMS	u	202	-	3,3,3	2.65	1 (33%)	3,3,3	1.29	0
36	LHG	E	103	-	46,46,48	1.03	2 (4%)	49,50,54	1.14	5 (10%)
36	LHG	d	408	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	5 (9%)
34	LMT	M	101	-	36,36,36	0.64	0	47,47,47	0.93	2 (4%)
30	OEX	a	419	3,41,1	0,14,14	-	-	-	-	-
22	BCR	B	617	-	41,41,41	0.98	0	56,56,56	1.62	11 (19%)
20	CLA	C	502	3	69,73,73	2.23	18 (26%)	83,113,113	2.33	29 (34%)
28	DMS	B	637	-	3,3,3	2.56	1 (33%)	3,3,3	0.73	0
28	DMS	V	205	-	3,3,3	2.71	1 (33%)	3,3,3	0.54	0
24	LMG	B	620	-	51,51,55	1.02	2 (3%)	59,59,63	1.31	5 (8%)
28	DMS	v	208	-	3,3,3	2.63	1 (33%)	3,3,3	0.66	0
32	HTG	d	401	-	19,19,19	1.08	1 (5%)	23,24,24	2.36	4 (17%)
20	CLA	b	610	2	69,73,73	2.25	18 (26%)	83,113,113	2.27	24 (28%)
28	DMS	A	415	-	3,3,3	2.75	1 (33%)	3,3,3	1.01	0
20	CLA	B	610	2	69,73,73	2.30	19 (27%)	83,113,113	2.22	27 (32%)
28	DMS	o	303	-	3,3,3	2.68	1 (33%)	3,3,3	0.50	0
36	LHG	D	408	-	48,48,48	0.82	2 (4%)	51,54,54	1.03	1 (1%)
20	CLA	c	510	3	69,73,73	1.99	20 (28%)	83,113,113	2.37	32 (38%)
28	DMS	C	529	-	3,3,3	2.69	1 (33%)	3,3,3	0.81	0
20	CLA	b	606	2	69,73,73	2.02	19 (27%)	83,113,113	2.40	26 (31%)
34	LMT	E	101	-	24,24,36	0.62	1 (4%)	29,29,47	1.01	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	601	2	69,73,73	2.07	18 (26%)	83,113,113	2.37	29 (34%)
20	CLA	C	511	3	69,73,73	2.32	21 (30%)	83,113,113	2.57	30 (36%)
28	DMS	d	415	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
32	HTG	B	632	-	19,19,19	1.02	1 (5%)	23,24,24	1.26	2 (8%)
28	DMS	U	902	-	3,3,3	2.66	1 (33%)	3,3,3	1.63	1 (33%)
34	LMT	B	627	-	15,15,36	0.48	0	14,14,47	0.67	0
20	CLA	C	507	41	69,73,73	2.40	21 (30%)	83,113,113	2.43	26 (31%)
20	CLA	C	512	3	59,63,73	2.76	24 (40%)	71,101,113	2.50	27 (38%)
20	CLA	b	618	2	69,73,73	2.18	21 (30%)	83,113,113	2.36	28 (33%)
28	DMS	c	533	-	3,3,3	2.74	1 (33%)	3,3,3	0.83	0
28	DMS	D	415	-	3,3,3	2.92	1 (33%)	3,3,3	0.73	0
20	CLA	a	403	1	69,73,73	1.85	15 (21%)	83,113,113	2.22	27 (32%)
28	DMS	c	528	-	3,3,3	2.57	1 (33%)	3,3,3	0.44	0
20	CLA	C	508	3	64,68,73	2.49	19 (29%)	77,107,113	2.50	27 (35%)
23	SQD	b	622	-	53,54,54	1.10	3 (5%)	62,65,65	1.55	11 (17%)
23	SQD	f	101	-	39,40,54	1.37	3 (7%)	48,51,65	3.70	12 (25%)
20	CLA	C	506	3	69,73,73	2.39	22 (31%)	83,113,113	2.35	23 (27%)
20	CLA	B	612	2	69,73,73	1.85	14 (20%)	83,113,113	2.39	29 (34%)
28	DMS	O	311	-	3,3,3	2.87	1 (33%)	3,3,3	0.92	0
28	DMS	j	105	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
32	HTG	u	201	-	7,7,19	0.43	0	6,6,24	0.70	0
20	CLA	D	404	4	69,73,73	2.11	22 (31%)	83,113,113	2.43	32 (38%)
28	DMS	O	307	-	3,3,3	2.68	1 (33%)	3,3,3	0.42	0
34	LMT	z	102	-	36,36,36	0.76	1 (2%)	47,47,47	1.49	8 (17%)
22	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.58	9 (16%)
28	DMS	V	204	-	3,3,3	2.65	1 (33%)	3,3,3	0.78	0
32	HTG	b	601	-	19,19,19	1.04	2 (10%)	23,24,24	1.27	2 (8%)
20	CLA	c	506	3	69,73,73	2.38	20 (28%)	83,113,113	2.41	28 (33%)
22	BCR	K	102	-	41,41,41	0.92	1 (2%)	56,56,56	1.48	6 (10%)
35	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	1.04	3 (3%)
28	DMS	O	305	-	3,3,3	2.63	1 (33%)	3,3,3	0.79	0
20	CLA	C	504	41	69,73,73	2.23	17 (24%)	83,113,113	2.33	24 (28%)
28	DMS	o	306	-	3,3,3	2.79	1 (33%)	3,3,3	1.03	0
28	DMS	O	310	-	3,3,3	2.70	1 (33%)	3,3,3	0.70	0
32	HTG	B	622	-	19,19,19	1.34	3 (15%)	23,24,24	1.93	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	b	608	2	69,73,73	2.33	18 (26%)	83,113,113	2.26	25 (30%)
22	BCR	j	102	-	41,41,41	0.85	0	56,56,56	1.38	9 (16%)
28	DMS	O	304	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
28	DMS	v	207	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
28	DMS	O	306	-	3,3,3	2.53	1 (33%)	3,3,3	0.64	0
34	LMT	B	625	-	24,24,36	0.53	0	29,29,47	1.26	4 (13%)
20	CLA	A	402	41	63,67,73	1.85	18 (28%)	75,105,113	2.96	31 (41%)
20	CLA	D	402	41	69,73,73	1.96	20 (28%)	83,113,113	2.27	23 (27%)
28	DMS	C	528	-	3,3,3	2.31	1 (33%)	3,3,3	0.59	0
20	CLA	c	511	3	69,73,73	2.48	19 (27%)	83,113,113	2.38	24 (28%)
32	HTG	v	210	-	14,14,19	0.62	0	18,19,24	2.19	4 (22%)
22	BCR	B	618	-	41,41,41	1.05	0	56,56,56	1.26	7 (12%)
28	DMS	b	637	-	3,3,3	2.66	1 (33%)	3,3,3	0.58	0
40	HEC	V	201	16	50,50,50	1.82	10 (20%)	68,82,82	1.59	11 (16%)
32	HTG	b	625	-	19,19,19	1.21	2 (10%)	23,24,24	1.34	4 (17%)
20	CLA	C	505	3	69,73,73	2.38	21 (30%)	83,113,113	2.11	23 (27%)
32	HTG	B	621	-	19,19,19	1.45	3 (15%)	23,24,24	1.79	6 (26%)
28	DMS	A	417	-	3,3,3	2.63	1 (33%)	3,3,3	0.45	0
28	DMS	O	303	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
28	DMS	d	414	-	3,3,3	2.50	1 (33%)	3,3,3	0.24	0
28	DMS	B	636	-	3,3,3	2.76	1 (33%)	3,3,3	0.78	0
35	DGD	D	406	-	51,51,67	1.11	2 (3%)	59,59,81	1.21	5 (8%)
22	BCR	b	620	-	41,41,41	1.08	1 (2%)	56,56,56	1.23	5 (8%)
20	CLA	D	401	4	69,73,73	1.93	20 (28%)	83,113,113	2.41	29 (34%)
24	LMG	J	101	39	45,45,55	1.01	2 (4%)	53,53,63	0.98	3 (5%)
22	BCR	k	101	-	41,41,41	0.94	0	56,56,56	1.12	6 (10%)
28	DMS	D	414	-	3,3,3	2.53	1 (33%)	3,3,3	0.25	0
28	DMS	b	636	-	3,3,3	2.71	1 (33%)	3,3,3	0.75	0
28	DMS	o	307	-	3,3,3	2.65	1 (33%)	3,3,3	0.85	0
34	LMT	b	627	-	33,33,36	0.88	1 (3%)	44,44,47	1.80	10 (22%)
20	CLA	B	615	2	69,73,73	2.08	19 (27%)	83,113,113	2.68	32 (38%)
32	HTG	B	631	-	19,19,19	0.94	2 (10%)	23,24,24	2.09	6 (26%)
30	OEX	A	420	3,41,1	0,14,14	-	-	-	-	-
34	LMT	a	418	-	36,36,36	0.68	2 (5%)	47,47,47	1.54	6 (12%)
28	DMS	v	202	-	3,3,3	2.50	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	HTG	B	623	-	19,19,19	0.96	1 (5%)	23,24,24	1.56	2 (8%)
34	LMT	T	102	-	24,24,36	0.45	0	29,29,47	1.15	2 (6%)
22	BCR	a	408	-	41,41,41	1.21	2 (4%)	56,56,56	1.44	7 (12%)
34	LMT	I	101	-	36,36,36	0.65	1 (2%)	47,47,47	1.28	6 (12%)
40	HEC	v	201	16	50,50,50	1.85	13 (26%)	68,82,82	1.55	13 (19%)
20	CLA	b	612	41	69,73,73	2.10	20 (28%)	83,113,113	2.38	27 (32%)
28	DMS	V	208	-	3,3,3	2.65	1 (33%)	3,3,3	0.74	0
22	BCR	C	514	-	41,41,41	0.85	0	56,56,56	1.31	7 (12%)
28	DMS	v	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.66	0
36	LHG	l	102	-	48,48,48	0.78	2 (4%)	51,54,54	1.00	2 (3%)
20	CLA	c	507	41	69,73,73	2.28	16 (23%)	83,113,113	2.52	27 (32%)
28	DMS	b	634	-	3,3,3	2.67	1 (33%)	3,3,3	0.68	0
28	DMS	b	631	-	3,3,3	2.88	1 (33%)	3,3,3	1.24	0
20	CLA	B	602	41	69,73,73	2.58	20 (28%)	83,113,113	2.67	30 (36%)
20	CLA	B	603	2	69,73,73	2.16	19 (27%)	83,113,113	2.29	25 (30%)
20	CLA	c	503	3	69,73,73	2.49	22 (31%)	83,113,113	2.39	26 (31%)
28	DMS	v	209	-	3,3,3	2.63	1 (33%)	3,3,3	0.56	0
35	DGD	d	416	-	51,51,67	1.11	3 (5%)	59,59,81	1.20	6 (10%)
24	LMG	C	524	-	45,45,55	1.10	3 (6%)	53,53,63	1.36	5 (9%)
34	LMT	f	102	-	24,24,36	0.79	1 (4%)	29,29,47	0.96	2 (6%)
28	DMS	c	527	-	3,3,3	2.31	1 (33%)	3,3,3	0.49	0
38	RRX	H	101	-	42,42,42	0.77	1 (2%)	57,58,58	1.49	8 (14%)
34	LMT	c	523	-	36,36,36	0.81	1 (2%)	47,47,47	1.60	6 (12%)
20	CLA	B	605	2	69,73,73	2.12	19 (27%)	83,113,113	2.07	26 (31%)
34	LMT	b	628	-	25,25,36	0.55	0	30,30,47	1.20	2 (6%)
23	SQD	a	401	-	53,54,54	1.12	3 (5%)	62,65,65	1.40	7 (11%)
28	DMS	b	638	-	3,3,3	2.78	1 (33%)	3,3,3	0.94	0
20	CLA	b	611	2	69,73,73	2.66	21 (30%)	83,113,113	2.00	24 (28%)
20	CLA	b	613	2	69,73,73	2.02	13 (18%)	83,113,113	2.34	29 (34%)
20	CLA	B	609	2	69,73,73	1.94	18 (26%)	83,113,113	2.47	28 (33%)
28	DMS	c	534	-	3,3,3	2.69	1 (33%)	3,3,3	0.76	0
35	DGD	C	517	-	56,56,67	0.98	2 (3%)	70,70,81	0.93	4 (5%)
22	BCR	A	405	-	41,41,41	0.95	3 (7%)	56,56,56	1.27	7 (12%)
28	DMS	C	525[A]	-	3,3,3	2.80	1 (33%)	3,3,3	0.85	0
37	HEM	e	102	5,6	50,50,50	1.97	10 (20%)	66,82,82	1.54	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	b	609	41	69,73,73	2.10	21 (30%)	83,113,113	2.17	30 (36%)
22	BCR	d	405	-	41,41,41	0.94	0	56,56,56	1.84	11 (19%)
31	BCT	a	413	29	2,3,3	0.65	0	2,3,3	1.47	0
20	CLA	C	509	3	69,73,73	2.22	17 (24%)	83,113,113	2.57	28 (33%)
24	LMG	C	519	-	51,51,55	1.03	2 (3%)	59,59,63	1.23	8 (13%)
28	DMS	U	904	-	3,3,3	2.85	1 (33%)	3,3,3	0.70	0
34	LMT	m	102	-	36,36,36	0.58	0	47,47,47	1.14	4 (8%)
32	HTG	V	202	-	12,13,19	0.76	1 (8%)	16,18,24	2.50	6 (37%)
32	HTG	c	520	-	19,19,19	0.89	2 (10%)	23,24,24	1.32	2 (8%)
20	CLA	b	604	2	69,73,73	2.14	20 (28%)	83,113,113	2.34	32 (38%)
36	LHG	d	406	-	48,48,48	0.94	2 (4%)	51,54,54	1.16	5 (9%)
36	LHG	d	407	-	48,48,48	0.73	2 (4%)	51,54,54	0.99	4 (7%)
28	DMS	c	535	-	3,3,3	2.78	1 (33%)	3,3,3	0.79	0
20	CLA	B	607	2	69,73,73	2.36	20 (28%)	83,113,113	2.60	29 (34%)
28	DMS	C	527	-	3,3,3	2.56	1 (33%)	3,3,3	0.49	0
28	DMS	F	102	-	3,3,3	2.63	1 (33%)	3,3,3	0.61	0
35	DGD	h	101	-	63,63,67	0.98	3 (4%)	77,77,81	1.04	4 (5%)
28	DMS	A	414	-	3,3,3	1.97	1 (33%)	3,3,3	0.54	0
28	DMS	C	533	-	3,3,3	2.64	1 (33%)	3,3,3	0.48	0
28	DMS	B	643	-	3,3,3	2.78	1 (33%)	3,3,3	0.74	0
20	CLA	c	512	3	69,73,73	2.37	22 (31%)	83,113,113	2.44	25 (30%)
20	CLA	A	401	1	69,73,73	1.94	19 (27%)	83,113,113	2.16	24 (28%)
28	DMS	C	525[B]	-	3,3,3	2.59	1 (33%)	3,3,3	0.79	0
28	DMS	O	309	-	3,3,3	2.67	1 (33%)	3,3,3	1.16	0
28	DMS	V	206	-	3,3,3	2.68	1 (33%)	3,3,3	0.67	0
20	CLA	B	616	2	69,73,73	2.15	18 (26%)	83,113,113	2.30	25 (30%)
20	CLA	C	513	3	69,73,73	2.53	20 (28%)	83,113,113	2.32	22 (26%)
35	DGD	C	516	-	63,63,67	0.89	2 (3%)	77,77,81	1.20	7 (9%)
28	DMS	C	531	-	3,3,3	2.66	1 (33%)	3,3,3	0.97	0
28	DMS	B	642	-	3,3,3	2.79	1 (33%)	3,3,3	0.75	0
28	DMS	C	526	-	3,3,3	2.56	1 (33%)	3,3,3	0.81	0
32	HTG	b	602	-	19,19,19	1.00	2 (10%)	23,24,24	1.15	1 (4%)
28	DMS	H	103	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
28	DMS	o	308	-	3,3,3	2.85	1 (33%)	3,3,3	0.81	0
20	CLA	B	604	2	69,73,73	2.08	21 (30%)	83,113,113	2.57	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	b	603	41	69,73,73	2.88	20 (28%)	83,113,113	2.50	29 (34%)
24	LMG	A	407	-	51,51,55	0.95	2 (3%)	59,59,63	1.06	3 (5%)
28	DMS	B	645	-	3,3,3	2.73	1 (33%)	3,3,3	0.93	0
28	DMS	o	304	-	3,3,3	2.64	1 (33%)	3,3,3	0.65	0
20	CLA	b	617	2	69,73,73	2.14	18 (26%)	83,113,113	2.31	25 (30%)
35	DGD	c	517	-	63,63,67	1.04	4 (6%)	77,77,81	1.19	8 (10%)
20	CLA	c	508	3	64,68,73	2.32	17 (26%)	77,107,113	2.49	28 (36%)
28	DMS	B	644	-	3,3,3	2.87	1 (33%)	3,3,3	1.26	0
35	DGD	c	515	-	63,63,67	0.85	3 (4%)	77,77,81	1.19	8 (10%)
23	SQD	a	409	-	53,54,54	1.01	4 (7%)	62,65,65	2.11	11 (17%)
20	CLA	c	509	3	69,73,73	2.22	19 (27%)	83,113,113	2.54	31 (37%)
20	CLA	b	615	2	69,73,73	1.95	19 (27%)	83,113,113	2.43	27 (32%)
27	PL9	a	415	-	55,55,55	0.83	3 (5%)	68,69,69	1.67	16 (23%)
28	DMS	b	641	-	3,3,3	2.79	1 (33%)	3,3,3	1.11	0
23	SQD	A	406	-	53,54,54	1.00	3 (5%)	62,65,65	1.75	14 (22%)
20	CLA	B	613	2	69,73,73	2.13	18 (26%)	83,113,113	2.37	28 (33%)
20	CLA	c	513	3	69,73,73	2.53	19 (27%)	83,113,113	2.35	26 (31%)
27	PL9	D	412	-	55,55,55	1.06	3 (5%)	68,69,69	1.51	12 (17%)
35	DGD	c	516	-	58,58,67	0.86	2 (3%)	72,72,81	1.13	6 (8%)
34	LMT	J	103	-	24,24,36	0.65	1 (4%)	29,29,47	1.12	1 (3%)
28	DMS	D	416	-	3,3,3	2.67	1 (33%)	3,3,3	0.57	0
20	CLA	c	504	41	69,73,73	2.14	22 (31%)	83,113,113	2.80	29 (34%)
23	SQD	F	101	-	34,35,54	1.01	2 (5%)	42,45,65	1.59	7 (16%)
28	DMS	O	308	-	3,3,3	2.76	1 (33%)	3,3,3	0.79	0
28	DMS	u	204	-	3,3,3	2.66	1 (33%)	3,3,3	0.49	0
20	CLA	d	404	4	69,73,73	2.00	19 (27%)	83,113,113	2.58	30 (36%)
37	HEM	E	104	5,6	50,50,50	2.19	9 (18%)	66,82,82	1.75	10 (15%)
22	BCR	T	101	-	41,41,41	0.81	0	56,56,56	1.50	11 (19%)
28	DMS	B	635	-	3,3,3	2.63	1 (33%)	3,3,3	0.46	0
36	LHG	L	101	-	48,48,48	0.90	3 (6%)	51,54,54	0.90	1 (1%)
34	LMT	Z	101	-	36,36,36	0.68	1 (2%)	47,47,47	0.98	3 (6%)
28	DMS	c	536	-	3,3,3	2.84	1 (33%)	3,3,3	1.23	0
20	CLA	d	403	41	69,73,73	2.01	18 (26%)	83,113,113	2.29	24 (28%)
24	LMG	b	623	-	49,49,55	0.96	2 (4%)	57,57,63	1.31	6 (10%)
21	PHO	a	406	-	58,69,69	2.55	13 (22%)	56,99,99	2.84	16 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	a	404	41	-	7/33/109/115	-
22	BCR	K	101	-	-	4/29/63/63	0/2/2/2
23	SQD	A	412	-	-	24/49/69/69	0/1/1/1
20	CLA	b	605	2	-	1/39/115/115	-
23	SQD	l	101	-	-	28/49/69/69	0/1/1/1
20	CLA	c	501	3	-	3/39/115/115	-
32	HTG	c	521	-	-	5/10/30/30	0/1/1/1
20	CLA	b	616	2	-	18/39/115/115	-
21	PHO	A	403	-	-	2/37/103/103	0/5/6/6
22	BCR	b	621	-	-	0/29/63/63	0/2/2/2
22	BCR	c	514	-	-	0/29/63/63	0/2/2/2
32	HTG	C	534	-	-	6/10/30/30	0/1/1/1
20	CLA	C	501	3	-	5/39/115/115	-
20	CLA	B	611	41	-	4/39/115/115	-
21	PHO	D	403	-	-	3/37/103/103	0/5/6/6
32	HTG	D	417	-	-	5/10/30/30	0/1/1/1
34	LMT	m	101	-	-	15/21/61/61	0/2/2/2
20	CLA	a	407	1	-	0/18/94/115	-
20	CLA	c	502	3	-	6/39/115/115	-
24	LMG	c	519	-	-	26/46/66/70	0/1/1/1
20	CLA	b	607	2	-	4/39/115/115	-
36	LHG	D	407	-	-	9/53/53/53	-
27	PL9	d	412	-	-	3/53/73/73	0/1/1/1
20	CLA	B	614	2	-	6/39/115/115	-
21	PHO	a	405	-	-	4/37/103/103	0/5/6/6
20	CLA	A	404	1	-	10/39/115/115	-
22	BCR	b	619	-	-	2/29/63/63	0/2/2/2
36	LHG	D	409	-	-	14/53/53/53	-
20	CLA	d	402	4	-	5/39/115/115	-
32	HTG	C	521	-	-	6/10/30/30	0/1/1/1
32	HTG	O	302	-	-	5/10/30/30	0/1/1/1
20	CLA	B	606	2	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	b	614	2	-	4/39/115/115	-
24	LMG	c	518	-	-	8/46/66/70	0/1/1/1
27	PL9	A	411	-	-	10/53/73/73	0/1/1/1
32	HTG	b	624	-	-	0/10/30/30	0/1/1/1
20	CLA	B	608	41	-	1/39/115/115	-
24	LMG	a	410	-	-	18/46/66/70	0/1/1/1
22	BCR	t	101	-	-	3/29/63/63	0/2/2/2
38	RRX	x	101	-	-	3/29/65/65	0/2/2/2
22	BCR	D	405	-	-	4/29/63/63	0/2/2/2
24	LMG	j	101	39	-	15/40/60/70	0/1/1/1
20	CLA	C	510	3	-	2/39/115/115	-
35	DGD	H	102	-	-	15/51/91/95	0/2/2/2
20	CLA	C	503	3	-	4/39/115/115	-
22	BCR	C	515	-	-	0/29/63/63	0/2/2/2
32	HTG	C	522	-	-	4/10/30/30	0/1/1/1
34	LMT	B	626	-	-	7/15/35/61	0/1/1/2
20	CLA	c	505	3	-	1/39/115/115	-
36	LHG	E	103	-	-	27/45/45/53	-
32	HTG	C	520	-	-	4/10/30/30	0/1/1/1
22	BCR	k	102	-	-	1/29/63/63	0/2/2/2
36	LHG	d	408	-	-	14/53/53/53	-
34	LMT	M	101	-	-	1/21/61/61	0/2/2/2
22	BCR	B	617	-	-	2/29/63/63	0/2/2/2
20	CLA	C	502	3	-	7/39/115/115	-
32	HTG	d	401	-	-	9/10/30/30	0/1/1/1
24	LMG	B	620	-	-	19/46/66/70	0/1/1/1
36	LHG	D	408	-	-	10/53/53/53	-
20	CLA	b	610	2	-	1/39/115/115	-
20	CLA	B	610	2	-	3/39/115/115	-
20	CLA	c	510	3	-	3/39/115/115	-
20	CLA	b	606	2	-	3/39/115/115	-
34	LMT	E	101	-	-	8/15/35/61	0/1/1/2
20	CLA	B	601	2	-	18/39/115/115	-
20	CLA	C	511	3	-	0/39/115/115	-
32	HTG	B	632	-	-	2/10/30/30	0/1/1/1
34	LMT	B	627	-	-	7/13/13/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	C	507	41	-	11/39/115/115	-
20	CLA	C	512	3	-	6/27/103/115	-
20	CLA	b	618	2	-	17/39/115/115	-
20	CLA	a	403	1	-	4/39/115/115	-
20	CLA	C	508	3	-	6/33/109/115	-
23	SQD	b	622	-	-	23/49/69/69	0/1/1/1
23	SQD	f	101	-	-	16/34/54/69	0/1/1/1
20	CLA	C	506	3	-	12/39/115/115	-
20	CLA	B	612	2	-	3/39/115/115	-
32	HTG	u	201	-	-	1/5/5/30	-
20	CLA	D	404	4	-	13/39/115/115	-
34	LMT	z	102	-	-	13/21/61/61	0/2/2/2
22	BCR	B	619	-	-	0/29/63/63	0/2/2/2
32	HTG	b	601	-	-	2/10/30/30	0/1/1/1
20	CLA	c	506	3	-	10/39/115/115	-
22	BCR	K	102	-	-	1/29/63/63	0/2/2/2
35	DGD	C	518	-	-	12/51/91/95	0/2/2/2
32	HTG	B	622	-	-	5/10/30/30	0/1/1/1
20	CLA	C	504	41	-	11/39/115/115	-
20	CLA	b	608	2	-	9/39/115/115	-
22	BCR	j	102	-	-	2/29/63/63	0/2/2/2
34	LMT	B	625	-	-	4/15/35/61	0/1/1/2
20	CLA	A	402	41	-	3/32/108/115	-
20	CLA	D	402	41	-	5/39/115/115	-
20	CLA	c	511	3	-	0/39/115/115	-
32	HTG	v	210	-	-	3/5/25/30	0/1/1/1
22	BCR	B	618	-	-	0/29/63/63	0/2/2/2
40	HEC	V	201	16	1/1/3/7	5/14/54/54	-
32	HTG	b	625	-	-	4/10/30/30	0/1/1/1
20	CLA	C	505	3	-	1/39/115/115	-
32	HTG	B	621	-	-	5/10/30/30	0/1/1/1
35	DGD	D	406	-	-	26/46/66/95	0/1/1/2
22	BCR	b	620	-	-	0/29/63/63	0/2/2/2
20	CLA	D	401	4	-	7/39/115/115	-
24	LMG	J	101	39	-	9/40/60/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	k	101	-	-	4/29/63/63	0/2/2/2
34	LMT	b	627	-	-	10/18/58/61	0/2/2/2
20	CLA	B	615	2	-	10/39/115/115	-
32	HTG	B	631	-	-	5/10/30/30	0/1/1/1
34	LMT	a	418	-	-	11/21/61/61	0/2/2/2
32	HTG	B	623	-	-	6/10/30/30	0/1/1/1
34	LMT	T	102	-	-	11/15/35/61	0/1/1/2
22	BCR	a	408	-	-	0/29/63/63	0/2/2/2
34	LMT	I	101	-	-	8/21/61/61	0/2/2/2
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
20	CLA	b	612	41	-	5/39/115/115	-
22	BCR	C	514	-	-	5/29/63/63	0/2/2/2
36	LHG	l	102	-	-	19/53/53/53	-
20	CLA	c	507	41	-	6/39/115/115	-
20	CLA	B	602	41	-	23/39/115/115	-
20	CLA	B	603	2	-	3/39/115/115	-
20	CLA	c	503	3	-	3/39/115/115	-
35	DGD	d	416	-	-	30/46/66/95	0/1/1/2
24	LMG	C	524	-	-	22/40/60/70	0/1/1/1
34	LMT	f	102	-	-	8/15/35/61	0/1/1/2
38	RRX	H	101	-	-	1/29/65/65	0/2/2/2
34	LMT	c	523	-	-	8/21/61/61	0/2/2/2
20	CLA	B	605	2	-	8/39/115/115	-
34	LMT	b	628	-	-	9/17/37/61	0/1/1/2
23	SQD	a	401	-	-	20/49/69/69	0/1/1/1
20	CLA	b	611	2	-	0/39/115/115	-
20	CLA	b	613	2	-	7/39/115/115	-
20	CLA	B	609	2	-	1/39/115/115	-
35	DGD	C	517	-	-	14/44/84/95	0/2/2/2
22	BCR	A	405	-	-	0/29/63/63	0/2/2/2
37	HEM	e	102	5,6	-	4/14/54/54	-
20	CLA	b	609	41	-	3/39/115/115	-
22	BCR	d	405	-	-	4/29/63/63	0/2/2/2
20	CLA	C	509	3	-	8/39/115/115	-
24	LMG	C	519	-	-	19/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMT	m	102	-	-	3/21/61/61	0/2/2/2
32	HTG	V	202	-	-	1/4/24/30	0/1/1/1
32	HTG	c	520	-	-	5/10/30/30	0/1/1/1
20	CLA	b	604	2	-	7/39/115/115	-
36	LHG	d	406	-	-	11/53/53/53	-
36	LHG	d	407	-	-	11/53/53/53	-
20	CLA	B	607	2	-	11/39/115/115	-
35	DGD	h	101	-	-	15/51/91/95	0/2/2/2
20	CLA	c	512	3	-	9/39/115/115	-
20	CLA	A	401	1	-	4/39/115/115	-
20	CLA	B	616	2	-	5/39/115/115	-
20	CLA	C	513	3	-	10/39/115/115	-
35	DGD	C	516	-	-	18/51/91/95	0/2/2/2
32	HTG	b	602	-	-	3/10/30/30	0/1/1/1
20	CLA	B	604	2	-	3/39/115/115	-
20	CLA	b	603	41	-	18/39/115/115	-
24	LMG	A	407	-	-	28/46/66/70	0/1/1/1
20	CLA	b	617	2	-	8/39/115/115	-
35	DGD	c	517	-	-	14/51/91/95	0/2/2/2
20	CLA	c	508	3	-	2/33/109/115	-
35	DGD	c	515	-	-	18/51/91/95	0/2/2/2
23	SQD	a	409	-	-	20/49/69/69	0/1/1/1
20	CLA	c	509	3	-	10/39/115/115	-
20	CLA	b	615	2	-	6/39/115/115	-
27	PL9	a	415	-	-	11/53/73/73	0/1/1/1
23	SQD	A	406	-	-	21/49/69/69	0/1/1/1
20	CLA	B	613	2	-	0/39/115/115	-
20	CLA	c	513	3	-	15/39/115/115	-
27	PL9	D	412	-	-	3/53/73/73	0/1/1/1
35	DGD	c	516	-	-	13/46/86/95	0/2/2/2
34	LMT	J	103	-	-	7/15/35/61	0/1/1/2
20	CLA	c	504	41	-	5/39/115/115	-
23	SQD	F	101	-	-	17/28/48/69	0/1/1/1
37	HEM	E	104	5,6	-	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	d	404	4	-	8/39/115/115	-
22	BCR	T	101	-	-	1/29/63/63	0/2/2/2
36	LHG	L	101	-	-	17/53/53/53	-
34	LMT	Z	101	-	-	8/21/61/61	0/2/2/2
20	CLA	d	403	41	-	5/39/115/115	-
24	LMG	b	623	-	-	14/44/64/70	0/1/1/1
21	PHO	a	406	-	-	2/37/103/103	0/5/6/6

All (1682) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	MG-NA	12.91	2.36	2.06
20	c	513	CLA	MG-NA	12.66	2.36	2.06
20	B	602	CLA	MG-NA	11.66	2.34	2.06
20	c	507	CLA	MG-NA	10.98	2.32	2.06
20	c	511	CLA	MG-NC	10.70	2.31	2.06
21	A	403	PHO	C1D-C2D	10.49	1.51	1.39
20	b	603	CLA	MG-NB	-10.46	1.85	2.05
20	C	502	CLA	MG-NA	10.10	2.30	2.06
20	C	506	CLA	MG-NA	10.02	2.30	2.06
20	b	608	CLA	MG-NA	9.93	2.29	2.06
20	c	502	CLA	MG-NA	9.90	2.29	2.06
20	C	511	CLA	MG-NA	9.62	2.29	2.06
20	C	508	CLA	MG-NA	9.57	2.29	2.06
20	B	605	CLA	MG-NA	9.52	2.28	2.06
20	c	503	CLA	MG-NA	9.50	2.28	2.06
20	b	603	CLA	MG-NC	9.40	2.28	2.06
20	b	617	CLA	MG-NA	9.30	2.28	2.06
20	B	613	CLA	MG-NA	9.26	2.28	2.06
21	a	406	PHO	C1B-C2B	9.16	1.49	1.39
21	D	403	PHO	C1B-C2B	9.10	1.49	1.39
20	c	509	CLA	MG-NA	9.07	2.27	2.06
20	C	509	CLA	MG-NA	9.01	2.27	2.06
20	C	503	CLA	MG-NA	8.95	2.27	2.06
21	a	406	PHO	C1D-C2D	8.91	1.49	1.39
20	b	613	CLA	MG-NA	8.84	2.27	2.06
21	D	403	PHO	C1D-C2D	8.78	1.49	1.39
20	b	603	CLA	MG-ND	8.72	2.23	2.05
20	c	508	CLA	MG-NA	8.69	2.26	2.06
20	d	403	CLA	MG-NA	8.65	2.26	2.06
20	c	506	CLA	MG-ND	-8.64	1.88	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	507	CLA	MG-NC	8.62	2.26	2.06
20	C	513	CLA	MG-NA	8.51	2.26	2.06
20	B	610	CLA	MG-NA	8.45	2.26	2.06
20	C	512	CLA	MG-NA	8.34	2.26	2.06
20	B	608	CLA	MG-NA	8.25	2.25	2.06
37	E	104	HEM	FE-NC	8.21	2.23	1.95
20	C	504	CLA	MG-NA	8.16	2.25	2.06
20	c	501	CLA	MG-NA	8.12	2.25	2.06
20	c	504	CLA	MG-NA	8.10	2.25	2.06
20	c	512	CLA	MG-NA	8.09	2.25	2.06
20	b	605	CLA	MG-NA	8.07	2.25	2.06
37	e	102	HEM	C3D-C2D	7.99	1.53	1.36
20	C	505	CLA	MG-NB	7.99	2.21	2.05
20	B	607	CLA	MG-NA	7.94	2.25	2.06
20	C	510	CLA	MG-NA	7.85	2.24	2.06
20	B	603	CLA	MG-NA	7.84	2.24	2.06
20	B	616	CLA	MG-NA	7.81	2.24	2.06
20	b	606	CLA	MG-NA	7.76	2.24	2.06
20	b	618	CLA	MG-NA	7.73	2.24	2.06
20	C	507	CLA	MG-NA	7.70	2.24	2.06
37	E	104	HEM	C3D-C2D	7.69	1.53	1.36
20	b	616	CLA	MG-NA	7.66	2.24	2.06
21	a	405	PHO	C1B-C2B	7.58	1.48	1.39
20	C	513	CLA	MG-NC	7.30	2.23	2.06
20	c	505	CLA	MG-NA	7.26	2.23	2.06
20	B	611	CLA	MG-NA	7.15	2.23	2.06
40	v	201	HEC	C3D-C2D	7.08	1.51	1.36
20	c	503	CLA	MG-NC	7.01	2.22	2.06
20	c	506	CLA	MG-NB	6.97	2.19	2.05
20	B	614	CLA	MG-NA	6.94	2.22	2.06
21	a	405	PHO	C1D-C2D	6.93	1.47	1.39
20	D	401	CLA	MG-NA	6.93	2.22	2.06
20	C	512	CLA	MG-NC	6.85	2.22	2.06
21	A	403	PHO	C1B-C2B	6.81	1.47	1.39
20	b	610	CLA	MG-NB	6.80	2.19	2.05
20	B	612	CLA	MG-NA	6.73	2.22	2.06
20	D	404	CLA	MG-NC	6.62	2.22	2.06
20	B	611	CLA	MG-NC	6.61	2.22	2.06
20	B	601	CLA	MG-NA	6.58	2.21	2.06
20	B	607	CLA	MG-NC	6.52	2.21	2.06
20	c	506	CLA	MG-NA	6.46	2.21	2.06
20	B	602	CLA	MG-ND	6.46	2.18	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	614	CLA	MG-NA	6.41	2.21	2.06
20	d	404	CLA	MG-NA	6.31	2.21	2.06
20	b	607	CLA	MG-NA	6.30	2.21	2.06
20	A	402	CLA	MG-NA	6.14	2.20	2.06
20	b	611	CLA	MG-NB	6.12	2.17	2.05
20	c	512	CLA	MG-NB	6.09	2.17	2.05
20	D	404	CLA	MG-NA	6.03	2.20	2.06
21	D	403	PHO	C3B-C2B	6.03	1.48	1.40
20	B	607	CLA	C3C-C2C	6.01	1.49	1.36
20	C	513	CLA	MG-ND	5.99	2.17	2.05
20	a	403	CLA	MG-NA	5.91	2.20	2.06
20	b	609	CLA	MG-NC	5.90	2.20	2.06
20	b	604	CLA	MG-NA	5.88	2.20	2.06
20	a	404	CLA	MG-NA	5.88	2.20	2.06
20	B	609	CLA	MG-NA	5.83	2.20	2.06
20	C	512	CLA	C3C-C2C	5.82	1.49	1.36
40	V	201	HEC	FE-NB	5.82	2.12	1.94
20	C	508	CLA	MG-ND	-5.81	1.94	2.05
20	b	609	CLA	MG-NA	5.81	2.20	2.06
20	B	607	CLA	CHC-C1C	5.78	1.50	1.38
20	b	610	CLA	C3C-C2C	5.77	1.49	1.36
20	d	402	CLA	CHC-C1C	5.75	1.50	1.38
20	c	503	CLA	C3C-C2C	5.75	1.49	1.36
20	b	610	CLA	CHC-C1C	5.74	1.50	1.38
20	b	607	CLA	MG-NB	5.72	2.17	2.05
20	c	503	CLA	MG-ND	5.71	2.17	2.05
20	C	513	CLA	C3C-C2C	5.69	1.48	1.36
20	a	407	CLA	CHC-C1C	5.67	1.50	1.38
20	b	608	CLA	MG-NC	5.65	2.19	2.06
20	b	605	CLA	CHC-C1C	5.62	1.49	1.38
20	b	606	CLA	C3C-C2C	5.61	1.48	1.36
28	C	532	DMS	O-S	5.56	1.87	1.50
20	C	503	CLA	CHC-C1C	5.56	1.49	1.38
20	C	512	CLA	MG-NB	5.54	2.16	2.05
20	C	505	CLA	C3C-C2C	5.53	1.48	1.36
20	B	606	CLA	MG-NA	5.50	2.19	2.06
20	b	612	CLA	O2D-CGD	5.50	1.46	1.33
20	b	615	CLA	CHC-C1C	5.49	1.49	1.38
20	B	615	CLA	MG-NA	5.48	2.19	2.06
20	B	601	CLA	CHC-C1C	5.47	1.49	1.38
20	C	509	CLA	C3C-C2C	5.47	1.48	1.36
20	c	512	CLA	C3C-C2C	5.47	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	511	CLA	O2D-CGD	5.46	1.46	1.33
20	C	503	CLA	C3C-C2C	5.44	1.48	1.36
20	b	615	CLA	MG-NA	5.43	2.19	2.06
20	c	504	CLA	C3C-C2C	5.42	1.48	1.36
20	b	611	CLA	C3C-C2C	5.42	1.48	1.36
20	b	612	CLA	C1B-NB	-5.39	1.31	1.37
20	C	512	CLA	O2D-CGD	5.39	1.46	1.33
23	f	101	SQD	O47-C7	5.37	1.47	1.35
20	b	611	CLA	CHC-C1C	5.35	1.49	1.38
20	B	610	CLA	MG-NB	5.35	2.16	2.05
20	C	504	CLA	C3C-C2C	5.34	1.48	1.36
20	A	402	CLA	CHC-C1C	5.34	1.49	1.38
21	a	406	PHO	C3B-C4B	5.34	1.47	1.41
20	C	506	CLA	CHC-C1C	5.34	1.49	1.38
20	c	511	CLA	MG-NA	5.33	2.18	2.06
20	b	604	CLA	C3C-C2C	5.32	1.48	1.36
20	D	402	CLA	MG-NA	5.32	2.18	2.06
20	B	601	CLA	C3C-C2C	5.31	1.48	1.36
20	C	507	CLA	CHD-C1D	5.30	1.48	1.38
20	C	501	CLA	C3C-C2C	5.30	1.48	1.36
20	B	614	CLA	CHC-C1C	5.29	1.49	1.38
20	c	508	CLA	CHD-C1D	5.28	1.48	1.38
20	c	507	CLA	C3C-C2C	5.28	1.48	1.36
20	B	602	CLA	C3C-C2C	5.27	1.47	1.36
20	B	603	CLA	CHD-C1D	5.26	1.48	1.38
20	C	513	CLA	CHD-C1D	5.26	1.48	1.38
21	D	403	PHO	C3D-C4D	-5.25	1.33	1.41
20	d	403	CLA	C3C-C2C	5.25	1.47	1.36
20	B	610	CLA	CHC-C1C	5.25	1.49	1.38
20	b	612	CLA	CHC-C1C	5.25	1.49	1.38
20	b	618	CLA	CHC-C1C	5.24	1.49	1.38
20	C	501	CLA	MG-NC	5.23	2.18	2.06
20	C	511	CLA	MG-NC	5.23	2.18	2.06
20	b	605	CLA	C3C-C2C	5.22	1.47	1.36
40	V	201	HEC	C3D-C2D	5.21	1.47	1.36
20	C	512	CLA	CHD-C1D	5.21	1.48	1.38
20	b	603	CLA	O2A-CGA	5.21	1.48	1.33
20	c	509	CLA	CHD-C1D	5.20	1.48	1.38
20	C	510	CLA	O2D-CGD	5.20	1.45	1.33
20	c	512	CLA	CHC-C1C	5.20	1.49	1.38
20	b	603	CLA	O2D-CGD	5.20	1.45	1.33
20	c	505	CLA	CHC-C1C	5.19	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	508	CLA	C3C-C2C	5.18	1.47	1.36
20	A	404	CLA	MG-NC	5.17	2.18	2.06
20	c	502	CLA	CHC-C1C	5.15	1.49	1.38
20	b	603	CLA	C3C-C2C	5.15	1.47	1.36
20	b	609	CLA	C3C-C2C	5.13	1.47	1.36
20	b	603	CLA	CHC-C1C	5.13	1.48	1.38
21	D	403	PHO	C4D-CHA	5.13	1.47	1.39
32	B	621	HTG	C1'-S1	-5.11	1.74	1.81
20	C	508	CLA	O2D-CGD	5.11	1.45	1.33
20	b	607	CLA	C3C-C2C	5.11	1.47	1.36
20	B	615	CLA	CHD-C1D	5.11	1.48	1.38
20	B	602	CLA	O2A-CGA	5.10	1.48	1.33
20	C	501	CLA	CHC-C1C	5.10	1.48	1.38
20	c	508	CLA	C3C-C2C	5.10	1.47	1.36
20	c	504	CLA	O2D-CGD	5.09	1.45	1.33
20	c	503	CLA	CHC-C1C	5.08	1.48	1.38
20	b	616	CLA	CHD-C1D	5.08	1.48	1.38
20	C	505	CLA	CHD-C1D	5.08	1.48	1.38
24	B	620	LMG	O8-C28	5.07	1.48	1.33
20	D	404	CLA	C3C-C2C	5.07	1.47	1.36
21	a	406	PHO	C4D-CHA	5.06	1.47	1.39
20	B	606	CLA	CHC-C1C	5.05	1.48	1.38
20	c	513	CLA	C3C-C2C	5.05	1.47	1.36
20	C	513	CLA	O2D-CGD	5.05	1.45	1.33
20	c	506	CLA	O2D-CGD	5.04	1.45	1.33
20	B	615	CLA	MG-NC	5.04	2.18	2.06
20	C	502	CLA	O2D-CGD	5.03	1.45	1.33
20	c	513	CLA	O2D-CGD	5.03	1.45	1.33
20	b	607	CLA	C1D-ND	-5.03	1.31	1.37
20	C	507	CLA	C3C-C2C	5.02	1.47	1.36
20	c	510	CLA	MG-ND	-5.02	1.95	2.05
20	B	604	CLA	C3C-C2C	5.01	1.47	1.36
20	a	403	CLA	C3C-C2C	5.01	1.47	1.36
20	c	505	CLA	C3C-C2C	5.01	1.47	1.36
20	C	506	CLA	C3C-C2C	5.01	1.47	1.36
20	b	614	CLA	C3C-C2C	5.01	1.47	1.36
20	C	511	CLA	O2D-CGD	5.00	1.45	1.33
20	b	604	CLA	MG-ND	5.00	2.15	2.05
20	C	506	CLA	O2D-CGD	4.99	1.45	1.33
20	C	504	CLA	O2D-CGD	4.98	1.45	1.33
20	c	501	CLA	OBD-CAD	4.96	1.31	1.22
20	B	604	CLA	O2D-CGD	4.96	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	512	CLA	O2D-CGD	4.95	1.45	1.33
20	B	610	CLA	CHD-C1D	4.95	1.48	1.38
20	B	611	CLA	C3C-C2C	4.95	1.47	1.36
21	D	403	PHO	C3C-C2C	4.95	1.47	1.36
20	C	509	CLA	CHD-C1D	4.94	1.48	1.38
20	c	511	CLA	CHC-C1C	4.93	1.48	1.38
28	b	631	DMS	O-S	4.92	1.83	1.50
20	B	604	CLA	MG-NB	-4.91	1.96	2.05
20	c	508	CLA	MG-NC	4.90	2.17	2.06
20	C	511	CLA	C3C-C2C	4.90	1.47	1.36
20	c	511	CLA	CHD-C1D	4.89	1.47	1.38
28	D	415	DMS	O-S	4.89	1.83	1.50
20	a	403	CLA	CHC-C1C	4.88	1.48	1.38
20	B	606	CLA	C3C-C2C	4.88	1.47	1.36
20	B	602	CLA	O2D-CGD	4.86	1.45	1.33
20	b	618	CLA	C3C-C2C	4.86	1.47	1.36
20	B	610	CLA	C3C-C2C	4.86	1.47	1.36
21	A	403	PHO	C3B-C2B	4.86	1.47	1.40
20	b	616	CLA	C3C-C2C	4.86	1.47	1.36
20	b	607	CLA	CHC-C1C	4.85	1.48	1.38
20	C	505	CLA	CHC-C1C	4.85	1.48	1.38
35	d	416	DGD	O2G-C1B	4.85	1.48	1.34
20	b	612	CLA	C3C-C2C	4.84	1.47	1.36
20	A	404	CLA	C3C-C2C	4.84	1.47	1.36
20	B	604	CLA	MG-NA	4.84	2.17	2.06
20	b	617	CLA	C3C-C2C	4.83	1.47	1.36
20	d	402	CLA	CHB-C1B	4.83	1.50	1.39
20	B	616	CLA	O2D-CGD	4.83	1.45	1.33
20	c	505	CLA	CHD-C1D	4.82	1.47	1.38
20	b	611	CLA	O2D-CGD	4.81	1.44	1.33
28	c	536	DMS	O-S	4.81	1.82	1.50
20	B	607	CLA	CHC-C4B	4.81	1.50	1.39
35	D	406	DGD	O2G-C1B	4.81	1.47	1.34
20	C	509	CLA	OBD-CAD	4.81	1.30	1.22
20	b	613	CLA	CHD-C1D	4.80	1.47	1.38
20	b	615	CLA	O2D-CGD	4.80	1.44	1.33
20	C	508	CLA	CHC-C1C	4.80	1.48	1.38
20	c	509	CLA	OBD-CAD	4.80	1.30	1.22
20	B	603	CLA	C3C-C2C	4.80	1.46	1.36
20	B	613	CLA	CHC-C1C	4.80	1.48	1.38
28	B	644	DMS	O-S	4.80	1.82	1.50
20	a	407	CLA	MG-ND	4.79	2.15	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	D	406	DGD	O1G-C1A	4.78	1.47	1.33
28	O	311	DMS	O-S	4.78	1.82	1.50
20	C	512	CLA	CHC-C1C	4.78	1.48	1.38
28	b	639	DMS	O-S	4.77	1.82	1.50
28	o	308	DMS	O-S	4.77	1.82	1.50
20	b	616	CLA	CHC-C1C	4.76	1.48	1.38
20	B	611	CLA	CHC-C1C	4.75	1.48	1.38
20	B	607	CLA	O2D-CGD	4.75	1.44	1.33
37	E	104	HEM	FE-ND	4.75	2.09	1.94
28	U	904	DMS	O-S	4.75	1.82	1.50
20	C	502	CLA	C3C-C2C	4.75	1.46	1.36
20	D	401	CLA	C3C-C2C	4.74	1.46	1.36
20	B	605	CLA	CHD-C1D	4.73	1.47	1.38
20	a	404	CLA	CHC-C1C	4.73	1.48	1.38
20	B	607	CLA	CHD-C1D	4.73	1.47	1.38
20	c	509	CLA	CHC-C1C	4.73	1.48	1.38
24	c	518	LMG	O8-C28	4.73	1.47	1.33
20	C	502	CLA	CHB-C1B	4.73	1.50	1.39
20	C	502	CLA	CHC-C1C	4.72	1.48	1.38
24	C	519	LMG	O8-C28	4.72	1.47	1.33
28	c	530	DMS	O-S	4.72	1.82	1.50
20	C	509	CLA	O2D-CGD	4.72	1.44	1.33
24	C	524	LMG	O8-C28	4.71	1.47	1.33
24	J	101	LMG	O7-C10	4.71	1.47	1.34
20	c	501	CLA	MG-ND	-4.71	1.96	2.05
20	c	506	CLA	CHC-C1C	4.71	1.48	1.38
35	d	416	DGD	O1G-C1A	4.71	1.47	1.33
20	b	618	CLA	O2D-CGD	4.70	1.44	1.33
20	b	608	CLA	C3C-C2C	4.70	1.46	1.36
21	D	403	PHO	C3D-C2D	4.70	1.47	1.39
20	b	613	CLA	C3C-C2C	4.70	1.46	1.36
20	b	608	CLA	O2D-CGD	4.70	1.44	1.33
20	C	510	CLA	CHD-C1D	4.70	1.47	1.38
23	a	401	SQD	O48-C23	4.69	1.47	1.33
28	C	525[A]	DMS	O-S	4.69	1.81	1.50
28	o	302	DMS	O-S	4.68	1.81	1.50
28	B	642	DMS	O-S	4.68	1.81	1.50
28	B	643	DMS	O-S	4.68	1.81	1.50
28	A	418	DMS	O-S	4.68	1.81	1.50
20	B	615	CLA	CHC-C1C	4.67	1.48	1.38
20	B	609	CLA	O2D-CGD	4.67	1.44	1.33
28	j	105	DMS	O-S	4.66	1.81	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	b	638	DMS	O-S	4.66	1.81	1.50
20	c	511	CLA	CHB-C1B	4.66	1.49	1.39
20	b	608	CLA	CHD-C1D	4.66	1.47	1.38
20	C	512	CLA	CHB-C1B	4.65	1.49	1.39
20	c	510	CLA	C3C-C2C	4.65	1.46	1.36
20	C	503	CLA	MG-NB	4.65	2.15	2.05
20	A	404	CLA	CHC-C1C	4.64	1.47	1.38
28	o	306	DMS	O-S	4.64	1.81	1.50
20	c	511	CLA	C3C-C2C	4.64	1.46	1.36
21	a	406	PHO	C3B-C2B	4.64	1.46	1.40
21	a	405	PHO	C3C-C2C	4.64	1.46	1.36
20	b	606	CLA	CHC-C1C	4.64	1.47	1.38
24	c	518	LMG	O7-C10	4.63	1.47	1.34
20	B	615	CLA	C3C-C2C	4.63	1.46	1.36
28	A	415	DMS	O-S	4.63	1.81	1.50
23	b	622	SQD	O47-C7	4.63	1.47	1.34
21	a	406	PHO	C3C-C2C	4.63	1.46	1.36
20	D	401	CLA	CHD-C1D	4.63	1.47	1.38
28	O	308	DMS	O-S	4.62	1.81	1.50
20	B	614	CLA	C3C-C2C	4.61	1.46	1.36
20	A	404	CLA	CHB-C1B	4.61	1.49	1.39
28	b	641	DMS	O-S	4.61	1.81	1.50
28	B	638	DMS	O-S	4.61	1.81	1.50
20	b	614	CLA	C4B-NB	-4.61	1.32	1.37
20	b	613	CLA	CHC-C1C	4.61	1.47	1.38
20	B	613	CLA	C3C-C2C	4.61	1.46	1.36
20	C	504	CLA	MG-ND	4.61	2.14	2.05
37	e	102	HEM	FE-ND	4.61	2.09	1.94
20	C	510	CLA	C3C-C2C	4.60	1.46	1.36
28	B	636	DMS	O-S	4.60	1.81	1.50
21	a	405	PHO	O2D-CGD	4.60	1.44	1.33
28	v	207	DMS	O-S	4.60	1.81	1.50
20	b	605	CLA	CHD-C1D	4.60	1.47	1.38
28	c	535	DMS	O-S	4.60	1.81	1.50
20	d	404	CLA	C3C-C2C	4.60	1.46	1.36
28	b	640	DMS	O-S	4.60	1.81	1.50
20	C	505	CLA	C1B-NB	-4.59	1.32	1.37
28	h	102	DMS	O-S	4.59	1.81	1.50
20	B	616	CLA	C3C-C2C	4.58	1.46	1.36
28	H	103	DMS	O-S	4.58	1.81	1.50
28	D	413	DMS	O-S	4.58	1.81	1.50
20	C	503	CLA	CHD-C4C	4.58	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	508	CLA	CHD-C1D	4.58	1.47	1.38
20	c	501	CLA	C3C-C2C	4.58	1.46	1.36
20	B	609	CLA	CHD-C1D	4.57	1.47	1.38
28	c	533	DMS	O-S	4.57	1.81	1.50
20	b	603	CLA	CHD-C1D	4.57	1.47	1.38
20	C	506	CLA	CHB-C1B	4.57	1.49	1.39
20	c	508	CLA	O2D-CGD	4.57	1.44	1.33
20	b	603	CLA	MG-NA	4.57	2.17	2.06
20	a	407	CLA	C1D-ND	-4.56	1.32	1.37
28	o	305	DMS	O-S	4.56	1.81	1.50
28	B	645	DMS	O-S	4.56	1.81	1.50
20	B	602	CLA	CHC-C1C	4.56	1.47	1.38
20	B	615	CLA	CHB-C1B	4.55	1.49	1.39
28	B	639	DMS	O-S	4.55	1.81	1.50
28	V	205	DMS	O-S	4.55	1.81	1.50
20	b	610	CLA	MG-NA	4.55	2.17	2.06
28	O	310	DMS	O-S	4.54	1.80	1.50
28	b	636	DMS	O-S	4.54	1.80	1.50
28	d	415	DMS	O-S	4.53	1.80	1.50
20	D	402	CLA	CHD-C4C	4.53	1.49	1.39
20	B	616	CLA	C1B-NB	-4.53	1.32	1.37
28	b	632	DMS	O-S	4.53	1.80	1.50
28	A	416	DMS	O-S	4.52	1.80	1.50
20	a	407	CLA	C3C-C2C	4.52	1.46	1.36
20	B	616	CLA	CHD-C1D	4.52	1.47	1.38
20	b	611	CLA	CHD-C1D	4.52	1.47	1.38
28	O	307	DMS	O-S	4.52	1.80	1.50
28	o	303	DMS	O-S	4.52	1.80	1.50
28	b	635	DMS	O-S	4.52	1.80	1.50
20	d	402	CLA	MG-NA	4.51	2.17	2.06
20	c	509	CLA	C3C-C2C	4.51	1.46	1.36
20	B	612	CLA	CHD-C1D	4.51	1.47	1.38
36	E	103	LHG	O8-C23	4.49	1.46	1.33
20	b	617	CLA	CHC-C1C	4.49	1.47	1.38
20	c	506	CLA	C3C-C2C	4.49	1.46	1.36
23	l	101	SQD	O47-C7	4.49	1.47	1.34
21	a	405	PHO	C4D-CHA	4.49	1.46	1.39
28	C	529	DMS	O-S	4.49	1.80	1.50
28	D	416	DMS	O-S	4.48	1.80	1.50
28	V	206	DMS	O-S	4.48	1.80	1.50
20	B	611	CLA	CHD-C1D	4.48	1.47	1.38
20	B	604	CLA	CHB-C1B	4.48	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	v	206	DMS	O-S	4.48	1.80	1.50
20	b	606	CLA	O2D-CGD	4.48	1.44	1.33
20	B	613	CLA	CHD-C1D	4.48	1.47	1.38
28	B	641	DMS	O-S	4.48	1.80	1.50
28	c	531	DMS	O-S	4.48	1.80	1.50
20	b	609	CLA	CHD-C1D	4.47	1.47	1.38
36	E	103	LHG	O7-C7	4.47	1.46	1.33
20	c	504	CLA	CHD-C1D	4.47	1.47	1.38
20	B	603	CLA	OBD-CAD	4.47	1.30	1.22
28	b	637	DMS	O-S	4.47	1.80	1.50
20	C	505	CLA	O2D-CGD	4.47	1.44	1.33
28	c	529	DMS	O-S	4.47	1.80	1.50
20	A	401	CLA	MG-ND	-4.47	1.96	2.05
21	a	406	PHO	C3D-C2D	4.47	1.47	1.39
28	c	534	DMS	O-S	4.46	1.80	1.50
20	C	505	CLA	MG-NA	4.46	2.16	2.06
20	B	611	CLA	O2D-CGD	4.46	1.44	1.33
20	C	505	CLA	CHD-C4C	4.46	1.49	1.39
28	o	307	DMS	O-S	4.46	1.80	1.50
28	v	204	DMS	O-S	4.46	1.80	1.50
20	c	502	CLA	O2D-CGD	4.46	1.44	1.33
20	b	608	CLA	CHC-C4B	4.46	1.49	1.39
20	b	613	CLA	O2D-CGD	4.45	1.44	1.33
20	C	513	CLA	CHB-C1B	4.45	1.49	1.39
20	B	603	CLA	O2D-CGD	4.45	1.44	1.33
20	c	510	CLA	O2D-CGD	4.45	1.44	1.33
28	C	531	DMS	O-S	4.44	1.80	1.50
20	B	604	CLA	CHC-C1C	4.44	1.47	1.38
28	F	102	DMS	O-S	4.44	1.80	1.50
23	b	622	SQD	O48-C23	4.44	1.46	1.33
20	C	511	CLA	CHB-C1B	4.44	1.49	1.39
28	b	634	DMS	O-S	4.44	1.80	1.50
20	C	504	CLA	CHC-C1C	4.44	1.47	1.38
28	i	104	DMS	O-S	4.44	1.80	1.50
28	u	204	DMS	O-S	4.44	1.80	1.50
20	c	509	CLA	O2D-CGD	4.44	1.44	1.33
20	B	602	CLA	CHD-C1D	4.43	1.47	1.38
20	b	604	CLA	CHC-C1C	4.43	1.47	1.38
20	B	612	CLA	CHC-C1C	4.43	1.47	1.38
20	C	513	CLA	CHC-C1C	4.43	1.47	1.38
28	V	208	DMS	O-S	4.43	1.80	1.50
21	a	406	PHO	O2D-CGD	4.43	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	612	CLA	CHD-C1D	4.42	1.47	1.38
28	O	305	DMS	O-S	4.42	1.80	1.50
28	V	204	DMS	O-S	4.42	1.80	1.50
28	v	205	DMS	O-S	4.42	1.80	1.50
28	B	635	DMS	O-S	4.41	1.80	1.50
24	C	524	LMG	O7-C10	4.41	1.46	1.34
28	O	309	DMS	O-S	4.41	1.80	1.50
28	A	417	DMS	O-S	4.41	1.80	1.50
23	a	401	SQD	O47-C7	4.41	1.46	1.34
21	A	403	PHO	C3B-C4B	4.41	1.46	1.41
20	c	508	CLA	CHC-C1C	4.41	1.47	1.38
23	F	101	SQD	O48-C23	4.41	1.46	1.33
28	C	533	DMS	O-S	4.40	1.80	1.50
28	v	208	DMS	O-S	4.40	1.79	1.50
20	a	407	CLA	O2D-CGD	4.40	1.43	1.33
20	C	507	CLA	CHC-C1C	4.39	1.47	1.38
20	c	503	CLA	CHB-C1B	4.39	1.49	1.39
28	o	304	DMS	O-S	4.39	1.79	1.50
20	B	606	CLA	O2D-CGD	4.39	1.43	1.33
40	v	201	HEC	FE-ND	4.39	2.08	1.94
28	v	209	DMS	O-S	4.38	1.79	1.50
20	c	511	CLA	OBD-CAD	4.37	1.30	1.22
20	C	503	CLA	O2D-CGD	4.37	1.43	1.33
20	c	513	CLA	CHD-C1D	4.37	1.46	1.38
20	b	618	CLA	CHD-C1D	4.37	1.46	1.38
21	a	405	PHO	C3D-C2D	4.37	1.47	1.39
20	c	512	CLA	CHD-C1D	4.36	1.46	1.38
20	C	505	CLA	MG-NC	4.36	2.16	2.06
20	C	506	CLA	O2A-CGA	4.36	1.46	1.33
24	A	407	LMG	O7-C10	4.35	1.46	1.34
20	C	509	CLA	CHC-C1C	4.35	1.47	1.38
20	C	510	CLA	CHC-C1C	4.35	1.47	1.38
20	a	407	CLA	CHB-C1B	4.35	1.49	1.39
20	b	607	CLA	C3B-C4B	4.34	1.52	1.42
28	c	532	DMS	O-S	4.34	1.79	1.50
23	f	101	SQD	O48-C23	4.34	1.46	1.33
28	O	303	DMS	O-S	4.34	1.79	1.50
28	V	209	DMS	O-S	4.34	1.79	1.50
37	E	104	HEM	FE-NA	4.34	2.09	1.95
28	C	525[B]	DMS	O-S	4.34	1.79	1.50
28	O	304	DMS	O-S	4.34	1.79	1.50
20	c	509	CLA	CHB-C1B	4.33	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	505	CLA	CHB-C1B	4.33	1.49	1.39
28	V	207	DMS	O-S	4.33	1.79	1.50
20	C	503	CLA	MG-ND	4.33	2.14	2.05
20	C	501	CLA	MG-NB	4.33	2.14	2.05
20	b	608	CLA	CHB-C1B	4.33	1.49	1.39
28	v	203	DMS	O-S	4.32	1.79	1.50
28	u	202	DMS	O-S	4.32	1.79	1.50
28	c	528	DMS	O-S	4.32	1.79	1.50
20	c	501	CLA	CHC-C4B	4.32	1.49	1.39
20	a	404	CLA	CHD-C4C	4.31	1.49	1.39
20	C	506	CLA	CHD-C1D	4.31	1.46	1.38
23	A	412	SQD	O48-C23	4.31	1.45	1.33
20	A	401	CLA	CHD-C4C	4.31	1.49	1.39
23	l	101	SQD	O48-C23	4.31	1.45	1.33
20	C	501	CLA	CHD-C1D	4.31	1.46	1.38
28	U	903[A]	DMS	O-S	4.30	1.79	1.50
37	e	102	HEM	FE-NB	4.30	2.08	1.94
28	C	526	DMS	O-S	4.29	1.79	1.50
28	C	527	DMS	O-S	4.29	1.79	1.50
28	D	414	DMS	O-S	4.29	1.79	1.50
20	C	506	CLA	CHC-C4B	4.29	1.49	1.39
20	b	610	CLA	C4B-NB	-4.28	1.32	1.37
20	B	608	CLA	CHD-C1D	4.28	1.46	1.38
20	b	605	CLA	O2D-CGD	4.28	1.43	1.33
20	c	506	CLA	CHD-C1D	4.28	1.46	1.38
36	D	407	LHG	O8-C23	4.28	1.45	1.33
20	c	513	CLA	MG-ND	4.27	2.14	2.05
20	c	513	CLA	CHC-C1C	4.27	1.47	1.38
20	a	407	CLA	O2A-CGA	4.27	1.45	1.33
28	b	633	DMS	O-S	4.27	1.79	1.50
28	U	902	DMS	O-S	4.27	1.79	1.50
20	C	504	CLA	CHD-C1D	4.27	1.46	1.38
28	d	413	DMS	O-S	4.26	1.79	1.50
20	C	507	CLA	CHD-C4C	4.26	1.49	1.39
24	c	519	LMG	O8-C28	4.26	1.45	1.33
28	C	530	DMS	O-S	4.26	1.79	1.50
20	b	604	CLA	C1B-NB	-4.26	1.32	1.37
20	b	610	CLA	C1D-ND	-4.26	1.32	1.37
24	b	623	LMG	O8-C28	4.25	1.45	1.33
28	B	637	DMS	O-S	4.25	1.78	1.50
20	B	605	CLA	CHC-C1C	4.25	1.47	1.38
28	d	414	DMS	O-S	4.25	1.78	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	505	CLA	C1B-NB	-4.24	1.32	1.37
20	d	404	CLA	CHD-C1D	4.23	1.46	1.38
20	b	613	CLA	CHB-C1B	4.23	1.48	1.39
21	D	403	PHO	O2D-CGD	4.23	1.43	1.33
23	A	406	SQD	O47-C7	4.23	1.46	1.34
20	C	512	CLA	O2A-CGA	4.22	1.45	1.33
28	u	203	DMS	O-S	4.22	1.78	1.50
20	B	608	CLA	CHB-C1B	4.22	1.48	1.39
20	C	507	CLA	MG-ND	4.22	2.14	2.05
20	d	403	CLA	CHC-C1C	4.21	1.47	1.38
20	c	507	CLA	CHC-C1C	4.21	1.47	1.38
20	d	403	CLA	CHD-C1D	4.21	1.46	1.38
21	D	403	PHO	C3B-C4B	4.21	1.46	1.41
20	b	604	CLA	C1D-ND	-4.21	1.32	1.37
20	B	603	CLA	CHC-C1C	4.20	1.47	1.38
28	O	306	DMS	O-S	4.20	1.78	1.50
20	C	508	CLA	MG-NB	4.19	2.14	2.05
20	b	617	CLA	CHB-C1B	4.19	1.48	1.39
20	c	513	CLA	CHB-C1B	4.18	1.48	1.39
20	c	501	CLA	CHD-C1D	4.18	1.46	1.38
20	B	608	CLA	C3C-C2C	4.18	1.45	1.36
20	c	501	CLA	CHC-C1C	4.18	1.47	1.38
20	B	613	CLA	CHB-C1B	4.18	1.48	1.39
20	c	502	CLA	CHD-C1D	4.18	1.46	1.38
20	C	509	CLA	O2A-CGA	4.17	1.45	1.33
20	b	604	CLA	CHD-C4C	4.17	1.48	1.39
20	B	603	CLA	CHB-C1B	4.17	1.48	1.39
20	D	404	CLA	CHB-C1B	4.17	1.48	1.39
24	A	407	LMG	O8-C28	4.17	1.45	1.33
20	A	401	CLA	CHC-C4B	4.17	1.48	1.39
20	B	601	CLA	C1D-ND	-4.17	1.32	1.37
20	B	610	CLA	C1B-NB	-4.17	1.32	1.37
20	c	510	CLA	CHC-C1C	4.17	1.47	1.38
28	v	202	DMS	O-S	4.16	1.78	1.50
20	c	507	CLA	O2D-CGD	4.16	1.43	1.33
20	C	504	CLA	CHD-C4C	4.16	1.48	1.39
20	b	614	CLA	CHC-C1C	4.15	1.47	1.38
20	c	507	CLA	CHD-C1D	4.15	1.46	1.38
20	b	610	CLA	OBD-CAD	4.15	1.29	1.22
20	C	505	CLA	C1D-ND	-4.15	1.32	1.37
20	A	404	CLA	CHC-C4B	4.15	1.48	1.39
20	b	610	CLA	CHB-C1B	4.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	405	PHO	C3B-C4B	4.14	1.46	1.41
24	j	101	LMG	O8-C28	4.14	1.45	1.33
20	b	617	CLA	O2D-CGD	4.14	1.43	1.33
20	B	616	CLA	CHC-C1C	4.14	1.46	1.38
20	B	613	CLA	O2D-CGD	4.14	1.43	1.33
20	c	512	CLA	CHC-C4B	4.13	1.48	1.39
24	b	623	LMG	O7-C10	4.13	1.45	1.34
24	a	410	LMG	O7-C10	4.13	1.45	1.34
20	c	512	CLA	CHD-C4C	4.12	1.48	1.39
28	U	903[B]	DMS	O-S	4.12	1.78	1.50
20	A	401	CLA	CHC-C1C	4.12	1.46	1.38
20	d	404	CLA	CHC-C1C	4.12	1.46	1.38
24	c	519	LMG	O7-C10	4.12	1.45	1.34
20	A	401	CLA	OBD-CAD	4.12	1.29	1.22
36	D	409	LHG	O8-C23	4.11	1.45	1.33
20	D	402	CLA	MG-NC	4.11	2.16	2.06
20	B	606	CLA	CHD-C1D	4.11	1.46	1.38
35	c	517	DGD	O1G-C1A	4.11	1.45	1.33
20	C	507	CLA	CHB-C1B	4.11	1.48	1.39
20	D	404	CLA	CHC-C1C	4.11	1.46	1.38
20	d	404	CLA	CHC-C4B	4.11	1.48	1.39
20	b	615	CLA	C3C-C2C	4.11	1.45	1.36
20	B	604	CLA	CHD-C1D	4.10	1.46	1.38
20	C	510	CLA	CHB-C1B	4.10	1.48	1.39
20	B	608	CLA	CHC-C4B	4.09	1.48	1.39
23	A	412	SQD	O47-C7	4.09	1.45	1.34
20	C	513	CLA	CHD-C4C	4.09	1.48	1.39
20	B	601	CLA	O2D-CGD	4.09	1.43	1.33
28	B	640	DMS	O-S	4.09	1.77	1.50
20	b	610	CLA	CHD-C4C	4.08	1.48	1.39
20	c	506	CLA	O2A-CGA	4.08	1.45	1.33
21	A	403	PHO	C3C-C2C	4.08	1.45	1.36
20	c	510	CLA	CHD-C1D	4.08	1.46	1.38
20	b	614	CLA	MG-NB	4.07	2.13	2.05
20	C	511	CLA	CHD-C1D	4.07	1.46	1.38
20	c	507	CLA	CHB-C1B	4.07	1.48	1.39
20	D	402	CLA	C3C-C2C	4.07	1.45	1.36
20	b	617	CLA	CHD-C4C	4.06	1.48	1.39
20	c	513	CLA	O2A-CGA	4.06	1.45	1.33
20	d	402	CLA	C3C-C2C	4.06	1.45	1.36
20	B	608	CLA	CHC-C1C	4.05	1.46	1.38
20	B	611	CLA	C4C-C3C	4.05	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	618	CLA	CHB-C1B	4.05	1.48	1.39
20	b	603	CLA	CHC-C4B	4.04	1.48	1.39
24	a	410	LMG	O8-C28	4.04	1.45	1.33
20	C	505	CLA	CHC-C4B	4.04	1.48	1.39
20	b	611	CLA	O2A-CGA	4.04	1.45	1.33
20	C	501	CLA	CHC-C4B	4.04	1.48	1.39
20	C	503	CLA	CHC-C4B	4.04	1.48	1.39
35	h	101	DGD	O2G-C1B	4.03	1.45	1.34
20	b	606	CLA	CHD-C1D	4.03	1.46	1.38
35	H	102	DGD	O2G-C1B	4.02	1.45	1.34
20	b	618	CLA	O2A-CGA	4.02	1.45	1.33
20	C	510	CLA	MG-NB	4.02	2.13	2.05
20	c	503	CLA	CHD-C1D	4.02	1.46	1.38
20	d	404	CLA	CHB-C1B	4.02	1.48	1.39
20	C	508	CLA	CHB-C1B	4.01	1.48	1.39
20	b	609	CLA	CHC-C1C	4.01	1.46	1.38
20	c	505	CLA	CHD-C4C	4.01	1.48	1.39
20	C	512	CLA	CHD-C4C	4.01	1.48	1.39
20	a	407	CLA	CHD-C1D	4.00	1.46	1.38
24	C	519	LMG	O7-C10	4.00	1.45	1.34
20	b	612	CLA	MG-NC	4.00	2.15	2.06
20	C	503	CLA	CHD-C1D	4.00	1.46	1.38
20	C	502	CLA	CHD-C1D	4.00	1.46	1.38
20	b	607	CLA	O2D-CGD	4.00	1.42	1.33
20	C	511	CLA	CHC-C1C	3.99	1.46	1.38
20	C	507	CLA	O2D-CGD	3.99	1.42	1.33
20	A	404	CLA	CHD-C1D	3.99	1.46	1.38
20	C	505	CLA	O2A-CGA	3.99	1.45	1.33
36	d	406	LHG	O8-C23	3.99	1.45	1.33
20	c	503	CLA	O2D-CGD	3.99	1.42	1.33
20	c	510	CLA	CHB-C1B	3.98	1.48	1.39
20	b	604	CLA	CHD-C1D	3.98	1.46	1.38
20	c	507	CLA	O2A-CGA	3.98	1.45	1.33
23	a	409	SQD	O48-C23	3.98	1.45	1.33
20	B	610	CLA	CHB-C1B	3.97	1.48	1.39
20	c	504	CLA	CHC-C1C	3.97	1.46	1.38
20	B	609	CLA	CHD-C4C	3.97	1.48	1.39
20	C	501	CLA	O2D-CGD	3.97	1.42	1.33
20	A	401	CLA	O2D-CGD	3.97	1.42	1.33
20	B	602	CLA	CHC-C4B	3.96	1.48	1.39
20	C	513	CLA	O2A-CGA	3.96	1.44	1.33
20	B	612	CLA	CHC-C4B	3.96	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	403	CLA	CHB-C1B	3.95	1.48	1.39
20	c	501	CLA	O2D-CGD	3.95	1.42	1.33
20	B	606	CLA	CHD-C4C	3.94	1.48	1.39
20	B	609	CLA	C3C-C2C	3.94	1.45	1.36
20	B	614	CLA	O2A-CGA	3.94	1.44	1.33
21	a	406	PHO	C3D-C4D	-3.93	1.35	1.41
20	C	508	CLA	O2A-CGA	3.93	1.44	1.33
20	B	616	CLA	MG-NC	3.92	2.15	2.06
35	C	516	DGD	O2G-C1B	3.92	1.45	1.34
20	a	407	CLA	OBD-CAD	3.92	1.29	1.22
20	D	402	CLA	CHC-C4B	3.91	1.48	1.39
20	C	501	CLA	MG-NA	3.91	2.15	2.06
20	B	602	CLA	CHB-C1B	3.90	1.48	1.39
20	b	610	CLA	O2D-CGD	3.90	1.42	1.33
20	c	512	CLA	O2A-CGA	3.90	1.44	1.33
20	b	611	CLA	CHB-C1B	3.90	1.48	1.39
20	c	513	CLA	CHD-C4C	3.90	1.48	1.39
20	D	402	CLA	C4B-NB	-3.90	1.33	1.37
20	b	615	CLA	CHD-C4C	3.89	1.48	1.39
20	c	507	CLA	CHC-C4B	3.89	1.48	1.39
20	B	604	CLA	CHD-C4C	3.89	1.48	1.39
20	b	611	CLA	CHC-C4B	3.88	1.48	1.39
20	a	403	CLA	O2D-CGD	3.88	1.42	1.33
20	B	606	CLA	CHB-C1B	3.88	1.48	1.39
20	b	608	CLA	CHC-C1C	3.88	1.46	1.38
20	D	401	CLA	CHD-C4C	3.88	1.48	1.39
35	c	517	DGD	O2G-C1B	3.88	1.45	1.34
35	C	517	DGD	O1G-C1A	3.87	1.44	1.33
28	c	527	DMS	O-S	3.87	1.76	1.50
20	B	605	CLA	C3C-C2C	3.87	1.44	1.36
20	c	502	CLA	CHB-C1B	3.87	1.48	1.39
20	C	503	CLA	O2A-CGA	3.86	1.44	1.33
20	b	609	CLA	O2D-CGD	3.86	1.42	1.33
20	b	603	CLA	CHB-C1B	3.85	1.48	1.39
20	d	404	CLA	O2A-CGA	3.85	1.44	1.33
20	d	404	CLA	C4C-C3C	3.84	1.51	1.45
20	C	508	CLA	CHC-C4B	3.84	1.48	1.39
21	A	403	PHO	C4D-CHA	3.84	1.45	1.39
20	B	611	CLA	CHC-C4B	3.84	1.48	1.39
40	V	201	HEC	FE-ND	3.84	2.06	1.94
20	C	503	CLA	MG-NC	3.84	2.15	2.06
32	B	622	HTG	C1'-S1	-3.84	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	506	CLA	CHD-C4C	3.83	1.48	1.39
35	C	518	DGD	O1G-C1A	3.83	1.44	1.33
20	b	604	CLA	C3B-C4B	3.83	1.51	1.42
20	C	513	CLA	CHC-C4B	3.82	1.48	1.39
20	B	614	CLA	CHB-C1B	3.82	1.48	1.39
20	B	605	CLA	O2D-CGD	3.82	1.42	1.33
20	C	508	CLA	OBD-CAD	3.82	1.29	1.22
20	b	614	CLA	C1B-NB	-3.82	1.33	1.37
20	b	612	CLA	CHC-C4B	3.81	1.48	1.39
20	a	403	CLA	CHD-C4C	3.81	1.47	1.39
20	b	617	CLA	CHD-C1D	3.81	1.45	1.38
20	b	605	CLA	C1D-ND	-3.81	1.33	1.37
20	C	503	CLA	C3B-C4B	3.81	1.51	1.42
20	B	601	CLA	MG-NC	3.80	2.15	2.06
20	C	501	CLA	CHD-C4C	3.80	1.47	1.39
20	A	404	CLA	MG-NA	3.79	2.15	2.06
32	D	417	HTG	C1'-S1	-3.79	1.76	1.81
20	B	612	CLA	C3C-C2C	3.79	1.44	1.36
21	D	403	PHO	OBD-CAD	3.79	1.27	1.22
20	b	614	CLA	O2D-CGD	3.79	1.42	1.33
20	C	504	CLA	MG-NC	3.79	2.15	2.06
20	B	612	CLA	OBD-CAD	3.79	1.29	1.22
20	b	613	CLA	O2A-CGA	3.79	1.44	1.33
20	C	501	CLA	C3B-C4B	3.78	1.51	1.42
28	C	528	DMS	O-S	3.78	1.75	1.50
20	C	513	CLA	C3D-C2D	3.78	1.49	1.39
20	C	502	CLA	O2A-CGA	3.77	1.44	1.33
20	b	603	CLA	OBD-CAD	3.77	1.29	1.22
20	c	511	CLA	CHC-C4B	3.77	1.47	1.39
20	B	602	CLA	OBD-CAD	3.77	1.29	1.22
20	B	601	CLA	CHC-C4B	3.76	1.47	1.39
20	a	404	CLA	CHB-C1B	3.76	1.47	1.39
20	b	617	CLA	OBD-CAD	3.76	1.29	1.22
32	b	624	HTG	C1'-S1	-3.76	1.76	1.81
20	C	509	CLA	C3D-C2D	3.76	1.49	1.39
20	B	616	CLA	CHD-C4C	3.75	1.47	1.39
20	b	616	CLA	O2D-CGD	3.75	1.42	1.33
32	O	302	HTG	C1'-S1	-3.74	1.76	1.81
20	c	512	CLA	CHB-C1B	3.74	1.47	1.39
23	a	409	SQD	O47-C7	3.74	1.44	1.34
20	a	403	CLA	CHD-C1D	3.74	1.45	1.38
20	A	401	CLA	C4C-C3C	3.74	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	616	CLA	CHC-C4B	3.74	1.47	1.39
24	j	101	LMG	O7-C10	3.74	1.44	1.34
20	c	508	CLA	CHC-C4B	3.73	1.47	1.39
20	D	404	CLA	O2D-CGD	3.73	1.42	1.33
20	b	605	CLA	CHD-C4C	3.73	1.47	1.39
20	c	512	CLA	OBD-CAD	3.73	1.28	1.22
20	B	602	CLA	CHD-C4C	3.72	1.47	1.39
24	J	101	LMG	O8-C28	3.72	1.44	1.33
21	a	405	PHO	OBD-CAD	3.72	1.27	1.22
20	D	404	CLA	CHC-C4B	3.72	1.47	1.39
20	B	603	CLA	C4C-C3C	3.72	1.51	1.45
21	D	403	PHO	O2A-CGA	3.72	1.44	1.33
20	c	508	CLA	C3D-C2D	3.72	1.49	1.39
20	c	508	CLA	CHB-C1B	3.71	1.47	1.39
20	b	611	CLA	OBD-CAD	3.71	1.28	1.22
20	c	504	CLA	O2A-CGA	3.70	1.44	1.33
20	B	605	CLA	MG-ND	3.70	2.13	2.05
20	c	504	CLA	OBD-CAD	3.70	1.28	1.22
20	A	404	CLA	OBD-CAD	3.70	1.28	1.22
20	c	501	CLA	CHB-C1B	3.69	1.47	1.39
20	C	510	CLA	OBD-CAD	3.69	1.28	1.22
20	c	510	CLA	O2A-CGA	3.69	1.44	1.33
20	B	605	CLA	CHD-C4C	3.69	1.47	1.39
20	b	608	CLA	C3D-C2D	3.68	1.49	1.39
35	c	516	DGD	O1G-C1A	3.68	1.44	1.33
20	C	501	CLA	CHB-C1B	3.68	1.47	1.39
20	b	615	CLA	O2A-CGA	3.68	1.44	1.33
20	B	605	CLA	CHB-C1B	3.68	1.47	1.39
20	c	503	CLA	C1D-ND	-3.68	1.33	1.37
20	b	610	CLA	CHD-C1D	3.68	1.45	1.38
32	C	534	HTG	C1'-S1	-3.68	1.76	1.81
21	A	403	PHO	C3D-C4D	-3.68	1.36	1.41
20	C	512	CLA	CHC-C4B	3.68	1.47	1.39
20	B	612	CLA	O2D-CGD	3.67	1.42	1.33
32	d	401	HTG	C1'-S1	-3.67	1.76	1.81
20	b	606	CLA	CHB-C1B	3.67	1.47	1.39
20	b	604	CLA	CHB-C1B	3.67	1.47	1.39
20	c	501	CLA	O2A-CGA	3.67	1.44	1.33
20	b	603	CLA	C3B-C4B	3.66	1.51	1.42
20	b	612	CLA	MG-NA	3.66	2.15	2.06
35	h	101	DGD	O5D-C1E	3.66	1.46	1.40
20	c	503	CLA	CHD-C4C	3.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	511	CLA	C3D-C2D	3.65	1.49	1.39
20	B	609	CLA	CHB-C1B	3.65	1.47	1.39
21	A	403	PHO	O2A-CGA	3.65	1.44	1.33
20	b	609	CLA	C3D-C2D	3.64	1.49	1.39
20	c	506	CLA	CHD-C4C	3.64	1.47	1.39
20	b	611	CLA	C3D-C2D	3.64	1.49	1.39
20	b	611	CLA	CHD-C4C	3.64	1.47	1.39
20	c	510	CLA	MG-NA	3.64	2.14	2.06
20	B	607	CLA	O2A-CGA	3.64	1.44	1.33
20	a	404	CLA	C4B-NB	-3.64	1.33	1.37
20	b	609	CLA	CHD-C4C	3.63	1.47	1.39
20	B	613	CLA	C1D-ND	-3.63	1.33	1.37
20	b	607	CLA	C4B-NB	-3.63	1.33	1.37
20	B	608	CLA	CHD-C4C	3.63	1.47	1.39
20	b	615	CLA	C3B-C4B	3.62	1.51	1.42
20	c	509	CLA	CHD-C4C	3.62	1.47	1.39
20	B	611	CLA	CHB-C1B	3.62	1.47	1.39
20	B	611	CLA	CHD-C4C	3.62	1.47	1.39
21	a	405	PHO	C3B-C2B	3.62	1.45	1.40
21	a	406	PHO	C3A-C2A	-3.62	1.51	1.54
20	B	616	CLA	CHB-C1B	3.62	1.47	1.39
20	c	511	CLA	CHD-C4C	3.61	1.47	1.39
20	b	614	CLA	CHD-C1D	3.61	1.45	1.38
21	D	403	PHO	C3A-C2A	-3.61	1.51	1.54
20	D	402	CLA	C3B-C4B	3.61	1.51	1.42
23	A	406	SQD	O48-C23	3.61	1.43	1.33
20	d	403	CLA	CHD-C4C	3.61	1.47	1.39
20	c	513	CLA	CHC-C4B	3.60	1.47	1.39
20	c	502	CLA	CHD-C4C	3.60	1.47	1.39
20	B	601	CLA	O2A-CGA	3.60	1.43	1.33
20	B	607	CLA	C1C-C2C	3.60	1.51	1.44
20	A	401	CLA	MG-NC	3.60	2.14	2.06
20	b	604	CLA	C1B-C2B	3.59	1.51	1.43
20	b	611	CLA	C3B-C4B	3.59	1.51	1.42
20	b	616	CLA	OBD-CAD	3.59	1.28	1.22
20	B	616	CLA	O2A-CGA	3.59	1.43	1.33
20	C	513	CLA	C3B-C4B	3.59	1.51	1.42
20	B	606	CLA	OBD-CAD	3.58	1.28	1.22
20	c	505	CLA	O2A-CGA	3.58	1.43	1.33
20	a	407	CLA	MG-NA	3.58	2.14	2.06
20	D	404	CLA	CHD-C4C	3.58	1.47	1.39
20	B	603	CLA	CHD-C4C	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	504	CLA	O2A-CGA	3.58	1.43	1.33
20	D	404	CLA	O2A-CGA	3.58	1.43	1.33
40	v	201	HEC	FE-NA	3.58	2.07	1.95
37	e	102	HEM	FE-NC	3.57	2.07	1.95
20	A	404	CLA	O2A-CGA	3.57	1.43	1.33
35	c	515	DGD	O1G-C1A	3.57	1.43	1.33
20	c	502	CLA	C1D-ND	-3.57	1.33	1.37
20	c	508	CLA	C1C-NC	-3.57	1.32	1.37
20	b	616	CLA	O2A-CGA	3.56	1.43	1.33
20	B	610	CLA	O2D-CGD	3.56	1.41	1.33
20	d	402	CLA	CHD-C1D	3.56	1.45	1.38
20	b	618	CLA	CHC-C4B	3.56	1.47	1.39
35	C	518	DGD	O2G-C1B	3.55	1.44	1.34
20	b	614	CLA	CHD-C4C	3.55	1.47	1.39
20	B	607	CLA	OBD-CAD	3.55	1.28	1.22
20	B	610	CLA	C3B-C4B	3.55	1.51	1.42
20	c	503	CLA	CHC-C4B	3.55	1.47	1.39
20	b	605	CLA	CHB-C1B	3.54	1.47	1.39
20	B	603	CLA	MG-NC	3.54	2.14	2.06
20	c	509	CLA	O2A-CGA	3.54	1.43	1.33
20	B	615	CLA	O2A-CGA	3.54	1.43	1.33
20	C	505	CLA	CHB-C1B	3.54	1.47	1.39
34	c	523	LMT	O1'-C1'	3.54	1.46	1.40
20	C	506	CLA	MG-NC	3.53	2.14	2.06
20	C	503	CLA	C1D-ND	-3.53	1.33	1.37
20	a	404	CLA	C3C-C2C	3.53	1.44	1.36
20	d	402	CLA	OBD-CAD	3.53	1.28	1.22
32	C	522	HTG	C1'-S1	-3.53	1.76	1.81
20	C	511	CLA	CHD-C4C	3.52	1.47	1.39
20	B	611	CLA	C3B-C4B	3.52	1.51	1.42
20	c	507	CLA	OBD-CAD	3.52	1.28	1.22
20	b	603	CLA	CHD-C4C	3.51	1.47	1.39
20	c	511	CLA	C3B-C4B	3.51	1.51	1.42
20	c	512	CLA	C4C-C3C	3.51	1.51	1.45
20	C	510	CLA	C3D-C2D	3.51	1.48	1.39
20	b	605	CLA	C1B-NB	-3.51	1.33	1.37
20	c	505	CLA	C3B-C4B	3.51	1.51	1.42
35	H	102	DGD	O1G-C1A	3.51	1.43	1.33
20	B	613	CLA	C4B-NB	-3.51	1.33	1.37
24	B	620	LMG	O7-C10	3.51	1.44	1.34
20	B	614	CLA	CHD-C4C	3.51	1.47	1.39
20	C	510	CLA	MG-ND	-3.51	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	612	CLA	CHD-C4C	3.50	1.47	1.39
20	C	507	CLA	O2A-CGA	3.50	1.43	1.33
21	a	406	PHO	O2A-CGA	3.49	1.43	1.33
20	B	615	CLA	CHC-C4B	3.49	1.47	1.39
20	C	511	CLA	OBD-CAD	3.49	1.28	1.22
20	B	608	CLA	C3B-C4B	3.48	1.50	1.42
20	C	509	CLA	CHB-C1B	3.48	1.47	1.39
32	B	632	HTG	C1'-S1	-3.48	1.77	1.81
20	C	512	CLA	C3B-C4B	3.48	1.50	1.42
20	c	502	CLA	C3C-C2C	3.48	1.44	1.36
20	c	507	CLA	CHD-C4C	3.48	1.47	1.39
20	b	617	CLA	C1D-ND	-3.47	1.33	1.37
20	A	402	CLA	C3C-C2C	3.47	1.44	1.36
20	b	604	CLA	O2A-CGA	3.47	1.43	1.33
20	b	616	CLA	CHB-C1B	3.47	1.47	1.39
20	C	501	CLA	O2A-CGA	3.47	1.43	1.33
20	C	511	CLA	CHC-C4B	3.46	1.47	1.39
20	C	507	CLA	CHC-C4B	3.46	1.47	1.39
35	H	102	DGD	O5D-C1E	3.46	1.46	1.40
20	D	402	CLA	O2D-CGD	3.45	1.41	1.33
20	c	506	CLA	CHC-C4B	3.45	1.47	1.39
20	b	616	CLA	CHD-C4C	3.45	1.47	1.39
20	D	402	CLA	CHC-C1C	3.45	1.45	1.38
20	c	513	CLA	C1D-ND	-3.45	1.33	1.37
22	b	620	BCR	C5-C6	3.45	1.40	1.34
20	C	504	CLA	C3D-C2D	3.44	1.48	1.39
20	B	610	CLA	CHC-C4B	3.44	1.47	1.39
20	c	510	CLA	C1D-ND	-3.44	1.33	1.37
20	D	401	CLA	O2A-CGA	3.44	1.43	1.33
20	B	609	CLA	CHC-C4B	3.44	1.47	1.39
36	d	408	LHG	O8-C23	3.44	1.43	1.33
20	b	610	CLA	C3B-C4B	3.44	1.50	1.42
20	D	404	CLA	CHD-C1D	3.43	1.45	1.38
20	A	404	CLA	O2D-CGD	3.43	1.41	1.33
20	D	402	CLA	CHD-C1D	3.43	1.45	1.38
20	c	508	CLA	O2A-CGA	3.43	1.43	1.33
20	C	510	CLA	CHD-C4C	3.43	1.47	1.39
20	B	613	CLA	CHD-C4C	3.42	1.47	1.39
20	B	604	CLA	MG-NC	3.41	2.14	2.06
20	b	609	CLA	CHB-C1B	3.41	1.47	1.39
27	d	412	PL9	C7-C3	3.41	1.54	1.51
20	C	510	CLA	O2A-CGA	3.41	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	602	CLA	C3B-C4B	3.41	1.50	1.42
20	B	614	CLA	C4C-C3C	3.41	1.50	1.45
20	b	612	CLA	C4C-C3C	3.41	1.50	1.45
20	B	610	CLA	O2A-CGA	3.40	1.43	1.33
20	b	606	CLA	CHD-C4C	3.40	1.47	1.39
20	C	504	CLA	CHB-C1B	3.40	1.47	1.39
20	B	615	CLA	C3B-C4B	3.40	1.50	1.42
20	C	504	CLA	C3B-C4B	3.40	1.50	1.42
20	D	401	CLA	C3B-C4B	3.40	1.50	1.42
20	B	610	CLA	C1D-ND	-3.40	1.33	1.37
35	C	516	DGD	O1G-C1A	3.40	1.43	1.33
20	c	510	CLA	CHD-C4C	3.39	1.47	1.39
20	B	607	CLA	CHB-C1B	3.39	1.47	1.39
20	c	511	CLA	O2A-CGA	3.39	1.43	1.33
20	c	502	CLA	OBD-CAD	3.39	1.28	1.22
20	C	508	CLA	C3D-C2D	3.39	1.48	1.39
20	b	618	CLA	C3D-C2D	3.38	1.48	1.39
20	B	609	CLA	CHC-C1C	3.38	1.45	1.38
20	a	404	CLA	O2A-CGA	3.38	1.43	1.33
20	c	502	CLA	O2A-CGA	3.38	1.43	1.33
20	B	614	CLA	CHD-C1D	3.38	1.44	1.38
20	C	508	CLA	CHD-C4C	3.37	1.46	1.39
20	C	501	CLA	C3D-C2D	3.37	1.48	1.39
20	b	608	CLA	CHD-C4C	3.37	1.46	1.39
20	B	615	CLA	O2D-CGD	3.37	1.41	1.33
20	C	507	CLA	OBD-CAD	3.37	1.28	1.22
20	c	505	CLA	CHC-C4B	3.35	1.46	1.39
20	b	618	CLA	MG-NC	3.35	2.14	2.06
36	D	408	LHG	O8-C23	3.35	1.43	1.33
36	L	101	LHG	O7-C7	3.35	1.43	1.34
20	B	609	CLA	MG-NB	-3.35	1.99	2.05
20	B	607	CLA	CHD-C4C	3.35	1.46	1.39
32	B	631	HTG	C1'-S1	-3.35	1.77	1.81
20	b	612	CLA	C3B-C4B	3.34	1.50	1.42
20	B	601	CLA	CHD-C1D	3.34	1.44	1.38
20	B	601	CLA	CHB-C1B	3.34	1.46	1.39
20	d	404	CLA	OBD-CAD	3.34	1.28	1.22
20	c	501	CLA	CHD-C4C	3.34	1.46	1.39
20	C	502	CLA	CHD-C4C	3.34	1.46	1.39
20	B	603	CLA	C1D-ND	-3.34	1.33	1.37
20	b	608	CLA	C4D-CHA	3.33	1.50	1.38
20	C	512	CLA	C1D-ND	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	101	LHG	O8-C23	3.33	1.43	1.33
20	d	404	CLA	MG-NC	3.32	2.14	2.06
20	c	509	CLA	CHC-C4B	3.32	1.46	1.39
20	b	605	CLA	OBD-CAD	3.32	1.28	1.22
20	B	608	CLA	C3D-C2D	3.32	1.48	1.39
40	V	201	HEC	CBC-CAC	-3.32	1.36	1.51
20	C	509	CLA	CHC-C4B	3.32	1.46	1.39
20	B	611	CLA	O2A-CGA	3.31	1.43	1.33
20	d	402	CLA	O2A-CGA	3.31	1.43	1.33
20	a	404	CLA	O2D-CGD	3.31	1.41	1.33
20	B	603	CLA	CHC-C4B	3.31	1.46	1.39
20	C	502	CLA	C4D-CHA	3.31	1.50	1.38
20	c	513	CLA	OBD-CAD	3.31	1.28	1.22
20	C	511	CLA	O2A-CGA	3.31	1.43	1.33
34	b	627	LMT	O1'-C1'	3.30	1.45	1.40
32	b	601	HTG	C1'-S1	-3.30	1.77	1.81
20	c	504	CLA	CHC-C4B	3.30	1.46	1.39
20	B	616	CLA	OBD-CAD	3.30	1.28	1.22
20	b	615	CLA	MG-NB	3.29	2.12	2.05
21	A	403	PHO	O2D-CGD	3.29	1.41	1.33
20	B	612	CLA	CHB-C1B	3.29	1.46	1.39
20	C	502	CLA	CHC-C4B	3.29	1.46	1.39
20	C	506	CLA	C4D-CHA	3.29	1.50	1.38
20	C	511	CLA	C3D-C2D	3.28	1.48	1.39
20	a	404	CLA	OBD-CAD	3.28	1.28	1.22
20	C	512	CLA	C4C-C3C	3.28	1.50	1.45
20	a	404	CLA	CHD-C1D	3.28	1.44	1.38
20	d	402	CLA	C3B-C4B	3.28	1.50	1.42
20	B	611	CLA	C3D-C2D	3.28	1.48	1.39
20	c	505	CLA	OBD-CAD	3.28	1.28	1.22
20	a	407	CLA	CHD-C4C	3.27	1.46	1.39
20	B	610	CLA	MG-NC	3.27	2.14	2.06
20	B	602	CLA	C4D-CHA	3.27	1.50	1.38
20	B	612	CLA	C1D-ND	-3.27	1.33	1.37
20	C	504	CLA	C4D-CHA	3.27	1.50	1.38
20	C	507	CLA	C3D-C2D	3.26	1.48	1.39
20	B	615	CLA	C1B-NB	-3.26	1.33	1.37
20	B	615	CLA	C1C-NC	-3.26	1.32	1.37
36	l	102	LHG	O8-C23	3.25	1.42	1.33
20	b	604	CLA	C4C-C3C	3.25	1.50	1.45
20	c	510	CLA	CHC-C4B	3.25	1.46	1.39
20	b	615	CLA	CHB-C1B	3.25	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	503	CLA	O2A-CGA	3.25	1.42	1.33
20	B	615	CLA	OBD-CAD	3.24	1.28	1.22
20	C	510	CLA	CHC-C4B	3.24	1.46	1.39
20	b	618	CLA	C1D-ND	-3.24	1.33	1.37
20	b	610	CLA	C1B-NB	-3.24	1.33	1.37
20	c	510	CLA	C1B-NB	-3.24	1.33	1.37
20	B	609	CLA	O2A-CGA	3.24	1.42	1.33
35	C	517	DGD	O2G-C1B	3.23	1.43	1.34
28	A	414	DMS	O-S	3.23	1.72	1.50
20	c	505	CLA	C4B-NB	-3.23	1.33	1.37
20	B	610	CLA	C3D-C2D	3.22	1.47	1.39
37	e	102	HEM	FE-NA	3.22	2.06	1.95
20	c	506	CLA	CHB-C1B	3.22	1.46	1.39
20	b	610	CLA	C4D-CHA	3.22	1.49	1.38
20	b	613	CLA	C3B-C4B	3.22	1.50	1.42
20	c	508	CLA	CHD-C4C	3.21	1.46	1.39
20	A	402	CLA	MG-NB	-3.21	1.99	2.05
20	C	502	CLA	C3D-C2D	3.21	1.47	1.39
20	B	601	CLA	CHD-C4C	3.21	1.46	1.39
20	b	618	CLA	CHD-C4C	3.21	1.46	1.39
20	d	402	CLA	C1D-ND	-3.21	1.33	1.37
20	d	402	CLA	CHD-C4C	3.21	1.46	1.39
20	C	506	CLA	C3B-C4B	3.21	1.50	1.42
20	b	606	CLA	C3B-C4B	3.21	1.50	1.42
20	b	615	CLA	CHD-C1D	3.20	1.44	1.38
20	C	505	CLA	C3D-C2D	3.19	1.47	1.39
20	B	604	CLA	O2A-CGA	3.19	1.42	1.33
20	b	607	CLA	CHD-C1D	3.19	1.44	1.38
20	A	402	CLA	CHB-C1B	3.19	1.46	1.39
20	D	401	CLA	O2D-CGD	3.19	1.41	1.33
20	c	502	CLA	C3D-C2D	3.19	1.47	1.39
20	C	509	CLA	CHD-C4C	3.19	1.46	1.39
20	C	512	CLA	C3D-C2D	3.19	1.47	1.39
20	C	503	CLA	CHB-C1B	3.18	1.46	1.39
20	c	510	CLA	OBD-CAD	3.18	1.28	1.22
20	b	618	CLA	C4D-CHA	3.18	1.49	1.38
20	C	503	CLA	C3D-C2D	3.18	1.47	1.39
20	c	508	CLA	C4C-C3C	3.18	1.50	1.45
20	C	507	CLA	C4D-CHA	3.17	1.49	1.38
36	D	408	LHG	O7-C7	3.17	1.43	1.34
20	a	407	CLA	C3D-C2D	3.17	1.47	1.39
20	C	508	CLA	C3B-C4B	3.17	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	507	CLA	C4D-CHA	3.17	1.49	1.38
20	D	401	CLA	CHB-C1B	3.17	1.46	1.39
20	b	614	CLA	MG-ND	-3.16	1.99	2.05
20	b	614	CLA	CHC-C4B	3.16	1.46	1.39
20	b	609	CLA	CHC-C4B	3.16	1.46	1.39
36	d	406	LHG	O7-C7	3.16	1.43	1.34
20	b	603	CLA	C3D-C2D	3.16	1.47	1.39
32	b	602	HTG	C1'-S1	-3.15	1.77	1.81
20	B	603	CLA	C3D-C2D	3.15	1.47	1.39
20	b	609	CLA	C3B-C4B	3.15	1.50	1.42
20	c	512	CLA	C3B-C4B	3.15	1.50	1.42
20	B	610	CLA	OBD-CAD	3.15	1.27	1.22
20	c	508	CLA	OBD-CAD	3.15	1.27	1.22
20	c	512	CLA	C3D-C2D	3.14	1.47	1.39
21	a	406	PHO	OBD-CAD	3.14	1.26	1.22
20	C	511	CLA	C3B-C4B	3.14	1.50	1.42
20	B	601	CLA	C3D-C2D	3.14	1.47	1.39
40	v	201	HEC	CBC-CAC	-3.14	1.37	1.51
23	a	409	SQD	C6-S	-3.14	1.65	1.77
20	d	404	CLA	CHD-C4C	3.14	1.46	1.39
20	A	402	CLA	C3B-C4B	3.14	1.50	1.42
20	b	613	CLA	CHC-C4B	3.13	1.46	1.39
20	b	608	CLA	MG-ND	3.13	2.12	2.05
20	C	513	CLA	C4D-CHA	3.13	1.49	1.38
20	C	505	CLA	OBD-CAD	3.13	1.27	1.22
20	c	509	CLA	C3D-C2D	3.12	1.47	1.39
20	C	513	CLA	C4C-C3C	3.12	1.50	1.45
20	A	404	CLA	MG-ND	-3.12	1.99	2.05
20	B	604	CLA	C3B-C4B	3.12	1.50	1.42
20	B	605	CLA	CHC-C4B	3.12	1.46	1.39
20	c	507	CLA	C4B-NB	-3.11	1.34	1.37
20	c	505	CLA	C4D-CHA	3.11	1.49	1.38
20	D	404	CLA	C3B-C4B	3.11	1.50	1.42
20	B	611	CLA	C4D-CHA	3.11	1.49	1.38
20	d	403	CLA	C1B-C2B	3.11	1.50	1.43
20	b	603	CLA	C4D-CHA	3.11	1.49	1.38
20	B	606	CLA	O2A-CGA	3.10	1.42	1.33
20	d	404	CLA	O2D-CGD	3.10	1.40	1.33
20	c	505	CLA	C3D-C2D	3.10	1.47	1.39
20	c	503	CLA	C4D-CHA	3.10	1.49	1.38
40	V	201	HEC	CMD-C2D	3.09	1.57	1.50
32	B	623	HTG	C1'-S1	-3.09	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	612	CLA	C1D-ND	-3.09	1.34	1.37
20	B	616	CLA	CHC-C4B	3.09	1.46	1.39
20	B	605	CLA	O2A-CGA	3.08	1.42	1.33
20	c	504	CLA	CHB-C1B	3.08	1.46	1.39
20	D	401	CLA	C4D-CHA	3.08	1.49	1.38
20	b	614	CLA	C1B-C2B	3.07	1.50	1.43
21	a	405	PHO	CBD-CGD	-3.07	1.48	1.52
20	C	502	CLA	C3B-C4B	3.07	1.49	1.42
20	b	606	CLA	C3D-C2D	3.07	1.47	1.39
36	D	409	LHG	O7-C7	3.07	1.43	1.34
20	b	612	CLA	CHB-C1B	3.07	1.46	1.39
20	b	614	CLA	O2A-CGA	3.07	1.42	1.33
20	C	512	CLA	C4D-CHA	3.07	1.49	1.38
20	b	609	CLA	C1B-NB	-3.06	1.34	1.37
35	c	516	DGD	O2G-C1B	3.06	1.42	1.34
20	c	503	CLA	C3D-C2D	3.06	1.47	1.39
22	a	408	BCR	C26-C25	3.06	1.39	1.34
20	c	503	CLA	C1B-NB	-3.06	1.34	1.37
20	b	604	CLA	O2D-CGD	3.06	1.40	1.33
20	B	607	CLA	C4D-CHA	3.06	1.49	1.38
20	B	616	CLA	C1B-C2B	3.05	1.50	1.43
20	c	506	CLA	OBD-CAD	3.05	1.27	1.22
32	c	521	HTG	C1'-S1	-3.05	1.77	1.81
20	B	614	CLA	O2D-CGD	3.05	1.40	1.33
40	v	201	HEC	FE-NC	3.05	2.05	1.95
20	D	404	CLA	C3D-C2D	3.04	1.47	1.39
20	c	504	CLA	C3D-C2D	3.04	1.47	1.39
20	C	506	CLA	OBD-CAD	3.04	1.27	1.22
20	c	505	CLA	C1D-ND	-3.04	1.34	1.37
37	E	104	HEM	CAB-C3B	3.03	1.55	1.47
32	b	625	HTG	C1-S1	3.03	1.85	1.80
20	D	401	CLA	CHC-C1C	3.03	1.44	1.38
20	c	511	CLA	MG-ND	3.03	2.11	2.05
20	C	511	CLA	C4C-C3C	3.03	1.50	1.45
20	c	504	CLA	C3B-C4B	3.03	1.49	1.42
20	B	613	CLA	O2A-CGA	3.03	1.42	1.33
20	A	401	CLA	C3C-C2C	3.02	1.43	1.36
20	B	606	CLA	C3B-C4B	3.02	1.49	1.42
20	b	607	CLA	CHB-C1B	3.02	1.46	1.39
36	d	408	LHG	O7-C7	3.02	1.42	1.34
20	B	602	CLA	C1D-ND	-3.02	1.34	1.37
20	b	618	CLA	C3B-C4B	3.00	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	614	CLA	CHB-C1B	3.00	1.46	1.39
20	C	503	CLA	C1B-NB	-3.00	1.34	1.37
35	h	101	DGD	O1G-C1A	3.00	1.42	1.33
28	B	634	DMS	O-S	3.00	1.70	1.50
37	E	104	HEM	CAC-C3C	3.00	1.55	1.47
20	c	513	CLA	C3D-C2D	3.00	1.47	1.39
20	b	617	CLA	C4D-CHA	3.00	1.49	1.38
20	B	606	CLA	C1B-NB	-3.00	1.34	1.37
20	B	606	CLA	C1B-C2B	3.00	1.50	1.43
20	A	404	CLA	C4D-ND	2.99	1.41	1.37
20	c	507	CLA	C3B-C4B	2.99	1.49	1.42
20	c	505	CLA	MG-NB	2.99	2.11	2.05
20	b	608	CLA	O2A-CGA	2.99	1.42	1.33
20	C	507	CLA	C3B-C4B	2.99	1.49	1.42
20	b	609	CLA	C4D-CHA	2.99	1.49	1.38
20	C	513	CLA	OBD-CAD	2.99	1.27	1.22
20	b	613	CLA	C3D-C2D	2.98	1.47	1.39
20	C	510	CLA	C4D-CHA	2.98	1.49	1.38
20	C	508	CLA	C4C-C3C	2.97	1.50	1.45
20	B	612	CLA	CHD-C4C	2.97	1.46	1.39
20	a	403	CLA	O2A-CGA	2.97	1.42	1.33
20	C	511	CLA	C4D-CHA	2.97	1.48	1.38
20	C	506	CLA	C3D-C2D	2.96	1.47	1.39
20	B	601	CLA	C4D-CHA	2.96	1.48	1.38
20	B	615	CLA	C4C-C3C	2.96	1.50	1.45
32	C	520	HTG	C1'-S1	-2.96	1.77	1.81
20	b	606	CLA	C4B-NB	-2.95	1.34	1.37
27	a	415	PL9	C7-C3	2.95	1.54	1.51
32	C	521	HTG	C1'-S1	-2.94	1.77	1.81
20	c	511	CLA	C4C-C3C	2.94	1.50	1.45
20	d	404	CLA	C3D-C2D	2.94	1.47	1.39
20	B	613	CLA	CHC-C4B	2.94	1.46	1.39
20	c	506	CLA	C4D-CHA	2.93	1.48	1.38
20	B	604	CLA	C1D-ND	-2.93	1.34	1.37
20	D	402	CLA	CHB-C1B	2.93	1.46	1.39
20	d	402	CLA	CHC-C4B	2.93	1.46	1.39
20	B	601	CLA	C3B-C4B	2.93	1.49	1.42
20	b	605	CLA	C3D-C2D	2.93	1.47	1.39
20	B	616	CLA	C4D-CHA	2.92	1.48	1.38
20	A	404	CLA	CHD-C4C	2.92	1.45	1.39
20	A	401	CLA	CHD-C1D	2.92	1.44	1.38
20	c	502	CLA	CHC-C4B	2.92	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	512	CLA	OBD-CAD	2.92	1.27	1.22
20	a	403	CLA	C4B-NB	-2.92	1.34	1.37
20	A	404	CLA	C3B-C4B	2.92	1.49	1.42
20	c	512	CLA	MG-NC	2.91	2.13	2.06
20	b	610	CLA	CHC-C4B	2.91	1.45	1.39
37	e	102	HEM	CAB-C3B	2.90	1.55	1.47
20	D	402	CLA	C1B-C2B	2.90	1.50	1.43
20	c	504	CLA	MG-NC	2.90	2.13	2.06
20	b	604	CLA	CHC-C4B	2.90	1.45	1.39
20	A	401	CLA	CHB-C1B	2.90	1.45	1.39
20	b	609	CLA	C1B-C2B	2.90	1.50	1.43
20	d	403	CLA	MG-ND	-2.89	2.00	2.05
20	c	501	CLA	C4D-CHA	2.89	1.48	1.38
32	b	624	HTG	C1-S1	-2.89	1.76	1.80
37	e	102	HEM	CAC-C3C	2.89	1.55	1.47
20	A	402	CLA	C1B-C2B	2.89	1.50	1.43
20	c	504	CLA	C4C-C3C	2.89	1.50	1.45
20	B	609	CLA	OBD-CAD	2.89	1.27	1.22
20	B	610	CLA	C1B-C2B	2.89	1.50	1.43
34	Z	101	LMT	O1'-C1'	2.88	1.45	1.40
20	C	501	CLA	OBD-CAD	2.88	1.27	1.22
20	c	506	CLA	C3B-C4B	2.88	1.49	1.42
20	D	404	CLA	OBD-CAD	2.88	1.27	1.22
20	a	404	CLA	C4D-ND	-2.88	1.33	1.37
20	B	607	CLA	C3D-C2D	2.88	1.47	1.39
20	A	401	CLA	C4D-CHA	2.88	1.48	1.38
20	b	615	CLA	CHC-C4B	2.88	1.45	1.39
20	b	603	CLA	C4D-ND	2.88	1.41	1.37
20	b	610	CLA	C3D-C2D	2.88	1.47	1.39
20	C	512	CLA	C1B-C2B	2.87	1.50	1.43
20	A	402	CLA	CHD-C1D	2.87	1.44	1.38
20	b	612	CLA	C4D-CHA	2.87	1.48	1.38
20	B	609	CLA	C1D-ND	-2.87	1.34	1.37
20	C	504	CLA	C1D-ND	-2.87	1.34	1.37
20	a	403	CLA	C4D-CHA	2.87	1.48	1.38
20	b	613	CLA	C4D-CHA	2.87	1.48	1.38
20	C	505	CLA	C3B-C4B	2.87	1.49	1.42
20	c	505	CLA	C1B-C2B	2.86	1.50	1.43
20	c	507	CLA	C3D-C2D	2.86	1.46	1.39
20	a	403	CLA	O2A-C1	-2.86	1.38	1.46
20	c	505	CLA	O2D-CGD	2.86	1.40	1.33
20	B	615	CLA	CHD-C4C	2.86	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	614	CLA	OBD-CAD	2.86	1.27	1.22
20	b	616	CLA	C3D-C2D	2.86	1.46	1.39
20	b	605	CLA	C3B-C4B	2.86	1.49	1.42
20	a	407	CLA	C3B-C4B	2.85	1.49	1.42
20	C	505	CLA	C4C-C3C	2.85	1.50	1.45
20	b	607	CLA	CHD-C4C	2.85	1.45	1.39
20	B	603	CLA	C1B-NB	-2.85	1.34	1.37
20	D	404	CLA	C4C-C3C	2.85	1.49	1.45
20	C	509	CLA	MG-NB	-2.84	2.00	2.05
20	C	507	CLA	C4C-C3C	2.84	1.49	1.45
20	c	501	CLA	C3D-C2D	2.84	1.46	1.39
20	B	609	CLA	MG-NC	2.84	2.13	2.06
20	b	614	CLA	C3D-C2D	2.84	1.46	1.39
20	c	502	CLA	C3B-C4B	2.84	1.49	1.42
20	A	402	CLA	C1C-NC	-2.84	1.33	1.37
20	C	505	CLA	C4D-CHA	2.83	1.48	1.38
20	c	506	CLA	C3D-C2D	2.83	1.46	1.39
20	C	510	CLA	C1C-NC	-2.83	1.33	1.37
20	d	403	CLA	OBD-CAD	2.83	1.27	1.22
20	B	606	CLA	C1D-ND	-2.83	1.34	1.37
20	b	616	CLA	C4C-C3C	2.82	1.49	1.45
20	A	404	CLA	C4D-CHA	2.82	1.48	1.38
20	C	505	CLA	C1B-C2B	2.82	1.49	1.43
20	B	603	CLA	C3B-C4B	2.82	1.49	1.42
20	B	612	CLA	C4D-CHA	2.82	1.48	1.38
20	C	501	CLA	C4D-CHA	2.82	1.48	1.38
20	b	609	CLA	O2A-CGA	2.81	1.41	1.33
20	c	508	CLA	C1D-ND	-2.81	1.34	1.37
20	a	407	CLA	C1B-NB	-2.81	1.34	1.37
20	b	612	CLA	C1B-C2B	2.81	1.49	1.43
20	b	611	CLA	C4D-CHA	2.80	1.48	1.38
20	C	506	CLA	C1D-ND	-2.80	1.34	1.37
20	B	605	CLA	C3B-C4B	2.80	1.49	1.42
20	c	512	CLA	C4D-CHA	2.79	1.48	1.38
20	b	617	CLA	O2A-CGA	2.79	1.41	1.33
20	a	404	CLA	C3D-C2D	2.79	1.46	1.39
20	b	606	CLA	O2A-CGA	2.79	1.41	1.33
20	a	404	CLA	C4D-CHA	2.78	1.48	1.38
20	c	513	CLA	C3B-C4B	2.78	1.49	1.42
20	c	512	CLA	C1B-NB	-2.78	1.34	1.37
20	B	610	CLA	C4B-NB	-2.78	1.34	1.37
23	A	412	SQD	C6-S	-2.78	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	402	CLA	C4D-CHA	2.78	1.48	1.38
20	b	617	CLA	MG-NC	2.78	2.12	2.06
20	C	503	CLA	OBD-CAD	2.78	1.27	1.22
20	c	504	CLA	C1B-NB	-2.78	1.34	1.37
20	C	504	CLA	C4B-NB	-2.77	1.34	1.37
20	C	503	CLA	C4D-CHA	2.77	1.48	1.38
20	B	611	CLA	OBD-CAD	2.77	1.27	1.22
20	c	505	CLA	MG-ND	2.76	2.11	2.05
20	d	404	CLA	C4D-CHA	2.76	1.48	1.38
40	v	201	HEC	CBB-CAB	-2.76	1.39	1.51
23	a	401	SQD	C6-S	-2.76	1.67	1.77
20	c	504	CLA	CHD-C4C	2.76	1.45	1.39
20	b	615	CLA	C1C-NC	-2.75	1.33	1.37
20	c	513	CLA	C4D-CHA	2.75	1.48	1.38
20	B	615	CLA	C1B-C2B	2.75	1.49	1.43
20	b	612	CLA	O2A-CGA	2.75	1.41	1.33
20	B	608	CLA	O2A-CGA	2.74	1.41	1.33
20	B	601	CLA	OBD-CAD	2.74	1.27	1.22
20	b	617	CLA	CHC-C4B	2.74	1.45	1.39
27	A	411	PL9	C7-C3	2.74	1.54	1.51
20	B	613	CLA	C1B-NB	-2.74	1.34	1.37
27	D	412	PL9	C6-C5	2.74	1.49	1.35
20	D	404	CLA	MG-ND	-2.74	2.00	2.05
20	b	609	CLA	MG-ND	2.73	2.11	2.05
20	B	613	CLA	C3B-C4B	2.73	1.49	1.42
32	B	622	HTG	O5-C1	2.73	1.46	1.42
20	A	402	CLA	C3D-C2D	2.73	1.46	1.39
20	C	510	CLA	C4C-C3C	2.73	1.49	1.45
20	c	511	CLA	C4D-CHA	2.73	1.48	1.38
20	B	610	CLA	C4D-CHA	2.73	1.48	1.38
20	D	404	CLA	C4D-CHA	2.72	1.48	1.38
20	C	510	CLA	C1D-ND	-2.72	1.34	1.37
20	B	612	CLA	C3D-C2D	2.72	1.46	1.39
20	a	404	CLA	C3B-C4B	2.72	1.49	1.42
20	B	609	CLA	C3D-C2D	2.71	1.46	1.39
20	b	607	CLA	O2A-CGA	2.71	1.41	1.33
20	B	607	CLA	C4C-C3C	2.71	1.49	1.45
20	b	608	CLA	C3B-C4B	2.70	1.49	1.42
20	b	614	CLA	C3B-C4B	2.70	1.49	1.42
20	C	509	CLA	C4D-CHA	2.70	1.48	1.38
20	c	512	CLA	C1D-ND	-2.70	1.34	1.37
20	b	607	CLA	OBD-CAD	2.70	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	401	CLA	MG-NB	2.70	2.11	2.05
21	A	403	PHO	C4B-NB	-2.69	1.33	1.38
20	c	509	CLA	C4C-C3C	2.69	1.49	1.45
20	b	615	CLA	OBD-CAD	2.69	1.27	1.22
32	c	520	HTG	C1'-S1	-2.69	1.78	1.81
20	A	402	CLA	O2D-CGD	2.69	1.39	1.33
20	C	511	CLA	C4D-ND	2.69	1.41	1.37
20	b	609	CLA	C1D-ND	-2.68	1.34	1.37
40	v	201	HEC	CMC-C2C	2.68	1.56	1.50
20	C	502	CLA	OBD-CAD	2.68	1.27	1.22
20	c	502	CLA	C4D-CHA	2.68	1.47	1.38
20	B	616	CLA	C3D-C2D	2.67	1.46	1.39
20	b	613	CLA	CHD-C4C	2.67	1.45	1.39
20	A	402	CLA	C1B-NB	-2.67	1.34	1.37
20	C	506	CLA	C4D-ND	2.67	1.41	1.37
20	c	503	CLA	C3B-C4B	2.67	1.49	1.42
20	D	402	CLA	C1D-ND	-2.67	1.34	1.37
20	b	612	CLA	C3D-C4D	-2.67	1.38	1.44
20	C	501	CLA	C1B-NB	-2.67	1.34	1.37
20	B	613	CLA	C3D-C2D	2.67	1.46	1.39
20	c	508	CLA	C3B-C4B	2.66	1.49	1.42
40	V	201	HEC	CBB-CAB	-2.66	1.39	1.51
20	B	614	CLA	C4D-CHA	2.66	1.47	1.38
20	C	511	CLA	C1D-ND	-2.66	1.34	1.37
20	B	614	CLA	CHC-C4B	2.66	1.45	1.39
20	B	604	CLA	C3D-C2D	2.66	1.46	1.39
20	c	510	CLA	C4D-CHA	2.66	1.47	1.38
40	V	201	HEC	CMC-C2C	2.66	1.56	1.50
35	c	515	DGD	O2G-C1B	2.65	1.41	1.34
21	a	406	PHO	CBD-CGD	-2.65	1.48	1.52
20	b	617	CLA	C1B-C2B	2.65	1.49	1.43
20	c	509	CLA	C4D-CHA	2.65	1.47	1.38
20	b	610	CLA	O2A-CGA	2.65	1.41	1.33
20	C	506	CLA	C4C-C3C	2.65	1.49	1.45
20	D	402	CLA	O2A-CGA	2.65	1.41	1.33
20	D	401	CLA	C1D-ND	-2.64	1.34	1.37
20	D	402	CLA	C1C-NC	-2.64	1.33	1.37
20	B	604	CLA	OBD-CAD	2.64	1.27	1.22
20	b	615	CLA	MG-NC	2.64	2.12	2.06
20	b	606	CLA	C1B-C2B	2.64	1.49	1.43
21	a	405	PHO	C3D-C4D	-2.64	1.37	1.41
40	V	201	HEC	CMA-C3A	2.64	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	405	PHO	C4B-NB	-2.63	1.33	1.38
20	c	513	CLA	C1C-C2C	2.63	1.49	1.44
20	b	617	CLA	C3B-C4B	2.63	1.48	1.42
20	D	401	CLA	CHC-C4B	2.63	1.45	1.39
20	B	602	CLA	C3D-C2D	2.63	1.46	1.39
20	D	401	CLA	C4B-NB	-2.63	1.34	1.37
20	b	603	CLA	C1C-NC	-2.63	1.33	1.37
23	A	406	SQD	C6-S	-2.63	1.67	1.77
20	c	513	CLA	C4B-NB	-2.63	1.34	1.37
20	a	407	CLA	CHC-C4B	2.62	1.45	1.39
20	B	604	CLA	C1B-C2B	2.62	1.49	1.43
20	b	617	CLA	C3D-C2D	2.62	1.46	1.39
27	a	415	PL9	C2-C3	2.62	1.41	1.34
20	b	605	CLA	C4D-CHA	2.62	1.47	1.38
36	l	102	LHG	O7-C7	2.62	1.41	1.34
27	a	415	PL9	C6-C5	2.61	1.48	1.35
20	D	402	CLA	C4C-C3C	2.61	1.49	1.45
20	b	605	CLA	C1B-C2B	2.61	1.49	1.43
20	B	602	CLA	C1B-C2B	2.61	1.49	1.43
20	B	605	CLA	C4D-CHA	2.61	1.47	1.38
20	c	509	CLA	C1D-ND	-2.61	1.34	1.37
20	c	510	CLA	MG-NC	2.60	2.12	2.06
20	b	618	CLA	C1C-C2C	2.60	1.49	1.44
27	A	411	PL9	C6-C5	2.60	1.48	1.35
20	B	609	CLA	MG-ND	2.60	2.10	2.05
20	B	601	CLA	MG-NB	-2.60	2.00	2.05
20	a	407	CLA	C4D-CHA	2.60	1.47	1.38
40	V	201	HEC	CMB-C2B	2.60	1.56	1.50
20	B	607	CLA	MG-ND	2.60	2.10	2.05
32	O	302	HTG	O5-C1	2.59	1.46	1.42
20	B	615	CLA	C4D-CHA	2.59	1.47	1.38
20	D	401	CLA	MG-NB	-2.59	2.00	2.05
20	c	503	CLA	C4C-C3C	2.59	1.49	1.45
20	b	616	CLA	C4D-CHA	2.58	1.47	1.38
20	B	616	CLA	C4C-C3C	2.58	1.49	1.45
20	b	615	CLA	C1B-NB	-2.58	1.34	1.37
20	b	604	CLA	OBD-CAD	2.58	1.26	1.22
20	A	404	CLA	C4C-C3C	2.58	1.49	1.45
20	b	606	CLA	C1B-NB	-2.58	1.34	1.37
20	B	611	CLA	C1C-C2C	2.57	1.49	1.44
20	b	612	CLA	C4B-NB	-2.57	1.34	1.37
37	e	102	HEM	CMC-C2C	2.57	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	E	104	HEM	CMD-C2D	2.57	1.56	1.50
20	B	602	CLA	MG-NC	2.56	2.12	2.06
32	b	601	HTG	C1-S1	-2.56	1.76	1.80
20	a	407	CLA	C1B-C2B	2.56	1.49	1.43
20	b	606	CLA	C1D-ND	-2.56	1.34	1.37
20	B	613	CLA	OBD-CAD	2.56	1.26	1.22
20	c	513	CLA	C4D-ND	2.55	1.41	1.37
20	B	605	CLA	C1D-ND	-2.55	1.34	1.37
20	A	401	CLA	C3D-C2D	2.55	1.46	1.39
24	c	519	LMG	O1-C1	2.55	1.44	1.40
20	C	503	CLA	C1C-C2C	2.55	1.49	1.44
20	c	504	CLA	C1C-NC	-2.54	1.34	1.37
20	A	404	CLA	C3D-C2D	2.54	1.46	1.39
20	b	605	CLA	O2A-CGA	2.54	1.40	1.33
20	b	606	CLA	C4D-CHA	2.54	1.47	1.38
34	f	102	LMT	O1'-C1'	2.54	1.44	1.40
20	b	607	CLA	C1B-NB	-2.54	1.34	1.37
20	B	616	CLA	C4D-ND	2.54	1.41	1.37
20	a	403	CLA	C3D-C2D	2.54	1.46	1.39
20	a	403	CLA	C3B-C4B	2.53	1.48	1.42
20	b	604	CLA	C3D-C2D	2.53	1.46	1.39
21	a	405	PHO	O2A-CGA	2.53	1.40	1.33
20	b	607	CLA	CHC-C4B	2.53	1.45	1.39
20	B	612	CLA	C3B-C4B	2.52	1.48	1.42
34	z	102	LMT	O1'-C1'	2.52	1.44	1.40
20	a	403	CLA	CHC-C4B	2.52	1.45	1.39
22	a	408	BCR	C40-C30	2.52	1.58	1.53
20	b	608	CLA	C4C-C3C	2.52	1.49	1.45
20	B	603	CLA	C1B-C2B	2.52	1.49	1.43
20	A	401	CLA	C4D-ND	2.52	1.41	1.37
20	c	501	CLA	C4B-NB	-2.52	1.34	1.37
20	A	401	CLA	O2A-CGA	2.52	1.40	1.33
20	B	604	CLA	C1C-NC	-2.52	1.34	1.37
20	c	509	CLA	C1B-C2B	2.52	1.49	1.43
20	C	507	CLA	C1B-C2B	2.51	1.49	1.43
20	B	609	CLA	C4D-CHA	2.51	1.47	1.38
27	d	412	PL9	C6-C5	2.51	1.48	1.35
20	C	511	CLA	C1B-C2B	2.51	1.49	1.43
20	C	509	CLA	C3B-C4B	2.51	1.48	1.42
23	b	622	SQD	C6-S	-2.51	1.68	1.77
20	B	613	CLA	C1B-C2B	2.51	1.49	1.43
20	A	401	CLA	C1D-C2D	2.50	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	510	CLA	C4B-NB	-2.50	1.34	1.37
20	c	509	CLA	C3B-C4B	2.50	1.48	1.42
20	B	605	CLA	C1B-C2B	2.50	1.49	1.43
20	d	404	CLA	C1B-NB	-2.50	1.34	1.37
20	c	509	CLA	MG-NC	2.49	2.12	2.06
20	B	607	CLA	C1D-ND	-2.49	1.34	1.37
20	A	402	CLA	CHD-C4C	2.49	1.44	1.39
20	c	507	CLA	C1C-C2C	2.49	1.49	1.44
20	c	505	CLA	C4C-C3C	2.49	1.49	1.45
20	C	510	CLA	C3D-C4D	-2.49	1.38	1.44
20	b	611	CLA	C1D-ND	-2.49	1.34	1.37
35	c	515	DGD	O5D-C1E	2.49	1.44	1.40
36	d	407	LHG	O8-C23	2.49	1.40	1.33
22	D	405	BCR	C12-C13	2.49	1.51	1.45
20	B	608	CLA	C4C-C3C	2.48	1.49	1.45
20	d	402	CLA	C4C-C3C	2.48	1.49	1.45
20	b	607	CLA	C4D-CHA	2.48	1.47	1.38
20	b	617	CLA	C4C-C3C	2.48	1.49	1.45
20	c	504	CLA	C1D-ND	-2.48	1.34	1.37
20	b	618	CLA	OBD-CAD	2.48	1.26	1.22
20	c	511	CLA	C1B-C2B	2.47	1.49	1.43
20	c	511	CLA	C1C-C2C	2.47	1.49	1.44
20	B	605	CLA	OBD-CAD	2.47	1.26	1.22
40	v	201	HEC	CAC-C3C	2.47	1.57	1.51
20	A	402	CLA	OBD-CAD	2.47	1.26	1.22
20	B	604	CLA	C4C-C3C	2.46	1.49	1.45
20	c	502	CLA	MG-NB	-2.46	2.00	2.05
20	B	602	CLA	C1C-C2C	2.46	1.49	1.44
20	A	402	CLA	CHC-C4B	2.46	1.44	1.39
20	B	615	CLA	C3D-C2D	2.46	1.45	1.39
20	B	609	CLA	C3B-C4B	2.46	1.48	1.42
20	C	503	CLA	C1B-C2B	2.46	1.49	1.43
20	A	402	CLA	C4D-CHA	2.46	1.47	1.38
20	c	506	CLA	C1C-NC	-2.46	1.34	1.37
20	c	508	CLA	C4D-CHA	2.46	1.47	1.38
23	l	101	SQD	O6-C1	2.46	1.44	1.40
20	C	509	CLA	C4C-C3C	2.45	1.49	1.45
20	c	504	CLA	C4D-CHA	2.45	1.47	1.38
20	b	612	CLA	C3D-C2D	2.45	1.45	1.39
20	C	512	CLA	C1C-C2C	2.45	1.49	1.44
27	A	411	PL9	C2-C3	2.45	1.41	1.34
20	c	510	CLA	MG-NB	2.44	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	611	CLA	C1B-C2B	2.44	1.49	1.43
21	A	403	PHO	CBD-CGD	-2.44	1.49	1.52
20	D	404	CLA	C1C-NC	-2.44	1.34	1.37
24	c	518	LMG	O1-C1	2.44	1.44	1.40
20	d	403	CLA	C3D-C2D	2.43	1.45	1.39
27	D	412	PL9	C2-C3	2.43	1.41	1.34
20	C	513	CLA	C1B-C2B	2.43	1.49	1.43
20	C	504	CLA	CHC-C4B	2.43	1.44	1.39
20	d	403	CLA	O2A-CGA	2.43	1.40	1.33
20	B	605	CLA	C3D-C2D	2.43	1.45	1.39
32	b	625	HTG	O5-C1	2.43	1.46	1.42
20	B	603	CLA	C4D-CHA	2.43	1.47	1.38
20	C	506	CLA	C1C-C2C	2.43	1.49	1.44
20	b	608	CLA	C1C-C2C	2.42	1.49	1.44
24	C	524	LMG	O1-C1	2.42	1.44	1.40
20	C	509	CLA	C4B-NB	-2.42	1.34	1.37
20	d	403	CLA	C3B-C4B	2.42	1.48	1.42
20	a	404	CLA	CHC-C4B	2.42	1.44	1.39
40	v	201	HEC	CMB-C2B	2.41	1.55	1.50
20	b	608	CLA	OBD-CAD	2.41	1.26	1.22
20	d	403	CLA	O2D-CGD	2.41	1.39	1.33
20	B	614	CLA	C3B-C4B	2.41	1.48	1.42
20	A	402	CLA	C3D-C4D	-2.41	1.38	1.44
20	b	605	CLA	CHC-C4B	2.41	1.44	1.39
35	d	416	DGD	O3G-C1D	2.41	1.44	1.40
20	d	403	CLA	C1B-NB	-2.41	1.34	1.37
20	B	606	CLA	C4D-CHA	2.40	1.46	1.38
20	c	512	CLA	C1B-C2B	2.40	1.48	1.43
20	D	404	CLA	C1B-C2B	2.40	1.48	1.43
20	d	403	CLA	CHB-C1B	2.40	1.44	1.39
20	d	403	CLA	CHC-C4B	2.40	1.44	1.39
20	c	502	CLA	C3D-C4D	-2.40	1.38	1.44
20	B	616	CLA	C3B-C4B	2.40	1.48	1.42
32	B	621	HTG	C1-C2	2.39	1.57	1.53
40	v	201	HEC	CMD-C2D	2.39	1.55	1.50
20	C	511	CLA	C1C-NC	-2.39	1.34	1.37
20	c	501	CLA	C4C-C3C	2.39	1.49	1.45
20	d	402	CLA	MG-NC	2.39	2.11	2.06
20	d	403	CLA	MG-NC	-2.38	2.00	2.06
34	E	101	LMT	O1'-C1'	2.38	1.44	1.40
37	e	102	HEM	CMA-C3A	2.38	1.55	1.50
20	c	510	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	509	CLA	C1B-C2B	2.38	1.48	1.43
32	C	522	HTG	C1-S1	-2.38	1.77	1.80
20	b	607	CLA	C1B-C2B	2.37	1.48	1.43
23	f	101	SQD	C6-S	-2.37	1.68	1.77
20	d	404	CLA	C1C-C2C	2.37	1.49	1.44
20	c	510	CLA	C3D-C2D	2.37	1.45	1.39
20	C	508	CLA	C4D-CHA	2.37	1.46	1.38
20	b	614	CLA	C4D-CHA	2.37	1.46	1.38
20	D	402	CLA	C1B-NB	-2.37	1.34	1.37
20	C	505	CLA	C4B-NB	-2.37	1.34	1.37
37	E	104	HEM	CMB-C2B	2.37	1.55	1.50
20	B	608	CLA	OBD-CAD	2.37	1.26	1.22
20	B	605	CLA	C4C-C3C	2.36	1.49	1.45
20	B	612	CLA	O2A-CGA	2.36	1.40	1.33
20	B	614	CLA	C3D-C2D	2.36	1.45	1.39
20	A	401	CLA	C1B-C2B	2.36	1.48	1.43
20	b	615	CLA	C1D-ND	-2.36	1.34	1.37
20	d	404	CLA	C3D-C4D	-2.36	1.38	1.44
20	c	510	CLA	C3B-C4B	2.36	1.48	1.42
20	c	504	CLA	MG-NB	2.36	2.10	2.05
37	E	104	HEM	CMC-C2C	2.36	1.55	1.50
20	c	506	CLA	C1B-C2B	2.35	1.48	1.43
20	b	605	CLA	C4B-NB	-2.35	1.34	1.37
20	A	404	CLA	C3D-C4D	-2.35	1.38	1.44
20	B	606	CLA	C3D-C2D	2.35	1.45	1.39
20	b	608	CLA	C3B-C2B	2.35	1.49	1.41
20	c	512	CLA	C1C-C2C	2.35	1.49	1.44
20	b	615	CLA	C3D-C2D	2.35	1.45	1.39
20	c	509	CLA	C1C-NC	-2.35	1.34	1.37
20	B	607	CLA	C3B-C4B	2.34	1.48	1.42
20	b	611	CLA	C4C-C3C	2.34	1.49	1.45
20	c	502	CLA	C4D-ND	2.34	1.40	1.37
20	B	601	CLA	MG-ND	2.34	2.10	2.05
20	b	606	CLA	C4C-C3C	2.34	1.49	1.45
20	c	502	CLA	C4C-C3C	2.34	1.49	1.45
20	a	404	CLA	C1D-ND	-2.34	1.34	1.37
20	B	604	CLA	C4D-CHA	2.33	1.46	1.38
20	B	614	CLA	OBD-CAD	2.33	1.26	1.22
27	d	412	PL9	C43-C44	2.33	1.38	1.33
20	B	604	CLA	CHC-C4B	2.33	1.44	1.39
23	F	101	SQD	C6-S	-2.32	1.68	1.77
20	c	505	CLA	C1D-C2D	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	501	CLA	C1B-C2B	2.31	1.48	1.43
20	C	502	CLA	C4B-NB	-2.31	1.34	1.37
20	b	611	CLA	C4B-NB	-2.31	1.34	1.37
20	C	507	CLA	C3B-C2B	2.31	1.49	1.41
20	b	612	CLA	OBD-CAD	2.31	1.26	1.22
20	b	610	CLA	MG-NC	2.31	2.11	2.06
20	C	504	CLA	C1B-NB	-2.30	1.35	1.37
20	b	616	CLA	MG-NC	2.30	2.11	2.06
20	c	507	CLA	C1D-ND	-2.30	1.35	1.37
20	b	606	CLA	MG-NB	2.30	2.10	2.05
21	a	405	PHO	C1B-NB	-2.30	1.34	1.38
20	B	605	CLA	C4B-NB	-2.30	1.35	1.37
35	c	517	DGD	O5D-C1E	2.29	1.44	1.40
20	B	606	CLA	CHC-C4B	2.29	1.44	1.39
20	b	607	CLA	C3D-C2D	2.29	1.45	1.39
20	C	506	CLA	C4B-NB	-2.29	1.35	1.37
20	C	513	CLA	C1D-ND	-2.29	1.35	1.37
20	b	618	CLA	MG-ND	2.29	2.10	2.05
36	d	407	LHG	O7-C7	2.29	1.40	1.34
20	b	611	CLA	C1C-C2C	2.28	1.49	1.44
20	b	604	CLA	C4D-CHA	2.28	1.46	1.38
20	b	609	CLA	OBD-CAD	2.28	1.26	1.22
20	C	506	CLA	C1B-NB	-2.28	1.35	1.37
36	L	101	LHG	O7-C5	-2.28	1.40	1.46
20	C	502	CLA	C1B-C2B	2.28	1.48	1.43
20	B	614	CLA	C1C-C2C	2.27	1.49	1.44
20	C	512	CLA	C1B-NB	-2.27	1.35	1.37
20	d	402	CLA	C3D-C2D	2.27	1.45	1.39
20	A	402	CLA	O2A-CGA	2.27	1.40	1.33
20	c	504	CLA	C4B-NB	-2.27	1.35	1.37
20	c	503	CLA	C1B-C2B	2.27	1.48	1.43
20	B	601	CLA	C4C-C3C	2.26	1.48	1.45
34	J	103	LMT	O1'-C1'	2.26	1.44	1.40
20	b	611	CLA	C1B-NB	-2.26	1.35	1.37
20	D	401	CLA	MG-ND	2.26	2.10	2.05
20	B	614	CLA	C1B-NB	-2.26	1.35	1.37
20	b	605	CLA	C4C-C3C	2.26	1.48	1.45
20	b	603	CLA	C4C-C3C	2.26	1.48	1.45
20	A	401	CLA	MG-NA	2.25	2.11	2.06
20	B	610	CLA	CHD-C4C	2.25	1.44	1.39
21	A	403	PHO	C3D-C2D	2.25	1.43	1.39
20	d	402	CLA	C1B-NB	-2.25	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	d	402	CLA	C1B-C2B	2.25	1.48	1.43
35	c	517	DGD	O2G-C2G	-2.25	1.41	1.46
20	C	513	CLA	C1C-C2C	2.24	1.48	1.44
32	c	520	HTG	C1-S1	-2.24	1.77	1.80
22	D	405	BCR	C21-C22	2.24	1.38	1.35
20	D	402	CLA	MG-NB	2.24	2.10	2.05
20	C	508	CLA	MG-NC	2.24	2.11	2.06
32	B	621	HTG	O5-C1	2.23	1.45	1.42
20	d	403	CLA	C1D-ND	-2.23	1.35	1.37
22	b	621	BCR	C26-C25	2.23	1.38	1.34
20	C	508	CLA	C1C-NC	-2.23	1.34	1.37
40	V	201	HEC	C4B-NB	-2.23	1.36	1.40
20	c	501	CLA	C1C-C2C	2.23	1.48	1.44
32	b	602	HTG	C1-S1	-2.22	1.77	1.80
20	b	615	CLA	C4B-NB	-2.22	1.35	1.37
20	b	605	CLA	MG-NB	2.22	2.10	2.05
20	C	506	CLA	MG-NB	2.22	2.10	2.05
20	B	611	CLA	C1C-NC	-2.21	1.34	1.37
20	D	401	CLA	C3D-C2D	2.21	1.45	1.39
20	b	613	CLA	C1B-NB	-2.21	1.35	1.37
22	A	405	BCR	C19-C18	2.21	1.50	1.45
20	B	607	CLA	C1B-C2B	2.21	1.48	1.43
20	C	506	CLA	C1B-C2B	2.21	1.48	1.43
40	v	201	HEC	CMA-C3A	2.21	1.55	1.50
20	B	602	CLA	C1C-NC	-2.21	1.34	1.37
20	A	404	CLA	C1C-NC	-2.21	1.34	1.37
20	c	503	CLA	OBD-CAD	2.21	1.26	1.22
20	c	512	CLA	C3B-C2B	2.20	1.48	1.41
20	c	503	CLA	C3D-C4D	-2.20	1.39	1.44
20	C	507	CLA	C1C-C2C	2.20	1.48	1.44
20	C	507	CLA	C1A-CHA	2.20	1.52	1.43
20	C	511	CLA	MG-NB	-2.20	2.01	2.05
20	C	512	CLA	C4D-ND	2.20	1.40	1.37
20	B	608	CLA	C4D-CHA	2.20	1.46	1.38
20	b	615	CLA	C4D-CHA	2.19	1.46	1.38
20	d	404	CLA	C4B-NB	-2.19	1.35	1.37
20	B	602	CLA	C4C-C3C	2.19	1.48	1.45
20	C	512	CLA	C3B-C2B	2.19	1.48	1.41
20	C	513	CLA	C3B-C2B	2.19	1.48	1.41
20	C	502	CLA	MG-NC	2.19	2.11	2.06
34	a	418	LMT	O5B-C1B	2.18	1.47	1.41
20	b	618	CLA	C1B-C2B	2.18	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	614	CLA	C4C-C3C	2.18	1.48	1.45
20	C	501	CLA	C1B-C2B	2.18	1.48	1.43
20	d	402	CLA	C4D-CHA	2.18	1.46	1.38
20	c	506	CLA	C1C-C2C	2.17	1.48	1.44
20	C	512	CLA	MG-ND	2.17	2.10	2.05
20	D	404	CLA	C1D-ND	-2.17	1.35	1.37
20	b	617	CLA	C3B-C2B	2.17	1.48	1.41
20	b	606	CLA	MG-NC	2.17	2.11	2.06
20	b	614	CLA	C1D-ND	-2.16	1.35	1.37
20	c	503	CLA	C1C-NC	-2.16	1.34	1.37
20	d	402	CLA	O2D-CGD	2.16	1.38	1.33
20	b	606	CLA	CHC-C4B	2.16	1.44	1.39
34	I	101	LMT	O1'-C1'	2.16	1.43	1.40
20	a	404	CLA	C3D-C4D	-2.16	1.39	1.44
20	D	404	CLA	C4B-NB	-2.15	1.35	1.37
20	b	604	CLA	C4D-ND	2.15	1.40	1.37
37	e	102	HEM	CMB-C2B	2.15	1.55	1.50
20	B	609	CLA	C3D-C4D	-2.15	1.39	1.44
20	c	504	CLA	C3D-C4D	-2.14	1.39	1.44
20	d	403	CLA	C4D-CHA	2.14	1.46	1.38
20	b	609	CLA	C1C-NC	-2.14	1.34	1.37
20	D	401	CLA	C4C-C3C	2.14	1.48	1.45
20	B	613	CLA	MG-NB	2.14	2.10	2.05
20	b	607	CLA	MG-ND	-2.14	2.01	2.05
20	C	502	CLA	CAA-C2A	2.14	1.58	1.54
20	B	615	CLA	C4B-NB	-2.14	1.35	1.37
24	j	101	LMG	O7-C8	-2.13	1.41	1.46
32	C	521	HTG	O5-C1	2.13	1.45	1.42
20	d	402	CLA	C1D-C2D	2.13	1.49	1.45
32	B	622	HTG	C1-S1	2.13	1.84	1.80
20	b	603	CLA	C1C-C2C	2.13	1.48	1.44
20	c	503	CLA	C1C-C2C	2.13	1.48	1.44
20	c	506	CLA	MG-NC	2.12	2.11	2.06
20	C	501	CLA	C4C-C3C	2.12	1.48	1.45
20	b	618	CLA	C4B-NB	-2.11	1.35	1.37
40	v	201	HEC	CAB-C3B	2.11	1.56	1.51
20	D	401	CLA	C1B-NB	-2.11	1.35	1.37
20	D	404	CLA	C4D-ND	2.11	1.40	1.37
20	B	611	CLA	C1B-C2B	2.11	1.48	1.43
20	a	403	CLA	C4C-C3C	2.10	1.48	1.45
20	C	502	CLA	C1C-C2C	2.10	1.48	1.44
20	B	607	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	K	101	BCR	C12-C13	2.09	1.50	1.45
20	d	404	CLA	C3B-C4B	2.09	1.47	1.42
40	v	201	HEC	FE-NB	2.09	2.01	1.94
22	A	405	BCR	C8-C9	2.09	1.50	1.45
20	B	614	CLA	C1-C2	2.09	1.55	1.49
22	t	101	BCR	C23-C22	2.09	1.50	1.45
20	c	504	CLA	C1B-C2B	2.09	1.48	1.43
20	C	511	CLA	C3D-C4D	-2.08	1.39	1.44
20	b	618	CLA	C3D-C4D	-2.08	1.39	1.44
34	a	418	LMT	O1'-C1'	2.08	1.43	1.40
20	b	609	CLA	C4C-C3C	2.08	1.48	1.45
20	B	604	CLA	C1B-NB	-2.07	1.35	1.37
23	a	409	SQD	O47-C45	-2.07	1.41	1.46
20	D	402	CLA	C3D-C2D	2.07	1.44	1.39
23	l	101	SQD	C6-S	-2.06	1.69	1.77
20	b	618	CLA	C1C-NC	-2.06	1.34	1.37
20	C	503	CLA	C4C-C3C	2.06	1.48	1.45
20	B	603	CLA	O2A-CGA	2.06	1.39	1.33
20	c	510	CLA	C5-C3	2.06	1.55	1.51
20	b	616	CLA	C3B-C4B	2.06	1.47	1.42
22	t	101	BCR	C20-C21	2.05	1.49	1.43
20	C	507	CLA	C4D-ND	2.05	1.40	1.37
20	b	611	CLA	C1A-CHA	2.05	1.51	1.43
20	D	404	CLA	C1C-C2C	2.05	1.48	1.44
27	D	412	PL9	C28-C29	2.05	1.37	1.33
20	c	509	CLA	C3B-C2B	2.05	1.48	1.41
20	C	501	CLA	C1D-ND	-2.05	1.35	1.37
20	c	506	CLA	C1D-ND	-2.04	1.35	1.37
22	D	405	BCR	C20-C21	2.04	1.49	1.43
22	c	514	BCR	C12-C13	2.04	1.50	1.45
20	B	613	CLA	C4C-C3C	2.04	1.48	1.45
20	c	513	CLA	MG-NC	2.04	2.11	2.06
20	C	510	CLA	C3B-C4B	2.03	1.47	1.42
20	b	604	CLA	CAB-C3B	2.03	1.53	1.47
20	B	603	CLA	MG-ND	2.03	2.09	2.05
22	B	619	BCR	C20-C21	2.03	1.49	1.43
20	d	402	CLA	C3B-C2B	2.03	1.48	1.41
20	C	505	CLA	C1C-C2C	2.03	1.48	1.44
20	b	609	CLA	C4B-NB	-2.03	1.35	1.37
20	C	508	CLA	C3B-C2B	2.02	1.48	1.41
20	c	511	CLA	C4D-ND	2.02	1.40	1.37
20	b	605	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	512	CLA	C3D-C4D	-2.02	1.39	1.44
32	B	631	HTG	C1-S1	-2.02	1.77	1.80
38	H	101	RRX	C5-C6	2.02	1.37	1.34
32	V	202	HTG	O5-C1	2.01	1.45	1.42
22	K	102	BCR	C23-C22	2.01	1.50	1.45
22	A	405	BCR	C15-C14	2.01	1.49	1.43
34	m	101	LMT	O1'-C1'	2.01	1.43	1.40
20	B	608	CLA	C3D-C4D	-2.01	1.39	1.44
20	c	512	CLA	C3D-C4D	-2.01	1.39	1.44
20	B	605	CLA	C1B-NB	-2.01	1.35	1.37
20	c	502	CLA	C1C-NC	-2.01	1.34	1.37
20	D	401	CLA	C1C-C2C	2.01	1.48	1.44
20	B	604	CLA	MG-ND	2.01	2.09	2.05
20	D	401	CLA	OBD-CAD	2.00	1.25	1.22

All (2619) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	f	101	SQD	O9-S-C6	-14.05	90.24	106.94
20	c	504	CLA	C4A-NA-C1A	12.19	112.19	106.71
20	C	511	CLA	C4A-NA-C1A	11.76	111.99	106.71
20	c	501	CLA	C4A-NA-C1A	11.42	111.84	106.71
21	A	403	PHO	C2D-C1D-ND	11.02	117.13	109.53
20	c	509	CLA	C4A-NA-C1A	10.78	111.55	106.71
23	f	101	SQD	O8-S-O9	-10.52	85.57	111.27
20	C	507	CLA	C4A-NA-C1A	10.48	111.42	106.71
20	c	503	CLA	C4A-NA-C1A	10.40	111.38	106.71
20	c	502	CLA	C4A-NA-C1A	10.20	111.29	106.71
23	f	101	SQD	O7-S-C6	10.17	119.03	106.94
21	a	405	PHO	C2D-C1D-ND	10.09	116.49	109.53
32	d	401	HTG	C1'-S1-C1	9.92	118.65	100.09
21	D	403	PHO	C2D-C1D-ND	9.74	116.25	109.53
20	B	611	CLA	C4A-NA-C1A	9.65	111.05	106.71
20	C	506	CLA	C4A-NA-C1A	9.63	111.04	106.71
23	f	101	SQD	O9-S-O7	-9.49	81.11	113.95
20	C	512	CLA	C4A-NA-C1A	9.49	110.97	106.71
21	A	403	PHO	C4D-ND-C1D	-9.48	99.19	108.83
20	c	511	CLA	C4A-NA-C1A	9.47	110.96	106.71
21	A	403	PHO	C2B-C1B-NB	9.43	116.04	109.53
20	A	404	CLA	C2D-C1D-ND	9.29	116.95	110.10
23	a	409	SQD	O6-C1-C2	9.27	122.78	108.30
21	D	403	PHO	C2B-C1B-NB	9.26	115.92	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	606	CLA	C4A-NA-C1A	9.18	110.83	106.71
21	a	406	PHO	C2D-C1D-ND	9.09	115.80	109.53
20	b	612	CLA	C2B-C1B-NB	8.98	116.25	110.23
20	A	402	CLA	C2B-C1B-NB	8.86	116.17	110.23
20	B	602	CLA	C4A-NA-C1A	8.77	110.65	106.71
20	A	404	CLA	C2B-C1B-NB	8.75	116.09	110.23
20	b	616	CLA	C4A-NA-C1A	8.71	110.62	106.71
21	a	406	PHO	C2B-C1B-NB	8.65	115.50	109.53
20	b	615	CLA	C4A-NA-C1A	8.61	110.58	106.71
20	b	603	CLA	C2B-C1B-NB	8.51	115.93	110.23
20	A	402	CLA	C4A-NA-C1A	8.41	110.49	106.71
20	A	404	CLA	C1D-ND-C4D	-8.35	100.40	106.33
20	c	504	CLA	C2B-C1B-NB	8.34	115.82	110.23
20	B	615	CLA	C4A-NA-C1A	8.32	110.45	106.71
20	B	604	CLA	C2B-C1B-NB	8.32	115.81	110.23
21	D	403	PHO	C4D-ND-C1D	-8.31	100.38	108.83
20	c	501	CLA	C2B-C1B-NB	8.27	115.78	110.23
20	c	508	CLA	C2B-C1B-NB	8.27	115.77	110.23
20	d	404	CLA	C2B-C1B-NB	8.10	115.66	110.23
20	c	501	CLA	C2D-C1D-ND	8.09	116.07	110.10
20	C	502	CLA	C4A-NA-C1A	8.09	110.34	106.71
20	C	509	CLA	C2B-C1B-NB	8.03	115.61	110.23
21	a	405	PHO	C2B-C1B-NB	7.97	115.03	109.53
20	c	504	CLA	C2D-C1D-ND	7.86	115.90	110.10
20	C	509	CLA	C4A-NA-C1A	7.86	110.24	106.71
20	c	508	CLA	C4A-NA-C1A	7.86	110.24	106.71
20	B	615	CLA	C2D-C1D-ND	7.79	115.85	110.10
20	C	508	CLA	C4A-NA-C1A	7.78	110.20	106.71
23	a	409	SQD	O9-S-C6	7.70	116.09	106.94
20	B	603	CLA	C4A-NA-C1A	7.68	110.16	106.71
21	a	406	PHO	C4D-ND-C1D	-7.67	101.03	108.83
21	A	403	PHO	C1C-C2C-C3C	-7.66	102.24	108.61
20	c	512	CLA	C4A-NA-C1A	7.63	110.14	106.71
20	c	502	CLA	C2B-C1B-NB	7.62	115.34	110.23
20	B	608	CLA	C2B-C1B-NB	7.61	115.33	110.23
20	A	401	CLA	C2B-C1B-NB	7.60	115.33	110.23
20	B	606	CLA	C2D-C1D-ND	7.56	115.68	110.10
20	B	609	CLA	C2D-C1D-ND	7.56	115.68	110.10
20	B	607	CLA	C4A-NA-C1A	7.53	110.09	106.71
20	b	605	CLA	C2C-C1C-NC	7.53	117.02	109.97
20	B	606	CLA	C2B-C1B-NB	7.52	115.27	110.23
20	B	604	CLA	C2C-C1C-NC	7.51	117.00	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	615	CLA	C2B-C1B-NB	7.49	115.25	110.23
20	b	616	CLA	C2B-C1B-NB	7.48	115.25	110.23
20	D	404	CLA	C2B-C1B-NB	7.48	115.24	110.23
20	C	513	CLA	C2B-C1B-NB	7.47	115.24	110.23
20	A	402	CLA	C2D-C1D-ND	7.46	115.61	110.10
32	c	521	HTG	C1'-S1-C1	7.37	113.87	100.09
20	B	609	CLA	C2B-C1B-NB	7.36	115.17	110.23
20	d	403	CLA	C2C-C1C-NC	7.36	116.87	109.97
20	C	513	CLA	C4A-NA-C1A	7.33	110.00	106.71
20	C	508	CLA	C2D-C1D-ND	7.33	115.50	110.10
20	d	404	CLA	C2D-C1D-ND	7.32	115.50	110.10
20	B	607	CLA	C2B-C1B-NB	7.31	115.13	110.23
20	c	507	CLA	C4A-NA-C1A	7.28	109.98	106.71
20	D	401	CLA	C4A-NA-C1A	7.21	109.95	106.71
20	c	510	CLA	C2B-C1B-NB	7.21	115.07	110.23
20	B	609	CLA	CHD-C1D-ND	-7.21	117.83	124.45
20	b	617	CLA	C4A-NA-C1A	7.20	109.94	106.71
20	B	611	CLA	C2B-C1B-NB	7.17	115.04	110.23
20	C	511	CLA	C2B-C1B-NB	7.15	115.03	110.23
20	D	404	CLA	C4A-NA-C1A	7.13	109.91	106.71
20	c	502	CLA	C2D-C1D-ND	7.12	115.35	110.10
20	c	509	CLA	C2B-C1B-NB	7.10	114.99	110.23
20	B	601	CLA	C2B-C1B-NB	7.09	114.98	110.23
21	a	405	PHO	C1C-C2C-C3C	-7.08	102.72	108.61
20	b	603	CLA	C4A-NA-C1A	7.08	109.89	106.71
20	b	616	CLA	C2D-C1D-ND	7.06	115.31	110.10
20	b	614	CLA	C2C-C1C-NC	7.05	116.58	109.97
20	b	607	CLA	C2C-C1C-NC	7.05	116.57	109.97
20	D	401	CLA	C2B-C1B-NB	7.04	114.95	110.23
20	c	513	CLA	C4A-NA-C1A	7.02	109.86	106.71
20	A	404	CLA	C4A-NA-C1A	7.01	109.86	106.71
20	b	610	CLA	C2B-C1B-NB	7.00	114.93	110.23
21	A	403	PHO	C3D-C4D-ND	6.99	117.25	107.72
20	B	612	CLA	C2B-C1B-NB	6.98	114.91	110.23
20	B	616	CLA	C2D-C1D-ND	6.94	115.22	110.10
20	C	508	CLA	C2B-C1B-NB	6.91	114.86	110.23
20	b	612	CLA	C2D-C1D-ND	6.90	115.19	110.10
20	b	613	CLA	C2D-C1D-ND	6.88	115.17	110.10
32	B	631	HTG	C1'-S1-C1	6.86	112.92	100.09
20	b	618	CLA	C4A-NA-C1A	6.84	109.78	106.71
20	B	616	CLA	C2B-C1B-NB	6.84	114.81	110.23
20	c	506	CLA	C2B-C1B-NB	6.83	114.81	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	615	CLA	C4D-CHA-C1A	-6.83	112.93	121.25
20	a	404	CLA	C2C-C1C-NC	6.80	116.34	109.97
22	d	405	BCR	C24-C23-C22	-6.80	115.96	126.23
20	B	613	CLA	C4A-NA-C1A	6.78	109.75	106.71
20	b	618	CLA	C2B-C1B-NB	6.78	114.78	110.23
20	B	612	CLA	CHD-C4C-C3C	-6.77	114.89	124.84
20	C	502	CLA	C2D-C1D-ND	6.75	115.08	110.10
20	B	602	CLA	O2D-CGD-CBD	6.74	123.25	111.27
20	b	618	CLA	O2D-CGD-CBD	6.74	123.24	111.27
32	C	522	HTG	C1'-S1-C1	6.74	112.70	100.09
21	D	403	PHO	C3D-C4D-ND	6.73	116.90	107.72
20	B	612	CLA	C2D-C1D-ND	6.73	115.06	110.10
20	b	603	CLA	C2D-C1D-ND	6.72	115.06	110.10
20	B	602	CLA	CHD-C1D-ND	-6.71	118.29	124.45
20	D	404	CLA	C2D-C1D-ND	6.70	115.04	110.10
20	B	606	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
20	B	604	CLA	C2D-C1D-ND	6.64	115.00	110.10
20	C	505	CLA	C4A-NA-C1A	6.58	109.67	106.71
20	C	511	CLA	C2D-C1D-ND	6.58	114.95	110.10
20	D	401	CLA	C2C-C1C-NC	6.57	116.12	109.97
20	C	510	CLA	C2C-C1C-NC	6.55	116.11	109.97
20	C	510	CLA	C2B-C1B-NB	6.55	114.62	110.23
20	c	512	CLA	C2B-C1B-NB	6.54	114.62	110.23
20	b	613	CLA	C4A-NA-C1A	6.54	109.65	106.71
20	b	606	CLA	C2C-C1C-NC	6.53	116.09	109.97
20	B	608	CLA	C2C-C1C-NC	6.52	116.08	109.97
20	C	501	CLA	O2D-CGD-CBD	6.50	122.82	111.27
20	B	616	CLA	C4A-NA-C1A	6.49	109.62	106.71
20	B	605	CLA	C2C-C1C-NC	6.48	116.04	109.97
20	c	507	CLA	C2B-C1B-NB	6.48	114.58	110.23
20	B	609	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	b	608	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	C	504	CLA	C2C-C1C-NC	6.42	115.98	109.97
20	B	601	CLA	C2D-C1D-ND	6.41	114.83	110.10
20	b	607	CLA	C2B-C1B-NB	6.40	114.53	110.23
20	c	513	CLA	C2D-C1D-ND	6.40	114.82	110.10
20	B	610	CLA	C4A-NA-C1A	6.39	109.58	106.71
20	b	604	CLA	C2B-C1B-NB	6.39	114.52	110.23
21	a	405	PHO	C4D-ND-C1D	-6.38	102.34	108.83
20	B	615	CLA	O2D-CGD-O1D	-6.38	111.37	123.84
20	C	504	CLA	C2B-C1B-NB	6.37	114.50	110.23
20	B	613	CLA	CAC-C3C-C4C	6.35	133.04	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	613	CLA	CHD-C1D-ND	-6.34	118.62	124.45
32	C	521	HTG	C1'-S1-C1	6.26	111.80	100.09
20	a	407	CLA	C2D-C1D-ND	6.26	114.72	110.10
20	c	510	CLA	C2D-C1D-ND	6.26	114.72	110.10
20	B	601	CLA	CHC-C4B-NB	6.26	130.88	124.26
20	A	402	CLA	CAC-C3C-C4C	6.25	132.92	124.81
21	D	403	PHO	C1C-C2C-C3C	-6.25	103.42	108.61
20	C	509	CLA	C2C-C1C-NC	6.23	115.81	109.97
20	b	617	CLA	C2D-C1D-ND	6.22	114.69	110.10
20	B	614	CLA	C2C-C1C-NC	6.21	115.79	109.97
20	C	504	CLA	CHD-C1D-ND	-6.19	118.76	124.45
20	D	402	CLA	C2C-C1C-NC	6.19	115.78	109.97
20	C	503	CLA	C2B-C1B-NB	6.19	114.38	110.23
20	c	509	CLA	C2D-C1D-ND	6.19	114.66	110.10
23	f	101	SQD	O47-C7-C8	6.18	122.47	111.09
20	B	611	CLA	C2D-C1D-ND	6.18	114.66	110.10
20	c	508	CLA	C2D-C1D-ND	6.18	114.66	110.10
20	b	613	CLA	C2B-C1B-NB	6.18	114.38	110.23
20	c	513	CLA	C2B-C1B-NB	6.15	114.36	110.23
20	b	606	CLA	C2D-C1D-ND	6.15	114.64	110.10
20	b	615	CLA	C2D-C1D-ND	6.13	114.62	110.10
20	b	610	CLA	C2D-C1D-ND	6.12	114.62	110.10
20	c	506	CLA	C2D-C1D-ND	6.12	114.62	110.10
20	C	510	CLA	C4A-NA-C1A	6.12	109.46	106.71
20	c	501	CLA	C1D-ND-C4D	-6.11	102.00	106.33
32	V	202	HTG	O5-C1-C2	-6.09	102.65	110.31
23	l	101	SQD	O7-S-C6	6.09	114.17	106.94
32	B	623	HTG	C1'-S1-C1	6.09	111.47	100.09
20	c	511	CLA	C2B-C1B-NB	6.07	114.30	110.23
20	C	508	CLA	C1D-ND-C4D	-6.06	102.03	106.33
32	C	520	HTG	C1'-S1-C1	6.03	111.36	100.09
20	c	505	CLA	C4A-NA-C1A	6.02	109.41	106.71
20	B	607	CLA	CHC-C4B-NB	6.01	130.62	124.26
20	a	404	CLA	C2B-C1B-NB	6.01	114.26	110.23
20	B	607	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
20	b	603	CLA	O2D-CGD-CBD	5.99	121.91	111.27
20	B	603	CLA	C2C-C1C-NC	5.96	115.56	109.97
20	b	607	CLA	C2D-C1D-ND	5.95	114.49	110.10
20	b	605	CLA	C2B-C1B-NB	5.95	114.22	110.23
20	c	507	CLA	C2D-C1D-ND	5.92	114.47	110.10
20	a	403	CLA	C4A-NA-C1A	5.92	109.37	106.71
20	A	402	CLA	CHD-C1D-ND	-5.91	119.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	V	201	HEC	C1D-ND-C4D	5.91	111.17	105.07
20	c	504	CLA	CHD-C1D-ND	-5.90	119.03	124.45
20	B	613	CLA	C2C-C1C-NC	5.90	115.50	109.97
20	C	510	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
20	A	402	CLA	C2C-C1C-NC	5.88	115.48	109.97
20	d	403	CLA	C2D-C1D-ND	5.87	114.43	110.10
20	B	614	CLA	C2D-C1D-ND	5.86	114.42	110.10
20	c	507	CLA	C2C-C1C-NC	5.85	115.46	109.97
20	C	504	CLA	C4A-NA-C1A	5.85	109.34	106.71
21	a	406	PHO	C3D-C4D-ND	5.85	115.69	107.72
23	f	101	SQD	O8-S-C6	5.84	115.04	105.74
20	b	618	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
20	b	604	CLA	CHD-C1D-ND	-5.81	119.11	124.45
20	d	402	CLA	C2C-C1C-NC	5.81	115.41	109.97
20	c	510	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
22	b	619	BCR	C7-C8-C9	-5.78	117.50	126.23
20	B	615	CLA	C1D-ND-C4D	-5.77	102.23	106.33
20	a	407	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	b	615	CLA	C2C-C1C-NC	5.77	115.38	109.97
20	b	614	CLA	C2D-C1D-ND	5.77	114.35	110.10
20	b	616	CLA	C4D-CHA-C1A	-5.77	114.23	121.25
20	C	512	CLA	C2B-C1B-NB	5.76	114.09	110.23
20	b	604	CLA	C2D-C1D-ND	5.76	114.35	110.10
20	b	614	CLA	C4A-NA-C1A	5.76	109.30	106.71
20	c	506	CLA	CHD-C1D-ND	-5.76	119.16	124.45
20	c	501	CLA	CHD-C4C-C3C	-5.76	116.38	124.84
20	D	402	CLA	C2D-C1D-ND	5.75	114.34	110.10
20	b	605	CLA	C1C-C2C-C3C	-5.74	100.92	106.96
20	C	501	CLA	C2B-C1B-NB	5.74	114.08	110.23
20	C	507	CLA	C2B-C1B-NB	5.73	114.08	110.23
20	a	404	CLA	C1C-C2C-C3C	-5.73	100.93	106.96
20	b	610	CLA	C2C-C1C-NC	5.73	115.34	109.97
20	C	511	CLA	C2C-C1C-NC	5.71	115.33	109.97
20	C	505	CLA	C2C-C1C-NC	5.71	115.32	109.97
20	B	603	CLA	C2B-C1B-NB	5.70	114.05	110.23
20	B	604	CLA	C1C-C2C-C3C	-5.69	100.97	106.96
20	B	609	CLA	C2C-C1C-NC	5.68	115.29	109.97
20	B	616	CLA	C2C-C1C-NC	5.68	115.29	109.97
32	b	624	HTG	C1'-S1-C1	5.68	110.71	100.09
20	B	602	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
20	B	610	CLA	C2C-C1C-NC	5.67	115.28	109.97
23	A	412	SQD	O9-S-C6	5.67	113.67	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	501	CLA	C3B-C2B-C1B	-5.66	100.33	107.16
20	d	404	CLA	C2C-C1C-NC	5.65	115.26	109.97
21	A	403	PHO	O2D-CGD-CBD	5.65	118.15	111.00
20	c	512	CLA	CHD-C1D-ND	-5.62	119.29	124.45
20	B	604	CLA	CHD-C1D-ND	-5.62	119.29	124.45
20	B	603	CLA	CHC-C4B-NB	5.61	130.20	124.26
20	B	608	CLA	C2D-C1D-ND	5.61	114.24	110.10
20	C	506	CLA	C2D-C1D-ND	5.61	114.24	110.10
20	b	605	CLA	O2D-CGD-O1D	-5.58	112.93	123.84
20	C	501	CLA	CHD-C1D-ND	-5.57	119.33	124.45
20	c	513	CLA	CHD-C4C-C3C	-5.57	116.66	124.84
20	b	609	CLA	CHC-C4B-NB	5.56	130.15	124.26
20	b	608	CLA	C2D-C1D-ND	5.56	114.20	110.10
20	B	602	CLA	C2D-C1D-ND	5.55	114.19	110.10
21	A	403	PHO	CBC-CAC-C3C	-5.55	104.76	112.88
21	a	406	PHO	C1C-C2C-C3C	-5.55	104.00	108.61
20	b	614	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
20	b	609	CLA	C2C-C1C-NC	5.54	115.16	109.97
34	c	523	LMT	C1'-O5'-C5'	5.53	124.55	113.69
20	B	602	CLA	C2B-C1B-NB	5.53	113.94	110.23
21	a	406	PHO	O2D-CGD-CBD	5.52	117.99	111.00
20	C	509	CLA	C2D-C1D-ND	5.52	114.17	110.10
20	d	403	CLA	C4A-NA-C1A	5.51	109.18	106.71
20	c	507	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	a	409	SQD	C1-O5-C5	-5.51	102.88	113.69
20	b	615	CLA	CHD-C1D-ND	-5.50	119.40	124.45
20	b	611	CLA	C2C-C1C-NC	5.50	115.12	109.97
20	C	507	CLA	O2D-CGD-CBD	5.50	121.04	111.27
38	H	101	RRX	C24-C23-C22	-5.50	117.93	126.23
23	l	101	SQD	O6-C1-C2	5.48	116.86	108.30
20	b	614	CLA	CHC-C4B-NB	5.48	130.06	124.26
20	b	607	CLA	CAC-C3C-C4C	5.48	131.91	124.81
20	c	501	CLA	C2C-C1C-NC	5.47	115.10	109.97
20	B	614	CLA	C2B-C1B-NB	5.47	113.90	110.23
20	B	612	CLA	C4A-NA-C1A	5.46	109.16	106.71
20	B	611	CLA	CHD-C4C-C3C	-5.46	116.82	124.84
20	C	504	CLA	C1C-C2C-C3C	-5.46	101.22	106.96
20	c	506	CLA	CHC-C4B-NB	5.45	130.03	124.26
20	B	604	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
20	B	610	CLA	CHC-C4B-NB	5.42	129.99	124.26
20	c	506	CLA	C4A-NA-C1A	5.42	109.14	106.71
32	C	521	HTG	C1-O5-C5	5.41	122.56	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	SQD	O6-C1-C2	5.40	116.73	108.30
20	B	602	CLA	CHC-C4B-NB	5.40	129.97	124.26
20	c	503	CLA	C2D-C1D-ND	5.40	114.08	110.10
20	B	607	CLA	CHD-C1D-ND	-5.40	119.50	124.45
20	b	614	CLA	CAC-C3C-C4C	5.40	131.81	124.81
20	C	509	CLA	CHC-C4B-NB	5.39	129.96	124.26
20	C	501	CLA	C2D-C1D-ND	5.39	114.08	110.10
32	v	210	HTG	C1'-S1-C1	5.39	110.47	100.16
20	D	402	CLA	C4A-NA-C1A	5.39	109.13	106.71
20	C	503	CLA	CHC-C4B-NB	5.37	129.94	124.26
20	a	407	CLA	CHC-C4B-NB	5.36	129.94	124.26
20	c	503	CLA	CHC-C4B-NB	5.36	129.93	124.26
24	C	524	LMG	O7-C10-C11	5.36	123.04	111.50
35	D	406	DGD	O2G-C1B-C2B	5.35	123.04	111.50
32	B	622	HTG	C1'-S1-C1	5.35	110.09	100.09
20	b	608	CLA	C2C-C1C-NC	5.35	114.98	109.97
20	a	407	CLA	O2D-CGD-CBD	5.33	120.74	111.27
20	A	404	CLA	C4D-CHA-C1A	-5.33	114.76	121.25
20	b	612	CLA	O2D-CGD-CBD	5.33	120.73	111.27
20	b	613	CLA	C2C-C1C-NC	5.32	114.95	109.97
20	a	403	CLA	C2D-C1D-ND	5.31	114.02	110.10
20	c	503	CLA	C2C-C1C-NC	5.31	114.94	109.97
20	C	502	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
20	b	608	CLA	C2B-C1B-NB	5.30	113.78	110.23
20	b	611	CLA	CHC-C4B-NB	5.28	129.85	124.26
20	d	404	CLA	CHD-C1D-ND	-5.28	119.60	124.45
40	V	201	HEC	C4B-NB-C1B	5.28	110.52	105.07
20	B	607	CLA	C2D-C1D-ND	5.27	113.99	110.10
20	b	609	CLA	C2B-C1B-NB	5.26	113.76	110.23
20	c	505	CLA	C2B-C1B-NB	5.26	113.76	110.23
20	a	407	CLA	CAC-C3C-C4C	5.26	131.63	124.81
20	d	404	CLA	C1D-ND-C4D	-5.25	102.61	106.33
23	f	101	SQD	O8-S-O7	5.24	124.09	111.27
20	B	607	CLA	CMB-C2B-C1B	5.24	133.35	125.37
20	c	511	CLA	C2D-C1D-ND	5.24	113.96	110.10
34	b	627	LMT	C3B-C4B-C5B	5.23	119.58	110.24
20	c	513	CLA	CHD-C1D-ND	-5.23	119.65	124.45
20	B	609	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
20	b	615	CLA	C2B-C1B-NB	5.22	113.73	110.23
22	D	405	BCR	C24-C23-C22	-5.22	118.35	126.23
20	B	606	CLA	C2C-C1C-NC	5.21	114.85	109.97
20	C	501	CLA	O2D-CGD-O1D	-5.21	113.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	407	CLA	C2B-C1B-NB	5.20	113.72	110.23
20	c	505	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
20	C	506	CLA	O2D-CGD-CBD	5.19	120.50	111.27
23	A	412	SQD	O6-C1-C2	5.19	116.40	108.30
20	c	502	CLA	CAC-C3C-C4C	5.19	131.54	124.81
20	b	606	CLA	CHD-C4C-C3C	-5.18	117.22	124.84
20	B	613	CLA	C2D-C1D-ND	5.18	113.92	110.10
20	c	507	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
20	c	507	CLA	O2D-CGD-CBD	5.18	120.47	111.27
22	B	617	BCR	C7-C8-C9	-5.16	118.44	126.23
22	D	405	BCR	C7-C8-C9	-5.16	118.44	126.23
37	e	102	HEM	C4D-ND-C1D	5.16	110.40	105.07
20	B	611	CLA	C2C-C1C-NC	5.15	114.80	109.97
34	c	523	LMT	C1B-O5B-C5B	5.15	123.80	113.69
20	D	402	CLA	CAC-C3C-C4C	5.15	131.49	124.81
20	d	404	CLA	C4A-NA-C1A	5.15	109.02	106.71
20	C	505	CLA	CHD-C4C-C3C	-5.15	117.28	124.84
20	a	403	CLA	CHD-C4C-C3C	-5.14	117.28	124.84
20	B	610	CLA	CHD-C4C-C3C	-5.13	117.29	124.84
20	c	505	CLA	CHD-C1D-ND	-5.13	119.74	124.45
20	c	507	CLA	CHC-C4B-NB	5.13	129.69	124.26
20	b	610	CLA	CAC-C3C-C4C	5.13	131.46	124.81
20	C	501	CLA	C2C-C1C-NC	5.12	114.77	109.97
20	d	404	CLA	CHD-C4C-C3C	-5.11	117.32	124.84
20	c	512	CLA	O2D-CGD-CBD	5.11	120.35	111.27
20	B	601	CLA	C2C-C1C-NC	5.11	114.76	109.97
20	b	606	CLA	C2B-C1B-NB	5.10	113.65	110.23
20	b	604	CLA	C2C-C1C-NC	5.10	114.75	109.97
20	C	504	CLA	C2D-C1D-ND	5.09	113.85	110.10
20	d	403	CLA	C2B-C1B-NB	5.09	113.64	110.23
20	A	402	CLA	C3B-C4B-NB	5.08	115.23	110.52
20	D	401	CLA	C2D-C1D-ND	5.08	113.85	110.10
20	b	614	CLA	C4D-CHA-C1A	-5.07	115.08	121.25
20	b	618	CLA	C2D-C1D-ND	5.07	113.84	110.10
34	I	101	LMT	O1B-C4'-C3'	5.06	120.75	107.28
20	c	512	CLA	C2D-C1D-ND	5.06	113.83	110.10
20	B	614	CLA	C4D-CHA-C1A	-5.06	115.09	121.25
20	C	509	CLA	C4D-CHA-C1A	-5.06	115.10	121.25
20	c	506	CLA	CHD-C4C-C3C	-5.05	117.42	124.84
20	b	607	CLA	CHD-C1D-ND	-5.05	119.82	124.45
20	d	402	CLA	C2B-C1B-NB	5.03	113.60	110.23
20	b	607	CLA	C1C-C2C-C3C	-5.01	101.69	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	513	CLA	CHC-C4B-NB	5.01	129.56	124.26
20	C	508	CLA	C4D-CHA-C1A	-5.01	115.15	121.25
20	c	505	CLA	C2C-C1C-NC	5.01	114.67	109.97
20	D	402	CLA	C2B-C1B-NB	5.00	113.59	110.23
32	v	210	HTG	O5-C1-C2	-4.99	104.03	110.31
20	b	607	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
20	c	507	CLA	C1C-C2C-C3C	-4.98	101.72	106.96
20	C	509	CLA	C1C-C2C-C3C	-4.98	101.73	106.96
20	D	402	CLA	CHD-C4C-C3C	-4.96	117.55	124.84
20	A	404	CLA	CHD-C1D-ND	-4.95	119.91	124.45
37	E	104	HEM	C4C-NC-C1C	4.94	110.19	105.35
20	C	513	CLA	C2C-C1C-NC	4.93	114.59	109.97
32	D	417	HTG	C1'-S1-C1	4.92	109.30	100.09
20	B	604	CLA	O2D-CGD-CBD	4.92	120.01	111.27
20	B	607	CLA	O2D-CGD-O1D	-4.92	114.22	123.84
20	a	407	CLA	CHD-C4C-C3C	-4.92	117.61	124.84
20	b	613	CLA	CHC-C4B-NB	4.92	129.46	124.26
20	D	404	CLA	CHD-C1D-ND	-4.91	119.94	124.45
20	a	404	CLA	C2D-C1D-ND	4.91	113.72	110.10
20	C	512	CLA	C2D-C1D-ND	4.91	113.72	110.10
20	B	614	CLA	CHD-C4C-C3C	-4.91	117.63	124.84
20	b	607	CLA	C4D-CHA-C1A	-4.90	115.28	121.25
20	b	617	CLA	CHC-C4B-NB	4.90	129.44	124.26
20	C	510	CLA	CHD-C1D-ND	-4.89	119.96	124.45
34	a	418	LMT	C3'-C4'-C5'	-4.89	99.72	110.93
20	a	407	CLA	CHD-C1D-ND	-4.88	119.97	124.45
20	d	404	CLA	C4D-CHA-C1A	-4.88	115.31	121.25
20	c	501	CLA	O2D-CGD-CBD	4.87	119.93	111.27
20	c	502	CLA	C2C-C1C-NC	4.87	114.54	109.97
20	b	608	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
20	B	605	CLA	C4A-NA-C1A	4.86	108.89	106.71
20	b	605	CLA	CHD-C1D-ND	-4.86	119.98	124.45
20	b	615	CLA	C1-C2-C3	-4.85	117.65	126.04
20	A	401	CLA	C2D-C1D-ND	4.84	113.67	110.10
23	A	406	SQD	C1-C2-C3	-4.84	99.91	110.00
20	c	506	CLA	C2C-C1C-NC	4.84	114.51	109.97
37	E	104	HEM	C4D-ND-C1D	4.84	110.07	105.07
20	B	607	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
27	D	412	PL9	C40-C39-C41	4.83	123.39	115.27
20	d	403	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
20	b	616	CLA	CMB-C2B-C1B	4.82	132.71	125.37
20	b	610	CLA	CHD-C4C-C3C	-4.82	117.76	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	605	CLA	CHD-C4C-C3C	-4.81	117.77	124.84
20	b	615	CLA	C1C-C2C-C3C	-4.81	101.90	106.96
20	b	611	CLA	C2B-C1B-NB	4.81	113.45	110.23
20	B	616	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
20	C	509	CLA	C3B-C2B-C1B	-4.79	101.38	107.16
20	B	614	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
20	B	611	CLA	O2D-CGD-CBD	4.78	119.76	111.27
20	A	401	CLA	C1D-CHD-C4C	-4.78	115.75	126.06
20	C	506	CLA	C2B-C1B-NB	4.77	113.43	110.23
20	D	401	CLA	C3C-C4C-NC	4.77	115.92	110.57
20	c	501	CLA	C4D-CHA-C1A	-4.77	115.44	121.25
20	C	506	CLA	CHD-C4C-C3C	-4.77	117.83	124.84
20	c	510	CLA	C4D-CHA-C1A	-4.77	115.45	121.25
20	B	614	CLA	C4A-NA-C1A	4.76	108.85	106.71
40	v	201	HEC	C1D-ND-C4D	4.76	109.99	105.07
20	D	402	CLA	C1C-C2C-C3C	-4.76	101.95	106.96
20	b	612	CLA	C2C-C1C-NC	4.75	114.42	109.97
20	B	608	CLA	C1C-C2C-C3C	-4.75	101.96	106.96
20	c	504	CLA	C1D-ND-C4D	-4.75	102.96	106.33
20	C	507	CLA	CHC-C4B-NB	4.75	129.28	124.26
34	z	102	LMT	O1B-C4'-C3'	4.74	119.89	107.28
22	b	619	BCR	C24-C23-C22	-4.74	119.07	126.23
20	C	503	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
20	c	512	CLA	CHD-C4C-C3C	-4.74	117.88	124.84
20	b	617	CLA	C2C-C1C-NC	4.73	114.41	109.97
20	C	503	CLA	CHD-C1D-ND	-4.73	120.11	124.45
20	C	501	CLA	CHD-C4C-C3C	-4.72	117.90	124.84
20	B	615	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
20	b	616	CLA	CHC-C4B-NB	4.72	129.26	124.26
37	E	104	HEM	C4A-NA-C1A	4.72	109.97	105.35
20	a	404	CLA	CHC-C4B-NB	4.72	129.25	124.26
20	c	513	CLA	CHC-C4B-NB	4.72	129.25	124.26
20	b	612	CLA	CHB-C1B-NB	-4.72	119.26	124.26
20	c	511	CLA	CHC-C4B-NB	4.72	129.25	124.26
20	b	617	CLA	C2B-C1B-NB	4.72	113.39	110.23
20	C	506	CLA	CHD-C1D-ND	-4.71	120.13	124.45
20	b	610	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
36	D	407	LHG	O8-C23-O10	-4.71	111.72	123.59
20	b	613	CLA	CHD-C4C-C3C	-4.70	117.93	124.84
20	a	404	CLA	O2D-CGD-CBD	4.70	119.62	111.27
20	C	507	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
20	C	503	CLA	C2C-C1C-NC	4.70	114.38	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	514	BCR	C24-C23-C22	-4.69	119.14	126.23
20	B	604	CLA	C4A-NA-C1A	4.69	108.81	106.71
20	c	509	CLA	CHC-C4B-NB	4.69	129.22	124.26
20	c	503	CLA	CHD-C4C-C3C	-4.69	117.95	124.84
20	c	509	CLA	CHD-C1D-ND	-4.69	120.15	124.45
37	E	104	HEM	CBD-CAD-C3D	-4.69	99.61	112.63
20	b	615	CLA	CHD-C4C-C3C	-4.68	117.96	124.84
20	C	509	CLA	CMB-C2B-C1B	4.68	132.49	125.37
20	c	502	CLA	CHC-C4B-NB	4.67	129.21	124.26
20	c	508	CLA	C2C-C1C-NC	4.67	114.35	109.97
20	c	503	CLA	CHD-C1D-ND	-4.67	120.16	124.45
20	b	612	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
20	A	402	CLA	O2D-CGD-CBD	4.66	119.55	111.27
20	c	501	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
20	c	501	CLA	CHD-C1D-ND	-4.65	120.18	124.45
20	b	616	CLA	C1D-ND-C4D	-4.65	103.03	106.33
23	A	406	SQD	O47-C7-C8	4.63	121.49	111.50
21	a	406	PHO	CMA-C3A-C4A	-4.63	104.24	114.38
20	c	501	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
20	C	511	CLA	CHC-C4B-NB	4.60	129.13	124.26
20	D	404	CLA	C3B-C2B-C1B	-4.60	101.60	107.16
20	B	606	CLA	C4D-CHA-C1A	-4.59	115.66	121.25
20	d	403	CLA	CHC-C4B-NB	4.59	129.11	124.26
20	c	511	CLA	CHD-C4C-C3C	-4.58	118.11	124.84
20	c	513	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
20	B	613	CLA	CHC-C4B-NB	4.58	129.10	124.26
20	c	504	CLA	C2C-C1C-NC	4.58	114.26	109.97
20	c	508	CLA	C4D-CHA-C1A	-4.57	115.68	121.25
20	b	617	CLA	CHD-C4C-C3C	-4.57	118.12	124.84
20	c	512	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
20	C	513	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
20	C	513	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
20	A	402	CLA	C1D-ND-C4D	-4.57	103.09	106.33
20	C	508	CLA	C2C-C1C-NC	4.56	114.24	109.97
20	A	402	CLA	CMD-C2D-C1D	4.56	132.74	124.71
23	a	409	SQD	C1-C2-C3	-4.55	100.52	110.00
20	b	608	CLA	O2D-CGD-CBD	4.55	119.35	111.27
20	B	608	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
20	c	503	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
20	B	604	CLA	C3B-C4B-NB	4.55	114.73	110.52
20	c	511	CLA	C2C-C1C-NC	4.55	114.23	109.97
36	D	407	LHG	O8-C23-C24	4.54	126.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	512	CLA	O2D-CGD-CBD	4.54	119.33	111.27
20	C	504	CLA	CHD-C4C-C3C	-4.54	118.17	124.84
20	A	404	CLA	C4-C3-C5	4.54	122.90	115.27
20	D	401	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
20	a	404	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
20	b	603	CLA	C3B-C2B-C1B	-4.53	101.70	107.16
22	b	621	BCR	C24-C23-C22	-4.52	119.40	126.23
20	c	511	CLA	O2D-CGD-CBD	4.52	119.30	111.27
20	b	608	CLA	CHD-C1D-ND	-4.52	120.30	124.45
20	a	403	CLA	C1D-CHD-C4C	-4.52	116.31	126.06
20	d	403	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
20	B	602	CLA	CHD-C4C-NC	4.51	131.31	124.20
20	c	509	CLA	CHD-C4C-C3C	-4.51	118.21	124.84
20	D	402	CLA	CHD-C1D-ND	-4.51	120.31	124.45
20	a	404	CLA	CAC-C3C-C4C	4.51	130.66	124.81
22	B	619	BCR	C38-C26-C25	-4.50	119.48	124.53
20	c	503	CLA	C2B-C1B-NB	4.49	113.24	110.23
24	c	518	LMG	O7-C10-C11	4.49	121.18	111.50
20	b	609	CLA	C4-C3-C5	4.48	122.81	115.27
20	B	601	CLA	CAC-C3C-C4C	4.48	130.62	124.81
20	B	613	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
20	b	603	CLA	CHD-C4C-C3C	-4.48	118.26	124.84
20	a	403	CLA	CHD-C4C-NC	4.48	131.26	124.20
20	b	603	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
20	C	503	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
20	b	605	CLA	CHC-C4B-NB	4.47	128.99	124.26
20	C	510	CLA	O2D-CGD-CBD	4.47	119.21	111.27
20	c	510	CLA	CHD-C1D-ND	-4.46	120.35	124.45
20	b	614	CLA	C3C-C4C-NC	4.46	115.57	110.57
20	b	606	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
20	C	510	CLA	CHD-C4C-NC	4.45	131.21	124.20
20	b	616	CLA	C1-C2-C3	-4.44	118.36	126.04
20	C	505	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
20	b	610	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
20	D	404	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
20	c	504	CLA	C4D-CHA-C1A	-4.43	115.86	121.25
20	B	605	CLA	CHC-C4B-NB	4.43	128.94	124.26
20	B	613	CLA	C4D-CHA-C1A	-4.42	115.86	121.25
20	c	511	CLA	C1C-C2C-C3C	-4.42	102.31	106.96
32	b	602	HTG	C1'-S1-C1	4.42	108.35	100.09
20	c	504	CLA	CHD-C4C-C3C	-4.41	118.35	124.84
35	d	416	DGD	O2G-C1B-C2B	4.41	121.02	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	601	HTG	C1'-S1-C1	4.41	108.35	100.09
20	d	404	CLA	CMB-C2B-C1B	4.41	132.09	125.37
20	c	513	CLA	C2C-C1C-NC	4.41	114.11	109.97
20	d	404	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
20	b	613	CLA	C4D-CHA-C1A	-4.41	115.88	121.25
20	A	402	CLA	CHD-C4C-C3C	-4.41	118.36	124.84
20	C	503	CLA	CHD-C4C-C3C	-4.40	118.37	124.84
20	B	614	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
27	A	411	PL9	C53-C6-C1	4.40	123.98	114.99
20	d	404	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
20	B	616	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
20	b	609	CLA	CHD-C4C-C3C	-4.39	118.39	124.84
20	c	502	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
20	C	501	CLA	C4A-NA-C1A	4.38	108.68	106.71
20	B	607	CLA	O2D-CGD-CBD	4.38	119.05	111.27
20	A	404	CLA	CHB-C1B-NB	-4.38	119.62	124.26
20	B	610	CLA	C2D-C1D-ND	4.37	113.33	110.10
20	C	502	CLA	C2C-C1C-NC	4.37	114.07	109.97
20	C	507	CLA	C2C-C1C-NC	4.37	114.07	109.97
20	B	602	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
23	A	412	SQD	C1-O5-C5	-4.37	105.10	113.69
20	b	615	CLA	CMD-C2D-C1D	4.37	132.42	124.71
20	d	402	CLA	C4-C3-C5	4.37	122.62	115.27
20	C	502	CLA	C4D-CHA-C1A	-4.36	115.94	121.25
20	c	510	CLA	C1C-C2C-C3C	-4.36	102.38	106.96
20	B	608	CLA	CHD-C4C-C3C	-4.36	118.44	124.84
20	b	612	CLA	C4A-NA-C1A	4.36	108.66	106.71
20	a	403	CLA	CAC-C3C-C4C	4.35	130.46	124.81
20	C	511	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	b	622	SQD	O47-C7-C8	4.34	120.86	111.50
20	b	616	CLA	O2D-CGD-CBD	4.34	118.98	111.27
22	B	617	BCR	C15-C14-C13	-4.34	121.12	127.31
20	B	606	CLA	C3B-C2B-C1B	-4.34	101.93	107.16
20	C	508	CLA	CAC-C3C-C4C	4.33	130.43	124.81
20	b	606	CLA	O2D-CGD-CBD	4.33	118.96	111.27
20	B	603	CLA	CHD-C1D-ND	-4.33	120.48	124.45
32	c	520	HTG	C1'-S1-C1	4.33	108.19	100.09
20	a	404	CLA	CMD-C2D-C1D	4.33	132.34	124.71
20	B	612	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
20	A	401	CLA	CAC-C3C-C4C	4.32	130.41	124.81
20	b	617	CLA	CAC-C3C-C4C	4.32	130.41	124.81
20	b	608	CLA	CHC-C4B-NB	4.32	128.83	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	512	CLA	C3B-C2B-C1B	-4.31	101.95	107.16
20	C	503	CLA	O2D-CGD-CBD	4.31	118.93	111.27
20	D	401	CLA	CHD-C4C-C3C	-4.31	118.50	124.84
22	K	101	BCR	C33-C5-C6	-4.31	119.69	124.53
21	a	405	PHO	C3D-C4D-ND	4.31	113.59	107.72
20	d	402	CLA	C4A-NA-C1A	4.31	108.64	106.71
20	c	507	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
20	b	604	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
20	C	505	CLA	CHC-C4B-NB	4.30	128.81	124.26
20	B	603	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
20	C	503	CLA	C4A-NA-C1A	4.30	108.64	106.71
20	B	601	CLA	CHD-C4C-C3C	-4.30	118.52	124.84
20	C	505	CLA	C2B-C1B-NB	4.29	113.11	110.23
20	A	404	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
20	C	501	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
20	B	601	CLA	CHD-C1D-ND	-4.28	120.52	124.45
20	C	504	CLA	O2D-CGD-CBD	4.28	118.87	111.27
20	c	509	CLA	C2C-C1C-NC	4.28	113.98	109.97
20	c	506	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
20	b	615	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
24	B	620	LMG	O7-C10-C11	4.27	120.70	111.50
20	A	402	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
20	b	616	CLA	C2C-C1C-NC	4.27	113.97	109.97
22	t	101	BCR	C29-C28-C27	-4.26	101.86	111.38
23	A	412	SQD	O47-C7-C8	4.26	120.68	111.50
20	c	510	CLA	C2C-C1C-NC	4.26	113.96	109.97
20	d	402	CLA	C2D-C1D-ND	4.26	113.24	110.10
20	B	612	CLA	CHD-C4C-NC	4.25	130.91	124.20
32	V	202	HTG	C1-C2-C3	-4.25	102.19	110.59
21	a	406	PHO	C1-C2-C3	-4.25	118.69	126.04
32	c	521	HTG	C1-O5-C5	4.25	120.41	112.58
20	B	605	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
20	D	404	CLA	C2C-C1C-NC	4.24	113.95	109.97
20	b	613	CLA	O2D-CGD-CBD	4.24	118.80	111.27
20	C	506	CLA	CHA-C4D-ND	4.23	141.36	132.50
20	b	607	CLA	CMC-C2C-C1C	4.23	131.48	125.04
20	c	512	CLA	C2C-C1C-NC	4.23	113.94	109.97
20	C	513	CLA	C2D-C1D-ND	4.23	113.22	110.10
32	V	202	HTG	C1-O5-C5	-4.23	104.78	112.58
20	D	401	CLA	C4D-CHA-C1A	-4.23	116.11	121.25
20	b	609	CLA	CHD-C1D-ND	-4.22	120.58	124.45
20	b	617	CLA	CHD-C1D-ND	-4.22	120.58	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	612	CLA	C2C-C1C-NC	4.22	113.92	109.97
20	A	401	CLA	C4-C3-C5	4.21	122.36	115.27
34	z	102	LMT	C1B-O1B-C4'	4.21	128.38	117.96
20	C	507	CLA	CHD-C1D-ND	-4.21	120.59	124.45
20	c	512	CLA	C1-C2-C3	-4.21	118.77	126.04
20	c	508	CLA	CHD-C4C-C3C	-4.21	118.66	124.84
20	b	612	CLA	CHD-C4C-C3C	-4.20	118.66	124.84
20	A	404	CLA	C2C-C1C-NC	4.20	113.91	109.97
20	C	506	CLA	C2C-C1C-NC	4.20	113.91	109.97
21	D	403	PHO	O2D-CGD-CBD	4.20	116.31	111.00
20	C	509	CLA	O2D-CGD-CBD	4.20	118.72	111.27
20	c	508	CLA	C3B-C2B-C1B	-4.19	102.10	107.16
20	c	505	CLA	CHC-C4B-NB	4.19	128.69	124.26
20	C	501	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
20	D	401	CLA	CMC-C2C-C1C	4.19	131.42	125.04
20	b	608	CLA	C1C-C2C-C3C	-4.18	102.56	106.96
20	B	605	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
35	C	516	DGD	O3G-C3G-C2G	-4.18	100.82	110.90
20	B	605	CLA	C2D-C1D-ND	4.18	113.18	110.10
20	C	512	CLA	CHD-C4C-C3C	-4.18	118.70	124.84
37	e	102	HEM	CBA-CAA-C2A	-4.17	101.04	112.63
20	C	512	CLA	C4D-CHA-C1A	-4.17	116.17	121.25
20	B	615	CLA	O2D-CGD-CBD	4.17	118.68	111.27
20	c	508	CLA	CHD-C1D-ND	-4.17	120.62	124.45
20	c	504	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
34	b	627	LMT	O5'-C5'-C4'	4.16	118.53	109.75
20	c	503	CLA	C3D-C2D-C1D	-4.15	100.16	105.83
20	B	606	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
22	K	102	BCR	C7-C8-C9	-4.15	119.96	126.23
20	B	614	CLA	CMD-C2D-C1D	4.15	132.03	124.71
20	B	616	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
20	b	617	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
20	B	609	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
20	b	617	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
20	C	510	CLA	CHC-C4B-NB	4.14	128.64	124.26
20	C	512	CLA	C1-O2A-CGA	4.14	127.31	116.44
20	c	513	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
20	b	604	CLA	CHC-C4B-NB	4.14	128.64	124.26
35	H	102	DGD	O1G-C1A-O1A	-4.14	113.15	123.59
22	d	405	BCR	C11-C10-C9	-4.14	121.41	127.31
20	b	606	CLA	C3C-C4C-NC	4.14	115.21	110.57
23	b	622	SQD	O7-S-C6	4.13	111.85	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	611	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
20	D	402	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
20	b	603	CLA	C4D-CHA-C1A	-4.13	116.22	121.25
20	C	506	CLA	CHC-C4B-NB	4.12	128.62	124.26
20	A	402	CLA	C1C-C2C-C3C	-4.12	102.63	106.96
20	b	612	CLA	C3D-C2D-C1D	-4.12	100.21	105.83
20	C	507	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
20	B	606	CLA	CAC-C3C-C4C	4.11	130.15	124.81
37	E	104	HEM	CHC-C4B-NB	4.11	128.88	124.42
20	B	602	CLA	O2A-CGA-CBA	4.11	124.81	111.91
20	B	615	CLA	CHC-C4B-NB	4.10	128.60	124.26
22	B	619	BCR	C24-C23-C22	-4.10	120.03	126.23
20	b	611	CLA	CAC-C3C-C4C	4.10	130.13	124.81
20	B	610	CLA	CAC-C3C-C4C	4.10	130.13	124.81
23	a	401	SQD	O47-C7-C8	4.10	120.34	111.50
20	c	506	CLA	C3B-C2B-C1B	-4.10	102.21	107.16
20	c	502	CLA	O2D-CGD-CBD	4.10	118.55	111.27
20	B	607	CLA	CMD-C2D-C1D	4.10	131.94	124.71
24	b	623	LMG	O7-C10-C11	4.10	120.33	111.50
23	F	101	SQD	O9-S-C6	4.10	111.81	106.94
20	b	618	CLA	CHD-C1D-ND	-4.09	120.69	124.45
20	C	505	CLA	CHD-C1D-ND	-4.09	120.69	124.45
35	C	516	DGD	O2G-C1B-C2B	4.09	120.31	111.50
23	F	101	SQD	O6-C1-C2	4.08	114.68	108.30
20	B	611	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
20	c	506	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
20	b	603	CLA	C2C-C1C-NC	4.08	113.80	109.97
20	A	402	CLA	CHB-C1B-NB	-4.08	119.94	124.26
20	B	616	CLA	C1D-CHD-C4C	-4.07	117.28	126.06
20	B	610	CLA	CHA-C4D-ND	4.06	141.00	132.50
20	b	604	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
20	c	512	CLA	CHC-C4B-NB	4.06	128.55	124.26
20	b	609	CLA	C4D-CHA-C1A	-4.05	116.31	121.25
20	B	610	CLA	C4D-CHA-C1A	-4.05	116.32	121.25
23	A	406	SQD	O9-S-C6	4.05	111.75	106.94
20	B	608	CLA	O2D-CGD-O1D	-4.05	115.92	123.84
20	b	614	CLA	C1C-C2C-C3C	-4.04	102.70	106.96
20	a	404	CLA	CHD-C4C-C3C	-4.04	118.90	124.84
20	A	402	CLA	C4D-CHA-C1A	-4.04	116.33	121.25
20	c	505	CLA	C2D-C1D-ND	4.04	113.08	110.10
20	a	403	CLA	C2C-C1C-NC	4.04	113.76	109.97
20	A	401	CLA	C3B-C4B-NB	4.04	114.26	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	510	CLA	C2D-C1D-ND	4.04	113.08	110.10
20	C	508	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
20	c	511	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
34	b	627	LMT	C1'-O5'-C5'	4.04	121.61	113.69
20	b	607	CLA	C4-C3-C5	4.04	122.06	115.27
20	B	603	CLA	C2D-C1D-ND	4.03	113.08	110.10
34	a	418	LMT	O5B-C5B-C6B	4.03	116.46	106.44
20	A	402	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
20	d	403	CLA	C4D-CHA-C1A	-4.03	116.34	121.25
20	A	404	CLA	CMB-C2B-C1B	4.03	131.50	125.37
20	c	504	CLA	C3B-C4B-NB	4.03	114.25	110.52
20	B	613	CLA	C2B-C1B-NB	4.02	112.93	110.23
20	b	608	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
20	C	507	CLA	CHD-C4C-C3C	-4.02	118.94	124.84
20	b	618	CLA	C4-C3-C5	4.01	122.02	115.27
20	B	606	CLA	CHC-C4B-NB	4.01	128.51	124.26
20	B	606	CLA	CHD-C4C-NC	4.01	130.52	124.20
20	C	503	CLA	CHA-C4D-ND	4.00	140.87	132.50
20	c	501	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
20	b	605	CLA	O2D-CGD-CBD	4.00	118.37	111.27
37	e	102	HEM	C4C-NC-C1C	3.99	109.26	105.35
20	D	402	CLA	O2D-CGD-CBD	3.99	118.36	111.27
20	d	403	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
20	b	609	CLA	CAC-C3C-C4C	3.99	129.99	124.81
20	d	404	CLA	CHD-C4C-NC	3.99	130.49	124.20
20	B	616	CLA	CHD-C4C-C3C	-3.99	118.98	124.84
20	B	609	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
20	C	506	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
20	b	616	CLA	CHB-C4A-NA	3.98	130.02	124.51
20	B	615	CLA	C2C-C1C-NC	3.98	113.70	109.97
20	c	509	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
23	a	401	SQD	C1-O5-C5	-3.98	105.89	113.69
20	B	610	CLA	C3C-C4C-NC	3.97	115.03	110.57
20	b	604	CLA	C1-C2-C3	-3.97	119.17	126.04
20	c	501	CLA	CHC-C4B-NB	3.97	128.46	124.26
20	C	512	CLA	C2C-C1C-NC	3.97	113.69	109.97
20	B	601	CLA	C3B-C2B-C1B	-3.97	102.38	107.16
20	b	616	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
20	c	504	CLA	CMD-C2D-C1D	3.96	131.70	124.71
20	A	402	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
20	A	401	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
20	c	507	CLA	CMB-C2B-C1B	3.96	131.39	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	513	CLA	CHD-C4C-C3C	-3.96	119.03	124.84
20	b	617	CLA	C3D-C2D-C1D	-3.95	100.44	105.83
20	b	607	CLA	C3C-C4C-NC	3.95	115.00	110.57
20	C	509	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
24	b	623	LMG	C9-C8-C7	-3.95	102.45	111.79
20	b	606	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
20	c	504	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
20	D	401	CLA	CHC-C4B-NB	3.94	128.43	124.26
20	C	504	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
20	A	404	CLA	CHD-C4C-C3C	-3.93	119.07	124.84
20	b	610	CLA	O2A-CGA-O1A	-3.93	113.69	123.59
32	B	621	HTG	C1'-S1-C1	3.92	107.43	100.09
34	c	523	LMT	O5B-C5B-C4B	3.92	116.81	109.69
20	C	508	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
20	B	612	CLA	C3D-C2D-C1D	-3.92	100.49	105.83
20	D	404	CLA	CHC-C4B-NB	3.92	128.40	124.26
20	b	604	CLA	CHA-C4D-ND	3.91	140.69	132.50
20	C	511	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
20	C	513	CLA	O2A-CGA-CBA	3.91	124.18	111.91
22	D	405	BCR	C29-C30-C25	3.91	116.50	110.48
20	C	510	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
20	C	509	CLA	CHD-C1D-ND	-3.91	120.86	124.45
27	A	411	PL9	C20-C19-C21	3.91	121.84	115.27
20	b	607	CLA	O2D-CGD-CBD	3.91	118.21	111.27
34	b	628	LMT	O5'-C5'-C4'	3.91	117.99	109.75
20	B	611	CLA	CMD-C2D-C1D	3.90	131.59	124.71
20	b	618	CLA	C2C-C1C-NC	3.90	113.63	109.97
20	b	615	CLA	CHC-C4B-NB	3.90	128.39	124.26
20	B	607	CLA	CHD-C4C-NC	3.89	130.34	124.20
20	c	509	CLA	C4D-CHA-C1A	-3.89	116.52	121.25
20	b	616	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
36	D	409	LHG	O4-P-O5	3.89	131.46	112.24
20	D	404	CLA	C4D-CHA-C1A	-3.88	116.52	121.25
20	c	505	CLA	C3B-C2B-C1B	-3.88	102.47	107.16
20	b	604	CLA	C3D-C2D-C1D	-3.88	100.53	105.83
20	B	616	CLA	CHA-C4D-ND	3.88	140.61	132.50
23	a	401	SQD	O6-C1-C2	3.88	114.35	108.30
20	c	504	CLA	C3B-C2B-C1B	-3.87	102.49	107.16
20	B	610	CLA	C3D-C2D-C1D	-3.87	100.55	105.83
20	C	513	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
20	b	613	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
23	l	101	SQD	O48-C23-C24	3.86	124.01	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	a	403	CLA	CHC-C4B-NB	3.86	128.34	124.26
20	c	508	CLA	CHC-C4B-NB	3.85	128.34	124.26
32	B	631	HTG	C3-C4-C5	3.85	117.11	110.24
20	b	616	CLA	C3B-C2B-C1B	-3.85	102.51	107.16
27	d	412	PL9	C40-C39-C41	3.85	121.75	115.27
20	a	404	CLA	C3B-C2B-C1B	-3.85	102.51	107.16
20	c	507	CLA	C4D-CHA-C1A	-3.85	116.56	121.25
32	B	632	HTG	C1'-S1-C1	3.85	107.28	100.09
20	c	512	CLA	CHD-C4C-NC	3.84	130.26	124.20
20	b	607	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	D	401	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
20	b	609	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	c	512	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
20	b	606	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
20	c	511	CLA	C3B-C2B-C1B	-3.84	102.53	107.16
20	C	502	CLA	C2B-C1B-NB	3.84	112.80	110.23
20	B	616	CLA	CHD-C1D-ND	-3.84	120.93	124.45
20	B	605	CLA	C4D-CHA-C1A	-3.83	116.59	121.25
20	b	617	CLA	O2D-CGD-CBD	3.83	118.07	111.27
35	H	102	DGD	O1G-C1A-C2A	3.83	123.91	111.91
20	b	611	CLA	CHD-C4C-C3C	-3.82	119.22	124.84
20	c	510	CLA	C3B-C2B-C1B	-3.82	102.55	107.16
20	a	403	CLA	C3D-C2D-C1D	-3.82	100.61	105.83
20	c	502	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
20	c	505	CLA	O2D-CGD-CBD	3.82	118.05	111.27
20	C	505	CLA	O2D-CGD-CBD	3.82	118.05	111.27
20	c	510	CLA	CHD-C4C-NC	3.82	130.22	124.20
20	b	610	CLA	O2D-CGD-CBD	3.81	118.04	111.27
20	B	615	CLA	CHD-C4C-C3C	-3.81	119.24	124.84
20	C	512	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
27	a	415	PL9	C53-C6-C1	3.81	122.78	114.99
20	a	404	CLA	CHD-C1D-ND	-3.81	120.95	124.45
20	b	606	CLA	C4D-CHA-C1A	-3.81	116.62	121.25
20	a	407	CLA	C3B-C2B-C1B	-3.80	102.57	107.16
20	c	506	CLA	O2D-CGD-CBD	3.80	118.03	111.27
20	c	507	CLA	C3D-C2D-C1D	-3.80	100.64	105.83
23	A	406	SQD	C1-O5-C5	-3.80	106.23	113.69
20	B	603	CLA	CHD-C4C-C3C	-3.80	119.26	124.84
20	B	601	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
20	c	506	CLA	CMD-C2D-C1D	3.80	131.40	124.71
20	B	610	CLA	C1-C2-C3	-3.80	119.48	126.04
20	B	612	CLA	C1-C2-C3	-3.80	119.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	LMG	O7-C10-C11	3.79	119.67	111.50
20	C	513	CLA	CHD-C1D-ND	-3.79	120.97	124.45
32	B	622	HTG	C1-C2-C3	3.78	118.06	110.59
27	a	415	PL9	C30-C29-C31	3.78	121.63	115.27
21	D	403	PHO	CED-O2D-CGD	3.78	124.49	115.94
20	B	602	CLA	CMD-C2D-C1D	3.78	131.37	124.71
20	b	610	CLA	C3B-C2B-C1B	-3.77	102.61	107.16
20	B	606	CLA	CHD-C1D-ND	-3.77	120.99	124.45
20	b	616	CLA	CHD-C1D-ND	-3.77	120.99	124.45
20	B	602	CLA	O2A-C1-C2	3.77	118.53	108.64
20	A	402	CLA	CHC-C4B-NB	3.77	128.24	124.26
20	b	605	CLA	C3B-C2B-C1B	-3.76	102.62	107.16
21	a	405	PHO	O2D-CGD-CBD	3.75	115.75	111.00
20	C	501	CLA	C4D-CHA-C1A	-3.75	116.68	121.25
20	B	602	CLA	C2C-C1C-NC	3.75	113.49	109.97
20	B	614	CLA	C3B-C4B-NB	3.75	113.99	110.52
20	B	601	CLA	CHA-C4D-ND	3.74	140.32	132.50
20	B	601	CLA	O2D-CGD-CBD	3.74	117.91	111.27
37	e	102	HEM	CBD-CAD-C3D	-3.73	102.25	112.63
20	b	610	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
20	B	605	CLA	O2D-CGD-CBD	3.73	117.90	111.27
20	B	602	CLA	CHB-C1B-NB	-3.73	120.31	124.26
20	c	510	CLA	O2D-CGD-CBD	3.73	117.89	111.27
20	a	403	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
20	C	513	CLA	C4D-CHA-C1A	-3.72	116.72	121.25
20	a	404	CLA	C4D-CHA-C1A	-3.72	116.72	121.25
20	c	501	CLA	CHD-C4C-NC	3.72	130.07	124.20
40	v	201	HEC	CBC-CAC-C3C	3.72	122.68	112.43
20	B	603	CLA	O2D-CGD-CBD	3.72	117.87	111.27
20	C	506	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
20	b	603	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
20	C	502	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
20	b	617	CLA	CHA-C4D-ND	3.71	140.26	132.50
34	c	523	LMT	O5'-C5'-C4'	3.71	117.58	109.75
35	c	515	DGD	O5D-C6D-C5D	-3.71	102.18	109.05
20	A	401	CLA	C7-C6-C5	-3.71	103.28	113.36
20	b	609	CLA	C2D-C1D-ND	3.70	112.83	110.10
23	l	101	SQD	O47-C7-C8	3.70	119.48	111.50
24	c	519	LMG	O7-C10-C11	3.70	119.48	111.50
20	b	607	CLA	C3B-C2B-C1B	-3.69	102.70	107.16
20	C	507	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
20	B	612	CLA	O2D-CGD-CBD	3.69	117.83	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	510	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
20	b	614	CLA	CMC-C2C-C1C	3.68	130.65	125.04
20	C	508	CLA	CHD-C1D-ND	-3.68	121.07	124.45
20	C	511	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
20	b	609	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	A	404	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
20	A	401	CLA	CHD-C4C-C3C	-3.68	119.44	124.84
20	B	604	CLA	C1D-ND-C4D	-3.68	103.72	106.33
20	c	504	CLA	O2D-CGD-CBD	3.67	117.79	111.27
20	c	508	CLA	CMB-C2B-C1B	3.67	130.96	125.37
20	B	607	CLA	CHB-C1B-NB	-3.67	120.38	124.26
20	c	506	CLA	CHA-C4D-ND	3.66	140.17	132.50
20	b	611	CLA	C3B-C2B-C1B	-3.66	102.74	107.16
20	c	510	CLA	CHA-C4D-ND	3.66	140.15	132.50
23	b	622	SQD	C3-C4-C5	3.66	116.77	110.24
20	b	603	CLA	CHA-C4D-ND	3.66	140.15	132.50
20	C	502	CLA	CMB-C2B-C1B	3.66	130.94	125.37
20	d	404	CLA	C3D-C2D-C1D	-3.66	100.84	105.83
20	C	502	CLA	C3D-C2D-C1D	-3.66	100.84	105.83
20	b	607	CLA	CHA-C4D-ND	3.65	140.15	132.50
20	a	407	CLA	O2D-CGD-O1D	-3.65	116.70	123.84
22	d	405	BCR	C39-C30-C25	-3.65	104.38	110.30
22	t	101	BCR	C33-C5-C6	-3.65	120.43	124.53
20	b	613	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
20	c	504	CLA	CHB-C1B-NB	-3.65	120.39	124.26
20	c	510	CLA	C4-C3-C5	3.65	121.41	115.27
20	c	501	CLA	CMB-C2B-C1B	3.64	130.92	125.37
20	C	502	CLA	CMD-C2D-C1D	3.64	131.13	124.71
20	B	610	CLA	CED-O2D-CGD	3.64	124.17	115.94
21	a	405	PHO	O2D-CGD-O1D	-3.64	116.72	123.84
20	B	608	CLA	CHD-C1D-ND	-3.64	121.11	124.45
20	b	617	CLA	CMC-C2C-C1C	3.64	130.58	125.04
20	b	615	CLA	CAC-C3C-C4C	3.63	129.52	124.81
20	C	503	CLA	C2D-C1D-ND	3.63	112.78	110.10
20	b	618	CLA	C3B-C4B-NB	3.63	113.88	110.52
20	b	603	CLA	CMB-C2B-C1B	3.63	130.89	125.37
20	b	606	CLA	CHA-C4D-ND	3.63	140.09	132.50
22	B	617	BCR	C24-C23-C22	-3.62	120.76	126.23
35	c	515	DGD	O2G-C1B-C2B	3.62	119.31	111.50
35	h	101	DGD	O2G-C1B-C2B	3.62	119.31	111.50
20	C	504	CLA	CHC-C4B-NB	3.62	128.09	124.26
27	a	415	PL9	O1-C4-C3	-3.62	116.73	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	401	CLA	CMD-C2D-C3D	3.62	135.94	127.61
20	C	513	CLA	O2D-CGD-CBD	3.62	117.69	111.27
20	c	508	CLA	C3D-C2D-C1D	-3.62	100.90	105.83
20	d	402	CLA	C2A-C1A-CHA	-3.61	117.54	123.86
20	b	618	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
20	B	601	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
20	B	607	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
20	c	503	CLA	C4-C3-C5	3.61	121.34	115.27
20	B	608	CLA	CBC-CAC-C3C	-3.61	102.49	112.43
20	C	505	CLA	C3B-C2B-C1B	-3.60	102.81	107.16
20	c	501	CLA	C3B-C4B-NB	3.60	113.86	110.52
32	B	621	HTG	C1-O5-C5	3.60	119.22	112.58
20	D	402	CLA	CHD-C4C-NC	3.60	129.88	124.20
20	B	602	CLA	C3D-C2D-C1D	-3.60	100.92	105.83
20	b	613	CLA	CHD-C1D-ND	-3.60	121.15	124.45
20	D	402	CLA	C3B-C2B-C1B	-3.59	102.83	107.16
20	B	607	CLA	C4D-CHA-C1A	-3.59	116.88	121.25
22	b	619	BCR	C33-C5-C6	-3.59	120.50	124.53
20	b	605	CLA	C4-C3-C5	3.59	121.31	115.27
20	C	509	CLA	C1-C2-C3	-3.59	119.84	126.04
20	C	506	CLA	C1-C2-C3	-3.59	119.84	126.04
20	a	404	CLA	C4A-NA-C1A	3.59	108.32	106.71
20	C	511	CLA	CHD-C4C-C3C	-3.58	119.57	124.84
20	c	509	CLA	CAC-C3C-C4C	3.58	129.46	124.81
20	B	611	CLA	C3B-C2B-C1B	-3.58	102.84	107.16
20	B	603	CLA	CHA-C4D-ND	3.58	139.99	132.50
20	B	614	CLA	CHD-C1D-ND	-3.58	121.16	124.45
20	C	512	CLA	CHA-C4D-ND	3.58	139.99	132.50
20	C	507	CLA	CHA-C4D-ND	3.58	139.98	132.50
20	d	402	CLA	C3B-C4B-NB	3.58	113.83	110.52
20	b	612	CLA	CHD-C1D-ND	-3.57	121.17	124.45
20	b	613	CLA	CMD-C2D-C1D	3.57	131.01	124.71
21	A	403	PHO	O2D-CGD-O1D	-3.57	116.86	123.84
20	B	602	CLA	O1D-CGD-CBD	-3.57	117.19	124.48
20	B	612	CLA	CHC-C4B-NB	3.57	128.03	124.26
20	C	511	CLA	CHD-C1D-ND	-3.56	121.18	124.45
35	c	517	DGD	O1G-C1A-O1A	-3.56	114.60	123.59
20	b	614	CLA	CHD-C1D-ND	-3.56	121.18	124.45
32	C	534	HTG	C1'-S1-C1	3.56	106.75	100.09
20	d	404	CLA	C4-C3-C5	3.56	121.26	115.27
23	A	412	SQD	O48-C23-C24	3.56	123.08	111.91
20	A	401	CLA	C2C-C1C-NC	3.56	113.31	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	604	CLA	C3D-C2D-C1D	-3.55	100.98	105.83
20	C	513	CLA	CHA-C4D-ND	3.55	139.92	132.50
20	b	617	CLA	CHD-C4C-NC	3.55	129.79	124.20
20	c	511	CLA	C4D-CHA-C1A	-3.55	116.93	121.25
20	c	503	CLA	CHA-C4D-ND	3.54	139.91	132.50
24	B	620	LMG	O8-C28-C29	3.54	123.02	111.91
20	A	404	CLA	CHC-C4B-NB	3.54	128.00	124.26
21	D	403	PHO	OBD-CAD-C3D	-3.54	122.11	127.98
20	B	601	CLA	C4A-NA-C1A	3.54	108.30	106.71
20	B	611	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
20	B	611	CLA	CHC-C4B-NB	3.53	128.00	124.26
20	b	603	CLA	CHD-C1D-ND	-3.53	121.21	124.45
21	D	403	PHO	C1-C2-C3	-3.53	119.94	126.04
20	c	508	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
20	d	402	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
20	b	603	CLA	C3D-C2D-C1D	-3.53	101.01	105.83
20	d	404	CLA	C3B-C4B-NB	3.53	113.79	110.52
20	B	603	CLA	C3B-C2B-C1B	-3.53	102.91	107.16
20	B	605	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
20	B	602	CLA	CMB-C2B-C1B	3.52	130.73	125.37
20	B	615	CLA	C3D-C2D-C1D	-3.52	101.03	105.83
20	D	404	CLA	CAC-C3C-C4C	3.52	129.38	124.81
20	B	606	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
20	B	613	CLA	C3B-C2B-C1B	-3.51	102.92	107.16
20	b	610	CLA	CHD-C1D-ND	-3.51	121.23	124.45
20	c	512	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
22	C	514	BCR	C38-C26-C25	-3.51	120.59	124.53
20	B	604	CLA	C3B-C2B-C1B	-3.51	102.93	107.16
22	b	620	BCR	C29-C30-C25	3.51	115.88	110.48
20	b	618	CLA	CAC-C3C-C4C	3.50	129.36	124.81
20	b	612	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
20	C	506	CLA	C3D-C2D-C1D	-3.50	101.06	105.83
20	B	610	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
36	d	406	LHG	O8-C23-O10	-3.50	114.77	123.59
20	D	404	CLA	O2D-CGD-CBD	3.50	117.48	111.27
20	B	611	CLA	C3C-C4C-NC	3.50	114.49	110.57
20	b	618	CLA	CBC-CAC-C3C	-3.50	102.79	112.43
40	V	201	HEC	CBD-CAD-C3D	-3.49	102.93	112.63
20	c	503	CLA	C3B-C2B-C1B	-3.49	102.95	107.16
20	B	608	CLA	C4D-CHA-C1A	-3.49	117.00	121.25
20	d	402	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
20	B	613	CLA	O2D-CGD-O1D	-3.49	117.02	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	511	CLA	CMC-C2C-C1C	3.49	130.35	125.04
22	k	101	BCR	C7-C8-C9	-3.48	120.97	126.23
20	b	609	CLA	C3B-C2B-C1B	-3.48	102.96	107.16
20	b	614	CLA	C3B-C2B-C1B	-3.48	102.96	107.16
20	b	610	CLA	CHA-C4D-ND	3.48	139.78	132.50
20	B	611	CLA	C4C-C3C-C2C	-3.48	101.83	106.90
20	C	507	CLA	CHD-C4C-NC	3.48	129.68	124.20
38	H	101	RRX	C7-C8-C9	-3.48	120.98	126.23
20	C	508	CLA	CHC-C4B-NB	3.47	127.93	124.26
20	b	617	CLA	O2D-CGD-O1D	-3.47	117.06	123.84
34	J	103	LMT	C3'-C4'-C5'	-3.47	104.05	110.24
36	d	406	LHG	O8-C23-C24	3.47	122.79	111.91
20	B	606	CLA	C1D-ND-C4D	-3.46	103.88	106.33
20	B	607	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
20	b	608	CLA	C4D-CHA-C1A	-3.46	117.04	121.25
20	B	606	CLA	CHA-C4D-ND	3.46	139.74	132.50
20	B	606	CLA	C3C-C4C-NC	3.46	114.45	110.57
20	a	404	CLA	CMC-C2C-C1C	3.46	130.30	125.04
20	d	403	CLA	C3C-C4C-NC	3.46	114.45	110.57
20	b	605	CLA	CMC-C2C-C1C	3.45	130.30	125.04
20	B	615	CLA	C2A-C1A-CHA	-3.45	117.82	123.86
20	b	610	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
20	B	608	CLA	C2A-C1A-CHA	-3.45	117.83	123.86
20	c	505	CLA	CAC-C3C-C4C	3.45	129.28	124.81
20	c	502	CLA	CHD-C4C-C3C	-3.45	119.77	124.84
22	b	619	BCR	C23-C22-C21	-3.44	113.66	118.94
20	B	601	CLA	CMB-C2B-C1B	3.44	130.61	125.37
20	b	604	CLA	C1-O2A-CGA	3.44	125.47	116.44
20	b	618	CLA	C3B-C2B-C1B	-3.44	103.01	107.16
20	B	606	CLA	C1-C2-C3	-3.44	120.09	126.04
20	A	404	CLA	CHB-C4A-NA	3.44	129.27	124.51
23	b	622	SQD	O6-C1-C2	3.44	113.67	108.30
23	b	622	SQD	O5-C1-C2	-3.44	103.07	110.35
20	d	404	CLA	CHC-C4B-NB	3.44	127.90	124.26
36	E	103	LHG	O7-C7-C8	3.44	122.69	111.91
22	b	620	BCR	C38-C26-C25	-3.44	120.67	124.53
20	B	606	CLA	C3D-C2D-C1D	-3.44	101.14	105.83
20	B	605	CLA	CHA-C4D-ND	3.43	139.69	132.50
20	b	608	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
20	c	510	CLA	CHB-C1B-NB	-3.43	120.62	124.26
20	c	506	CLA	CHD-C4C-NC	3.43	129.61	124.20
23	l	101	SQD	C1-O5-C5	-3.43	106.96	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	512	CLA	C4D-CHA-C1A	-3.42	117.08	121.25
24	B	620	LMG	O7-C10-O9	-3.42	115.43	123.70
22	d	405	BCR	C29-C30-C25	3.42	115.75	110.48
20	a	403	CLA	C2B-C1B-NB	3.42	112.52	110.23
20	c	502	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
21	D	403	PHO	C4B-NB-C1B	-3.42	103.54	108.83
20	d	403	CLA	CBC-CAC-C3C	-3.41	103.03	112.43
20	B	603	CLA	C3D-C2D-C1D	-3.41	101.18	105.83
20	b	611	CLA	C4A-NA-C1A	3.41	108.24	106.71
23	A	406	SQD	O8-S-C6	3.41	111.17	105.74
40	v	201	HEC	C2A-C1A-NA	-3.40	107.01	110.32
20	D	401	CLA	C3B-C2B-C1B	-3.40	103.05	107.16
20	a	403	CLA	C4D-CHA-C1A	-3.40	117.11	121.25
34	b	627	LMT	O5B-C5B-C6B	3.40	114.90	106.44
20	c	502	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
22	B	618	BCR	C29-C30-C25	3.40	115.72	110.48
20	c	510	CLA	C4A-NA-C1A	3.40	108.23	106.71
23	F	101	SQD	C1-C2-C3	-3.39	102.93	110.00
20	D	401	CLA	CHA-C4D-ND	3.39	139.59	132.50
20	C	510	CLA	C3B-C2B-C1B	-3.39	103.07	107.16
20	c	505	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
20	b	608	CLA	C1-O2A-CGA	3.38	125.32	116.44
27	A	411	PL9	C30-C29-C31	3.38	120.96	115.27
20	d	402	CLA	C4D-CHA-C1A	-3.38	117.13	121.25
24	C	519	LMG	O7-C10-C11	3.38	118.79	111.50
20	d	403	CLA	C3D-C2D-C1D	-3.38	101.22	105.83
20	B	609	CLA	O2D-CGD-CBD	3.38	117.27	111.27
20	c	509	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
20	C	507	CLA	C2D-C1D-ND	3.37	112.59	110.10
20	B	610	CLA	O2D-CGD-CBD	3.37	117.26	111.27
20	C	510	CLA	C4D-CHA-C1A	-3.37	117.15	121.25
20	C	512	CLA	C3D-C2D-C1D	-3.37	101.23	105.83
20	D	404	CLA	C3D-C2D-C1D	-3.37	101.23	105.83
20	C	506	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
20	C	504	CLA	C3B-C2B-C1B	-3.37	103.10	107.16
20	b	605	CLA	CHA-C4D-ND	3.37	139.54	132.50
20	C	504	CLA	CHD-C4C-NC	3.36	129.50	124.20
20	b	616	CLA	C3B-C4B-NB	3.36	113.64	110.52
20	D	402	CLA	CHC-C4B-NB	3.36	127.82	124.26
24	C	519	LMG	O8-C28-C29	3.36	122.46	111.91
20	d	404	CLA	CMD-C2D-C1D	3.36	130.64	124.71
20	b	618	CLA	CHD-C4C-NC	3.36	129.49	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	611	CLA	CHA-C4D-ND	3.36	139.52	132.50
20	c	510	CLA	CHC-C4B-NB	3.36	127.81	124.26
20	B	608	CLA	CAC-C3C-C4C	3.36	129.16	124.81
20	C	507	CLA	C4-C3-C5	3.36	120.92	115.27
20	c	513	CLA	O2D-CGD-CBD	3.35	117.23	111.27
20	c	513	CLA	CHD-C4C-NC	3.35	129.49	124.20
20	a	407	CLA	C4D-CHA-C1A	-3.35	117.17	121.25
21	D	403	PHO	C4D-CHA-CBD	3.35	110.03	108.52
20	C	505	CLA	CHA-C4D-ND	3.35	139.50	132.50
20	c	509	CLA	CHD-C4C-NC	3.35	129.48	124.20
32	b	624	HTG	O5-C1-C2	-3.34	106.11	110.31
20	C	505	CLA	CHD-C4C-NC	3.34	129.47	124.20
20	b	603	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
20	C	511	CLA	CMB-C2B-C1B	3.34	130.45	125.37
20	B	611	CLA	CHA-C4D-ND	3.34	139.48	132.50
22	b	621	BCR	C38-C26-C25	-3.33	120.78	124.53
20	b	612	CLA	CHA-C4D-ND	3.33	139.47	132.50
32	B	631	HTG	O5-C5-C4	3.33	115.75	109.69
20	B	604	CLA	CHC-C1C-NC	-3.33	119.15	124.20
20	b	603	CLA	CHC-C4B-NB	3.33	127.78	124.26
20	B	615	CLA	CHD-C1D-ND	-3.33	121.40	124.45
20	a	404	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
24	c	518	LMG	C4-C3-C2	3.33	116.63	110.82
20	C	508	CLA	C3D-C4D-ND	3.32	115.62	110.24
20	b	611	CLA	CMB-C2B-C1B	3.32	130.43	125.37
23	f	101	SQD	O48-C23-C24	3.32	122.33	111.91
38	H	101	RRX	C16-C15-C14	-3.32	116.67	123.47
20	C	502	CLA	C1D-ND-C4D	-3.32	103.98	106.33
20	b	604	CLA	CMC-C2C-C1C	3.32	130.09	125.04
20	a	407	CLA	C3D-C2D-C1D	-3.31	101.31	105.83
20	C	502	CLA	C3B-C4B-NB	3.31	113.59	110.52
27	a	415	PL9	C25-C24-C26	3.31	120.84	115.27
20	D	404	CLA	CHA-C4D-ND	3.31	139.43	132.50
20	C	501	CLA	C3B-C2B-C1B	-3.31	103.16	107.16
20	B	615	CLA	CHB-C4A-NA	3.31	129.09	124.51
20	B	601	CLA	C3C-C4C-NC	3.31	114.28	110.57
20	c	506	CLA	CMB-C2B-C1B	3.31	130.41	125.37
34	B	625	LMT	O5'-C5'-C4'	3.31	115.70	109.69
22	K	102	BCR	C38-C26-C25	-3.30	120.82	124.53
20	c	506	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
20	B	604	CLA	C2A-C1A-CHA	-3.30	118.09	123.86
20	B	604	CLA	C4D-CHA-C1A	-3.30	117.23	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	406	PHO	C4B-NB-C1B	-3.30	103.72	108.83
20	c	505	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	b	622	SQD	O9-S-C6	3.30	110.86	106.94
21	A	403	PHO	C4B-NB-C1B	-3.30	103.73	108.83
22	K	102	BCR	C24-C23-C22	-3.30	121.26	126.23
20	c	512	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
20	c	504	CLA	CHD-C4C-NC	3.29	129.39	124.20
20	c	501	CLA	CHB-C1B-NB	-3.29	120.77	124.26
20	a	407	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
20	C	505	CLA	C4D-CHA-C1A	-3.29	117.24	121.25
40	v	201	HEC	CHB-C1B-NB	3.29	127.99	124.42
20	D	404	CLA	CMD-C2D-C1D	3.29	130.51	124.71
20	B	604	CLA	CHD-C4C-NC	3.29	129.38	124.20
22	T	101	BCR	C35-C13-C12	3.29	123.26	118.08
20	C	509	CLA	C4-C3-C5	3.28	120.80	115.27
20	c	506	CLA	C4D-CHA-C1A	-3.28	117.25	121.25
20	C	509	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
20	C	513	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
20	b	614	CLA	C3D-C2D-C1D	-3.28	101.35	105.83
20	B	605	CLA	C3C-C4C-NC	3.28	114.25	110.57
20	c	512	CLA	CMD-C2D-C1D	3.28	130.50	124.71
24	c	519	LMG	O8-C28-C29	3.28	122.20	111.91
22	c	514	BCR	C32-C1-C6	-3.28	104.98	110.30
22	C	515	BCR	C7-C8-C9	-3.28	121.28	126.23
37	E	104	HEM	CMD-C2D-C1D	3.28	130.03	125.04
20	C	508	CLA	CHD-C4C-C3C	-3.28	120.02	124.84
20	C	502	CLA	O2D-CGD-CBD	3.28	117.09	111.27
20	c	501	CLA	CMD-C2D-C1D	3.28	130.49	124.71
20	c	505	CLA	CMC-C2C-C1C	3.28	130.03	125.04
20	c	513	CLA	C3D-C2D-C1D	-3.27	101.36	105.83
20	B	609	CLA	C3B-C2B-C1B	-3.27	103.21	107.16
20	B	614	CLA	C2A-C1A-CHA	-3.27	118.14	123.86
40	v	201	HEC	CBD-CAD-C3D	-3.27	103.54	112.63
20	c	504	CLA	CAC-C3C-C4C	3.27	129.05	124.81
27	D	412	PL9	C10-C9-C11	3.27	120.77	115.27
20	c	507	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
22	B	619	BCR	C2-C1-C6	3.27	115.51	110.48
20	b	616	CLA	CHD-C4C-NC	3.27	129.35	124.20
20	b	617	CLA	C3B-C2B-C1B	-3.27	103.22	107.16
20	B	615	CLA	CMB-C2B-C1B	3.27	130.34	125.37
20	b	616	CLA	C3D-C2D-C1D	-3.27	101.38	105.83
20	C	503	CLA	C3D-C2D-C1D	-3.26	101.38	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	605	CLA	C2D-C1D-ND	3.26	112.51	110.10
20	c	505	CLA	C3D-C2D-C1D	-3.26	101.38	105.83
20	c	511	CLA	C3D-C2D-C1D	-3.26	101.38	105.83
20	D	404	CLA	C1D-ND-C4D	-3.26	104.02	106.33
35	C	517	DGD	O2G-C1B-C2B	3.26	118.52	111.50
20	B	602	CLA	CHA-C4D-ND	3.26	139.31	132.50
20	B	609	CLA	C3B-C4B-NB	3.26	113.54	110.52
20	b	611	CLA	CHD-C1D-ND	-3.26	121.46	124.45
20	C	503	CLA	CHB-C1B-NB	-3.25	120.81	124.26
24	b	623	LMG	O8-C28-C29	3.25	122.12	111.91
20	b	614	CLA	C2B-C1B-NB	3.25	112.41	110.23
20	B	613	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
20	b	604	CLA	C1D-CHD-C4C	-3.24	119.06	126.06
22	T	101	BCR	C38-C26-C25	-3.24	120.89	124.53
20	c	507	CLA	CHA-C4D-ND	3.24	139.28	132.50
20	B	602	CLA	C3B-C2B-C1B	-3.24	103.25	107.16
20	b	618	CLA	C3C-C4C-NC	3.24	114.21	110.57
20	B	615	CLA	CAC-C3C-C4C	3.24	129.01	124.81
20	A	404	CLA	C3D-C2D-C1D	-3.24	101.41	105.83
20	C	508	CLA	C4-C3-C5	3.24	120.72	115.27
35	c	516	DGD	O2G-C1B-C2B	3.24	118.48	111.50
20	a	403	CLA	CHA-C4D-ND	3.24	139.27	132.50
22	a	408	BCR	C15-C16-C17	-3.23	116.85	123.47
20	C	501	CLA	CHD-C4C-NC	3.23	129.30	124.20
20	B	612	CLA	C3C-C4C-NC	3.23	114.20	110.57
20	c	508	CLA	O2D-CGD-CBD	3.23	117.01	111.27
20	b	612	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
34	m	101	LMT	C1'-O5'-C5'	3.23	120.03	113.69
20	d	403	CLA	O2D-CGD-CBD	3.23	117.00	111.27
20	B	611	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
20	b	611	CLA	C2D-C1D-ND	3.23	112.48	110.10
20	D	401	CLA	C2A-C1A-CHA	-3.22	118.22	123.86
20	c	511	CLA	CHA-C4D-ND	3.22	139.25	132.50
24	C	519	LMG	O1-C7-C8	-3.22	103.12	110.90
38	H	101	RRX	C10-C11-C12	-3.22	113.16	123.22
20	b	610	CLA	CED-O2D-CGD	3.22	123.22	115.94
20	B	604	CLA	CHC-C4B-NB	3.22	127.66	124.26
20	C	503	CLA	CMC-C2C-C1C	3.22	129.94	125.04
23	A	412	SQD	C1-C2-C3	-3.21	103.31	110.00
20	c	509	CLA	C3B-C4B-NB	3.21	113.49	110.52
20	C	507	CLA	CBC-CAC-C3C	-3.21	103.59	112.43
20	D	401	CLA	C1D-CHD-C4C	-3.21	119.14	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	616	CLA	CHC-C4B-NB	3.21	127.65	124.26
20	b	606	CLA	C3B-C2B-C1B	-3.20	103.29	107.16
20	c	513	CLA	CMC-C2C-C1C	3.20	129.92	125.04
20	B	615	CLA	CMD-C2D-C1D	3.20	130.36	124.71
20	B	605	CLA	C2B-C1B-NB	3.20	112.38	110.23
20	b	611	CLA	C4D-CHA-C1A	-3.20	117.35	121.25
20	c	509	CLA	CMC-C2C-C1C	3.20	129.91	125.04
20	C	502	CLA	CHD-C4C-NC	3.20	129.25	124.20
20	c	503	CLA	CHD-C4C-NC	3.20	129.24	124.20
40	V	201	HEC	C3B-C4B-NB	-3.20	106.61	110.17
27	d	412	PL9	C7-C8-C9	-3.20	121.47	126.79
20	B	613	CLA	C3D-C2D-C1D	-3.19	101.47	105.83
20	b	606	CLA	CHC-C4B-NB	3.19	127.64	124.26
20	C	505	CLA	C2D-C1D-ND	3.19	112.46	110.10
22	B	617	BCR	C33-C5-C6	-3.19	120.95	124.53
20	B	607	CLA	C2C-C1C-NC	3.19	112.96	109.97
20	C	504	CLA	C4D-CHA-C1A	-3.19	117.37	121.25
20	c	510	CLA	C1D-ND-C4D	-3.19	104.07	106.33
20	c	511	CLA	C1-O2A-CGA	3.18	124.80	116.44
20	a	403	CLA	CHD-C1D-ND	-3.18	121.53	124.45
20	C	504	CLA	CAC-C3C-C4C	3.18	128.94	124.81
20	C	504	CLA	CHA-C4D-ND	3.18	139.15	132.50
23	b	622	SQD	O48-C23-C24	3.18	121.88	111.91
20	A	401	CLA	C3D-C2D-C1D	-3.18	101.49	105.83
22	a	408	BCR	C29-C30-C25	3.18	115.37	110.48
20	C	501	CLA	CHC-C4B-NB	3.18	127.62	124.26
20	C	501	CLA	C2A-C1A-CHA	-3.18	118.31	123.86
20	B	614	CLA	O2A-CGA-CBA	3.17	121.87	111.91
20	b	609	CLA	CHA-C4D-ND	3.17	139.14	132.50
20	B	609	CLA	CHD-C4C-NC	3.17	129.20	124.20
22	D	405	BCR	C38-C26-C25	-3.17	120.97	124.53
20	C	502	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
20	D	401	CLA	C3D-C2D-C1D	-3.17	101.50	105.83
20	C	512	CLA	C4-C3-C5	3.17	120.60	115.27
20	c	511	CLA	C4-C3-C5	3.17	120.60	115.27
20	B	603	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
20	C	511	CLA	CHB-C1B-NB	-3.16	120.92	124.26
21	a	405	PHO	CMB-C2B-C3B	3.16	130.58	124.68
20	C	505	CLA	C3D-C2D-C1D	-3.15	101.53	105.83
20	C	502	CLA	CHA-C4D-ND	3.15	139.09	132.50
20	D	401	CLA	CMD-C2D-C1D	3.15	130.26	124.71
20	C	512	CLA	CHB-C1B-NB	-3.15	120.92	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	609	CLA	C1D-ND-C4D	-3.15	104.10	106.33
32	v	210	HTG	C1-C2-C3	-3.15	104.37	110.59
20	b	613	CLA	C3C-C4C-NC	3.15	114.10	110.57
35	c	517	DGD	O1G-C1A-C2A	3.15	121.79	111.91
22	B	619	BCR	C23-C24-C25	-3.15	118.36	127.20
22	T	101	BCR	C23-C24-C25	-3.15	118.36	127.20
27	d	412	PL9	O1-C4-C3	-3.14	117.26	120.72
20	b	616	CLA	CHB-C1B-NB	-3.14	120.93	124.26
20	B	601	CLA	C4D-CHA-C1A	-3.14	117.43	121.25
22	b	620	BCR	C8-C7-C6	-3.14	118.39	127.20
22	t	101	BCR	C12-C13-C14	-3.14	114.13	118.94
34	b	627	LMT	C4B-C3B-C2B	3.13	116.30	110.82
22	K	102	BCR	C34-C9-C8	3.13	123.01	118.08
20	b	605	CLA	C4D-CHA-C1A	-3.13	117.44	121.25
20	b	618	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
22	B	619	BCR	C33-C5-C6	-3.13	121.01	124.53
20	a	403	CLA	C4-C3-C5	3.13	120.53	115.27
20	B	609	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	B	612	CLA	CAC-C3C-C4C	3.13	128.87	124.81
20	b	603	CLA	CHD-C4C-NC	3.13	129.13	124.20
20	b	604	CLA	CMB-C2B-C3B	3.12	134.15	126.59
20	b	616	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
20	c	509	CLA	C1-C2-C3	-3.12	120.64	126.04
20	b	605	CLA	C3D-C2D-C1D	-3.12	101.57	105.83
20	b	604	CLA	C16-C17-C18	-3.12	101.28	115.98
20	c	510	CLA	C3D-C2D-C1D	-3.12	101.58	105.83
20	c	511	CLA	CHD-C4C-NC	3.11	129.11	124.20
34	B	625	LMT	C1-O1'-C1'	-3.11	108.68	113.84
27	a	415	PL9	C3-C4-C5	3.11	122.65	118.60
20	C	511	CLA	O2D-CGD-CBD	3.11	116.79	111.27
20	C	507	CLA	CHB-C1B-NB	-3.10	120.97	124.26
20	b	604	CLA	C4-C3-C5	3.10	120.49	115.27
32	b	625	HTG	C1-O5-C5	3.10	118.29	112.58
20	B	611	CLA	CMB-C2B-C1B	3.09	130.08	125.37
21	a	406	PHO	O2D-CGD-O1D	-3.09	117.79	123.84
20	C	507	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
20	D	402	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
20	C	502	CLA	CAC-C3C-C4C	3.09	128.82	124.81
22	C	514	BCR	C15-C14-C13	-3.09	122.90	127.31
20	b	616	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
27	d	412	PL9	C3-C4-C5	3.09	122.62	118.60
20	B	606	CLA	C3B-C4B-NB	3.08	113.38	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	512	CLA	CBC-CAC-C3C	-3.08	103.93	112.43
20	c	507	CLA	CMD-C2D-C1D	3.08	130.14	124.71
20	c	505	CLA	CHD-C4C-NC	3.08	129.06	124.20
20	C	512	CLA	CHC-C4B-NB	3.08	127.52	124.26
38	x	101	RRX	C16-C17-C18	-3.08	122.91	127.31
20	A	401	CLA	C3C-C4C-NC	3.08	114.02	110.57
20	b	612	CLA	CAC-C3C-C4C	3.08	128.80	124.81
27	d	412	PL9	C36-C37-C38	-3.08	101.77	111.88
20	D	402	CLA	CBC-CAC-C3C	-3.08	103.95	112.43
20	B	613	CLA	C2A-C1A-CHA	-3.08	118.48	123.86
21	D	403	PHO	O2D-CGD-O1D	-3.07	117.83	123.84
22	B	617	BCR	C20-C21-C22	-3.07	122.92	127.31
22	T	101	BCR	C7-C8-C9	-3.07	121.59	126.23
20	b	618	CLA	O1D-CGD-CBD	-3.07	118.20	124.48
34	T	102	LMT	C1'-C2'-C3'	3.07	116.38	110.00
34	b	627	LMT	C3'-C4'-C5'	3.07	117.96	110.93
22	b	621	BCR	C33-C5-C6	-3.07	121.08	124.53
20	D	404	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
20	B	609	CLA	CHA-C4D-ND	3.06	138.91	132.50
24	j	101	LMG	O2-C2-C1	-3.06	102.60	110.05
20	a	407	CLA	C3C-C4C-NC	3.06	114.00	110.57
20	b	603	CLA	C1-O2A-CGA	3.06	124.48	116.44
35	c	517	DGD	O2G-C1B-C2B	3.06	118.10	111.50
24	c	518	LMG	O1-C1-C2	3.06	113.08	108.30
20	b	604	CLA	C2A-C1A-CHA	-3.06	118.52	123.86
20	b	612	CLA	CMB-C2B-C1B	3.05	130.02	125.37
24	B	620	LMG	C9-C8-C7	-3.05	104.57	111.79
20	c	513	CLA	CHA-C4D-ND	3.05	138.88	132.50
22	d	405	BCR	C38-C26-C25	-3.05	121.10	124.53
20	C	511	CLA	CHA-C4D-ND	3.05	138.88	132.50
20	C	510	CLA	C4-C3-C5	3.05	120.40	115.27
20	c	511	CLA	CHD-C1D-ND	-3.05	121.66	124.45
22	t	101	BCR	C15-C16-C17	-3.04	117.24	123.47
20	B	608	CLA	C3B-C2B-C1B	-3.04	103.49	107.16
20	C	506	CLA	CAC-C3C-C4C	3.04	128.76	124.81
20	B	612	CLA	C3B-C2B-C1B	-3.04	103.49	107.16
23	A	412	SQD	O6-C44-C45	-3.04	103.56	110.90
36	L	101	LHG	O4-P-O5	3.04	127.26	112.24
20	D	401	CLA	C3B-C4B-NB	3.04	113.33	110.52
20	c	502	CLA	C1D-ND-C4D	-3.03	104.18	106.33
20	b	615	CLA	CHD-C4C-NC	3.03	128.98	124.20
20	B	603	CLA	O2D-CGD-O1D	-3.03	117.91	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	610	CLA	C2B-C1B-NB	3.03	112.26	110.23
20	B	605	CLA	CMD-C2D-C1D	3.03	130.04	124.71
20	B	604	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
22	C	515	BCR	C23-C24-C25	-3.02	118.71	127.20
20	c	507	CLA	O2A-CGA-CBA	3.02	121.39	111.91
24	A	407	LMG	O7-C10-C11	3.02	118.01	111.50
20	B	601	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
20	B	609	CLA	CMC-C2C-C1C	3.02	129.64	125.04
20	a	403	CLA	CHC-C1C-C2C	-3.02	118.34	126.73
20	C	510	CLA	C3D-C2D-C1D	-3.02	101.71	105.83
20	b	606	CLA	CAC-C3C-C4C	3.02	128.73	124.81
35	C	517	DGD	O5D-C6D-C5D	3.02	114.63	109.05
20	C	512	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
20	b	614	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
20	c	507	CLA	CHD-C4C-NC	3.02	128.96	124.20
20	d	402	CLA	C1D-CHD-C4C	-3.02	119.55	126.06
36	d	408	LHG	O7-C7-O9	-3.02	116.41	123.70
23	A	406	SQD	C44-O6-C1	-3.02	107.85	113.74
20	C	509	CLA	C3B-C4B-NB	3.01	113.31	110.52
20	C	506	CLA	C4-C3-C5	3.01	120.34	115.27
20	c	502	CLA	CHD-C1D-ND	-3.01	121.69	124.45
22	b	619	BCR	C11-C10-C9	-3.01	123.01	127.31
20	b	617	CLA	C1-O2A-CGA	3.01	124.34	116.44
20	a	404	CLA	C3C-C4C-NC	3.01	113.94	110.57
32	C	521	HTG	O5-C5-C4	3.01	115.16	109.69
20	B	611	CLA	CAA-CBA-CGA	-3.01	104.47	113.25
20	C	506	CLA	CMC-C2C-C1C	3.00	129.61	125.04
22	A	405	BCR	C38-C26-C25	-3.00	121.16	124.53
20	C	507	CLA	C1-O2A-CGA	3.00	124.31	116.44
20	B	613	CLA	CMD-C2D-C1D	3.00	130.00	124.71
20	D	404	CLA	CMA-C3A-C4A	-3.00	103.72	111.77
20	b	605	CLA	C3C-C4C-NC	3.00	113.93	110.57
40	V	201	HEC	CBC-CAC-C3C	3.00	120.69	112.43
20	B	601	CLA	C1-O2A-CGA	3.00	124.31	116.44
20	C	508	CLA	CHB-C4A-NA	2.99	128.65	124.51
20	d	403	CLA	C3B-C2B-C1B	-2.99	103.55	107.16
20	C	511	CLA	C4D-CHA-C1A	-2.99	117.61	121.25
20	B	602	CLA	C2A-C1A-CHA	-2.99	118.62	123.86
22	a	408	BCR	C7-C8-C9	-2.99	121.71	126.23
20	d	402	CLA	CAC-C3C-C4C	2.99	128.69	124.81
20	C	508	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
20	B	615	CLA	C1C-C2C-C3C	-2.99	103.81	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	613	CLA	CBC-CAC-C3C	-2.98	104.20	112.43
24	b	623	LMG	O8-C28-O10	-2.98	116.06	123.59
20	b	612	CLA	C3B-C4B-NB	2.98	113.28	110.52
22	K	101	BCR	C38-C26-C25	-2.98	121.18	124.53
20	B	613	CLA	C4B-CHC-C1C	-2.98	119.27	126.34
35	d	416	DGD	O1G-C1A-C2A	2.98	121.26	111.91
20	B	613	CLA	O2D-CGD-CBD	2.98	116.56	111.27
23	a	409	SQD	O47-C7-C8	2.98	117.92	111.50
20	B	614	CLA	C3C-C4C-NC	2.98	113.91	110.57
20	B	613	CLA	C4-C3-C5	2.98	120.28	115.27
20	b	614	CLA	O2D-CGD-CBD	2.98	116.56	111.27
36	E	103	LHG	O8-C23-C24	2.98	121.25	111.91
20	C	509	CLA	O2A-CGA-CBA	2.98	121.24	111.91
22	b	621	BCR	C7-C8-C9	-2.97	121.74	126.23
27	a	415	PL9	C7-C8-C9	-2.97	121.84	126.79
40	v	201	HEC	C4A-NA-C1A	2.97	108.26	105.35
20	c	510	CLA	C2A-C1A-CHA	-2.97	118.66	123.86
20	c	513	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
20	B	605	CLA	C3D-C2D-C1D	-2.97	101.78	105.83
20	c	509	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
20	b	606	CLA	C3B-C4B-NB	2.97	113.27	110.52
35	d	416	DGD	C3D-C4D-C5D	2.97	115.53	110.24
20	C	503	CLA	C1D-CHD-C4C	-2.96	119.67	126.06
20	b	608	CLA	C3B-C2B-C1B	-2.96	103.58	107.16
20	b	618	CLA	CHA-C4D-ND	2.96	138.70	132.50
20	a	407	CLA	CMC-C2C-C1C	2.96	129.55	125.04
20	b	608	CLA	CHD-C4C-NC	2.96	128.87	124.20
34	a	418	LMT	C1B-O5B-C5B	2.96	119.50	113.69
20	B	607	CLA	CHA-C4D-ND	2.96	138.69	132.50
20	C	509	CLA	CMD-C2D-C1D	2.96	129.93	124.71
20	b	603	CLA	C1D-ND-C4D	-2.96	104.23	106.33
20	b	613	CLA	C3B-C2B-C1B	-2.96	103.59	107.16
20	C	512	CLA	CHD-C1D-ND	-2.96	121.74	124.45
20	b	616	CLA	CAC-C3C-C4C	2.95	128.64	124.81
20	c	513	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
20	C	501	CLA	CHA-C4D-ND	2.95	138.67	132.50
32	B	621	HTG	O5-C5-C6	2.95	113.77	106.44
20	c	504	CLA	C4-C3-C5	2.95	120.23	115.27
20	B	606	CLA	O2D-CGD-CBD	2.95	116.51	111.27
20	c	508	CLA	C2A-C1A-CHA	-2.94	118.71	123.86
34	m	102	LMT	C3'-C4'-C5'	-2.94	104.18	110.93
20	b	607	CLA	CMD-C2D-C1D	2.94	129.90	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	611	CLA	C3C-C4C-NC	2.94	113.87	110.57
20	A	401	CLA	CHA-C4D-ND	2.94	138.65	132.50
20	b	611	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
35	c	515	DGD	O2G-C1B-O1B	-2.94	116.60	123.70
20	B	615	CLA	CHD-C4C-NC	2.94	128.83	124.20
27	D	412	PL9	C22-C23-C24	-2.94	120.59	127.66
20	C	510	CLA	C3B-C4B-NB	2.94	113.24	110.52
20	D	402	CLA	C3B-C4B-NB	2.94	113.24	110.52
20	C	503	CLA	CHD-C4C-NC	2.93	128.83	124.20
34	a	418	LMT	O1'-C1'-C2'	2.93	112.88	108.30
20	B	601	CLA	C1C-C2C-C3C	-2.93	103.87	106.96
27	A	411	PL9	C3-C4-C5	2.93	122.42	118.60
20	B	601	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
20	c	508	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	f	101	SQD	C1-O5-C5	2.93	119.43	113.69
20	b	610	CLA	CHD-C4C-NC	2.92	128.81	124.20
27	A	411	PL9	C45-C44-C46	2.92	120.19	115.27
34	b	628	LMT	C1'-O5'-C5'	2.92	119.42	113.69
20	A	401	CLA	CMB-C2B-C1B	2.92	129.82	125.37
20	B	602	CLA	C1D-CHD-C4C	-2.92	119.76	126.06
20	C	508	CLA	C5-C3-C2	-2.92	115.22	121.12
20	a	403	CLA	CMB-C2B-C1B	2.92	129.81	125.37
20	c	509	CLA	C3D-C2D-C1D	-2.92	101.85	105.83
32	V	202	HTG	O5-C1-S1	2.92	117.24	110.14
20	A	401	CLA	C4D-CHA-C1A	-2.91	117.70	121.25
20	B	610	CLA	C4C-C3C-C2C	-2.91	102.65	106.90
20	b	611	CLA	CBC-CAC-C3C	-2.91	104.40	112.43
20	c	513	CLA	C3C-C4C-NC	2.91	113.84	110.57
20	B	611	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
20	C	510	CLA	C4B-CHC-C1C	-2.91	119.43	126.34
35	c	515	DGD	O3G-C3G-C2G	-2.91	103.88	110.90
34	b	627	LMT	O2'-C2'-C3'	-2.91	103.62	110.35
20	C	510	CLA	O2A-CGA-O1A	-2.91	116.25	123.59
20	B	606	CLA	CMC-C2C-C1C	2.91	129.47	125.04
24	C	524	LMG	O8-C28-C29	2.91	121.03	111.91
32	D	417	HTG	O5-C5-C6	2.91	113.66	106.44
27	d	412	PL9	C36-C34-C33	-2.91	115.24	121.12
22	T	101	BCR	C15-C16-C17	-2.91	117.52	123.47
20	c	509	CLA	CHB-C4A-NA	2.90	128.53	124.51
20	a	403	CLA	C5-C3-C2	-2.90	115.25	121.12
20	b	604	CLA	CBB-CAB-C3B	-2.90	113.20	127.62
20	D	404	CLA	C6-C7-C8	-2.90	106.56	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	507	CLA	CMC-C2C-C1C	2.90	129.45	125.04
20	d	402	CLA	CHA-C4D-ND	2.89	138.55	132.50
20	c	507	CLA	O2A-CGA-O1A	-2.89	116.29	123.59
34	E	101	LMT	C1'-C2'-C3'	2.89	116.02	110.00
20	c	502	CLA	CHA-C4D-ND	2.89	138.54	132.50
20	b	604	CLA	O2D-CGD-CBD	2.89	116.40	111.27
20	b	605	CLA	CAC-C3C-C4C	2.89	128.56	124.81
20	C	502	CLA	CHD-C1D-ND	-2.89	121.80	124.45
23	a	401	SQD	O48-C23-C24	2.89	120.97	111.91
22	t	101	BCR	C28-C27-C26	-2.89	108.92	114.08
32	B	631	HTG	C1-O5-C5	2.89	117.90	112.58
22	B	619	BCR	C32-C1-C6	-2.88	105.62	110.30
37	E	104	HEM	C3B-C2B-C1B	2.88	108.62	106.49
35	c	517	DGD	O3G-C3G-C2G	-2.88	103.94	110.90
20	c	512	CLA	CHA-C4D-ND	2.88	138.53	132.50
20	B	605	CLA	CHD-C1D-ND	-2.88	121.81	124.45
20	b	613	CLA	CHA-C4D-ND	2.88	138.53	132.50
20	D	404	CLA	CHD-C4C-C3C	-2.88	120.61	124.84
21	a	406	PHO	C4-C3-C5	2.88	120.11	115.27
20	c	508	CLA	CHB-C1B-NB	-2.88	121.21	124.26
20	b	604	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
20	c	502	CLA	C1-C2-C3	-2.88	121.06	126.04
38	x	101	RRX	C33-C5-C6	-2.88	121.30	124.53
20	c	504	CLA	CHB-C4A-NA	2.88	128.49	124.51
20	B	609	CLA	C4D-CHA-C1A	-2.88	117.75	121.25
23	a	409	SQD	C44-O6-C1	-2.88	108.12	113.74
20	b	614	CLA	C1D-ND-C4D	-2.88	104.29	106.33
22	B	618	BCR	C11-C10-C9	-2.88	123.21	127.31
20	a	407	CLA	CHB-C1B-NB	-2.88	121.21	124.26
20	a	407	CLA	CED-O2D-CGD	2.88	122.44	115.94
35	c	516	DGD	O6E-C5E-C6E	2.87	113.58	106.44
20	B	610	CLA	OBD-CAD-C3D	-2.87	121.61	128.52
20	C	501	CLA	CMD-C2D-C1D	2.87	129.78	124.71
20	B	612	CLA	CHA-C4D-ND	2.87	138.51	132.50
20	B	615	CLA	CHA-C4D-ND	2.87	138.51	132.50
22	k	102	BCR	C33-C5-C6	-2.87	121.30	124.53
20	b	612	CLA	C4D-CHA-C1A	-2.87	117.75	121.25
22	b	619	BCR	C15-C16-C17	-2.87	117.60	123.47
20	c	507	CLA	C3C-C4C-NC	2.87	113.78	110.57
20	d	403	CLA	C1D-ND-C4D	-2.86	104.30	106.33
20	c	502	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
20	B	606	CLA	C4-C3-C5	2.86	120.09	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	Z	101	LMT	C1'-O5'-C5'	2.86	119.31	113.69
20	b	618	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
20	D	402	CLA	C4-C3-C5	2.86	120.08	115.27
20	d	403	CLA	C3B-C4B-NB	2.86	113.17	110.52
27	D	412	PL9	C40-C39-C38	-2.86	116.34	123.68
20	A	404	CLA	C3B-C4B-NB	2.86	113.17	110.52
20	d	402	CLA	C3D-C2D-C1D	-2.86	101.93	105.83
20	b	606	CLA	C1D-CHD-C4C	-2.86	119.90	126.06
20	B	606	CLA	CHB-C1B-NB	-2.85	121.23	124.26
20	c	512	CLA	CHB-C1B-NB	-2.85	121.23	124.26
20	c	507	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
20	B	607	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
27	A	411	PL9	C17-C18-C19	-2.85	120.81	127.66
21	D	403	PHO	CMB-C2B-C3B	2.84	129.99	124.68
34	B	625	LMT	C1'-O5'-C5'	2.84	119.27	113.69
20	b	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
20	B	612	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
37	e	102	HEM	C1B-NB-C4B	2.83	108.00	105.07
21	a	405	PHO	C4B-NB-C1B	-2.83	104.44	108.83
22	t	101	BCR	C11-C10-C9	-2.83	123.27	127.31
20	B	610	CLA	C3B-C2B-C1B	-2.83	103.74	107.16
20	B	602	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
20	c	511	CLA	CBC-CAC-C3C	-2.83	104.62	112.43
32	O	302	HTG	C1-O5-C5	2.83	117.80	112.58
22	D	405	BCR	C36-C18-C19	2.83	122.54	118.08
20	b	607	CLA	C1-C2-C3	-2.83	121.15	126.04
20	b	612	CLA	CMC-C2C-C1C	2.83	129.34	125.04
23	a	409	SQD	O8-S-C6	2.83	110.24	105.74
20	B	604	CLA	C3C-C4C-NC	2.82	113.74	110.57
20	a	407	CLA	CHA-C4D-ND	2.82	138.41	132.50
20	c	505	CLA	C3C-C4C-NC	2.82	113.73	110.57
20	B	613	CLA	CHA-C4D-ND	2.82	138.40	132.50
20	c	504	CLA	CHC-C4B-NB	2.82	127.24	124.26
32	v	210	HTG	O5-C1-S1	2.82	116.57	109.82
20	c	504	CLA	CMB-C2B-C1B	2.82	129.66	125.37
20	C	510	CLA	CAC-C3C-C4C	2.82	128.47	124.81
20	C	504	CLA	C1-C2-C3	-2.82	121.17	126.04
32	b	625	HTG	C1-C2-C3	2.82	116.15	110.59
20	b	608	CLA	CAC-C3C-C4C	2.82	128.46	124.81
22	k	101	BCR	C3-C4-C5	-2.82	109.05	114.08
20	b	605	CLA	O2A-CGA-O1A	-2.81	116.49	123.59
20	b	615	CLA	C4D-CHA-C1A	-2.81	117.83	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	534	HTG	O5-C5-C4	2.81	114.80	109.69
20	b	604	CLA	C4D-CHA-C1A	-2.81	117.83	121.25
20	b	609	CLA	CHD-C4C-NC	2.81	128.63	124.20
27	d	412	PL9	C21-C19-C18	-2.81	115.44	121.12
24	c	518	LMG	C3-C4-C5	2.81	115.25	110.24
34	B	626	LMT	O1'-C1'-C2'	2.81	112.68	108.30
20	c	512	CLA	C1-O2A-CGA	2.81	123.81	116.44
24	C	519	LMG	O8-C28-O10	-2.81	116.51	123.59
20	C	508	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
22	c	514	BCR	C21-C20-C19	-2.80	114.47	123.22
20	C	502	CLA	C16-C17-C18	-2.80	102.78	115.98
20	b	613	CLA	C1D-ND-C4D	-2.80	104.34	106.33
20	C	512	CLA	CED-O2D-CGD	2.80	122.27	115.94
20	B	611	CLA	C4D-CHA-C1A	-2.80	117.84	121.25
20	a	403	CLA	C4B-CHC-C1C	-2.80	119.70	126.34
20	B	602	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	A	406	SQD	O48-C23-O10	-2.80	116.53	123.59
20	C	503	CLA	C5-C3-C2	-2.80	115.46	121.12
35	c	516	DGD	O1G-C1A-O1A	-2.80	116.53	123.59
37	e	102	HEM	C4A-NA-C1A	2.80	108.09	105.35
22	B	619	BCR	C21-C20-C19	-2.80	114.49	123.22
20	C	512	CLA	CMB-C2B-C1B	2.79	129.62	125.37
20	b	613	CLA	C2A-C1A-CHA	-2.79	118.97	123.86
20	A	404	CLA	C3D-C4D-ND	2.79	114.75	110.24
20	B	611	CLA	CHD-C4C-NC	2.79	128.60	124.20
20	A	404	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
34	z	102	LMT	O5'-C1'-C2'	-2.79	104.44	110.35
20	a	403	CLA	C3B-C2B-C1B	-2.79	103.80	107.16
20	C	511	CLA	C1-O2A-CGA	2.79	123.76	116.44
20	c	509	CLA	C1D-ND-C4D	-2.79	104.36	106.33
22	t	101	BCR	C34-C9-C8	2.78	122.46	118.08
20	C	510	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
20	C	510	CLA	CMB-C2B-C1B	2.78	129.61	125.37
20	C	513	CLA	CHD-C4C-NC	2.78	128.59	124.20
20	B	603	CLA	C1-O2A-CGA	2.78	123.73	116.44
20	b	604	CLA	OBD-CAD-C3D	-2.78	121.83	128.52
20	c	510	CLA	CMB-C2B-C1B	2.78	129.60	125.37
20	b	608	CLA	CHA-C4D-ND	2.78	138.31	132.50
20	b	608	CLA	CMB-C2B-C1B	2.77	129.59	125.37
20	A	404	CLA	C1D-CHD-C4C	-2.77	120.08	126.06
20	a	404	CLA	C1-C2-C3	-2.77	121.25	126.04
38	H	101	RRX	C16-C17-C18	-2.77	123.35	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	v	201	HEC	C4B-NB-C1B	2.77	107.93	105.07
27	a	415	PL9	C40-C39-C41	2.77	119.93	115.27
20	b	616	CLA	CMD-C2D-C1D	2.77	129.59	124.71
35	c	517	DGD	O6D-C1D-O3G	-2.76	103.43	109.97
20	B	607	CLA	CAC-C3C-C2C	2.76	132.26	127.53
27	a	415	PL9	C42-C43-C44	-2.76	121.00	127.66
20	c	509	CLA	CHA-C4D-ND	2.76	138.28	132.50
20	B	612	CLA	C1D-ND-C4D	-2.76	104.37	106.33
35	C	516	DGD	C3D-C4D-C5D	-2.76	105.31	110.24
38	x	101	RRX	C38-C26-C25	-2.76	121.43	124.53
22	K	101	BCR	C7-C8-C9	-2.76	122.07	126.23
20	b	618	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
20	B	606	CLA	C2A-C1A-CHA	-2.76	119.04	123.86
20	c	506	CLA	CED-O2D-CGD	2.76	122.17	115.94
20	B	612	CLA	CMB-C2B-C1B	2.76	129.57	125.37
22	t	101	BCR	C21-C20-C19	-2.75	114.62	123.22
20	C	506	CLA	CHD-C4C-NC	2.75	128.54	124.20
27	d	412	PL9	C15-C14-C16	2.75	119.90	115.27
40	v	201	HEC	CMD-C2D-C1D	2.75	129.23	125.04
20	C	502	CLA	CHC-C4B-NB	2.75	127.17	124.26
20	c	504	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
20	B	605	CLA	CAC-C3C-C4C	2.75	128.38	124.81
27	D	412	PL9	C36-C37-C38	-2.75	102.85	111.88
38	H	101	RRX	C34-C9-C8	2.74	122.40	118.08
32	B	632	HTG	C1-O5-C5	2.74	117.64	112.58
20	d	403	CLA	CHA-C4D-ND	2.74	138.24	132.50
20	B	604	CLA	C1D-CHD-C4C	-2.74	120.14	126.06
22	k	102	BCR	C11-C10-C9	-2.74	123.40	127.31
20	b	604	CLA	CHD-C4C-C3C	-2.74	120.81	124.84
20	C	509	CLA	C3C-C4C-NC	2.74	113.64	110.57
20	c	508	CLA	CMA-C3A-C4A	-2.74	104.41	111.77
20	A	404	CLA	CHD-C4C-NC	2.74	128.52	124.20
20	C	507	CLA	C1D-CHD-C4C	-2.74	120.15	126.06
38	x	101	RRX	C24-C23-C22	-2.74	122.10	126.23
20	C	507	CLA	C4D-CHA-C1A	-2.74	117.92	121.25
23	F	101	SQD	O48-C23-C24	2.74	120.50	111.91
20	B	607	CLA	C3C-C4C-NC	2.74	113.64	110.57
20	C	511	CLA	C3B-C4B-NB	2.74	113.05	110.52
20	D	401	CLA	CAC-C3C-C4C	2.73	128.36	124.81
20	B	610	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	b	622	SQD	C4-C3-C2	2.73	115.59	110.82
20	b	603	CLA	O2A-CGA-CBA	2.73	120.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	102	LMT	O5'-C5'-C6'	2.73	113.22	106.44
20	B	611	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
20	C	502	CLA	C3C-C4C-NC	2.72	113.63	110.57
27	D	412	PL9	C36-C34-C33	-2.72	115.60	121.12
20	A	401	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
20	c	513	CLA	O2A-CGA-CBA	2.72	120.45	111.91
34	B	626	LMT	O5'-C5'-C6'	2.72	113.20	106.44
20	B	604	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
20	B	614	CLA	CHA-C4D-ND	2.72	138.19	132.50
22	c	514	BCR	C38-C26-C25	-2.72	121.47	124.53
20	C	501	CLA	C1-O2A-CGA	2.72	123.58	116.44
35	D	406	DGD	O1G-C1A-C2A	2.72	120.44	111.91
20	B	616	CLA	C4D-CHA-C1A	-2.72	117.94	121.25
20	C	506	CLA	C3C-C4C-NC	2.72	113.62	110.57
20	b	616	CLA	C4-C3-C5	2.72	119.84	115.27
20	C	509	CLA	CHA-C4D-ND	2.72	138.18	132.50
20	D	404	CLA	CHB-C1B-NB	-2.72	121.38	124.26
20	b	617	CLA	C4-C3-C5	2.72	119.84	115.27
20	B	609	CLA	C3C-C4C-NC	2.72	113.62	110.57
22	B	617	BCR	C21-C20-C19	-2.71	114.75	123.22
20	b	609	CLA	O2D-CGD-CBD	2.71	116.09	111.27
20	D	404	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
20	A	401	CLA	CHD-C1D-ND	-2.71	121.96	124.45
20	C	507	CLA	CMD-C2D-C1D	2.71	129.49	124.71
20	c	505	CLA	C4D-CHA-C1A	-2.71	117.95	121.25
34	c	523	LMT	O1'-C1'-C2'	2.71	112.53	108.30
20	B	612	CLA	CHD-C1D-ND	-2.71	121.97	124.45
20	C	504	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
20	c	512	CLA	CBA-CAA-C2A	-2.71	105.87	113.86
36	d	406	LHG	C6-O8-C23	2.71	127.14	117.12
20	b	606	CLA	C4-C3-C5	2.71	119.82	115.27
20	c	503	CLA	C1-C2-C3	-2.70	121.36	126.04
20	c	508	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	B	606	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
23	a	409	SQD	O5-C1-C2	-2.70	104.63	110.35
20	B	614	CLA	CHD-C4C-NC	2.70	128.46	124.20
20	B	603	CLA	CMA-C3A-C4A	-2.70	104.52	111.77
20	D	404	CLA	CBC-CAC-C3C	-2.70	105.00	112.43
22	t	101	BCR	C35-C13-C12	2.70	122.33	118.08
20	a	407	CLA	CMD-C2D-C3D	2.69	133.81	127.61
20	C	511	CLA	C1D-ND-C4D	-2.69	104.42	106.33
24	C	519	LMG	C8-O7-C10	-2.69	111.17	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	504	CLA	C1-O2A-CGA	2.69	123.50	116.44
20	b	612	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
20	C	508	CLA	CMD-C2D-C1D	2.69	129.45	124.71
20	c	512	CLA	CMC-C2C-C1C	2.69	129.13	125.04
20	C	513	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
20	b	608	CLA	C1-C2-C3	-2.69	121.40	126.04
20	d	404	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
20	A	402	CLA	CAC-C3C-C2C	-2.68	122.94	127.53
22	K	102	BCR	C20-C21-C22	-2.68	123.48	127.31
20	c	508	CLA	C1-C2-C3	-2.68	121.40	126.04
20	b	617	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
20	B	605	CLA	C6-C5-C3	-2.68	106.42	113.45
24	C	524	LMG	O1-C1-C2	2.68	112.49	108.30
22	A	405	BCR	C15-C16-C17	-2.68	117.98	123.47
20	A	402	CLA	CMB-C2B-C1B	2.68	129.45	125.37
20	C	512	CLA	CHD-C4C-NC	2.68	128.43	124.20
32	c	521	HTG	O5-C5-C4	2.68	114.56	109.69
20	c	502	CLA	C4D-CHA-C1A	-2.68	117.99	121.25
36	D	407	LHG	C11-C10-C9	-2.68	100.83	114.42
20	c	501	CLA	C3D-C4D-ND	2.68	114.57	110.24
35	H	102	DGD	O3G-C3G-C2G	-2.68	104.44	110.90
20	B	615	CLA	CHB-C1B-NB	-2.67	121.43	124.26
22	t	101	BCR	C23-C24-C25	-2.67	119.69	127.20
20	D	404	CLA	C4-C3-C5	2.67	119.77	115.27
20	B	611	CLA	CHD-C1D-ND	-2.67	122.00	124.45
20	c	512	CLA	O2A-CGA-CBA	2.67	120.29	111.91
20	d	403	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
20	B	612	CLA	C3B-C4B-NB	2.67	112.99	110.52
22	B	618	BCR	C24-C23-C22	-2.67	122.20	126.23
20	b	614	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
20	B	602	CLA	C4-C3-C2	-2.66	116.85	123.68
27	A	411	PL9	C25-C24-C26	2.66	119.75	115.27
20	c	501	CLA	C3C-C4C-NC	2.66	113.55	110.57
22	t	101	BCR	C38-C26-C25	-2.66	121.54	124.53
35	h	101	DGD	O1G-C1A-O1A	-2.66	116.89	123.59
20	C	504	CLA	CMC-C2C-C1C	2.66	129.08	125.04
20	A	402	CLA	C4-C3-C5	2.66	119.74	115.27
20	b	616	CLA	C4-C3-C2	-2.65	116.87	123.68
20	b	612	CLA	CHD-C4C-NC	2.65	128.38	124.20
20	C	504	CLA	C3B-C4B-NB	2.65	112.98	110.52
20	C	503	CLA	CAC-C3C-C4C	2.65	128.25	124.81
20	a	407	CLA	CHD-C4C-NC	2.65	128.38	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	511	CLA	CMB-C2B-C1B	2.65	129.40	125.37
32	B	622	HTG	O2-C2-C3	-2.64	104.24	110.35
20	C	513	CLA	C4-C3-C5	2.64	119.72	115.27
20	b	605	CLA	C4A-NA-C1A	2.64	107.89	106.71
20	B	610	CLA	CHD-C1D-ND	-2.64	122.03	124.45
21	D	403	PHO	C4-C3-C5	2.64	119.71	115.27
20	c	505	CLA	CHA-C4D-ND	2.64	138.02	132.50
27	a	415	PL9	C10-C9-C11	2.64	119.71	115.27
20	C	505	CLA	O2A-CGA-O1A	-2.64	116.93	123.59
20	b	609	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
20	B	609	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
20	A	402	CLA	CHD-C4C-NC	2.63	128.34	124.20
20	D	401	CLA	C4-C3-C5	2.63	119.69	115.27
22	a	408	BCR	C35-C13-C12	2.63	122.22	118.08
20	C	505	CLA	C7-C6-C5	-2.63	106.22	113.36
20	b	606	CLA	C6-C5-C3	-2.63	106.57	113.45
20	a	403	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
36	D	408	LHG	C13-C12-C11	-2.63	101.10	114.42
20	b	609	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
20	b	615	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
21	a	406	PHO	CED-O2D-CGD	2.62	121.87	115.94
20	B	612	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
20	B	604	CLA	CMC-C2C-C1C	2.62	129.03	125.04
20	a	403	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
20	c	503	CLA	C4D-CHA-C1A	-2.62	118.06	121.25
27	a	415	PL9	C37-C38-C39	-2.62	121.36	127.66
20	B	605	CLA	C3B-C2B-C1B	-2.62	104.00	107.16
37	E	104	HEM	C2A-C1A-NA	-2.62	107.22	110.15
23	A	406	SQD	O3-C3-C4	2.62	116.40	110.35
20	d	402	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
21	a	405	PHO	C4D-CHA-CBD	-2.62	107.33	108.52
20	B	616	CLA	C1D-ND-C4D	-2.61	104.48	106.33
23	b	622	SQD	O47-C7-O49	-2.61	117.39	123.70
20	B	613	CLA	CAC-C3C-C2C	-2.61	123.06	127.53
20	a	404	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
20	b	612	CLA	C1D-ND-C4D	-2.61	104.48	106.33
20	b	615	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
35	C	517	DGD	O2G-C1B-O1B	-2.60	117.41	123.70
20	c	508	CLA	C7-C6-C5	-2.60	106.30	113.36
20	B	607	CLA	C1-O2A-CGA	2.60	123.27	116.44
22	j	102	BCR	C16-C17-C18	-2.60	123.60	127.31
35	H	102	DGD	C2G-O2G-C1B	-2.60	111.40	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	518	LMG	O8-C28-C29	2.60	120.06	111.91
23	F	101	SQD	O6-C44-C45	2.60	113.73	108.76
22	j	102	BCR	C33-C5-C6	-2.59	121.62	124.53
20	c	513	CLA	C1D-ND-C4D	-2.59	104.49	106.33
20	A	401	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
20	D	401	CLA	CHD-C1D-ND	-2.59	122.07	124.45
20	b	605	CLA	CHD-C4C-NC	2.59	128.29	124.20
20	b	618	CLA	O2A-CGA-CBA	2.59	120.04	111.91
20	b	606	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
20	B	607	CLA	C4-C3-C5	2.59	119.63	115.27
20	d	403	CLA	CAC-C3C-C4C	2.59	128.17	124.81
20	A	404	CLA	O2D-CGD-CBD	2.59	115.87	111.27
20	C	507	CLA	C7-C6-C5	-2.59	106.33	113.36
20	B	613	CLA	CHD-C4C-NC	2.59	128.28	124.20
20	A	402	CLA	CHC-C1C-C2C	-2.59	119.54	126.73
20	D	401	CLA	CAA-CBA-CGA	-2.59	105.69	113.25
20	C	506	CLA	CMD-C2D-C1D	2.59	129.27	124.71
22	A	405	BCR	C24-C23-C22	-2.59	122.33	126.23
20	C	513	CLA	C1D-CHD-C4C	-2.59	120.48	126.06
24	c	519	LMG	O5-C6-C5	-2.59	102.42	111.29
20	B	614	CLA	C16-C15-C13	-2.58	107.56	115.92
20	B	605	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
40	V	201	HEC	CBB-CAB-C3B	2.58	119.55	112.43
20	b	605	CLA	CHC-C1C-NC	-2.58	120.28	124.20
20	C	508	CLA	O2D-CGD-CBD	2.58	115.86	111.27
20	c	506	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
20	b	603	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
20	B	608	CLA	C3C-C4C-NC	2.58	113.46	110.57
20	B	608	CLA	C3B-C4B-NB	2.58	112.91	110.52
20	B	613	CLA	C3C-C4C-NC	2.58	113.46	110.57
22	B	617	BCR	C34-C9-C10	-2.57	119.32	122.92
20	d	404	CLA	O2D-CGD-CBD	2.57	115.84	111.27
20	c	510	CLA	C3C-C4C-NC	2.57	113.46	110.57
22	k	101	BCR	C20-C21-C22	-2.57	123.64	127.31
32	b	601	HTG	C2'-C1'-S1	-2.57	104.09	112.40
20	c	503	CLA	CMC-C2C-C1C	2.57	128.96	125.04
32	C	534	HTG	C1-O5-C5	2.57	117.32	112.58
20	B	614	CLA	O2A-CGA-O1A	-2.57	117.12	123.59
20	c	510	CLA	CMC-C2C-C1C	2.57	128.95	125.04
20	B	605	CLA	C1D-CHD-C4C	-2.56	120.53	126.06
20	b	607	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
20	c	503	CLA	O2D-CGD-O1D	-2.56	118.83	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	E	101	LMT	C4'-C3'-C2'	2.56	115.30	110.82
35	C	518	DGD	O2G-C1B-C2B	2.56	117.02	111.50
20	b	607	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
20	c	509	CLA	CMD-C2D-C1D	2.56	129.22	124.71
20	b	608	CLA	C3C-C4C-NC	2.56	113.44	110.57
35	d	416	DGD	O6D-C5D-C4D	2.56	114.34	109.69
20	c	509	CLA	O2D-CGD-CBD	2.56	115.81	111.27
20	A	404	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
20	c	513	CLA	C4D-CHA-C1A	-2.55	118.14	121.25
20	c	508	CLA	CHA-C4D-ND	2.55	137.84	132.50
22	d	405	BCR	C10-C11-C12	-2.55	115.25	123.22
20	B	612	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
24	C	524	LMG	O7-C10-O9	-2.55	117.54	123.70
22	C	515	BCR	C33-C5-C6	-2.55	121.67	124.53
20	b	618	CLA	C4D-CHA-C1A	-2.55	118.15	121.25
22	t	101	BCR	C7-C6-C5	-2.55	115.29	121.46
20	d	404	CLA	CHB-C4A-NA	2.55	128.03	124.51
20	B	605	CLA	CGD-CBD-CAD	-2.55	102.48	110.73
20	b	614	CLA	C4-C3-C5	2.55	119.56	115.27
21	A	403	PHO	CMB-C2B-C3B	2.55	129.44	124.68
20	b	603	CLA	O2A-C1-C2	2.54	115.32	108.64
20	C	511	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
20	b	615	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
20	B	609	CLA	C1-O2A-CGA	2.54	123.11	116.44
20	B	607	CLA	O2A-CGA-CBA	2.54	119.88	111.91
20	D	401	CLA	O2D-CGD-CBD	2.54	115.78	111.27
22	D	405	BCR	C10-C11-C12	-2.54	115.29	123.22
20	A	404	CLA	CAC-C3C-C4C	2.54	128.10	124.81
20	C	502	CLA	CED-O2D-CGD	2.54	121.67	115.94
34	I	101	LMT	C3'-C4'-C5'	-2.54	105.11	110.93
20	a	403	CLA	O2A-CGA-CBA	2.53	119.86	111.91
20	C	509	CLA	CAC-C3C-C4C	2.53	128.10	124.81
23	A	412	SQD	O48-C46-C45	2.53	115.80	108.43
24	B	620	LMG	O6-C5-C6	2.53	112.73	106.44
20	D	402	CLA	CMC-C2C-C1C	2.53	128.89	125.04
20	B	606	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
20	b	610	CLA	C3C-C4C-NC	2.53	113.41	110.57
20	B	608	CLA	CHC-C4B-NB	2.53	126.93	124.26
20	b	609	CLA	C1D-ND-C4D	2.53	108.13	106.33
20	c	512	CLA	CMB-C2B-C1B	2.53	129.22	125.37
20	B	603	CLA	CHD-C4C-NC	2.53	128.19	124.20
20	D	404	CLA	CED-O2D-CGD	2.53	121.65	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	606	CLA	CHD-C1D-ND	-2.52	122.13	124.45
20	D	404	CLA	C3B-C4B-NB	2.52	112.86	110.52
24	A	407	LMG	O1-C1-C2	2.52	112.24	108.30
20	B	604	CLA	C4-C3-C5	2.52	119.52	115.27
20	B	614	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
20	c	504	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
20	b	611	CLA	C1-O2A-CGA	2.52	123.06	116.44
20	b	613	CLA	C1D-CHD-C4C	-2.52	120.62	126.06
22	j	102	BCR	C38-C26-C25	-2.52	121.70	124.53
20	B	608	CLA	C4A-NA-C1A	2.52	107.84	106.71
20	a	404	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
20	b	614	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
20	b	605	CLA	C5-C3-C2	-2.52	116.02	121.12
20	c	512	CLA	CAC-C3C-C4C	2.52	128.08	124.81
20	A	402	CLA	CHC-C4B-C3B	-2.52	116.52	127.71
22	c	514	BCR	C11-C10-C9	-2.52	123.72	127.31
34	T	102	LMT	O1'-C1'-C2'	-2.51	104.38	108.30
20	a	404	CLA	C3B-C4B-NB	2.51	112.85	110.52
27	A	411	PL9	C15-C14-C16	2.51	119.50	115.27
20	d	402	CLA	O2A-CGA-CBA	2.51	119.79	111.91
20	B	612	CLA	C4D-CHA-C1A	-2.51	118.19	121.25
20	B	616	CLA	CHB-C1B-NB	-2.51	121.60	124.26
37	E	104	HEM	C1B-NB-C4B	2.51	107.66	105.07
20	b	615	CLA	O2D-CGD-CBD	2.51	115.72	111.27
20	C	509	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
20	c	501	CLA	C2A-C1A-CHA	-2.51	119.48	123.86
20	B	614	CLA	CHC-C4B-NB	2.51	126.91	124.26
20	c	508	CLA	C4-C3-C5	2.51	119.49	115.27
20	c	502	CLA	C16-C17-C18	-2.50	104.18	115.98
36	D	407	LHG	O4-P-O5	2.50	124.62	112.24
20	c	510	CLA	CMD-C2D-C1D	2.50	129.12	124.71
21	D	403	PHO	CMA-C3A-C4A	-2.50	108.90	114.38
20	d	403	CLA	CMD-C2D-C1D	2.50	129.12	124.71
20	D	404	CLA	O2A-C1-C2	-2.50	102.07	108.64
20	C	511	CLA	C1D-CHD-C4C	-2.50	120.67	126.06
20	b	610	CLA	C6-C5-C3	-2.50	106.91	113.45
20	C	510	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
22	d	405	BCR	C2-C1-C6	2.49	114.32	110.48
20	B	611	CLA	C3B-C4B-NB	2.49	112.83	110.52
20	a	407	CLA	C1D-CHD-C4C	-2.49	120.68	126.06
20	b	607	CLA	CHC-C1C-NC	-2.49	120.42	124.20
22	t	101	BCR	C1-C6-C7	2.49	122.82	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	101	LMG	O8-C28-O10	-2.49	117.31	123.59
20	C	512	CLA	CAC-C3C-C4C	2.49	128.04	124.81
22	d	405	BCR	C34-C9-C10	-2.49	119.44	122.92
23	F	101	SQD	C1-O5-C5	-2.49	108.81	113.69
23	F	101	SQD	C3-C4-C5	2.49	114.67	110.24
20	A	402	CLA	C4B-CHC-C1C	-2.49	120.44	126.34
20	c	505	CLA	C4C-C3C-C2C	-2.49	103.27	106.90
20	B	616	CLA	O2D-CGD-CBD	2.49	115.69	111.27
20	B	610	CLA	O2A-CGA-O1A	-2.49	117.32	123.59
20	d	404	CLA	CHB-C1B-NB	-2.48	121.63	124.26
23	a	409	SQD	C45-O47-C7	-2.48	111.67	117.79
22	j	102	BCR	C37-C22-C23	2.48	121.99	118.08
20	c	507	CLA	C4-C3-C5	2.48	119.45	115.27
20	c	505	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
22	K	101	BCR	C37-C22-C23	2.48	121.99	118.08
20	B	607	CLA	C4B-CHC-C1C	-2.48	120.45	126.34
20	B	614	CLA	C7-C6-C5	-2.48	106.62	113.36
20	B	608	CLA	CMD-C2D-C1D	2.48	129.08	124.71
20	c	513	CLA	C4-C3-C5	2.48	119.44	115.27
20	B	615	CLA	CMA-C3A-C4A	-2.48	105.11	111.77
34	m	102	LMT	C1'-O5'-C5'	-2.48	108.82	113.69
24	c	518	LMG	C8-O7-C10	-2.48	111.69	117.79
20	B	607	CLA	C4C-C3C-C2C	-2.48	103.29	106.90
22	T	101	BCR	C33-C5-C6	-2.47	121.75	124.53
34	Z	101	LMT	O1B-C4'-C3'	2.47	113.86	107.28
20	C	501	CLA	CMB-C2B-C1B	2.47	129.14	125.37
32	C	534	HTG	C1-C2-C3	-2.47	105.71	110.59
20	b	608	CLA	O2A-CGA-CBA	2.47	119.67	111.91
21	D	403	PHO	C3D-CAD-CBD	2.47	110.86	107.61
20	C	509	CLA	CHC-C4B-C3B	-2.47	116.72	127.71
20	C	509	CLA	CHB-C1B-NB	-2.47	121.64	124.26
27	a	415	PL9	C45-C44-C46	2.47	119.43	115.27
21	a	406	PHO	CMB-C2B-C3B	2.47	129.30	124.68
20	B	616	CLA	C11-C10-C8	-2.47	107.94	115.92
20	D	402	CLA	CMD-C2D-C3D	2.47	133.29	127.61
20	b	604	CLA	CHB-C1B-NB	-2.47	121.64	124.26
27	d	412	PL9	C31-C32-C33	-2.47	103.77	111.88
20	b	617	CLA	C11-C10-C8	-2.47	107.94	115.92
20	B	608	CLA	CHA-C4D-ND	2.47	137.66	132.50
20	a	407	CLA	C4C-C3C-C2C	-2.47	103.30	106.90
20	B	608	CLA	C1D-CHD-C4C	-2.47	120.74	126.06
20	C	508	CLA	C2A-C1A-CHA	-2.47	119.55	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	618	CLA	CHC-C4B-NB	2.46	126.86	124.26
20	B	608	CLA	CHD-C4C-NC	2.46	128.09	124.20
23	A	406	SQD	C45-O47-C7	-2.46	111.73	117.79
20	c	511	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
20	C	502	CLA	C1D-CHD-C4C	-2.46	120.75	126.06
22	K	101	BCR	C24-C23-C22	-2.46	122.52	126.23
34	z	102	LMT	O1B-C1B-C2B	2.46	114.47	108.10
20	B	601	CLA	CHC-C4B-C3B	-2.46	116.78	127.71
20	b	615	CLA	O2A-CGA-CBA	2.46	119.61	111.91
20	C	505	CLA	CAC-C3C-C4C	2.46	128.00	124.81
20	B	615	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
35	C	518	DGD	O3G-C3G-C2G	-2.45	104.98	110.90
20	b	618	CLA	C4-C3-C2	-2.45	117.39	123.68
36	E	103	LHG	O7-C7-O9	-2.45	117.40	123.59
27	A	411	PL9	C7-C3-C4	2.45	118.87	116.88
20	b	616	CLA	CMC-C2C-C1C	2.45	128.77	125.04
27	d	412	PL9	C25-C24-C26	2.45	119.39	115.27
24	a	410	LMG	O8-C28-C29	2.45	119.59	111.91
20	b	610	CLA	CMD-C2D-C3D	2.45	133.24	127.61
20	B	601	CLA	C4-C3-C5	2.45	119.39	115.27
22	K	101	BCR	C8-C9-C10	-2.45	115.19	118.94
20	C	510	CLA	C1-C2-C3	-2.44	121.82	126.04
20	d	404	CLA	CAC-C3C-C4C	2.44	127.98	124.81
20	c	504	CLA	C1D-CHD-C4C	-2.44	120.79	126.06
22	k	101	BCR	C38-C26-C25	-2.44	121.78	124.53
20	b	604	CLA	CAC-C3C-C4C	2.44	127.98	124.81
20	B	602	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
20	a	404	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
34	I	101	LMT	O3'-C3'-C4'	2.44	116.41	109.94
20	C	505	CLA	C1D-ND-C4D	2.44	108.07	106.33
20	C	506	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
40	v	201	HEC	CHA-C1A-NA	2.44	127.08	124.44
20	a	403	CLA	C1-C2-C3	-2.44	121.83	126.04
20	b	609	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
22	C	515	BCR	C38-C26-C25	-2.44	121.79	124.53
20	A	402	CLA	C1-O2A-CGA	2.44	122.83	116.44
20	A	401	CLA	OBD-CAD-C3D	-2.44	122.66	128.52
32	c	520	HTG	C3-C4-C5	2.44	114.58	110.24
23	A	412	SQD	O5-C1-C2	-2.43	105.20	110.35
20	b	612	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
20	c	506	CLA	CAC-C3C-C4C	2.43	127.97	124.81
20	a	404	CLA	O2A-CGA-CBA	2.43	119.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	D	406	DGD	C3D-C4D-C5D	2.43	114.57	110.24
35	H	102	DGD	C6D-C5D-C4D	2.43	117.16	112.09
20	a	407	CLA	CBC-CAC-C3C	-2.43	105.74	112.43
20	C	505	CLA	O2A-CGA-CBA	2.43	119.52	111.91
22	b	621	BCR	C16-C15-C14	-2.43	118.50	123.47
27	D	412	PL9	C35-C34-C36	2.43	119.35	115.27
20	c	508	CLA	C3B-C4B-NB	2.43	112.77	110.52
20	B	609	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
20	B	616	CLA	CHD-C4C-NC	2.42	128.02	124.20
21	a	405	PHO	CMD-C2D-C3D	2.42	129.21	124.68
22	B	617	BCR	C8-C7-C6	-2.42	120.40	127.20
20	b	609	CLA	CBC-CAC-C3C	-2.42	105.76	112.43
20	b	611	CLA	CMD-C2D-C1D	2.42	128.98	124.71
20	b	615	CLA	C7-C6-C5	-2.42	106.79	113.36
38	H	101	RRX	C38-C26-C25	-2.42	121.81	124.53
23	A	406	SQD	O48-C23-C24	2.41	119.49	111.91
20	d	404	CLA	C3D-C4D-ND	2.41	114.14	110.24
20	c	502	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
22	B	619	BCR	C23-C22-C21	-2.41	115.24	118.94
20	b	615	CLA	CHB-C1B-NB	-2.41	121.70	124.26
20	c	511	CLA	O2A-CGA-CBA	2.41	119.48	111.91
27	A	411	PL9	C32-C33-C34	-2.41	121.85	127.66
20	b	615	CLA	C3B-C2B-C1B	-2.41	104.25	107.16
35	D	406	DGD	O2G-C1B-O1B	-2.41	117.87	123.70
32	d	401	HTG	C1-C2-C3	2.41	115.35	110.59
27	D	412	PL9	C53-C6-C1	2.41	119.92	114.99
20	c	504	CLA	CHA-C4D-ND	2.41	137.54	132.50
36	E	103	LHG	O4-P-O5	2.41	120.11	110.68
20	B	603	CLA	C4D-CHA-C1A	-2.41	118.32	121.25
22	D	405	BCR	C15-C14-C13	-2.41	123.87	127.31
27	d	412	PL9	C42-C41-C39	-2.41	105.06	112.98
20	B	607	CLA	CHC-C4B-C3B	-2.41	117.00	127.71
20	b	613	CLA	C1-C2-C3	-2.41	121.88	126.04
35	h	101	DGD	C6D-C5D-C4D	2.41	117.12	112.09
27	d	412	PL9	C20-C19-C21	2.40	119.32	115.27
20	b	617	CLA	CMD-C2D-C3D	2.40	133.15	127.61
20	D	402	CLA	C1D-CHD-C4C	-2.40	120.87	126.06
22	B	617	BCR	C16-C15-C14	-2.40	118.56	123.47
20	A	401	CLA	C1D-ND-C4D	-2.40	104.63	106.33
20	d	402	CLA	C3B-C2B-C1B	-2.40	104.27	107.16
20	B	612	CLA	C4C-C3C-C2C	-2.40	103.41	106.90
22	B	618	BCR	C28-C27-C26	-2.40	109.80	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	l	101	SQD	O48-C23-O10	-2.40	117.55	123.59
20	B	603	CLA	O2A-CGA-CBA	2.40	119.42	111.91
35	c	516	DGD	O1G-C1A-C2A	2.40	119.42	111.91
20	c	511	CLA	C1D-CHD-C4C	-2.39	120.89	126.06
20	B	616	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	c	519	LMG	O3-C3-C4	-2.39	104.81	110.35
24	j	101	LMG	C9-C8-C7	-2.39	106.13	111.79
35	H	102	DGD	O4D-C4D-C3D	-2.39	104.82	110.35
27	a	415	PL9	C20-C19-C21	2.39	119.29	115.27
20	B	611	CLA	CAC-C3C-C2C	2.39	131.62	127.53
20	b	616	CLA	CHC-C4B-C3B	-2.39	117.08	127.71
20	a	403	CLA	CHC-C1C-NC	2.39	127.83	124.20
20	b	607	CLA	CHC-C4B-NB	2.39	126.78	124.26
22	T	101	BCR	C12-C13-C14	-2.39	115.28	118.94
20	C	505	CLA	C3C-C4C-NC	2.39	113.25	110.57
20	b	605	CLA	C3B-C4B-NB	2.39	112.73	110.52
22	K	102	BCR	C37-C22-C21	-2.39	119.58	122.92
20	b	609	CLA	O2A-CGA-CBA	2.39	119.39	111.91
23	A	412	SQD	O48-C23-O10	-2.39	117.57	123.59
20	C	513	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
20	b	618	CLA	C1D-CHD-C4C	-2.38	120.92	126.06
27	a	415	PL9	C15-C14-C16	2.38	119.28	115.27
20	b	614	CLA	CHC-C1C-NC	-2.38	120.59	124.20
22	d	405	BCR	C2-C3-C4	2.38	116.70	111.38
20	b	614	CLA	C3B-C4B-NB	2.38	112.73	110.52
27	A	411	PL9	O2-C1-C2	-2.38	116.32	121.78
20	c	510	CLA	C3D-C4D-CHA	-2.38	107.27	112.72
28	b	640	DMS	C2-S-C1	2.38	110.69	98.44
20	a	404	CLA	CHA-C4D-ND	2.38	137.48	132.50
20	b	611	CLA	CED-O2D-CGD	2.38	121.32	115.94
20	C	505	CLA	CMC-C2C-C1C	2.38	128.66	125.04
20	B	603	CLA	C1D-CHD-C4C	-2.38	120.92	126.06
35	c	517	DGD	C3A-C2A-C1A	2.38	122.27	113.62
23	a	401	SQD	O9-S-C6	2.38	109.76	106.94
23	A	406	SQD	O9-S-O7	-2.37	105.73	113.95
20	b	608	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
20	c	513	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
20	B	612	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
22	d	405	BCR	C7-C8-C9	-2.37	122.65	126.23
20	B	601	CLA	C4B-CHC-C1C	-2.37	120.71	126.34
20	B	607	CLA	C1-C2-C3	-2.37	121.94	126.04
20	B	609	CLA	C6-C5-C3	-2.37	107.23	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C	534	HTG	C3-C4-C5	2.37	114.47	110.24
20	B	603	CLA	CMB-C2B-C3B	2.37	132.33	126.59
20	A	402	CLA	C3C-C4C-NC	2.37	113.23	110.57
20	B	615	CLA	C1D-CHD-C4C	-2.37	120.94	126.06
20	c	510	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
20	b	611	CLA	C4C-C3C-C2C	-2.37	103.44	106.90
21	a	405	PHO	CMC-C2C-C1C	2.37	129.20	124.73
20	c	507	CLA	C4B-CHC-C1C	-2.37	120.72	126.34
20	d	403	CLA	CHC-C1C-C2C	-2.37	120.16	126.73
20	C	502	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
24	c	519	LMG	O7-C10-O9	-2.37	117.99	123.70
20	b	611	CLA	O2D-CGD-CBD	2.36	115.47	111.27
20	c	509	CLA	O2A-CGA-CBA	2.36	119.33	111.91
20	B	611	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	b	614	CLA	CHC-C4B-C3B	-2.36	117.20	127.71
20	B	616	CLA	C1-O2A-CGA	2.36	122.64	116.44
20	b	613	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
20	C	503	CLA	C4-C3-C5	2.36	119.24	115.27
20	b	605	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
34	Z	101	LMT	O1B-C4'-C5'	2.36	115.91	109.45
27	d	412	PL9	C11-C9-C8	-2.36	116.35	121.12
34	b	627	LMT	C2'-C3'-C4'	2.36	115.06	109.68
20	d	402	CLA	O1D-CGD-CBD	2.35	129.30	124.48
20	B	612	CLA	CMC-C2C-C1C	2.35	128.62	125.04
27	A	411	PL9	C16-C14-C13	-2.35	116.36	121.12
20	b	606	CLA	CMC-C2C-C1C	2.35	128.62	125.04
20	C	511	CLA	CHB-C4A-NA	2.35	127.76	124.51
22	a	408	BCR	C8-C7-C6	-2.35	120.60	127.20
20	C	502	CLA	O2A-CGA-CBA	2.35	119.29	111.91
20	B	615	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
20	c	503	CLA	CMB-C2B-C1B	2.35	128.94	125.37
22	D	405	BCR	C28-C27-C26	-2.35	109.89	114.08
20	C	511	CLA	C4-C3-C5	2.34	119.21	115.27
20	c	509	CLA	CHC-C4B-C3B	-2.34	117.29	127.71
20	C	508	CLA	CMB-C2B-C1B	2.34	128.94	125.37
22	B	618	BCR	C33-C5-C6	-2.34	121.90	124.53
22	B	619	BCR	C37-C22-C21	2.34	126.20	122.92
20	b	612	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
32	V	202	HTG	O2-C2-C1	2.34	114.56	110.27
20	C	501	CLA	CAC-C3C-C4C	2.34	127.84	124.81
36	d	408	LHG	O8-C23-O10	-2.34	117.69	123.59
24	c	519	LMG	O1-C7-C8	-2.34	105.26	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	404	CLA	O2A-CGA-CBA	2.34	119.25	111.91
20	c	503	CLA	C1D-CHD-C4C	-2.34	121.01	126.06
20	c	509	CLA	CHB-C1B-NB	-2.34	121.78	124.26
20	c	506	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
20	b	605	CLA	O2A-CGA-CBA	2.34	119.24	111.91
20	B	609	CLA	CBB-CAB-C3B	-2.34	116.00	127.62
36	d	408	LHG	O8-C23-C24	2.34	119.24	111.91
20	B	609	CLA	C1D-CHD-C4C	-2.33	121.02	126.06
20	A	401	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
20	B	615	CLA	C4-C3-C5	2.33	119.19	115.27
23	a	409	SQD	O9-S-O7	-2.33	105.89	113.95
20	c	503	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
20	b	604	CLA	CMA-C3A-C4A	-2.33	105.52	111.77
20	b	605	CLA	C7-C6-C5	-2.33	107.04	113.36
20	b	616	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
20	A	404	CLA	CMD-C2D-C1D	2.32	128.81	124.71
20	B	602	CLA	C1-O2A-CGA	2.32	122.54	116.44
27	A	411	PL9	O1-C4-C3	-2.32	118.16	120.72
20	B	614	CLA	CAC-C3C-C4C	2.32	127.82	124.81
20	c	501	CLA	C1D-CHD-C4C	-2.32	121.05	126.06
20	d	402	CLA	CMB-C2B-C1B	2.32	128.90	125.37
36	d	408	LHG	O7-C7-C8	2.32	116.50	111.50
20	b	613	CLA	CHD-C4C-NC	2.32	127.86	124.20
20	b	609	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
20	d	403	CLA	CHC-C4B-C3B	-2.32	117.39	127.71
22	C	514	BCR	C23-C24-C25	-2.32	120.69	127.20
20	c	502	CLA	OBD-CAD-C3D	-2.32	122.94	128.52
27	D	412	PL9	C27-C28-C29	-2.31	122.09	127.66
20	C	504	CLA	C4-C3-C5	2.31	119.17	115.27
20	B	601	CLA	C1D-CHD-C4C	-2.31	121.06	126.06
22	A	405	BCR	C37-C22-C21	2.31	126.16	122.92
22	c	514	BCR	C34-C9-C10	-2.31	119.68	122.92
35	c	516	DGD	C6D-O5D-C1E	2.31	118.26	113.74
35	H	102	DGD	O2G-C1B-C2B	2.31	116.48	111.50
20	B	615	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
20	D	401	CLA	C4C-C3C-C2C	-2.31	103.53	106.90
20	d	404	CLA	C6-C7-C8	-2.31	108.45	115.92
22	t	101	BCR	C33-C5-C4	2.31	118.06	113.62
24	J	101	LMG	O7-C10-C11	2.31	116.48	111.50
20	D	401	CLA	CMB-C2B-C3B	2.31	132.18	126.59
22	B	618	BCR	C30-C25-C26	-2.31	119.36	122.61
20	A	404	CLA	C5-C3-C2	-2.31	116.44	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	415	PL9	C35-C34-C36	2.31	119.16	115.27
20	c	502	CLA	CMD-C2D-C3D	2.31	132.93	127.61
20	b	615	CLA	CHA-C4D-ND	2.31	137.33	132.50
20	C	503	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
40	V	201	HEC	CHB-C1B-NB	2.31	126.92	124.42
20	b	603	CLA	CED-O2D-CGD	2.31	121.16	115.94
34	z	102	LMT	O2'-C2'-C3'	2.31	115.68	110.35
27	A	411	PL9	C40-C39-C41	2.31	119.15	115.27
38	x	101	RRX	C16-C15-C14	-2.31	118.75	123.47
20	b	609	CLA	C4C-C3C-C2C	-2.31	103.54	106.90
23	A	406	SQD	O47-C7-O49	-2.30	118.14	123.70
20	d	404	CLA	C1D-CHD-C4C	-2.30	121.10	126.06
20	c	503	CLA	CMD-C2D-C1D	2.30	128.77	124.71
20	d	402	CLA	CMC-C2C-C1C	2.30	128.54	125.04
20	b	617	CLA	C6-C5-C3	-2.30	107.43	113.45
20	B	604	CLA	CHA-C4D-ND	2.30	137.31	132.50
20	b	611	CLA	CHC-C1C-NC	-2.30	120.72	124.20
20	b	605	CLA	C1D-CHD-C4C	-2.30	121.10	126.06
32	V	202	HTG	O5-C5-C6	2.30	112.14	106.44
20	B	613	CLA	CBC-CAC-C3C	-2.30	106.10	112.43
34	M	101	LMT	C3'-C4'-C5'	-2.30	105.66	110.93
20	C	508	CLA	CHD-C4C-NC	2.29	127.82	124.20
35	d	416	DGD	O3G-C1D-C2D	2.29	111.88	108.30
32	d	401	HTG	C2'-C1'-S1	-2.29	104.99	112.40
20	b	616	CLA	CHA-C4D-ND	2.29	137.29	132.50
22	k	101	BCR	C8-C7-C6	-2.29	120.77	127.20
20	c	504	CLA	C3D-C4D-ND	2.29	113.94	110.24
20	C	506	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
20	b	610	CLA	C4A-NA-C1A	2.29	107.73	106.71
22	k	102	BCR	C37-C22-C23	2.29	121.68	118.08
20	C	503	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
34	a	418	LMT	O1B-C4'-C5'	2.28	115.71	109.45
34	m	102	LMT	O1'-C1'-C2'	2.28	111.87	108.30
20	c	513	CLA	CHC-C1C-NC	-2.28	120.74	124.20
20	D	402	CLA	CHA-C4D-ND	2.28	137.27	132.50
20	c	509	CLA	C4-C3-C5	2.28	119.11	115.27
20	B	603	CLA	CHB-C4A-NA	2.28	127.67	124.51
24	C	519	LMG	O6-C5-C6	2.28	112.10	106.44
20	C	506	CLA	O1D-CGD-CBD	-2.28	119.83	124.48
20	C	504	CLA	CMD-C2D-C1D	2.28	128.72	124.71
20	c	501	CLA	O2A-CGA-O1A	-2.27	117.85	123.59
20	B	603	CLA	C4-C3-C5	2.27	119.10	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	501	CLA	CHC-C4B-C3B	-2.27	117.60	127.71
24	C	519	LMG	C9-C8-C7	-2.27	106.41	111.79
20	B	604	CLA	CHC-C4B-C3B	-2.27	117.60	127.71
20	C	503	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
20	B	609	CLA	CHC-C4B-NB	2.27	126.66	124.26
20	b	605	CLA	C1-O2A-CGA	2.27	122.40	116.44
35	c	515	DGD	O1G-C1G-C2G	-2.27	101.83	108.43
20	b	611	CLA	CMC-C2C-C1C	2.27	128.50	125.04
20	C	509	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
20	B	611	CLA	CHB-C1B-NB	-2.27	121.85	124.26
20	B	606	CLA	C4C-C3C-C2C	-2.27	103.59	106.90
20	c	503	CLA	CAC-C3C-C4C	2.27	127.75	124.81
22	D	405	BCR	C40-C30-C25	-2.27	106.62	110.30
20	c	509	CLA	C1-O2A-CGA	2.26	122.39	116.44
20	A	404	CLA	CHA-C4D-ND	2.26	137.24	132.50
32	B	622	HTG	C1-O5-C5	2.26	116.75	112.58
20	b	616	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
20	C	510	CLA	CMC-C2C-C3C	2.26	132.26	126.12
20	C	502	CLA	C3B-C2B-C1B	-2.26	104.43	107.16
36	d	407	LHG	O8-C23-O10	-2.26	117.88	123.59
20	b	612	CLA	CMD-C2D-C1D	2.26	128.70	124.71
20	B	601	CLA	O2A-CGA-CBA	2.26	119.00	111.91
20	c	502	CLA	CMB-C2B-C1B	2.26	128.81	125.37
20	C	503	CLA	C1D-ND-C4D	2.26	107.94	106.33
20	C	502	CLA	C4B-CHC-C1C	-2.26	120.98	126.34
22	j	102	BCR	C8-C9-C10	-2.26	115.48	118.94
20	B	610	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
20	d	403	CLA	CHD-C4C-NC	2.26	127.76	124.20
24	A	407	LMG	O8-C28-C29	2.26	118.99	111.91
20	C	511	CLA	O2A-C1-C2	-2.26	102.70	108.64
20	C	503	CLA	CHC-C1C-NC	-2.26	120.78	124.20
20	c	511	CLA	CHC-C1C-NC	-2.26	120.78	124.20
22	t	101	BCR	C7-C8-C9	-2.26	122.83	126.23
20	B	602	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
20	c	510	CLA	C4D-C3D-CAD	2.25	110.75	108.10
20	b	610	CLA	O2A-CGA-CBA	2.25	118.98	111.91
24	c	519	LMG	O8-C28-O10	-2.25	117.91	123.59
20	b	614	CLA	O2A-CGA-CBA	2.25	118.98	111.91
20	c	510	CLA	O2A-C1-C2	-2.25	102.72	108.64
20	B	606	CLA	OBD-CAD-C3D	-2.25	123.10	128.52
20	B	611	CLA	O2A-CGA-CBA	2.25	118.97	111.91
20	c	510	CLA	C4-C3-C2	-2.25	117.91	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	e	102	HEM	CHD-C4C-NC	2.25	126.87	124.44
20	D	404	CLA	CHD-C4C-NC	2.25	127.75	124.20
23	l	101	SQD	O5-C5-C4	-2.25	105.61	109.69
40	V	201	HEC	CMD-C2D-C1D	2.25	128.46	125.04
20	c	501	CLA	CMC-C2C-C1C	2.25	128.46	125.04
35	C	516	DGD	O1G-C1A-O1A	-2.25	117.92	123.59
20	b	616	CLA	C1D-CHD-C4C	-2.24	121.22	126.06
27	A	411	PL9	C37-C38-C39	-2.24	122.26	127.66
20	b	612	CLA	C4-C3-C5	2.24	119.04	115.27
22	C	515	BCR	C24-C23-C22	-2.24	122.85	126.23
20	B	606	CLA	CMD-C2D-C3D	2.24	132.76	127.61
24	b	623	LMG	C13-C12-C11	2.24	121.24	113.19
36	d	407	LHG	O7-C7-O9	-2.24	118.29	123.70
20	B	616	CLA	C1-C2-C3	-2.24	122.17	126.04
34	a	418	LMT	O3'-C3'-C2'	2.24	115.52	110.35
20	C	511	CLA	C4C-C3C-C2C	-2.24	103.64	106.90
20	C	511	CLA	CBC-CAC-C3C	-2.24	106.27	112.43
20	D	401	CLA	CHB-C1B-C2B	-2.24	120.92	127.24
36	D	409	LHG	O8-C23-O10	-2.24	117.95	123.59
20	B	601	CLA	CMC-C2C-C3C	2.23	132.18	126.12
20	B	615	CLA	C3D-C4D-ND	2.23	113.85	110.24
21	A	403	PHO	C7-C6-C5	-2.23	107.30	113.36
20	c	506	CLA	CHC-C4B-C3B	-2.23	117.79	127.71
32	B	631	HTG	O5-C1-C2	-2.23	107.51	110.31
20	c	508	CLA	CHB-C4A-NA	2.23	127.59	124.51
20	B	610	CLA	C1D-ND-C4D	2.23	107.92	106.33
37	e	102	HEM	C4C-C3C-C2C	2.23	108.58	106.75
20	c	513	CLA	CBB-CAB-C3B	-2.23	116.53	127.62
20	C	512	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
20	B	602	CLA	C4D-CHA-C1A	-2.23	118.54	121.25
20	C	511	CLA	CHC-C4B-C3B	-2.23	117.80	127.71
22	C	514	BCR	C29-C30-C25	2.22	113.91	110.48
35	C	517	DGD	O1G-C1A-O1A	-2.22	117.98	123.59
20	a	403	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
20	C	512	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
20	b	604	CLA	CHC-C1C-NC	-2.22	120.83	124.20
22	T	101	BCR	C20-C21-C22	-2.22	124.14	127.31
20	C	513	CLA	CHB-C1B-NB	-2.22	121.91	124.26
20	B	616	CLA	CBB-CAB-C3B	-2.22	116.57	127.62
20	c	507	CLA	CHC-C4B-C3B	-2.22	117.83	127.71
32	D	417	HTG	C1-C2-C3	2.22	114.97	110.59
36	d	406	LHG	O4-P-O5	2.22	123.22	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	517	DGD	C3E-C4E-C5E	-2.22	106.28	110.24
40	v	201	HEC	C1D-C2D-C3D	-2.22	104.62	106.96
20	B	615	CLA	C3D-C4D-CHA	-2.22	107.65	112.72
34	b	627	LMT	O2'-C2'-C1'	2.22	115.44	110.05
32	B	621	HTG	O4-C4-C3	-2.22	105.22	110.35
20	b	614	CLA	CHD-C4C-NC	2.22	127.70	124.20
22	k	102	BCR	C20-C21-C22	-2.22	124.15	127.31
24	j	101	LMG	O7-C10-C11	2.22	116.28	111.50
27	D	412	PL9	C11-C9-C8	-2.22	116.63	121.12
22	K	101	BCR	C10-C11-C12	-2.21	116.31	123.22
27	A	411	PL9	C51-C49-C50	2.21	119.49	114.60
20	b	603	CLA	O1D-CGD-CBD	-2.21	119.95	124.48
20	d	404	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
35	C	516	DGD	C4A-C3A-C2A	-2.21	105.23	113.19
20	B	610	CLA	C7-C6-C5	-2.21	107.35	113.36
32	B	621	HTG	O3-C3-C4	-2.21	105.24	110.35
20	C	510	CLA	CHC-C1C-C2C	-2.21	120.59	126.73
21	a	406	PHO	C4D-CHA-CBD	2.21	109.52	108.52
20	c	502	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
22	K	101	BCR	C7-C6-C5	-2.21	116.11	121.46
20	C	510	CLA	CHA-C4D-ND	2.21	137.12	132.50
20	a	404	CLA	CHC-C4B-C3B	-2.21	117.89	127.71
20	b	609	CLA	CGD-CBD-CAD	-2.21	103.59	110.73
20	B	610	CLA	CHD-C4C-NC	2.21	127.68	124.20
20	C	505	CLA	O2D-CGD-O1D	-2.21	119.53	123.84
20	C	501	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
22	A	405	BCR	C39-C30-C25	-2.20	106.72	110.30
22	k	102	BCR	C24-C23-C22	-2.20	122.91	126.23
20	c	503	CLA	OBD-CAD-C3D	-2.20	123.22	128.52
36	E	103	LHG	O7-C5-C6	2.20	115.12	108.61
20	D	402	CLA	CHC-C1C-C2C	-2.20	120.61	126.73
24	c	518	LMG	O7-C10-O9	-2.20	118.38	123.70
32	b	625	HTG	C4-C3-C2	2.20	114.67	110.82
20	b	605	CLA	CMD-C2D-C1D	2.20	128.59	124.71
34	z	102	LMT	C1B-O5B-C5B	2.20	118.00	113.69
22	K	101	BCR	C1-C6-C7	2.20	122.00	115.78
20	c	504	CLA	C2A-C1A-CHA	-2.20	120.02	123.86
20	B	610	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
20	B	603	CLA	CHC-C4B-C3B	-2.20	117.94	127.71
36	l	102	LHG	O4-P-O5	2.20	123.10	112.24
20	b	608	CLA	CMD-C2D-C1D	2.20	128.58	124.71
22	K	101	BCR	C21-C20-C19	-2.19	116.37	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	z	102	LMT	O1'-C1'-C2'	2.19	111.73	108.30
20	c	510	CLA	C3B-C4B-NB	2.19	112.55	110.52
20	b	606	CLA	CMD-C2D-C1D	2.19	128.58	124.71
23	f	101	SQD	O48-C23-O10	-2.19	118.06	123.59
20	B	612	CLA	CMD-C2D-C1D	2.19	128.58	124.71
20	A	402	CLA	CHA-C4D-ND	2.19	137.08	132.50
20	C	512	CLA	C1D-CHD-C4C	-2.19	121.34	126.06
20	D	404	CLA	C6-C5-C3	-2.19	107.72	113.45
20	b	609	CLA	CMD-C2D-C1D	2.19	128.57	124.71
20	B	608	CLA	CMC-C2C-C3C	2.19	132.05	126.12
20	b	613	CLA	O2A-C1-C2	-2.19	102.89	108.64
20	b	615	CLA	C3C-C4C-NC	2.18	113.02	110.57
20	C	507	CLA	CED-O2D-CGD	2.18	120.88	115.94
20	B	605	CLA	C4-C3-C5	2.18	118.94	115.27
20	B	608	CLA	CHB-C1B-C2B	-2.18	121.07	127.24
22	t	101	BCR	C2-C1-C6	2.18	113.84	110.48
22	D	405	BCR	C29-C28-C27	-2.18	106.50	111.38
20	c	509	CLA	C4D-C3D-CAD	2.18	110.67	108.10
20	B	601	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
20	c	506	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
35	D	406	DGD	O6D-C5D-C4D	2.18	113.65	109.69
20	c	508	CLA	C1-O2A-CGA	2.18	122.16	116.44
22	b	620	BCR	C33-C5-C6	2.18	126.97	124.53
20	d	404	CLA	CHA-C4D-ND	2.18	137.05	132.50
27	A	411	PL9	C10-C9-C11	2.18	118.93	115.27
36	d	408	LHG	O4-P-O5	2.18	123.00	112.24
20	B	612	CLA	C16-C15-C13	2.18	122.95	115.92
20	a	407	CLA	CHC-C4B-C3B	-2.17	118.03	127.71
20	c	502	CLA	C6-C5-C3	-2.17	107.75	113.45
35	d	416	DGD	C4D-C3D-C2D	2.17	114.62	110.82
22	k	101	BCR	C24-C23-C22	-2.17	122.95	126.23
22	b	621	BCR	C23-C24-C25	-2.17	121.10	127.20
20	b	611	CLA	C4-C3-C5	2.17	118.92	115.27
20	c	506	CLA	O2A-CGA-CBA	2.17	118.72	111.91
20	C	505	CLA	C1D-CHD-C4C	-2.17	121.38	126.06
32	b	625	HTG	C3-C4-C5	-2.17	106.37	110.24
22	c	514	BCR	C29-C30-C25	2.17	113.82	110.48
20	b	610	CLA	C3B-C4B-NB	2.17	112.53	110.52
32	B	621	HTG	O3-C3-C2	2.16	115.35	110.35
20	D	404	CLA	C2A-C1A-CHA	-2.16	120.08	123.86
20	c	509	CLA	C4C-C3C-C2C	-2.16	103.74	106.90
20	c	503	CLA	CHC-C1C-NC	-2.16	120.92	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	402	CLA	CHC-C1C-C2C	-2.16	120.72	126.73
32	B	622	HTG	C3-C4-C5	-2.16	106.38	110.24
34	B	625	LMT	C3'-C4'-C5'	2.16	114.09	110.24
20	B	606	CLA	CHC-C4B-C3B	-2.16	118.09	127.71
20	b	618	CLA	C1-O2A-CGA	2.16	122.11	116.44
20	b	614	CLA	C3D-C4D-ND	2.16	113.73	110.24
20	b	606	CLA	CGD-CBD-CAD	-2.16	103.74	110.73
23	a	401	SQD	C44-O6-C1	-2.16	109.52	113.74
20	b	604	CLA	O2A-CGA-CBA	2.16	118.68	111.91
22	D	405	BCR	C30-C25-C24	2.16	121.88	115.78
22	b	619	BCR	C21-C20-C19	-2.16	116.48	123.22
20	C	510	CLA	CHC-C4B-C3B	-2.16	118.11	127.71
20	d	402	CLA	C3C-C4C-NC	2.16	112.99	110.57
20	a	404	CLA	C4-C3-C5	2.16	118.90	115.27
22	b	621	BCR	C24-C25-C26	-2.16	116.24	121.46
20	a	403	CLA	CMD-C2D-C1D	2.15	128.51	124.71
22	A	405	BCR	C3-C4-C5	-2.15	110.23	114.08
22	k	102	BCR	C16-C17-C18	-2.15	124.24	127.31
20	B	611	CLA	C1D-ND-C4D	-2.15	104.81	106.33
20	b	613	CLA	CAC-C3C-C4C	2.15	127.60	124.81
20	b	616	CLA	C3D-C4D-ND	2.15	113.72	110.24
20	B	605	CLA	C3B-C4B-NB	2.15	112.51	110.52
20	b	604	CLA	C3C-C4C-NC	2.15	112.98	110.57
20	b	609	CLA	C3C-C4C-NC	2.15	112.98	110.57
20	b	614	CLA	CMD-C2D-C1D	2.15	128.50	124.71
24	C	524	LMG	O6-C5-C6	2.15	111.78	106.44
20	D	401	CLA	CHC-C4B-C3B	-2.15	118.16	127.71
20	c	501	CLA	O2A-CGA-CBA	2.15	118.64	111.91
36	l	102	LHG	O7-C7-C8	2.15	116.13	111.50
20	c	506	CLA	C1-C2-C3	-2.14	122.33	126.04
22	B	617	BCR	C40-C30-C25	-2.14	106.83	110.30
20	C	508	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	B	616	CLA	C3C-C4C-NC	2.14	112.97	110.57
32	B	623	HTG	O5-C1-C2	2.14	113.00	110.31
20	C	509	CLA	CHC-C1C-NC	-2.14	120.96	124.20
22	t	101	BCR	C8-C9-C10	-2.14	115.66	118.94
20	b	617	CLA	CHC-C4B-C3B	-2.14	118.20	127.71
20	B	602	CLA	C5-C3-C2	2.14	125.44	121.12
28	U	902	DMS	O-S-C1	2.14	117.44	106.54
20	b	603	CLA	C3D-C4D-CHA	-2.14	107.84	112.72
20	c	510	CLA	CED-O2D-CGD	2.13	120.76	115.94
23	b	622	SQD	O48-C23-O10	-2.13	118.21	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	607	CLA	C7-C6-C5	-2.13	107.57	113.36
20	c	506	CLA	C3C-C4C-NC	2.13	112.96	110.57
20	b	610	CLA	CHC-C1C-C2C	-2.13	120.81	126.73
20	D	402	CLA	CAC-C3C-C2C	-2.13	123.88	127.53
20	b	614	CLA	C4B-CHC-C1C	-2.13	121.28	126.34
20	B	601	CLA	C4-C3-C2	-2.13	118.21	123.68
20	A	402	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
20	B	603	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
20	d	404	CLA	CHC-C4B-C3B	-2.13	118.23	127.71
23	f	101	SQD	O47-C7-O49	-2.13	118.73	122.96
21	a	406	PHO	C1A-C2A-C3A	-2.13	100.81	102.84
27	a	415	PL9	C26-C24-C23	-2.13	116.81	121.12
27	d	412	PL9	C22-C23-C24	-2.13	122.54	127.66
40	v	201	HEC	CMB-C2B-C1B	-2.13	121.80	125.04
23	a	401	SQD	C1-C2-C3	-2.13	105.57	110.00
24	j	101	LMG	O8-C28-O10	-2.13	118.23	123.59
20	C	503	CLA	CMB-C2B-C1B	2.12	128.60	125.37
20	b	605	CLA	CHC-C4B-C3B	-2.12	118.27	127.71
24	J	101	LMG	O7-C10-O9	-2.12	118.57	123.70
27	D	412	PL9	C2-C3-C4	2.12	121.72	118.80
27	d	412	PL9	C35-C34-C36	2.12	118.84	115.27
20	c	505	CLA	CMD-C2D-C1D	2.12	128.45	124.71
20	B	613	CLA	CBB-CAB-C3B	-2.12	117.07	127.62
20	c	510	CLA	O2A-CGA-CBA	2.12	118.56	111.91
20	C	502	CLA	C1-C2-C3	-2.12	122.38	126.04
22	a	408	BCR	C38-C26-C25	-2.12	122.15	124.53
20	A	402	CLA	C3D-C4D-ND	2.12	113.67	110.24
20	c	505	CLA	C7-C6-C5	-2.12	107.61	113.36
20	b	609	CLA	C5-C3-C2	-2.12	116.83	121.12
22	a	408	BCR	C33-C5-C6	-2.12	122.15	124.53
20	C	512	CLA	CHB-C4A-NA	2.12	127.44	124.51
32	C	521	HTG	O5-C1-C2	2.12	112.97	110.31
20	c	507	CLA	C3B-C4B-NB	2.12	112.48	110.52
35	H	102	DGD	O5E-C6E-C5E	-2.12	104.03	111.29
20	C	502	CLA	C4C-C3C-C2C	-2.11	103.81	106.90
20	B	613	CLA	O2A-CGA-CBA	2.11	118.54	111.91
20	D	401	CLA	C14-C13-C15	-2.11	103.64	111.29
20	b	612	CLA	C3C-C4C-NC	2.11	112.94	110.57
20	B	609	CLA	C11-C10-C8	-2.11	109.09	115.92
20	C	508	CLA	O2A-CGA-CBA	2.11	118.54	111.91
20	b	606	CLA	CHD-C4C-NC	2.11	127.53	124.20
20	b	612	CLA	CHC-C4B-NB	2.11	126.49	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	623	LMG	O7-C10-O9	-2.11	118.60	123.70
35	c	516	DGD	O2G-C1B-O1B	-2.11	118.60	123.70
20	c	513	CLA	C4C-C3C-C2C	-2.11	103.82	106.90
21	a	406	PHO	CBC-CAC-C3C	2.11	115.97	112.88
20	d	404	CLA	C1-C2-C3	-2.11	122.39	126.04
20	c	505	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
20	C	503	CLA	CBB-CAB-C3B	-2.11	117.12	127.62
20	B	605	CLA	CHC-C4B-C3B	-2.11	118.33	127.71
35	c	515	DGD	C6D-O5D-C1E	-2.11	109.62	113.74
23	l	101	SQD	O8-S-C6	2.11	109.10	105.74
22	K	101	BCR	C15-C16-C17	-2.11	119.16	123.47
35	h	101	DGD	O3G-C3G-C2G	-2.11	105.82	110.90
20	b	617	CLA	C5-C3-C2	-2.11	116.86	121.12
20	A	401	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	c	507	CLA	CMC-C2C-C3C	2.10	131.83	126.12
20	b	615	CLA	CBC-CAC-C3C	-2.10	106.63	112.43
22	T	101	BCR	C21-C20-C19	-2.10	116.65	123.22
22	k	102	BCR	C35-C13-C12	2.10	121.39	118.08
20	a	407	CLA	C2A-C1A-CHA	-2.10	120.18	123.86
36	D	409	LHG	O8-C23-C24	2.10	118.50	111.91
34	E	101	LMT	O5'-C5'-C6'	2.10	111.66	106.44
20	c	502	CLA	CHC-C4B-C3B	-2.10	118.37	127.71
20	B	605	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
20	b	613	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
20	d	404	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	C	511	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
20	b	616	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
22	j	102	BCR	C10-C11-C12	-2.10	116.67	123.22
22	T	101	BCR	C7-C6-C5	-2.10	116.38	121.46
20	c	504	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
20	A	401	CLA	C5-C3-C2	-2.10	116.88	121.12
20	C	511	CLA	CHD-C4C-NC	2.09	127.50	124.20
20	B	605	CLA	O2A-CGA-CBA	2.09	118.47	111.91
20	B	614	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
20	c	509	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	a	407	CLA	O2A-CGA-CBA	2.09	118.47	111.91
20	C	504	CLA	C7-C6-C5	-2.09	107.68	113.36
20	b	608	CLA	C7-C6-C5	-2.09	107.68	113.36
24	j	101	LMG	O8-C28-C29	2.09	118.47	111.91
27	a	415	PL9	C17-C18-C19	-2.09	122.62	127.66
20	C	507	CLA	CMB-C2B-C1B	2.09	128.55	125.37
20	B	609	CLA	C2A-C3A-C4A	-2.09	98.49	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	608	CLA	C4B-CHC-C1C	-2.09	121.38	126.34
35	c	515	DGD	CDB-CCB-CBB	-2.09	103.82	114.42
21	D	403	PHO	C1A-C2A-C3A	-2.09	100.85	102.84
40	V	201	HEC	C2B-C1B-NB	-2.09	107.38	109.88
22	B	618	BCR	C8-C7-C6	-2.09	121.34	127.20
35	C	518	DGD	O1G-C1A-C2A	2.09	118.46	111.91
20	C	513	CLA	CHC-C4B-C3B	-2.09	118.43	127.71
20	b	607	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
20	c	506	CLA	CHB-C1B-NB	-2.08	122.05	124.26
20	b	618	CLA	CED-O2D-CGD	2.08	120.65	115.94
20	b	609	CLA	C4B-CHC-C1C	-2.08	121.39	126.34
38	x	101	RRX	O2-C28-C27	-2.08	105.21	109.68
20	C	508	CLA	C4C-C3C-C2C	-2.08	103.86	106.90
37	E	104	HEM	CAD-C3D-C4D	2.08	128.30	124.66
20	b	604	CLA	C3D-C4D-CHA	-2.08	107.96	112.72
20	C	509	CLA	CED-O2D-CGD	2.08	120.65	115.94
20	D	404	CLA	C3D-C4D-CHA	-2.08	107.96	112.72
34	I	101	LMT	C2'-C3'-C4'	-2.08	104.93	109.68
34	z	102	LMT	O2B-C2B-C3B	2.08	115.16	110.35
20	B	613	CLA	CHC-C4B-C3B	-2.08	118.46	127.71
40	V	201	HEC	O2D-CGD-CBD	2.08	120.70	114.03
20	C	508	CLA	C3B-C4B-NB	2.08	112.44	110.52
20	b	609	CLA	C3B-C4B-NB	2.08	112.44	110.52
34	m	102	LMT	O5B-C5B-C6B	2.07	111.59	106.44
22	b	619	BCR	C15-C14-C13	-2.07	124.35	127.31
20	c	501	CLA	C4-C3-C5	2.07	118.76	115.27
34	M	101	LMT	O5B-C5B-C6B	2.07	111.59	106.44
20	c	509	CLA	CMB-C2B-C1B	2.07	128.53	125.37
22	B	617	BCR	C16-C17-C18	-2.07	124.35	127.31
22	b	619	BCR	C37-C22-C21	2.07	125.82	122.92
20	c	504	CLA	CHC-C4B-C3B	-2.07	118.51	127.71
36	d	407	LHG	O7-C7-C8	2.07	115.96	111.50
20	C	504	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
22	C	514	BCR	C11-C10-C9	-2.07	124.36	127.31
20	b	607	CLA	CHD-C4C-NC	2.07	127.46	124.20
20	d	402	CLA	CHD-C4C-C3C	-2.07	121.80	124.84
20	A	404	CLA	C3D-C4D-CHA	-2.07	108.00	112.72
20	B	613	CLA	C4C-C3C-C2C	-2.07	103.89	106.90
20	b	609	CLA	O2A-C1-C2	-2.07	103.21	108.64
34	c	523	LMT	O5B-C1B-C2B	2.06	114.72	110.35
20	c	501	CLA	CBB-CAB-C3B	-2.06	117.35	127.62
20	B	613	CLA	C3B-C4B-NB	2.06	112.43	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	609	CLA	O2A-CGA-CBA	2.06	118.39	111.91
35	c	515	DGD	O2D-C2D-C1D	-2.06	105.03	110.05
24	j	101	LMG	O1-C7-C8	-2.06	105.92	110.90
20	c	508	CLA	CMD-C2D-C1D	2.06	128.35	124.71
20	B	612	CLA	C4B-CHC-C1C	-2.06	121.45	126.34
20	c	513	CLA	C1-O2A-CGA	2.06	121.85	116.44
20	b	613	CLA	C7-C6-C5	-2.06	107.76	113.36
20	b	618	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
20	c	508	CLA	C3C-C4C-NC	2.06	112.88	110.57
20	C	510	CLA	C4C-C3C-C2C	-2.06	103.90	106.90
22	T	101	BCR	C29-C30-C25	2.05	113.64	110.48
22	K	101	BCR	C20-C21-C22	-2.05	124.38	127.31
22	D	405	BCR	C32-C1-C6	2.05	113.63	110.30
20	b	613	CLA	C6-C5-C3	2.05	118.84	113.45
27	D	412	PL9	C31-C32-C33	-2.05	105.13	111.88
23	a	409	SQD	O48-C23-C24	2.05	118.35	111.91
23	f	101	SQD	O5-C5-C4	2.05	113.42	109.69
22	t	101	BCR	C40-C30-C25	-2.05	106.97	110.30
40	v	201	HEC	CHA-C4D-ND	2.05	126.65	124.42
22	j	102	BCR	C1-C6-C7	2.05	121.58	115.78
22	b	619	BCR	C23-C24-C25	-2.05	121.44	127.20
22	C	514	BCR	C33-C5-C6	-2.05	122.23	124.53
23	b	622	SQD	O9-S-O7	-2.05	106.86	113.95
20	d	402	CLA	CHB-C1B-NB	-2.05	122.09	124.26
20	C	511	CLA	CAC-C3C-C4C	2.05	127.47	124.81
20	C	511	CLA	C3C-C4C-NC	2.05	112.87	110.57
38	H	101	RRX	C34-C9-C10	-2.05	120.06	122.92
28	C	532	DMS	O-S-C2	2.05	116.98	106.54
32	d	401	HTG	C1-O5-C5	2.05	116.35	112.58
22	b	619	BCR	C35-C13-C12	2.05	121.30	118.08
34	I	101	LMT	O1B-C4'-C5'	2.05	115.05	109.45
22	j	102	BCR	C35-C13-C14	-2.05	120.06	122.92
20	B	614	CLA	CBB-CAB-C3B	-2.05	117.44	127.62
20	B	615	CLA	O2A-CGA-CBA	2.04	118.33	111.91
20	B	610	CLA	C1D-CHD-C4C	-2.04	121.65	126.06
20	b	605	CLA	C2A-C3A-C4A	-2.04	98.57	101.87
20	B	604	CLA	C3D-C4D-ND	2.04	113.55	110.24
20	a	404	CLA	C7-C6-C5	-2.04	107.81	113.36
35	C	516	DGD	O1G-C1G-C2G	-2.04	102.48	108.43
34	f	102	LMT	O1B-C4'-C5'	2.04	114.37	109.30
20	b	615	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	c	502	CLA	CBB-CAB-C3B	-2.04	117.47	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	d	403	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
20	C	512	CLA	CMD-C2D-C3D	2.04	132.31	127.61
20	C	509	CLA	C1-O2A-CGA	2.04	121.80	116.44
20	c	502	CLA	CMC-C2C-C1C	2.04	128.15	125.04
20	B	615	CLA	C4D-C3D-CAD	2.04	110.50	108.10
40	V	201	HEC	CHD-C1D-ND	2.04	126.89	124.37
36	D	407	LHG	O7-C7-O9	-2.04	118.78	123.70
20	b	603	CLA	CMC-C2C-C1C	2.04	128.14	125.04
32	O	302	HTG	C4-C3-C2	2.04	114.38	110.82
20	B	601	CLA	O2A-C1-C2	2.04	113.99	108.64
22	k	102	BCR	C15-C14-C13	-2.04	124.40	127.31
20	c	508	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
34	B	626	LMT	O3'-C3'-C4'	-2.04	105.64	110.35
24	C	519	LMG	O7-C10-O9	-2.04	118.78	123.70
20	c	502	CLA	C3B-C4B-NB	2.04	112.40	110.52
22	C	514	BCR	C20-C21-C22	-2.03	124.41	127.31
34	I	101	LMT	C1B-O1B-C4'	2.03	123.00	117.96
35	c	517	DGD	C3D-C4D-C5D	-2.03	106.61	110.24
21	a	405	PHO	CAC-C3C-C4C	2.03	129.43	124.27
20	D	401	CLA	CHC-C1C-C2C	-2.03	121.08	126.73
20	c	506	CLA	O2A-C1-C2	2.03	113.98	108.64
27	d	412	PL9	C37-C36-C34	-2.03	106.29	112.98
22	j	102	BCR	C21-C20-C19	-2.03	116.87	123.22
22	A	405	BCR	C8-C7-C6	-2.03	121.50	127.20
22	b	621	BCR	C23-C22-C21	-2.03	115.83	118.94
20	b	604	CLA	C4B-CHC-C1C	2.03	131.15	126.34
20	b	616	CLA	O2A-CGA-CBA	2.03	118.27	111.91
20	c	503	CLA	C4C-C3C-C2C	-2.03	103.94	106.90
20	c	503	CLA	CHC-C4B-C3B	-2.03	118.69	127.71
22	d	405	BCR	C34-C9-C8	2.03	121.27	118.08
20	C	507	CLA	CHC-C4B-C3B	-2.03	118.69	127.71
27	A	411	PL9	C7-C8-C9	-2.03	123.42	126.79
20	A	402	CLA	CHB-C4A-NA	2.03	127.31	124.51
20	b	603	CLA	CHB-C1B-NB	-2.02	122.11	124.26
20	B	606	CLA	C3D-C4D-CHA	-2.02	108.09	112.72
22	b	620	BCR	C15-C16-C17	-2.02	119.33	123.47
20	b	613	CLA	CHC-C4B-C3B	-2.02	118.71	127.71
20	B	604	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
21	A	403	PHO	C1A-C2A-C3A	-2.02	100.92	102.84
20	C	501	CLA	CHC-C1C-NC	-2.02	121.14	124.20
36	d	407	LHG	C13-C12-C11	-2.02	104.17	114.42
20	A	404	CLA	CBC-CAC-C3C	-2.02	106.86	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	512	CLA	C3C-C4C-NC	2.02	112.83	110.57
34	b	627	LMT	C1-O1'-C1'	2.02	117.19	113.84
22	k	102	BCR	C7-C8-C9	-2.02	123.19	126.23
20	B	616	CLA	CMD-C2D-C3D	2.02	132.25	127.61
32	B	622	HTG	O4-C4-C5	2.02	114.31	109.30
20	A	404	CLA	C4C-C3C-C2C	-2.02	103.96	106.90
20	D	404	CLA	CHC-C4B-C3B	-2.02	118.74	127.71
22	t	101	BCR	C3-C4-C5	-2.02	110.48	114.08
20	b	606	CLA	CHB-C4A-NA	2.01	127.30	124.51
20	b	610	CLA	C5-C3-C2	-2.01	117.05	121.12
20	B	602	CLA	CED-O2D-CGD	2.01	120.49	115.94
21	a	405	PHO	OBD-CAD-C3D	-2.01	124.64	127.98
22	K	101	BCR	C23-C22-C21	-2.01	115.86	118.94
36	d	406	LHG	C11-C10-C9	-2.01	104.22	114.42
22	C	515	BCR	C3-C4-C5	-2.01	110.49	114.08
20	c	502	CLA	C4C-C3C-C2C	-2.01	103.97	106.90
32	B	631	HTG	C6-C5-C4	-2.01	108.30	113.00
22	D	405	BCR	C30-C25-C26	-2.01	119.79	122.61
20	c	510	CLA	CHB-C4A-NA	2.01	127.29	124.51
35	C	516	DGD	C1E-O6E-C5E	2.01	117.63	113.69
20	b	603	CLA	C1-C2-C3	-2.01	122.57	126.04
20	b	615	CLA	C12-C11-C10	-2.01	104.02	113.24
40	v	201	HEC	C4C-NC-C1C	2.01	107.31	105.35
23	A	406	SQD	O5-C1-C2	-2.00	106.11	110.35
20	b	604	CLA	CAA-CBA-CGA	-2.00	107.40	113.25
20	C	503	CLA	C7-C6-C5	-2.00	107.92	113.36
20	B	604	CLA	CMD-C2D-C1D	2.00	128.24	124.71
20	B	616	CLA	C4C-C3C-C2C	-2.00	103.98	106.90
21	A	403	PHO	CBA-CAA-C2A	-2.00	107.96	113.81
20	c	507	CLA	CED-O2D-CGD	2.00	120.46	115.94
20	a	407	CLA	C1-O2A-CGA	2.00	122.54	116.73
20	d	402	CLA	C5-C3-C2	-2.00	117.07	121.12
20	b	603	CLA	CMD-C2D-C1D	2.00	128.24	124.71

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	201	HEC	NA
40	v	201	HEC	NA

All (1416) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	B	601	CLA	C11-C10-C8-C9
20	B	602	CLA	CBA-CGA-O2A-C1
20	B	602	CLA	O1A-CGA-O2A-C1
20	B	602	CLA	CHA-CBD-CGD-O1D
20	B	602	CLA	CHA-CBD-CGD-O2D
20	B	602	CLA	CAD-CBD-CGD-O2D
20	B	606	CLA	C2-C3-C5-C6
20	B	607	CLA	C11-C12-C13-C14
20	B	610	CLA	C2B-C3B-CAB-CBB
20	B	615	CLA	CHA-CBD-CGD-O2D
20	B	615	CLA	CAD-CBD-CGD-O1D
20	C	502	CLA	CHA-CBD-CGD-O1D
20	C	502	CLA	CAD-CBD-CGD-O1D
20	C	508	CLA	CHA-CBD-CGD-O1D
20	C	509	CLA	C11-C10-C8-C9
20	D	402	CLA	CHA-CBD-CGD-O1D
20	b	603	CLA	CHA-CBD-CGD-O2D
20	b	603	CLA	C11-C10-C8-C9
20	b	604	CLA	CHA-CBD-CGD-O1D
20	b	608	CLA	CHA-CBD-CGD-O1D
20	b	608	CLA	CHA-CBD-CGD-O2D
20	b	608	CLA	C6-C7-C8-C10
20	b	616	CLA	CHA-CBD-CGD-O1D
20	b	616	CLA	CHA-CBD-CGD-O2D
20	b	616	CLA	CAD-CBD-CGD-O1D
20	b	616	CLA	CAD-CBD-CGD-O2D
20	b	616	CLA	C4-C3-C5-C6
20	b	618	CLA	C2-C3-C5-C6
20	b	618	CLA	C4-C3-C5-C6
20	c	502	CLA	CHA-CBD-CGD-O2D
20	c	508	CLA	CHA-CBD-CGD-O1D
22	D	405	BCR	C21-C22-C23-C24
22	D	405	BCR	C37-C22-C23-C24
22	D	405	BCR	C23-C24-C25-C30
22	K	101	BCR	C36-C18-C19-C20
22	d	405	BCR	C37-C22-C23-C24
22	k	101	BCR	C7-C8-C9-C10
22	k	101	BCR	C7-C8-C9-C34
22	t	101	BCR	C11-C12-C13-C14
22	t	101	BCR	C11-C12-C13-C35
23	A	412	SQD	C2-C1-O6-C44
23	A	412	SQD	O5-C1-O6-C44
23	F	101	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
23	a	401	SQD	C2-C1-O6-C44
23	a	401	SQD	O6-C44-C45-O47
23	b	622	SQD	O5-C1-O6-C44
23	b	622	SQD	C46-C45-O47-C7
23	b	622	SQD	O49-C7-O47-C45
23	b	622	SQD	C8-C7-O47-C45
23	f	101	SQD	C8-C7-O47-C45
23	f	101	SQD	C5-C6-S-O8
23	l	101	SQD	C8-C7-O47-C45
23	l	101	SQD	O10-C23-O48-C46
23	l	101	SQD	C24-C23-O48-C46
23	l	101	SQD	O5-C5-C6-S
24	C	524	LMG	C11-C10-O7-C8
27	A	411	PL9	C9-C11-C12-C13
27	a	415	PL9	C9-C11-C12-C13
27	a	415	PL9	C14-C16-C17-C18
27	a	415	PL9	C23-C24-C26-C27
27	a	415	PL9	C25-C24-C26-C27
32	B	622	HTG	C2'-C1'-S1-C1
32	B	623	HTG	C2-C1-S1-C1'
32	B	623	HTG	O5-C1-S1-C1'
32	C	520	HTG	C2'-C1'-S1-C1
32	C	521	HTG	C2-C1-S1-C1'
32	C	522	HTG	O5-C1-S1-C1'
32	C	534	HTG	C2'-C1'-S1-C1
32	V	202	HTG	C2-C1-S1-C1'
32	c	520	HTG	C2-C1-S1-C1'
32	c	520	HTG	O5-C1-S1-C1'
32	c	521	HTG	C2'-C1'-S1-C1
32	d	401	HTG	C2-C1-S1-C1'
32	d	401	HTG	O5-C1-S1-C1'
34	B	627	LMT	C2-C1-O1'-C1'
34	a	418	LMT	C2'-C1'-O1'-C1
34	a	418	LMT	O5'-C1'-O1'-C1
34	f	102	LMT	C2'-C1'-O1'-C1
34	f	102	LMT	O5'-C1'-O1'-C1
34	m	101	LMT	O5'-C1'-O1'-C1
34	m	101	LMT	C2-C1-O1'-C1'
35	D	406	DGD	C2B-C1B-O2G-C2G
35	D	406	DGD	C2D-C1D-O3G-C3G
35	D	406	DGD	O6D-C1D-O3G-C3G
36	D	408	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
36	E	103	LHG	O1-C1-C2-C3
36	E	103	LHG	C6-C5-O7-C7
36	L	101	LHG	C4-O6-P-O3
36	L	101	LHG	C4-O6-P-O4
36	L	101	LHG	C4-O6-P-O5
36	d	407	LHG	O1-C1-C2-C3
36	d	407	LHG	C3-O3-P-O5
36	l	102	LHG	C4-O6-P-O3
36	l	102	LHG	C4-O6-P-O4
36	l	102	LHG	C4-O6-P-O5
20	B	611	CLA	C15-C16-C17-C18
23	f	101	SQD	O49-C7-O47-C45
23	F	101	SQD	O10-C23-O48-C46
36	E	103	LHG	O10-C23-O8-C6
34	z	102	LMT	O5B-C1B-O1B-C4'
36	E	103	LHG	C8-C7-O7-C5
36	E	103	LHG	C24-C23-O8-C6
35	d	416	DGD	O1A-C1A-O1G-C1G
36	E	103	LHG	O9-C7-O7-C5
20	b	617	CLA	C13-C15-C16-C17
34	b	627	LMT	C2B-C1B-O1B-C4'
23	l	101	SQD	O49-C7-O47-C45
24	C	524	LMG	O9-C10-O7-C8
34	I	101	LMT	C3'-C4'-O1B-C1B
20	B	601	CLA	C3-C5-C6-C7
20	B	602	CLA	C3-C5-C6-C7
20	b	603	CLA	C3-C5-C6-C7
23	F	101	SQD	C24-C23-O48-C46
20	A	404	CLA	C4-C3-C5-C6
20	B	606	CLA	C4-C3-C5-C6
20	A	404	CLA	C2-C3-C5-C6
20	b	616	CLA	C2-C3-C5-C6
20	C	513	CLA	CBD-CGD-O2D-CED
20	B	615	CLA	C3-C5-C6-C7
23	b	622	SQD	C24-C23-O48-C46
35	d	416	DGD	C2A-C1A-O1G-C1G
32	c	521	HTG	O5-C5-C6-O6
32	v	210	HTG	O5-C5-C6-O6
34	Z	101	LMT	O5B-C5B-C6B-O6B
32	C	520	HTG	S1-C1'-C2'-C3'
32	D	417	HTG	S1-C1'-C2'-C3'
35	D	406	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
32	C	534	HTG	O5-C5-C6-O6
34	m	101	LMT	O5'-C5'-C6'-O6'
34	z	102	LMT	C4'-C5'-C6'-O6'
20	B	605	CLA	C3-C5-C6-C7
20	b	618	CLA	CBD-CGD-O2D-CED
34	b	627	LMT	O5'-C5'-C6'-O6'
34	c	523	LMT	O5'-C5'-C6'-O6'
32	B	622	HTG	C3'-C4'-C5'-C6'
35	c	515	DGD	C2A-C3A-C4A-C5A
36	D	409	LHG	C31-C32-C33-C34
23	b	622	SQD	C31-C32-C33-C34
24	a	410	LMG	C37-C38-C39-C40
32	c	520	HTG	C4-C5-C6-O6
24	b	623	LMG	C10-C11-C12-C13
23	l	101	SQD	C31-C32-C33-C34
34	z	102	LMT	C3'-C4'-O1B-C1B
32	B	623	HTG	O5-C5-C6-O6
34	J	103	LMT	O5'-C5'-C6'-O6'
34	a	418	LMT	O5'-C5'-C6'-O6'
35	d	416	DGD	O6D-C5D-C6D-O5D
32	v	210	HTG	C4-C5-C6-O6
34	b	627	LMT	C4B-C5B-C6B-O6B
23	b	622	SQD	O10-C23-O48-C46
34	B	627	LMT	O1'-C1'-O5'-C5'
32	D	417	HTG	O5-C5-C6-O6
32	c	520	HTG	O5-C5-C6-O6
34	z	102	LMT	O5'-C5'-C6'-O6'
20	B	601	CLA	C4-C3-C5-C6
27	a	415	PL9	C30-C29-C31-C32
20	B	601	CLA	C2-C3-C5-C6
20	b	607	CLA	C2-C3-C5-C6
27	a	415	PL9	C28-C29-C31-C32
24	j	101	LMG	C10-C11-C12-C13
32	B	631	HTG	O5-C5-C6-O6
34	T	102	LMT	O5'-C5'-C6'-O6'
34	f	102	LMT	O5'-C5'-C6'-O6'
24	A	407	LMG	O10-C28-O8-C9
34	Z	101	LMT	C4B-C5B-C6B-O6B
24	a	410	LMG	O6-C1-O1-C7
34	z	102	LMT	O5'-C1'-O1'-C1
27	A	411	PL9	C24-C26-C27-C28
20	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	A	407	LMG	C29-C28-O8-C9
34	f	102	LMT	C4'-C5'-C6'-O6'
40	V	201	HEC	C2C-C3C-CAC-CBC
24	A	407	LMG	C15-C16-C17-C18
34	T	102	LMT	C4'-C5'-C6'-O6'
20	C	513	CLA	O1A-CGA-O2A-C1
24	c	519	LMG	O10-C28-O8-C9
23	f	101	SQD	C24-C23-O48-C46
24	c	519	LMG	C29-C28-O8-C9
35	c	516	DGD	C1A-C2A-C3A-C4A
36	d	408	LHG	C11-C12-C13-C14
32	B	631	HTG	C4-C5-C6-O6
34	b	627	LMT	C4'-C5'-C6'-O6'
32	D	417	HTG	C4-C5-C6-O6
20	B	602	CLA	C10-C11-C12-C13
20	b	618	CLA	C8-C10-C11-C12
36	d	407	LHG	O2-C2-C3-O3
23	A	412	SQD	O6-C44-C45-O47
23	a	409	SQD	C9-C10-C11-C12
24	B	620	LMG	C37-C38-C39-C40
34	J	103	LMT	C4'-C5'-C6'-O6'
20	B	602	CLA	C11-C10-C8-C9
20	C	504	CLA	C11-C12-C13-C14
20	b	603	CLA	C14-C13-C15-C16
20	b	604	CLA	C14-C13-C15-C16
20	c	506	CLA	C6-C7-C8-C9
20	c	513	CLA	C11-C10-C8-C9
20	c	513	CLA	C14-C13-C15-C16
35	D	406	DGD	C7B-C8B-C9B-CAB
32	C	521	HTG	S1-C1'-C2'-C3'
22	d	405	BCR	C21-C22-C23-C24
23	F	101	SQD	O47-C45-C46-O48
35	C	517	DGD	C1B-C2B-C3B-C4B
23	f	101	SQD	O10-C23-O48-C46
20	C	506	CLA	C10-C11-C12-C13
32	B	623	HTG	C4-C5-C6-O6
32	c	521	HTG	C4-C5-C6-O6
20	A	404	CLA	C13-C15-C16-C17
20	A	404	CLA	C15-C16-C17-C18
20	B	612	CLA	C15-C16-C17-C18
20	b	616	CLA	C10-C11-C12-C13
20	c	513	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
20	B	615	CLA	C5-C6-C7-C8
20	D	404	CLA	C8-C10-C11-C12
20	b	616	CLA	C8-C10-C11-C12
20	b	618	CLA	C15-C16-C17-C18
20	c	509	CLA	C13-C15-C16-C17
23	A	412	SQD	C23-C24-C25-C26
23	a	409	SQD	C7-C8-C9-C10
23	b	622	SQD	C23-C24-C25-C26
24	c	519	LMG	C10-C11-C12-C13
24	c	519	LMG	C28-C29-C30-C31
20	B	601	CLA	C10-C11-C12-C13
34	m	101	LMT	O1'-C1-C2-C3
23	a	401	SQD	C23-C24-C25-C26
24	a	410	LMG	C10-C11-C12-C13
32	B	621	HTG	C4-C5-C6-O6
20	B	615	CLA	C8-C10-C11-C12
20	b	614	CLA	C13-C15-C16-C17
20	c	506	CLA	C10-C11-C12-C13
20	A	404	CLA	C12-C13-C15-C16
20	D	401	CLA	C12-C13-C15-C16
20	b	615	CLA	C11-C12-C13-C15
22	T	101	BCR	C13-C14-C15-C16
22	t	101	BCR	C13-C14-C15-C16
20	B	607	CLA	C2A-CAA-CBA-CGA
20	B	602	CLA	O1D-CGD-O2D-CED
34	a	418	LMT	C4'-C5'-C6'-O6'
23	a	401	SQD	O5-C1-O6-C44
34	B	626	LMT	O5'-C1'-O1'-C1
27	A	411	PL9	C19-C21-C22-C23
34	T	102	LMT	O1'-C1-C2-C3
32	b	625	HTG	S1-C1'-C2'-C3'
32	B	621	HTG	O5-C5-C6-O6
36	D	408	LHG	O2-C2-C3-O3
20	A	404	CLA	C3-C5-C6-C7
20	C	507	CLA	C5-C6-C7-C8
20	a	404	CLA	C8-C10-C11-C12
24	A	407	LMG	C10-C11-C12-C13
35	d	416	DGD	C4D-C5D-C6D-O5D
20	B	601	CLA	C13-C15-C16-C17
20	c	513	CLA	C10-C11-C12-C13
20	c	513	CLA	C13-C15-C16-C17
20	C	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
32	C	534	HTG	C4-C5-C6-O6
20	b	606	CLA	C15-C16-C17-C18
20	b	608	CLA	C15-C16-C17-C18
35	D	406	DGD	C2A-C1A-O1G-C1G
32	C	522	HTG	C1'-C2'-C3'-C4'
20	c	506	CLA	C15-C16-C17-C18
32	B	622	HTG	S1-C1'-C2'-C3'
35	c	517	DGD	C1A-C2A-C3A-C4A
36	d	406	LHG	C23-C24-C25-C26
36	D	408	LHG	C1-C2-C3-O3
36	d	407	LHG	C1-C2-C3-O3
36	E	103	LHG	C11-C10-C9-C8
20	B	616	CLA	C10-C11-C12-C13
20	b	605	CLA	C5-C6-C7-C8
20	C	503	CLA	CBD-CGD-O2D-CED
20	b	608	CLA	C16-C17-C18-C20
24	C	524	LMG	O6-C5-C6-O5
40	V	201	HEC	C4C-C3C-CAC-CBC
34	Z	101	LMT	C5'-C4'-O1B-C1B
35	C	517	DGD	C8B-C9B-CAB-CBB
20	B	602	CLA	C13-C15-C16-C17
32	B	622	HTG	C1'-C2'-C3'-C4'
23	A	412	SQD	C28-C29-C30-C31
23	F	101	SQD	C28-C29-C30-C31
23	l	101	SQD	C15-C16-C17-C18
24	A	407	LMG	C11-C12-C13-C14
24	A	407	LMG	C18-C19-C20-C21
24	a	410	LMG	C34-C35-C36-C37
24	c	519	LMG	C16-C17-C18-C19
24	c	519	LMG	C32-C33-C34-C35
24	c	519	LMG	C39-C40-C41-C42
34	m	101	LMT	C7-C8-C9-C10
35	C	518	DGD	CBB-CCB-CDB-CEB
35	c	515	DGD	C5A-C6A-C7A-C8A
35	d	416	DGD	C2A-C3A-C4A-C5A
35	d	416	DGD	C7A-C8A-C9A-CAA
35	h	101	DGD	C6B-C7B-C8B-C9B
36	d	406	LHG	C29-C30-C31-C32
20	C	502	CLA	C16-C17-C18-C20
20	c	502	CLA	C16-C17-C18-C19
23	A	412	SQD	C27-C28-C29-C30
23	a	401	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	a	401	SQD	C29-C30-C31-C32
24	B	620	LMG	C31-C32-C33-C34
24	B	620	LMG	C32-C33-C34-C35
34	b	628	LMT	C5-C6-C7-C8
35	D	406	DGD	C5A-C6A-C7A-C8A
35	D	406	DGD	C8B-C9B-CAB-CBB
36	E	103	LHG	C28-C29-C30-C31
36	L	101	LHG	C27-C28-C29-C30
36	d	408	LHG	C10-C11-C12-C13
23	l	101	SQD	C46-C45-O47-C7
24	C	524	LMG	C9-C8-O7-C10
24	J	101	LMG	O6-C5-C6-O5
24	A	407	LMG	O9-C10-O7-C8
35	C	516	DGD	C7A-C8A-C9A-CAA
35	D	406	DGD	C6A-C7A-C8A-C9A
36	D	407	LHG	C27-C28-C29-C30
36	d	408	LHG	C28-C29-C30-C31
36	l	102	LHG	C27-C28-C29-C30
23	A	406	SQD	C11-C12-C13-C14
23	A	412	SQD	C26-C27-C28-C29
24	B	620	LMG	C15-C16-C17-C18
24	a	410	LMG	C17-C18-C19-C20
24	a	410	LMG	C35-C36-C37-C38
35	D	406	DGD	C2A-C3A-C4A-C5A
35	c	515	DGD	C7A-C8A-C9A-CAA
35	d	416	DGD	C3B-C4B-C5B-C6B
36	D	409	LHG	C15-C16-C17-C18
23	A	406	SQD	C18-C19-C20-C21
24	C	519	LMG	C17-C18-C19-C20
24	C	524	LMG	C33-C34-C35-C36
34	I	101	LMT	O1'-C1-C2-C3
34	z	102	LMT	C5-C6-C7-C8
35	d	416	DGD	CAB-CBB-CCB-CDB
24	J	101	LMG	C10-C11-C12-C13
36	D	407	LHG	C23-C24-C25-C26
20	c	501	CLA	O1D-CGD-O2D-CED
23	b	622	SQD	C2-C1-O6-C44
24	A	407	LMG	C2-C1-O1-C7
34	B	626	LMT	C2'-C1'-O1'-C1
23	l	101	SQD	C29-C30-C31-C32
24	A	407	LMG	C21-C22-C23-C24
24	A	407	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
35	d	416	DGD	C7B-C8B-C9B-CAB
20	d	404	CLA	C13-C15-C16-C17
20	C	506	CLA	C16-C17-C18-C20
20	b	615	CLA	C16-C17-C18-C19
20	b	618	CLA	C16-C17-C18-C20
20	B	607	CLA	O1D-CGD-O2D-CED
34	b	627	LMT	O5B-C5B-C6B-O6B
23	A	406	SQD	C34-C35-C36-C37
23	F	101	SQD	C32-C33-C34-C35
23	b	622	SQD	C24-C25-C26-C27
24	C	519	LMG	C34-C35-C36-C37
34	B	627	LMT	C11-C10-C9-C8
35	h	101	DGD	C6A-C7A-C8A-C9A
36	D	407	LHG	C28-C29-C30-C31
36	D	409	LHG	C28-C29-C30-C31
20	B	604	CLA	C6-C7-C8-C9
20	D	404	CLA	C11-C10-C8-C9
20	b	608	CLA	C6-C7-C8-C9
20	b	612	CLA	C14-C13-C15-C16
24	C	519	LMG	C10-C11-C12-C13
24	c	518	LMG	C10-C11-C12-C13
35	C	517	DGD	C1A-C2A-C3A-C4A
20	A	402	CLA	C10-C11-C12-C13
23	f	101	SQD	C25-C26-C27-C28
24	A	407	LMG	C17-C18-C19-C20
24	C	524	LMG	C19-C20-C21-C22
24	a	410	LMG	C30-C31-C32-C33
34	c	523	LMT	C5-C6-C7-C8
35	C	516	DGD	C8B-C9B-CAB-CBB
35	C	517	DGD	C3A-C4A-C5A-C6A
35	D	406	DGD	C9B-CAB-CBB-CCB
35	c	515	DGD	C8A-C9A-CAA-CBA
20	D	402	CLA	O1D-CGD-O2D-CED
23	A	412	SQD	C9-C10-C11-C12
23	a	401	SQD	C24-C25-C26-C27
23	l	101	SQD	C11-C12-C13-C14
24	C	519	LMG	C14-C15-C16-C17
24	C	519	LMG	C39-C40-C41-C42
34	b	628	LMT	C2-C3-C4-C5
35	c	517	DGD	C8A-C9A-CAA-CBA
36	d	406	LHG	O1-C1-C2-C3
24	A	407	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
24	c	519	LMG	C11-C10-O7-C8
23	A	406	SQD	C31-C32-C33-C34
24	B	620	LMG	C17-C18-C19-C20
24	C	519	LMG	C20-C21-C22-C23
24	C	524	LMG	C34-C35-C36-C37
24	a	410	LMG	C16-C17-C18-C19
34	f	102	LMT	C3-C4-C5-C6
35	D	406	DGD	CCB-CDB-CEB-CFB
36	d	408	LHG	C17-C18-C19-C20
23	F	101	SQD	C23-C24-C25-C26
23	A	406	SQD	C30-C31-C32-C33
23	F	101	SQD	C27-C28-C29-C30
23	a	401	SQD	C27-C28-C29-C30
23	a	409	SQD	C30-C31-C32-C33
24	A	407	LMG	C13-C14-C15-C16
24	B	620	LMG	C35-C36-C37-C38
24	C	519	LMG	C33-C34-C35-C36
24	C	524	LMG	C18-C19-C20-C21
24	b	623	LMG	C32-C33-C34-C35
32	B	623	HTG	C3'-C4'-C5'-C6'
32	B	632	HTG	C3'-C4'-C5'-C6'
32	C	520	HTG	C3'-C4'-C5'-C6'
34	I	101	LMT	C5-C6-C7-C8
35	C	517	DGD	C4B-C5B-C6B-C7B
35	C	518	DGD	CCB-CDB-CEB-CFB
35	D	406	DGD	C6B-C7B-C8B-C9B
35	d	416	DGD	CCB-CDB-CEB-CFB
40	v	201	HEC	C2B-C3B-CAB-CBB
20	B	610	CLA	C4B-C3B-CAB-CBB
20	B	605	CLA	C16-C17-C18-C20
20	C	506	CLA	C16-C17-C18-C19
20	C	507	CLA	C16-C17-C18-C20
20	b	608	CLA	C16-C17-C18-C19
20	b	617	CLA	C16-C17-C18-C19
20	b	617	CLA	C16-C17-C18-C20
20	c	509	CLA	C16-C17-C18-C19
24	A	407	LMG	O6-C1-O1-C7
20	b	617	CLA	C10-C11-C12-C13
23	A	412	SQD	C25-C26-C27-C28
23	a	401	SQD	C25-C26-C27-C28
23	a	409	SQD	C26-C27-C28-C29
24	B	620	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
24	j	101	LMG	C18-C19-C20-C21
34	B	625	LMT	C7-C8-C9-C10
35	d	416	DGD	C6A-C7A-C8A-C9A
36	D	407	LHG	C25-C26-C27-C28
34	b	627	LMT	C1-C2-C3-C4
24	b	623	LMG	C35-C36-C37-C38
34	J	103	LMT	C5-C6-C7-C8
35	C	518	DGD	C9A-CAA-CBA-CCA
35	D	406	DGD	CBB-CCB-CDB-CEB
36	E	103	LHG	C34-C35-C36-C37
20	b	603	CLA	C10-C11-C12-C13
35	D	406	DGD	O1A-C1A-O1G-C1G
23	a	401	SQD	C28-C29-C30-C31
23	b	622	SQD	C33-C34-C35-C36
24	b	623	LMG	C33-C34-C35-C36
24	c	519	LMG	C12-C13-C14-C15
24	j	101	LMG	C32-C33-C34-C35
32	B	623	HTG	C2'-C3'-C4'-C5'
34	E	101	LMT	C2-C3-C4-C5
34	z	102	LMT	C6-C7-C8-C9
35	H	102	DGD	C8A-C9A-CAA-CBA
24	c	519	LMG	C15-C16-C17-C18
24	c	519	LMG	C35-C36-C37-C38
32	B	621	HTG	C3'-C4'-C5'-C6'
34	z	102	LMT	C5'-C4'-O1B-C1B
20	C	512	CLA	O1D-CGD-O2D-CED
23	a	409	SQD	C29-C30-C31-C32
32	B	631	HTG	C2'-C3'-C4'-C5'
32	b	601	HTG	C3'-C4'-C5'-C6'
36	D	408	LHG	C11-C10-C9-C8
20	B	605	CLA	C16-C17-C18-C19
20	C	507	CLA	C16-C17-C18-C19
20	b	618	CLA	C16-C17-C18-C19
23	A	412	SQD	C11-C10-C9-C8
23	a	409	SQD	C11-C10-C9-C8
23	a	409	SQD	C27-C28-C29-C30
23	l	101	SQD	C17-C18-C19-C20
35	c	516	DGD	C3A-C4A-C5A-C6A
35	c	517	DGD	C8B-C9B-CAB-CBB
36	d	406	LHG	C27-C28-C29-C30
34	z	102	LMT	C2B-C1B-O1B-C4'
20	C	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	A	412	SQD	C10-C11-C12-C13
24	A	407	LMG	C20-C21-C22-C23
32	d	401	HTG	C3'-C4'-C5'-C6'
34	I	101	LMT	C4-C5-C6-C7
23	a	409	SQD	C18-C19-C20-C21
23	l	101	SQD	C28-C29-C30-C31
34	T	102	LMT	C6-C7-C8-C9
34	I	101	LMT	C11-C10-C9-C8
34	B	627	LMT	O5'-C1'-O1'-C1
36	E	103	LHG	O1-C1-C2-O2
20	B	616	CLA	C5-C6-C7-C8
20	a	403	CLA	C2C-C3C-CAC-CBC
23	b	622	SQD	C18-C19-C20-C21
23	f	101	SQD	C24-C25-C26-C27
24	A	407	LMG	C29-C30-C31-C32
32	C	520	HTG	C2'-C3'-C4'-C5'
32	O	302	HTG	C3'-C4'-C5'-C6'
35	C	516	DGD	C3B-C4B-C5B-C6B
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	515	DGD	C4B-C5B-C6B-C7B
36	E	103	LHG	C29-C30-C31-C32
32	C	521	HTG	O5-C5-C6-O6
23	A	412	SQD	C31-C32-C33-C34
24	b	623	LMG	C14-C15-C16-C17
32	D	417	HTG	C2'-C3'-C4'-C5'
23	l	101	SQD	C14-C15-C16-C17
24	c	519	LMG	C29-C30-C31-C32
34	m	101	LMT	C6-C7-C8-C9
23	a	409	SQD	C17-C18-C19-C20
23	b	622	SQD	C27-C28-C29-C30
24	c	519	LMG	C34-C35-C36-C37
36	E	103	LHG	C26-C27-C28-C29
36	l	102	LHG	C28-C29-C30-C31
24	B	620	LMG	C33-C34-C35-C36
24	c	519	LMG	O9-C10-O7-C8
34	J	103	LMT	C1-C2-C3-C4
20	C	509	CLA	C2-C1-O2A-CGA
35	c	515	DGD	O6D-C5D-C6D-O5D
32	c	521	HTG	C1'-C2'-C3'-C4'
35	h	101	DGD	CBB-CCB-CDB-CEB
20	B	601	CLA	C15-C16-C17-C18
24	B	620	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	c	518	LMG	C39-C40-C41-C42
20	c	509	CLA	C16-C17-C18-C20
35	C	516	DGD	C1B-C2B-C3B-C4B
22	B	617	BCR	C1-C6-C7-C8
22	B	617	BCR	C5-C6-C7-C8
22	C	514	BCR	C23-C24-C25-C26
22	C	514	BCR	C23-C24-C25-C30
22	D	405	BCR	C23-C24-C25-C26
22	d	405	BCR	C23-C24-C25-C26
22	d	405	BCR	C23-C24-C25-C30
20	d	403	CLA	C2C-C3C-CAC-CBC
24	a	410	LMG	C18-C19-C20-C21
24	c	519	LMG	C18-C19-C20-C21
34	b	628	LMT	C7-C8-C9-C10
35	c	517	DGD	C7B-C8B-C9B-CAB
36	L	101	LHG	C31-C32-C33-C34
20	B	607	CLA	C15-C16-C17-C18
20	b	608	CLA	C10-C11-C12-C13
23	l	101	SQD	C12-C13-C14-C15
24	C	519	LMG	C19-C20-C21-C22
34	f	102	LMT	C4-C5-C6-C7
35	C	518	DGD	C2A-C3A-C4A-C5A
35	c	517	DGD	CAA-CBA-CCA-CDA
23	b	622	SQD	C7-C8-C9-C10
34	b	627	LMT	C6-C7-C8-C9
35	C	517	DGD	C5B-C6B-C7B-C8B
35	C	517	DGD	C6B-C7B-C8B-C9B
35	c	516	DGD	C5A-C6A-C7A-C8A
35	d	416	DGD	C3A-C4A-C5A-C6A
20	b	607	CLA	C4-C3-C5-C6
20	B	601	CLA	C12-C13-C15-C16
20	C	504	CLA	C11-C12-C13-C15
20	b	604	CLA	C12-C13-C15-C16
20	b	612	CLA	C12-C13-C15-C16
20	b	613	CLA	C12-C13-C15-C16
20	b	616	CLA	C11-C10-C8-C7
20	c	509	CLA	C12-C13-C15-C16
23	a	401	SQD	C33-C34-C35-C36
32	d	401	HTG	C2'-C3'-C4'-C5'
34	B	625	LMT	C11-C10-C9-C8
35	d	416	DGD	O1B-C1B-O2G-C2G
34	b	628	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
35	C	518	DGD	CAA-CBA-CCA-CDA
35	C	518	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CCA-CDA-CEA-CFA
20	b	608	CLA	C2A-CAA-CBA-CGA
20	C	504	CLA	C13-C15-C16-C17
20	b	610	CLA	C13-C15-C16-C17
24	j	101	LMG	C34-C35-C36-C37
34	B	627	LMT	C4-C5-C6-C7
35	C	516	DGD	C6B-C7B-C8B-C9B
36	d	408	LHG	C30-C31-C32-C33
23	b	622	SQD	C29-C30-C31-C32
34	B	626	LMT	C7-C8-C9-C10
36	d	408	LHG	C32-C33-C34-C35
20	B	607	CLA	C13-C15-C16-C17
20	c	509	CLA	C15-C16-C17-C18
24	a	410	LMG	C19-C20-C21-C22
24	c	519	LMG	C20-C21-C22-C23
24	j	101	LMG	C13-C14-C15-C16
32	b	625	HTG	C3'-C4'-C5'-C6'
35	c	515	DGD	C2B-C3B-C4B-C5B
34	E	101	LMT	C1-C2-C3-C4
20	b	609	CLA	C3-C5-C6-C7
34	c	523	LMT	C7-C8-C9-C10
20	b	616	CLA	C16-C17-C18-C19
20	B	607	CLA	C8-C10-C11-C12
23	f	101	SQD	C26-C27-C28-C29
34	I	101	LMT	C6-C7-C8-C9
34	T	102	LMT	C2-C3-C4-C5
34	z	102	LMT	C2-C3-C4-C5
35	d	416	DGD	C2B-C1B-O2G-C2G
32	v	210	HTG	C2'-C1'-S1-C1
20	b	615	CLA	C8-C10-C11-C12
24	C	524	LMG	C20-C21-C22-C23
23	l	101	SQD	C26-C27-C28-C29
24	J	101	LMG	C12-C13-C14-C15
24	b	623	LMG	C29-C30-C31-C32
35	c	516	DGD	CBB-CCB-CDB-CEB
23	A	406	SQD	O6-C44-C45-O47
35	C	518	DGD	C7B-C8B-C9B-CAB
23	f	101	SQD	C27-C28-C29-C30
23	l	101	SQD	C11-C10-C9-C8
36	l	102	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
20	C	510	CLA	C8-C10-C11-C12
20	c	504	CLA	C13-C15-C16-C17
20	C	507	CLA	C4-C3-C5-C6
20	C	507	CLA	C2-C3-C5-C6
27	a	415	PL9	C4-C3-C7-C8
23	a	401	SQD	C18-C19-C20-C21
34	T	102	LMT	C1-C2-C3-C4
34	a	418	LMT	C1-C2-C3-C4
20	B	601	CLA	C14-C13-C15-C16
20	a	404	CLA	C6-C7-C8-C9
20	c	506	CLA	C14-C13-C15-C16
20	c	509	CLA	C14-C13-C15-C16
24	c	519	LMG	C33-C34-C35-C36
35	h	101	DGD	C8A-C9A-CAA-CBA
20	b	618	CLA	C3-C5-C6-C7
34	B	627	LMT	C1-C2-C3-C4
24	a	410	LMG	C36-C37-C38-C39
34	T	102	LMT	C3-C4-C5-C6
23	A	406	SQD	C14-C15-C16-C17
35	C	516	DGD	CBA-CCA-CDA-CEA
20	C	506	CLA	C1A-C2A-CAA-CBA
20	C	502	CLA	C16-C17-C18-C19
20	b	615	CLA	C16-C17-C18-C20
23	A	406	SQD	C28-C29-C30-C31
23	l	101	SQD	C27-C28-C29-C30
24	B	620	LMG	C18-C19-C20-C21
34	m	101	LMT	C4'-C5'-C6'-O6'
34	f	102	LMT	C1-C2-C3-C4
23	a	409	SQD	C33-C34-C35-C36
23	b	622	SQD	C30-C31-C32-C33
36	D	407	LHG	C34-C35-C36-C37
36	E	103	LHG	C23-C24-C25-C26
23	b	622	SQD	C34-C35-C36-C37
20	D	404	CLA	C13-C15-C16-C17
34	T	102	LMT	C9-C10-C11-C12
24	B	620	LMG	C10-C11-C12-C13
35	D	406	DGD	CCA-CDA-CEA-CFA
23	A	412	SQD	C16-C17-C18-C19
23	b	622	SQD	C11-C10-C9-C8
36	d	408	LHG	C16-C17-C18-C19
20	B	615	CLA	O1D-CGD-O2D-CED
35	c	517	DGD	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
36	D	409	LHG	C17-C18-C19-C20
32	O	302	HTG	C2'-C3'-C4'-C5'
35	C	516	DGD	C5B-C6B-C7B-C8B
24	j	101	LMG	O6-C5-C6-O5
27	a	415	PL9	C15-C14-C16-C17
24	c	518	LMG	C38-C39-C40-C41
36	d	407	LHG	C34-C35-C36-C37
23	a	409	SQD	C14-C15-C16-C17
23	l	101	SQD	C10-C11-C12-C13
34	E	101	LMT	C6-C7-C8-C9
36	l	102	LHG	C32-C33-C34-C35
20	b	604	CLA	C16-C17-C18-C19
23	A	412	SQD	O6-C44-C45-C46
23	F	101	SQD	C30-C31-C32-C33
23	a	409	SQD	O6-C44-C45-C46
24	A	407	LMG	C32-C33-C34-C35
24	c	519	LMG	C7-C8-C9-O8
35	c	517	DGD	C9A-CAA-CBA-CCA
23	a	401	SQD	C19-C20-C21-C22
23	a	409	SQD	C35-C36-C37-C38
32	b	601	HTG	C4'-C5'-C6'-C7'
35	D	406	DGD	C4B-C5B-C6B-C7B
23	F	101	SQD	C45-C44-O6-C1
24	C	524	LMG	C8-C7-O1-C1
24	c	518	LMG	C8-C7-O1-C1
35	C	517	DGD	C2G-C3G-O3G-C1D
35	C	517	DGD	C5D-C6D-O5D-C1E
40	v	201	HEC	C2C-C3C-CAC-CBC
23	l	101	SQD	C16-C17-C18-C19
34	J	103	LMT	C7-C8-C9-C10
35	h	101	DGD	C7A-C8A-C9A-CAA
23	a	401	SQD	C26-C27-C28-C29
21	D	403	PHO	C2C-C3C-CAC-CBC
24	A	407	LMG	C40-C41-C42-C43
35	C	518	DGD	CAB-CBB-CCB-CDB
35	H	102	DGD	CDB-CEB-CFB-CGB
36	L	101	LHG	C33-C34-C35-C36
23	A	406	SQD	C15-C16-C17-C18
23	a	409	SQD	C31-C32-C33-C34
24	c	519	LMG	C40-C41-C42-C43
35	h	101	DGD	CDB-CEB-CFB-CGB
36	E	103	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
36	d	406	LHG	O1-C1-C2-O2
24	j	101	LMG	C12-C13-C14-C15
21	a	405	PHO	C8-C10-C11-C12
34	m	101	LMT	C9-C10-C11-C12
35	D	406	DGD	O6D-C5D-C6D-O5D
35	c	515	DGD	O6E-C5E-C6E-O5E
32	B	631	HTG	C1'-C2'-C3'-C4'
21	a	405	PHO	C4-C3-C5-C6
23	f	101	SQD	C35-C36-C37-C38
20	c	513	CLA	C16-C17-C18-C19
20	b	603	CLA	CBA-CGA-O2A-C1
24	C	519	LMG	C21-C22-C23-C24
24	C	519	LMG	C22-C23-C24-C25
24	C	524	LMG	C17-C18-C19-C20
34	b	628	LMT	C1-C2-C3-C4
23	a	401	SQD	C31-C32-C33-C34
24	c	519	LMG	C22-C23-C24-C25
34	a	418	LMT	C9-C10-C11-C12
35	H	102	DGD	CAA-CBA-CCA-CDA
36	D	408	LHG	C32-C33-C34-C35
32	B	632	HTG	O5-C5-C6-O6
20	B	601	CLA	C2-C1-O2A-CGA
20	c	509	CLA	C2-C1-O2A-CGA
35	H	102	DGD	CDA-CEA-CFA-CGA
36	d	406	LHG	C31-C32-C33-C34
34	I	101	LMT	O5B-C5B-C6B-O6B
35	C	516	DGD	O6E-C5E-C6E-O5E
24	b	623	LMG	C12-C13-C14-C15
34	b	627	LMT	O5B-C1B-O1B-C4'
36	E	103	LHG	C3-O3-P-O5
32	B	631	HTG	C4'-C5'-C6'-C7'
35	h	101	DGD	O2G-C1B-C2B-C3B
20	B	602	CLA	C16-C17-C18-C20
24	A	407	LMG	C12-C13-C14-C15
23	F	101	SQD	C33-C34-C35-C36
36	d	408	LHG	C35-C36-C37-C38
20	C	509	CLA	C15-C16-C17-C18
23	a	401	SQD	C35-C36-C37-C38
34	Z	101	LMT	C3'-C4'-O1B-C1B
35	D	406	DGD	C4A-C5A-C6A-C7A
35	d	416	DGD	CBB-CCB-CDB-CEB
23	a	409	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
21	a	406	PHO	C2C-C3C-CAC-CBC
24	B	620	LMG	C19-C20-C21-C22
34	B	625	LMT	C6-C7-C8-C9
35	d	416	DGD	C4A-C5A-C6A-C7A
23	A	406	SQD	C27-C28-C29-C30
23	a	401	SQD	C16-C17-C18-C19
20	A	404	CLA	C6-C7-C8-C10
20	B	601	CLA	C11-C10-C8-C7
20	B	602	CLA	C11-C12-C13-C15
20	B	607	CLA	C11-C12-C13-C15
20	C	506	CLA	C11-C12-C13-C15
20	C	507	CLA	C11-C10-C8-C7
20	C	508	CLA	C11-C10-C8-C7
20	C	513	CLA	C11-C10-C8-C7
20	D	404	CLA	C6-C7-C8-C10
20	a	404	CLA	C6-C7-C8-C10
20	b	603	CLA	C12-C13-C15-C16
20	c	506	CLA	C12-C13-C15-C16
20	c	507	CLA	C11-C10-C8-C7
20	c	513	CLA	C11-C10-C8-C7
32	b	625	HTG	C2'-C3'-C4'-C5'
34	I	101	LMT	C9-C10-C11-C12
20	A	404	CLA	C6-C7-C8-C9
20	B	602	CLA	C11-C12-C13-C14
20	B	602	CLA	C14-C13-C15-C16
20	B	607	CLA	C11-C10-C8-C9
20	C	506	CLA	C11-C12-C13-C14
20	C	507	CLA	C11-C10-C8-C9
20	C	508	CLA	C11-C10-C8-C9
20	D	401	CLA	C14-C13-C15-C16
20	b	615	CLA	C11-C12-C13-C14
34	B	625	LMT	C4'-C5'-C6'-O6'
35	c	515	DGD	C4A-C5A-C6A-C7A
20	B	615	CLA	C10-C11-C12-C13
35	C	517	DGD	C5A-C6A-C7A-C8A
22	C	514	BCR	C37-C22-C23-C24
20	d	404	CLA	C16-C17-C18-C20
23	A	406	SQD	C9-C10-C11-C12
36	d	407	LHG	C11-C10-C9-C8
36	d	407	LHG	C32-C33-C34-C35
23	F	101	SQD	O6-C44-C45-O47
23	a	401	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
24	A	407	LMG	C22-C23-C24-C25
35	d	416	DGD	C8A-C9A-CAA-CBA
36	D	409	LHG	C35-C36-C37-C38
36	d	408	LHG	C19-C20-C21-C22
35	C	518	DGD	CDB-CEB-CFB-CGB
20	C	506	CLA	C5-C6-C7-C8
24	J	101	LMG	C36-C37-C38-C39
20	c	512	CLA	C4B-C3B-CAB-CBB
36	l	102	LHG	O6-C4-C5-C6
35	c	515	DGD	CAA-CBA-CCA-CDA
34	a	418	LMT	C4-C5-C6-C7
35	c	516	DGD	C6A-C7A-C8A-C9A
20	B	605	CLA	C13-C15-C16-C17
34	M	101	LMT	O5'-C5'-C6'-O6'
35	C	516	DGD	C8A-C9A-CAA-CBA
34	c	523	LMT	C4'-C5'-C6'-O6'
27	a	415	PL9	C13-C14-C16-C17
23	A	412	SQD	C7-C8-C9-C10
24	c	519	LMG	C21-C22-C23-C24
20	d	404	CLA	C8-C10-C11-C12
23	A	406	SQD	C26-C27-C28-C29
24	C	524	LMG	C31-C32-C33-C34
34	T	102	LMT	C7-C8-C9-C10
34	m	101	LMT	C5-C6-C7-C8
36	d	406	LHG	C25-C26-C27-C28
36	l	102	LHG	C31-C32-C33-C34
20	a	403	CLA	C4C-C3C-CAC-CBC
23	a	409	SQD	C13-C14-C15-C16
24	j	101	LMG	C36-C37-C38-C39
20	c	513	CLA	CBA-CGA-O2A-C1
24	C	519	LMG	C29-C28-O8-C9
36	E	103	LHG	C13-C14-C15-C16
34	T	102	LMT	C2-C1-O1'-C1'
34	m	102	LMT	C2-C1-O1'-C1'
34	z	102	LMT	C2-C1-O1'-C1'
24	J	101	LMG	C35-C36-C37-C38
24	c	519	LMG	C14-C15-C16-C17
20	b	616	CLA	C16-C17-C18-C20
23	A	406	SQD	C32-C33-C34-C35
24	C	519	LMG	C30-C31-C32-C33
35	d	416	DGD	C4B-C5B-C6B-C7B
23	A	406	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
23	f	101	SQD	C44-C45-C46-O48
24	A	407	LMG	O1-C7-C8-C9
24	A	407	LMG	C7-C8-C9-O8
35	d	416	DGD	O1G-C1G-C2G-C3G
34	Z	101	LMT	C2-C3-C4-C5
24	B	620	LMG	C11-C12-C13-C14
23	F	101	SQD	O6-C44-C45-C46
24	C	524	LMG	C21-C22-C23-C24
34	B	626	LMT	C11-C10-C9-C8
20	B	602	CLA	C4-C3-C5-C6
27	D	412	PL9	C30-C29-C31-C32
20	c	502	CLA	C16-C17-C18-C20
35	H	102	DGD	C3B-C4B-C5B-C6B
40	v	201	HEC	C4B-C3B-CAB-CBB
20	d	402	CLA	C2C-C3C-CAC-CBC
32	d	401	HTG	C4-C5-C6-O6
34	c	523	LMT	C4B-C5B-C6B-O6B
36	D	408	LHG	C4-O6-P-O3
20	b	603	CLA	O1A-CGA-O2A-C1
20	B	601	CLA	C8-C10-C11-C12
20	b	618	CLA	C13-C15-C16-C17
23	A	406	SQD	C12-C13-C14-C15
24	j	101	LMG	C31-C32-C33-C34
35	H	102	DGD	CBB-CCB-CDB-CEB
35	d	416	DGD	C9A-CAA-CBA-CCA
35	c	515	DGD	C4D-C5D-C6D-O5D
20	B	602	CLA	C16-C17-C18-C19
34	m	101	LMT	C1-C2-C3-C4
34	b	628	LMT	C2'-C1'-O1'-C1
23	b	622	SQD	O47-C45-C46-O48
23	l	101	SQD	O6-C44-C45-O47
24	C	524	LMG	O7-C8-C9-O8
24	c	519	LMG	O7-C8-C9-O8
35	D	406	DGD	O2G-C2G-C3G-O3G
35	d	416	DGD	O1G-C1G-C2G-O2G
23	A	406	SQD	C35-C36-C37-C38
34	B	626	LMT	C6-C7-C8-C9
34	T	102	LMT	C5-C6-C7-C8
24	b	623	LMG	C31-C32-C33-C34
20	b	617	CLA	C5-C6-C7-C8
20	c	510	CLA	C8-C10-C11-C12
20	b	616	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
20	b	618	CLA	C10-C11-C12-C13
20	B	605	CLA	C6-C7-C8-C9
20	B	614	CLA	C14-C13-C15-C16
20	C	513	CLA	C11-C10-C8-C9
20	b	612	CLA	C11-C12-C13-C14
20	b	618	CLA	C11-C10-C8-C9
20	a	404	CLA	C11-C12-C13-C15
20	C	513	CLA	C3-C5-C6-C7
38	x	101	RRX	C23-C24-C25-C30
38	x	101	RRX	C23-C24-C25-C26
24	a	410	LMG	C29-C30-C31-C32
22	C	514	BCR	C21-C22-C23-C24
20	b	613	CLA	C13-C15-C16-C17
23	b	622	SQD	C28-C29-C30-C31
34	E	101	LMT	O1'-C1-C2-C3
35	C	516	DGD	O6D-C5D-C6D-O5D
36	d	407	LHG	C26-C27-C28-C29
20	D	404	CLA	C16-C17-C18-C19
20	b	604	CLA	C16-C17-C18-C20
20	b	613	CLA	C16-C17-C18-C20
20	c	513	CLA	C16-C17-C18-C20
36	L	101	LHG	C7-C8-C9-C10
32	b	602	HTG	C4-C5-C6-O6
32	B	621	HTG	C4'-C5'-C6'-C7'
35	c	515	DGD	CCA-CDA-CEA-CFA
24	j	101	LMG	C15-C16-C17-C18
20	B	605	CLA	C6-C7-C8-C10
20	B	607	CLA	C11-C10-C8-C7
20	B	614	CLA	C12-C13-C15-C16
20	C	504	CLA	C11-C10-C8-C7
20	C	504	CLA	C12-C13-C15-C16
20	C	509	CLA	C11-C10-C8-C7
20	b	603	CLA	C11-C12-C13-C15
20	b	617	CLA	C12-C13-C15-C16
20	b	618	CLA	C11-C10-C8-C7
20	c	512	CLA	C11-C10-C8-C7
20	c	513	CLA	C12-C13-C15-C16
20	d	404	CLA	C6-C7-C8-C10
23	a	409	SQD	C28-C29-C30-C31
20	B	612	CLA	C16-C17-C18-C20
23	A	412	SQD	C15-C16-C17-C18
32	C	521	HTG	O5-C1-S1-C1'

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Mol	Chain	Res	Type	Atoms
32	C	534	HTG	O5-C1-S1-C1'
32	d	401	HTG	C2'-C1'-S1-C1
32	O	302	HTG	C1'-C2'-C3'-C4'
35	d	416	DGD	C5B-C6B-C7B-C8B
20	d	404	CLA	C16-C17-C18-C19
20	B	614	CLA	C10-C11-C12-C13
24	j	101	LMG	C17-C18-C19-C20
35	c	515	DGD	CDA-CEA-CFA-CGA
23	a	409	SQD	C12-C13-C14-C15
34	c	523	LMT	C4-C5-C6-C7
32	d	401	HTG	S1-C1'-C2'-C3'
20	B	611	CLA	C8-C10-C11-C12
20	c	506	CLA	C5-C6-C7-C8
34	m	101	LMT	C2-C3-C4-C5
20	A	401	CLA	CAD-CBD-CGD-O2D
20	B	605	CLA	CAD-CBD-CGD-O2D
20	B	615	CLA	CAD-CBD-CGD-O2D
20	C	503	CLA	CAD-CBD-CGD-O2D
20	C	509	CLA	CAD-CBD-CGD-O2D
20	C	512	CLA	CAD-CBD-CGD-O2D
20	D	404	CLA	CAD-CBD-CGD-O2D
20	a	403	CLA	CAD-CBD-CGD-O2D
20	b	606	CLA	CAD-CBD-CGD-O2D
20	b	612	CLA	CAD-CBD-CGD-O2D
20	c	513	CLA	CAD-CBD-CGD-O2D
21	a	406	PHO	CAD-CBD-CGD-O2D
37	E	104	HEM	C2C-C3C-CAC-CBC
23	A	412	SQD	C17-C18-C19-C20
35	c	516	DGD	C2B-C3B-C4B-C5B
35	c	517	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CCB-CDB-CEB-CFB
35	d	416	DGD	O6D-C1D-O3G-C3G
20	c	512	CLA	C15-C16-C17-C18
23	a	401	SQD	O6-C44-C45-C46
35	C	516	DGD	C9A-CAA-CBA-CCA
36	L	101	LHG	O6-C4-C5-O7
36	l	102	LHG	O6-C4-C5-O7
35	H	102	DGD	O2G-C1B-C2B-C3B
24	B	620	LMG	C30-C31-C32-C33
24	j	101	LMG	C14-C15-C16-C17
20	a	404	CLA	C11-C12-C13-C14
20	B	603	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	607	CLA	CHA-CBD-CGD-O1D
20	B	608	CLA	CHA-CBD-CGD-O2D
20	C	504	CLA	CHA-CBD-CGD-O1D
20	C	506	CLA	CHA-CBD-CGD-O1D
20	C	507	CLA	CHA-CBD-CGD-O1D
20	C	507	CLA	CHA-CBD-CGD-O2D
20	C	508	CLA	CHA-CBD-CGD-O2D
20	b	603	CLA	CHA-CBD-CGD-O1D
20	b	607	CLA	CHA-CBD-CGD-O1D
20	c	502	CLA	CHA-CBD-CGD-O1D
20	c	504	CLA	CHA-CBD-CGD-O1D
20	c	507	CLA	CHA-CBD-CGD-O1D
20	c	508	CLA	CHA-CBD-CGD-O2D
20	c	509	CLA	CHA-CBD-CGD-O1D
20	C	509	CLA	C13-C15-C16-C17
20	c	513	CLA	O1A-CGA-O2A-C1
23	f	101	SQD	O47-C45-C46-O48
23	l	101	SQD	O47-C45-C46-O48
24	A	407	LMG	O1-C7-C8-O7
24	A	407	LMG	O7-C8-C9-O8
35	d	416	DGD	O2G-C2G-C3G-O3G
20	D	404	CLA	C10-C11-C12-C13
24	C	519	LMG	O10-C28-O8-C9
34	m	102	LMT	O5'-C5'-C6'-O6'
23	l	101	SQD	C35-C36-C37-C38
20	D	401	CLA	C2C-C3C-CAC-CBC
27	A	411	PL9	C4-C3-C7-C8
20	B	601	CLA	C11-C12-C13-C14
20	C	502	CLA	C14-C13-C15-C16
20	C	504	CLA	C11-C10-C8-C9
20	c	512	CLA	C11-C10-C8-C9
23	b	622	SQD	C11-C12-C13-C14
24	A	407	LMG	C39-C40-C41-C42
34	m	101	LMT	C4-C5-C6-C7
36	l	102	LHG	C30-C31-C32-C33
35	C	516	DGD	CDA-CEA-CFA-CGA
20	c	506	CLA	C13-C15-C16-C17
24	a	410	LMG	C20-C21-C22-C23
35	C	516	DGD	CBB-CCB-CDB-CEB
20	c	507	CLA	C5-C6-C7-C8
24	C	524	LMG	C29-C28-O8-C9
34	E	101	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	C	534	HTG	C4'-C5'-C6'-C7'
36	D	409	LHG	C2-C3-O3-P
36	d	408	LHG	C2-C3-O3-P
34	c	523	LMT	C11-C10-C9-C8
35	H	102	DGD	C6A-C7A-C8A-C9A
20	B	602	CLA	C4B-C3B-CAB-CBB
20	C	501	CLA	C4B-C3B-CAB-CBB
36	D	408	LHG	C4-O6-P-O5
20	b	603	CLA	C16-C17-C18-C19
34	b	628	LMT	O5'-C1'-O1'-C1
35	D	406	DGD	CAB-CBB-CCB-CDB
24	C	524	LMG	O10-C28-O8-C9
20	B	602	CLA	CAD-CBD-CGD-O1D
20	B	606	CLA	CAD-CBD-CGD-O1D
20	C	504	CLA	CAD-CBD-CGD-O1D
20	C	506	CLA	CAD-CBD-CGD-O1D
20	b	603	CLA	CAD-CBD-CGD-O1D
20	b	607	CLA	CAD-CBD-CGD-O1D
20	c	501	CLA	CAD-CBD-CGD-O1D
20	c	502	CLA	CAD-CBD-CGD-O1D
20	c	504	CLA	CAD-CBD-CGD-O1D
36	E	103	LHG	C7-C8-C9-C10
35	c	515	DGD	CBA-CCA-CDA-CEA
36	D	409	LHG	C34-C35-C36-C37
36	l	102	LHG	C10-C11-C12-C13
34	m	101	LMT	O5B-C5B-C6B-O6B
35	c	515	DGD	C5B-C6B-C7B-C8B
20	C	508	CLA	C11-C12-C13-C14
20	B	601	CLA	C6-C7-C8-C10
20	B	601	CLA	C11-C12-C13-C15
20	C	509	CLA	C6-C7-C8-C10
20	D	404	CLA	C11-C12-C13-C15
20	b	603	CLA	C11-C10-C8-C7
20	c	513	CLA	C11-C12-C13-C15
20	d	404	CLA	C11-C12-C13-C15
21	a	405	PHO	C2-C3-C5-C6
23	l	101	SQD	C7-C8-C9-C10
32	C	522	HTG	C2-C1-S1-C1'
32	C	534	HTG	C2-C1-S1-C1'
32	D	417	HTG	C2-C1-S1-C1'
23	l	101	SQD	C25-C26-C27-C28
34	Z	101	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
32	O	302	HTG	C4'-C5'-C6'-C7'
20	C	503	CLA	C8-C10-C11-C12
36	D	409	LHG	C12-C13-C14-C15
36	L	101	LHG	C30-C31-C32-C33
34	m	101	LMT	C4B-C5B-C6B-O6B
34	m	102	LMT	C5-C6-C7-C8
24	a	410	LMG	C7-C8-C9-O8
35	d	416	DGD	C1G-C2G-C3G-O3G
24	a	410	LMG	O7-C8-C9-O8
36	D	409	LHG	C10-C11-C12-C13
36	L	101	LHG	C28-C29-C30-C31
35	h	101	DGD	C7B-C8B-C9B-CAB
24	B	620	LMG	C14-C15-C16-C17
24	J	101	LMG	C34-C35-C36-C37
32	C	521	HTG	C2'-C3'-C4'-C5'
35	c	516	DGD	C2G-C3G-O3G-C1D
35	c	516	DGD	C5D-C6D-O5D-C1E
35	d	416	DGD	CDB-CEB-CFB-CGB
20	b	603	CLA	C11-C12-C13-C14
20	c	507	CLA	C11-C10-C8-C9
20	c	513	CLA	C11-C12-C13-C14
20	d	404	CLA	C6-C7-C8-C9
20	d	404	CLA	C11-C12-C13-C14
24	C	519	LMG	C28-C29-C30-C31
23	b	622	SQD	C9-C10-C11-C12
36	d	406	LHG	C15-C16-C17-C18
23	A	406	SQD	C11-C10-C9-C8
24	B	620	LMG	O8-C28-C29-C30
35	d	416	DGD	CAA-CBA-CCA-CDA
36	D	408	LHG	C14-C15-C16-C17
32	B	622	HTG	C4'-C5'-C6'-C7'
20	B	602	CLA	C2B-C3B-CAB-CBB
20	c	512	CLA	C2B-C3B-CAB-CBB
20	d	402	CLA	C2B-C3B-CAB-CBB
24	b	623	LMG	C13-C14-C15-C16
20	B	609	CLA	C13-C15-C16-C17
34	B	626	LMT	C4-C5-C6-C7
36	d	408	LHG	C33-C34-C35-C36
23	A	412	SQD	C24-C25-C26-C27
35	h	101	DGD	C9B-CAB-CBB-CCB
35	D	406	DGD	CBA-CCA-CDA-CEA
36	L	101	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
20	b	618	CLA	CBA-CGA-O2A-C1
20	D	401	CLA	C2-C1-O2A-CGA
20	d	402	CLA	C2-C1-O2A-CGA
24	C	524	LMG	C32-C33-C34-C35
36	L	101	LHG	C11-C12-C13-C14
24	C	519	LMG	C12-C13-C14-C15
35	D	406	DGD	C8A-C9A-CAA-CBA
20	b	618	CLA	O1A-CGA-O2A-C1
22	b	619	BCR	C1-C6-C7-C8
32	u	201	HTG	C3'-C4'-C5'-C6'
24	C	519	LMG	C11-C12-C13-C14
34	a	418	LMT	C11-C10-C9-C8
34	J	103	LMT	C2-C3-C4-C5
24	c	519	LMG	O1-C7-C8-O7
34	b	627	LMT	C3-C4-C5-C6
35	h	101	DGD	C5B-C6B-C7B-C8B
36	D	408	LHG	C3-O3-P-O6
36	d	407	LHG	C3-O3-P-O6
24	c	518	LMG	C11-C12-C13-C14
21	D	403	PHO	CHA-CBD-CGD-O1D
23	F	101	SQD	C24-C25-C26-C27
24	A	407	LMG	C37-C38-C39-C40
36	l	102	LHG	C5-C6-O8-C23
24	B	620	LMG	C28-C29-C30-C31
20	d	403	CLA	C4C-C3C-CAC-CBC
35	C	516	DGD	C5A-C6A-C7A-C8A
36	D	407	LHG	C35-C36-C37-C38
35	C	518	DGD	O6D-C5D-C6D-O5D
23	b	622	SQD	C44-C45-C46-O48
24	C	524	LMG	C7-C8-C9-O8
35	D	406	DGD	C1G-C2G-C3G-O3G
34	E	101	LMT	C11-C10-C9-C8
20	B	602	CLA	C2-C3-C5-C6
20	B	602	CLA	C11-C10-C8-C7
20	B	602	CLA	C12-C13-C15-C16
20	B	604	CLA	C6-C7-C8-C10
20	B	615	CLA	C12-C13-C15-C16
20	D	404	CLA	C11-C10-C8-C7
20	b	616	CLA	C12-C13-C15-C16
24	C	524	LMG	C29-C30-C31-C32
35	c	517	DGD	CBB-CCB-CDB-CEB
20	A	404	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	C	504	CLA	C14-C13-C15-C16
20	D	404	CLA	C6-C7-C8-C9
20	D	404	CLA	C11-C12-C13-C14
20	b	617	CLA	C14-C13-C15-C16
20	D	404	CLA	C16-C17-C18-C20
32	c	521	HTG	C2'-C3'-C4'-C5'
35	H	102	DGD	C5B-C6B-C7B-C8B
36	L	101	LHG	C17-C18-C19-C20
23	A	412	SQD	C24-C23-O48-C46
20	D	401	CLA	C15-C16-C17-C18
23	f	101	SQD	C31-C32-C33-C34
32	b	602	HTG	C3'-C4'-C5'-C6'
24	b	623	LMG	C30-C31-C32-C33
36	d	406	LHG	C11-C10-C9-C8
34	c	523	LMT	O1'-C1-C2-C3
20	b	614	CLA	C10-C11-C12-C13
20	b	616	CLA	C15-C16-C17-C18
23	l	101	SQD	C32-C33-C34-C35
34	a	418	LMT	C7-C8-C9-C10
36	E	103	LHG	C1-C2-C3-O3
27	D	412	PL9	C28-C29-C31-C32
23	A	406	SQD	C10-C11-C12-C13
20	b	613	CLA	C16-C17-C18-C19
32	d	401	HTG	O5-C5-C6-O6
24	c	519	LMG	C31-C32-C33-C34
20	C	508	CLA	CBD-CGD-O2D-CED
35	d	416	DGD	C6B-C7B-C8B-C9B
20	d	402	CLA	C4B-C3B-CAB-CBB
35	c	516	DGD	O6E-C1E-O5D-C6D
27	A	411	PL9	C14-C16-C17-C18
27	D	412	PL9	C39-C41-C42-C43
36	d	406	LHG	C7-C8-C9-C10
35	c	517	DGD	O6D-C5D-C6D-O5D
20	C	513	CLA	C8-C10-C11-C12
20	b	617	CLA	C8-C10-C11-C12
35	h	101	DGD	CCB-CDB-CEB-CFB
20	C	504	CLA	C5-C6-C7-C8
24	J	101	LMG	C30-C31-C32-C33
27	d	412	PL9	C43-C44-C46-C47
36	D	409	LHG	C29-C30-C31-C32
20	b	603	CLA	C13-C15-C16-C17
20	c	506	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	a	410	LMG	C31-C32-C33-C34
34	b	627	LMT	C2-C3-C4-C5
36	E	103	LHG	C32-C33-C34-C35
34	Z	101	LMT	C3-C4-C5-C6
36	D	409	LHG	C11-C12-C13-C14
24	C	524	LMG	O1-C7-C8-O7
24	C	524	LMG	C11-C12-C13-C14
36	E	103	LHG	C2-C3-O3-P
35	C	518	DGD	CCA-CDA-CEA-CFA
32	C	521	HTG	C4-C5-C6-O6
36	l	102	LHG	C17-C18-C19-C20
20	c	504	CLA	C11-C12-C13-C14
20	d	402	CLA	C4C-C3C-CAC-CBC
34	f	102	LMT	C5-C6-C7-C8
20	A	401	CLA	C2C-C3C-CAC-CBC
37	E	104	HEM	CAD-CBD-CGD-O2D
36	E	103	LHG	O2-C2-C3-O3
23	a	409	SQD	C11-C12-C13-C14
36	D	409	LHG	C14-C15-C16-C17
32	B	621	HTG	S1-C1'-C2'-C3'
20	c	503	CLA	C10-C11-C12-C13
24	b	623	LMG	C36-C37-C38-C39
20	C	506	CLA	C6-C7-C8-C10
20	C	507	CLA	C11-C12-C13-C15
20	b	615	CLA	C15-C16-C17-C18
34	E	101	LMT	C5-C6-C7-C8
23	A	412	SQD	O10-C23-O48-C46
37	E	104	HEM	CAD-CBD-CGD-O1D
40	v	201	HEC	C4C-C3C-CAC-CBC
20	b	616	CLA	O1D-CGD-O2D-CED
36	d	407	LHG	O1-C1-C2-O2
35	d	416	DGD	C5A-C6A-C7A-C8A
36	l	102	LHG	C29-C30-C31-C32
27	A	411	PL9	C3-C7-C8-C9
36	d	408	LHG	C13-C14-C15-C16
20	D	402	CLA	C2C-C3C-CAC-CBC
20	B	614	CLA	C15-C16-C17-C18
20	C	513	CLA	C4-C3-C5-C6
27	A	411	PL9	C15-C14-C16-C17
36	D	407	LHG	C29-C30-C31-C32
20	C	501	CLA	C2B-C3B-CAB-CBB
37	E	104	HEM	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
34	a	418	LMT	C6-C7-C8-C9
32	O	302	HTG	O5-C5-C6-O6
34	z	102	LMT	O5B-C5B-C6B-O6B
23	A	412	SQD	C11-C12-C13-C14
24	a	410	LMG	C39-C40-C41-C42
35	D	406	DGD	CDA-CEA-CFA-CGA
35	H	102	DGD	O1G-C1G-C2G-O2G
20	a	403	CLA	O1D-CGD-O2D-CED
22	k	101	BCR	C19-C20-C21-C22
38	x	101	RRX	C9-C10-C11-C12
36	E	103	LHG	C30-C31-C32-C33
32	c	520	HTG	C2'-C3'-C4'-C5'
36	d	408	LHG	C14-C15-C16-C17
36	E	103	LHG	C5-C6-O8-C23
20	c	503	CLA	C8-C10-C11-C12
27	A	411	PL9	C39-C41-C42-C43
23	F	101	SQD	C25-C26-C27-C28
24	b	623	LMG	C38-C39-C40-C41
35	D	406	DGD	C5B-C6B-C7B-C8B
20	A	402	CLA	C6-C7-C8-C9
20	b	616	CLA	C14-C13-C15-C16
24	a	410	LMG	C11-C12-C13-C14
36	l	102	LHG	C11-C12-C13-C14
27	a	415	PL9	C2-C3-C7-C8
34	J	103	LMT	C6-C7-C8-C9
24	J	101	LMG	C32-C33-C34-C35
35	C	516	DGD	C4D-C5D-C6D-O5D
35	h	101	DGD	O1B-C1B-C2B-C3B
20	b	603	CLA	CAA-CBA-CGA-O2A
36	D	407	LHG	C17-C18-C19-C20
20	A	404	CLA	C8-C10-C11-C12
20	C	504	CLA	C15-C16-C17-C18
40	V	201	HEC	CAD-CBD-CGD-O2D
22	b	619	BCR	C5-C6-C7-C8
22	k	102	BCR	C1-C6-C7-C8
23	l	101	SQD	O6-C44-C45-C46
24	C	519	LMG	C32-C33-C34-C35
34	E	101	LMT	C3-C4-C5-C6
35	c	515	DGD	C5D-C6D-O5D-C1E
24	B	620	LMG	C20-C21-C22-C23
34	B	626	LMT	C4'-C5'-C6'-O6'
24	c	518	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	616	CLA	C13-C15-C16-C17
20	C	502	CLA	C4B-C3B-CAB-CBB
23	f	101	SQD	C30-C31-C32-C33
27	a	415	PL9	C39-C41-C42-C43
35	C	517	DGD	C2E-C1E-O5D-C6D
35	c	517	DGD	C6A-C7A-C8A-C9A
36	D	409	LHG	C33-C34-C35-C36
20	b	612	CLA	C16-C17-C18-C20
20	C	513	CLA	C10-C11-C12-C13
20	c	509	CLA	O1D-CGD-O2D-CED
27	A	411	PL9	C20-C19-C21-C22
20	d	403	CLA	C13-C15-C16-C17
27	A	411	PL9	C13-C14-C16-C17
34	Z	101	LMT	C11-C10-C9-C8
32	b	602	HTG	O5-C5-C6-O6
23	A	406	SQD	O47-C7-C8-C9
24	A	407	LMG	C38-C39-C40-C41
20	B	601	CLA	C6-C7-C8-C9
20	B	616	CLA	C14-C13-C15-C16
20	C	507	CLA	C11-C12-C13-C14
20	C	509	CLA	C6-C7-C8-C9
20	b	616	CLA	C11-C10-C8-C9
20	D	401	CLA	C4C-C3C-CAC-CBC
24	j	101	LMG	C35-C36-C37-C38
36	d	408	LHG	C31-C32-C33-C34
20	B	601	CLA	CAD-CBD-CGD-O2D
20	B	611	CLA	CAD-CBD-CGD-O2D
20	C	501	CLA	CAD-CBD-CGD-O2D
20	b	603	CLA	CAD-CBD-CGD-O2D
20	c	503	CLA	CAD-CBD-CGD-O2D
20	c	509	CLA	CAD-CBD-CGD-O2D
20	c	512	CLA	CAD-CBD-CGD-O2D
21	A	403	PHO	CAD-CBD-CGD-O2D
21	D	403	PHO	CAD-CBD-CGD-O2D
21	a	405	PHO	CAD-CBD-CGD-O2D
20	B	601	CLA	C16-C17-C18-C19
23	A	412	SQD	C14-C15-C16-C17
20	C	506	CLA	C15-C16-C17-C18
20	C	512	CLA	CAA-CBA-CGA-O2A
23	F	101	SQD	O48-C23-C24-C25
36	L	101	LHG	C32-C33-C34-C35
32	b	625	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
37	E	104	HEM	CAA-CBA-CGA-O1A
40	v	201	HEC	CAD-CBD-CGD-O2D
24	C	519	LMG	C15-C16-C17-C18
20	C	513	CLA	C2-C3-C5-C6
36	E	103	LHG	O7-C5-C6-O8
35	d	416	DGD	CCA-CDA-CEA-CFA
23	l	101	SQD	C44-C45-C46-O48
24	c	519	LMG	O1-C7-C8-C9
20	B	612	CLA	C16-C17-C18-C19
40	V	201	HEC	CAD-CBD-CGD-O1D
40	v	201	HEC	CAD-CBD-CGD-O1D
36	d	407	LHG	C31-C32-C33-C34
20	B	605	CLA	O2A-C1-C2-C3
20	B	614	CLA	O2A-C1-C2-C3
20	C	512	CLA	O2A-C1-C2-C3
20	D	401	CLA	O2A-C1-C2-C3
20	b	606	CLA	O2A-C1-C2-C3
20	b	618	CLA	O2A-C1-C2-C3
21	A	403	PHO	O2A-C1-C2-C3
20	B	611	CLA	C4C-C3C-CAC-CBC
37	E	104	HEM	C4C-C3C-CAC-CBC
36	l	102	LHG	C9-C10-C11-C12
36	E	103	LHG	O8-C23-C24-C25
37	e	102	HEM	CAA-CBA-CGA-O1A
24	C	524	LMG	C4-C5-C6-O5
20	c	510	CLA	C16-C17-C18-C19
34	b	628	LMT	C6-C7-C8-C9
20	A	402	CLA	CHA-CBD-CGD-O1D
20	B	603	CLA	CHA-CBD-CGD-O1D
20	B	606	CLA	CHA-CBD-CGD-O1D
20	B	607	CLA	CHA-CBD-CGD-O2D
20	D	402	CLA	CHA-CBD-CGD-O2D
20	b	613	CLA	CHA-CBD-CGD-O2D
20	b	618	CLA	CHA-CBD-CGD-O1D
20	c	507	CLA	CHA-CBD-CGD-O2D
20	d	403	CLA	CHA-CBD-CGD-O1D
20	d	403	CLA	CHA-CBD-CGD-O2D
37	e	102	HEM	CAD-CBD-CGD-O1D
20	c	512	CLA	CAA-CBA-CGA-O2A
20	A	401	CLA	C4C-C3C-CAC-CBC
20	b	614	CLA	C8-C10-C11-C12
37	E	104	HEM	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	e	102	HEM	CAA-CBA-CGA-O2A
37	e	102	HEM	CAD-CBD-CGD-O2D
32	d	401	HTG	C4'-C5'-C6'-C7'
23	f	101	SQD	O48-C23-C24-C25
24	j	101	LMG	O7-C10-C11-C12
36	L	101	LHG	C25-C26-C27-C28
24	b	623	LMG	C17-C18-C19-C20
34	b	628	LMT	C11-C10-C9-C8
20	B	616	CLA	C12-C13-C15-C16
20	D	404	CLA	C12-C13-C15-C16
27	d	412	PL9	C28-C29-C31-C32
20	B	615	CLA	C14-C13-C15-C16
20	b	613	CLA	C14-C13-C15-C16
38	H	101	RRX	C9-C10-C11-C12
20	C	502	CLA	C2B-C3B-CAB-CBB
20	a	404	CLA	C2B-C3B-CAB-CBB
20	c	513	CLA	C2B-C3B-CAB-CBB
23	A	412	SQD	C33-C34-C35-C36
36	L	101	LHG	C13-C14-C15-C16
20	b	616	CLA	C2A-CAA-CBA-CGA
35	H	102	DGD	C6B-C7B-C8B-C9B
35	h	101	DGD	CDA-CEA-CFA-CGA
23	a	401	SQD	C30-C31-C32-C33
22	K	101	BCR	C17-C18-C19-C20
22	K	102	BCR	C7-C8-C9-C10
34	a	418	LMT	O1'-C1-C2-C3
20	c	512	CLA	C1A-C2A-CAA-CBA
23	A	406	SQD	O49-C7-C8-C9
36	E	103	LHG	O10-C23-C24-C25
35	C	516	DGD	C7B-C8B-C9B-CAB
36	l	102	LHG	C26-C27-C28-C29
20	b	604	CLA	C8-C10-C11-C12
23	F	101	SQD	O10-C23-C24-C25
22	C	514	BCR	C9-C10-C11-C12
35	c	516	DGD	C4E-C5E-C6E-O5E
35	C	517	DGD	C4A-C5A-C6A-C7A
20	C	501	CLA	C2A-CAA-CBA-CGA
20	b	604	CLA	C2A-CAA-CBA-CGA
35	C	518	DGD	C4B-C5B-C6B-C7B
20	c	512	CLA	CAA-CBA-CGA-O1A
35	c	516	DGD	C2E-C1E-O5D-C6D
20	b	609	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
36	D	408	LHG	C3-O3-P-O5
20	C	512	CLA	CAA-CBA-CGA-O1A
24	A	407	LMG	C19-C20-C21-C22
20	b	614	CLA	C3-C5-C6-C7
22	K	101	BCR	C1-C6-C7-C8
22	K	101	BCR	C5-C6-C7-C8
22	j	102	BCR	C1-C6-C7-C8
22	j	102	BCR	C5-C6-C7-C8
22	k	101	BCR	C23-C24-C25-C30
35	H	102	DGD	CCB-CDB-CEB-CFB
35	h	101	DGD	C9A-CAA-CBA-CCA
40	V	201	HEC	C2B-C3B-CAB-CBB
20	A	401	CLA	C15-C16-C17-C18
20	B	604	CLA	C5-C6-C7-C8
20	b	613	CLA	C8-C10-C11-C12
23	A	412	SQD	C13-C14-C15-C16
35	H	102	DGD	CCA-CDA-CEA-CFA
20	B	610	CLA	CAD-CBD-CGD-O1D
20	C	512	CLA	CAD-CBD-CGD-O1D
20	a	404	CLA	CAD-CBD-CGD-O1D
20	b	609	CLA	CAD-CBD-CGD-O1D
20	c	506	CLA	CAD-CBD-CGD-O1D
35	H	102	DGD	O1B-C1B-C2B-C3B
20	C	505	CLA	CAA-CBA-CGA-O2A
20	C	506	CLA	C6-C7-C8-C9
36	d	406	LHG	C32-C33-C34-C35
24	c	518	LMG	C32-C33-C34-C35
35	C	516	DGD	C2A-C3A-C4A-C5A
24	j	101	LMG	O9-C10-C11-C12
34	z	102	LMT	C4-C5-C6-C7
20	B	614	CLA	C13-C15-C16-C17
24	B	620	LMG	C36-C37-C38-C39
34	B	627	LMT	C2-C3-C4-C5
35	c	515	DGD	C6A-C7A-C8A-C9A
34	m	101	LMT	C11-C10-C9-C8
35	h	101	DGD	CAA-CBA-CCA-CDA
24	b	623	LMG	O8-C28-C29-C30
35	c	516	DGD	C4A-C5A-C6A-C7A
20	c	510	CLA	C16-C17-C18-C20
23	A	406	SQD	C33-C34-C35-C36
20	B	603	CLA	C11-C12-C13-C15
20	b	618	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	c	502	CLA	C11-C12-C13-C15
20	c	504	CLA	C12-C13-C15-C16
20	c	506	CLA	C11-C10-C8-C7
20	c	507	CLA	C11-C12-C13-C15
23	f	101	SQD	O10-C23-C24-C25
20	c	505	CLA	CAA-CBA-CGA-O2A
24	J	101	LMG	O7-C10-C11-C12
35	C	517	DGD	O2G-C1B-C2B-C3B
24	C	519	LMG	C16-C17-C18-C19
35	c	516	DGD	C7A-C8A-C9A-CAA
36	l	102	LHG	C7-C8-C9-C10
24	c	518	LMG	O6-C5-C6-O5
36	L	101	LHG	C26-C27-C28-C29
35	C	516	DGD	O6E-C1E-O5D-C6D
35	C	517	DGD	O6E-C1E-O5D-C6D
35	c	515	DGD	O6E-C1E-O5D-C6D
20	B	602	CLA	C5-C6-C7-C8
36	D	407	LHG	C11-C10-C9-C8
32	C	522	HTG	C4-C5-C6-O6
20	C	501	CLA	CAA-CBA-CGA-O2A
20	c	501	CLA	CAA-CBA-CGA-O2A
35	c	517	DGD	O1G-C1A-C2A-C3A
36	E	103	LHG	C24-C25-C26-C27
20	b	603	CLA	C8-C10-C11-C12
20	D	402	CLA	C15-C16-C17-C18
23	l	101	SQD	C19-C20-C21-C22
27	d	412	PL9	C45-C44-C46-C47
23	a	409	SQD	O47-C7-C8-C9
36	D	409	LHG	O8-C23-C24-C25

There are no ring outliers.

186 monomers are involved in 488 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	a	404	CLA	1	0
22	K	101	BCR	2	0
28	U	903[B]	DMS	10	0
28	b	635	DMS	1	0
23	A	412	SQD	2	0
20	b	605	CLA	2	0
23	l	101	SQD	2	0
20	c	501	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	641	DMS	3	0
20	b	616	CLA	1	0
21	A	403	PHO	1	0
22	b	621	BCR	4	0
22	c	514	BCR	1	0
28	D	413	DMS	2	0
32	C	534	HTG	1	0
20	C	501	CLA	3	0
20	B	611	CLA	4	0
21	D	403	PHO	1	0
32	D	417	HTG	3	0
28	u	203	DMS	1	0
20	c	502	CLA	3	0
20	b	607	CLA	4	0
28	A	418	DMS	3	0
20	B	614	CLA	1	0
21	a	405	PHO	1	0
28	i	104	DMS	4	0
36	D	409	LHG	19	0
28	C	530	DMS	1	0
28	b	632	DMS	2	0
20	B	606	CLA	6	0
20	b	614	CLA	1	0
27	A	411	PL9	11	0
31	A	421	BCT	5	0
28	A	416	DMS	3	0
24	a	410	LMG	4	0
28	U	903[A]	DMS	2	0
28	c	530	DMS	7	0
22	t	101	BCR	4	0
38	x	101	RRX	3	0
22	D	405	BCR	3	0
28	o	302	DMS	9	0
20	C	510	CLA	3	0
35	H	102	DGD	2	0
20	C	503	CLA	2	0
22	C	515	BCR	1	0
28	b	639	DMS	9	0
34	B	626	LMT	2	0
28	C	532	DMS	6	0
20	c	505	CLA	1	0
28	b	640	DMS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	d	413	DMS	3	0
32	C	520	HTG	1	0
22	k	102	BCR	3	0
28	u	202	DMS	2	0
36	E	103	LHG	6	0
36	d	408	LHG	20	0
20	C	502	CLA	2	0
28	B	637	DMS	1	0
28	V	205	DMS	1	0
20	b	610	CLA	1	0
28	A	415	DMS	2	0
28	o	303	DMS	4	0
20	c	510	CLA	2	0
20	b	606	CLA	3	0
20	B	601	CLA	4	0
20	C	511	CLA	1	0
32	B	632	HTG	2	0
28	U	902	DMS	1	0
34	B	627	LMT	1	0
20	C	507	CLA	2	0
20	b	618	CLA	5	0
28	c	533	DMS	1	0
28	D	415	DMS	2	0
20	a	403	CLA	4	0
20	C	508	CLA	3	0
23	b	622	SQD	3	0
23	f	101	SQD	2	0
20	C	506	CLA	2	0
20	B	612	CLA	1	0
28	O	307	DMS	2	0
34	z	102	LMT	5	0
22	B	619	BCR	3	0
28	V	204	DMS	1	0
20	c	506	CLA	4	0
22	K	102	BCR	1	0
28	O	305	DMS	1	0
20	C	504	CLA	3	0
28	o	306	DMS	5	0
28	O	310	DMS	2	0
32	B	622	HTG	8	0
20	b	608	CLA	4	0
22	j	102	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	O	306	DMS	1	0
34	B	625	LMT	1	0
20	A	402	CLA	2	0
20	D	402	CLA	3	0
20	c	511	CLA	1	0
32	v	210	HTG	1	0
22	B	618	BCR	3	0
32	b	625	HTG	6	0
32	B	621	HTG	6	0
28	A	417	DMS	1	0
28	d	414	DMS	5	0
35	D	406	DGD	5	0
22	b	620	BCR	1	0
20	D	401	CLA	1	0
22	k	101	BCR	3	0
28	D	414	DMS	8	0
28	o	307	DMS	3	0
34	b	627	LMT	2	0
32	B	631	HTG	1	0
34	a	418	LMT	10	0
22	a	408	BCR	1	0
34	I	101	LMT	2	0
20	b	612	CLA	3	0
28	V	208	DMS	1	0
22	C	514	BCR	2	0
28	v	206	DMS	4	0
36	l	102	LHG	1	0
20	c	507	CLA	3	0
28	b	634	DMS	2	0
28	b	631	DMS	6	0
20	B	602	CLA	2	0
20	B	603	CLA	1	0
20	c	503	CLA	2	0
35	d	416	DGD	2	0
24	C	524	LMG	2	0
34	c	523	LMT	2	0
20	B	605	CLA	2	0
34	b	628	LMT	1	0
23	a	401	SQD	4	0
28	b	638	DMS	3	0
20	b	611	CLA	2	0
20	b	613	CLA	1	0

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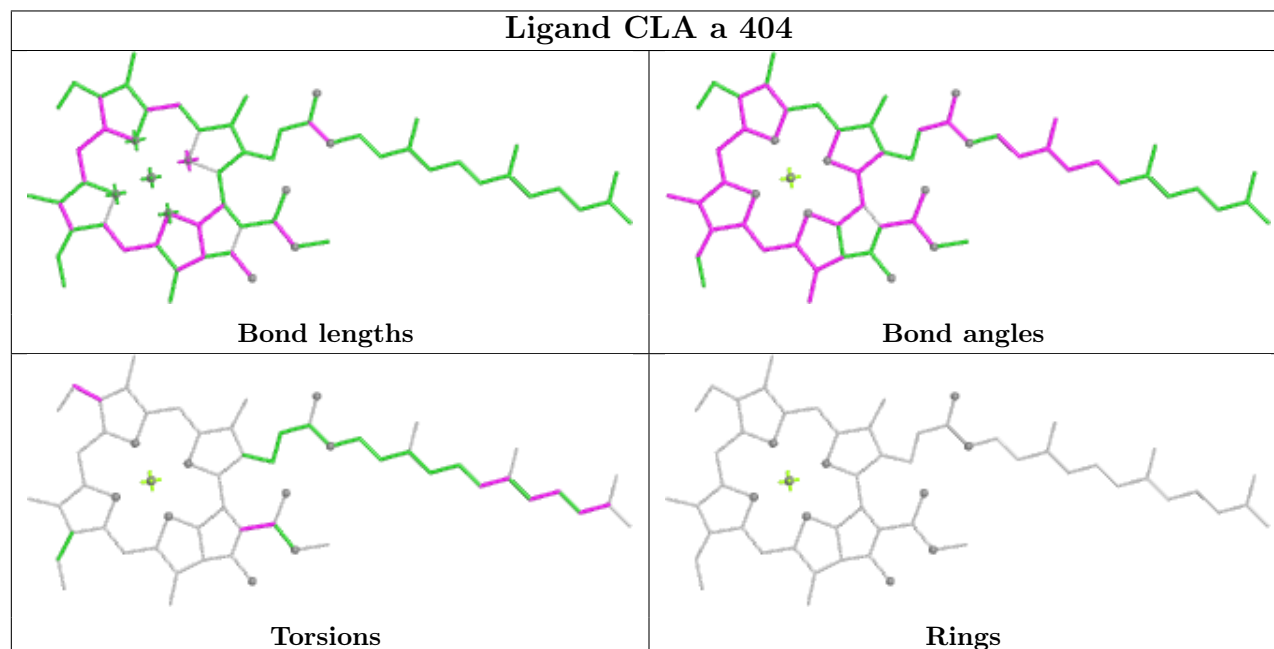
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22	A	405	BCR	5	0
37	e	102	HEM	3	0
20	b	609	CLA	2	0
22	d	405	BCR	3	0
20	C	509	CLA	5	0
24	C	519	LMG	3	0
28	U	904	DMS	3	0
34	m	102	LMT	1	0
32	c	520	HTG	1	0
20	b	604	CLA	3	0
36	d	406	LHG	2	0
20	B	607	CLA	1	0
28	C	527	DMS	3	0
28	F	102	DMS	3	0
35	h	101	DGD	1	0
28	B	643	DMS	1	0
20	c	512	CLA	3	0
20	A	401	CLA	6	0
28	V	206	DMS	2	0
20	B	616	CLA	2	0
20	C	513	CLA	2	0
28	C	531	DMS	5	0
28	B	642	DMS	8	0
28	o	308	DMS	1	0
20	B	604	CLA	2	0
20	b	603	CLA	1	0
24	A	407	LMG	4	0
28	B	645	DMS	2	0
20	b	617	CLA	2	0
35	c	517	DGD	2	0
20	c	508	CLA	6	0
28	B	644	DMS	5	0
23	a	409	SQD	5	0
20	c	509	CLA	2	0
20	b	615	CLA	2	0
27	a	415	PL9	10	0
28	b	641	DMS	2	0
23	A	406	SQD	3	0
20	c	513	CLA	3	0
35	c	516	DGD	2	0
34	J	103	LMT	1	0
20	c	504	CLA	3	0

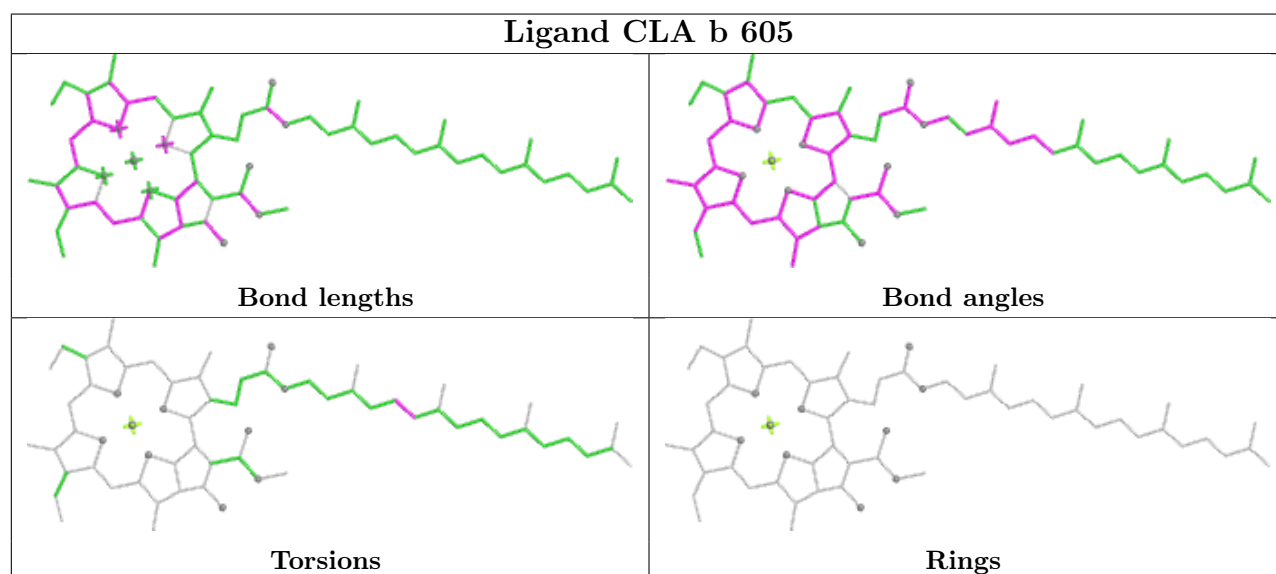
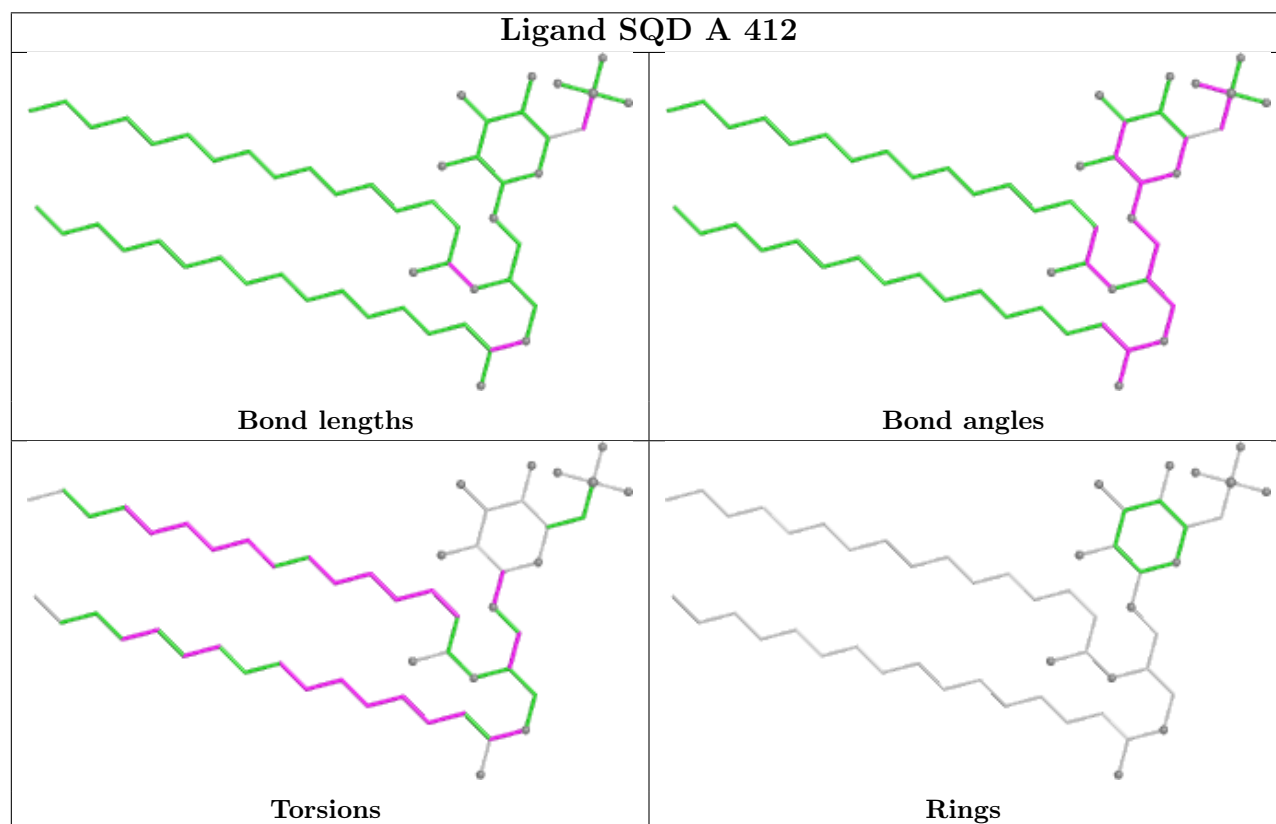
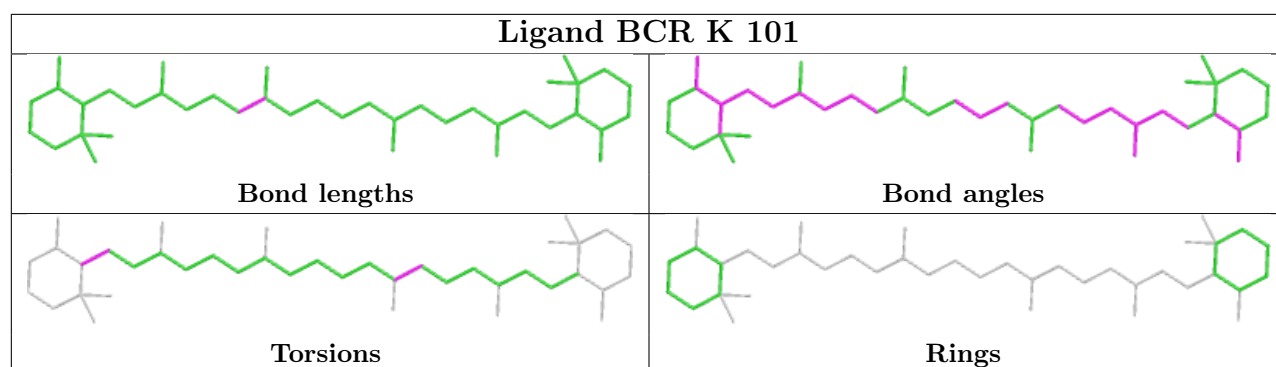
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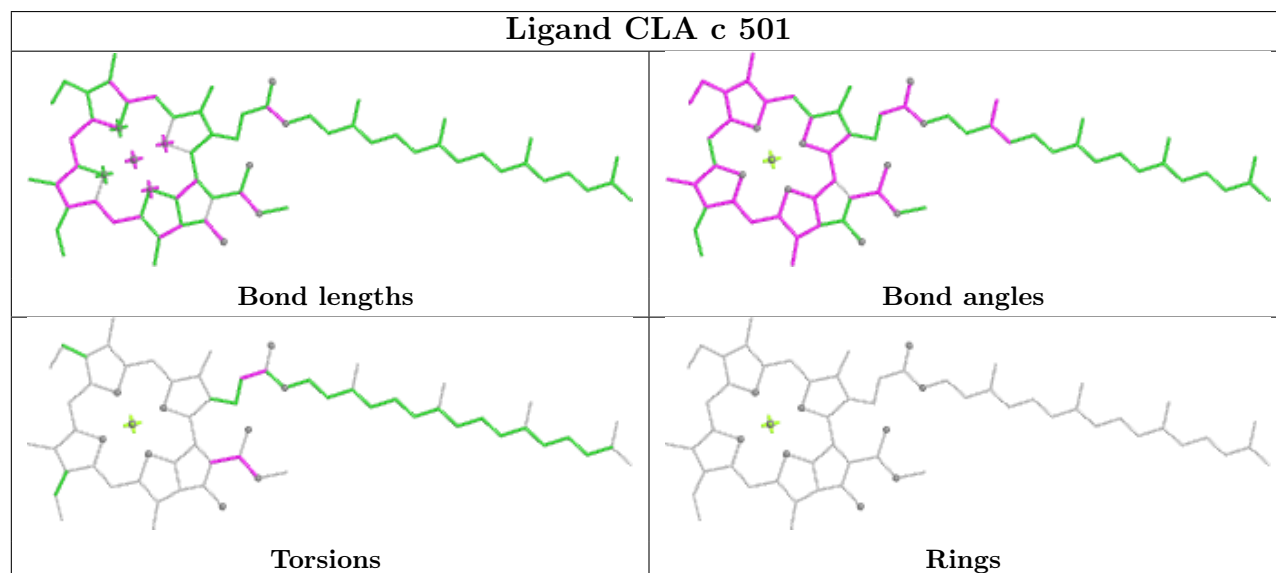
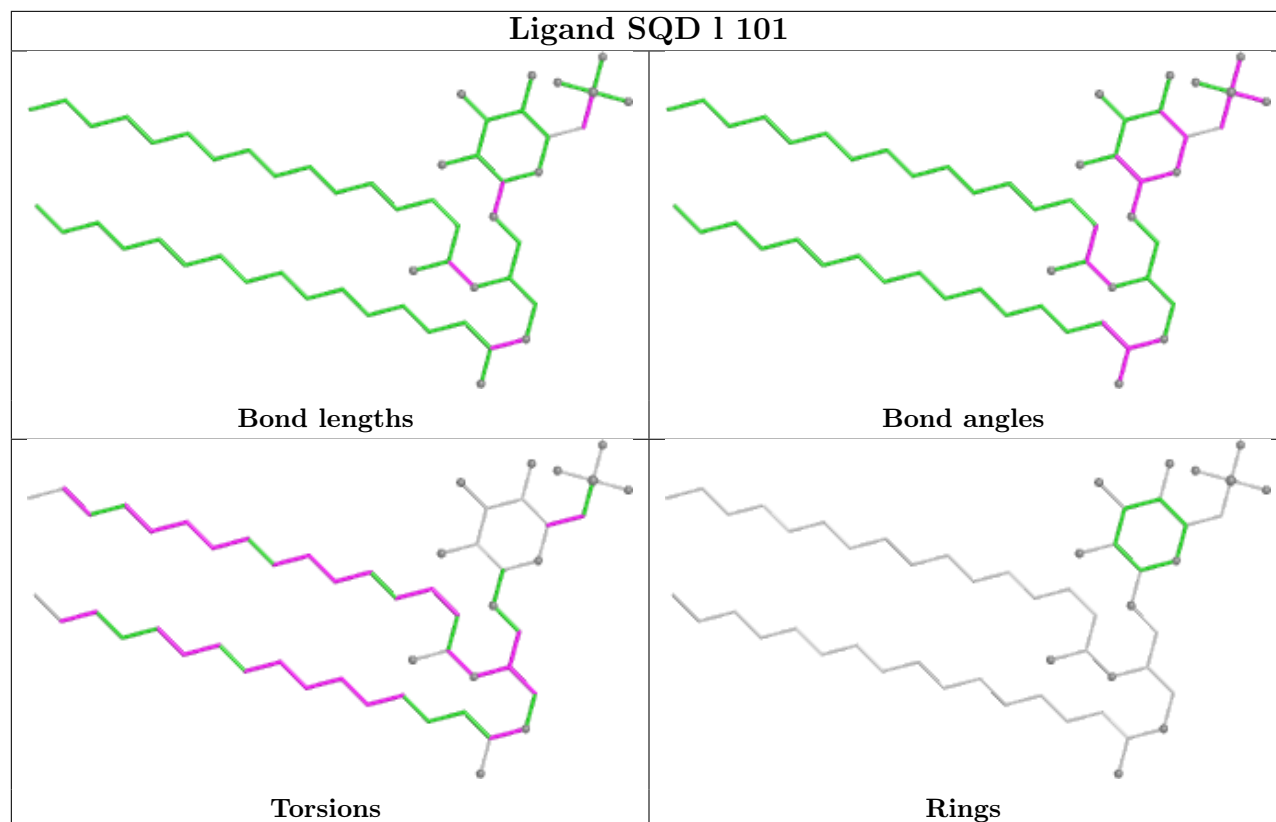
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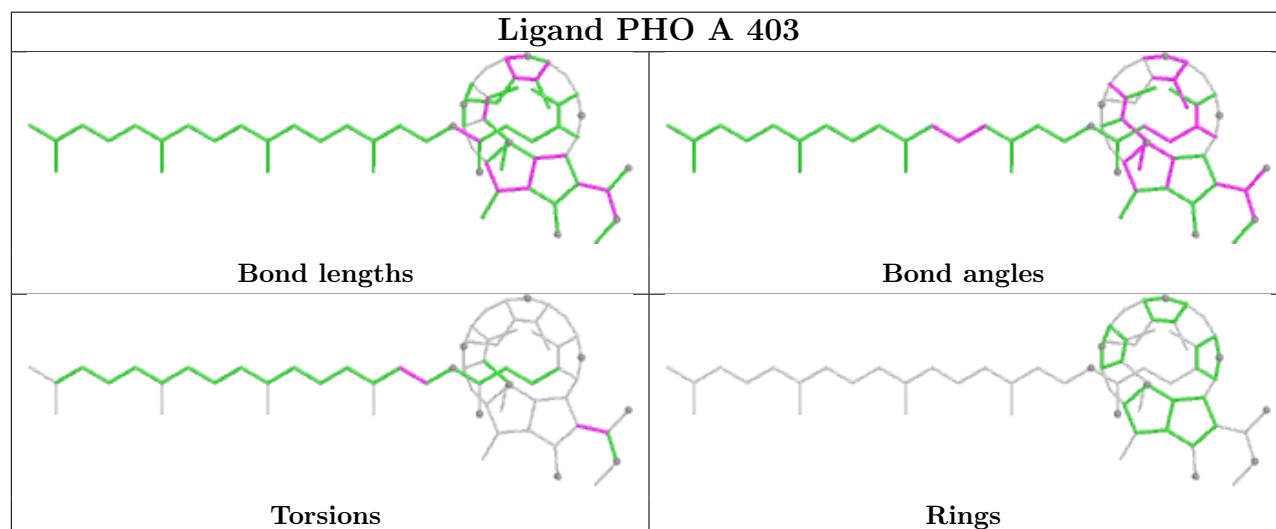
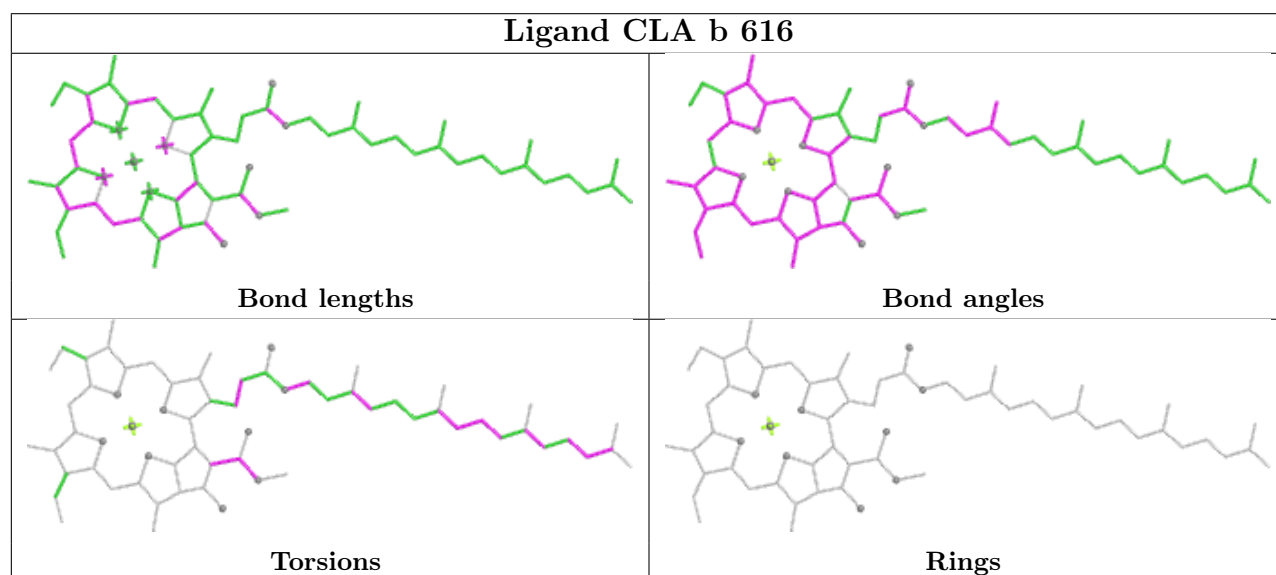
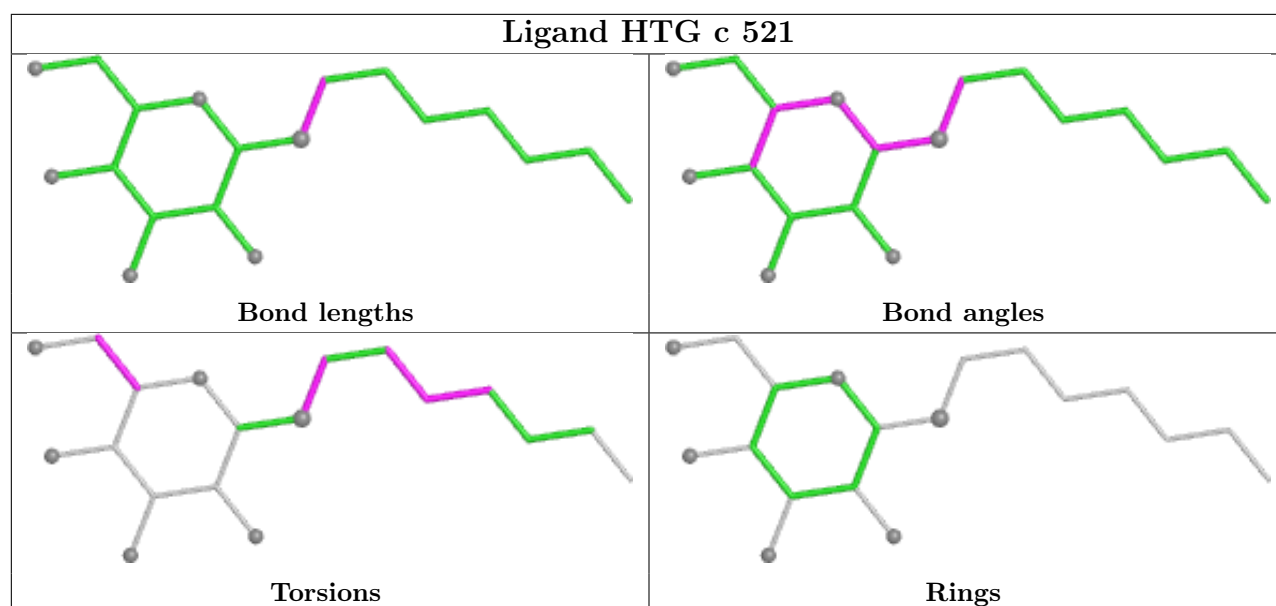
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	F	101	SQD	1	0
28	O	308	DMS	1	0
20	d	404	CLA	2	0
37	E	104	HEM	1	0
22	T	101	BCR	4	0
28	B	635	DMS	4	0
28	c	536	DMS	8	0
20	d	403	CLA	2	0
24	b	623	LMG	2	0
21	a	406	PHO	1	0

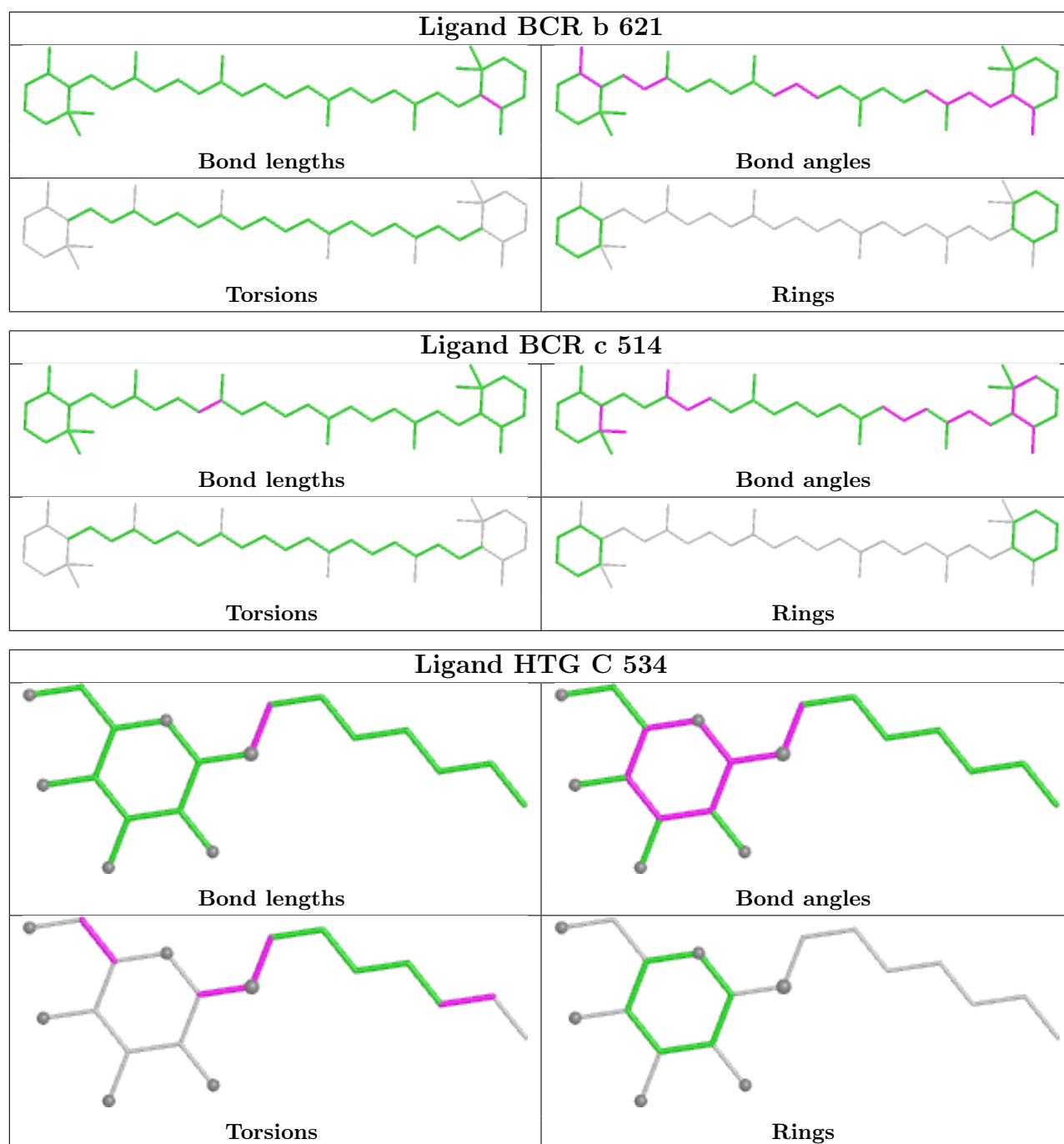
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

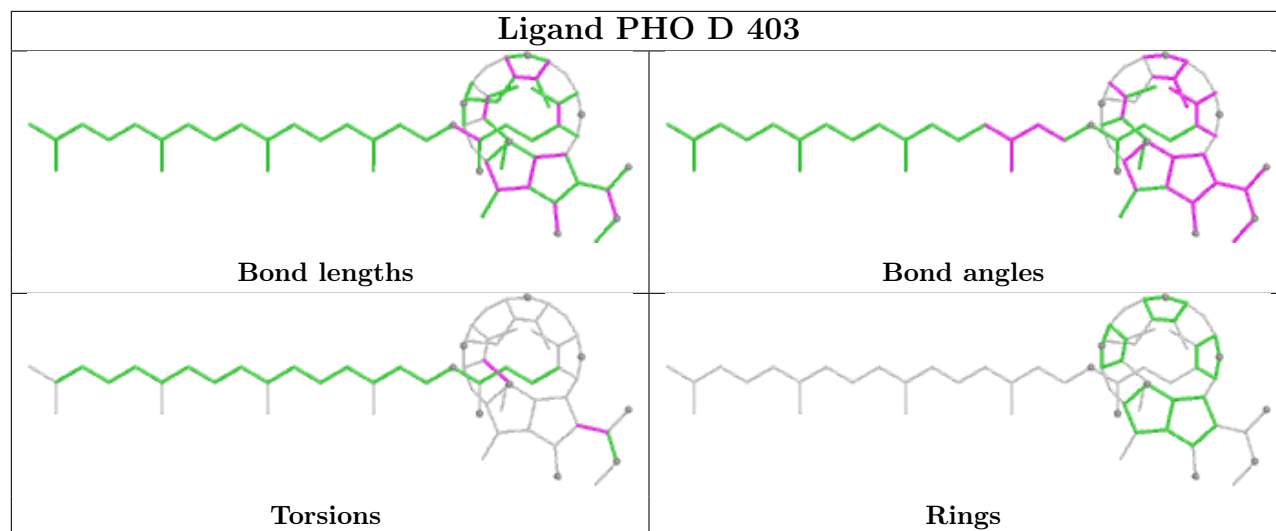
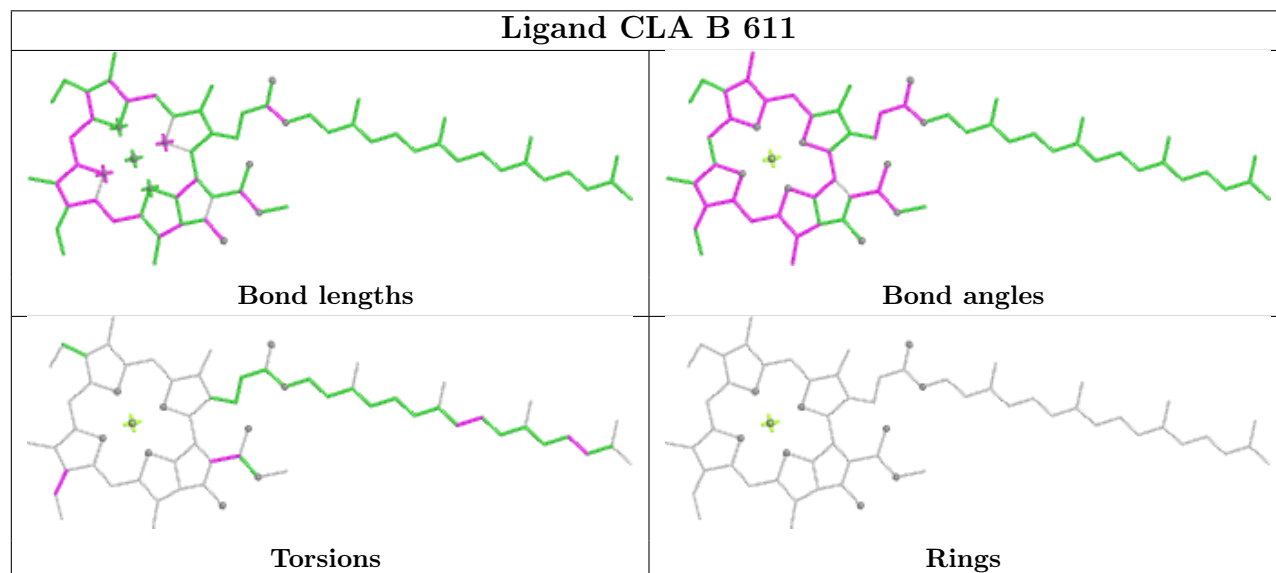
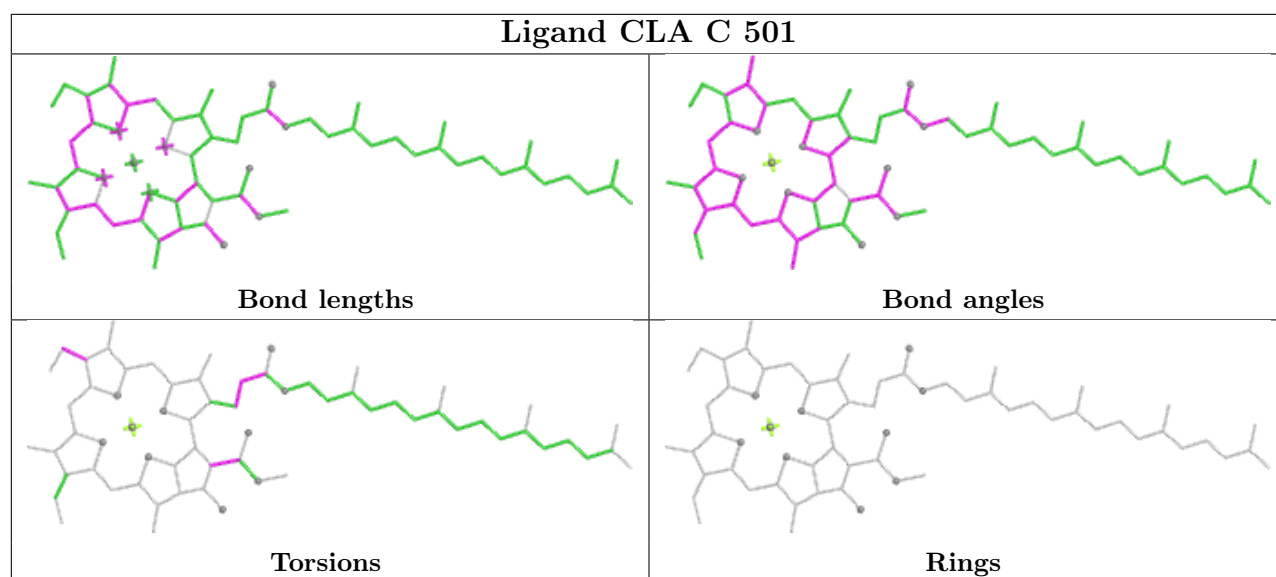


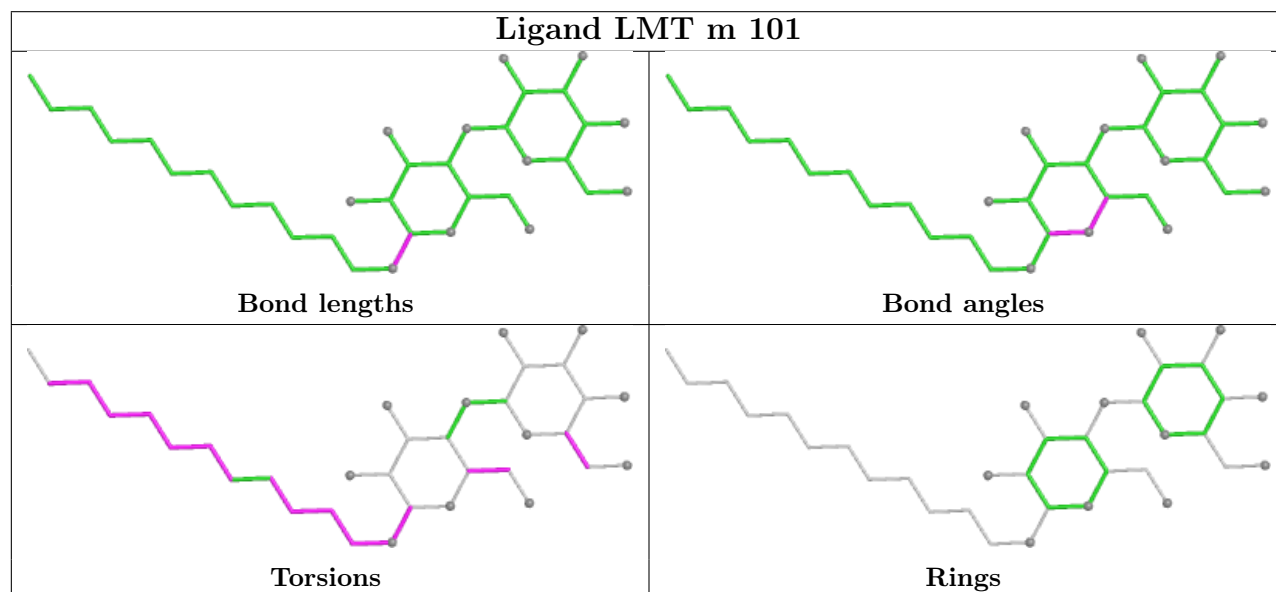
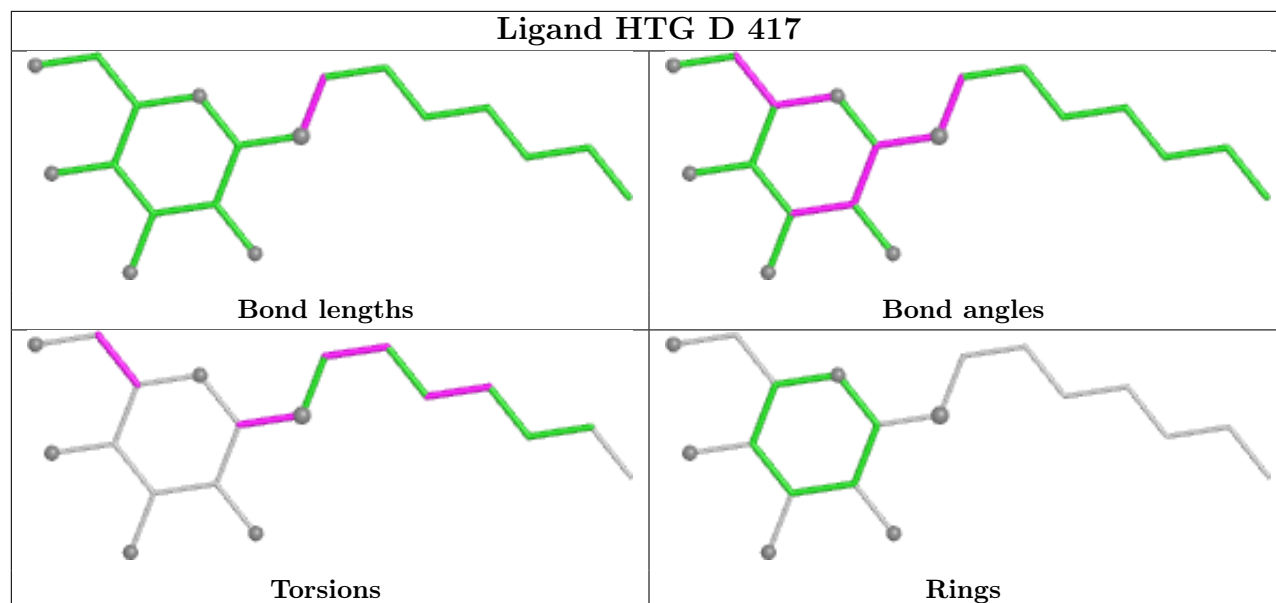




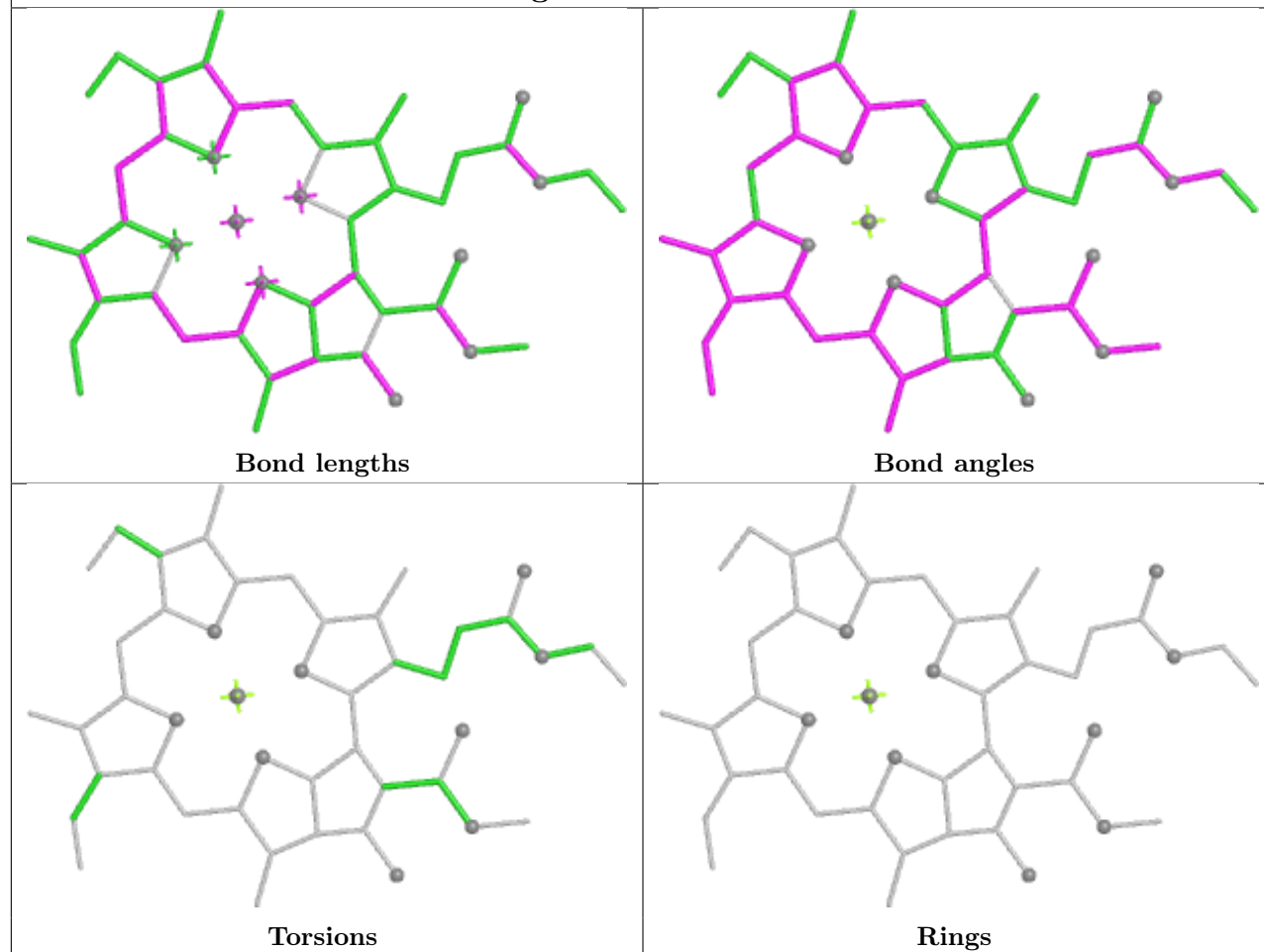




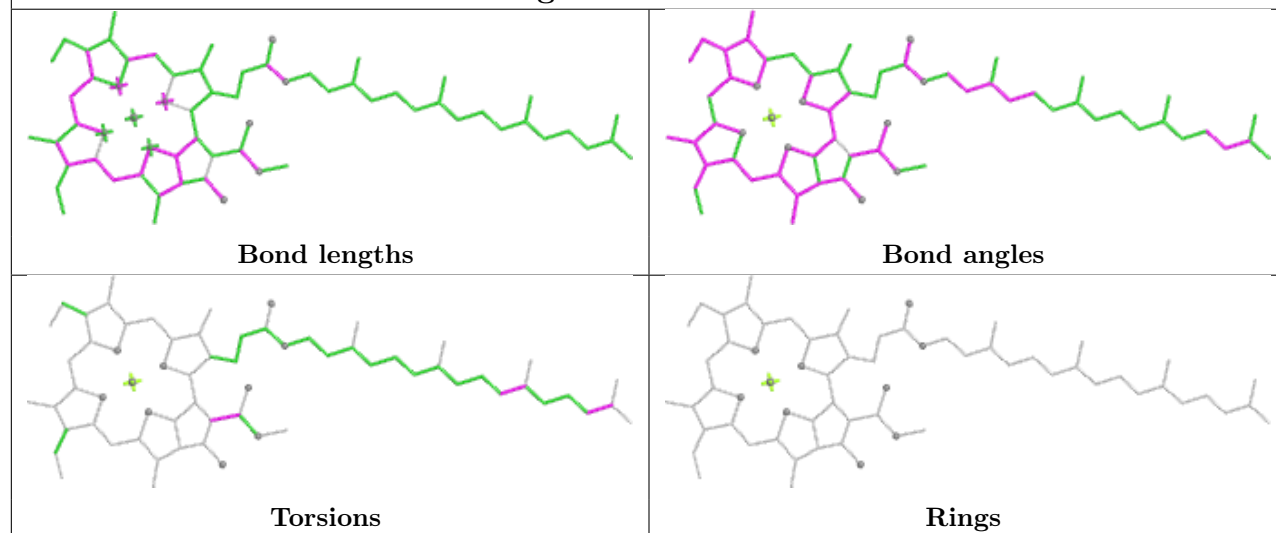


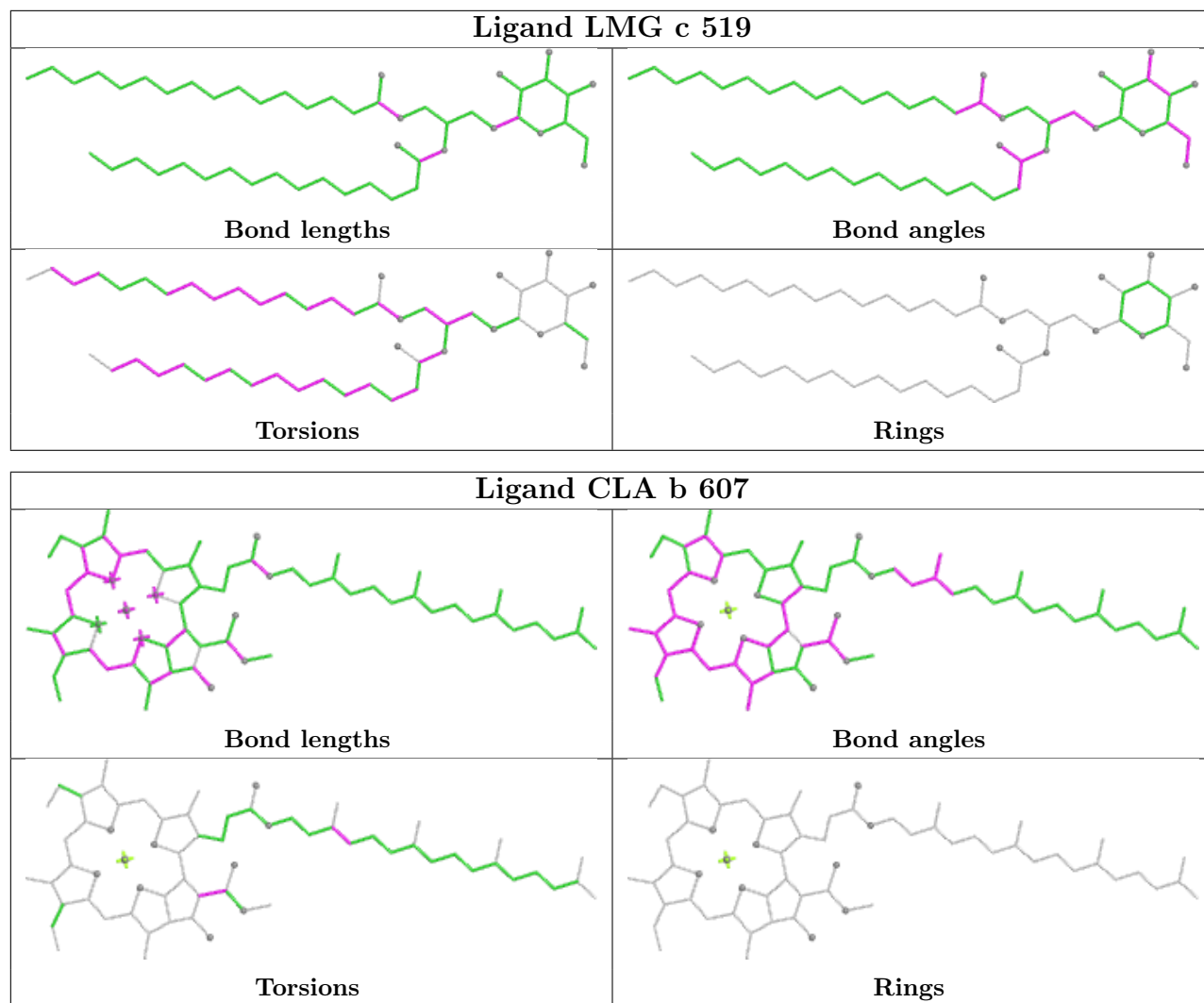


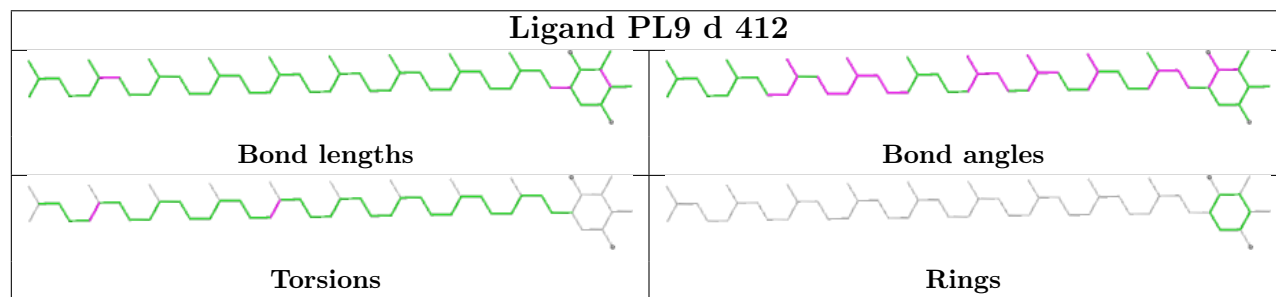
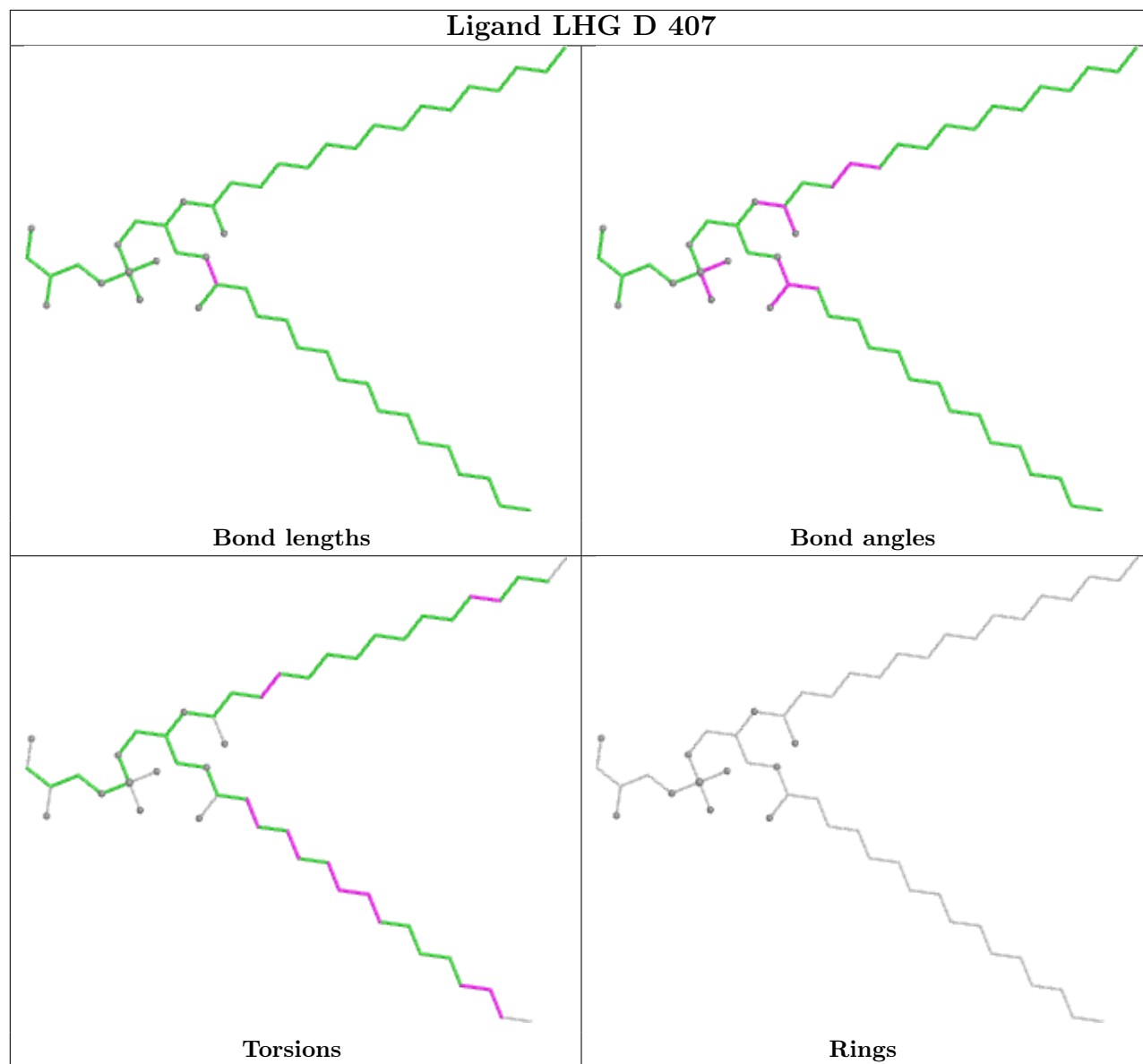
Ligand CLA a 407

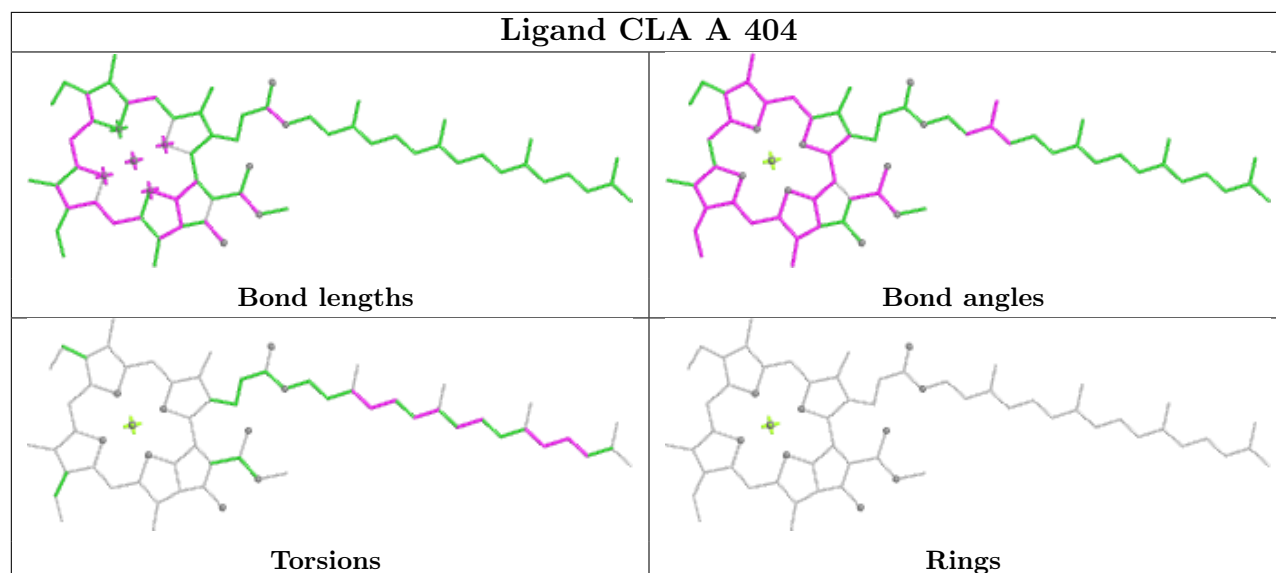
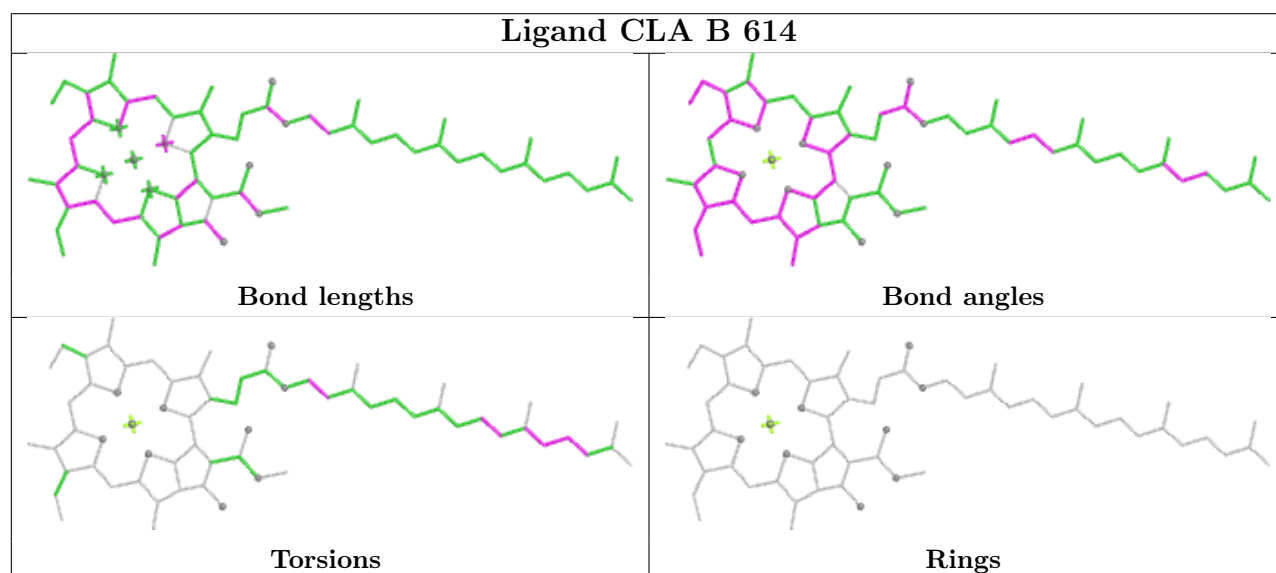
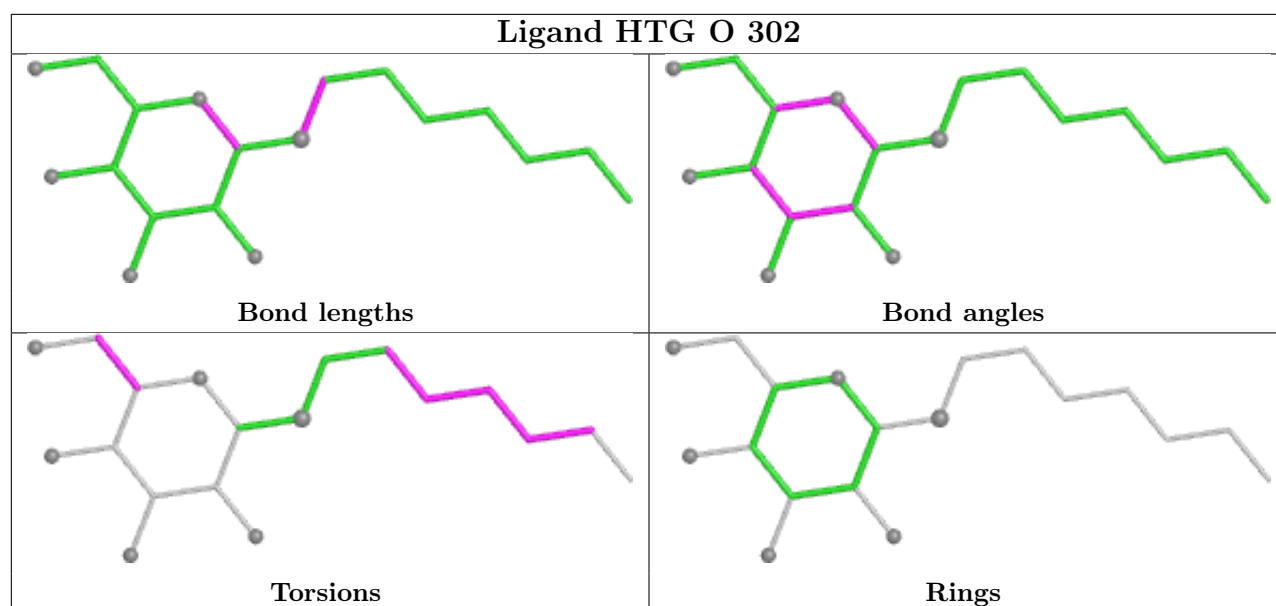


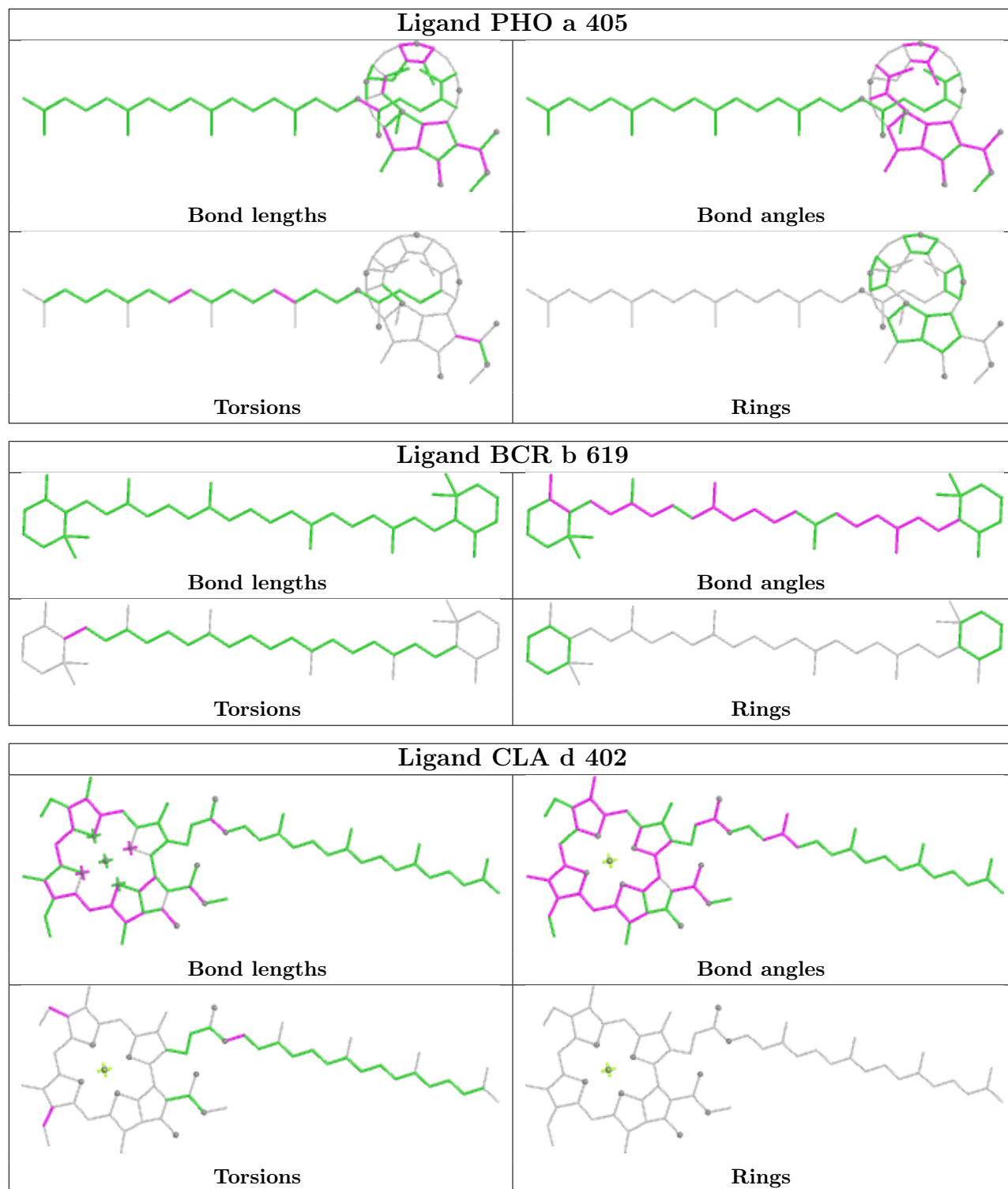
Ligand CLA c 502

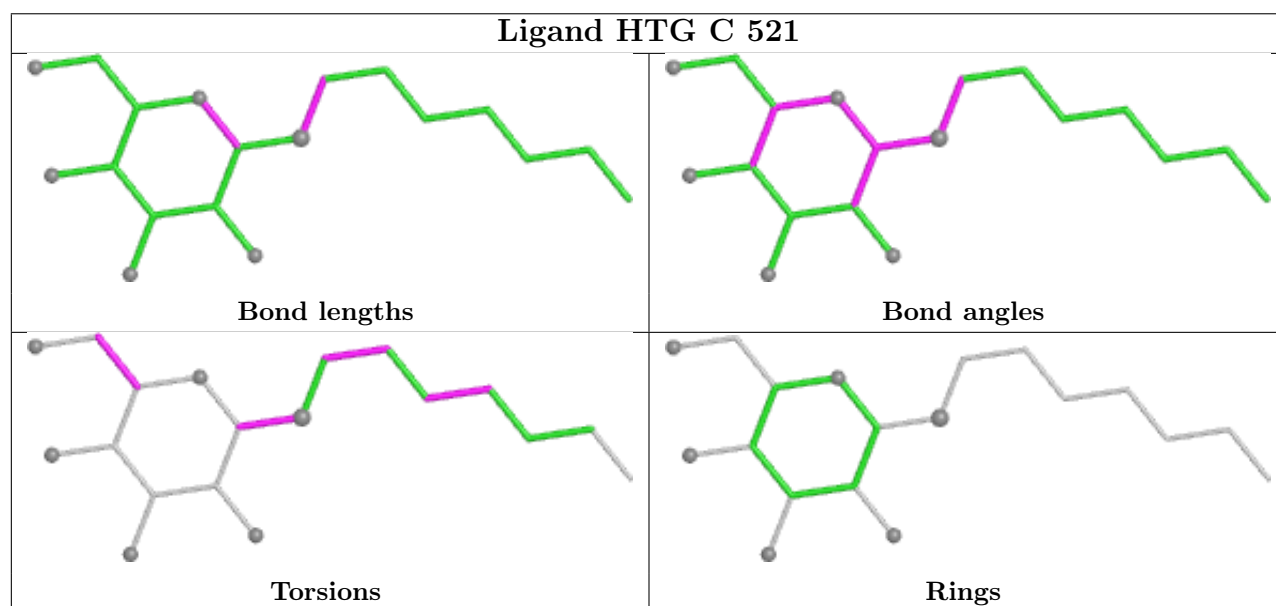
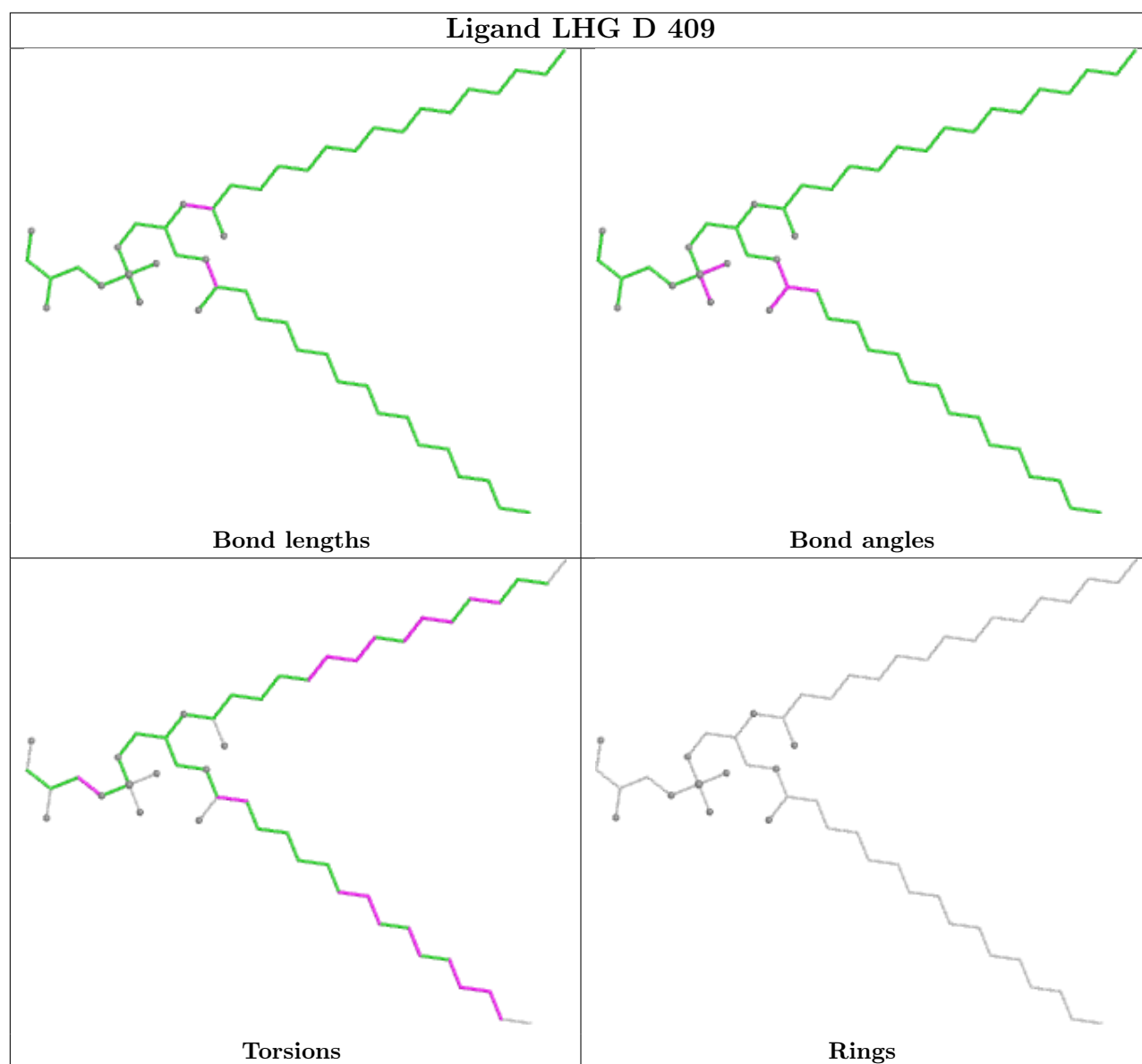


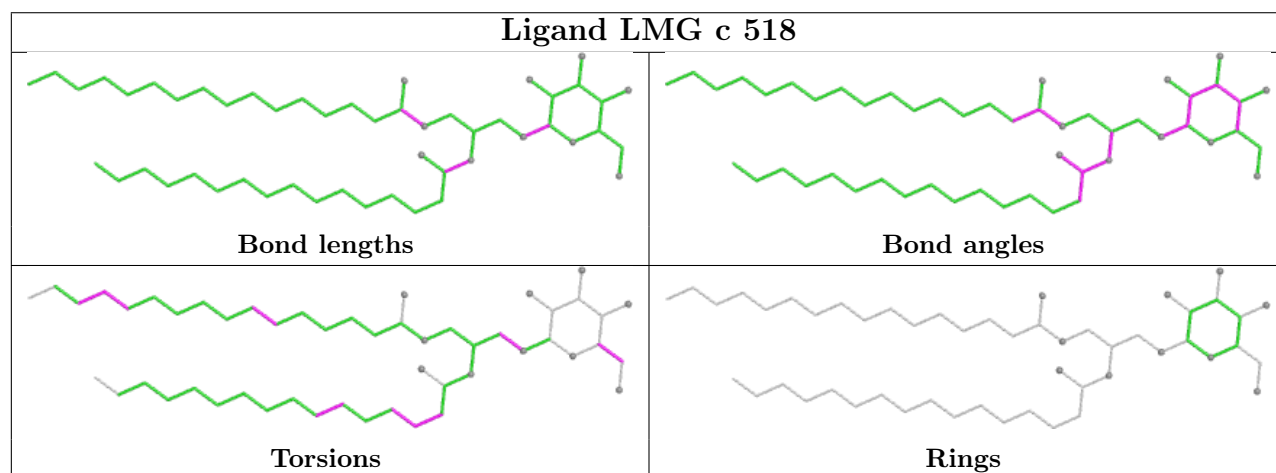
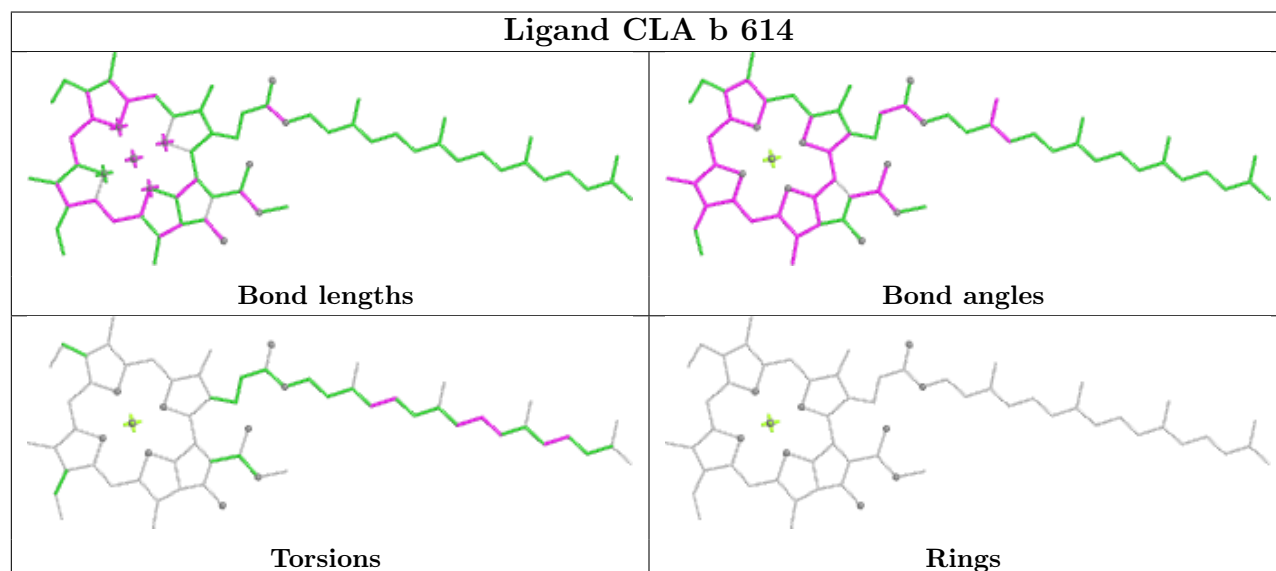
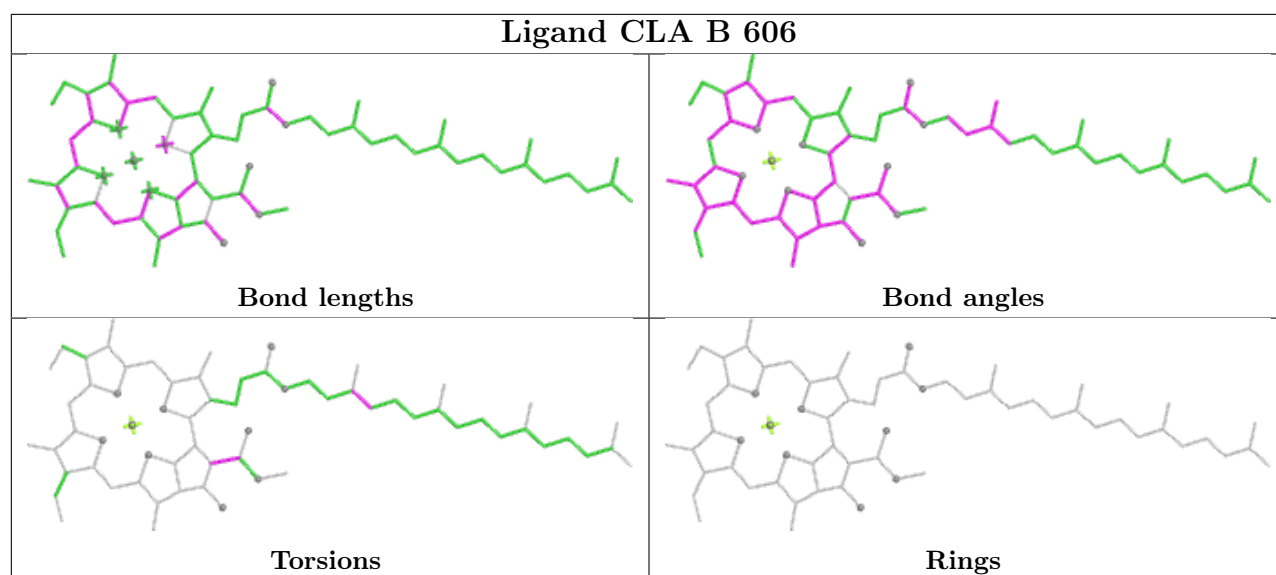


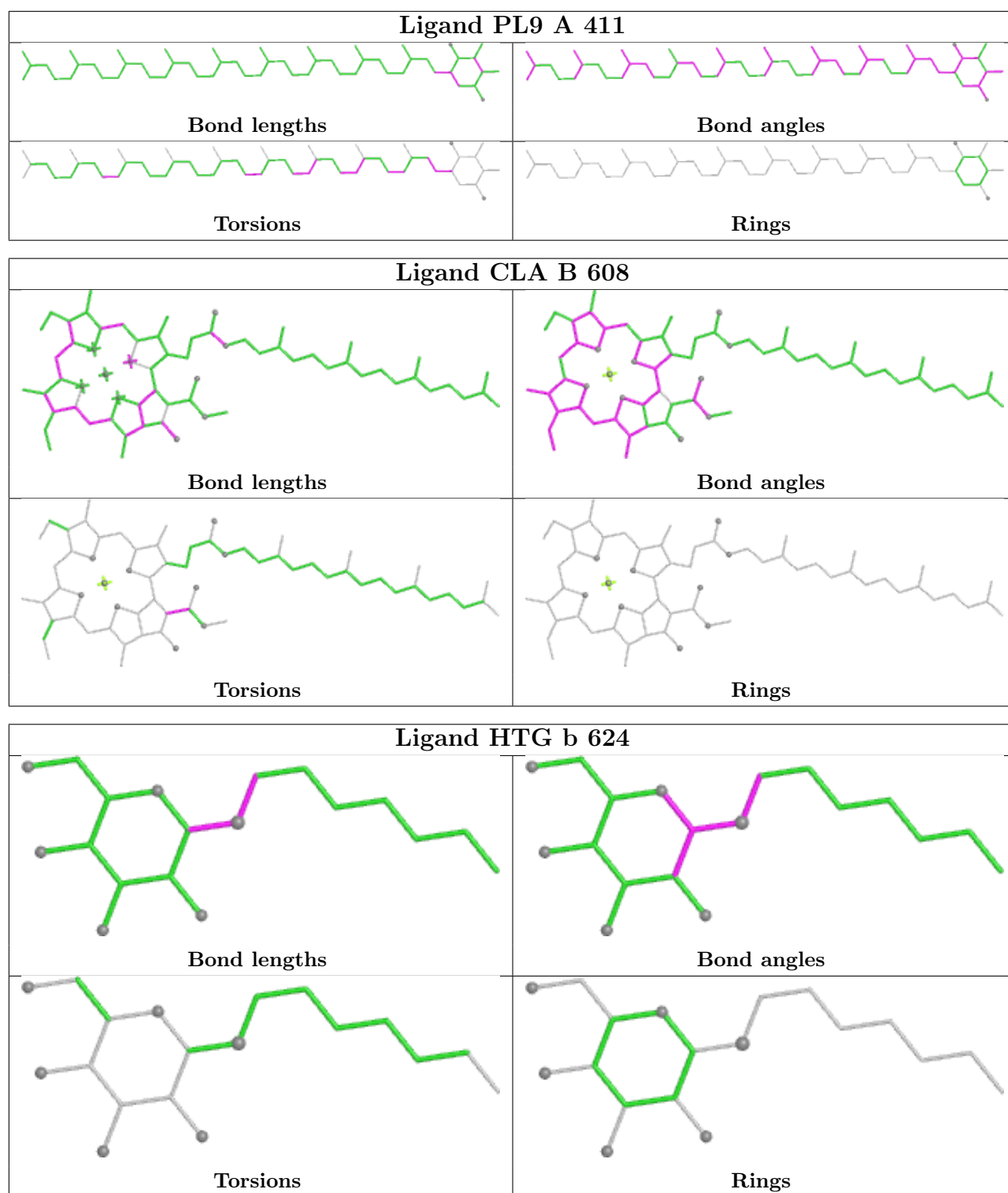


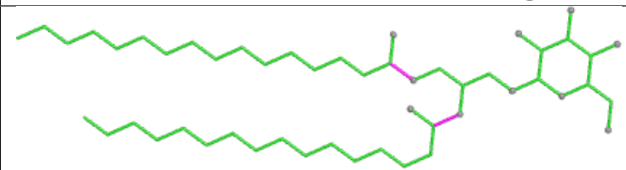
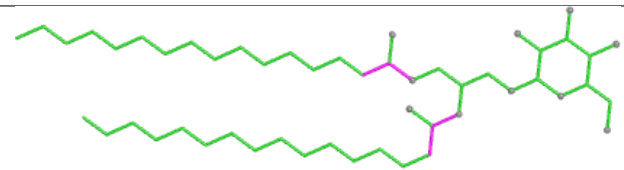
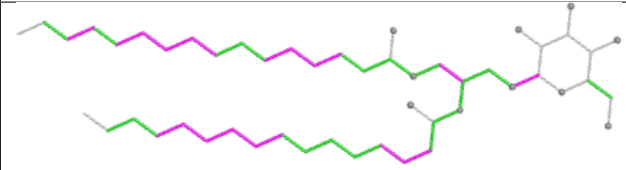
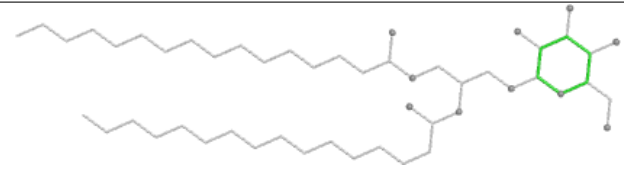
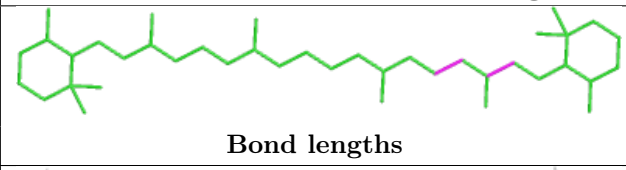
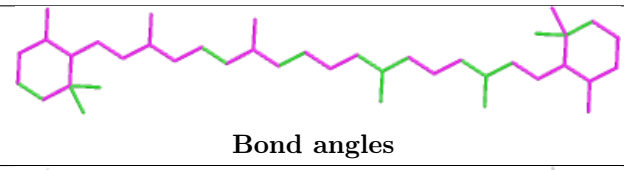
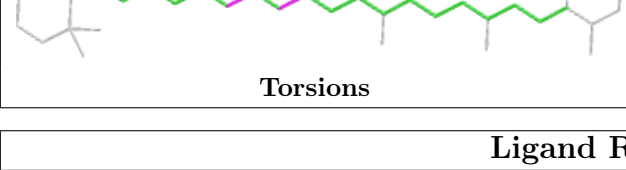
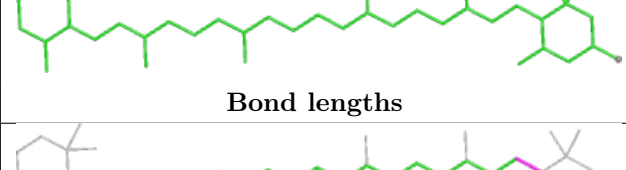
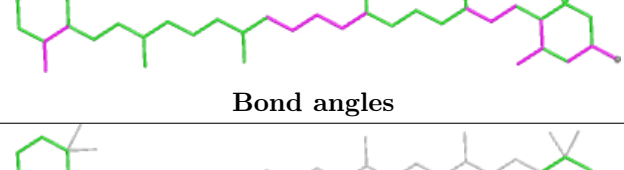
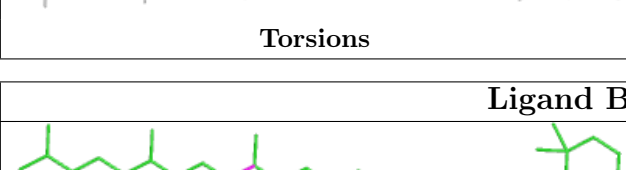
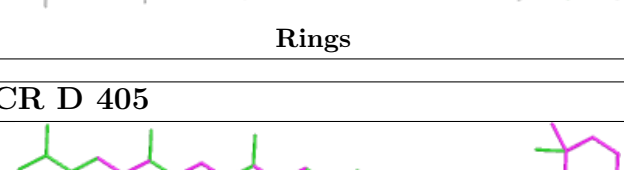
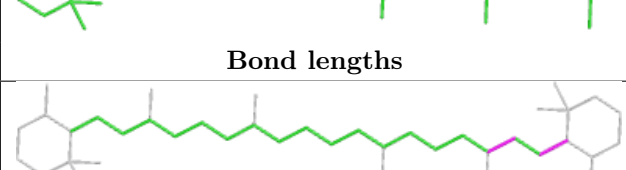
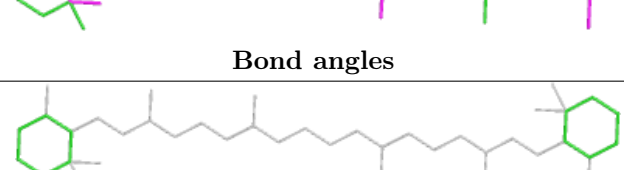


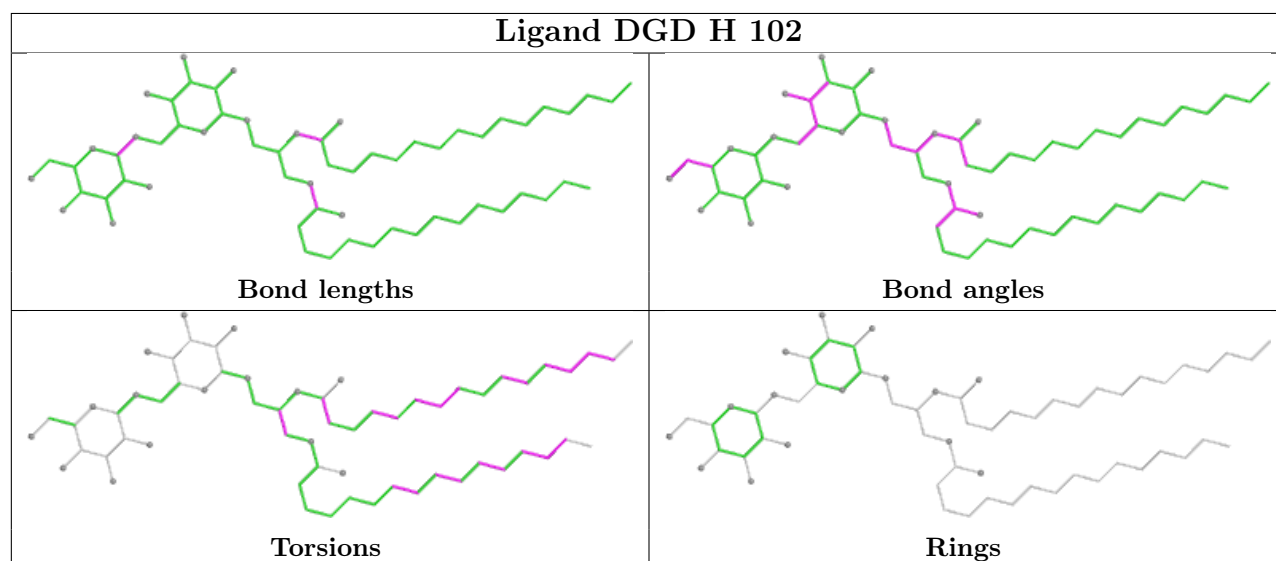
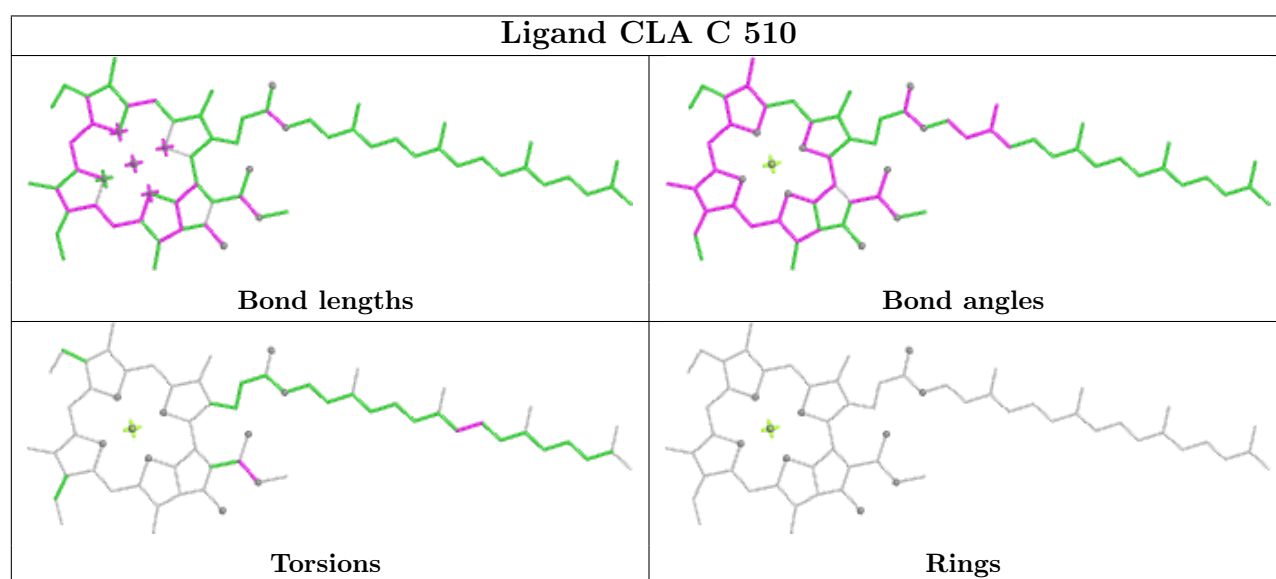
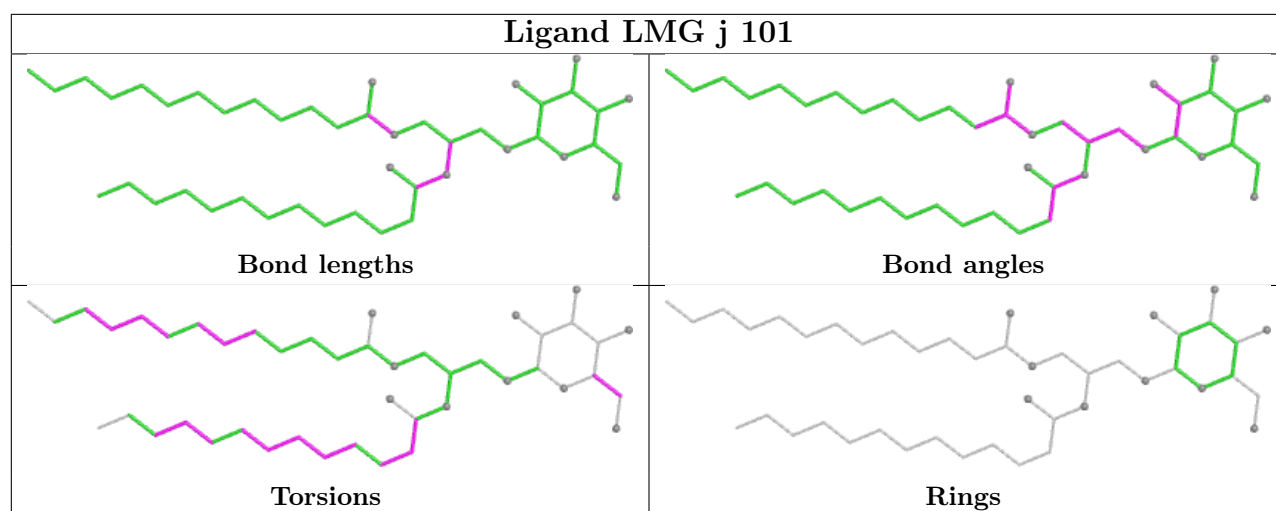


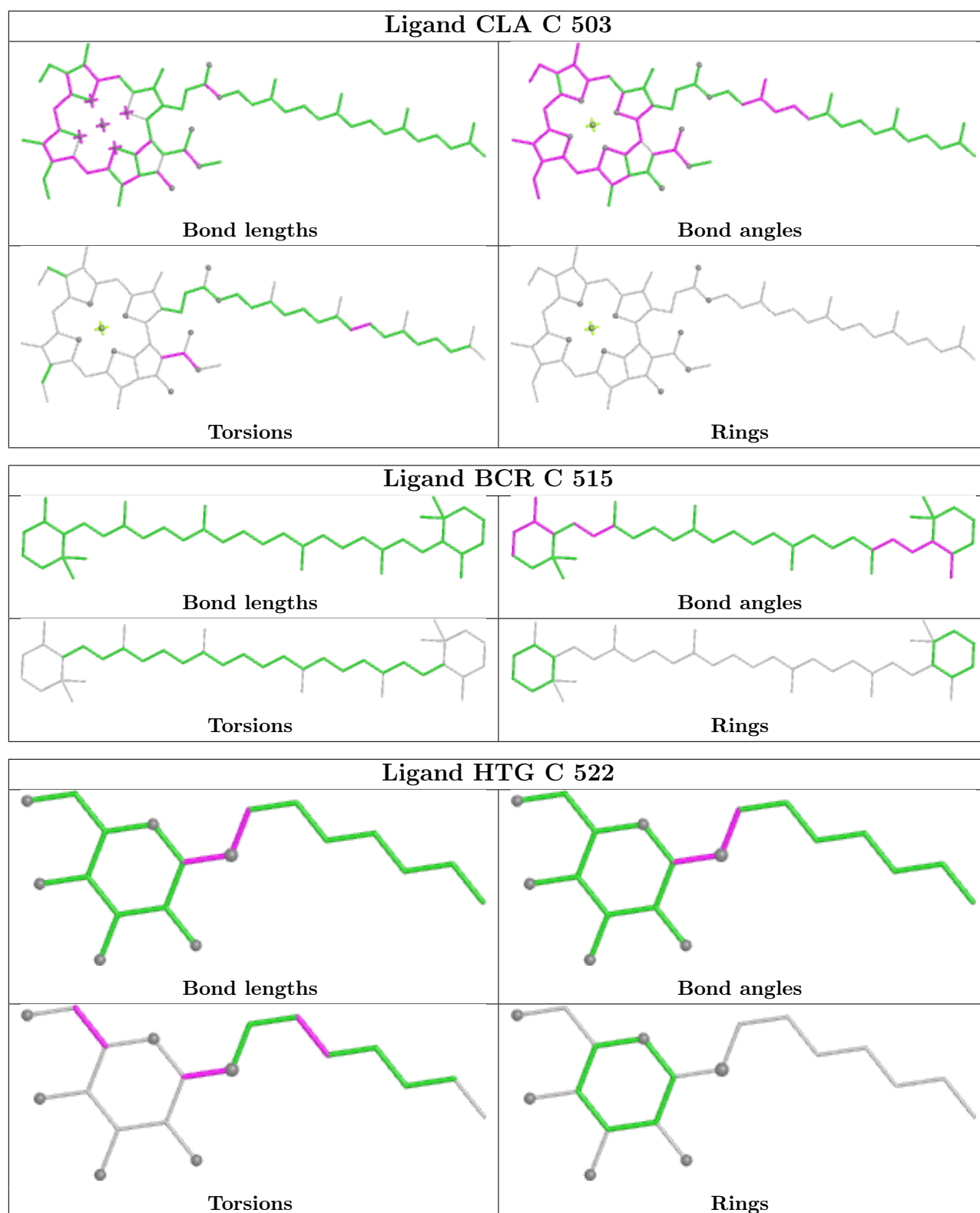


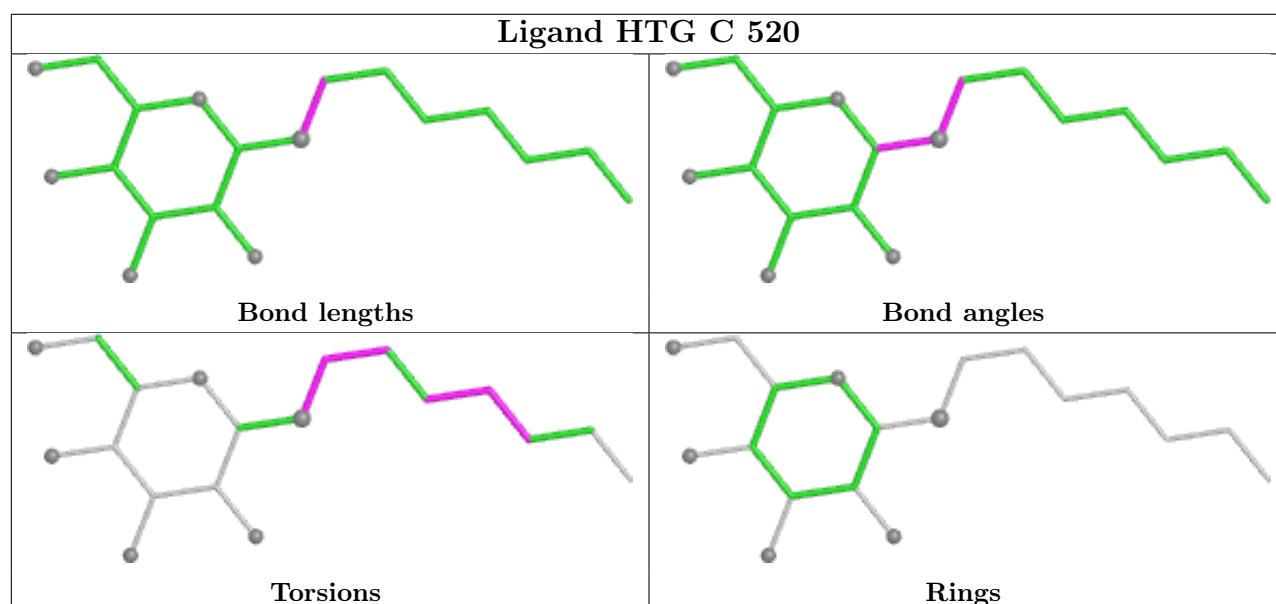
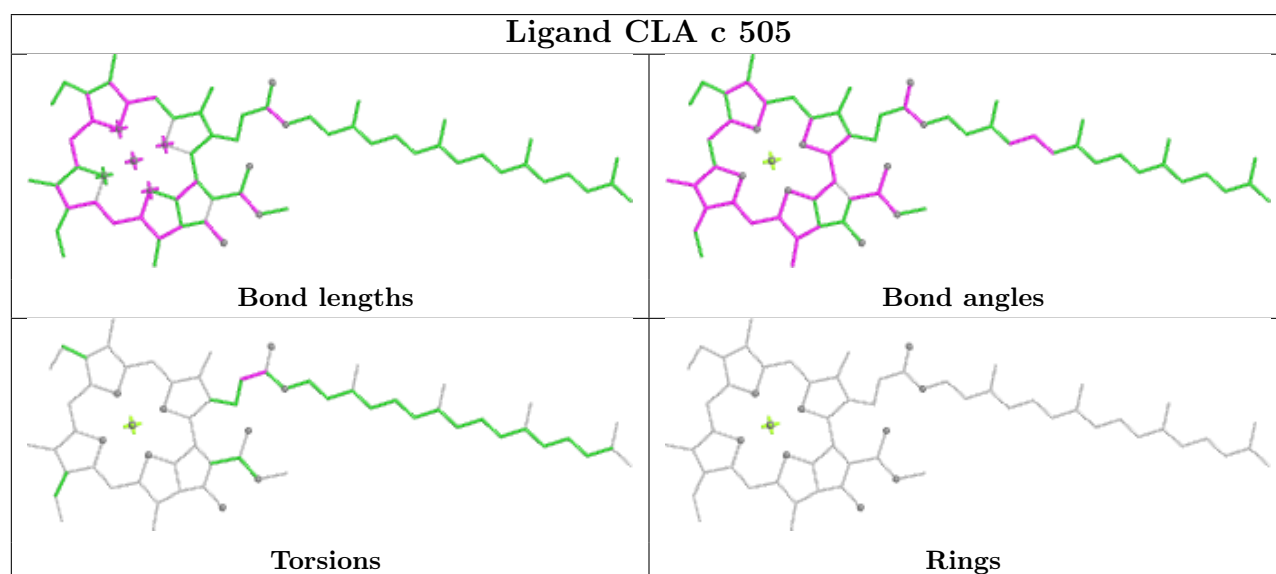
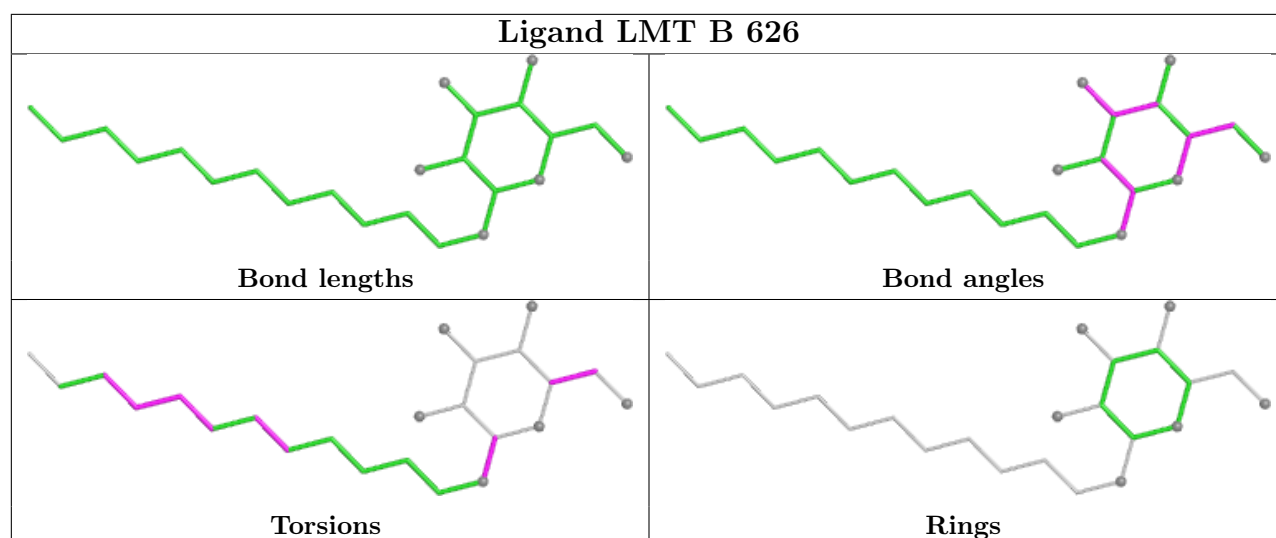


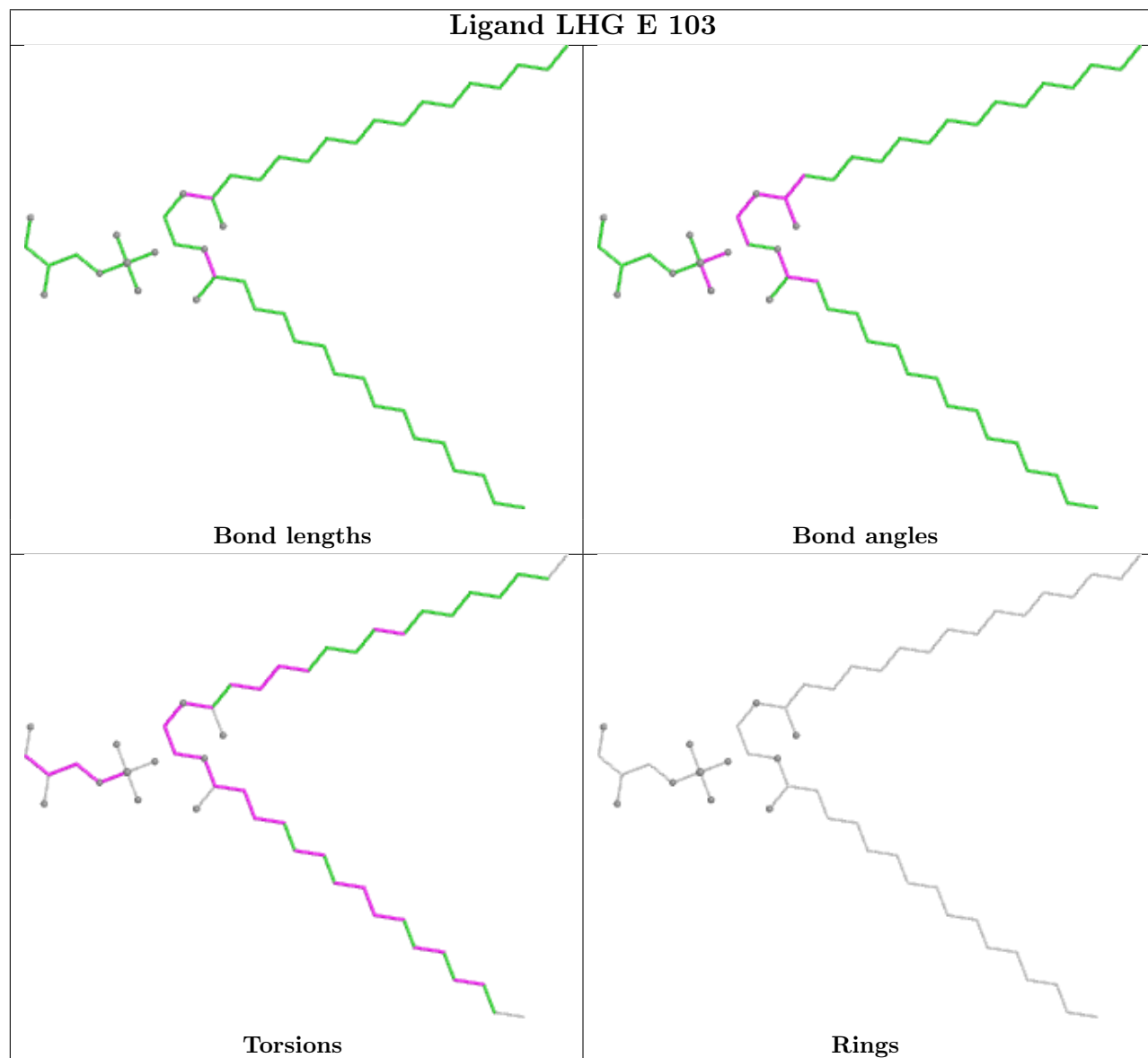
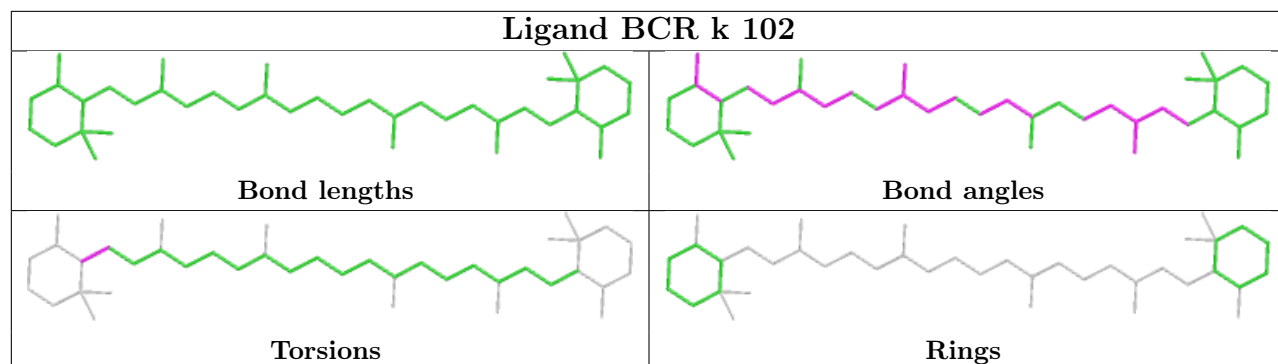


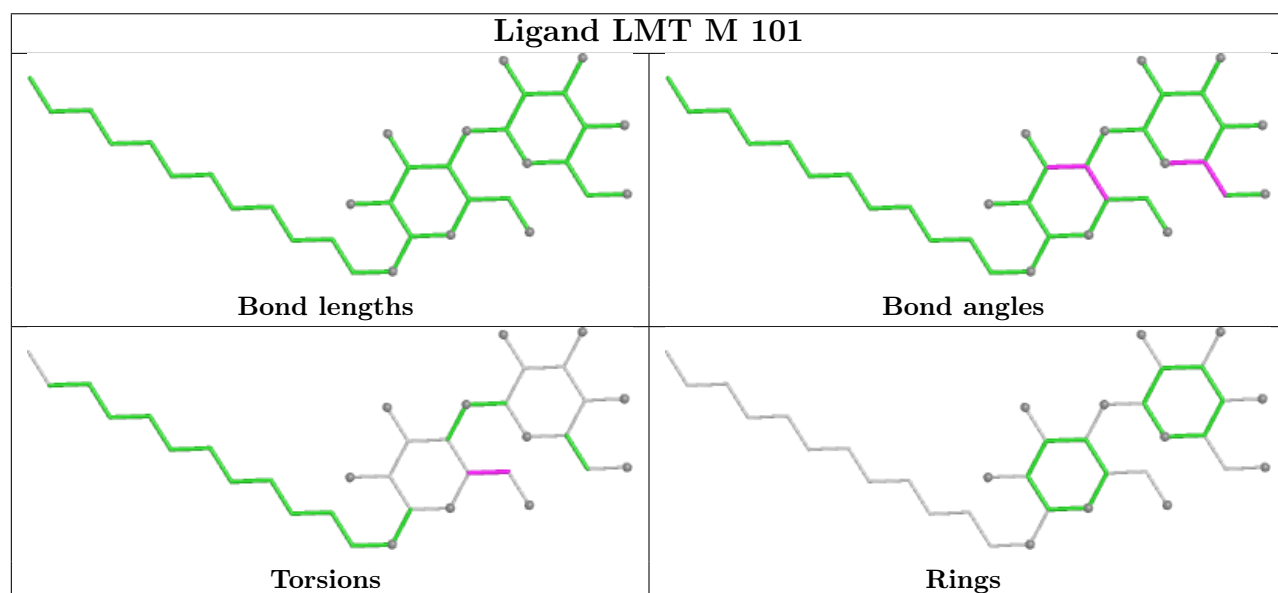
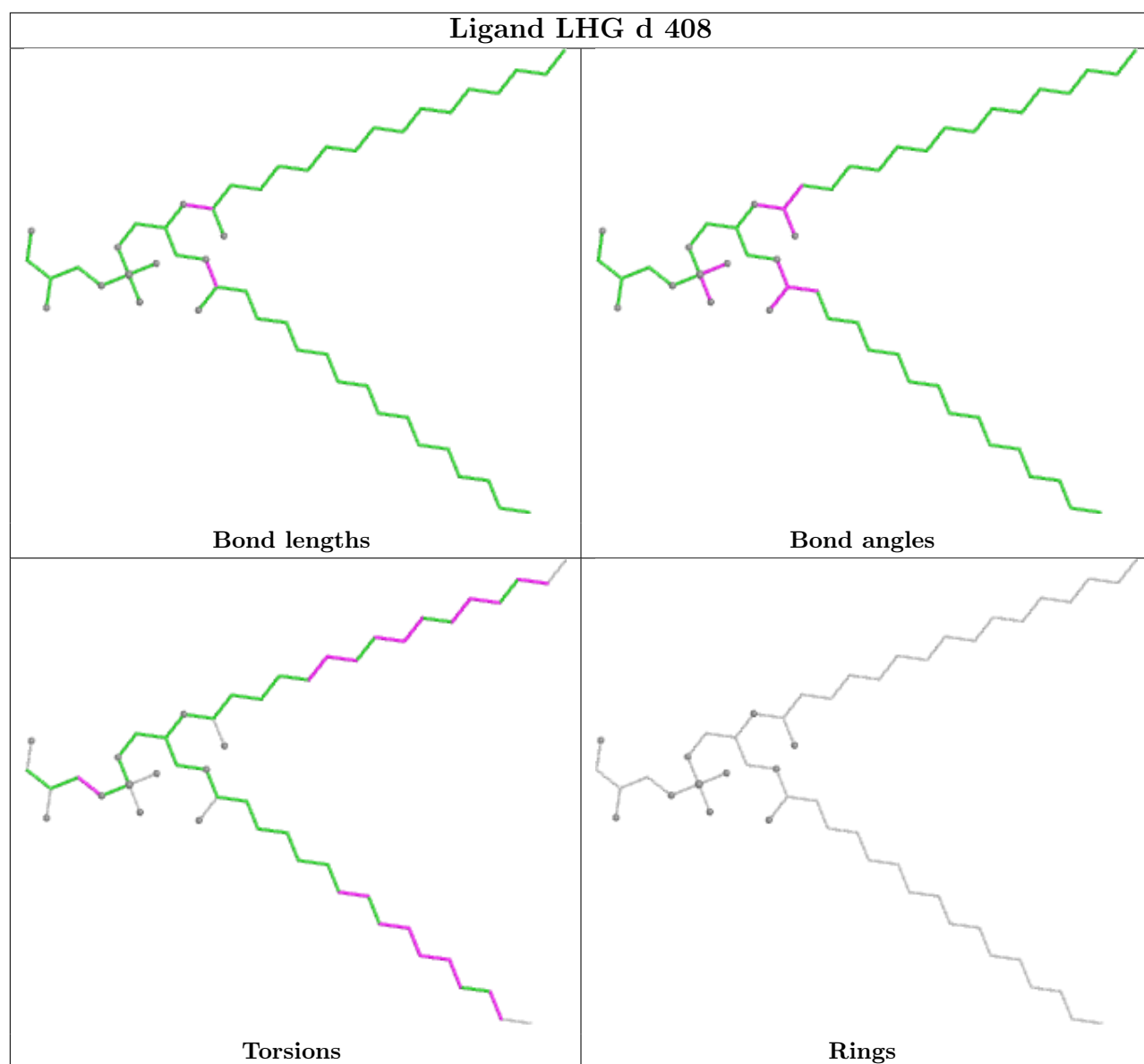
Ligand LMG a 410	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings

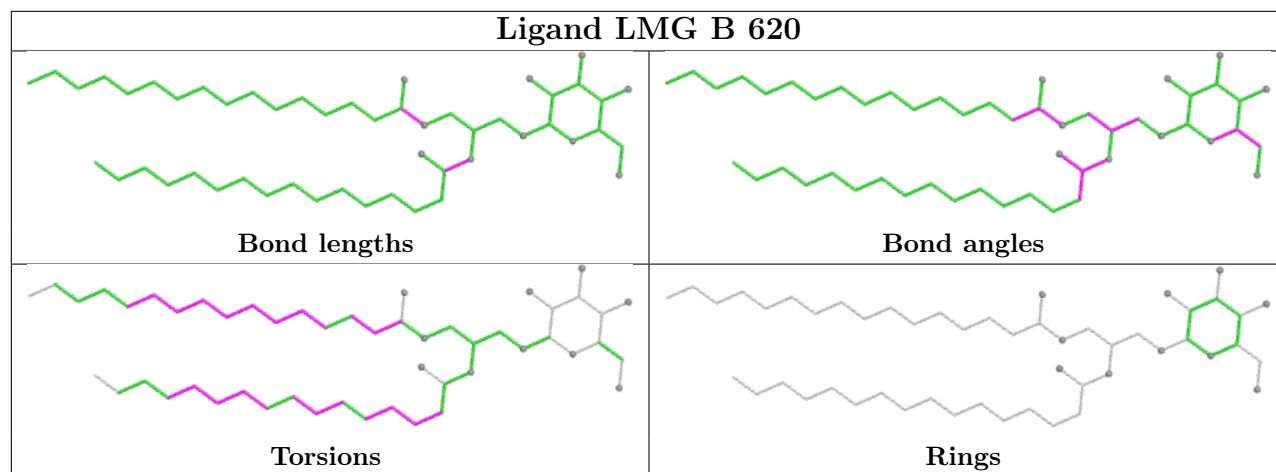
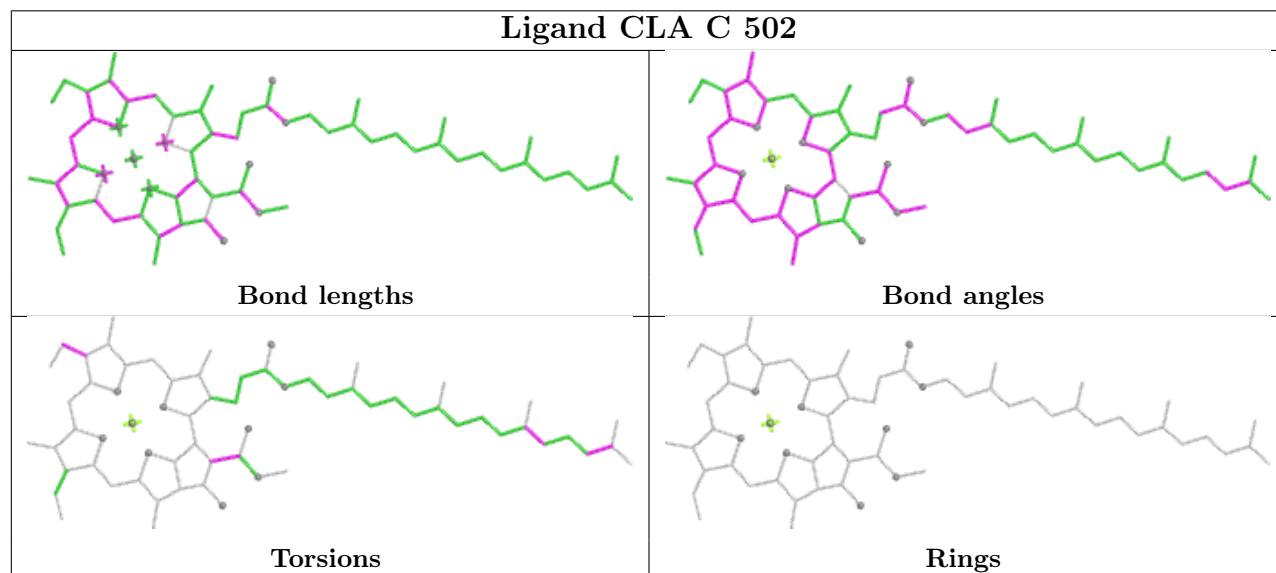
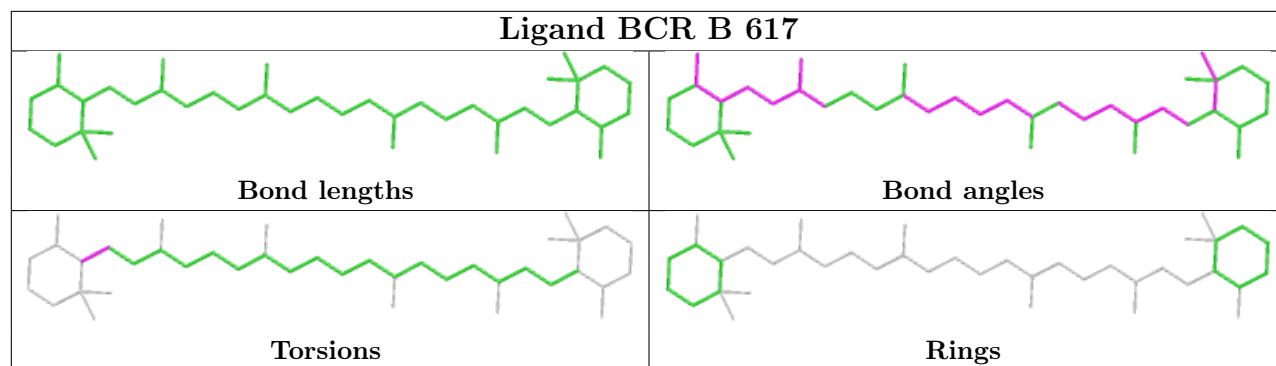


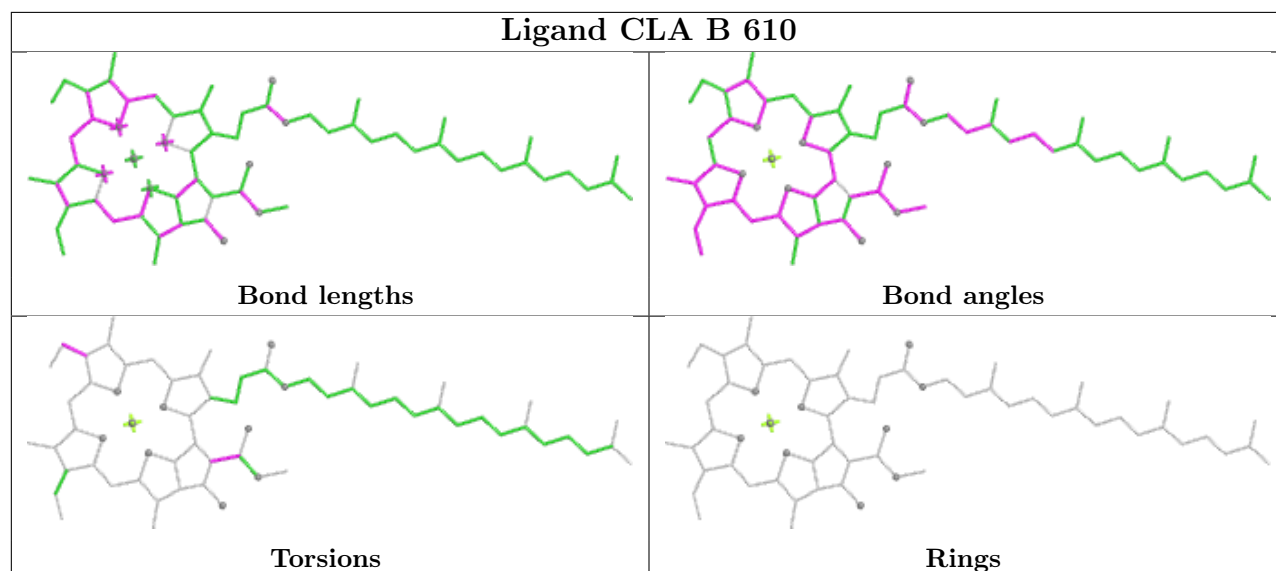
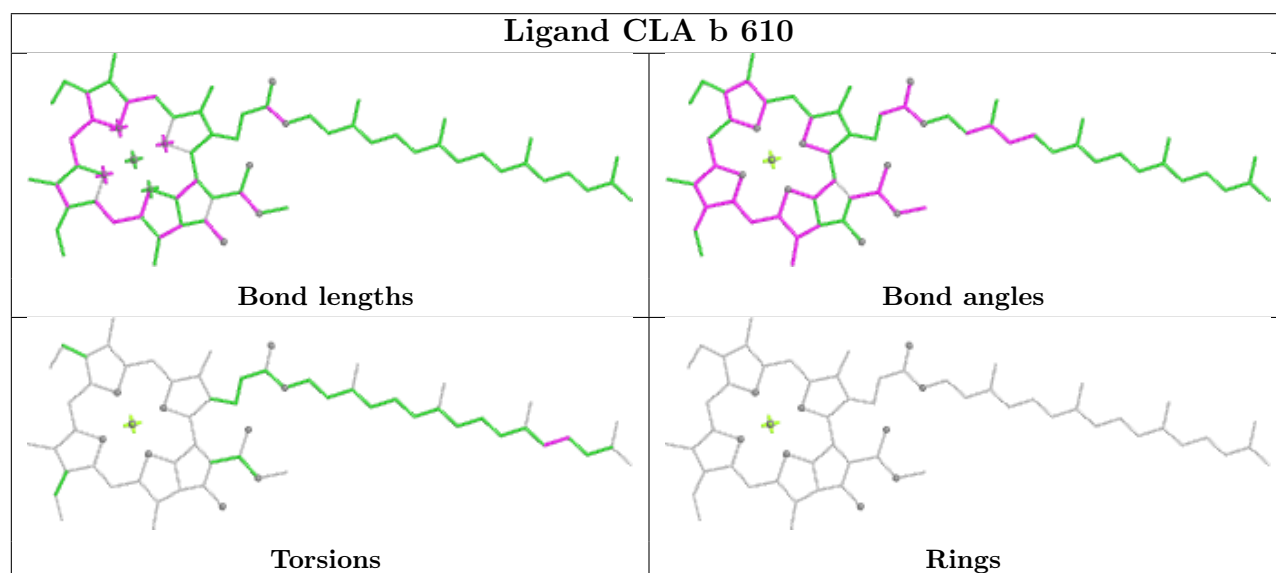
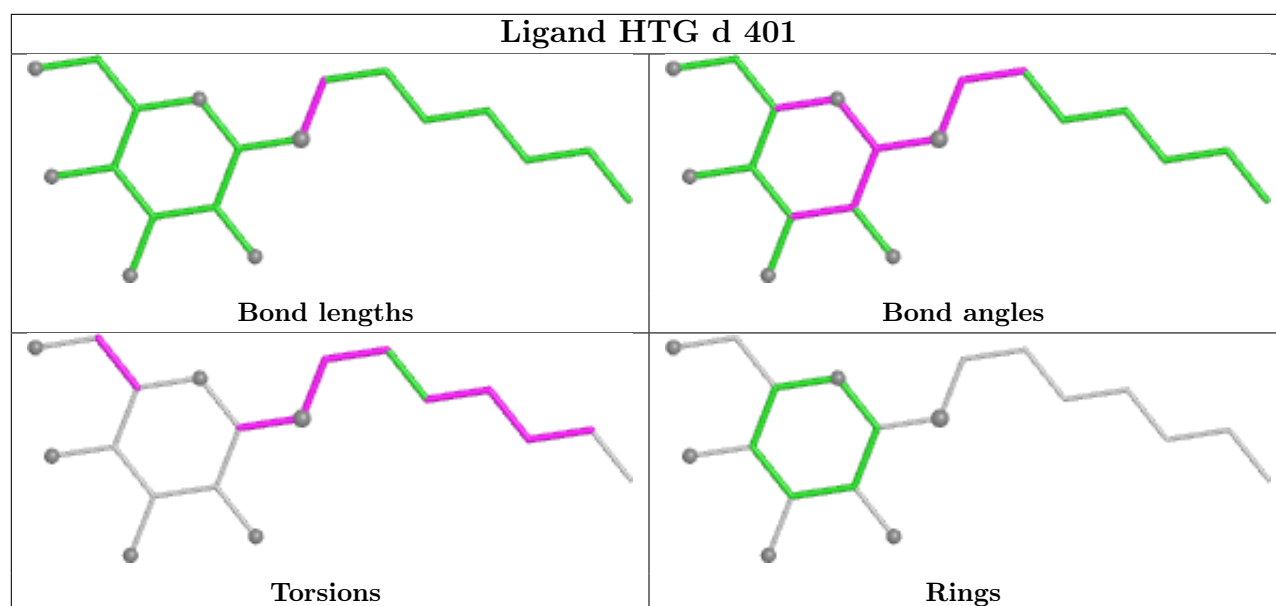


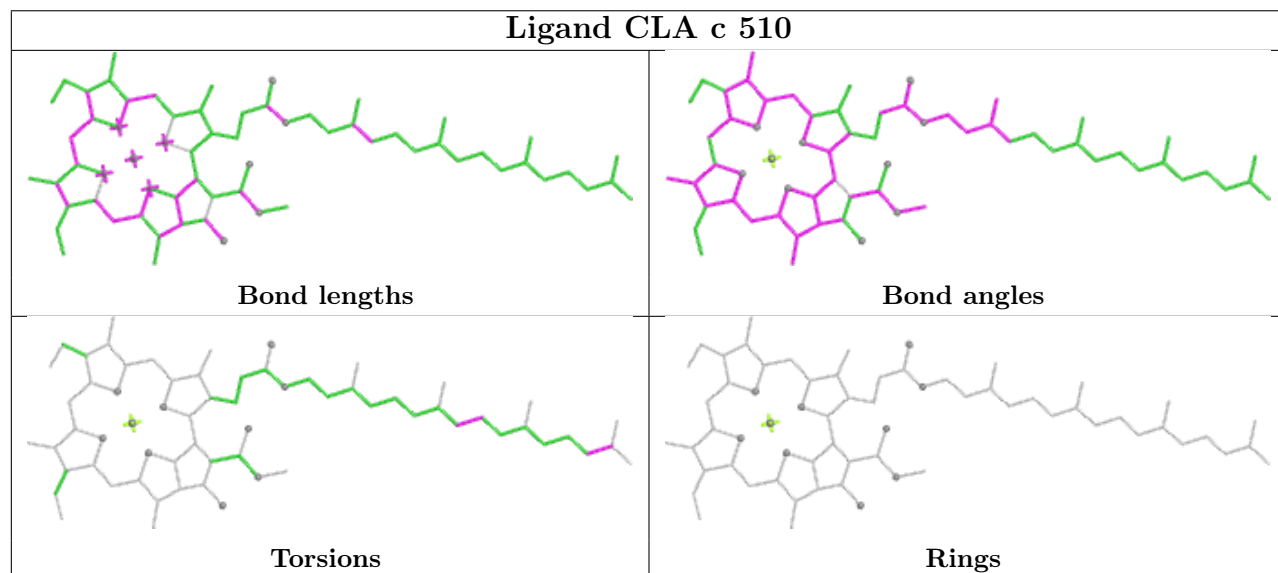
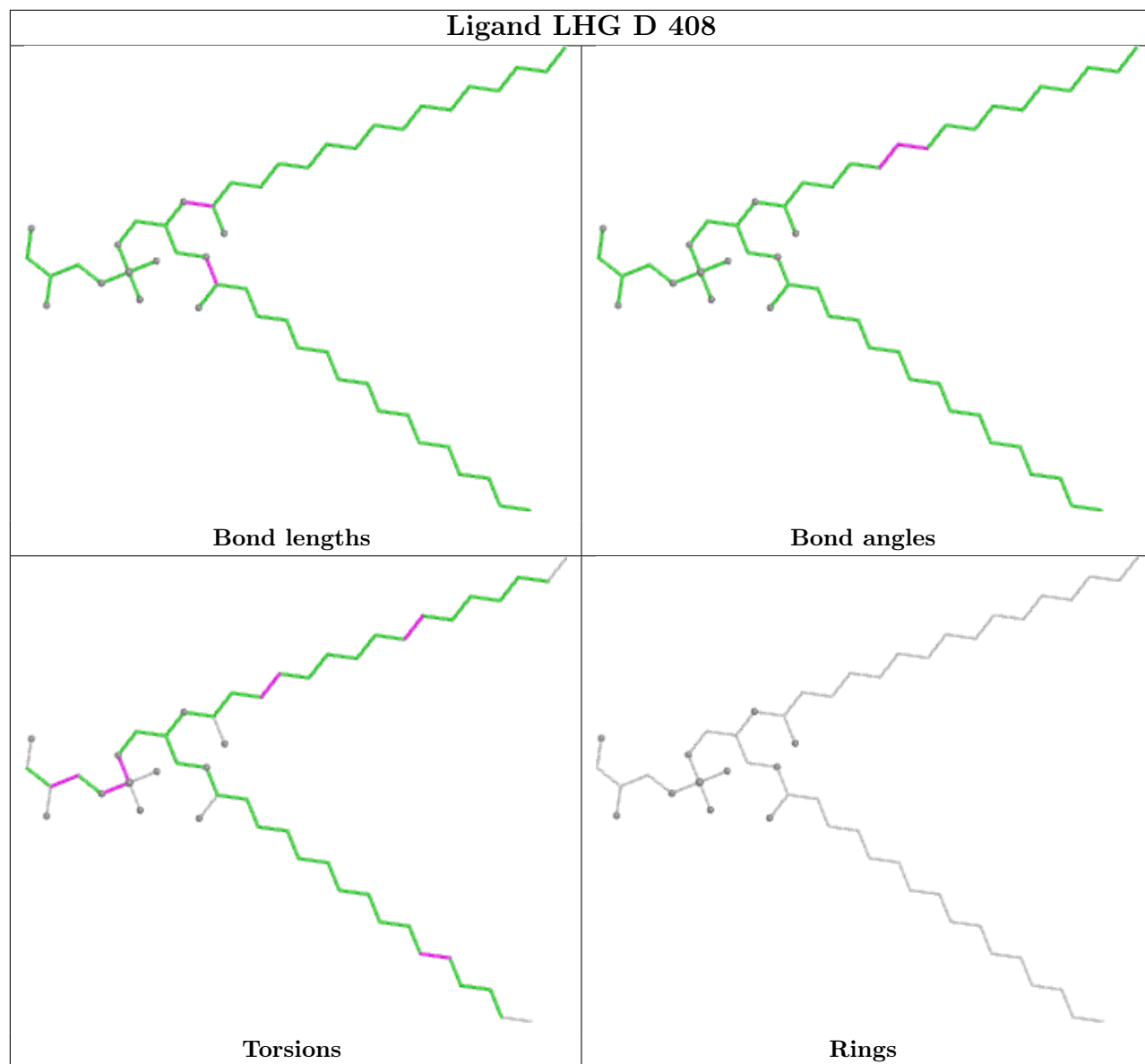




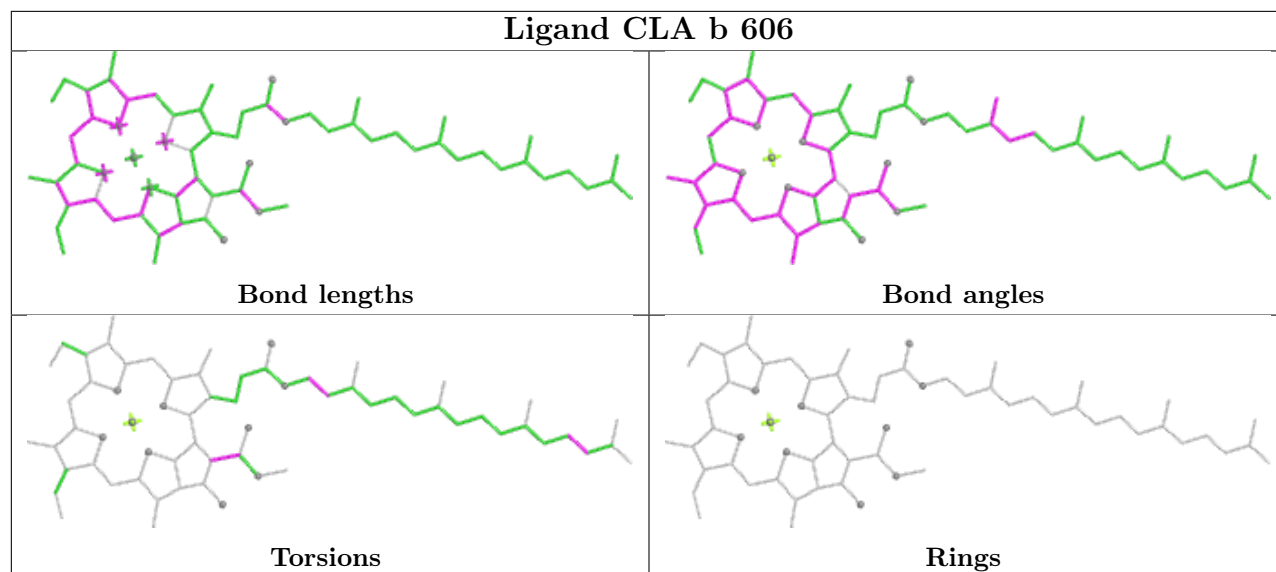




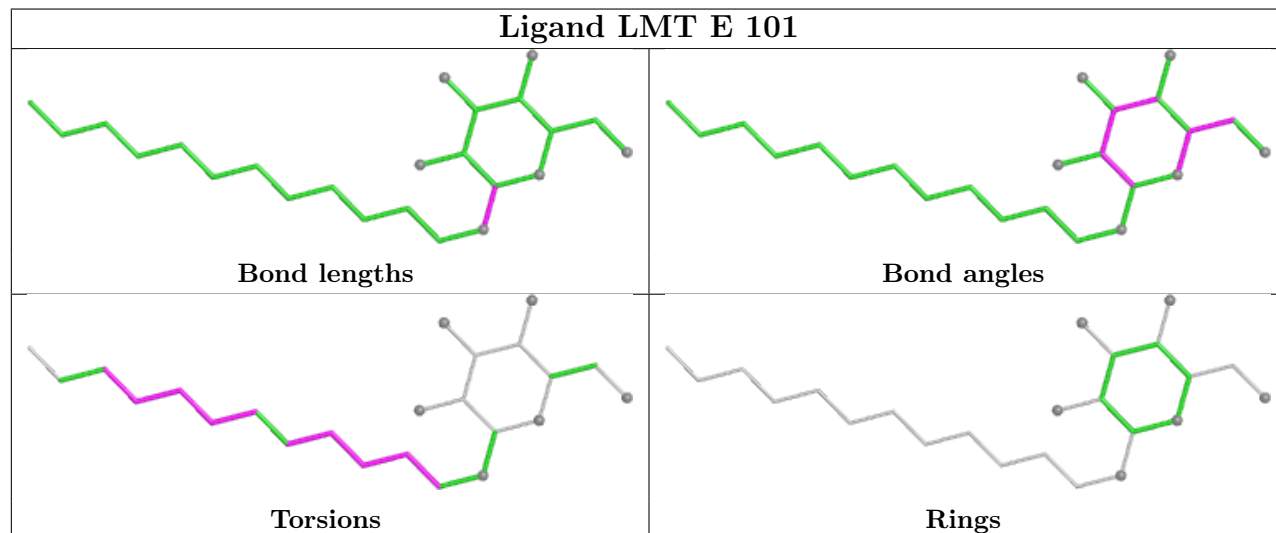




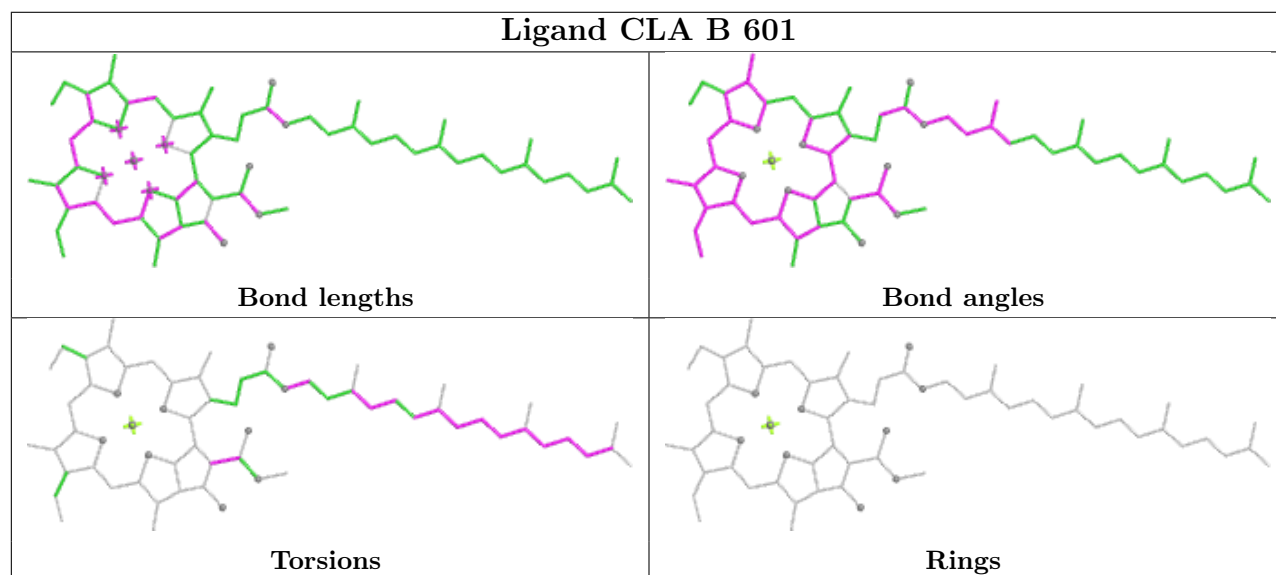
Ligand CLA b 606

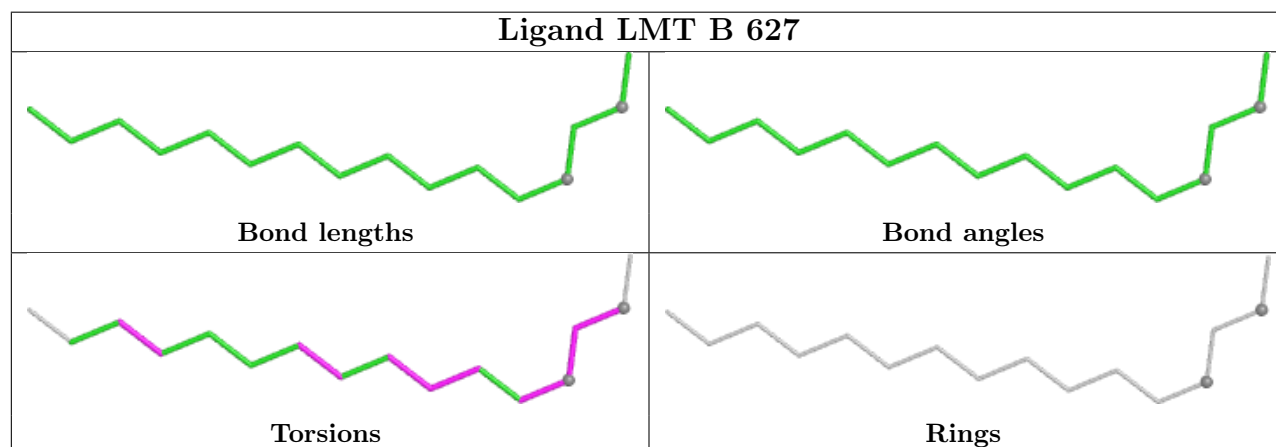
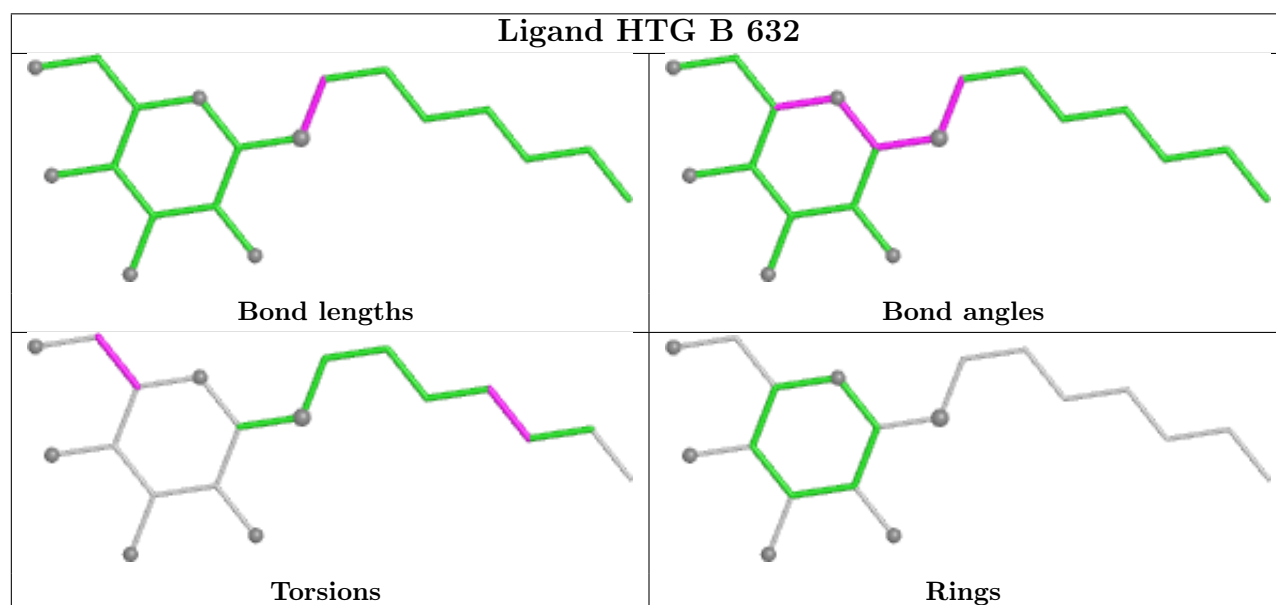
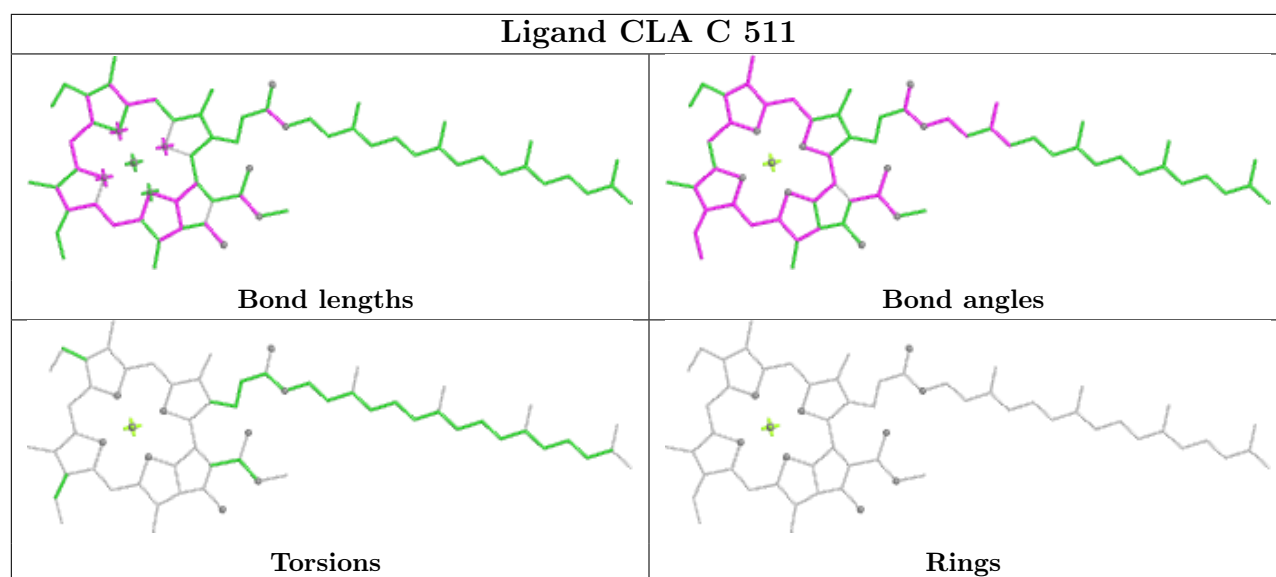


Ligand LMT E 101

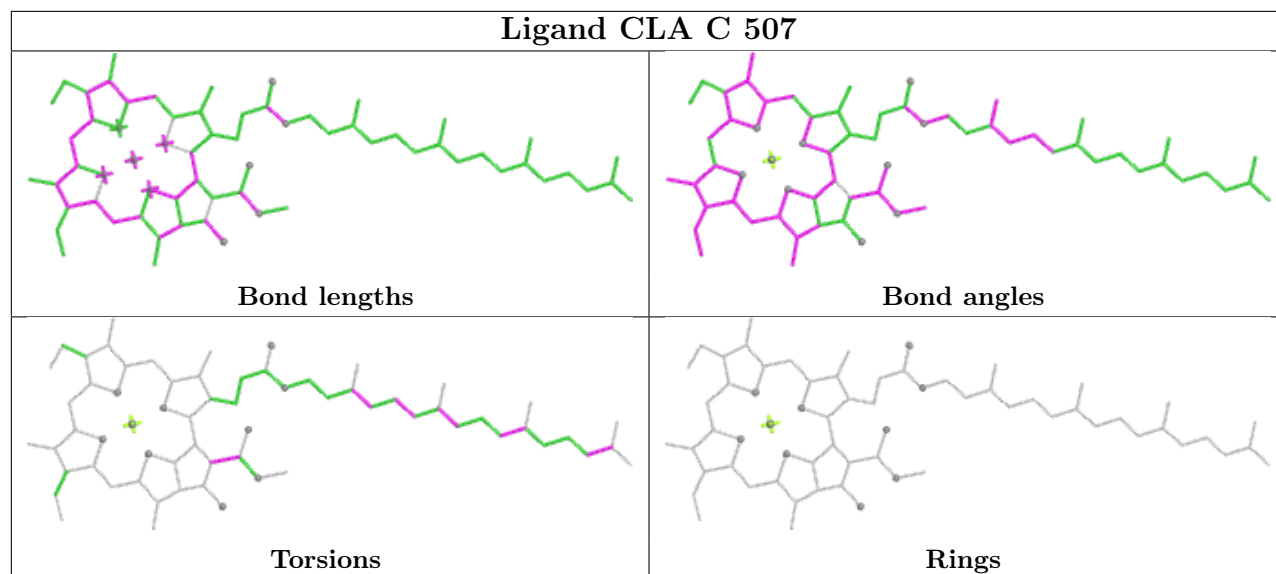


Ligand CLA B 601

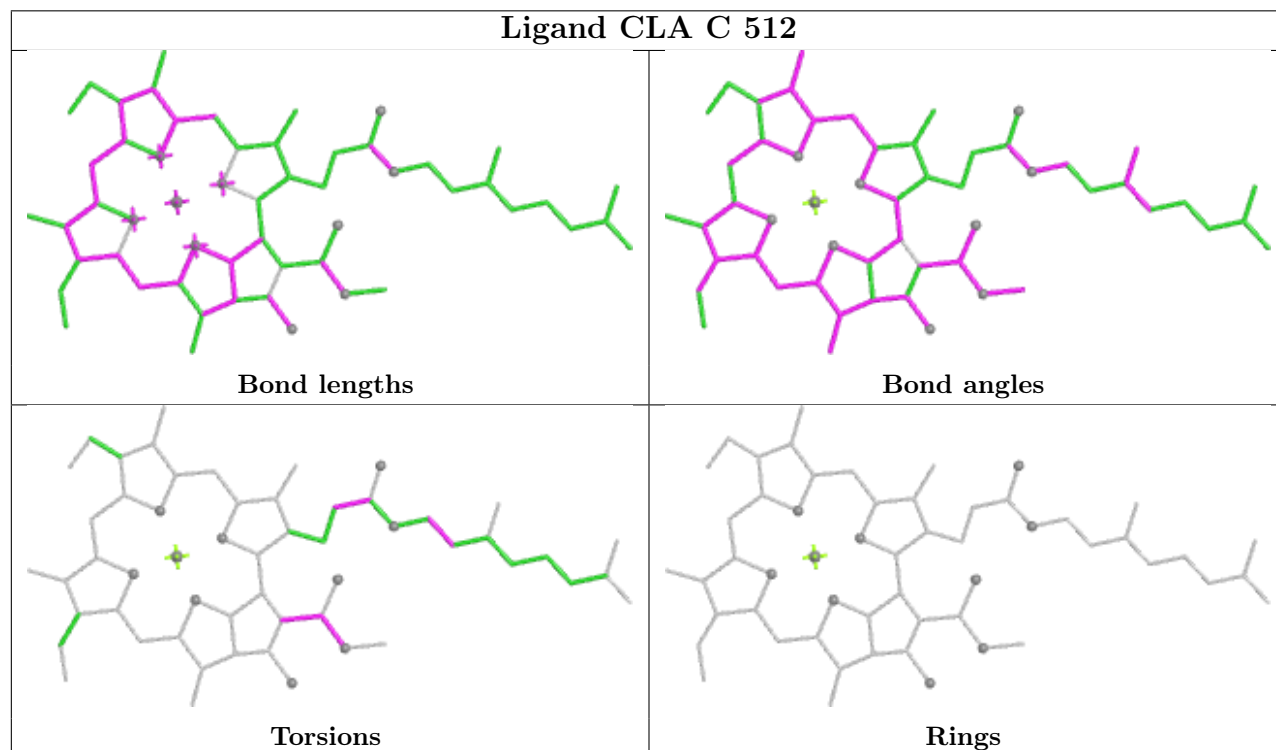


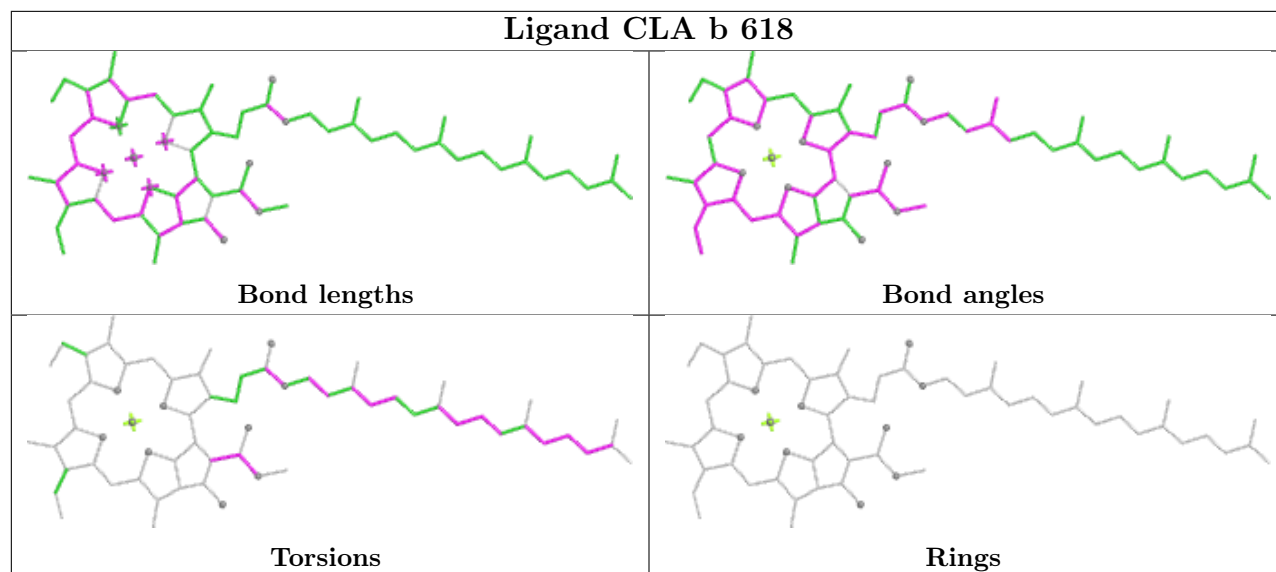
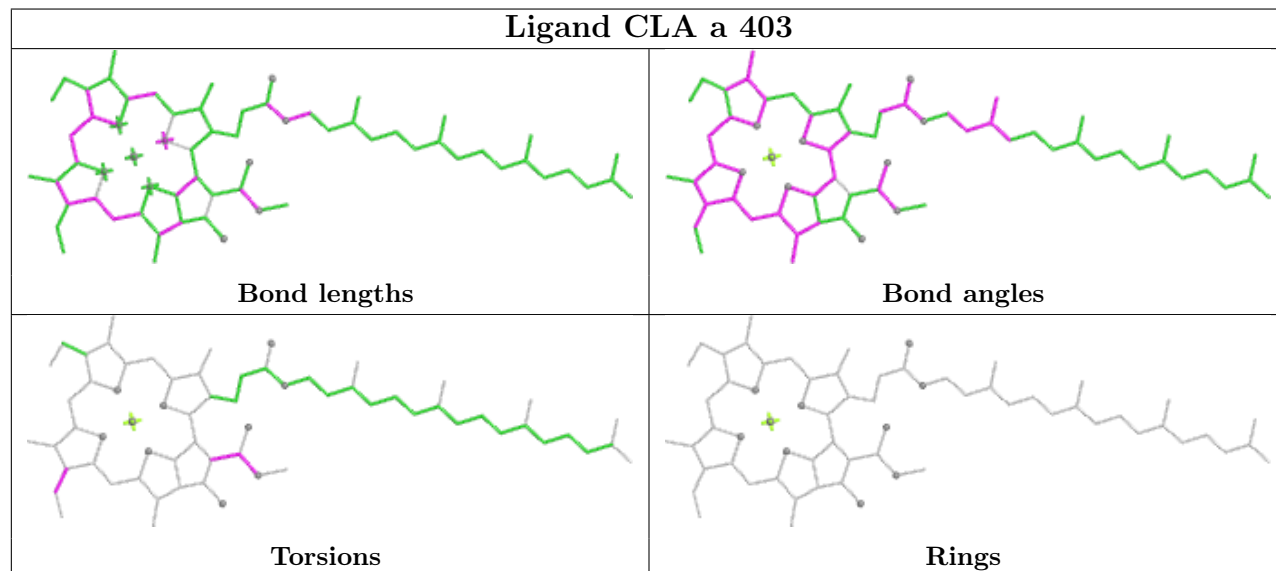


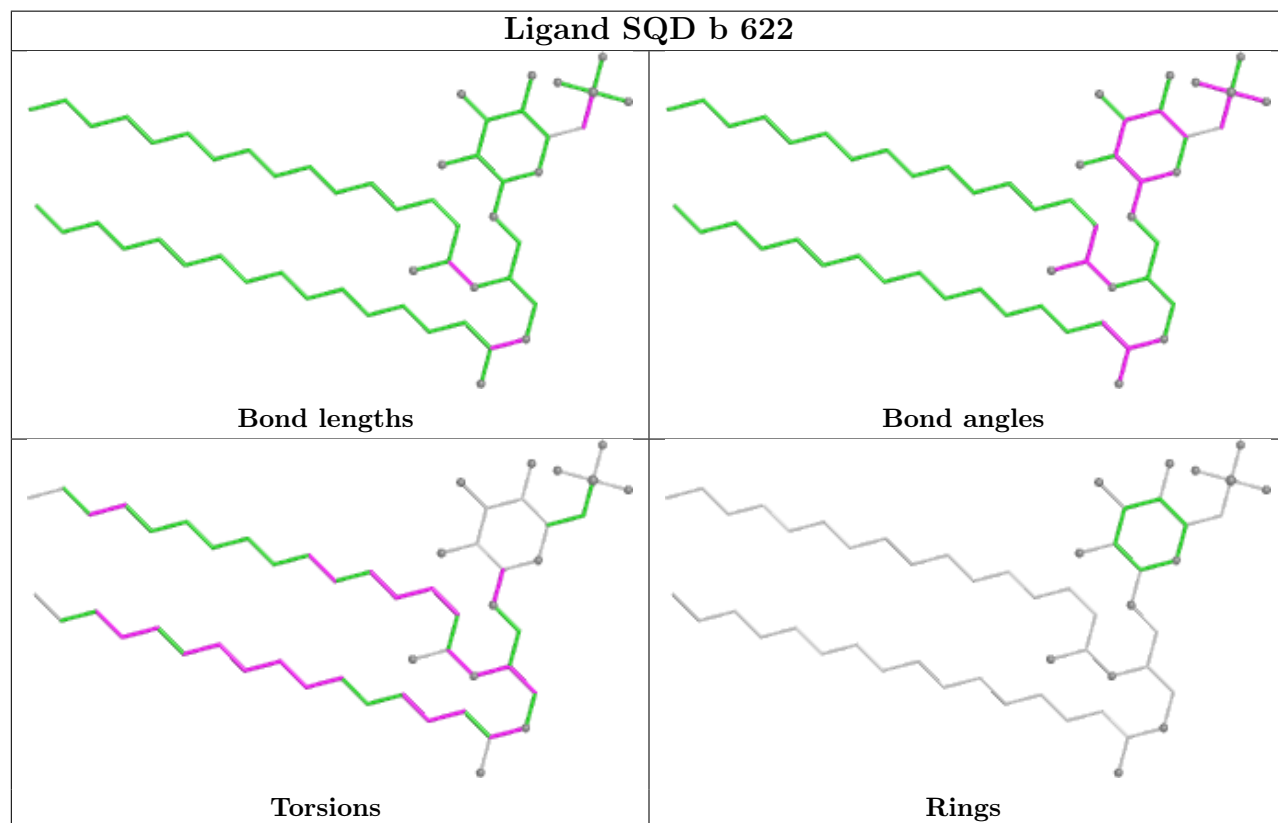
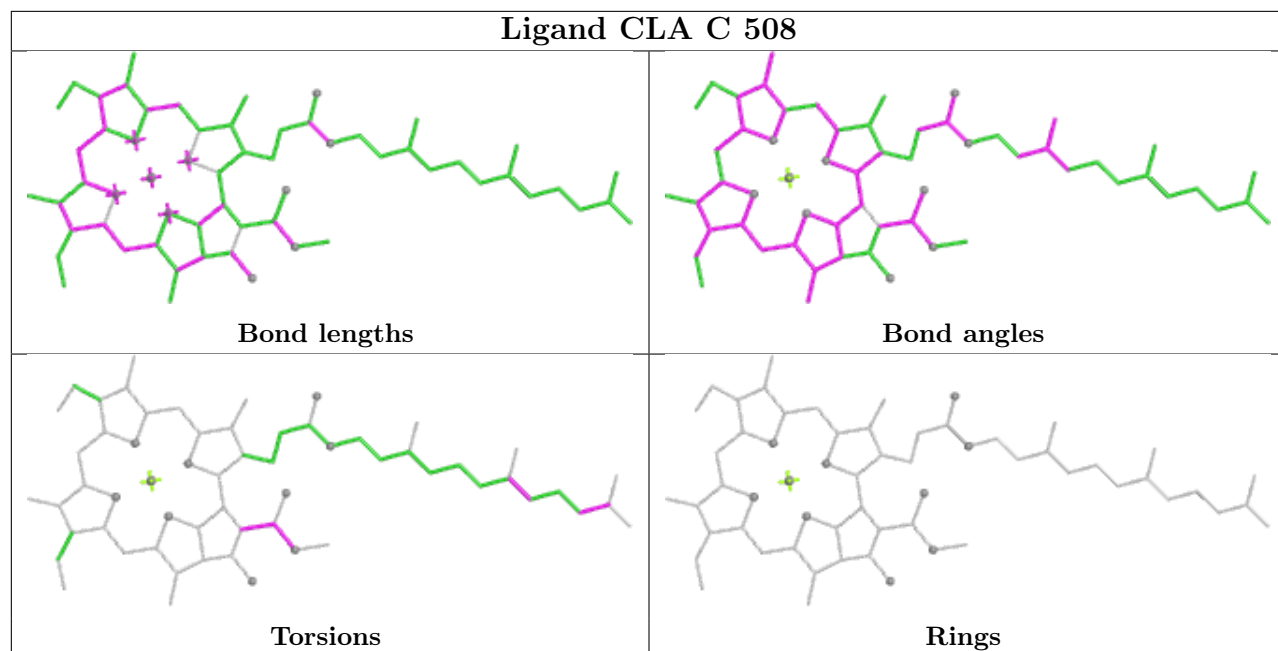
Ligand CLA C 507

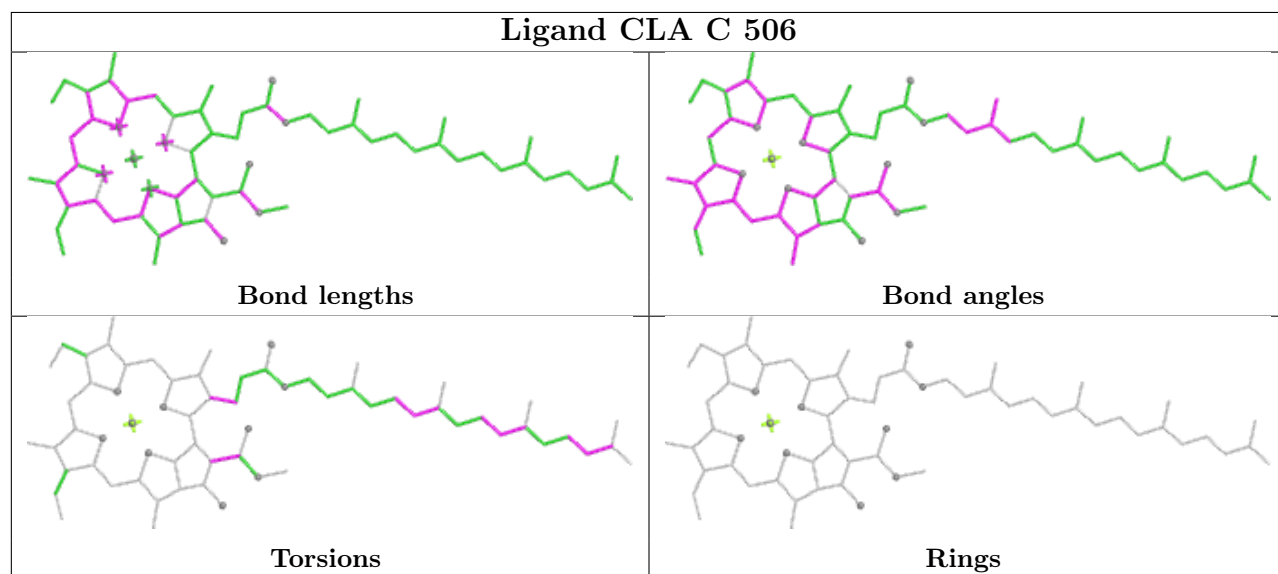
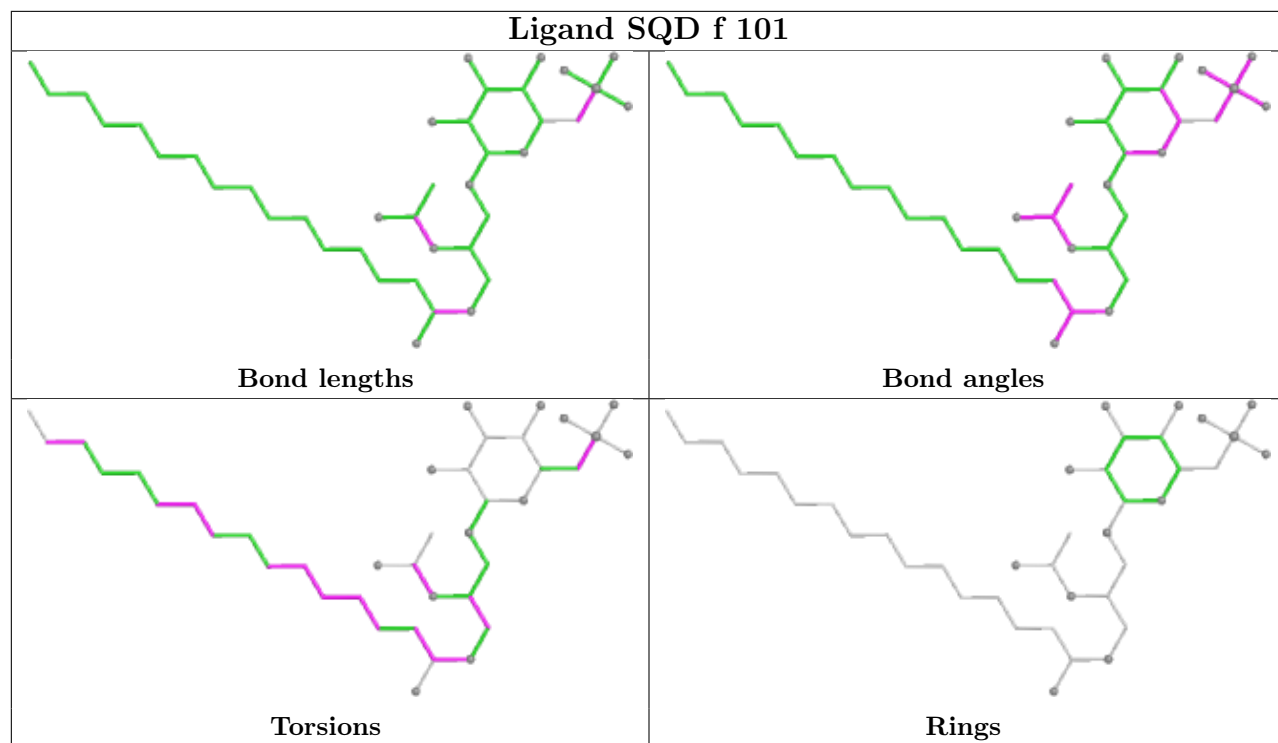


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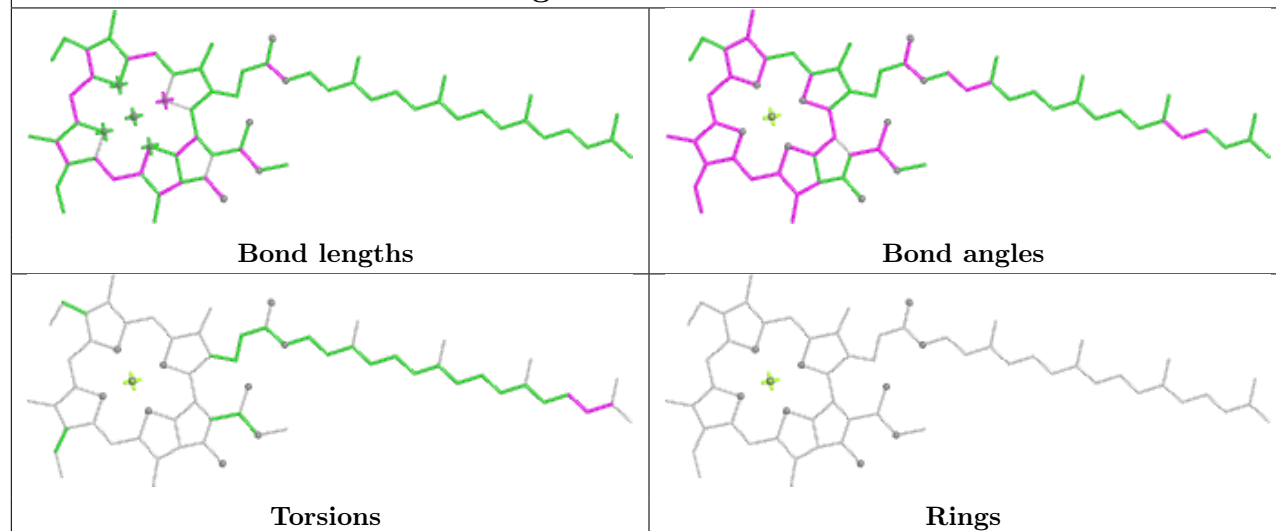


Ligand CLA b 618**Ligand CLA a 403**

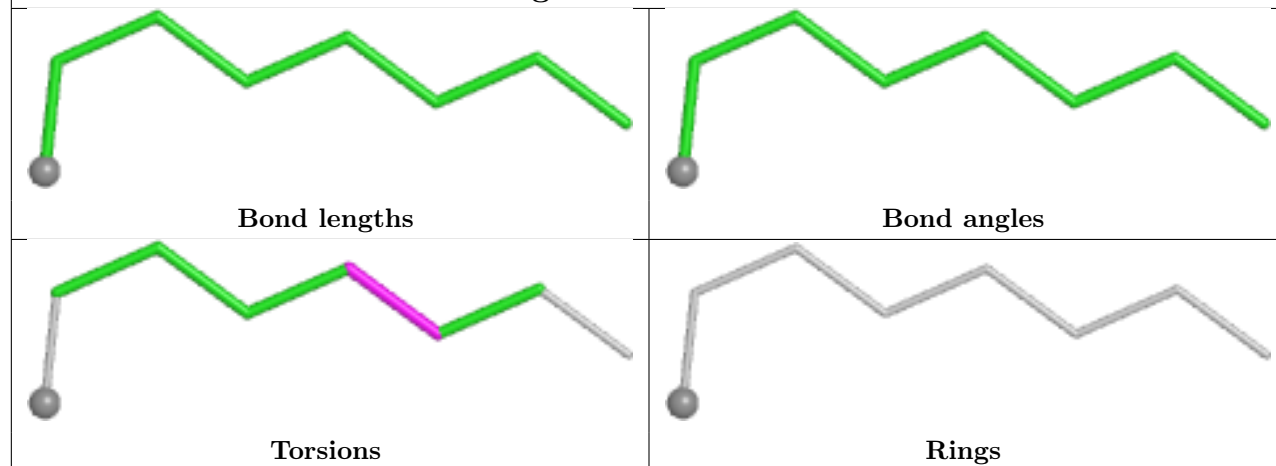




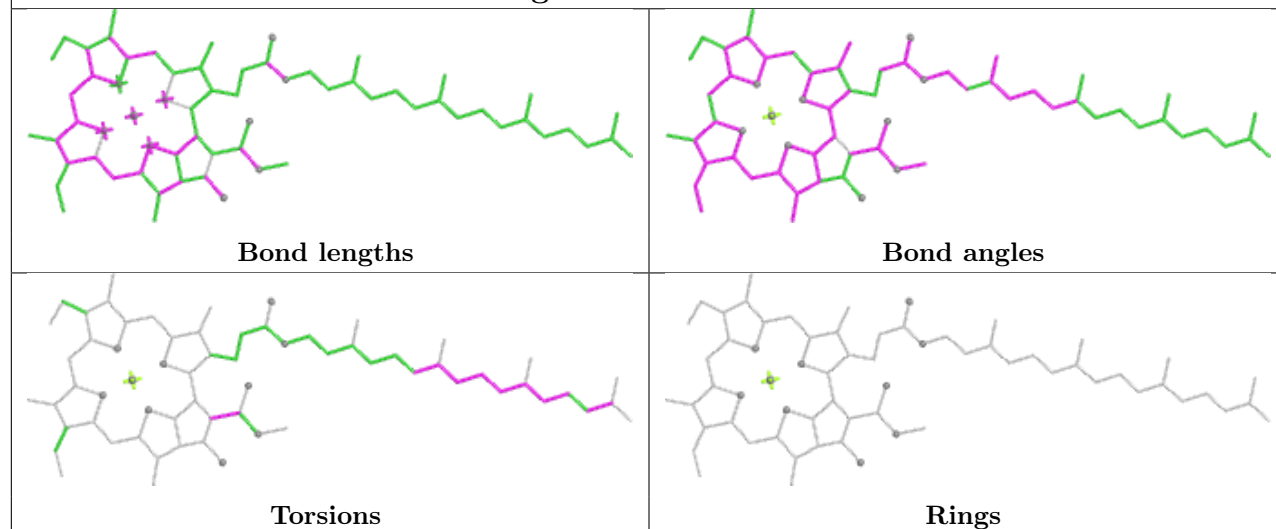
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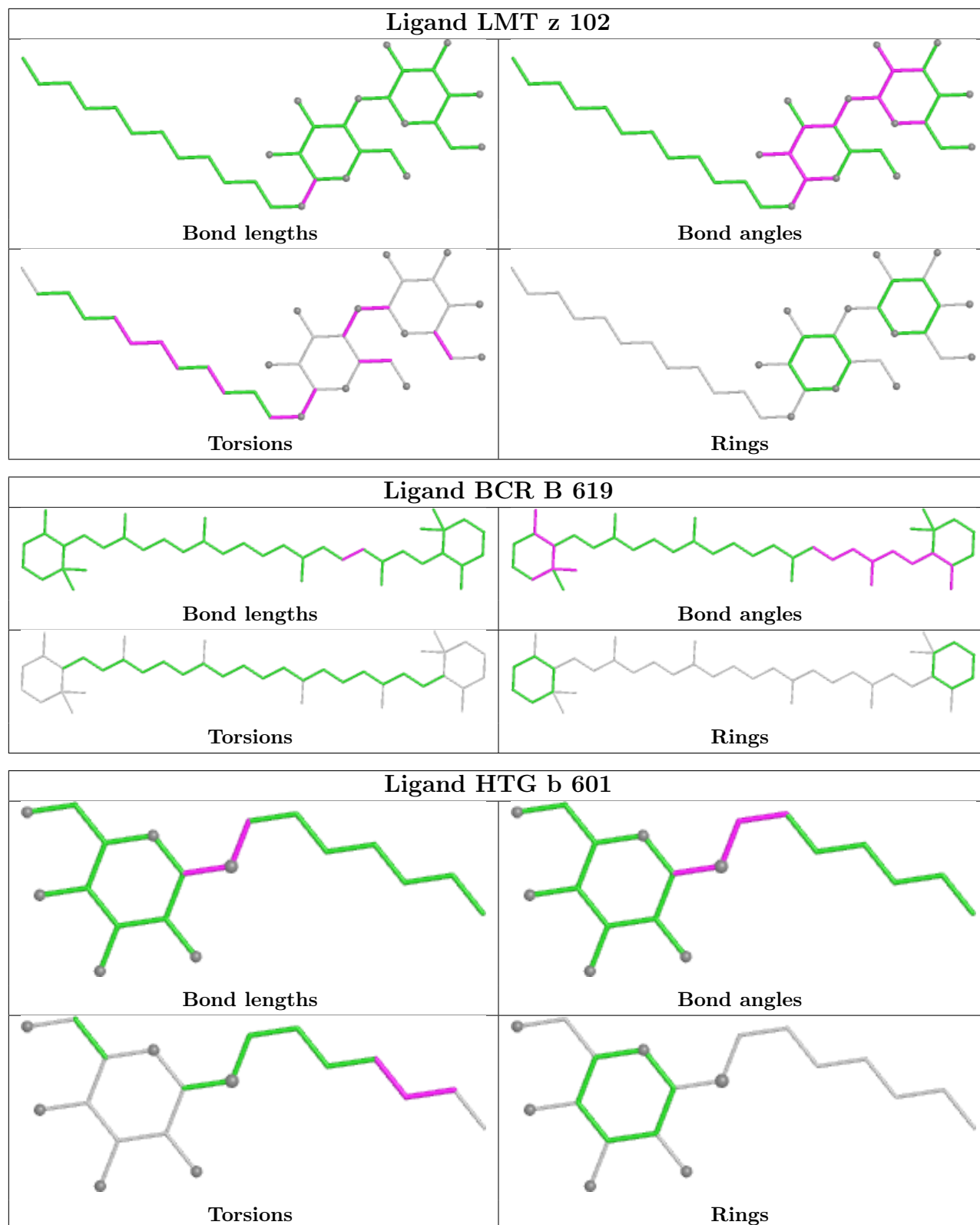


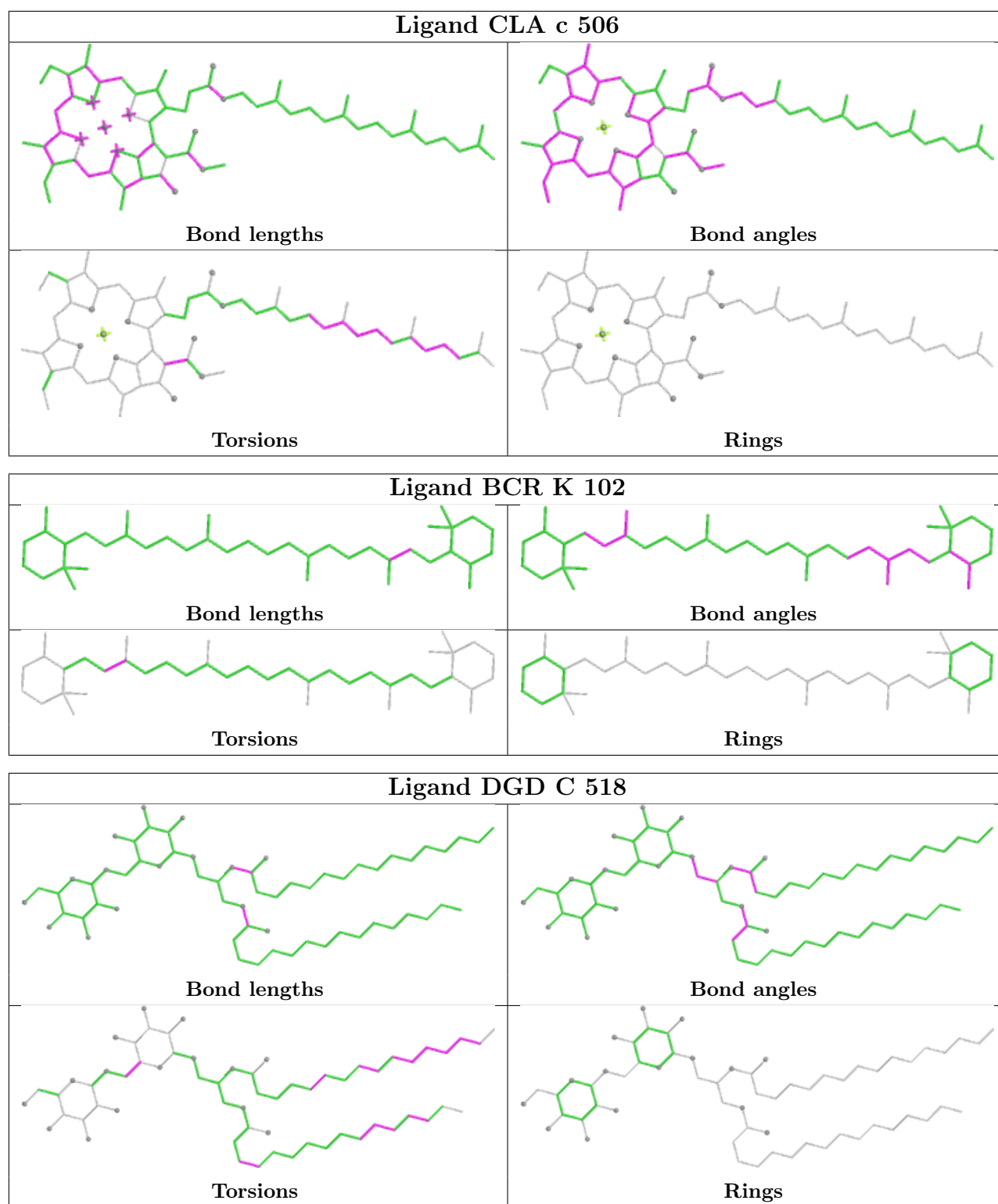
Ligand HTG u 201

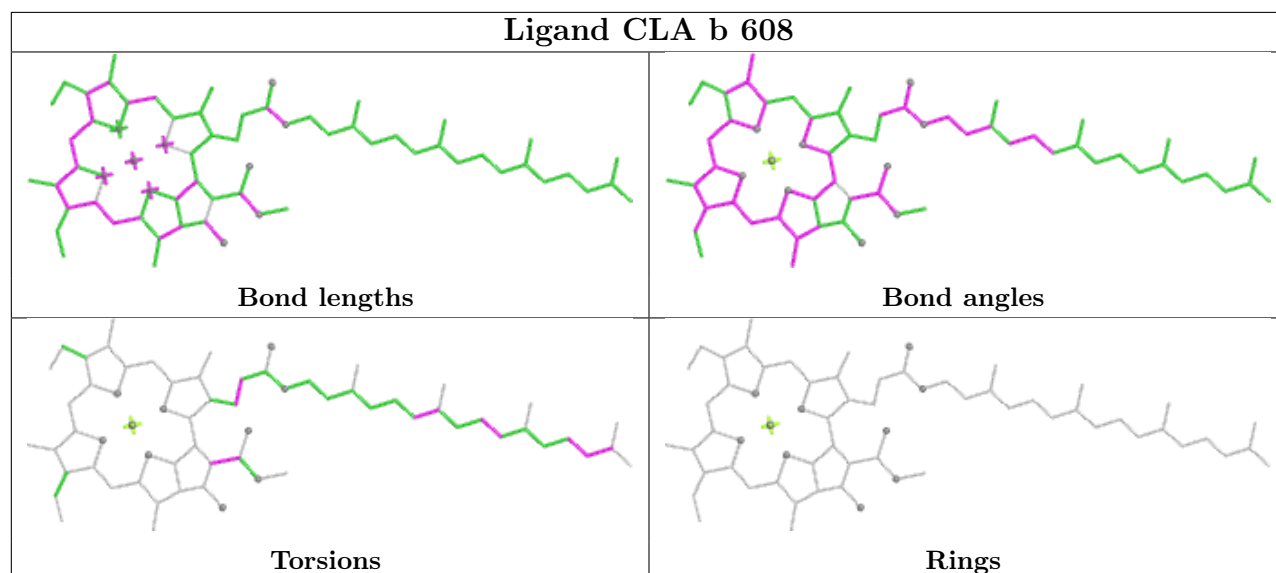
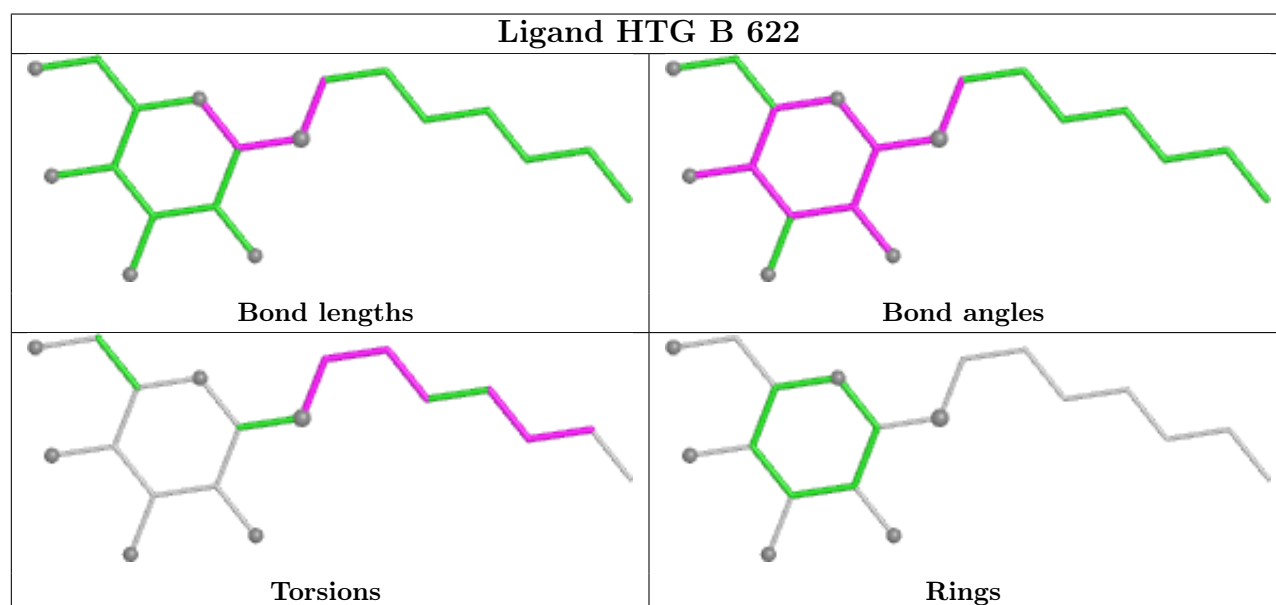
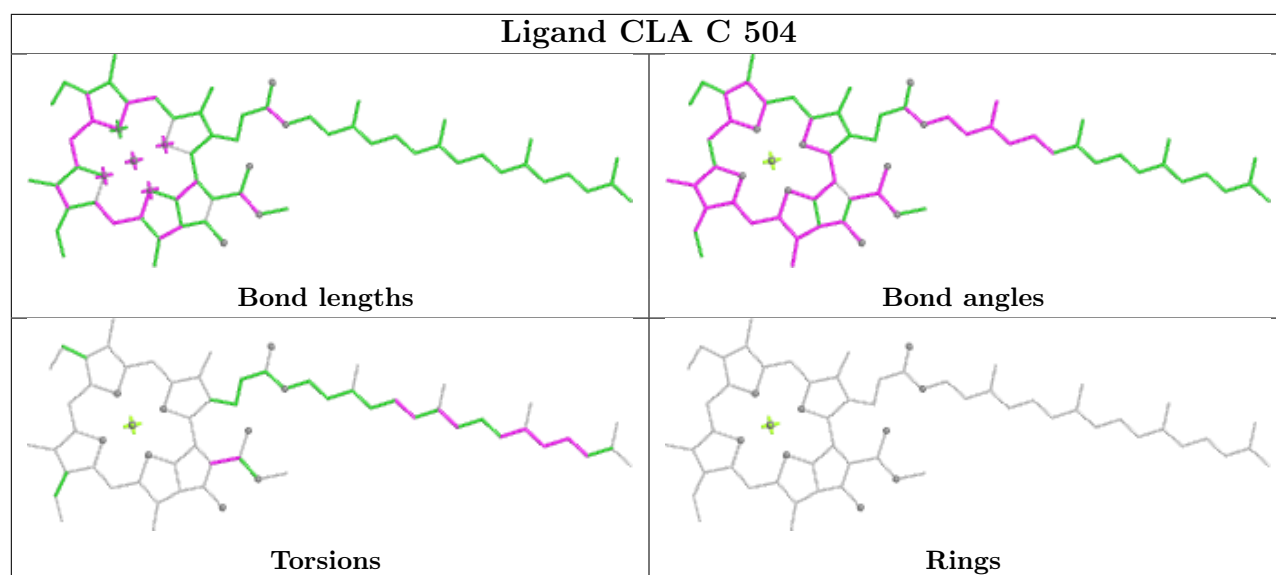


Ligand CLA D 404

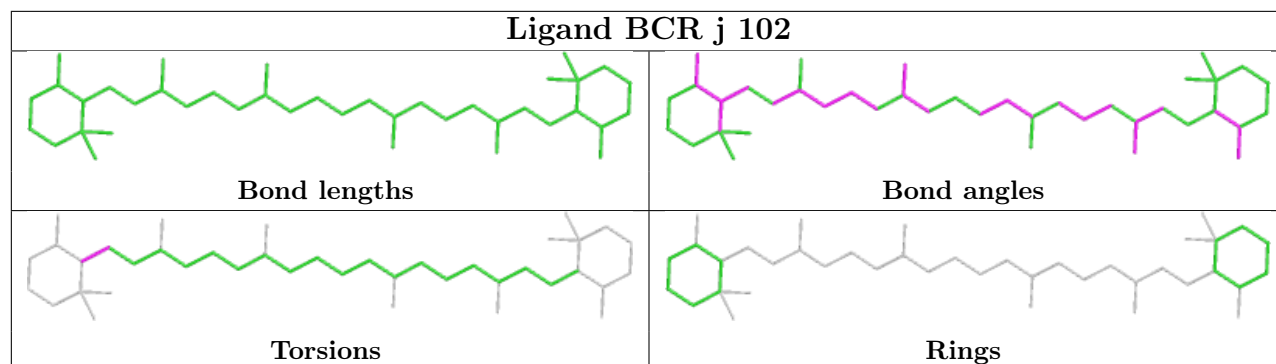




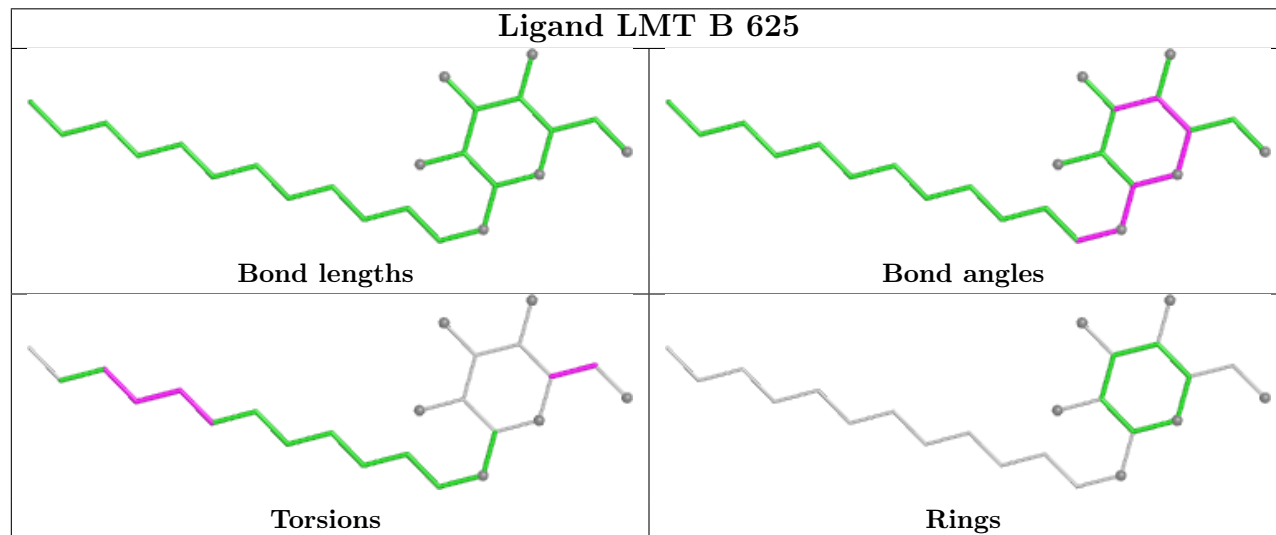




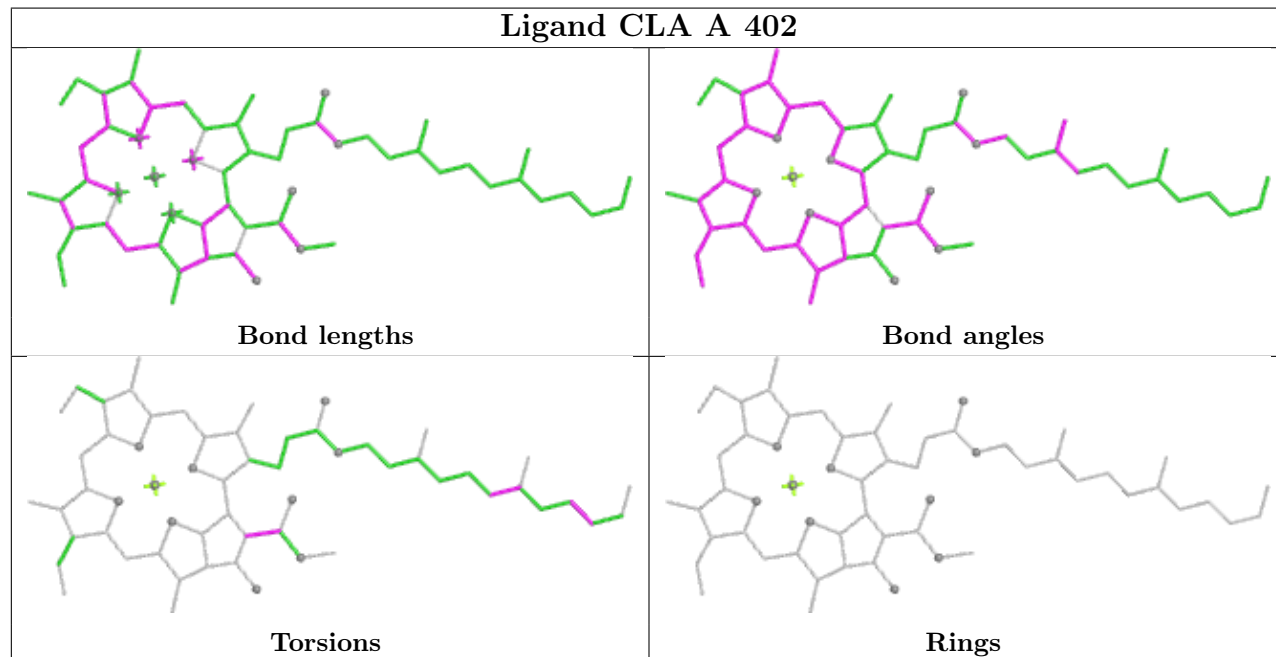
Ligand BCR j 102

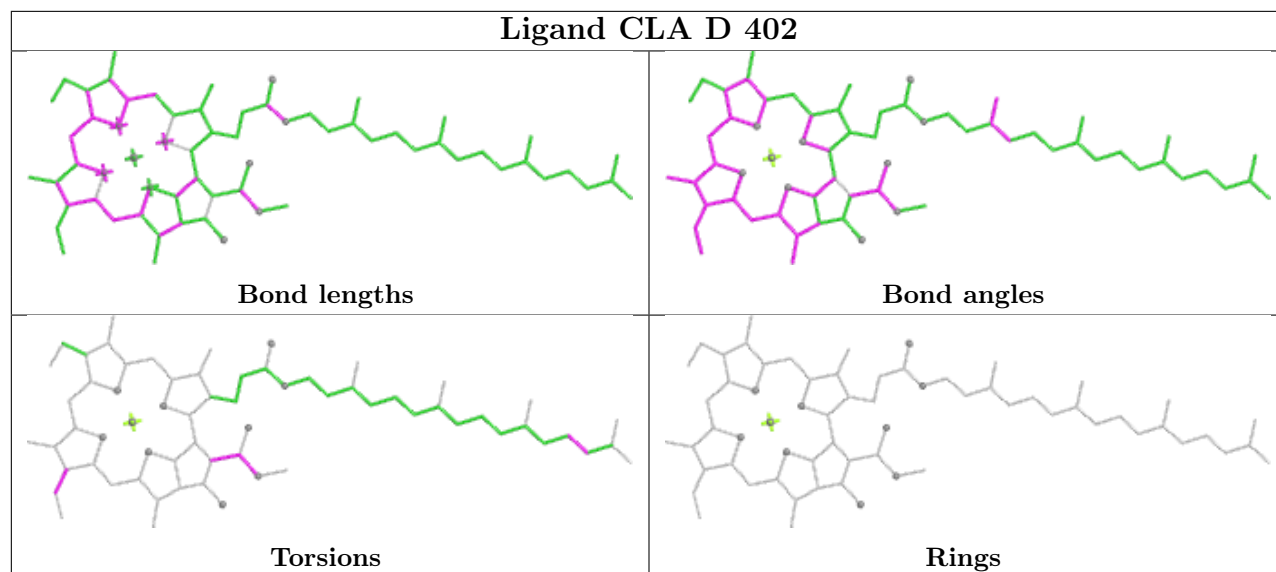
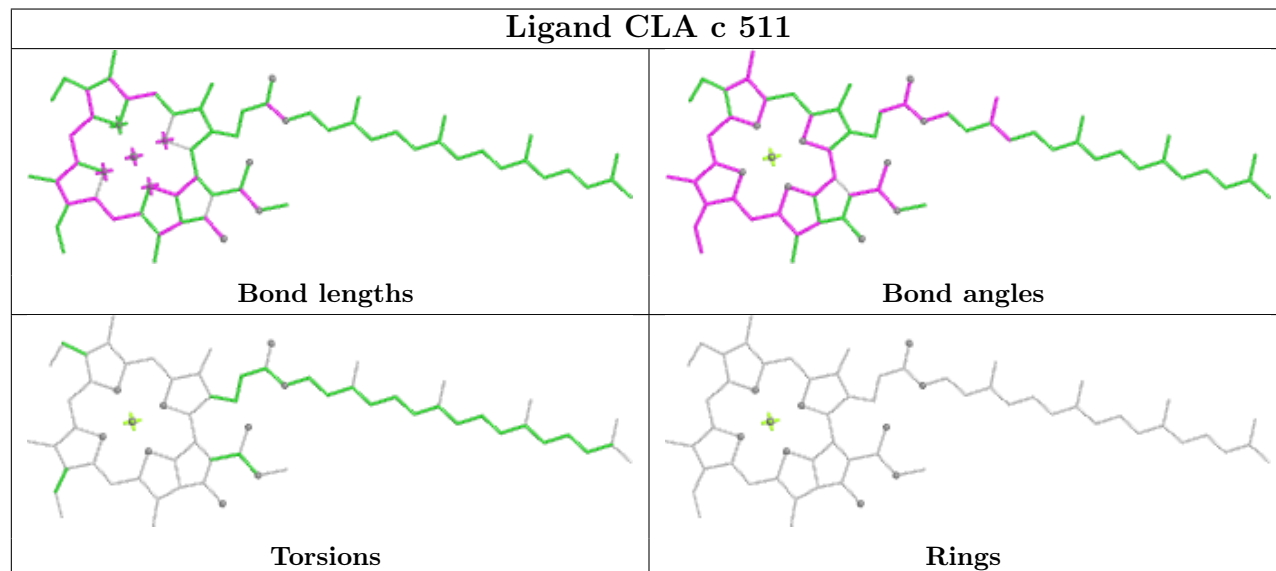


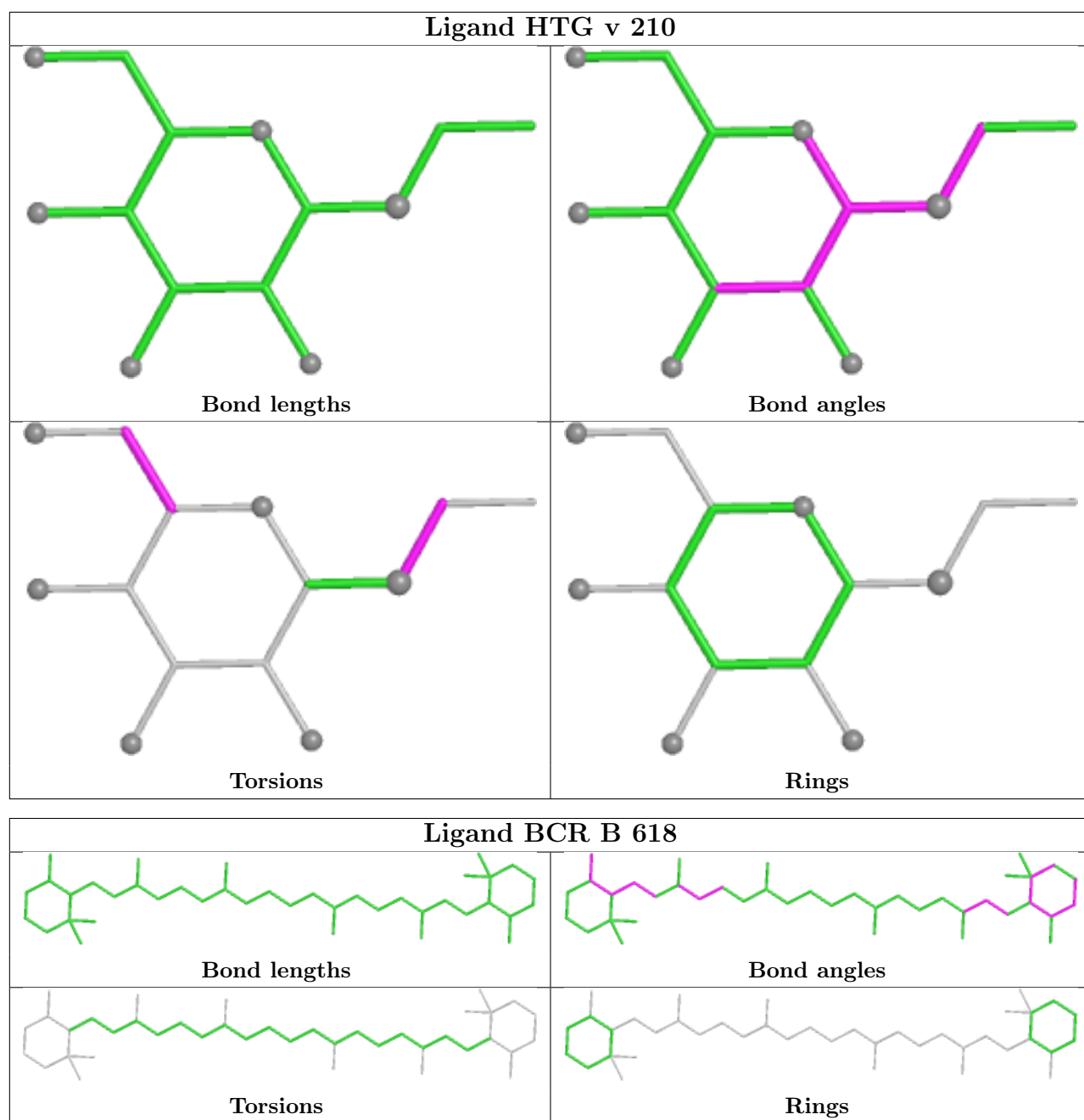
Ligand LMT B 625



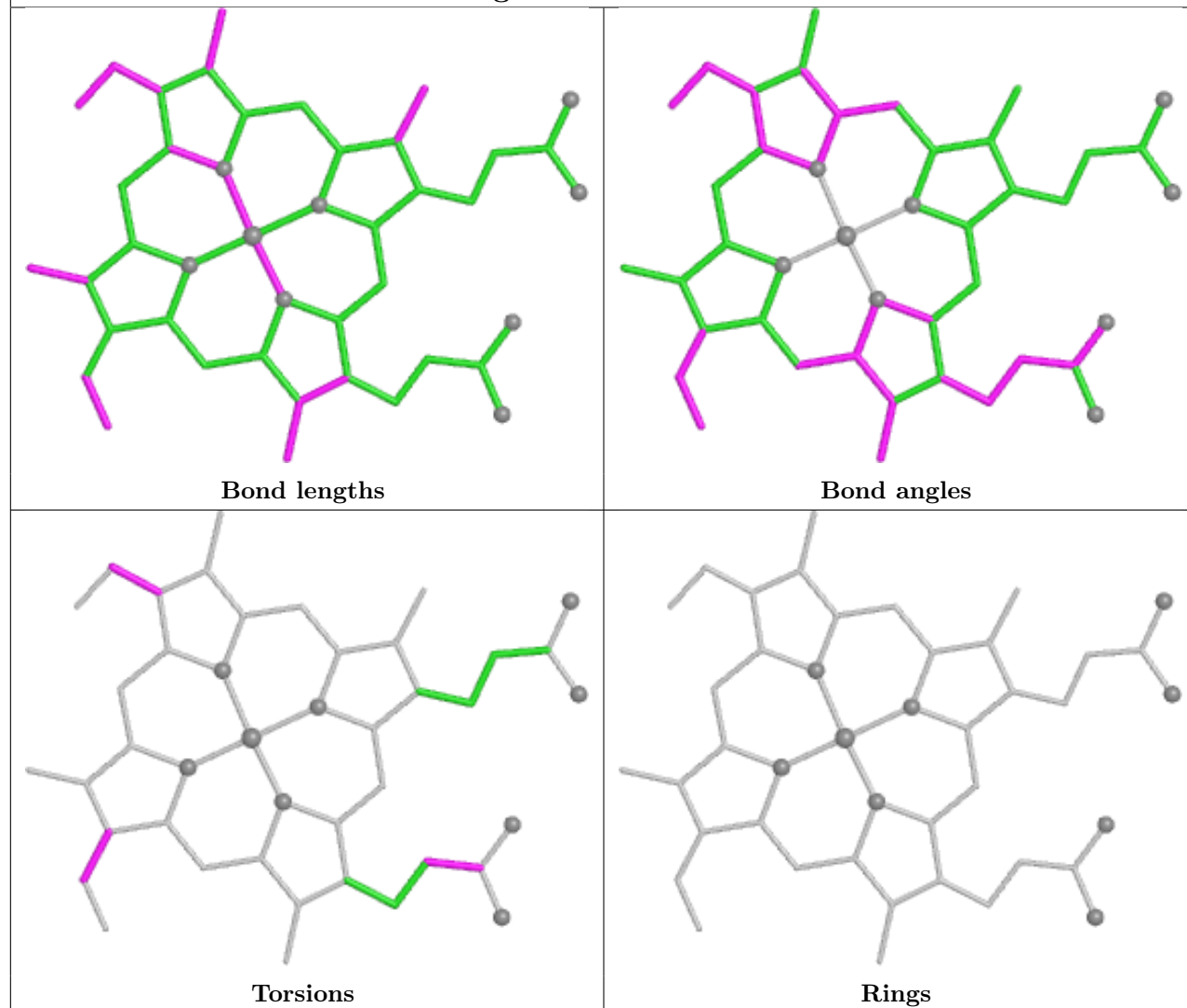
Ligand CLA A 402



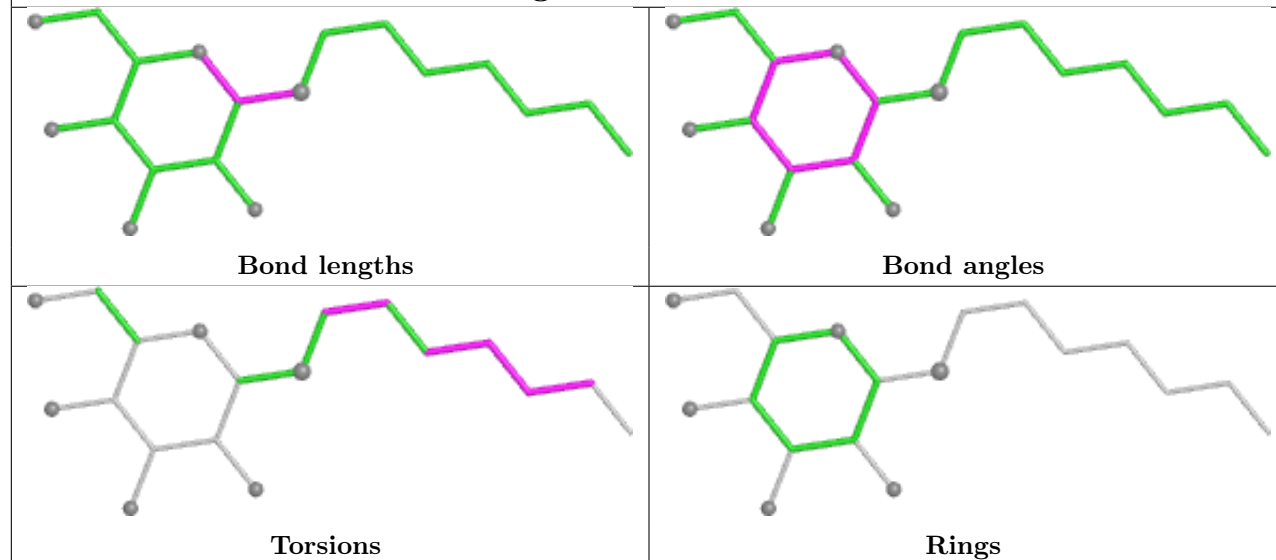
Ligand CLA D 402**Ligand CLA c 511**

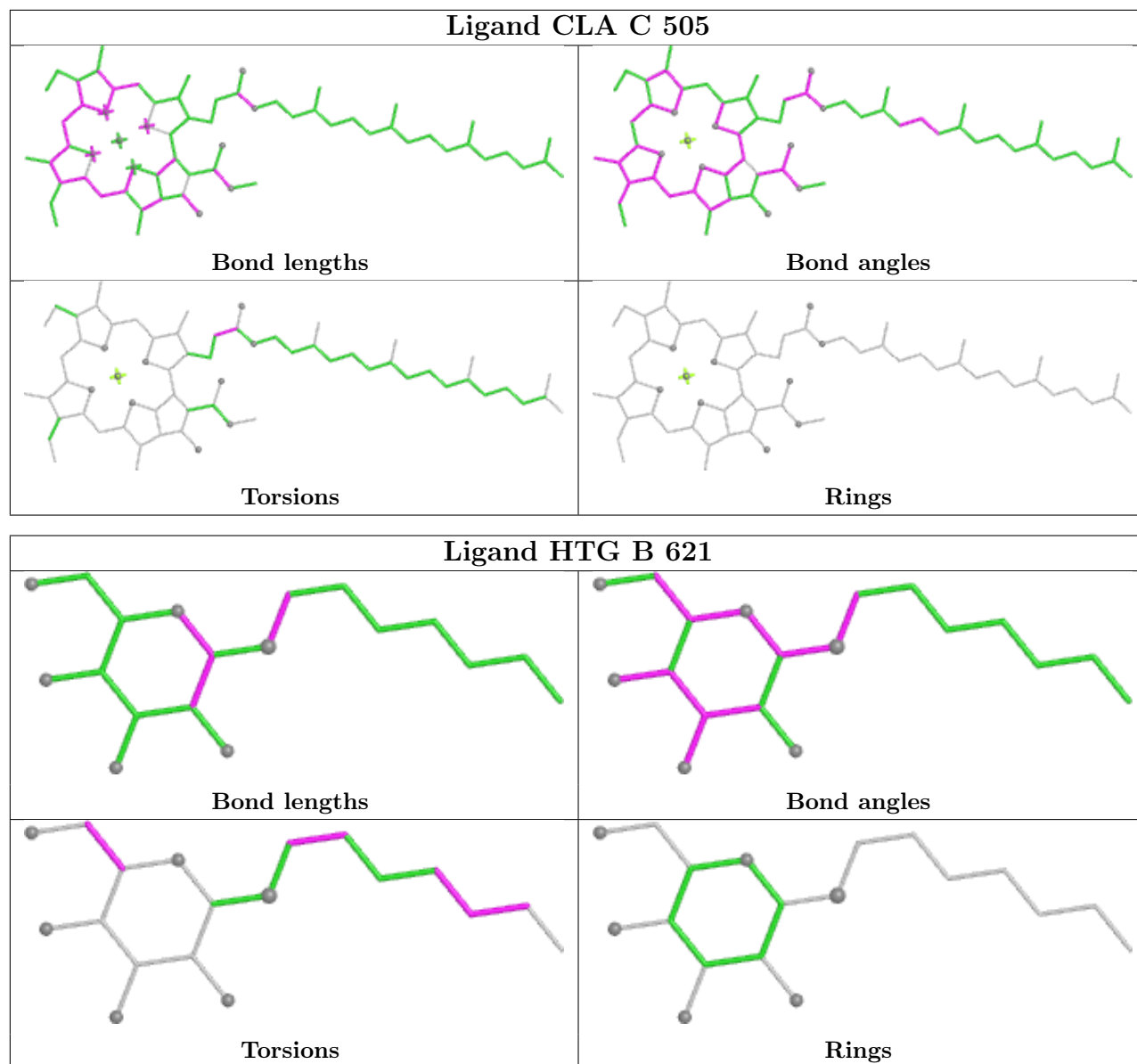


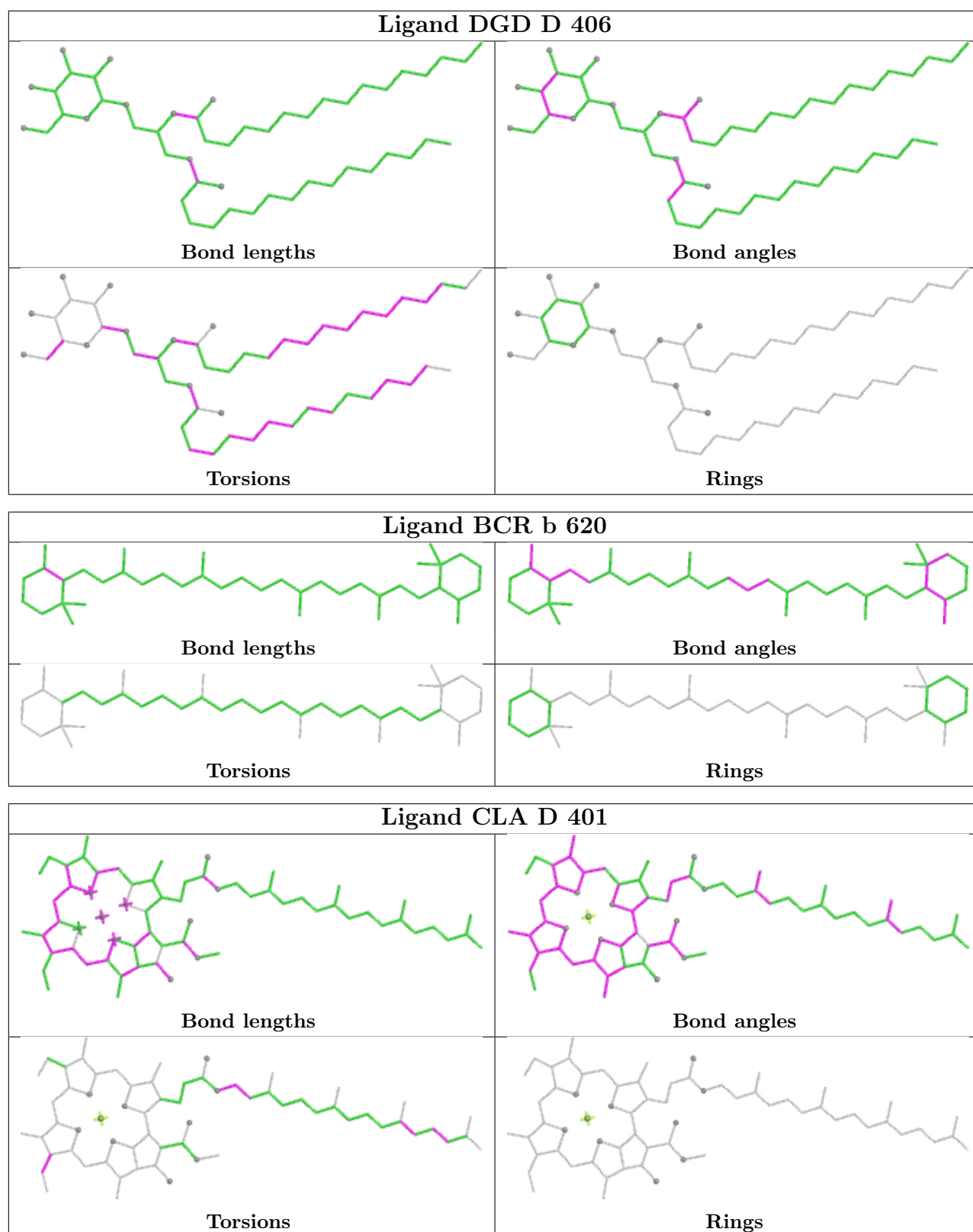
Ligand HEC V 201

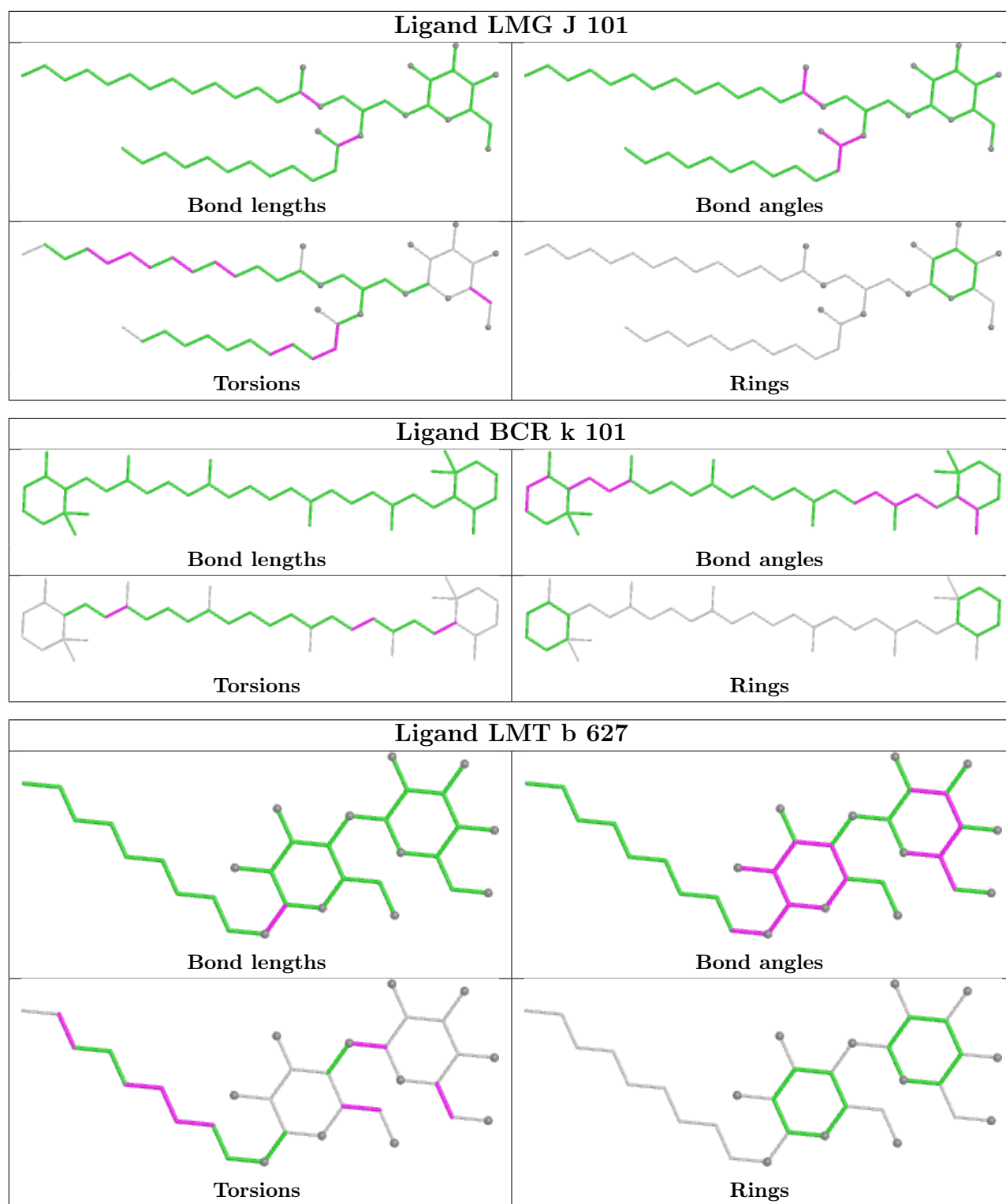


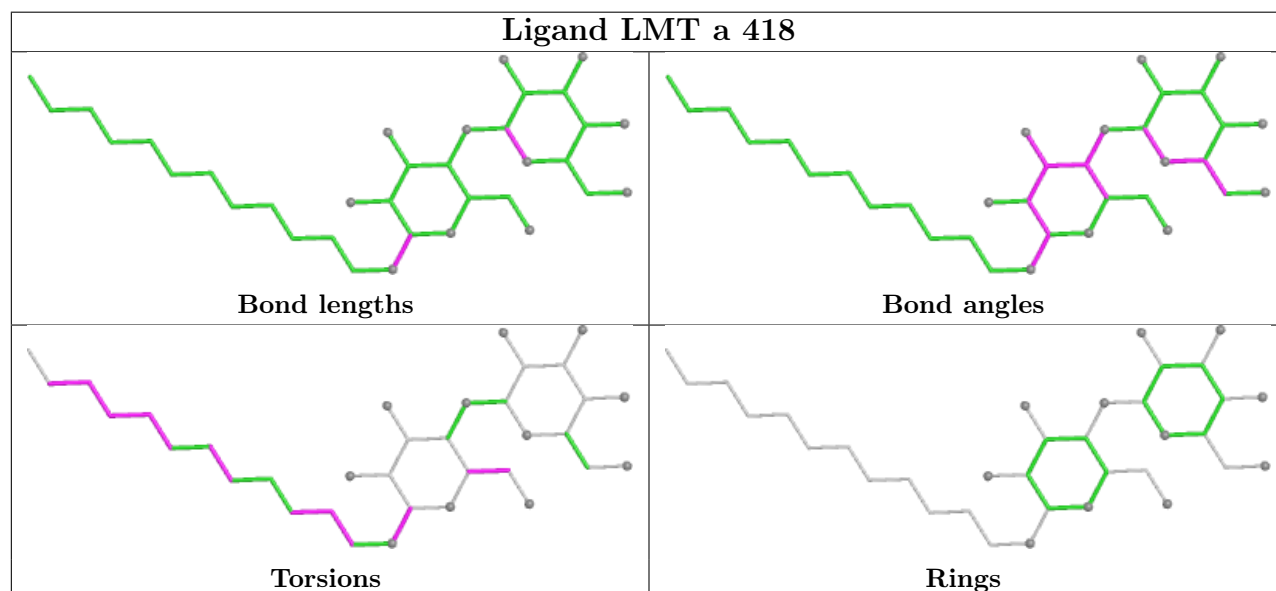
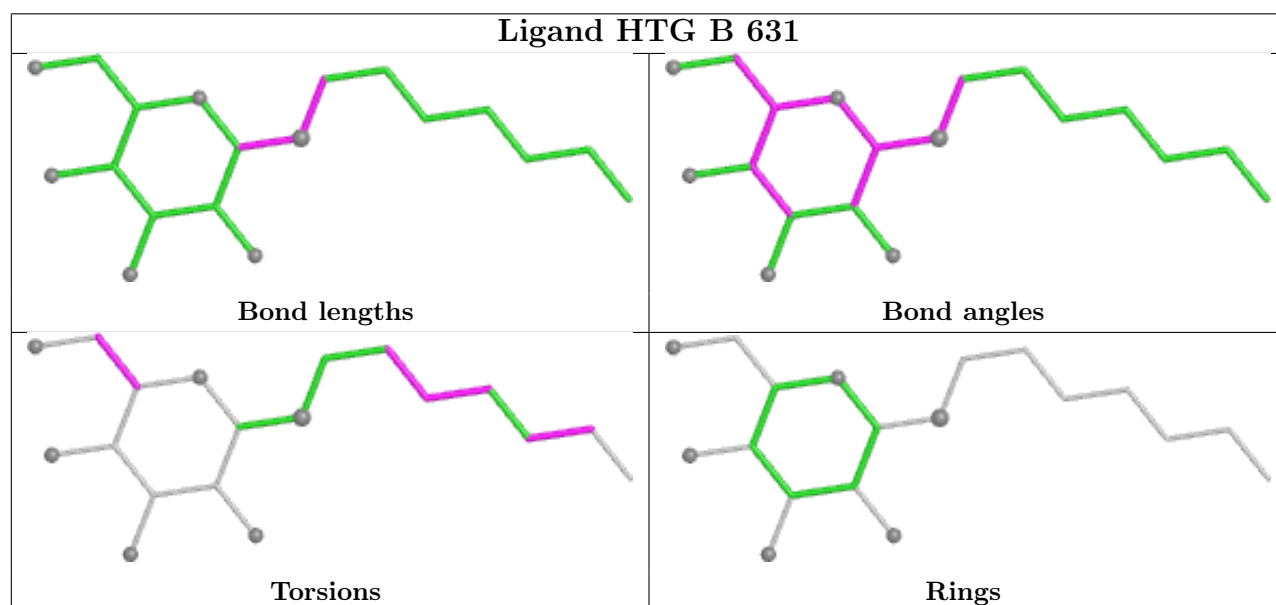
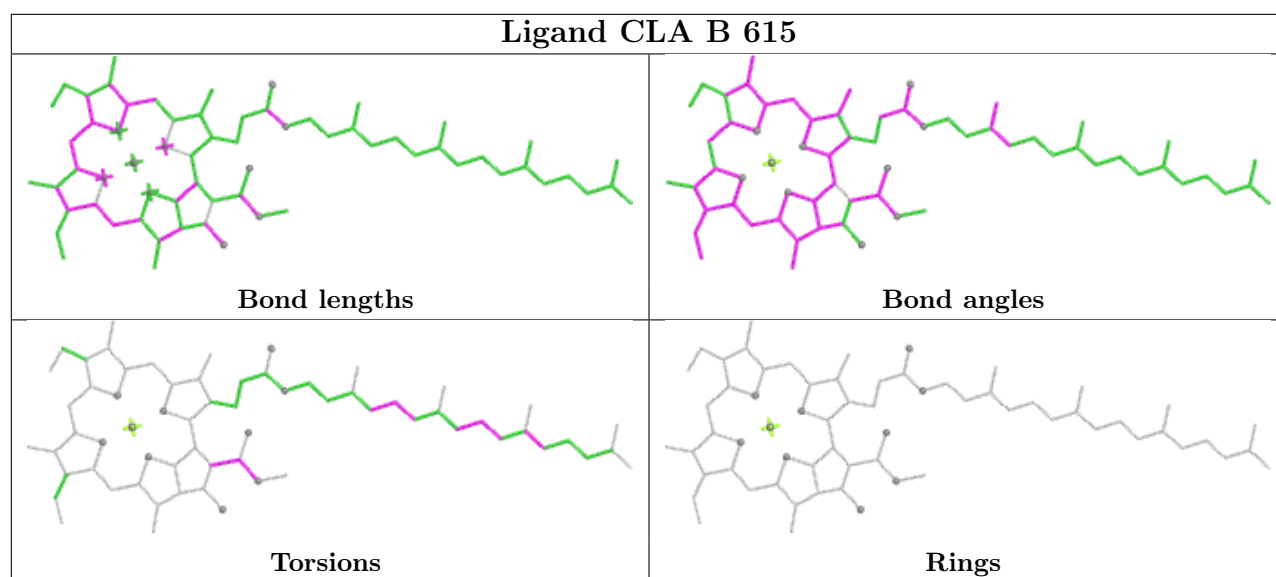
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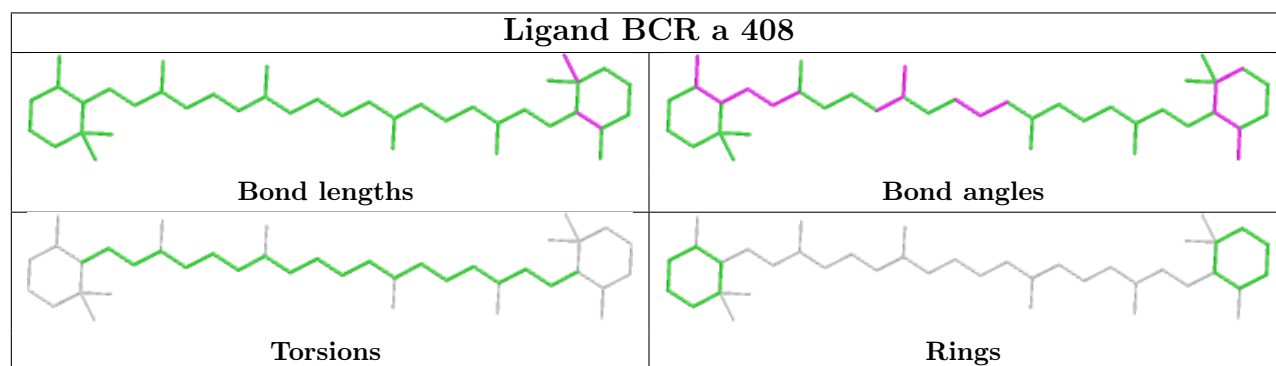
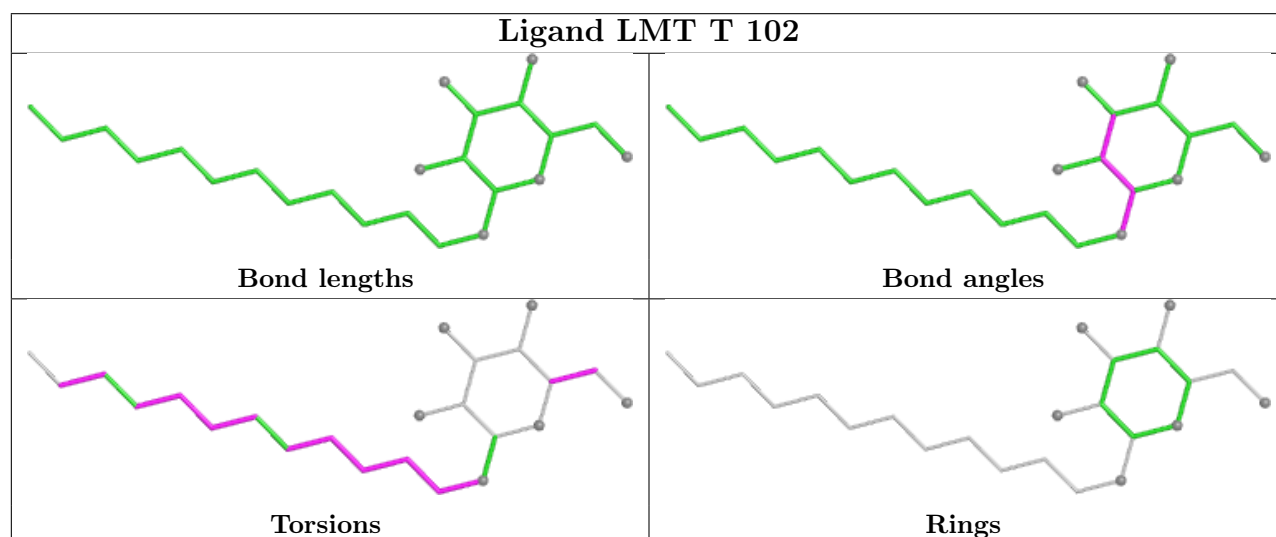
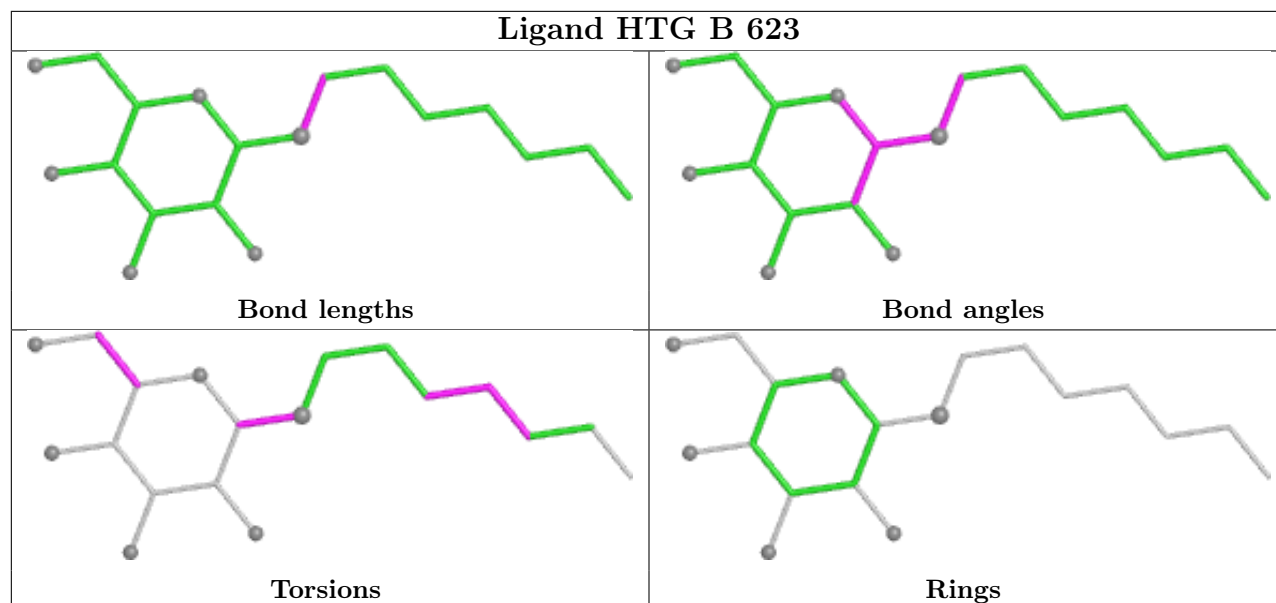


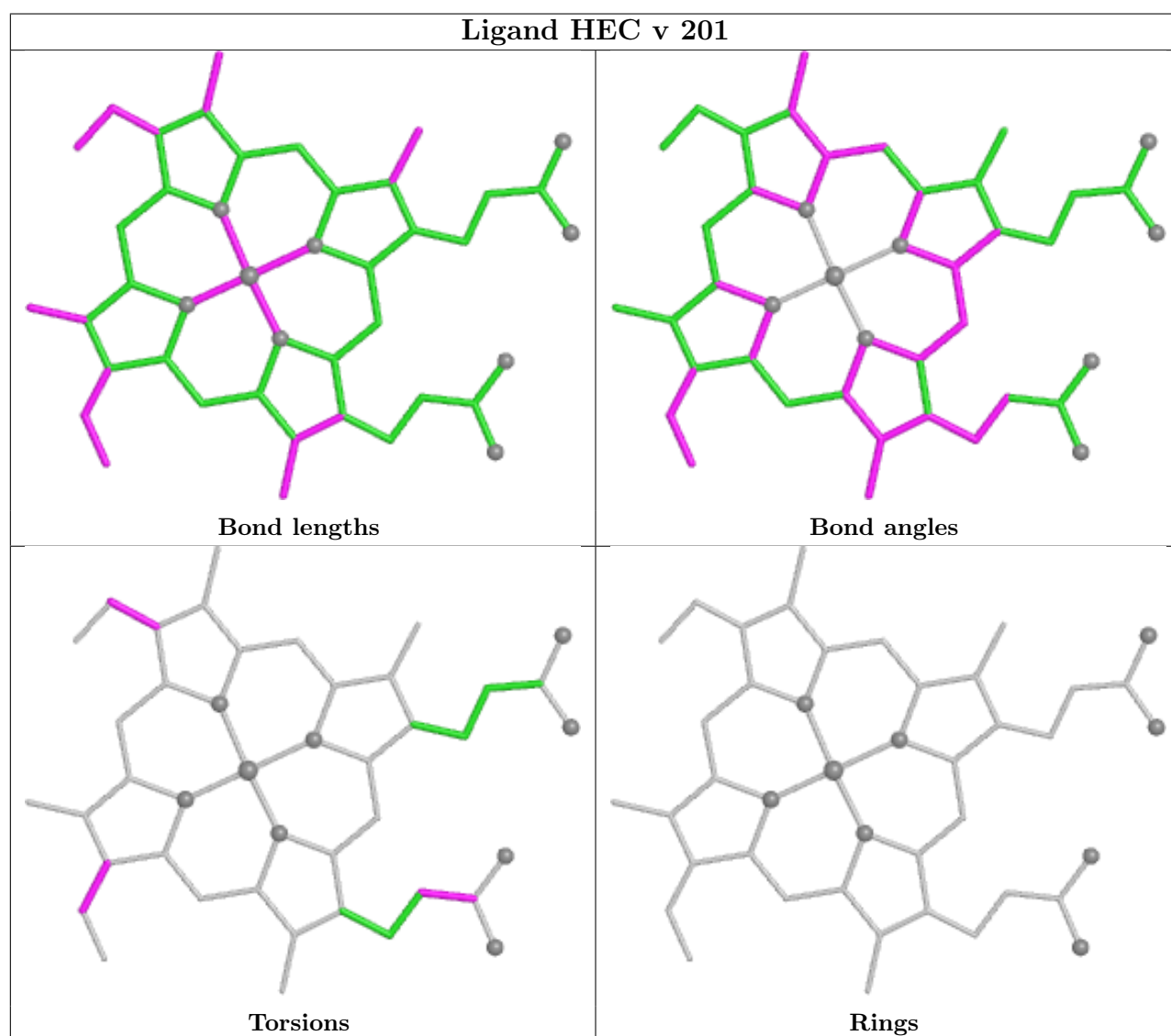
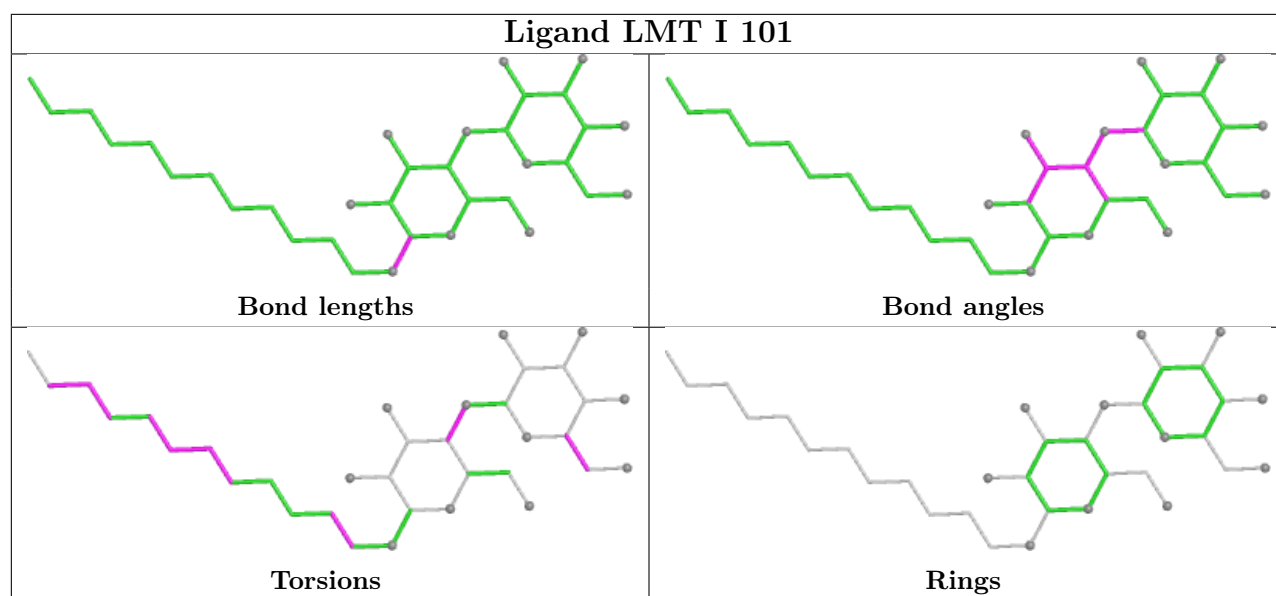


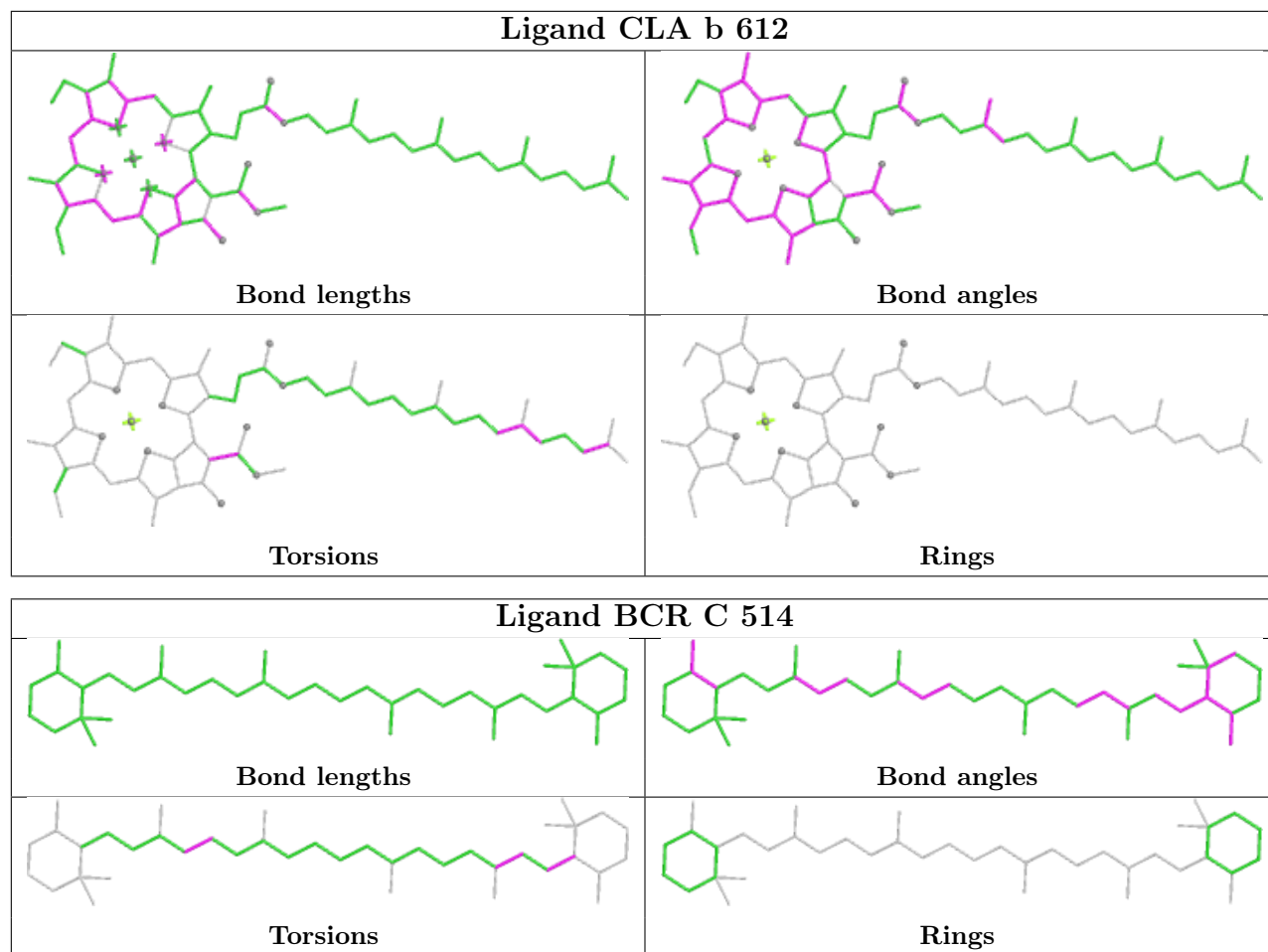


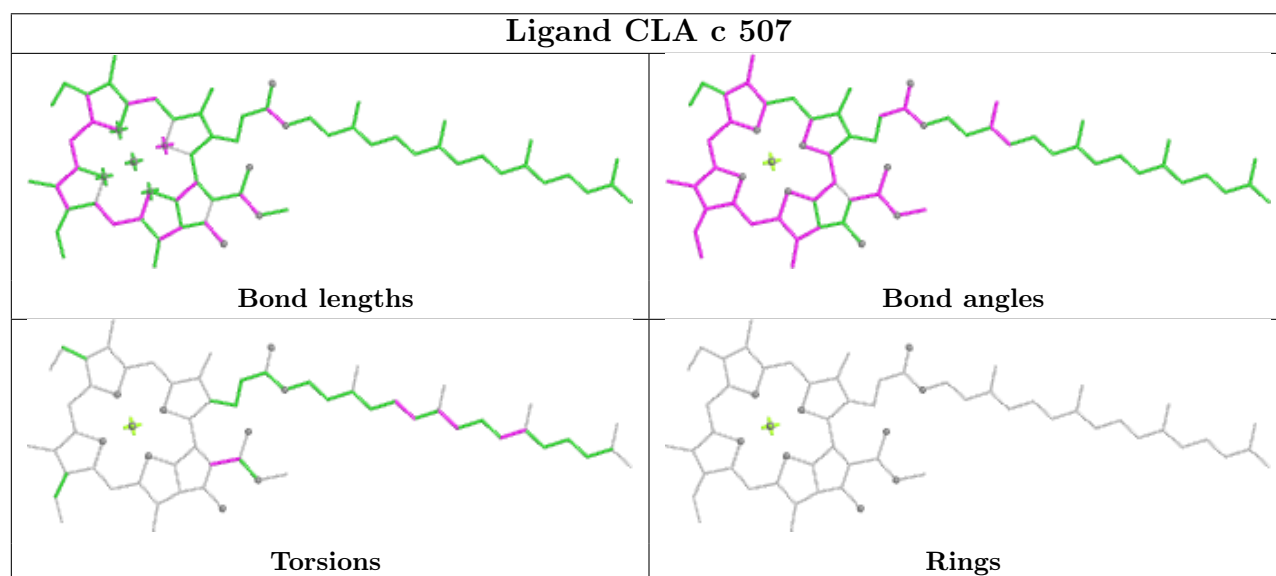
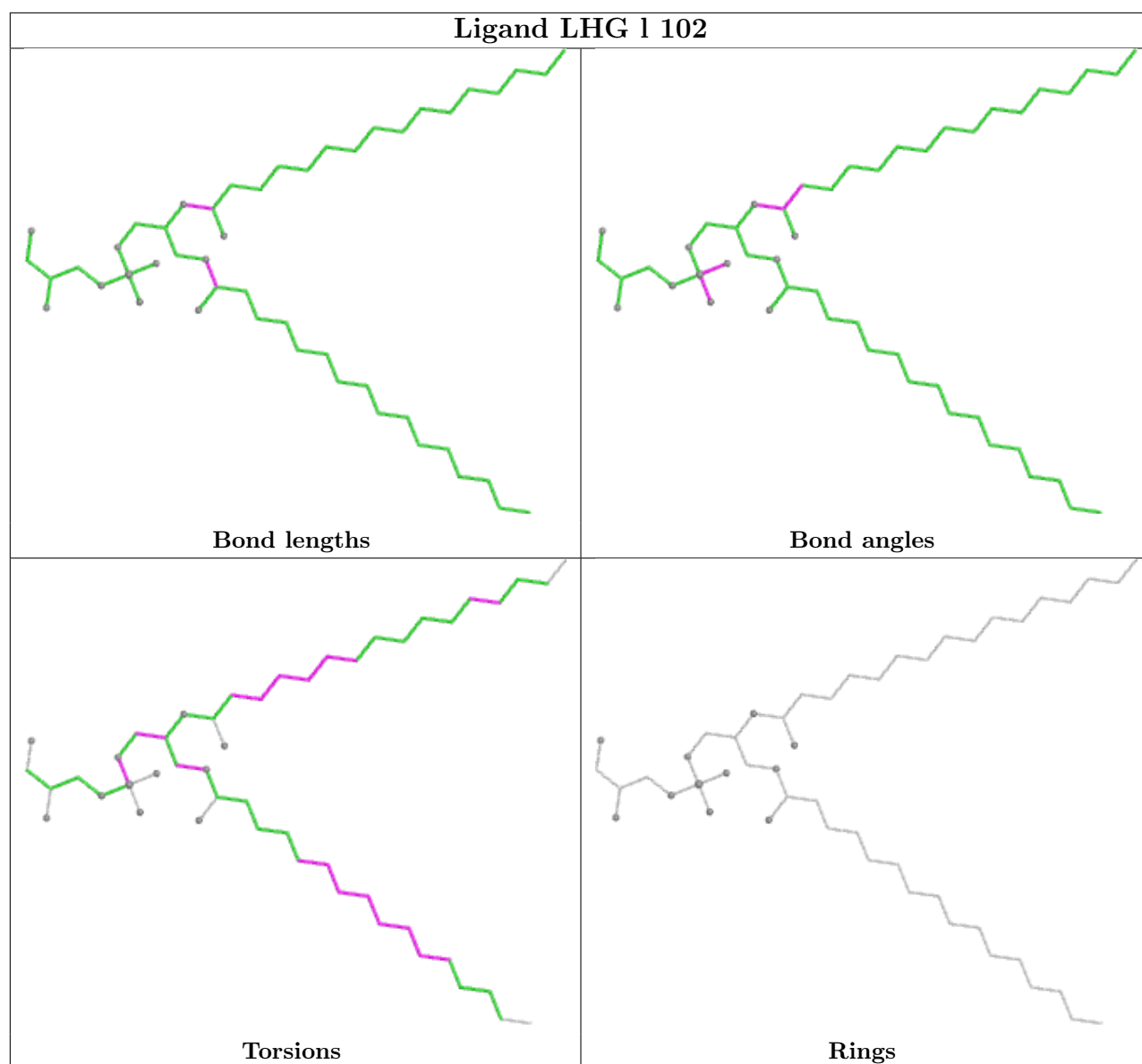


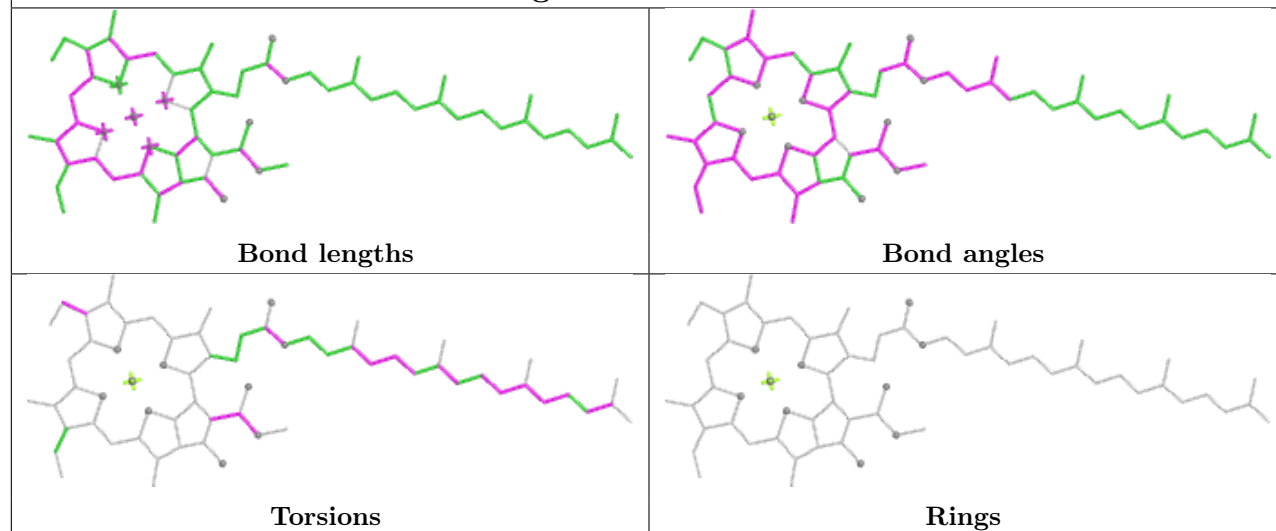
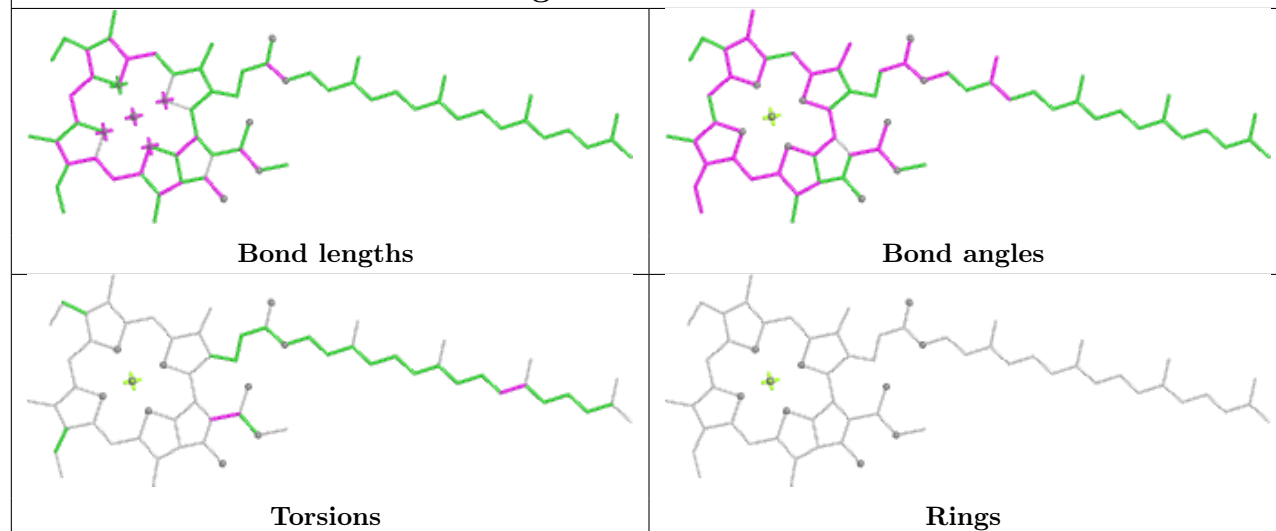
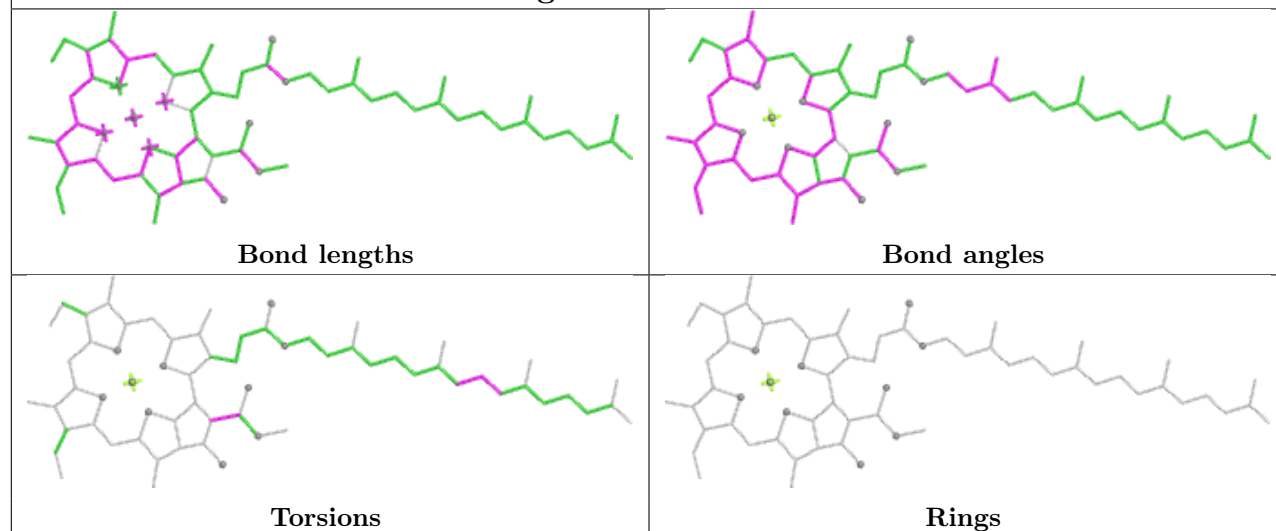


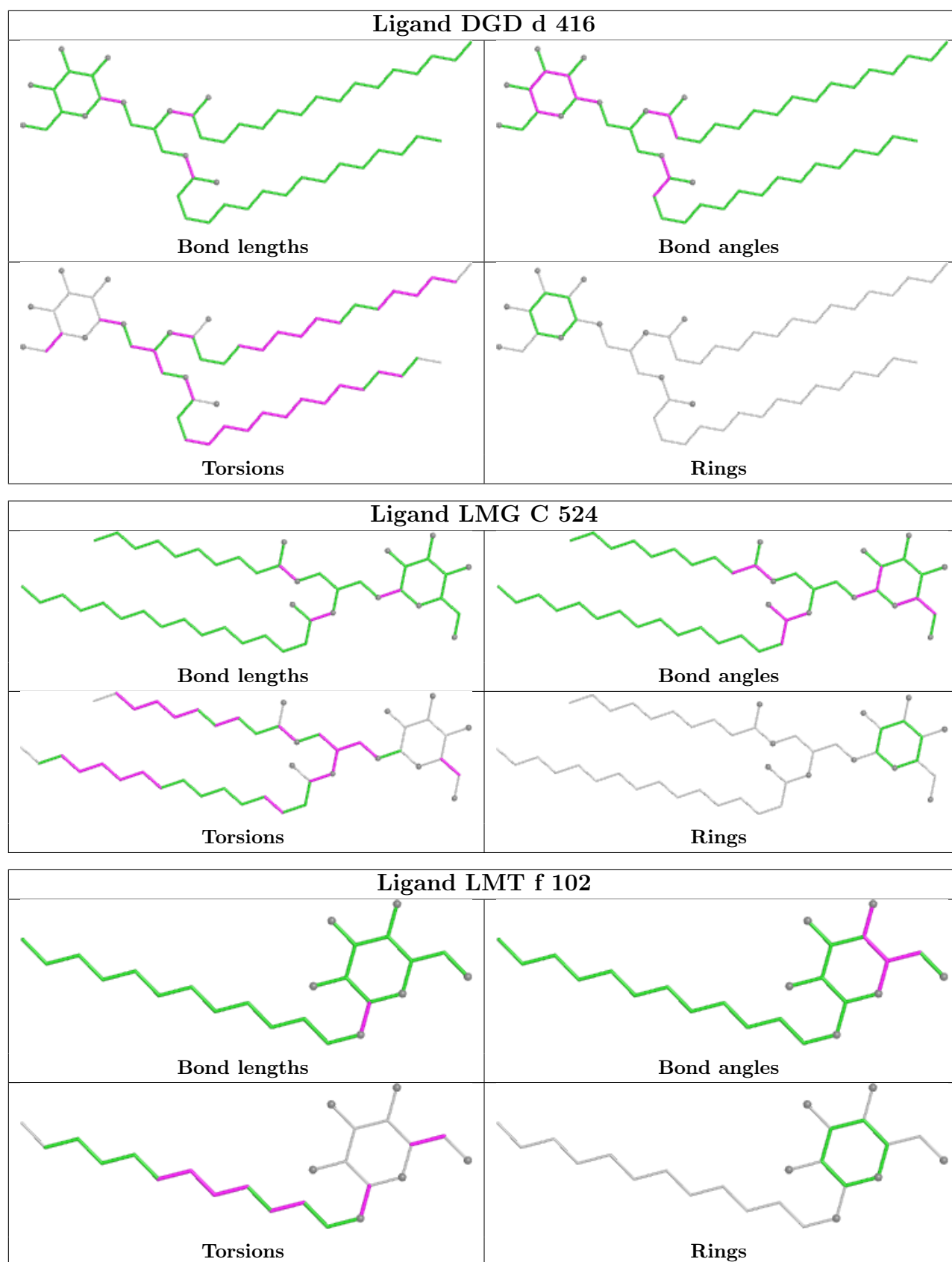


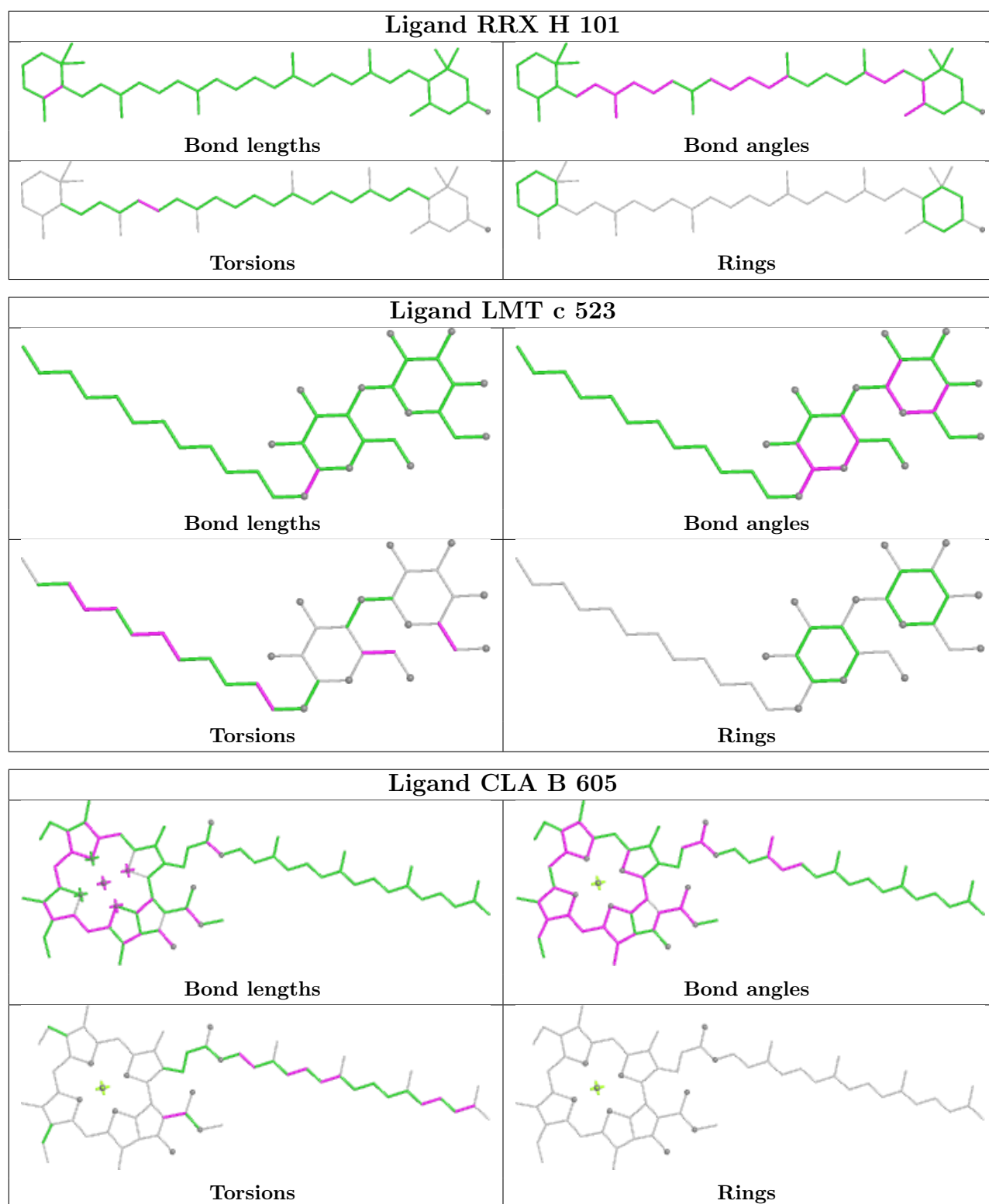


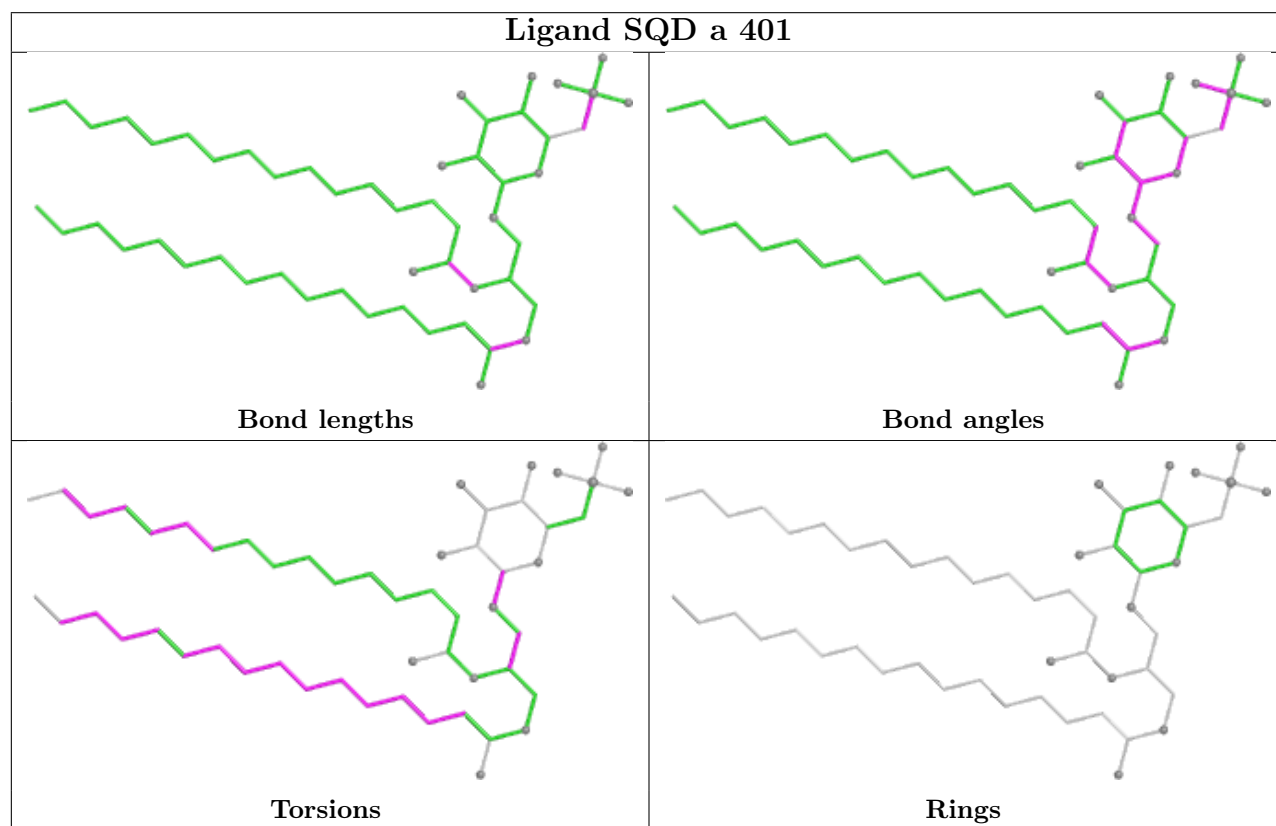
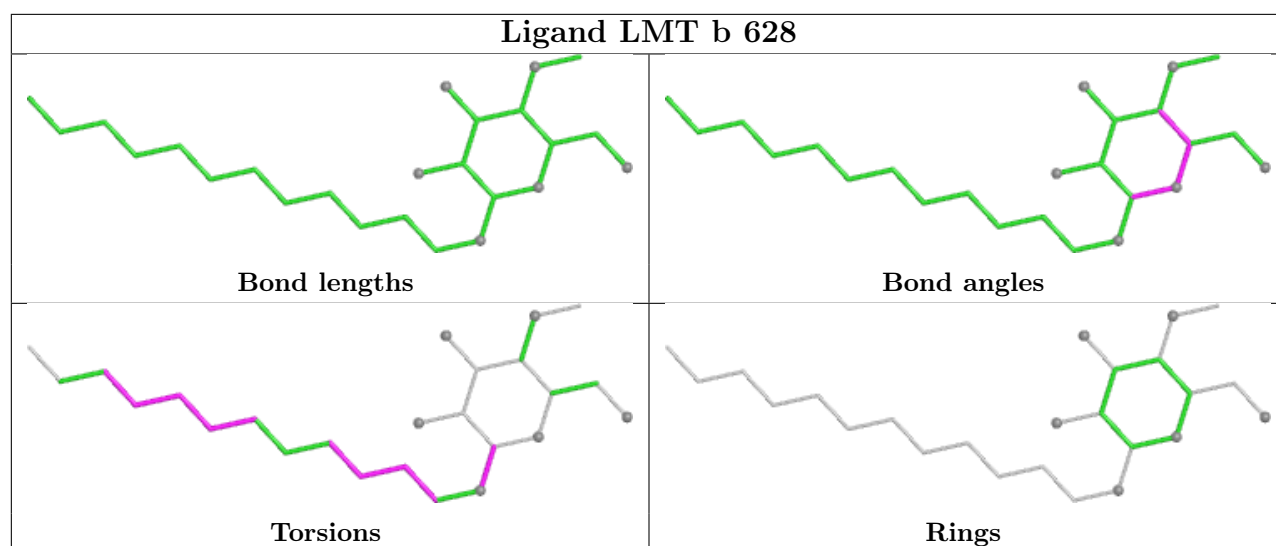


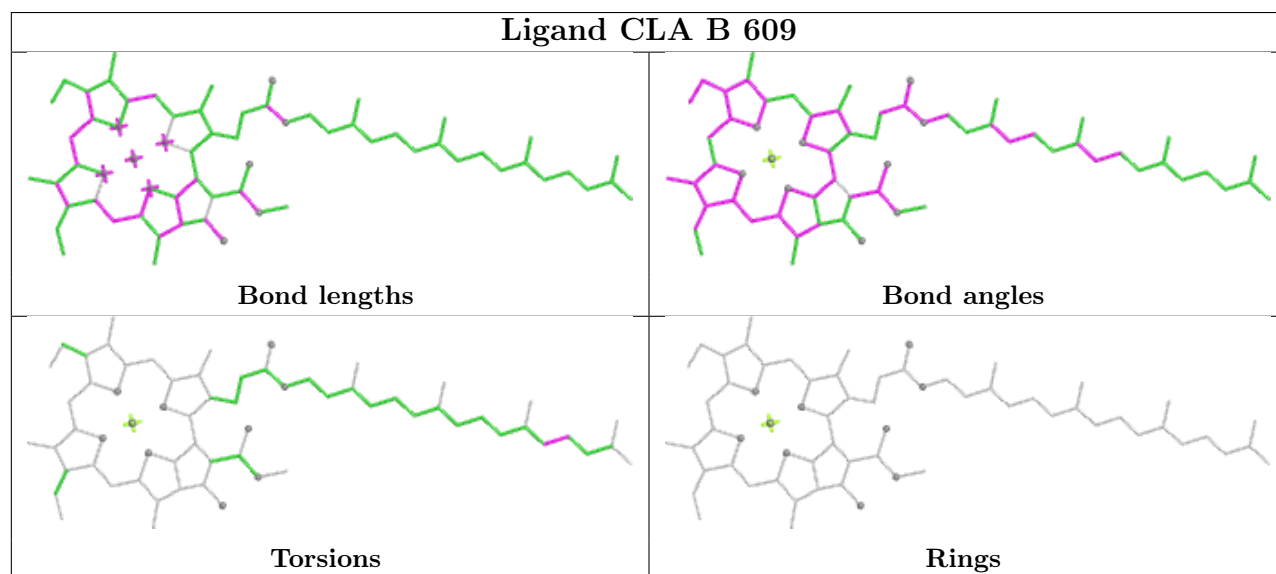
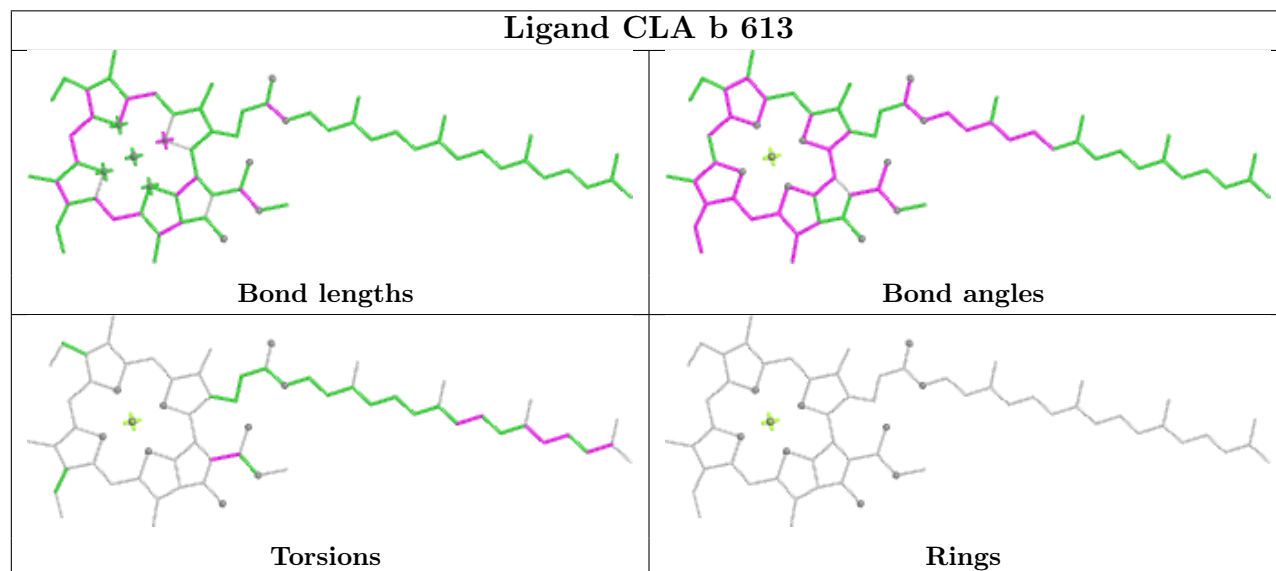
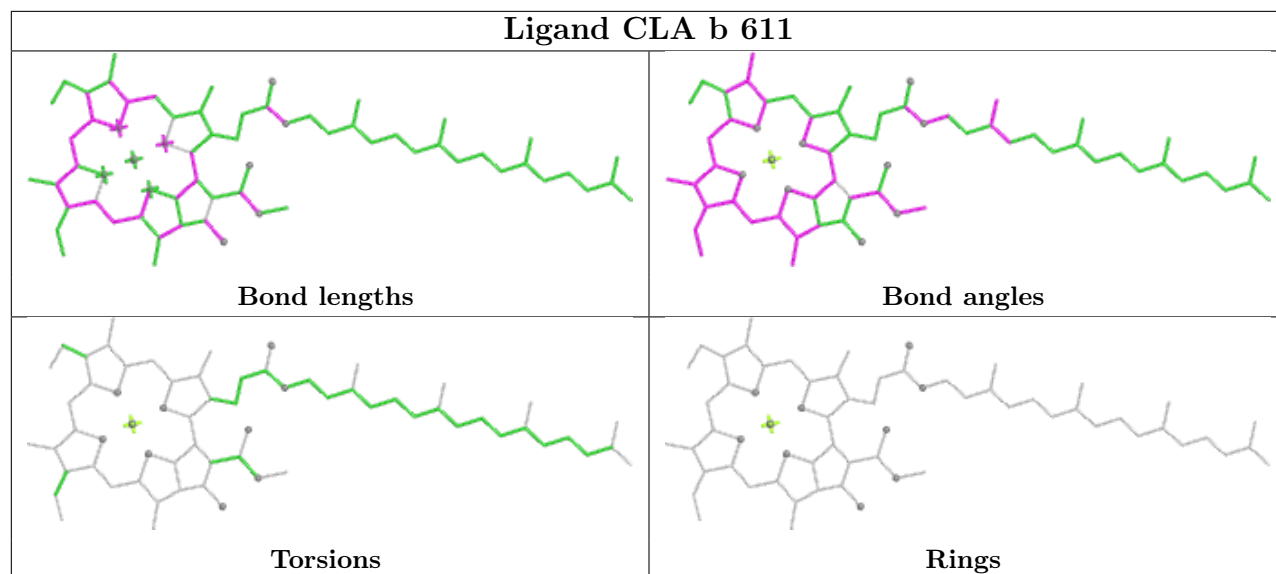


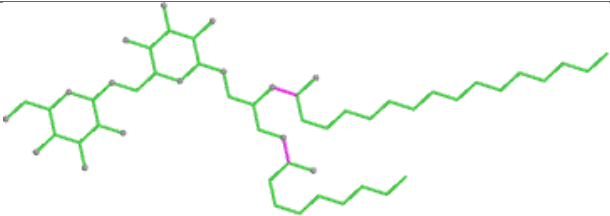
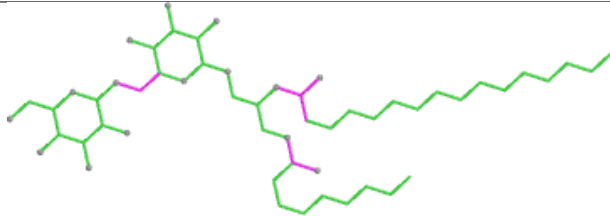
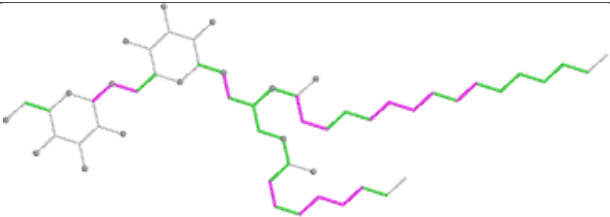
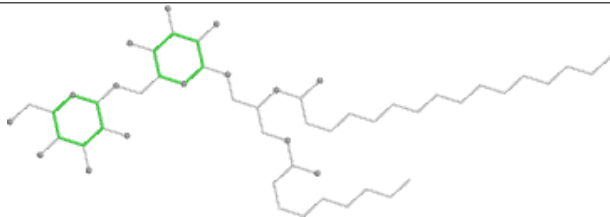
Ligand CLA B 602**Ligand CLA B 603****Ligand CLA c 503**

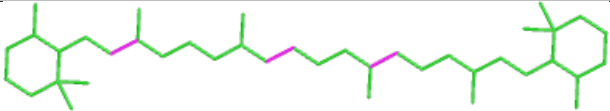
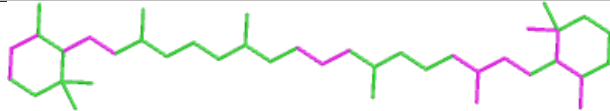
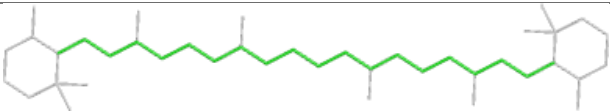
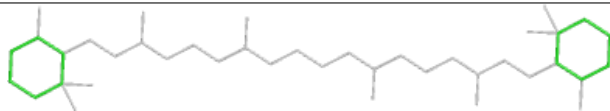




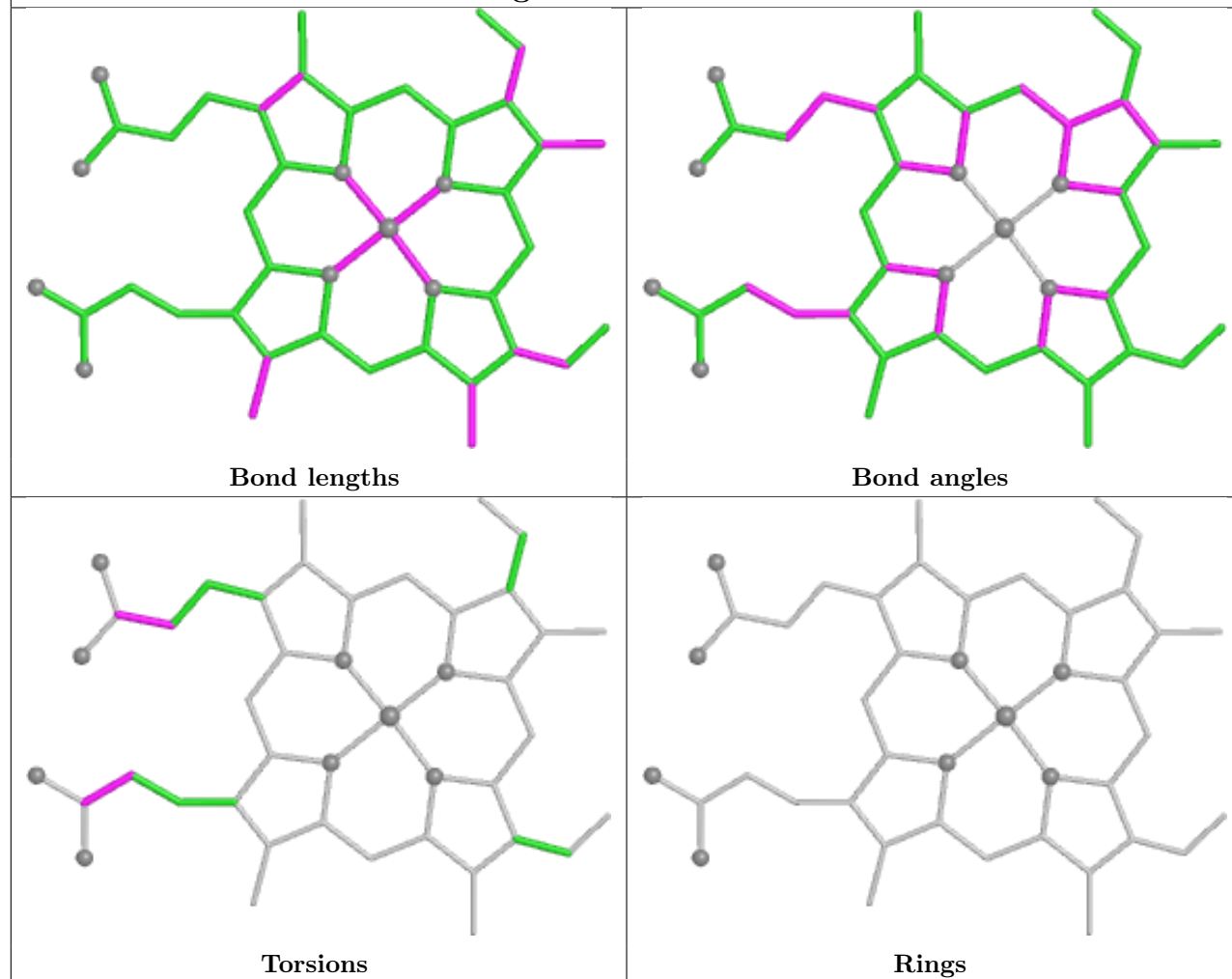




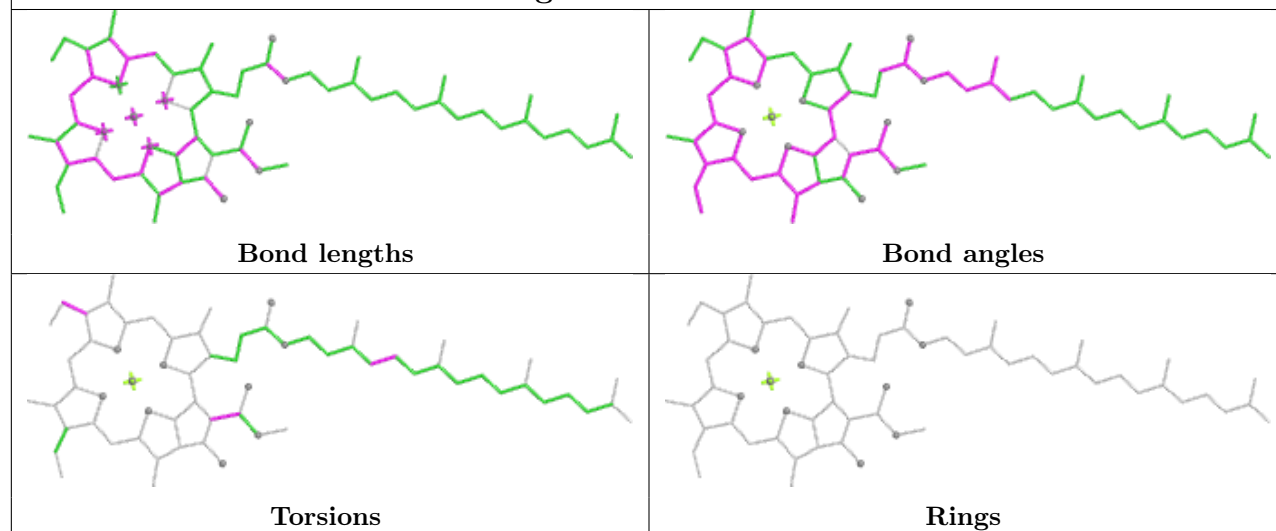
Ligand DGD C 517			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

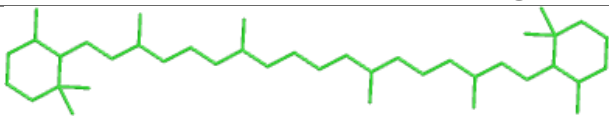
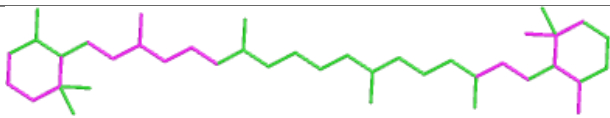
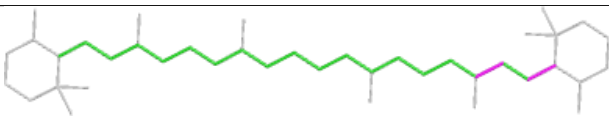
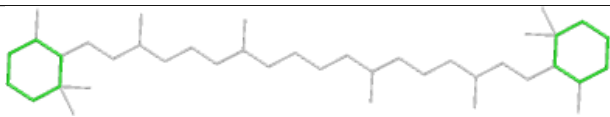
Ligand BCR A 405			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

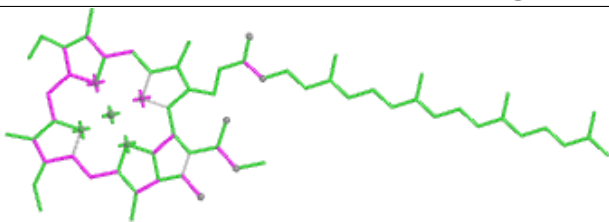
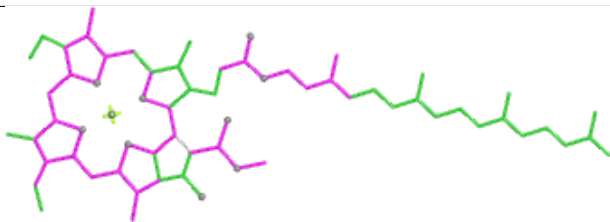
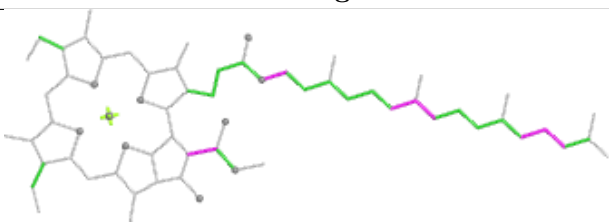
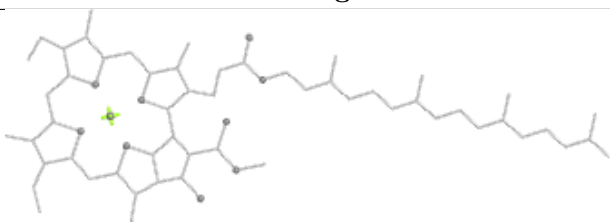
Ligand HEM e 102

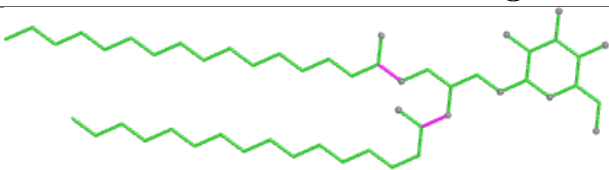
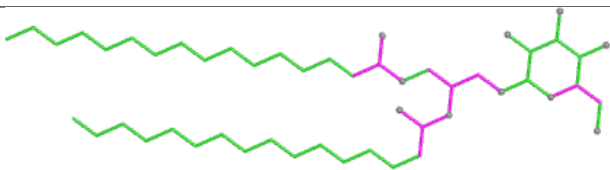
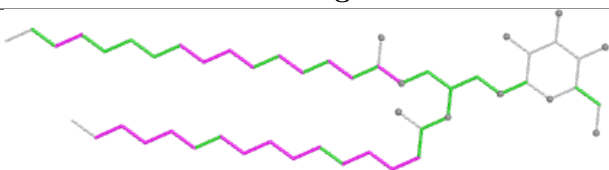
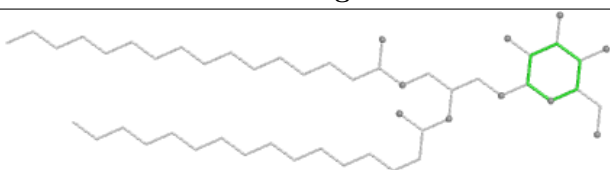


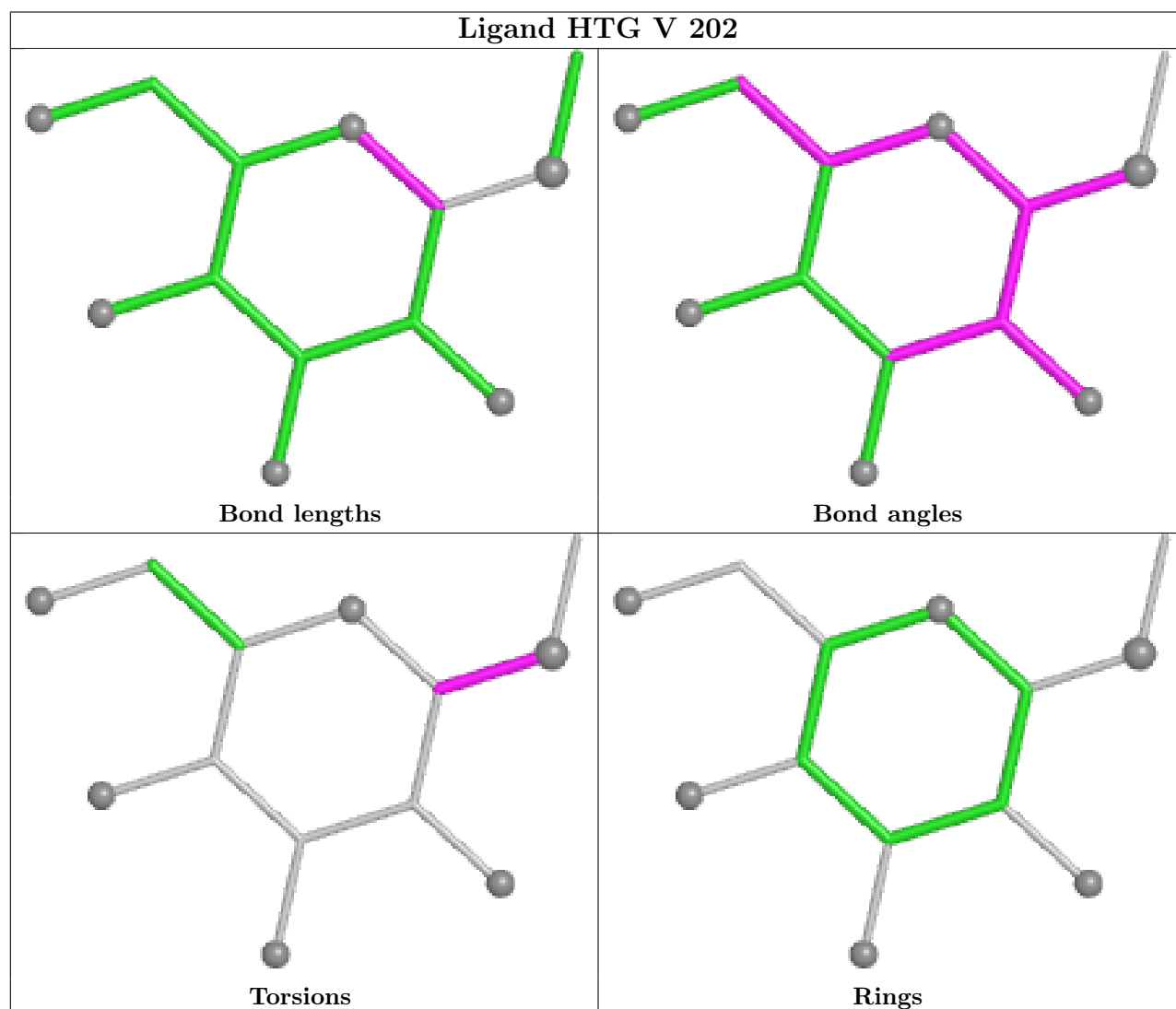
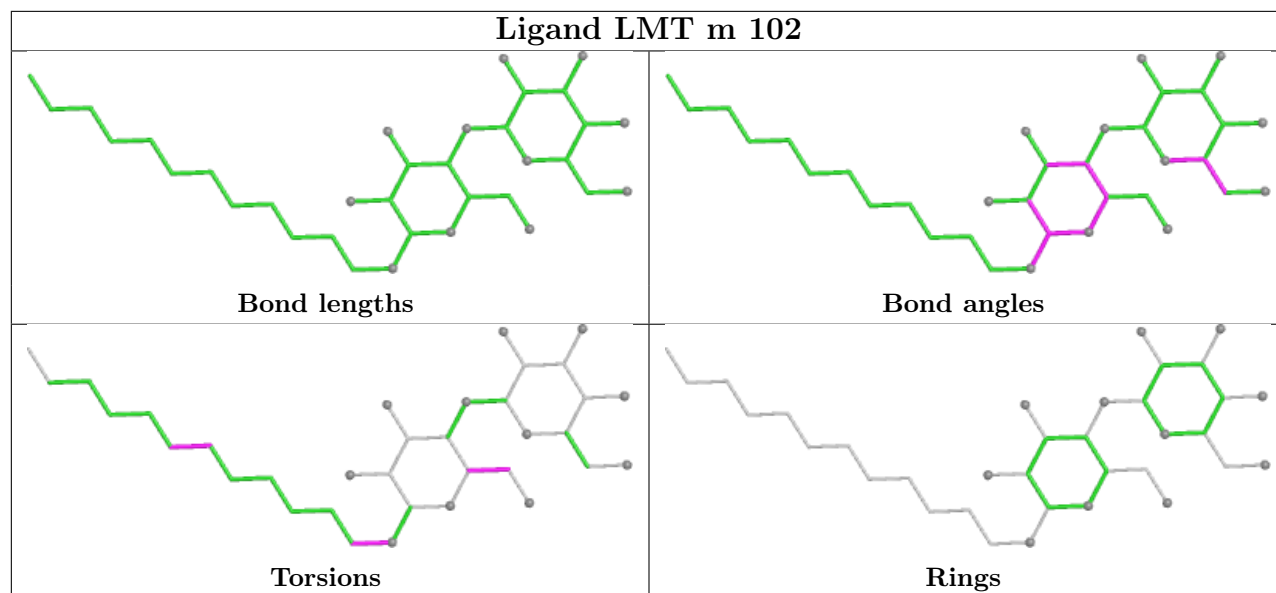
Ligand CLA b 609

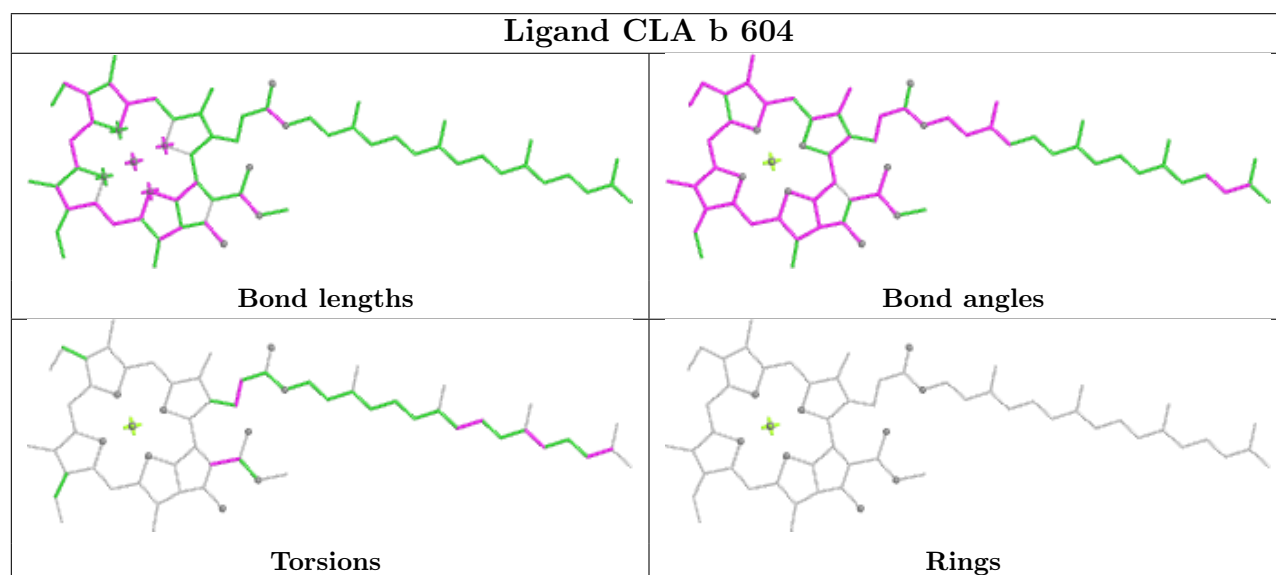
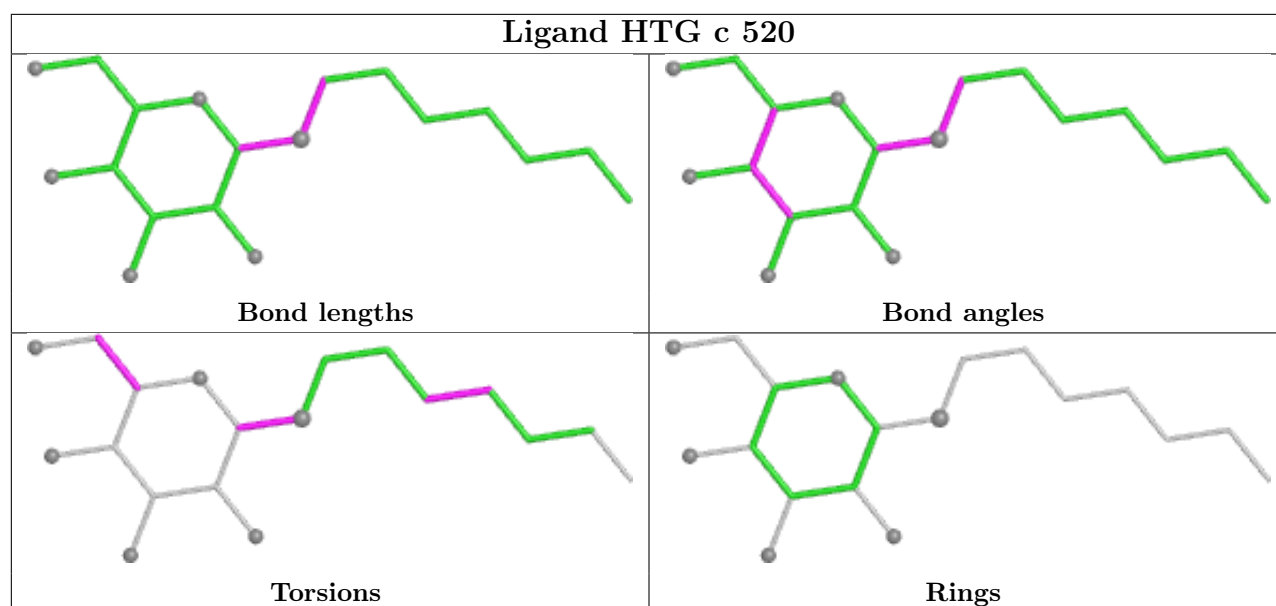


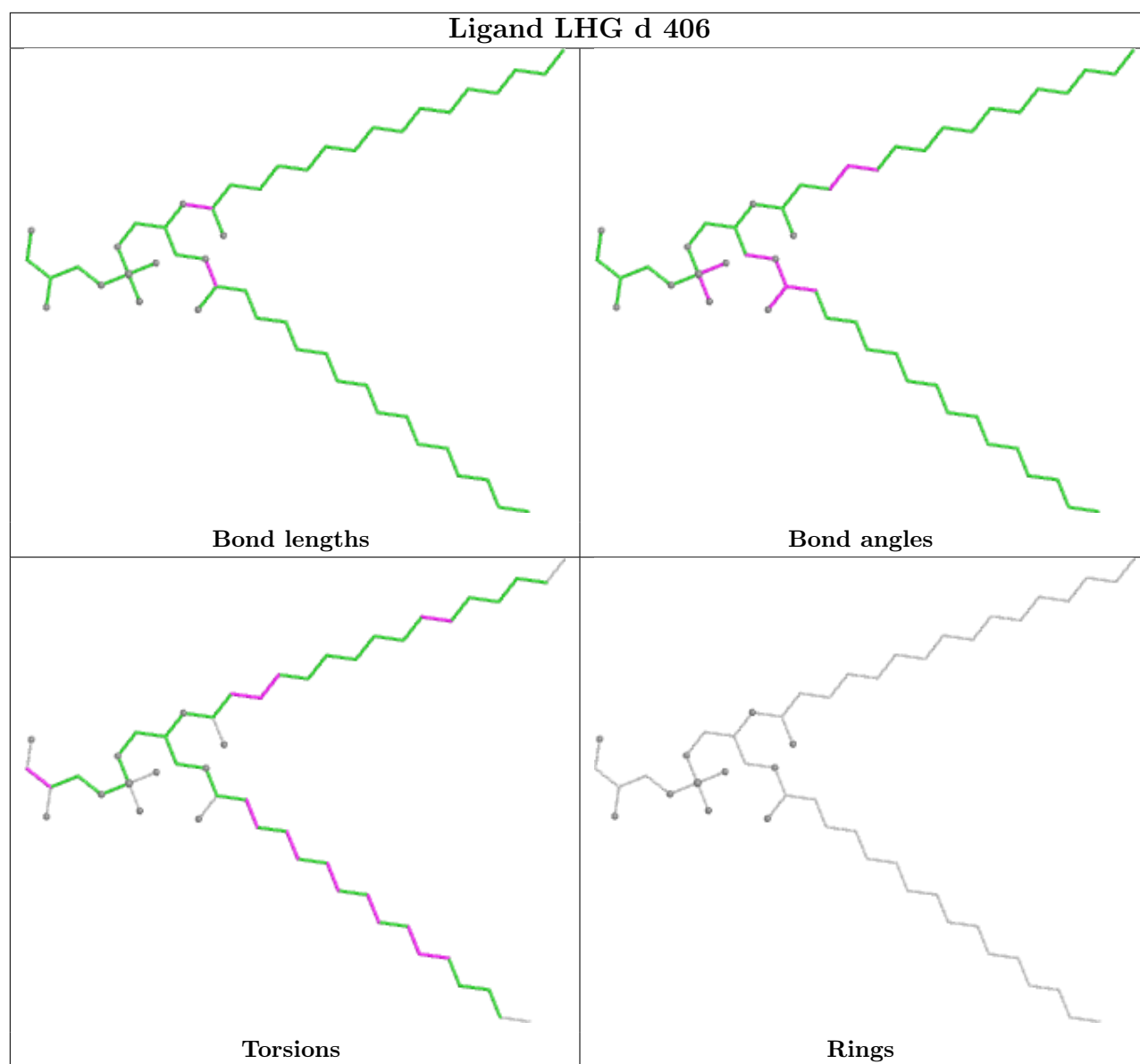
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

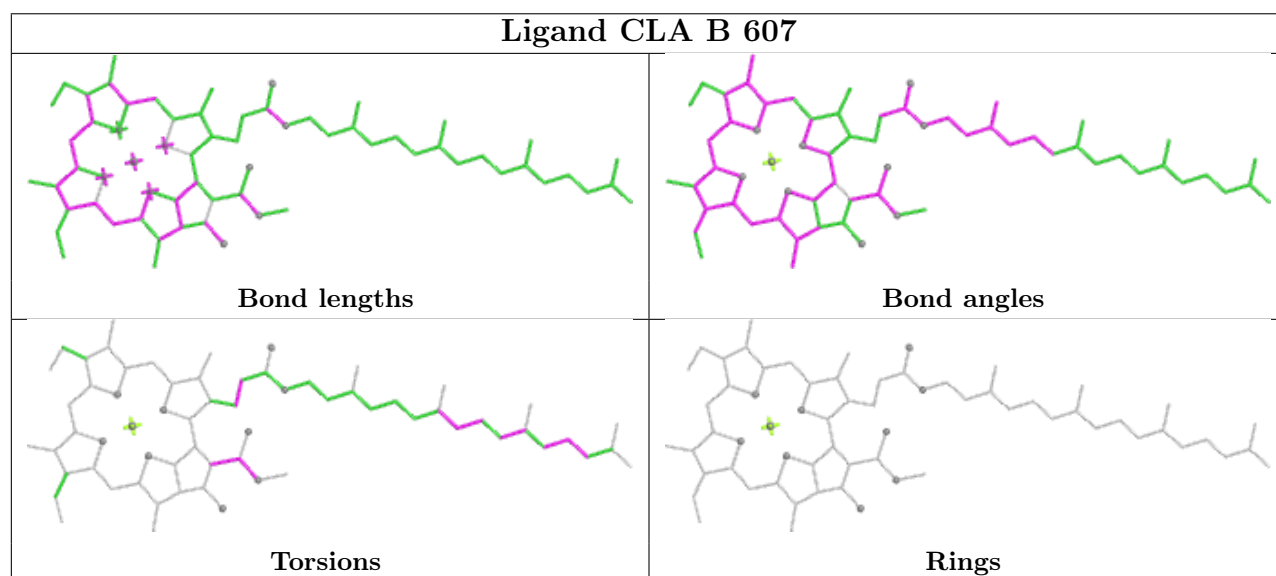
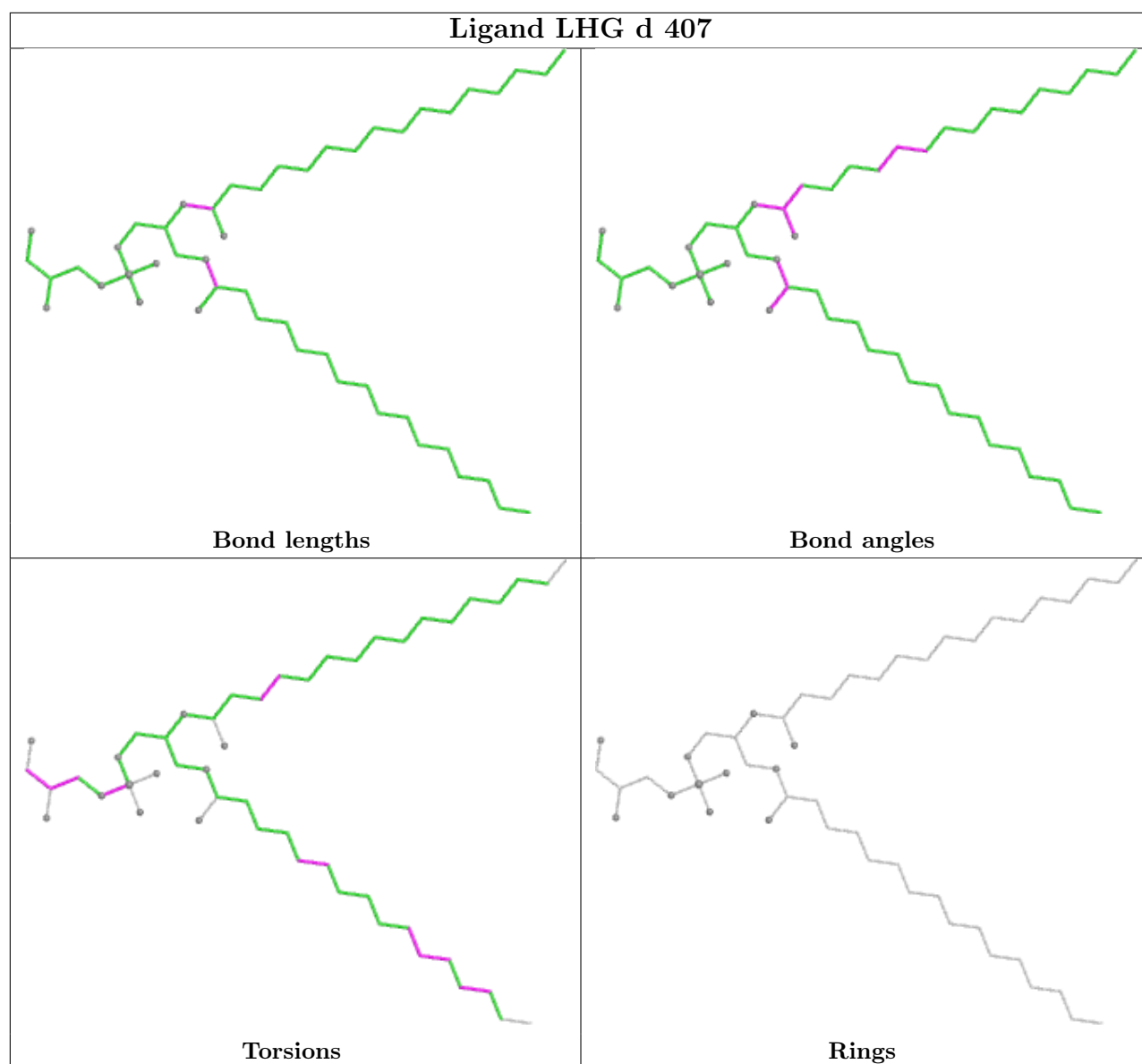
Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

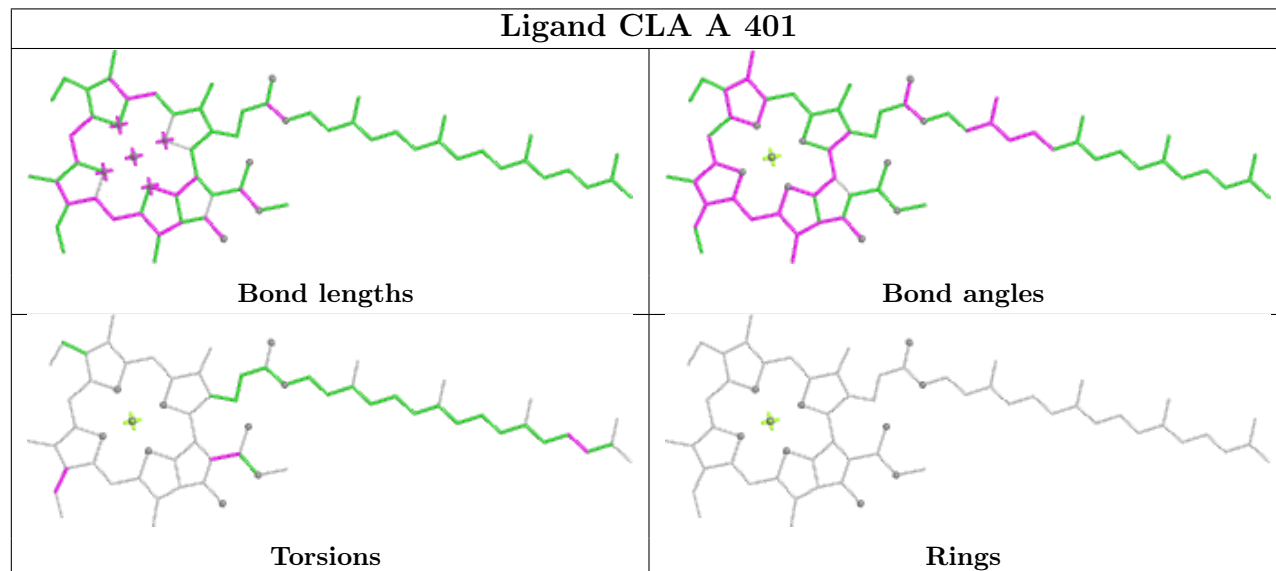
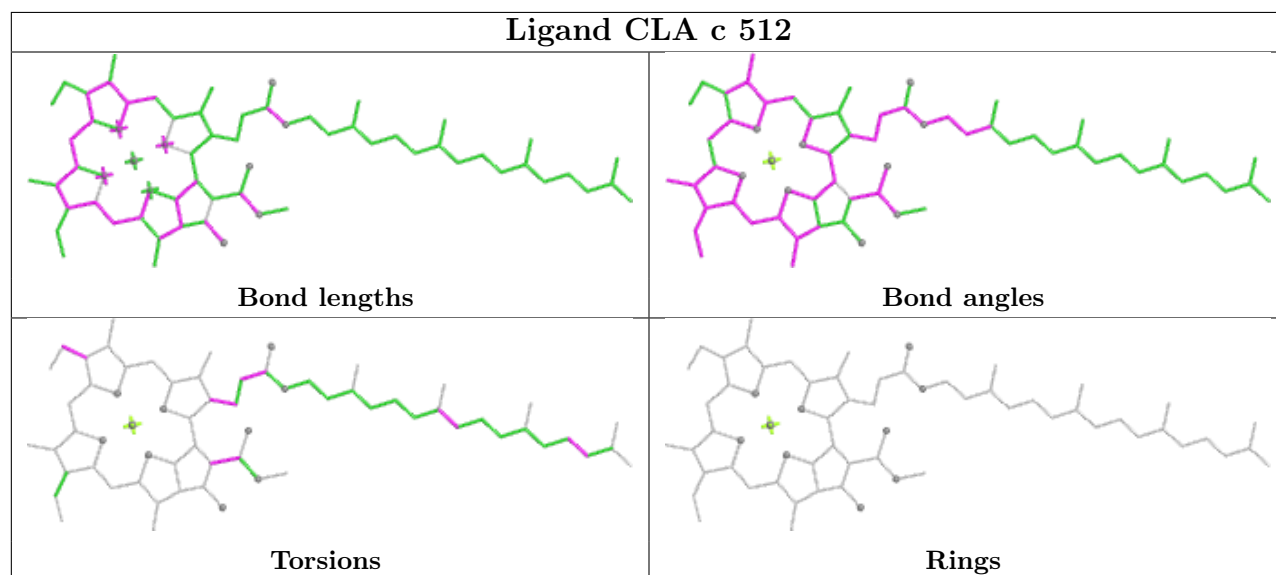
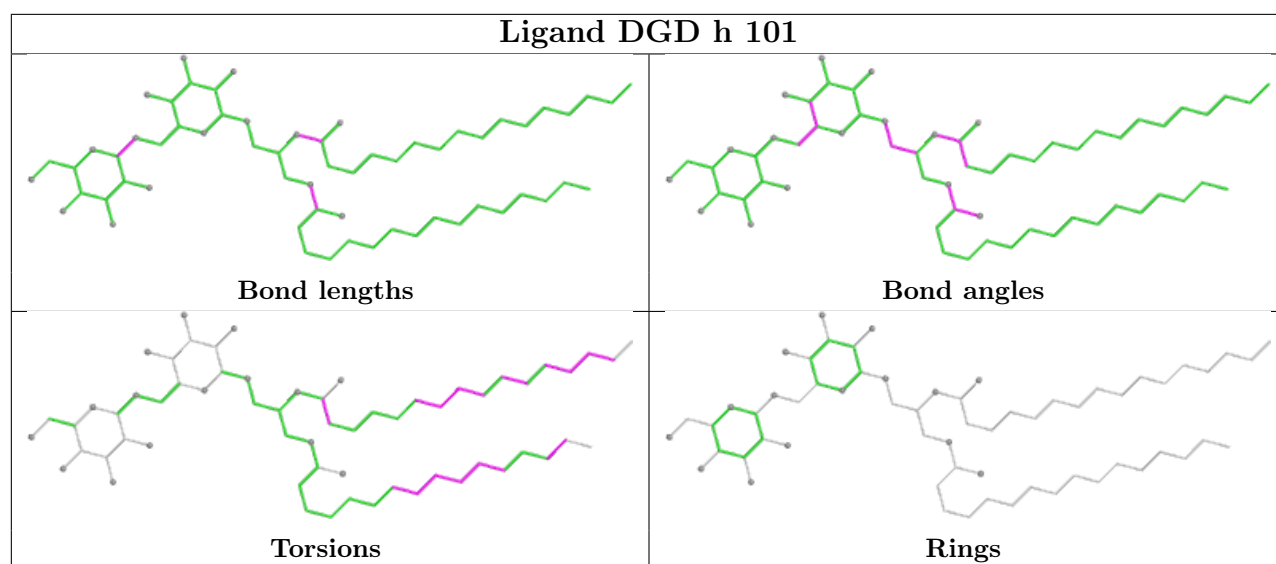
Ligand LMG C 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

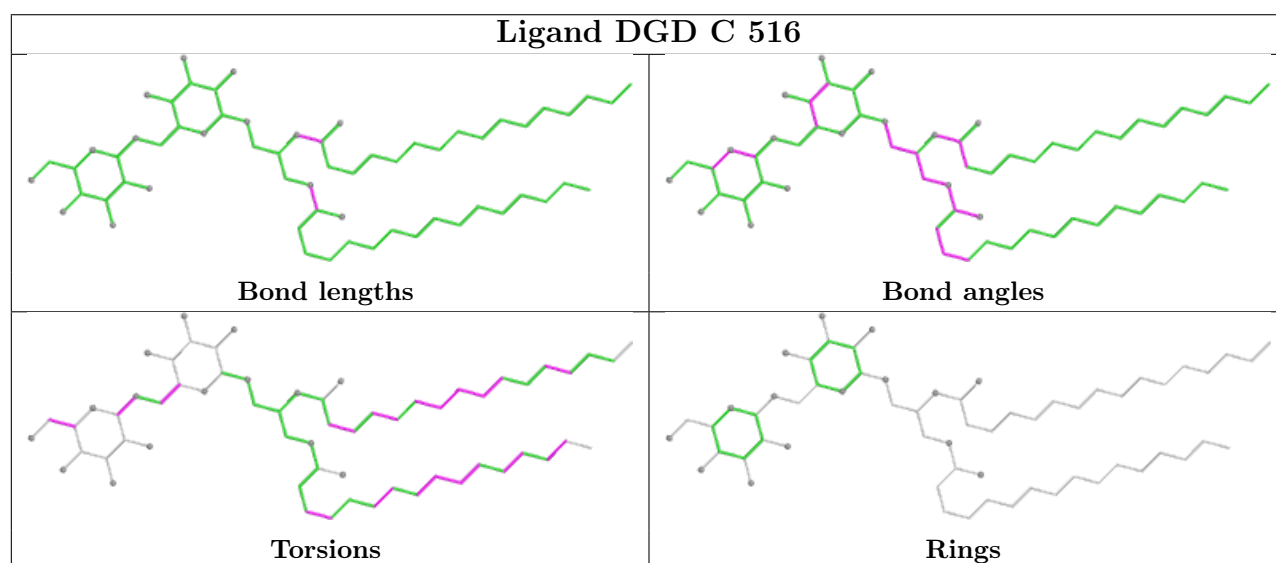
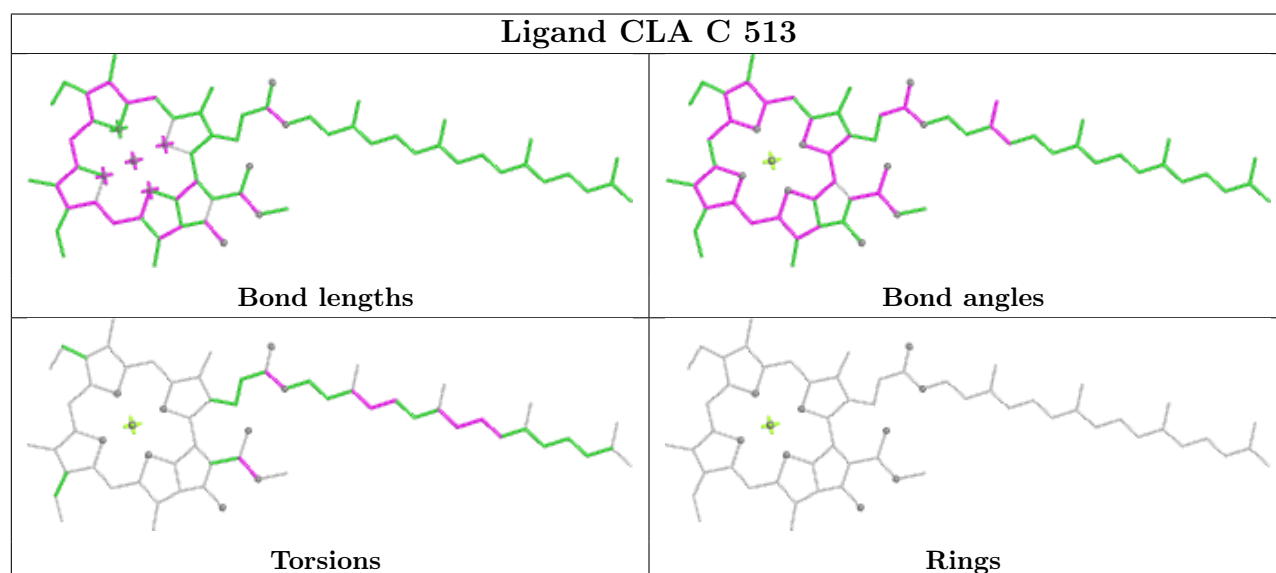
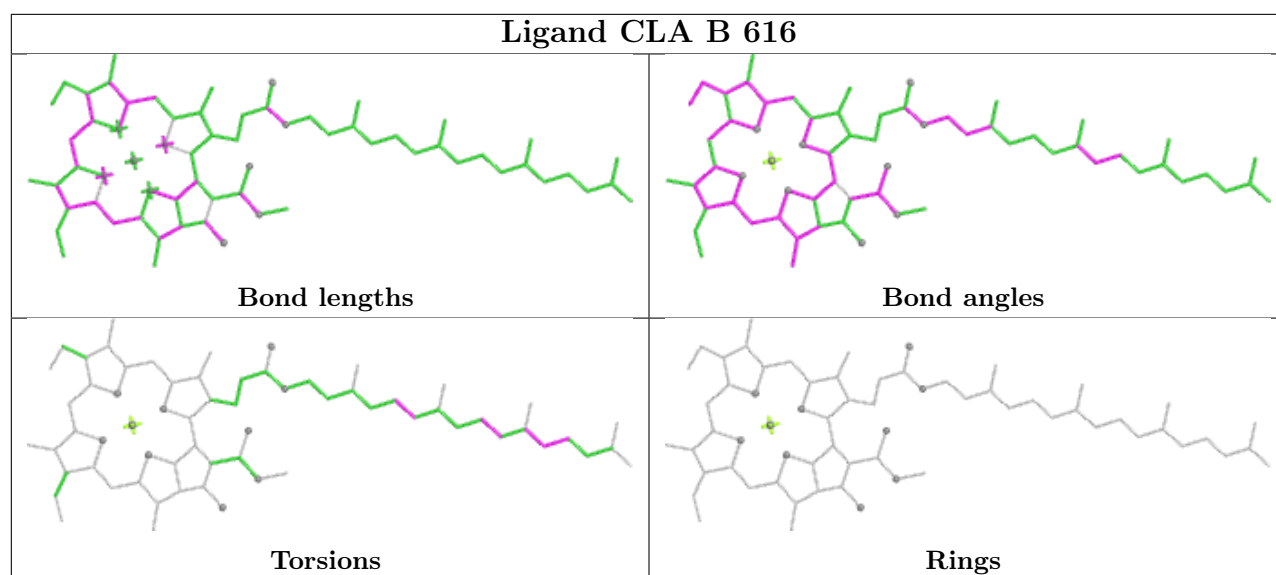


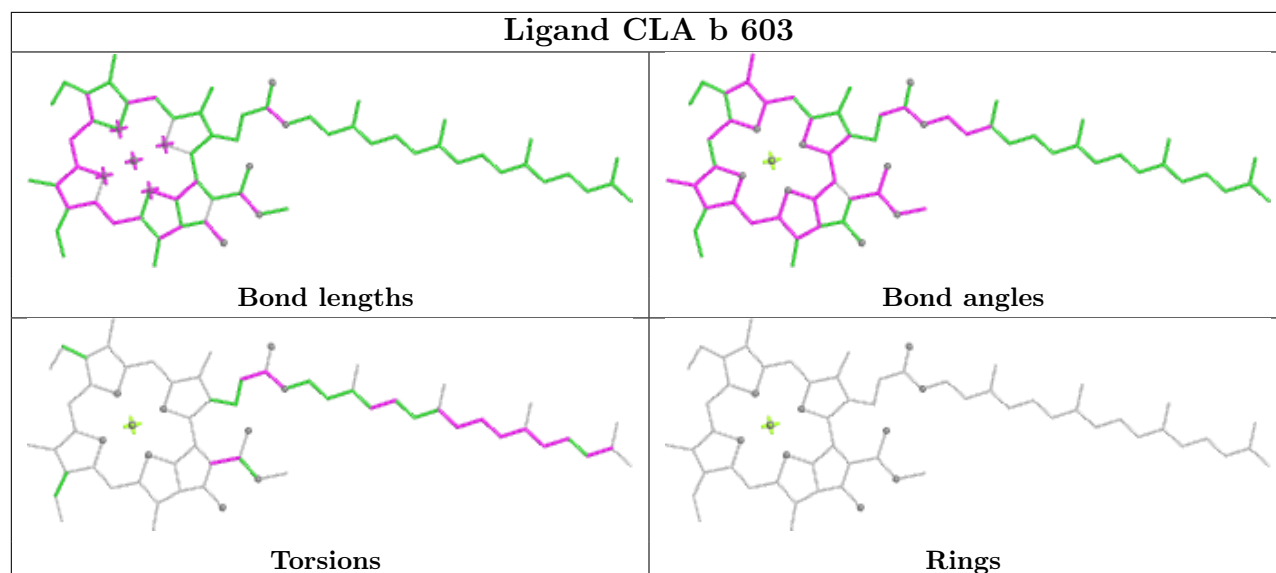
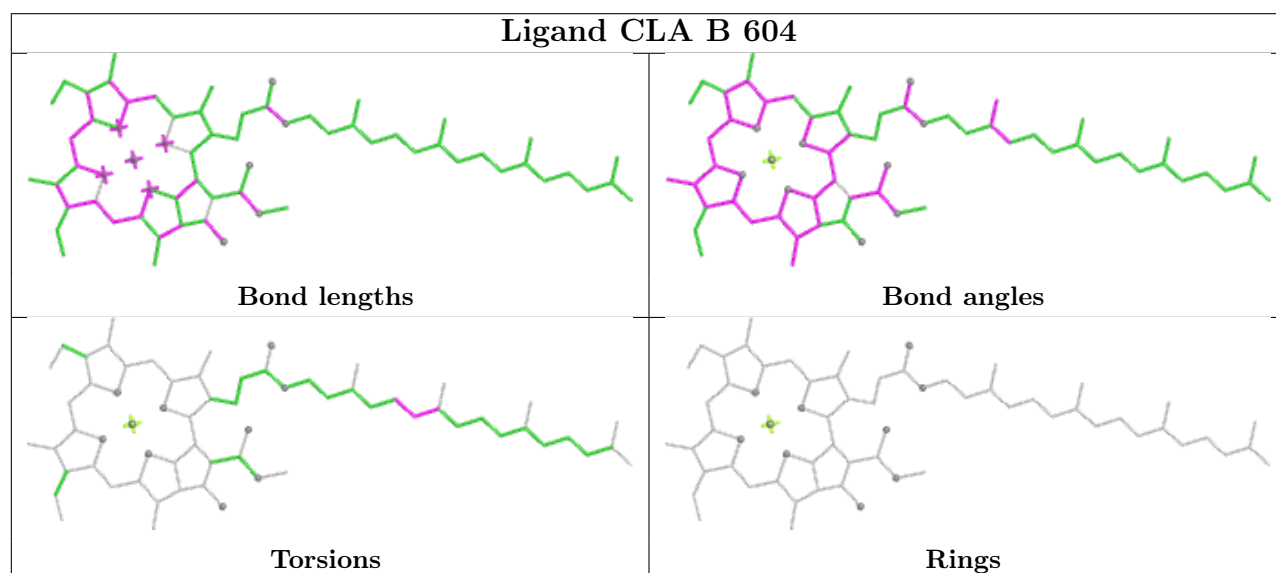
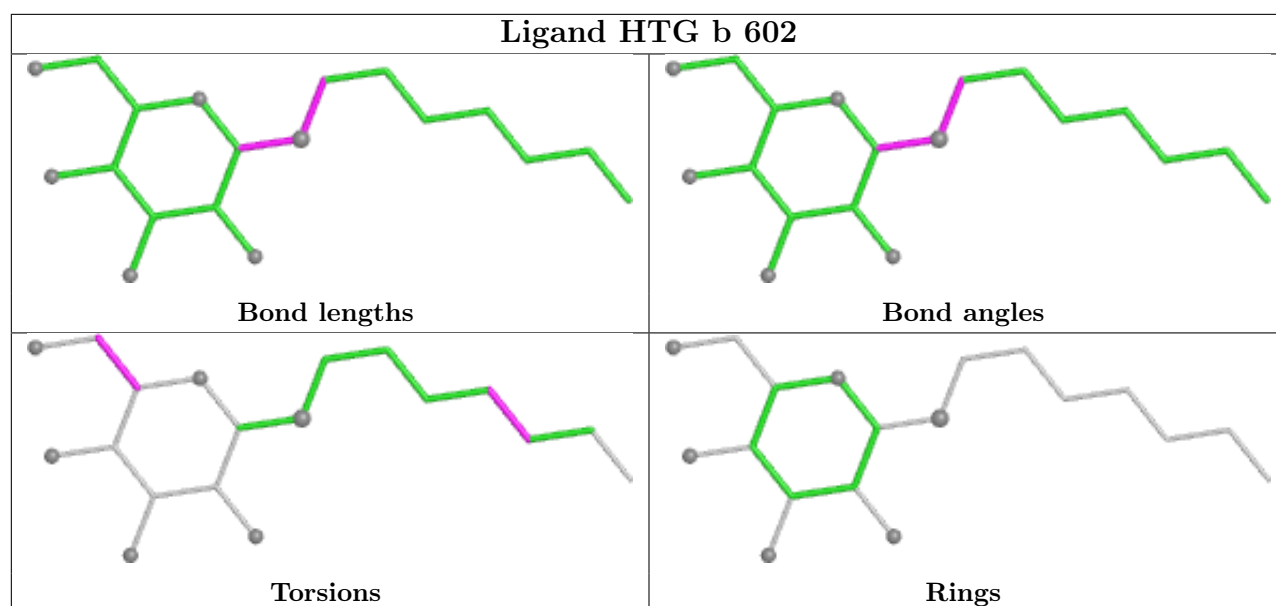


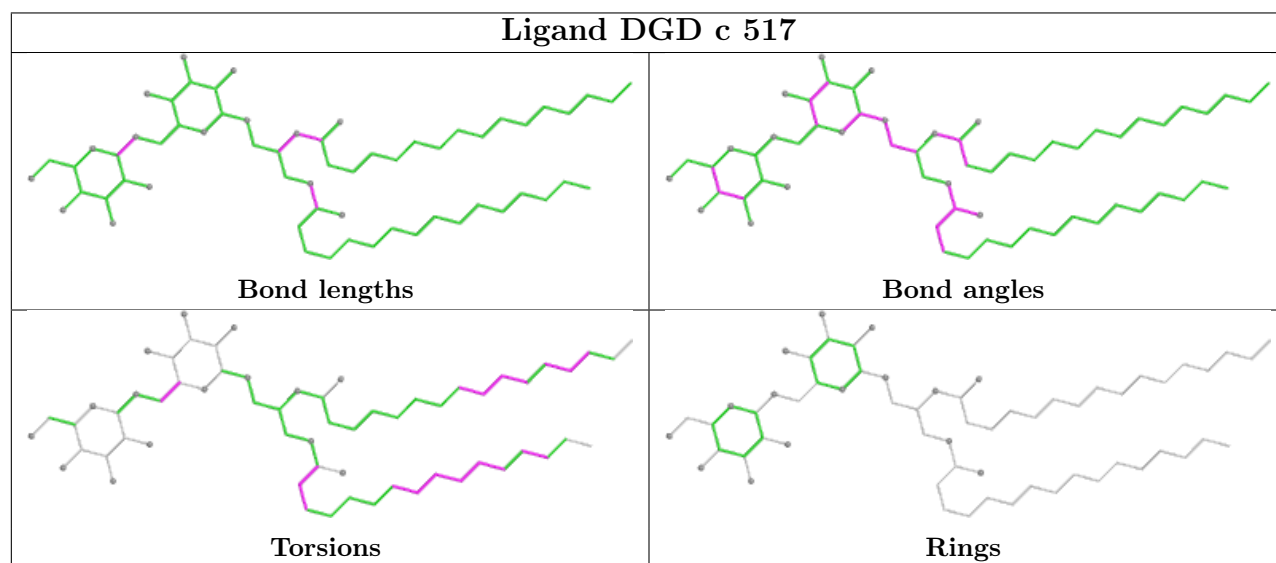
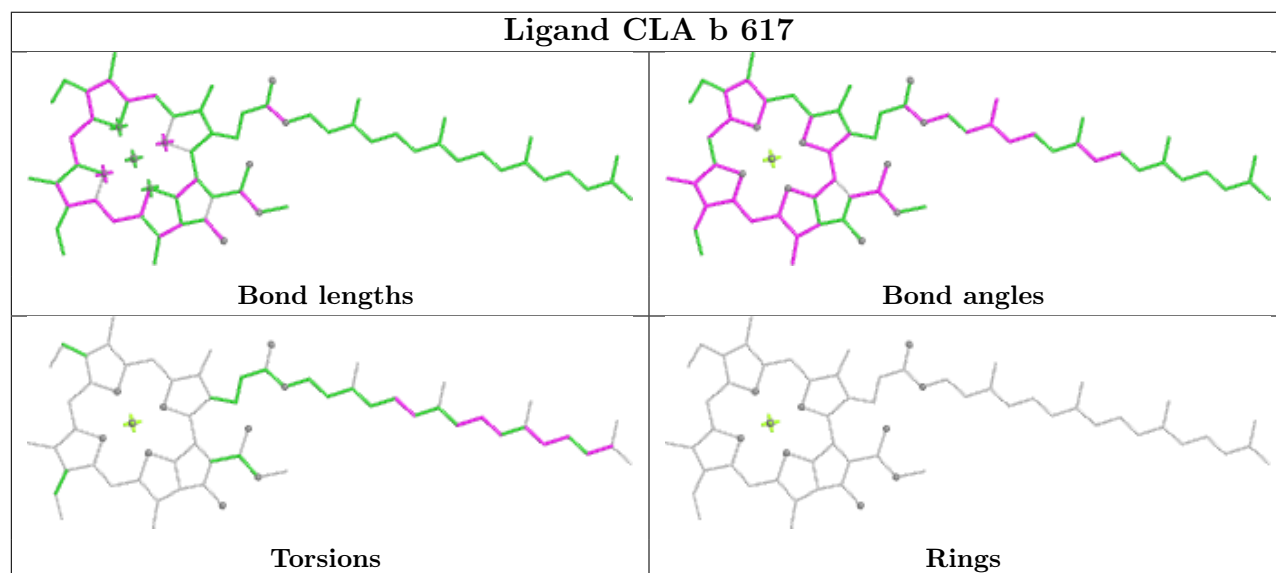
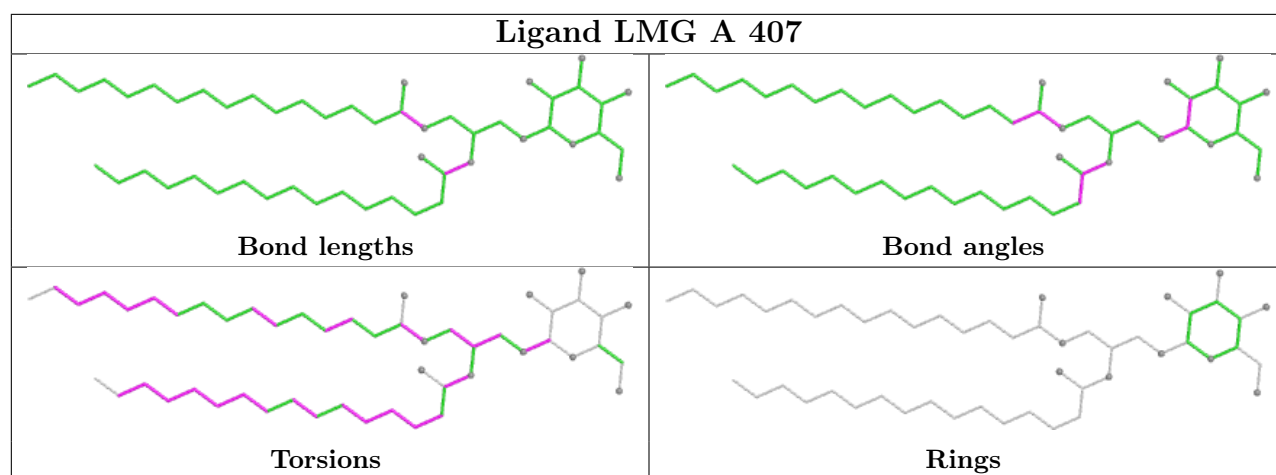




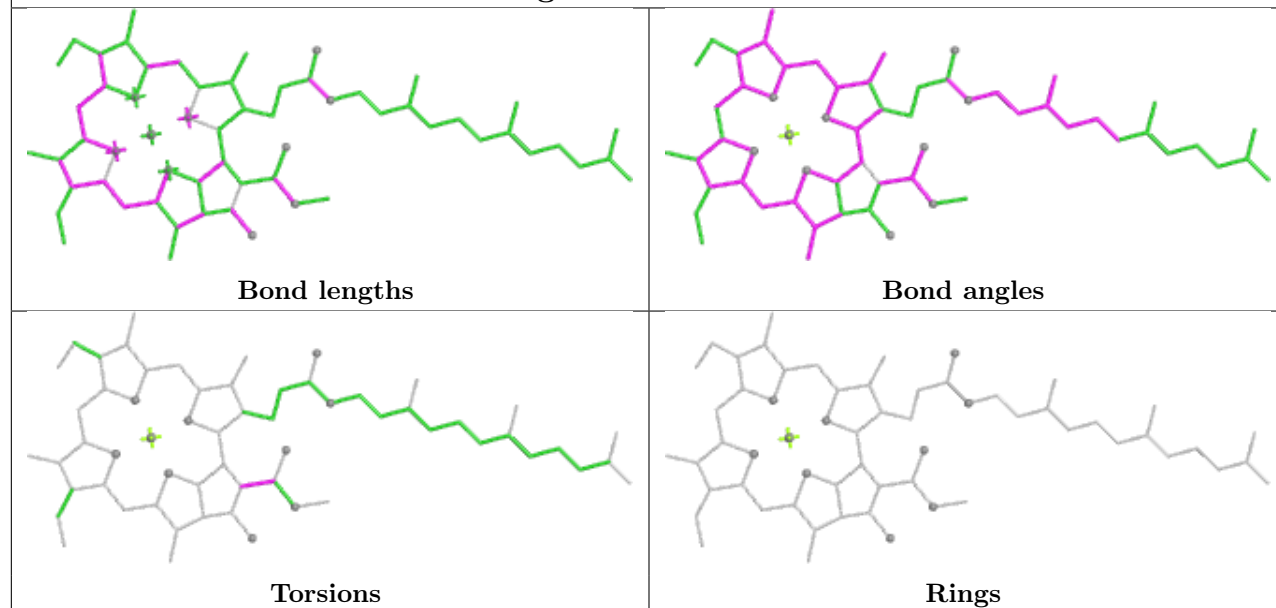




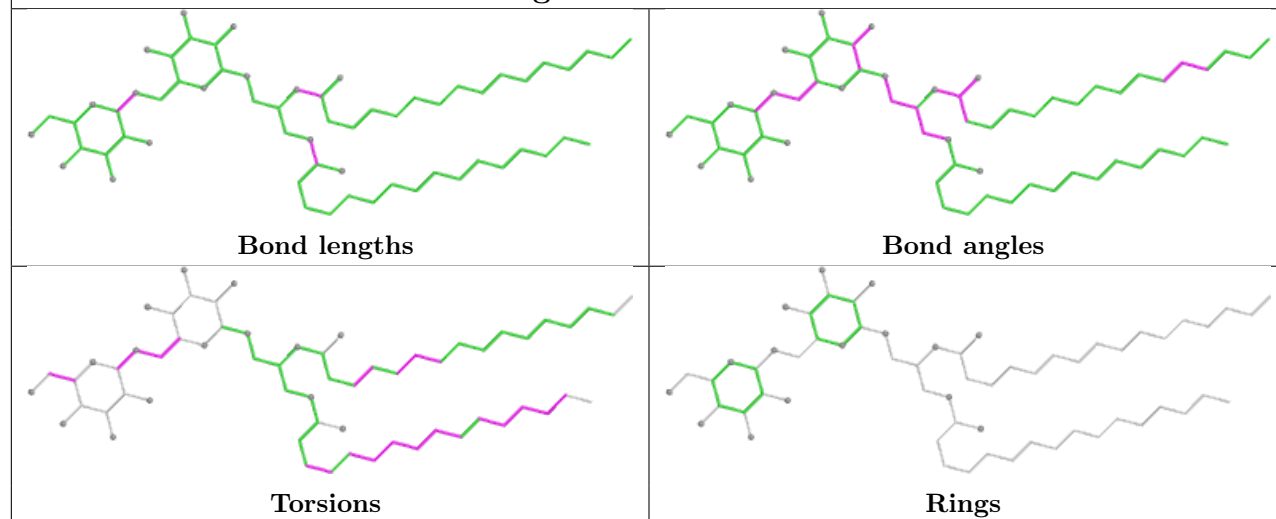


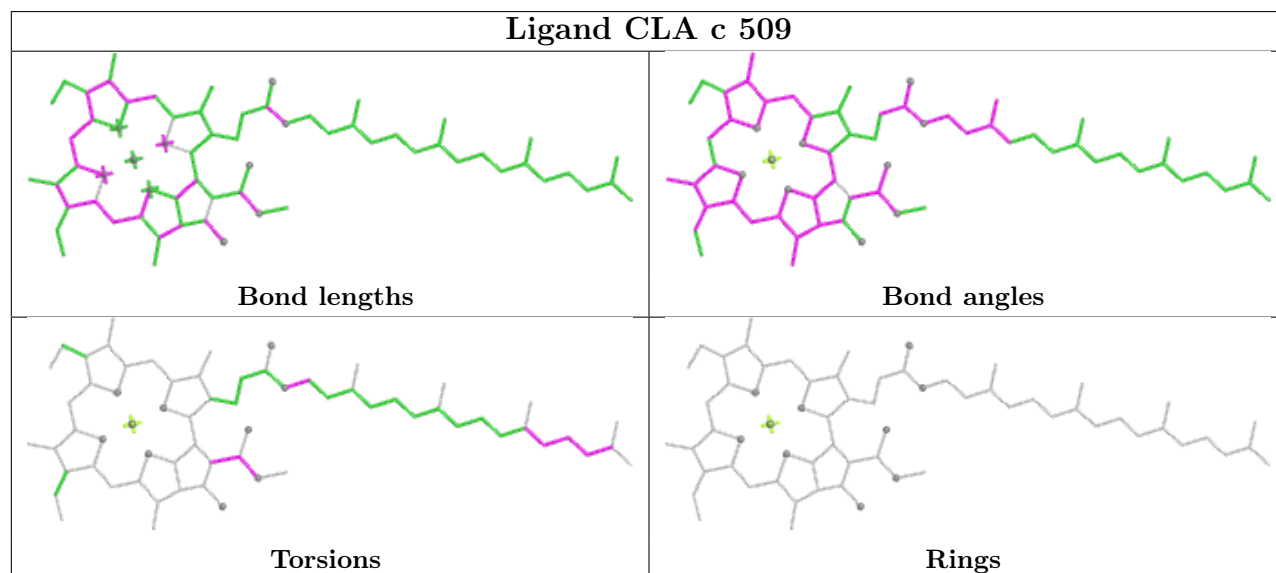
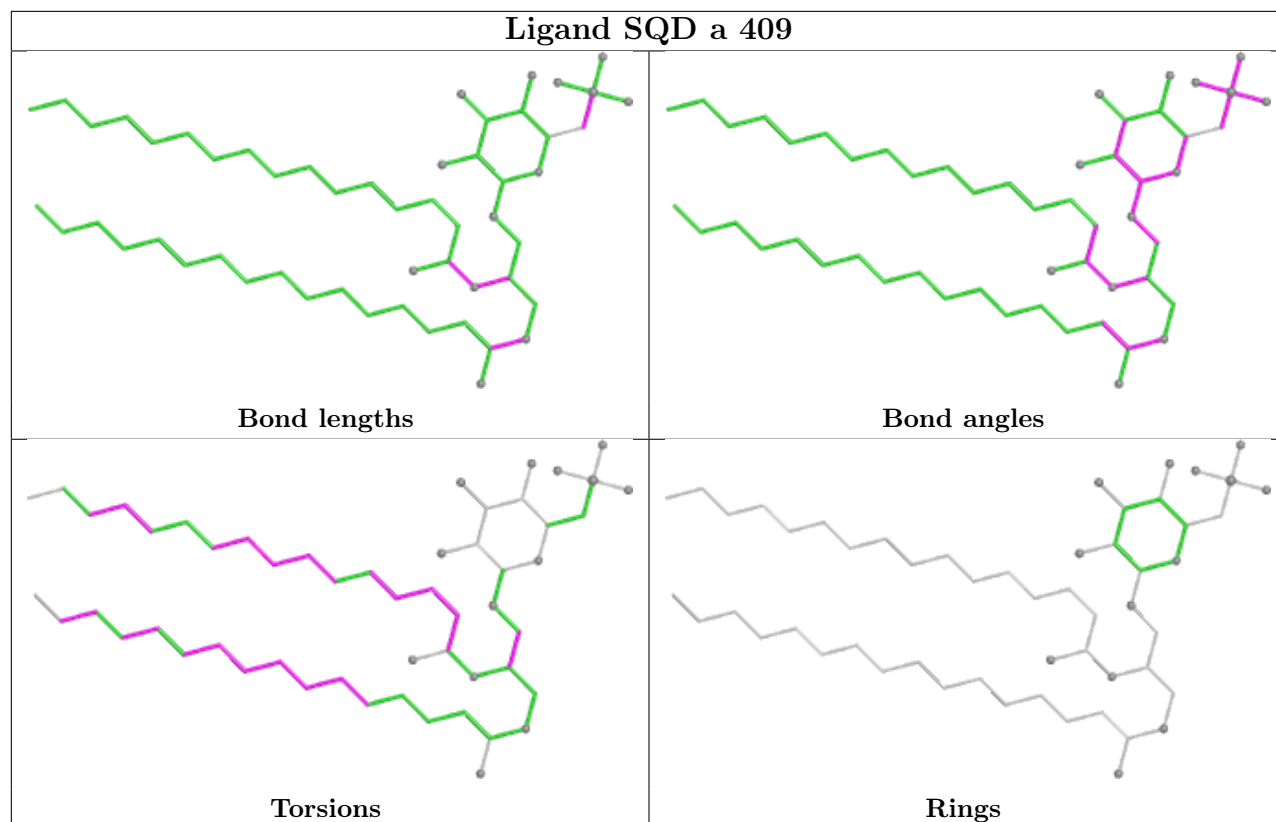


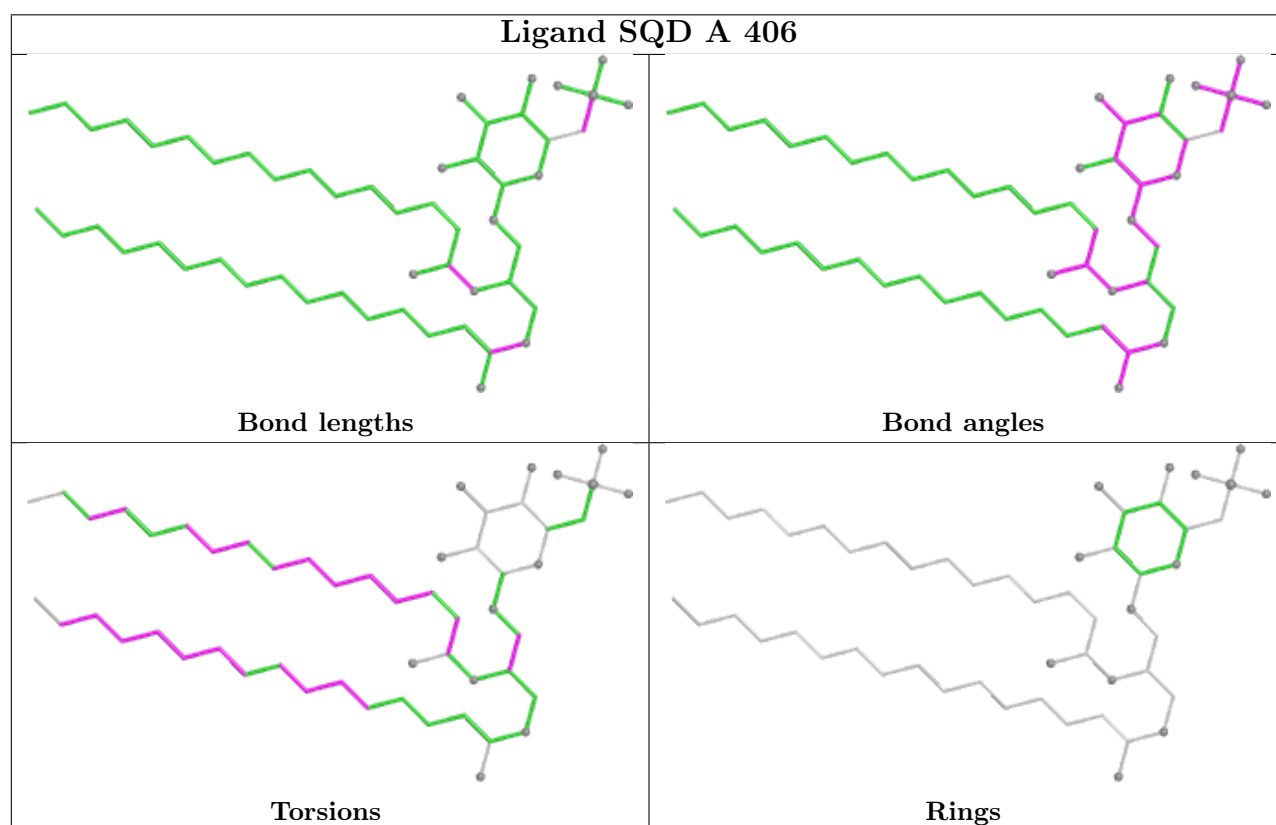
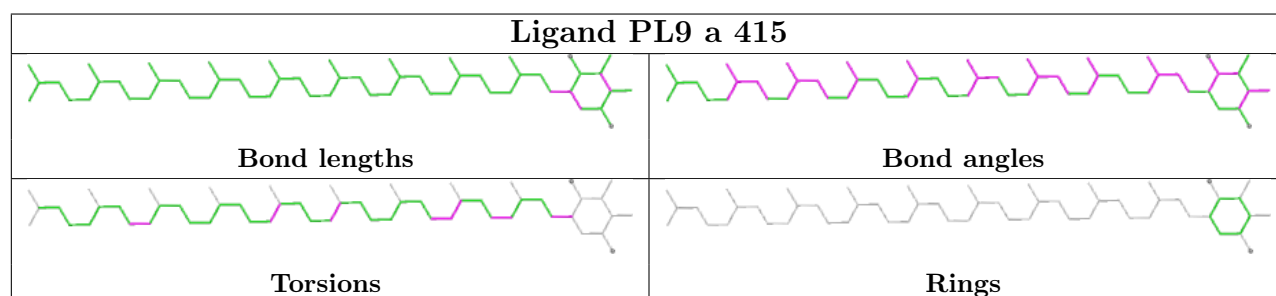
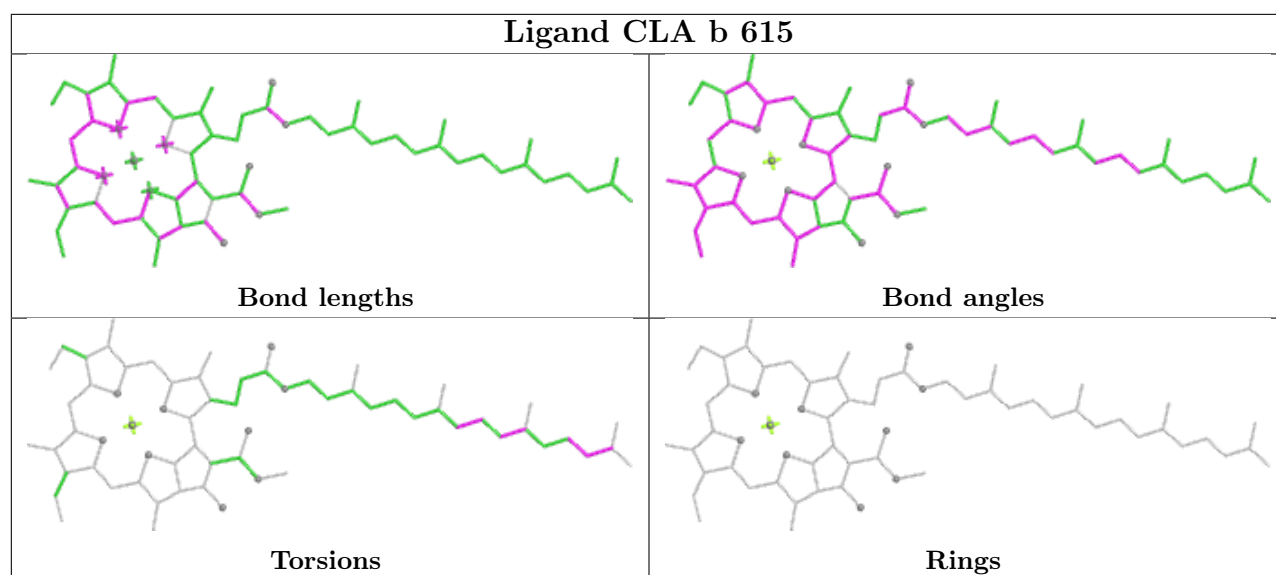
Ligand CLA c 508

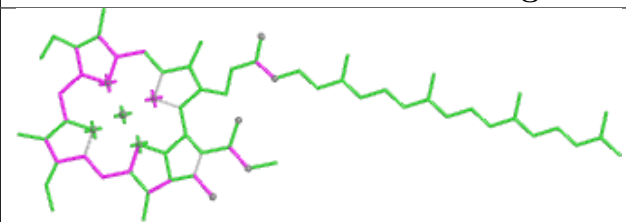
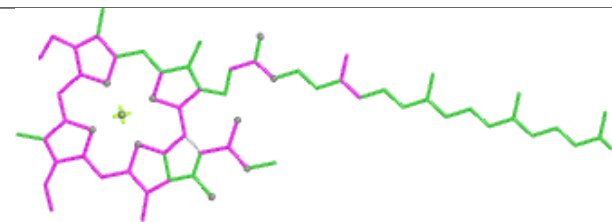
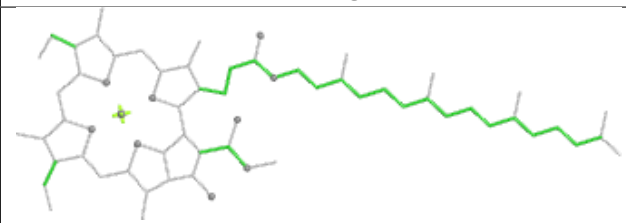
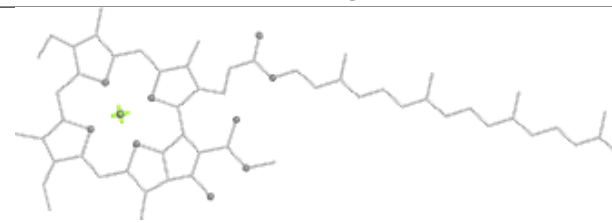


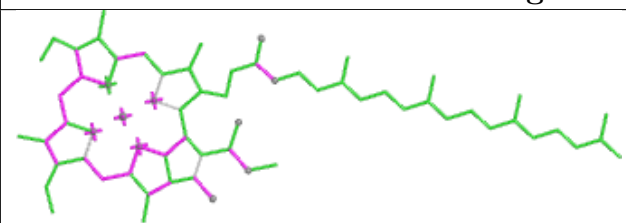
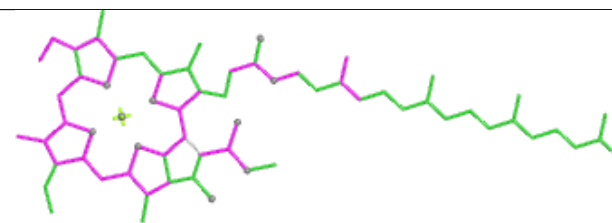
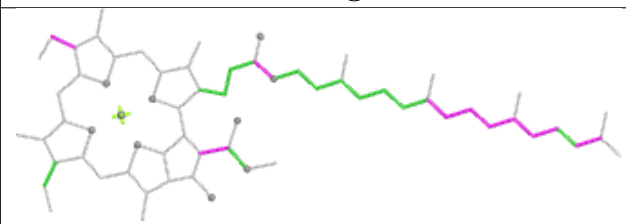
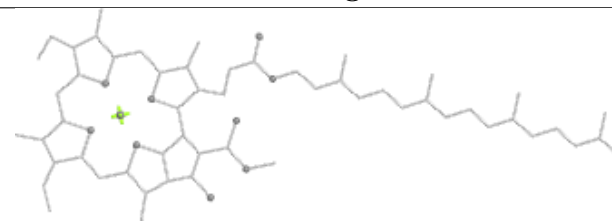
Ligand DGD c 515



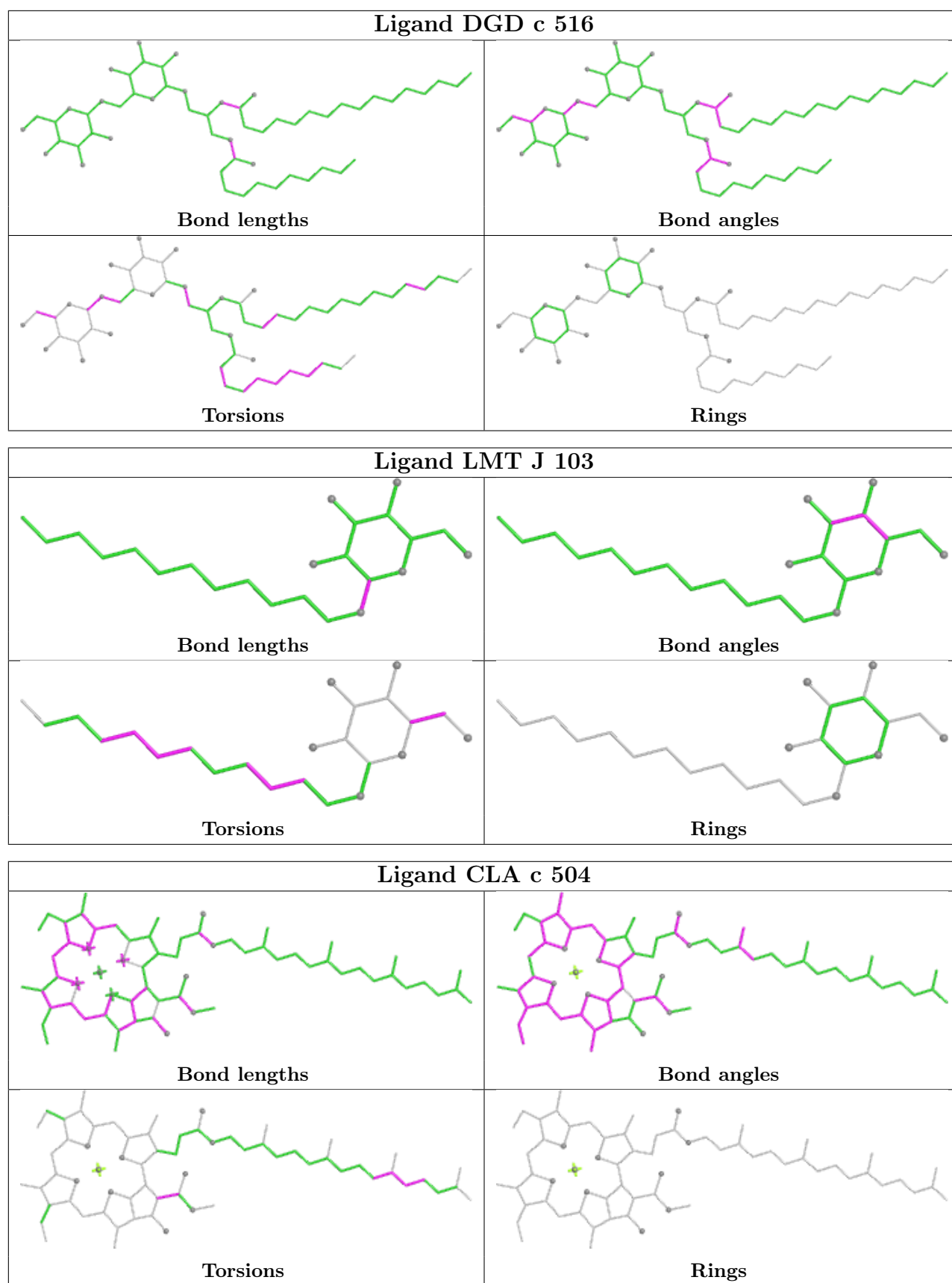


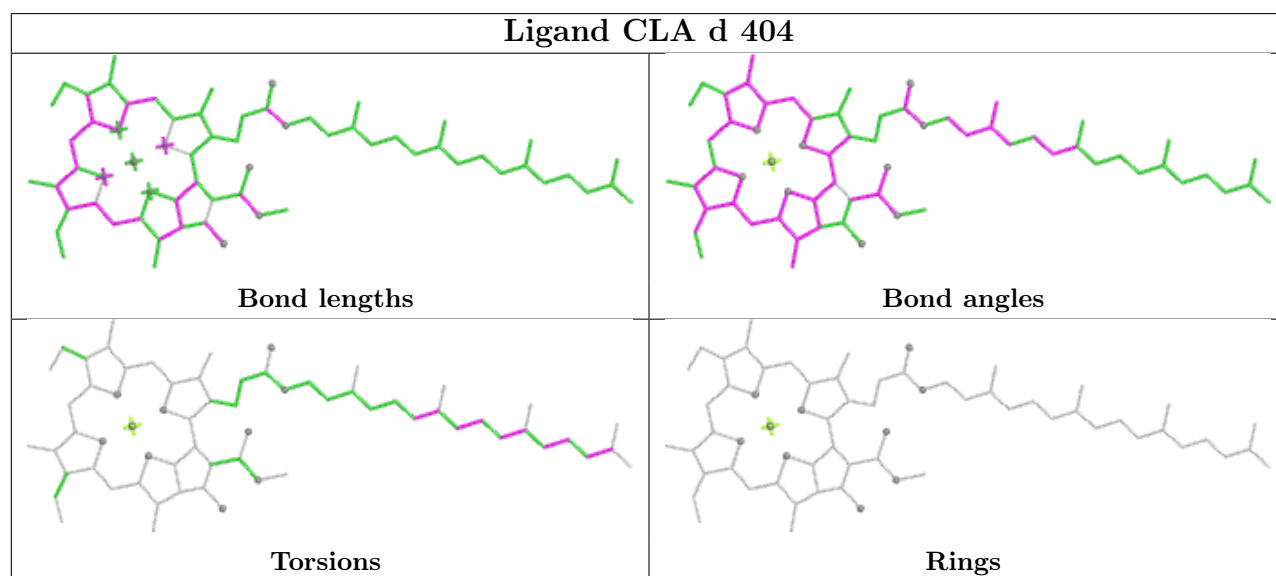
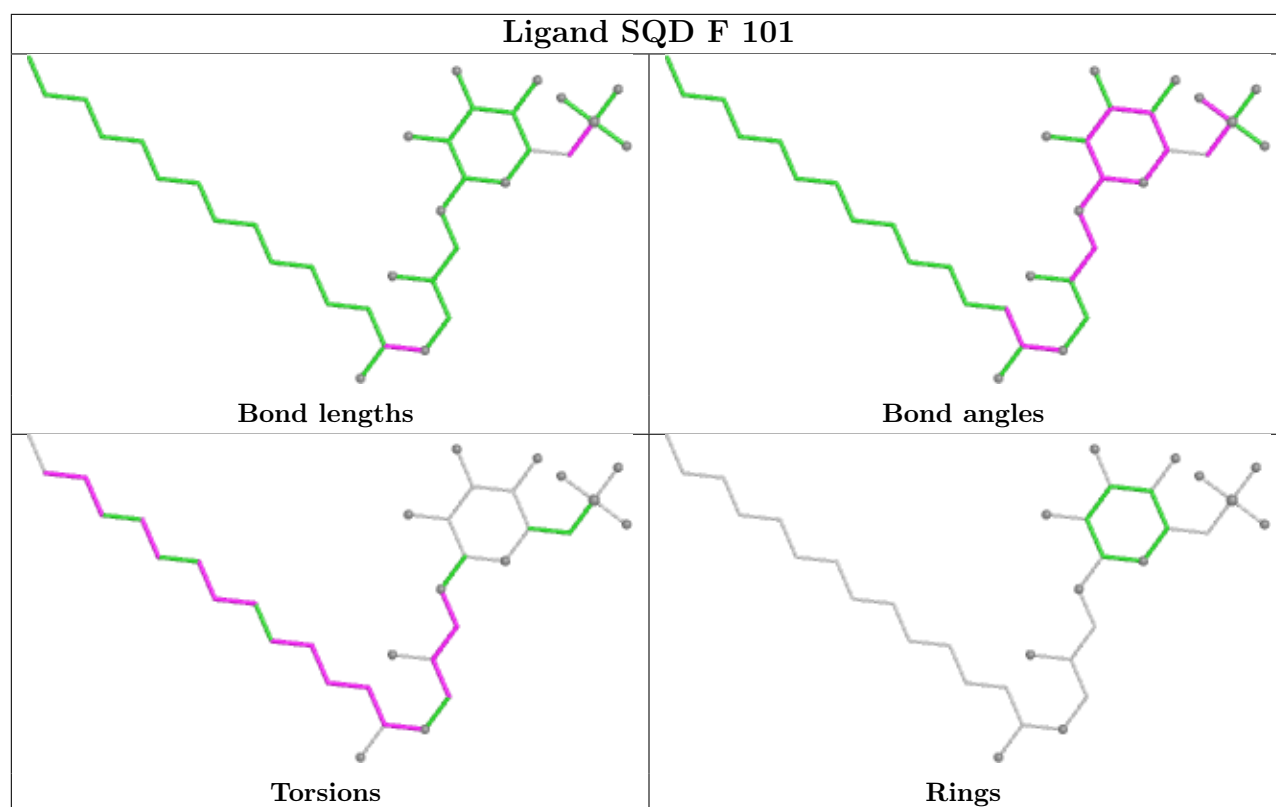


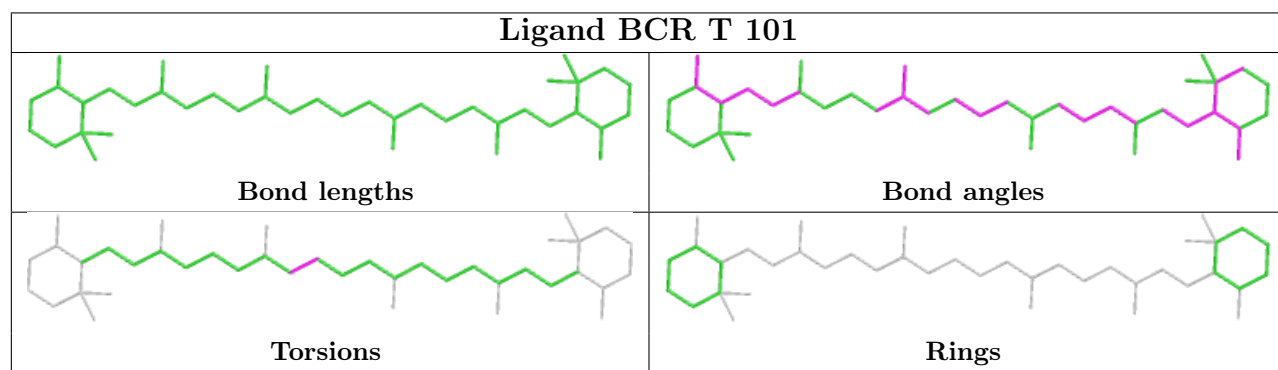
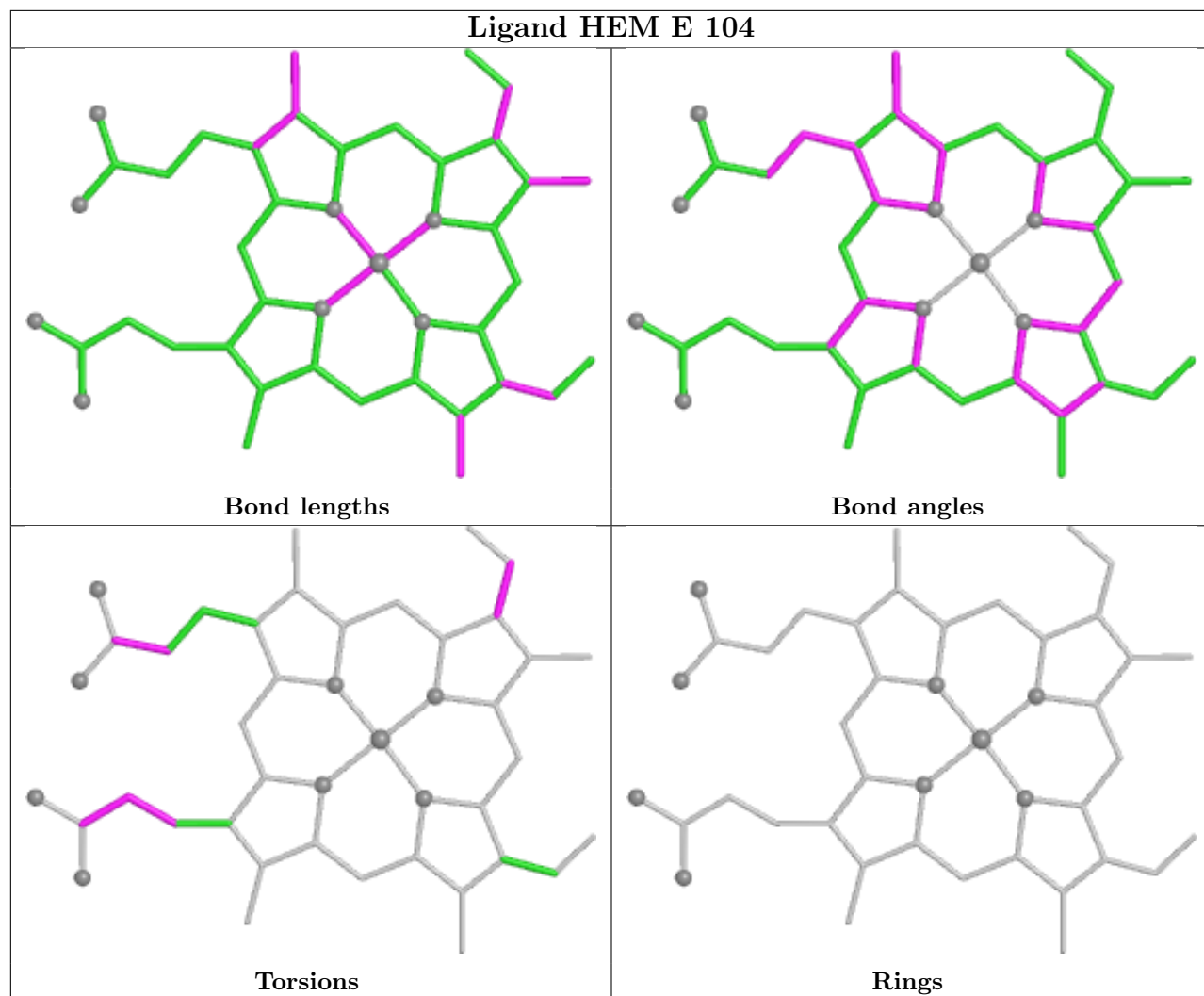
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

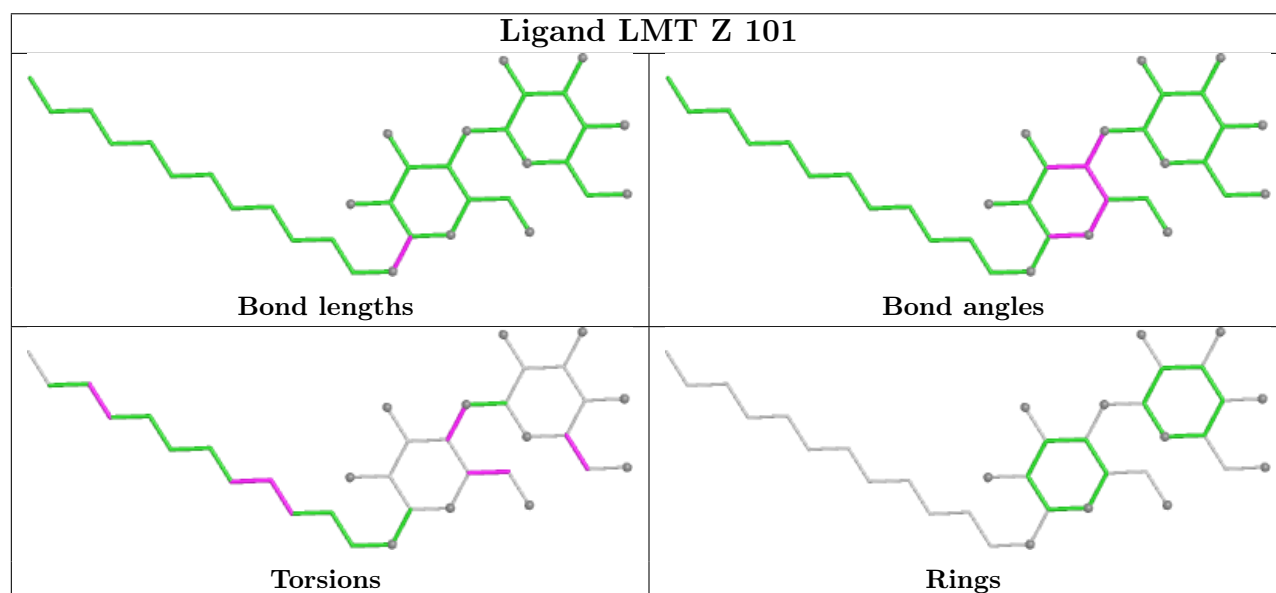
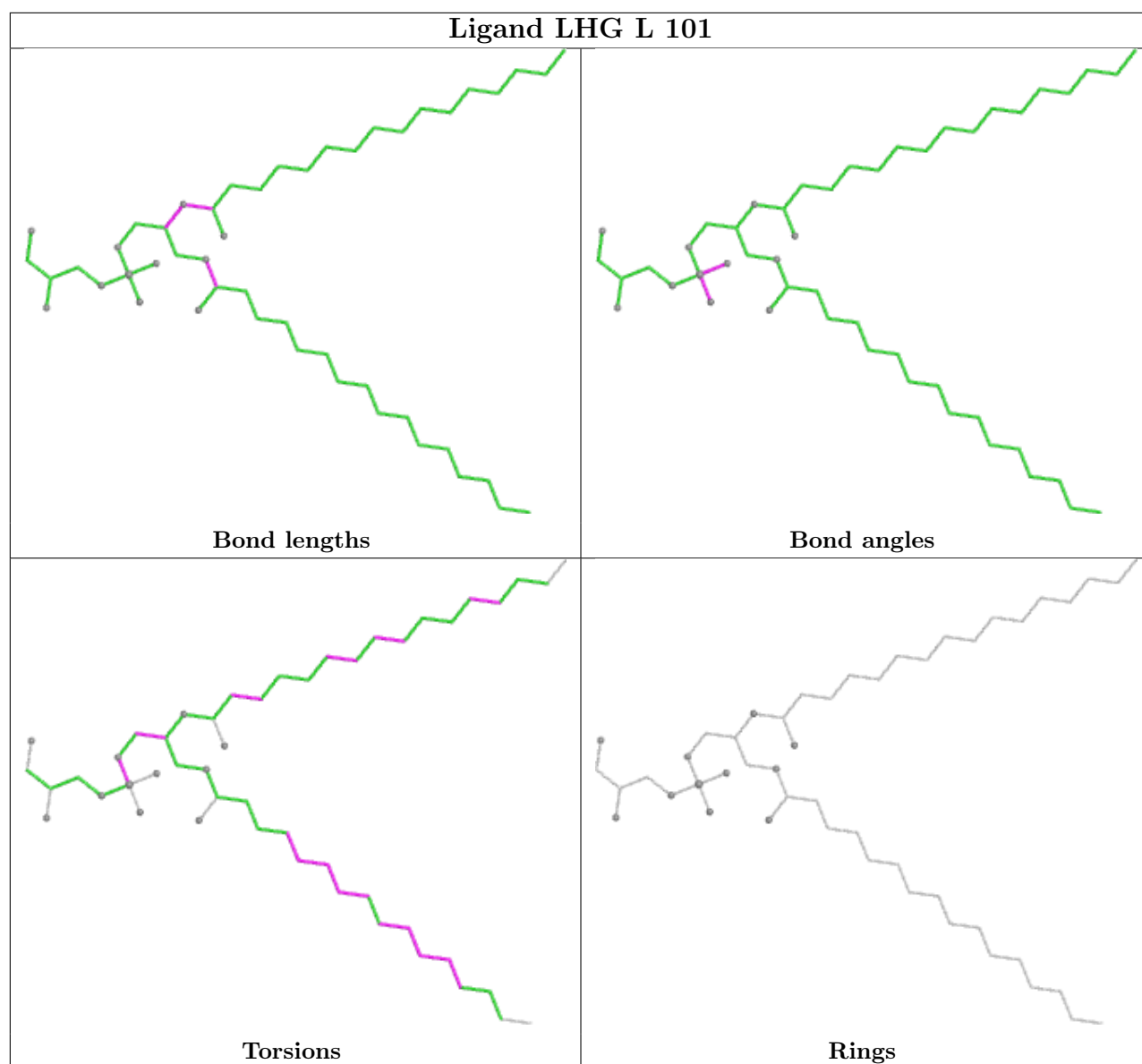
Ligand CLA c 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

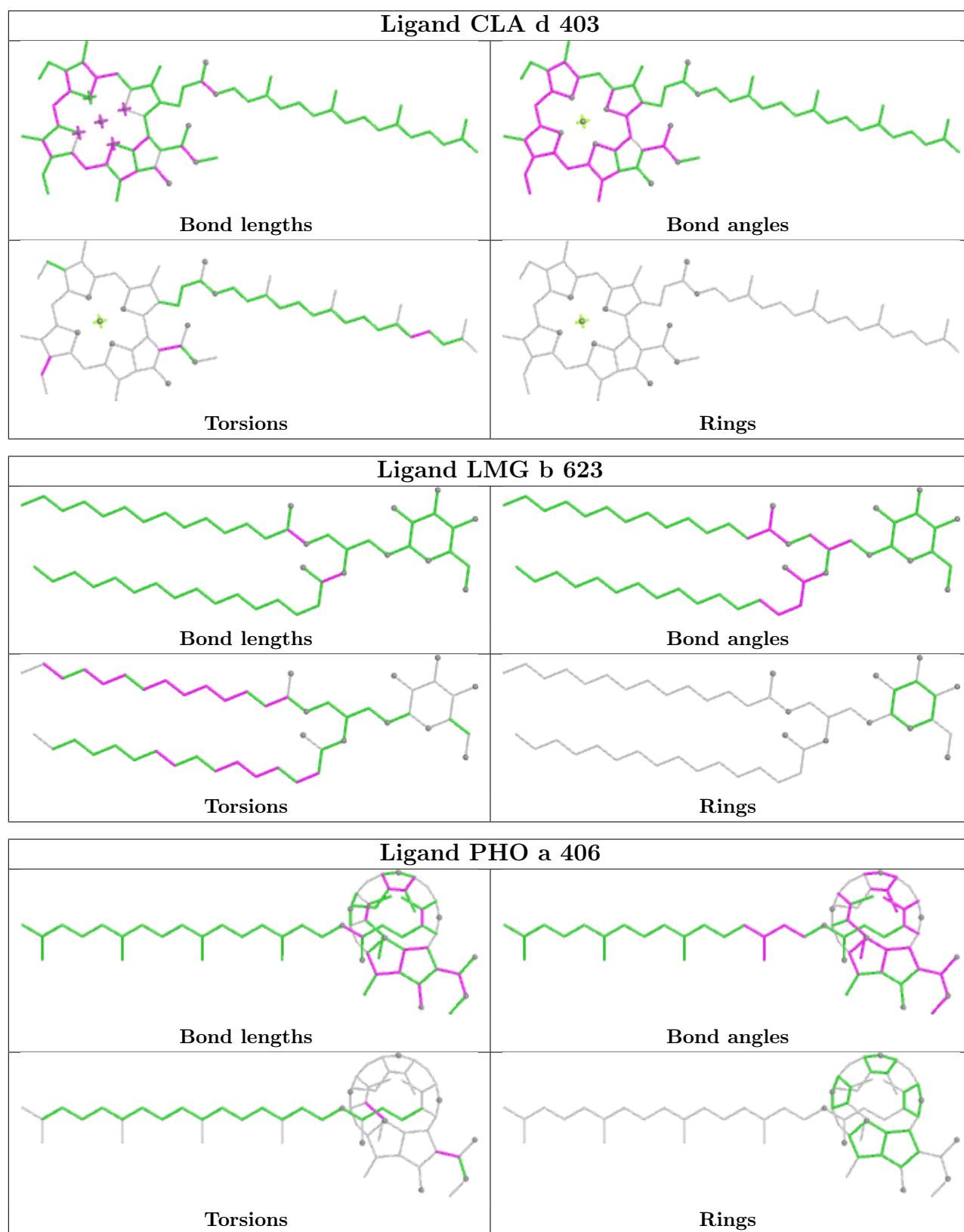
Ligand PL9 D 412	
	
Bond lengths	Bond angles
	
Torsions	Rings











5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	334/344 (97%)	-0.66	2 (0%) 85 88	15, 23, 46, 68	3 (0%)
1	a	334/344 (97%)	-0.64	0 100 100	14, 23, 48, 78	4 (1%)
2	B	505/505 (100%)	-0.49	10 (1%) 65 68	15, 28, 54, 85	11 (2%)
2	b	495/505 (98%)	-0.42	13 (2%) 57 61	16, 27, 53, 95	4 (0%)
3	C	451/455 (99%)	-0.31	1 (0%) 91 93	21, 33, 49, 83	1 (0%)
3	c	455/455 (100%)	-0.34	0 100 100	22, 33, 46, 79	1 (0%)
4	D	342/342 (100%)	-0.66	1 (0%) 90 92	17, 24, 44, 90	1 (0%)
4	d	342/342 (100%)	-0.72	1 (0%) 90 92	18, 25, 42, 86	0
5	E	78/83 (93%)	0.44	6 (7%) 19 20	28, 47, 75, 87	1 (1%)
5	e	78/83 (93%)	0.20	2 (2%) 57 61	29, 43, 63, 81	2 (2%)
6	F	33/44 (75%)	-0.05	2 (6%) 27 29	28, 36, 63, 66	0
6	f	32/44 (72%)	-0.11	1 (3%) 51 55	28, 34, 72, 90	0
7	H	64/65 (98%)	0.07	2 (3%) 51 55	26, 36, 50, 78	1 (1%)
7	h	62/65 (95%)	-0.06	0 100 100	25, 36, 48, 58	1 (1%)
8	I	34/38 (89%)	-0.05	0 100 100	29, 36, 60, 78	0
8	i	35/38 (92%)	-0.14	0 100 100	29, 34, 47, 85	1 (2%)
9	J	36/40 (90%)	-0.01	1 (2%) 55 58	26, 41, 74, 90	0
9	j	40/40 (100%)	0.09	2 (5%) 34 37	27, 39, 56, 65	0
10	K	37/37 (100%)	-0.22	0 100 100	33, 40, 52, 59	0
10	k	37/37 (100%)	-0.06	0 100 100	32, 40, 56, 64	0
11	L	37/37 (100%)	-0.65	0 100 100	12, 22, 65, 81	1 (2%)
11	l	37/37 (100%)	-0.67	0 100 100	12, 22, 76, 91	1 (2%)
12	M	33/36 (91%)	-0.67	1 (3%) 52 56	15, 25, 39, 57	1 (3%)
12	m	34/36 (94%)	-0.64	0 100 100	16, 26, 53, 74	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.26	2 (0%) 82 86	17, 32, 56, 85	6 (2%)
13	o	243/244 (99%)	-0.21	2 (0%) 82 86	17, 35, 67, 89	2 (0%)
14	T	28/32 (87%)	-0.70	0 100 100	19, 23, 37, 54	1 (3%)
14	t	29/32 (90%)	-0.52	0 100 100	20, 23, 49, 74	0
15	U	97/104 (93%)	-0.38	0 100 100	22, 29, 49, 67	0
15	u	97/104 (93%)	-0.39	0 100 100	24, 29, 44, 75	0
16	V	137/137 (100%)	-0.55	0 100 100	17, 28, 43, 60	3 (2%)
16	v	137/137 (100%)	-0.18	0 100 100	25, 36, 53, 74	0
17	Y	29/30 (96%)	0.52	2 (6%) 23 25	41, 51, 72, 79	0
17	y	29/30 (96%)	0.30	0 100 100	41, 50, 66, 70	0
18	X	38/40 (95%)	0.38	1 (2%) 57 61	32, 42, 68, 72	0
18	x	35/40 (87%)	0.18	1 (2%) 53 57	33, 40, 63, 67	0
19	Z	62/62 (100%)	0.61	4 (6%) 25 27	38, 48, 86, 98	0
19	z	61/62 (98%)	0.88	6 (9%) 13 13	45, 54, 86, 96	0
All	All	5230/5350 (97%)	-0.36	63 (1%) 76 80	12, 30, 57, 98	47 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	496	TYR	5.1
7	H	65	LEU	4.9
2	b	495	PHE	4.3
2	b	499	VAL	4.3
2	b	502	VAL	3.9
19	Z	33	TRP	3.8
2	b	484	PRO	3.8
2	b	504	THR	3.6
5	e	61	ARG	3.4
19	z	61	VAL	3.4
5	E	73	LYS	3.3
2	B	495	PHE	3.2
5	e	83	LEU	3.0
3	C	23	ALA	3.0
7	H	64	ALA	3.0
2	B	486	LEU	2.9
5	E	80	LEU	2.9
19	z	36	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	494	GLY	2.9
2	b	503	THR	2.9
19	Z	32	ASP	2.9
13	O	60	ARG	2.8
6	f	14	PRO	2.8
19	z	33	TRP	2.7
2	b	491	VAL	2.6
2	B	479	PHE	2.6
2	b	479	PHE	2.6
17	Y	18	VAL	2.5
19	Z	30	PRO	2.5
1	A	262	TYR	2.5
2	B	500	GLY	2.5
2	b	500	GLY	2.5
5	E	79	PHE	2.4
2	b	497	GLN	2.4
17	Y	19	ILE	2.4
2	B	487	SER	2.4
5	E	4	THR	2.4
19	z	4	LEU	2.3
1	A	11	ALA	2.3
19	z	30	PRO	2.3
4	D	11	GLU	2.3
2	b	501	ASP	2.3
2	B	293	ALA	2.2
2	B	496	TYR	2.2
4	d	11	GLU	2.2
6	F	16	PHE	2.2
6	F	13	TYR	2.2
13	o	36	GLN	2.2
2	b	129	GLY	2.2
9	J	5	GLY	2.2
13	O	59	LYS	2.2
9	j	2	MET	2.1
2	B	499	VAL	2.1
18	X	2	THR	2.1
13	o	246	ALA	2.1
5	E	76	VAL	2.1
9	j	1	MET	2.1
18	x	2	THR	2.1
19	z	2	THR	2.1
2	B	501	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	61	ARG	2.1
19	Z	35	ARG	2.1
12	M	33	GLN	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
14	FME	t	1	10/11	0.96	0.06	23,27,49,50	0
14	FME	T	1	10/11	0.97	0.06	23,29,48,51	0
8	FME	i	1	10/11	0.98	0.06	30,31,34,35	0
8	FME	I	1	10/11	0.98	0.05	26,32,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	UNL	b	642	13/-	0.59	0.14	71,80,87,90	0
35	DGD	D	406	51/66	0.62	0.16	57,74,100,108	0
26	UNL	B	646	16/-	0.64	0.14	85,89,93,94	0
28	DMS	j	105	4/4	0.66	0.18	70,74,75,88	0
26	UNL	B	629	10/-	0.66	0.15	54,69,74,74	0
28	DMS	O	308	4/4	0.67	0.17	66,74,76,87	0
26	UNL	Z	102	4/-	0.67	0.20	59,61,62,63	0
32	HTG	C	534	19/19	0.67	0.14	68,110,128,130	0
26	UNL	b	643	9/-	0.67	0.12	67,67,74,74	0
28	DMS	b	638	4/4	0.68	0.20	67,75,77,86	0
28	DMS	o	306	4/4	0.68	0.19	55,58,65,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMT	f	102	24/35	0.69	0.15	62,77,94,98	0
28	DMS	U	904	4/4	0.69	0.18	58,66,66,83	0
28	DMS	O	305	4/4	0.70	0.22	64,66,77,86	0
32	HTG	D	417	19/19	0.70	0.15	67,105,119,120	0
28	DMS	B	636	4/4	0.71	0.17	77,86,90,96	0
28	DMS	O	309	4/4	0.71	0.23	58,65,72,73	0
35	DGD	d	416	51/66	0.71	0.14	56,75,96,103	0
28	DMS	H	103	4/4	0.72	0.21	84,101,109,112	0
26	UNL	B	647	13/-	0.72	0.13	71,81,90,91	0
28	DMS	b	640	4/4	0.72	0.18	49,58,71,73	0
26	UNL	A	413	4/-	0.72	0.13	64,64,64,66	0
26	UNL	a	402	6/-	0.72	0.14	50,57,62,63	0
32	HTG	v	210	14/19	0.73	0.16	60,80,92,100	0
26	UNL	T	103	13/-	0.73	0.13	64,68,72,72	0
26	UNL	a	414	28/-	0.73	0.14	59,68,84,87	0
32	HTG	c	521	19/19	0.73	0.14	57,85,102,105	0
26	UNL	b	645	6/-	0.74	0.16	57,65,76,76	0
26	UNL	h	103	16/-	0.74	0.14	61,69,73,76	0
32	HTG	c	520	19/19	0.74	0.15	77,88,99,100	0
26	UNL	A	410	36/-	0.74	0.15	57,78,84,91	0
26	UNL	c	526	8/-	0.75	0.17	54,59,64,65	0
28	DMS	D	415	4/4	0.75	0.23	57,58,63,65	0
34	LMT	I	101	35/35	0.75	0.13	67,82,91,92	0
28	DMS	O	310	4/4	0.76	0.19	76,78,82,94	0
26	UNL	E	102	15/-	0.76	0.17	55,62,76,77	0
28	DMS	o	308	4/4	0.76	0.19	60,61,62,63	0
34	LMT	b	627	32/35	0.77	0.14	42,67,84,87	0
26	UNL	J	107	3/-	0.77	0.12	61,61,63,64	0
32	HTG	b	602	19/19	0.77	0.13	51,103,117,118	0
28	DMS	b	641	4/4	0.77	0.20	63,65,75,80	0
36	LHG	E	103	48/49	0.77	0.15	44,99,108,119	0
34	LMT	E	101	24/35	0.78	0.12	64,78,84,90	0
26	UNL	I	105	10/-	0.78	0.10	60,66,71,72	0
26	UNL	I	106	11/-	0.78	0.17	61,73,81,81	0
26	UNL	B	633	16/-	0.78	0.16	53,61,69,70	0
26	UNL	I	104	11/-	0.78	0.13	53,56,59,62	0
32	HTG	u	201	8/19	0.78	0.17	45,52,69,89	0
26	UNL	j	104	16/-	0.78	0.14	49,58,64,66	0
32	HTG	B	623	19/19	0.79	0.12	53,88,93,94	0
26	UNL	J	104	14/-	0.79	0.13	67,77,80,81	0
26	UNL	I	103	13/-	0.79	0.14	47,53,84,87	0
26	UNL	H	104	4/-	0.79	0.14	60,62,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMT	c	523	35/35	0.79	0.12	67,77,83,85	0
26	UNL	t	102	16/-	0.79	0.12	61,71,80,80	0
26	UNL	c	524	30/-	0.79	0.14	59,74,86,87	0
32	HTG	d	401	19/19	0.79	0.14	58,99,111,120	0
26	UNL	c	525	10/-	0.79	0.13	58,65,66,67	0
26	UNL	U	901	14/-	0.80	0.15	40,49,59,59	0
28	DMS	B	638	4/4	0.80	0.18	53,61,63,68	0
26	UNL	C	523	34/-	0.80	0.12	59,80,92,101	0
26	UNL	b	644	7/-	0.80	0.11	64,65,70,70	0
26	UNL	H	105	6/-	0.80	0.13	51,55,63,65	0
34	LMT	a	418	35/35	0.80	0.13	45,69,78,81	0
26	UNL	j	106	6/-	0.80	0.16	52,55,58,59	0
23	SQD	f	101	40/54	0.80	0.14	57,86,102,107	0
27	PL9	A	411	55/55	0.80	0.15	43,67,89,92	0
34	LMT	m	101	35/35	0.80	0.13	48,94,110,114	0
27	PL9	a	415	55/55	0.80	0.16	52,67,89,94	0
28	DMS	b	637	4/4	0.80	0.17	77,79,84,93	0
28	DMS	A	418	4/4	0.80	0.21	68,74,80,85	0
34	LMT	b	628	25/35	0.81	0.12	54,79,95,96	0
28	DMS	u	204	4/4	0.81	0.18	71,78,83,86	0
28	DMS	B	642	4/4	0.81	0.22	43,51,68,71	0
32	HTG	B	632	19/19	0.81	0.12	51,97,108,114	0
34	LMT	z	102	35/35	0.81	0.12	46,85,99,101	0
34	LMT	Z	101	35/35	0.81	0.14	44,90,107,109	0
24	LMG	C	524	45/55	0.81	0.20	22,46,51,56	45
26	UNL	b	630	11/-	0.81	0.13	55,60,67,68	0
28	DMS	d	415	4/4	0.82	0.17	68,71,71,72	0
28	DMS	O	306	4/4	0.82	0.18	66,73,73,75	0
32	HTG	C	521	19/19	0.82	0.12	46,78,89,90	0
28	DMS	V	205	4/4	0.82	0.15	67,76,77,79	0
28	DMS	B	639	4/4	0.82	0.18	65,70,71,76	0
28	DMS	c	533	4/4	0.82	0.16	73,75,77,87	0
26	UNL	M	102	12/-	0.83	0.13	49,53,95,98	0
26	UNL	B	630	14/-	0.83	0.12	67,74,83,84	0
26	UNL	a	416	11/-	0.83	0.14	66,68,76,78	0
34	LMT	J	103	24/35	0.83	0.12	53,61,81,85	0
26	UNL	x	102	9/-	0.83	0.14	56,68,72,72	0
26	UNL	L	102	14/-	0.84	0.15	56,60,84,84	0
24	LMG	c	518	51/55	0.84	0.11	37,72,84,87	0
23	SQD	l	101	54/54	0.84	0.13	47,68,101,106	0
28	DMS	b	636	4/4	0.84	0.18	66,71,72,79	0
26	UNL	d	409	36/-	0.84	0.12	36,60,91,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	DMS	v	207	4/4	0.84	0.15	53,66,72,87	0
23	SQD	b	622	54/54	0.84	0.12	46,63,95,100	0
34	LMT	B	627	16/35	0.84	0.12	52,60,78,78	0
26	UNL	i	101	16/-	0.84	0.12	41,45,65,65	0
26	UNL	i	103	11/-	0.84	0.11	58,61,65,66	0
26	UNL	b	629	16/-	0.84	0.13	41,48,60,60	0
28	DMS	C	532	4/4	0.85	0.17	33,40,41,48	0
32	HTG	C	520	19/19	0.85	0.11	64,70,76,79	0
28	DMS	O	311	4/4	0.85	0.16	57,65,69,72	0
32	HTG	C	522	19/19	0.85	0.11	66,83,104,107	0
28	DMS	c	534	4/4	0.85	0.14	70,71,75,81	0
23	SQD	F	101	35/54	0.85	0.13	51,76,89,90	0
26	UNL	e	101	7/-	0.85	0.12	54,58,64,65	0
32	HTG	b	624	19/19	0.85	0.12	49,74,80,85	0
28	DMS	b	634	4/4	0.85	0.16	59,67,67,75	0
28	DMS	A	417	4/4	0.85	0.16	70,72,77,81	0
26	UNL	J	105	12/-	0.85	0.13	63,67,71,71	0
28	DMS	v	203	4/4	0.85	0.18	67,69,76,79	0
28	DMS	B	644	4/4	0.85	0.16	52,53,61,69	0
28	DMS	C	527	4/4	0.85	0.17	73,76,79,87	0
26	UNL	z	101	6/-	0.86	0.10	49,55,55,57	0
28	DMS	C	533	4/4	0.86	0.13	72,73,73,74	0
23	SQD	a	401	54/54	0.86	0.11	39,58,82,86	0
28	DMS	v	204	4/4	0.86	0.17	48,54,57,69	0
28	DMS	U	902	4/4	0.86	0.18	35,44,49,58	0
28	DMS	c	532	4/4	0.86	0.18	65,70,76,77	0
23	SQD	A	412	54/54	0.86	0.11	41,60,78,81	0
26	UNL	B	628	15/-	0.86	0.12	45,50,60,66	0
34	LMT	B	625	24/35	0.86	0.10	48,67,86,89	0
28	DMS	V	208	4/4	0.86	0.18	75,77,82,85	0
26	UNL	D	410	37/-	0.86	0.11	42,57,93,98	0
28	DMS	B	635	4/4	0.86	0.17	90,94,95,96	0
32	HTG	B	622	19/19	0.87	0.14	28,46,54,54	0
32	HTG	b	625	19/19	0.87	0.14	30,44,66,70	0
28	DMS	B	640	4/4	0.87	0.23	45,48,49,50	0
26	UNL	b	646	6/-	0.87	0.12	54,58,60,62	0
28	DMS	u	203	4/4	0.87	0.20	47,55,56,65	0
28	DMS	c	535	4/4	0.87	0.14	58,59,65,68	0
28	DMS	O	304	4/4	0.87	0.15	63,68,72,73	0
26	UNL	D	411	16/-	0.87	0.11	39,45,58,62	0
34	LMT	m	102	35/35	0.87	0.10	34,53,58,59	0
34	LMT	B	626	24/35	0.87	0.11	37,54,86,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	DMS	o	303	4/4	0.87	0.15	66,69,75,79	0
32	HTG	V	202	13/19	0.87	0.10	45,49,70,82	0
28	DMS	v	208	4/4	0.87	0.17	89,92,92,95	0
34	LMT	T	102	24/35	0.88	0.12	36,53,78,85	0
28	DMS	o	305	4/4	0.88	0.14	73,75,77,87	0
28	DMS	C	529	4/4	0.88	0.15	70,73,74,74	0
28	DMS	C	531	4/4	0.88	0.17	53,54,58,74	0
24	LMG	a	410	51/55	0.88	0.09	44,55,65,67	0
28	DMS	B	643	4/4	0.88	0.13	51,53,62,71	0
28	DMS	A	415	4/4	0.88	0.15	55,58,65,71	0
28	DMS	D	416	4/4	0.88	0.14	83,87,89,91	0
26	UNL	I	102	16/-	0.88	0.11	38,47,63,64	0
28	DMS	O	303	4/4	0.88	0.14	63,72,77,78	0
28	DMS	v	209	4/4	0.88	0.13	71,78,79,79	0
28	DMS	o	304	4/4	0.88	0.15	68,79,82,83	0
34	LMT	M	101	35/35	0.88	0.10	34,53,63,64	0
26	UNL	i	102	11/-	0.89	0.10	48,54,64,65	0
26	UNL	d	411	16/-	0.89	0.09	33,42,55,55	0
26	UNL	J	106	4/-	0.89	0.12	57,60,61,67	0
24	LMG	B	620	51/55	0.89	0.09	33,43,55,58	0
28	DMS	v	205	4/4	0.89	0.12	67,70,72,73	0
26	UNL	X	101	16/-	0.89	0.11	37,40,59,59	0
28	DMS	C	525[A]	4/4	0.89	0.17	48,49,51,57	4
28	DMS	V	209	4/4	0.89	0.14	57,73,77,81	0
28	DMS	C	525[B]	4/4	0.89	0.17	32,33,35,35	4
24	LMG	c	519	51/55	0.90	0.11	29,59,86,88	0
28	DMS	O	307	4/4	0.90	0.15	69,76,77,88	0
24	LMG	C	519	51/55	0.90	0.11	31,67,83,84	0
28	DMS	B	645	4/4	0.90	0.13	56,59,64,71	0
20	CLA	C	513	65/65	0.90	0.09	40,48,72,77	0
28	DMS	A	416	4/4	0.90	0.12	59,60,69,77	0
24	LMG	A	407	51/55	0.90	0.09	40,55,70,78	0
28	DMS	U	903[A]	4/4	0.90	0.16	32,34,40,41	4
28	DMS	U	903[B]	4/4	0.90	0.16	26,28,29,32	4
28	DMS	B	641	4/4	0.90	0.12	68,69,75,80	0
28	DMS	V	204	4/4	0.90	0.12	58,64,64,72	0
20	CLA	C	506	65/65	0.90	0.09	32,45,86,87	0
28	DMS	c	536	4/4	0.90	0.18	33,33,45,46	0
28	DMS	V	207	4/4	0.91	0.14	62,63,63,70	0
20	CLA	b	603	65/65	0.91	0.10	30,45,75,82	0
24	LMG	b	623	49/55	0.91	0.09	33,42,54,61	0
33	CA	V	203	1/1	0.91	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	DMS	v	206	4/4	0.91	0.13	52,53,61,66	0
28	DMS	u	202	4/4	0.91	0.18	40,46,52,54	0
28	DMS	b	639	4/4	0.91	0.13	46,49,49,50	0
23	SQD	A	406	54/54	0.91	0.10	34,59,71,76	0
28	DMS	o	307	4/4	0.92	0.13	53,58,63,65	0
22	BCR	C	514	40/40	0.92	0.07	36,45,49,50	0
28	DMS	V	206	4/4	0.92	0.12	59,61,63,65	0
26	UNL	d	410	16/-	0.92	0.10	33,45,63,63	0
28	DMS	d	413	4/4	0.92	0.14	47,53,55,57	0
28	DMS	d	414	4/4	0.92	0.17	57,62,64,68	0
20	CLA	B	602	65/65	0.92	0.10	29,42,77,81	0
28	DMS	B	637	4/4	0.92	0.14	53,53,54,60	0
28	DMS	b	632	4/4	0.92	0.12	55,58,66,70	0
32	HTG	b	601	19/19	0.92	0.09	45,61,67,80	0
28	DMS	c	529	4/4	0.92	0.11	79,82,86,87	0
28	DMS	C	530	4/4	0.92	0.17	44,44,46,50	0
28	DMS	b	635	4/4	0.92	0.12	58,62,69,73	0
28	DMS	h	102	4/4	0.93	0.15	50,51,53,62	0
33	CA	o	301	1/1	0.93	0.06	48,48,48,48	0
28	DMS	i	104	4/4	0.93	0.11	63,66,67,71	0
28	DMS	C	526	4/4	0.93	0.13	59,60,63,65	0
32	HTG	B	631	19/19	0.93	0.08	41,57,69,73	0
20	CLA	C	512	55/65	0.93	0.07	37,44,49,54	0
28	DMS	D	413	4/4	0.93	0.11	50,56,60,61	0
22	BCR	K	101	40/40	0.93	0.07	33,37,42,45	0
22	BCR	k	102	40/40	0.93	0.07	41,46,51,51	0
28	DMS	c	530	4/4	0.93	0.20	36,43,45,49	0
35	DGD	h	101	62/66	0.93	0.08	25,34,41,49	0
20	CLA	b	618	65/65	0.93	0.09	23,33,92,98	0
22	BCR	D	405	40/40	0.94	0.07	26,30,58,60	0
20	CLA	c	513	65/65	0.94	0.08	36,46,81,87	0
31	BCT	A	421	4/4	0.94	0.07	31,34,40,44	0
31	BCT	a	413	4/4	0.94	0.07	32,32,38,42	0
32	HTG	B	621	19/19	0.94	0.08	36,41,48,52	0
22	BCR	K	102	40/40	0.94	0.07	31,36,40,41	0
22	BCR	d	405	40/40	0.94	0.07	24,30,56,58	0
28	DMS	F	102	4/4	0.94	0.12	51,52,56,64	0
23	SQD	a	409	54/54	0.94	0.09	33,56,75,78	0
22	BCR	k	101	40/40	0.94	0.07	28,36,41,42	0
28	DMS	c	528	4/4	0.94	0.13	58,62,63,65	0
20	CLA	c	506	65/65	0.94	0.07	24,39,71,74	0
28	DMS	b	633	4/4	0.94	0.12	45,48,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	DGD	H	102	62/66	0.94	0.08	25,33,40,43	0
28	DMS	c	531	4/4	0.94	0.11	73,78,85,86	0
32	HTG	O	302	19/19	0.94	0.08	34,42,50,53	0
36	LHG	D	407	49/49	0.94	0.07	28,37,44,52	0
36	LHG	D	409	49/49	0.94	0.10	27,33,81,83	0
22	BCR	t	101	40/40	0.94	0.06	22,29,41,43	0
38	RRX	H	101	41/41	0.94	0.07	27,31,41,46	0
38	RRX	x	101	41/41	0.94	0.07	26,32,47,58	0
20	CLA	C	505	65/65	0.95	0.06	28,33,44,48	0
20	CLA	B	601	65/65	0.95	0.08	23,29,82,86	0
20	CLA	c	511	65/65	0.95	0.06	27,33,40,43	0
20	CLA	c	512	65/65	0.95	0.07	28,41,70,72	0
28	DMS	D	414	4/4	0.95	0.12	55,56,57,58	0
20	CLA	C	507	65/65	0.95	0.07	28,37,52,57	0
35	DGD	C	517	55/66	0.95	0.06	26,34,59,62	0
24	LMG	j	101	45/55	0.95	0.07	27,32,60,64	0
20	CLA	C	508	60/65	0.95	0.06	23,31,47,51	0
35	DGD	c	517	62/66	0.95	0.07	23,30,56,71	0
22	BCR	C	515	40/40	0.95	0.06	31,37,43,45	0
20	CLA	C	511	65/65	0.95	0.07	30,37,42,45	0
20	CLA	B	610	65/65	0.95	0.06	26,31,35,38	0
20	CLA	C	503	65/65	0.95	0.06	28,33,37,42	0
22	BCR	T	101	40/40	0.95	0.06	24,32,43,45	0
20	CLA	C	504	65/65	0.95	0.07	27,30,59,61	0
20	CLA	b	608	65/65	0.95	0.07	24,31,59,63	0
20	CLA	c	507	65/65	0.96	0.07	25,30,49,57	0
20	CLA	c	508	60/65	0.96	0.06	24,28,52,54	0
28	DMS	b	631	4/4	0.96	0.09	23,24,27,35	0
33	CA	O	301	1/1	0.96	0.05	47,47,47,47	0
20	CLA	c	509	65/65	0.96	0.07	25,30,53,58	0
20	CLA	C	509	65/65	0.96	0.07	29,34,52,55	0
28	DMS	v	202	4/4	0.96	0.11	50,51,53,55	0
20	CLA	C	510	65/65	0.96	0.06	26,31,38,44	0
20	CLA	C	502	65/65	0.96	0.06	24,29,41,48	0
22	BCR	A	405	40/40	0.96	0.05	21,26,32,35	0
22	BCR	B	618	40/40	0.96	0.06	21,28,42,45	0
24	LMG	J	101	45/55	0.96	0.07	27,32,64,70	0
22	BCR	B	619	40/40	0.96	0.06	22,30,42,44	0
20	CLA	B	607	65/65	0.96	0.07	22,29,55,62	0
20	CLA	B	603	65/65	0.96	0.06	23,28,35,39	0
27	PL9	D	412	55/55	0.96	0.05	19,23,29,34	0
20	CLA	B	611	65/65	0.96	0.06	21,26,34,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
27	PL9	d	412	55/55	0.96	0.05	18,23,29,35	0
20	CLA	b	604	65/65	0.96	0.06	23,27,33,35	0
20	CLA	B	615	65/65	0.96	0.07	20,24,70,79	0
20	CLA	b	611	65/65	0.96	0.06	24,30,34,41	0
22	BCR	a	408	40/40	0.96	0.05	21,25,30,31	0
22	BCR	b	619	40/40	0.96	0.05	23,26,32,35	0
35	DGD	C	516	62/66	0.96	0.07	22,32,74,79	0
22	BCR	b	620	40/40	0.96	0.05	22,27,43,46	0
35	DGD	C	518	62/66	0.96	0.07	24,30,62,73	0
22	BCR	c	514	40/40	0.96	0.06	28,36,39,39	0
20	CLA	b	612	65/65	0.96	0.06	21,27,36,41	0
35	DGD	c	515	62/66	0.96	0.07	23,32,71,75	0
35	DGD	c	516	57/66	0.96	0.06	27,32,62,68	0
22	BCR	j	102	40/40	0.96	0.06	30,35,42,45	0
20	CLA	b	616	65/65	0.96	0.07	20,26,73,80	0
20	CLA	B	616	65/65	0.96	0.06	25,29,48,52	0
20	CLA	c	501	65/65	0.96	0.06	26,30,41,48	0
20	CLA	c	503	65/65	0.96	0.06	25,35,40,43	0
20	CLA	c	504	65/65	0.96	0.06	25,29,55,60	0
36	LHG	d	406	49/49	0.96	0.06	29,36,43,48	0
36	LHG	d	408	49/49	0.96	0.09	24,31,83,88	0
20	CLA	c	505	65/65	0.96	0.06	25,30,46,50	0
20	CLA	C	501	65/65	0.96	0.06	27,33,45,52	0
21	PHO	A	403	64/64	0.97	0.04	18,22,24,25	0
21	PHO	D	403	64/64	0.97	0.04	18,24,29,35	0
21	PHO	a	405	64/64	0.97	0.04	17,20,22,25	0
21	PHO	a	406	64/64	0.97	0.04	19,24,29,32	0
20	CLA	b	610	65/65	0.97	0.05	20,26,31,33	0
22	BCR	B	617	40/40	0.97	0.05	22,26,32,33	0
20	CLA	B	608	65/65	0.97	0.05	18,21,34,39	0
20	CLA	B	609	65/65	0.97	0.04	22,25,31,33	0
20	CLA	b	613	65/65	0.97	0.05	20,22,38,44	0
20	CLA	b	614	65/65	0.97	0.05	21,25,31,37	0
20	CLA	A	402	59/65	0.97	0.05	18,22,52,58	0
20	CLA	b	617	65/65	0.97	0.05	23,30,44,50	0
20	CLA	B	604	65/65	0.97	0.05	21,24,33,39	0
20	CLA	B	612	65/65	0.97	0.05	19,22,36,42	0
20	CLA	c	502	65/65	0.97	0.06	22,26,39,48	0
20	CLA	D	401	65/65	0.97	0.05	16,20,35,41	0
20	CLA	D	404	65/65	0.97	0.07	26,29,77,81	0
22	BCR	b	621	40/40	0.97	0.05	27,32,42,44	0
20	CLA	a	403	65/65	0.97	0.05	17,20,29,38	0

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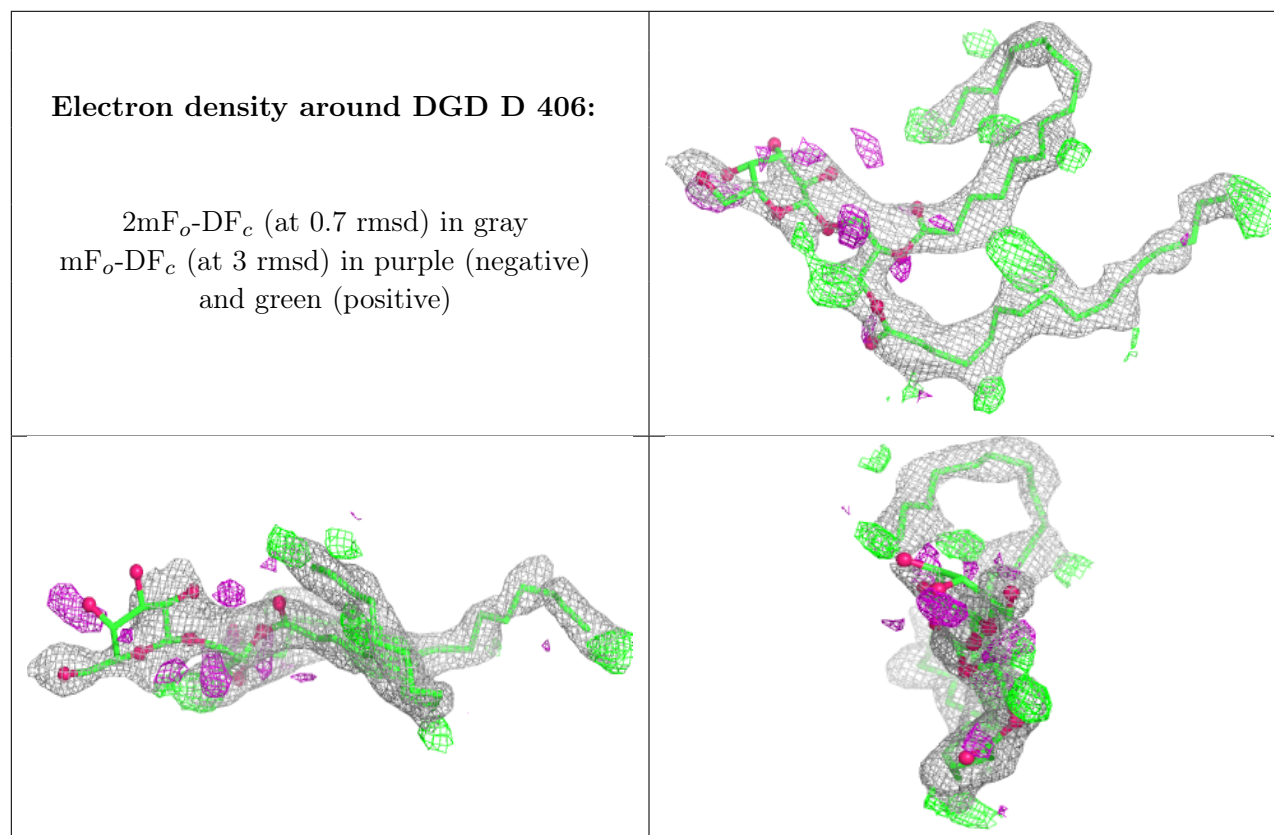
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	a	407	47/65	0.97	0.05	19,22,41,48	0
20	CLA	B	613	65/65	0.97	0.05	21,25,30,34	0
20	CLA	B	606	65/65	0.97	0.05	19,24,35,37	0
33	CA	b	626	1/1	0.97	0.06	42,42,42,42	0
36	LHG	D	408	49/49	0.97	0.06	23,30,44,49	0
20	CLA	b	605	65/65	0.97	0.05	21,25,34,37	0
20	CLA	c	510	65/65	0.97	0.05	23,29,39,42	0
36	LHG	L	101	49/49	0.97	0.06	24,31,49,53	0
20	CLA	b	606	65/65	0.97	0.05	20,24,54,59	0
36	LHG	d	407	49/49	0.97	0.06	22,27,46,50	0
20	CLA	A	404	65/65	0.97	0.07	20,25,88,90	0
36	LHG	l	102	49/49	0.97	0.06	22,30,51,54	0
37	HEM	E	104	43/43	0.97	0.08	39,44,52,56	0
37	HEM	e	102	43/43	0.97	0.08	34,41,56,68	0
20	CLA	b	609	65/65	0.97	0.05	19,22,33,37	0
20	CLA	d	404	65/65	0.97	0.07	24,29,78,87	0
20	CLA	b	615	65/65	0.98	0.05	18,22,53,59	0
20	CLA	D	402	65/65	0.98	0.04	15,19,30,36	0
20	CLA	B	605	65/65	0.98	0.06	19,23,55,58	0
33	CA	c	522	1/1	0.98	0.05	41,41,41,41	0
28	DMS	B	634	4/4	0.98	0.07	23,24,25,26	0
20	CLA	d	402	65/65	0.98	0.04	16,20,35,41	0
20	CLA	d	403	65/65	0.98	0.04	17,19,27,34	0
20	CLA	B	614	65/65	0.98	0.04	19,22,48,53	0
28	DMS	c	527	4/4	0.98	0.06	33,33,34,38	0
20	CLA	a	404	60/65	0.98	0.06	18,22,66,75	0
20	CLA	b	607	65/65	0.98	0.05	20,24,33,35	0
28	DMS	C	528	4/4	0.98	0.07	33,37,39,41	0
28	DMS	o	302	4/4	0.98	0.08	20,28,31,36	0
20	CLA	A	401	65/65	0.98	0.04	16,19,30,36	0
33	CA	B	624	1/1	0.98	0.11	43,43,43,43	0
39	MG	J	102	1/1	0.98	0.05	33,33,33,33	0
40	HEC	v	201	43/43	0.98	0.06	25,29,34,37	0
25	CL	A	409	1/1	0.99	0.03	22,22,22,22	0
28	DMS	A	414	4/4	0.99	0.06	25,28,28,29	0
29	FE2	A	419	1/1	0.99	0.02	29,29,29,29	0
29	FE2	a	417	1/1	0.99	0.02	27,27,27,27	0
39	MG	j	103	1/1	0.99	0.08	31,31,31,31	0
40	HEC	V	201	43/43	0.99	0.04	21,23,27,31	0
25	CL	a	412	1/1	0.99	0.03	24,24,24,24	0
25	CL	A	408	1/1	1.00	0.01	22,22,22,22	0
30	OEX	A	420	10/10	1.00	0.03	21,23,24,24	0

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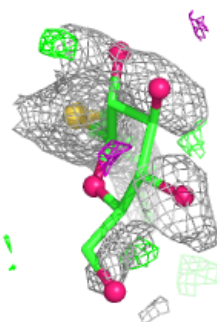
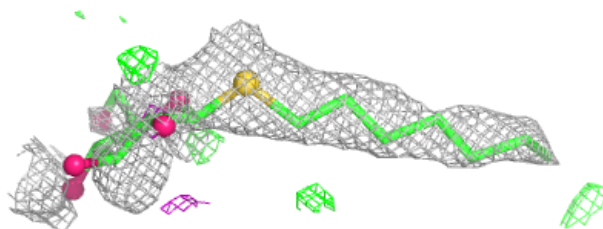
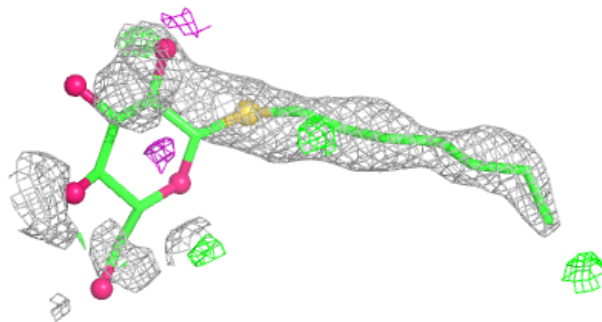
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	OEX	a	419	10/10	1.00	0.02	21,24,26,26	0
25	CL	a	411	1/1	1.00	0.03	22,22,22,22	0

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.

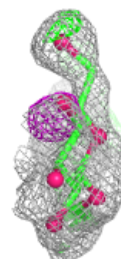
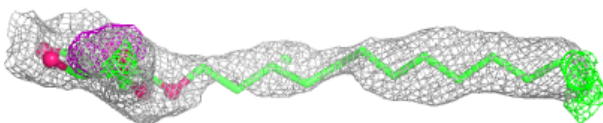
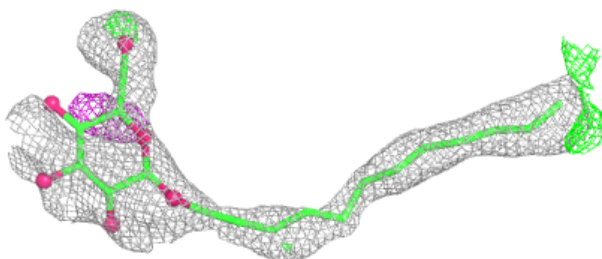


Electron density around HTG C 534:

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

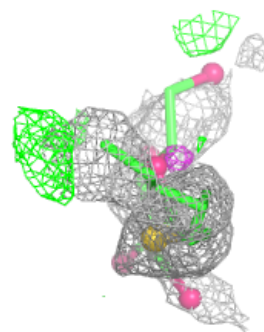
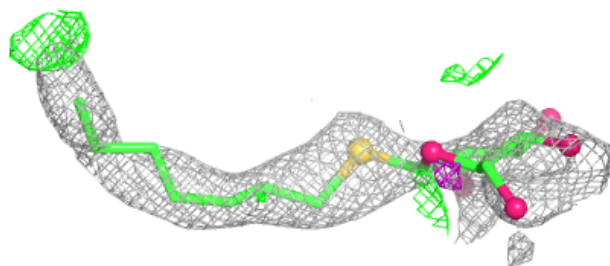
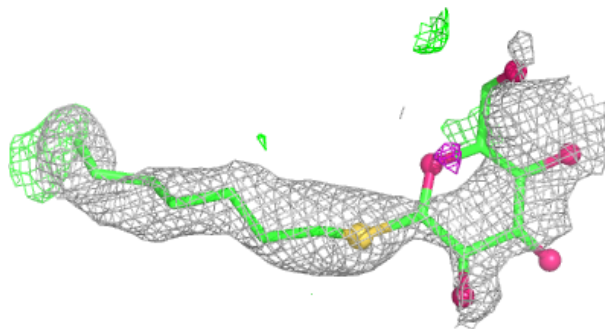
**Electron density around LMT f 102:**

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

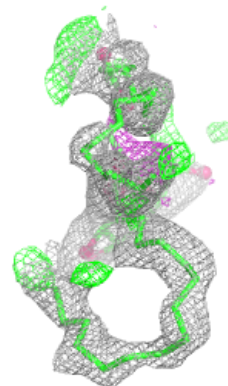
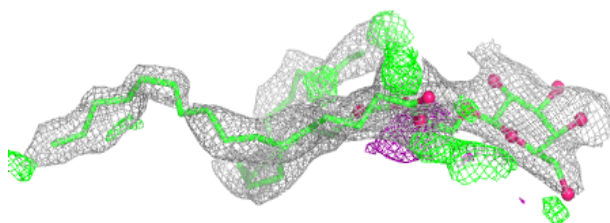
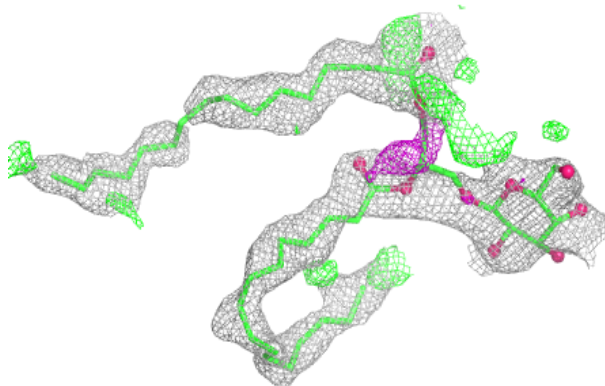


Electron density around HTG D 417:

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

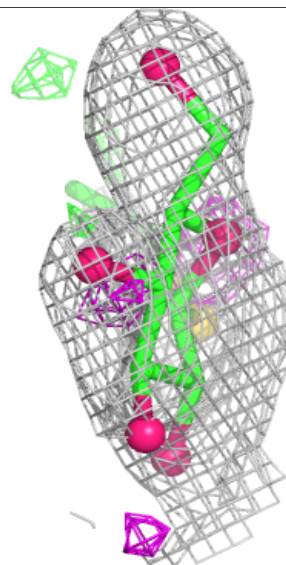
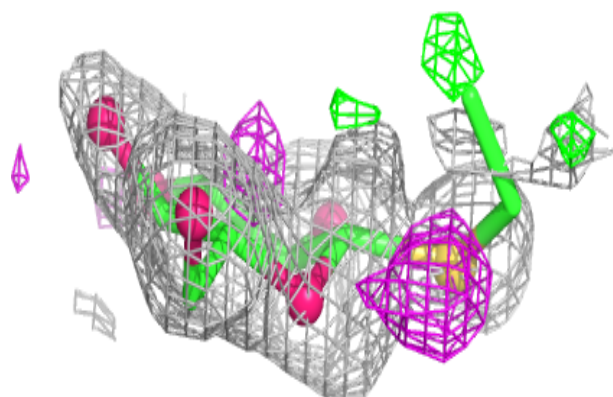
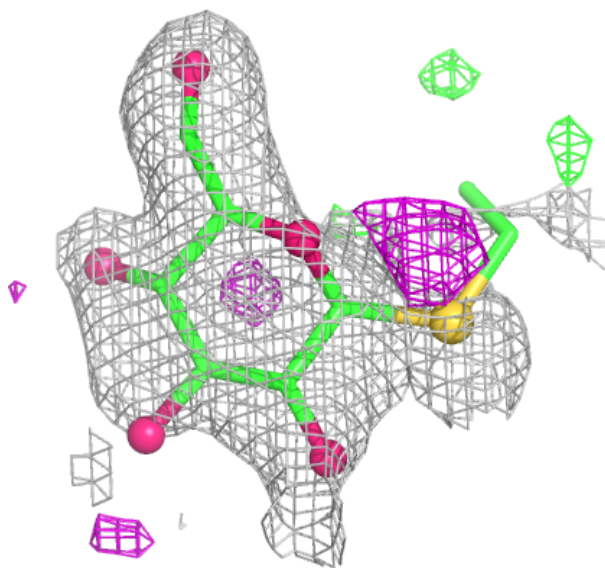
**Electron density around DGD d 416:**

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



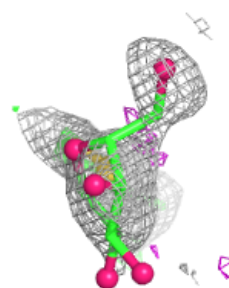
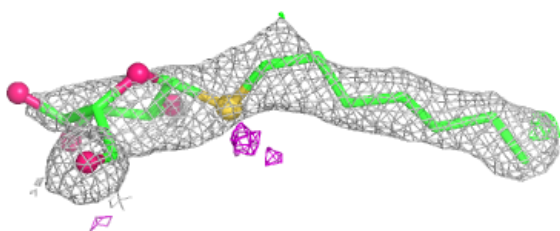
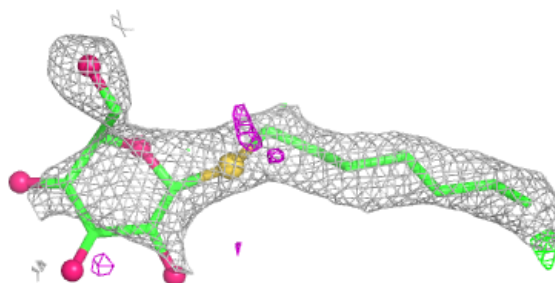
Electron density around HTG v 210:

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

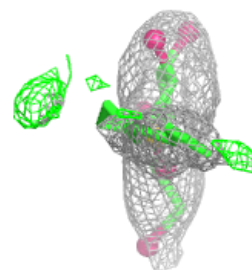
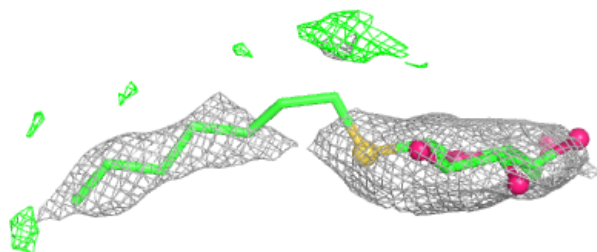
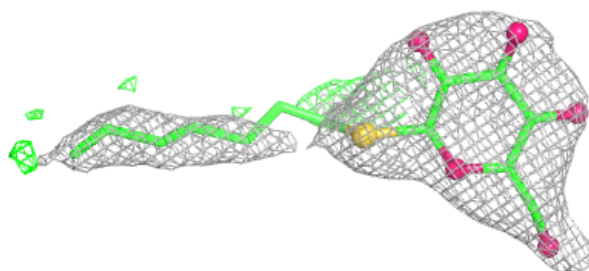


Electron density around HTG c 521:

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

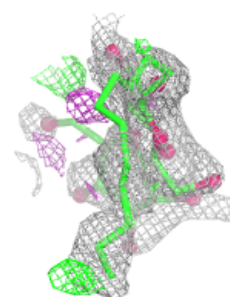
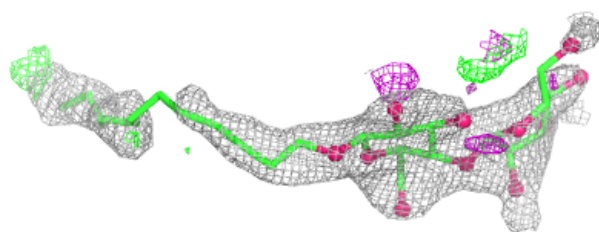
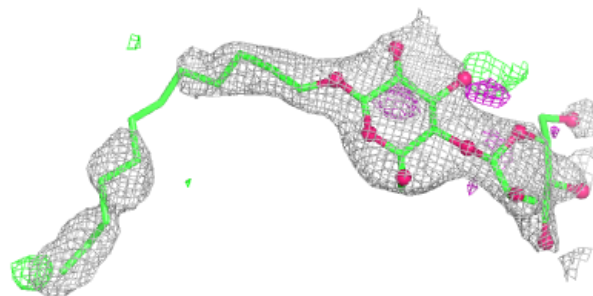
**Electron density around HTG c 520:**

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

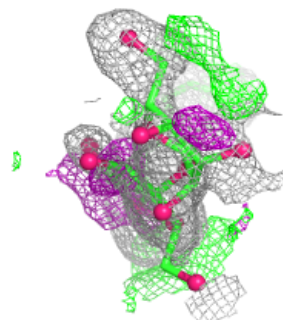
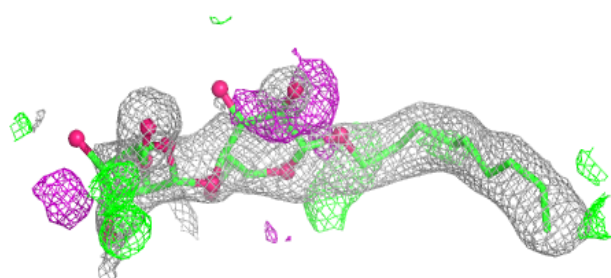
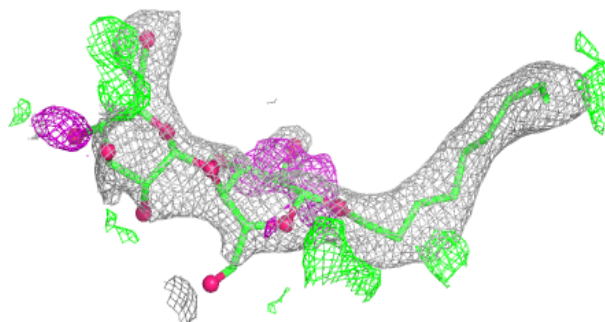


Electron density around LMT I 101:

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

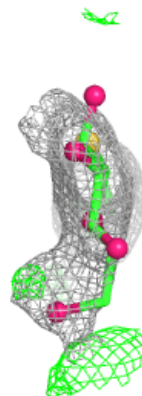
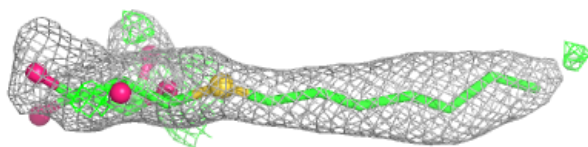
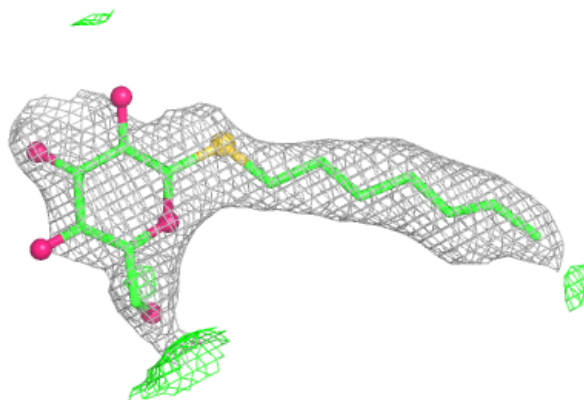
**Electron density around LMT b 627:**

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



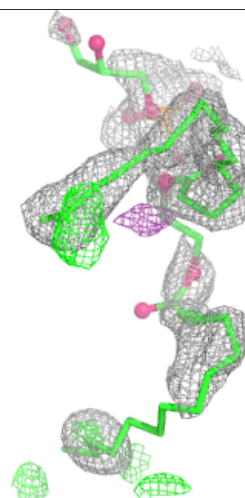
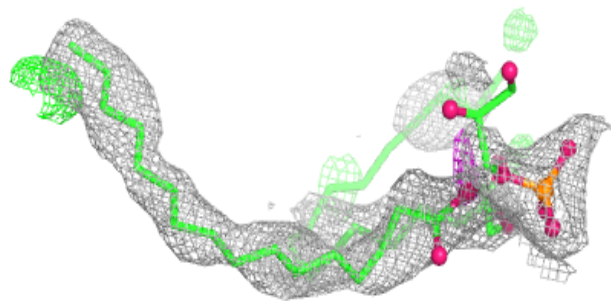
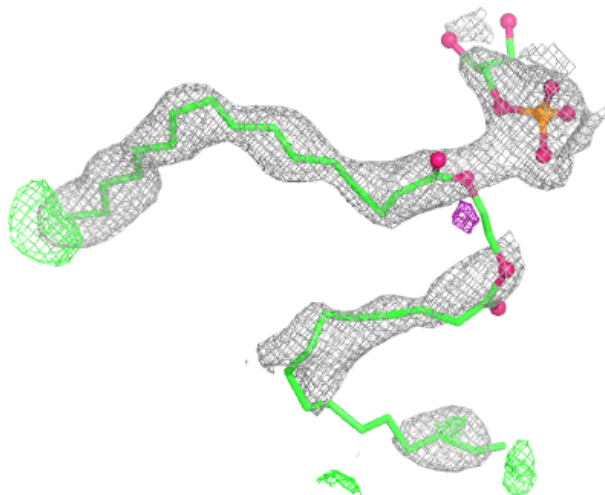
Electron density around HTG b 602:

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



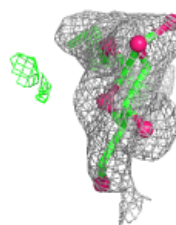
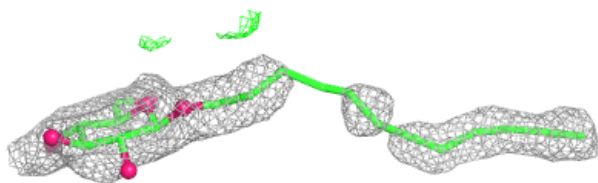
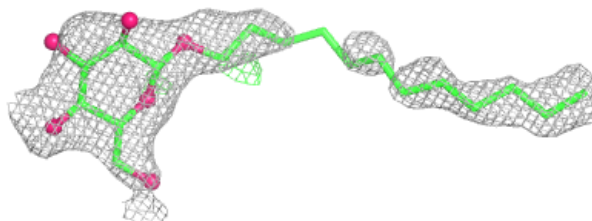
Electron density around LHG E 103:

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

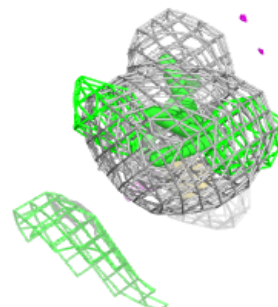
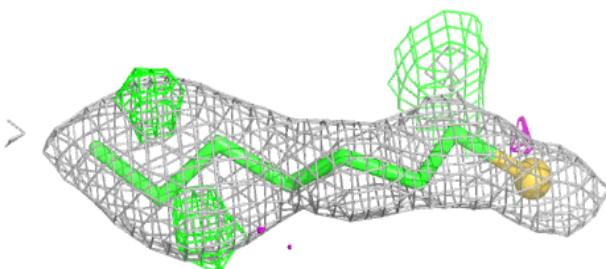
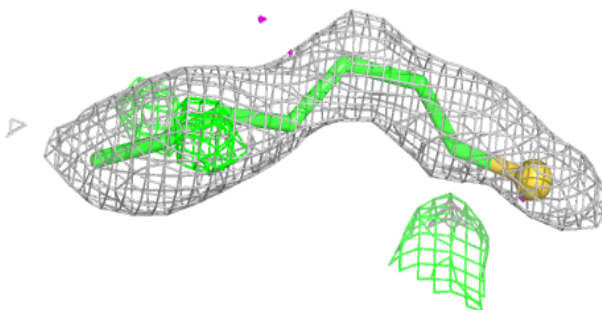


Electron density around LMT E 101:

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

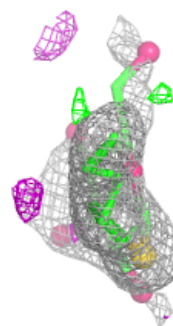
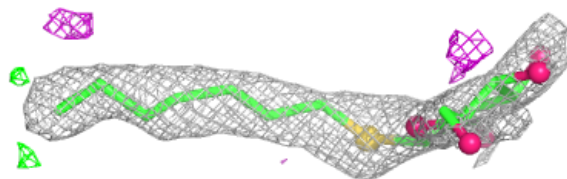
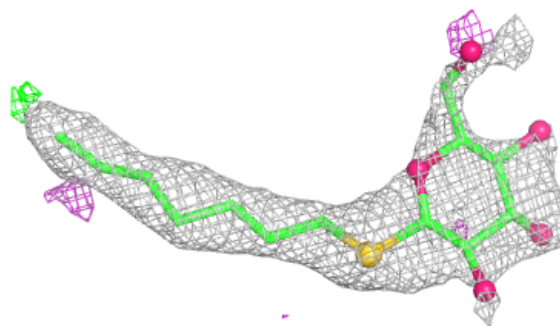
**Electron density around HTG u 201:**

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

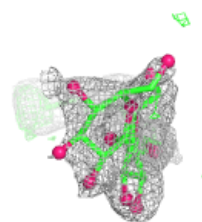
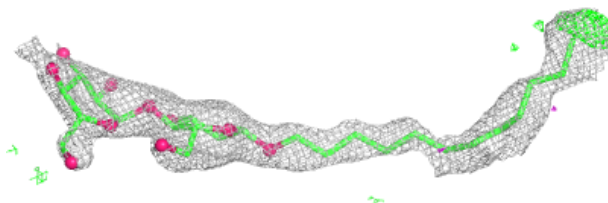
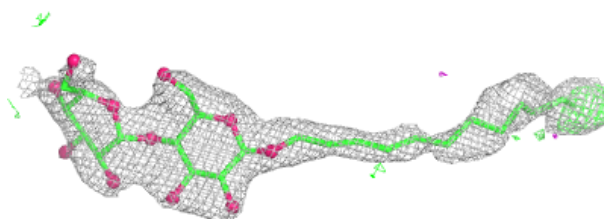


Electron density around HTG B 623:

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

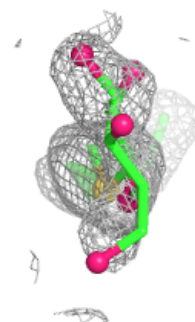
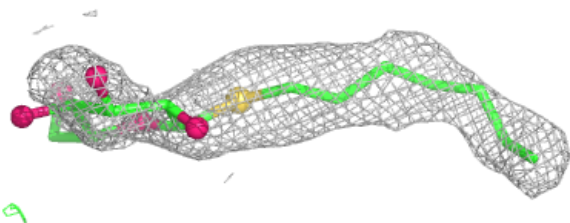
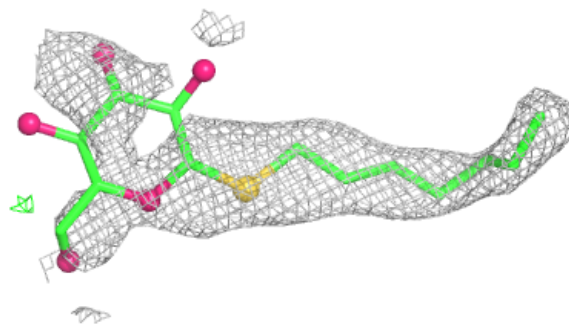
**Electron density around LMT c 523:**

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

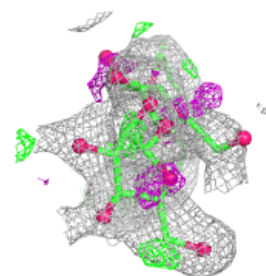
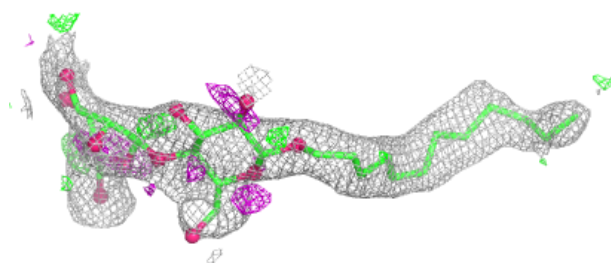
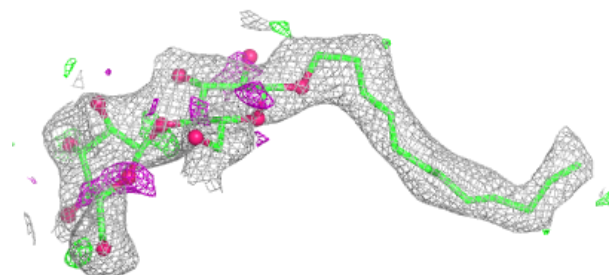


Electron density around HTG d 401:

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

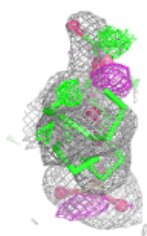
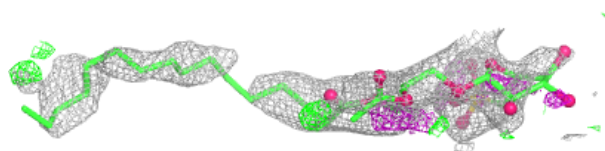
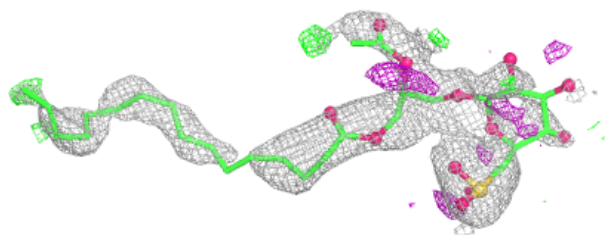
**Electron density around LMT a 418:**

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

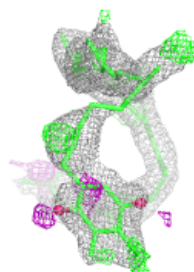
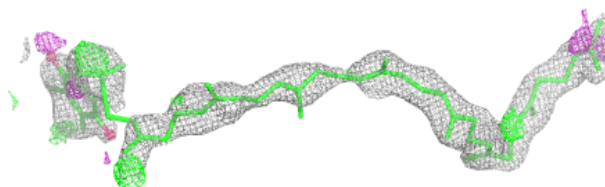
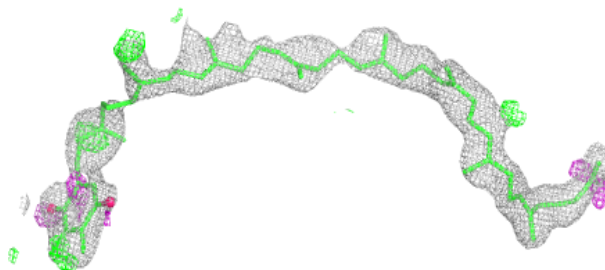


Electron density around SQD f 101:

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

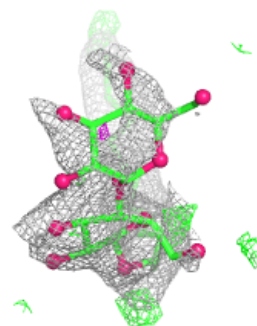
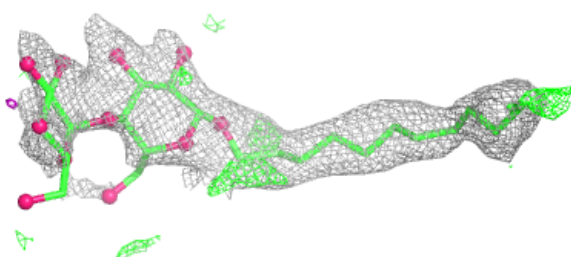
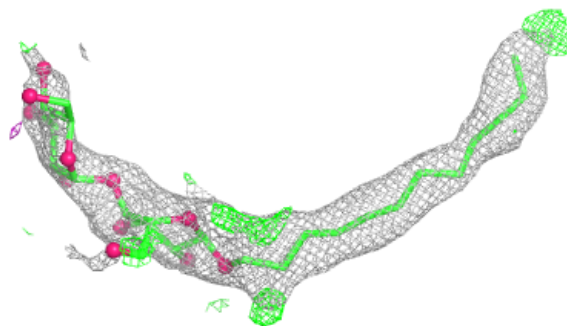
**Electron density around PL9 A 411:**

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

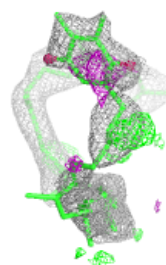
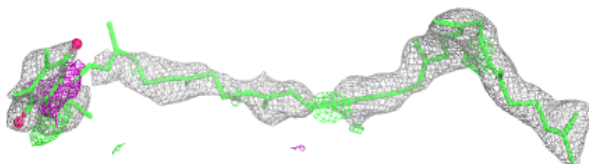
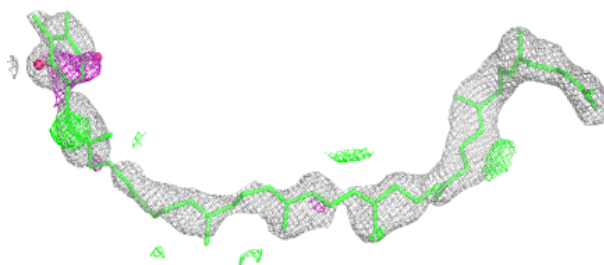


Electron density around LMT m 101:

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

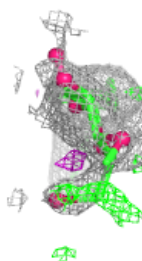
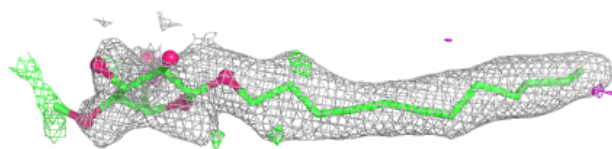
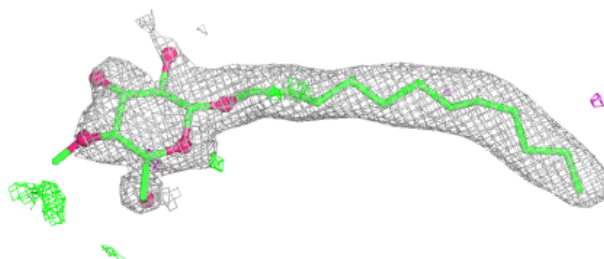
**Electron density around PL9 a 415:**

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

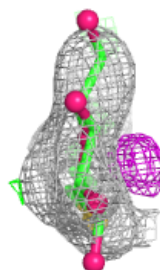
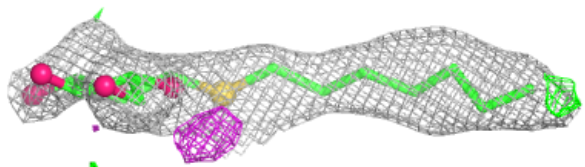
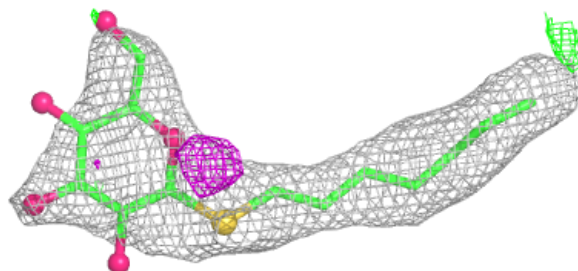


Electron density around LMT b 628:

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

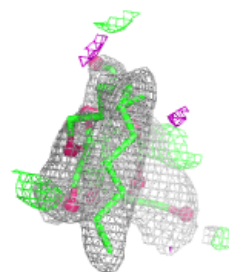
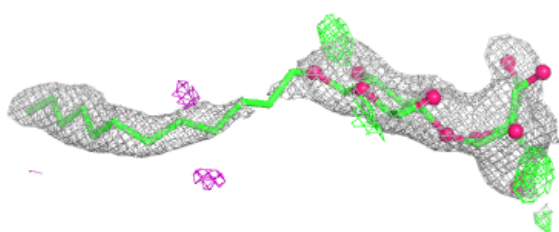
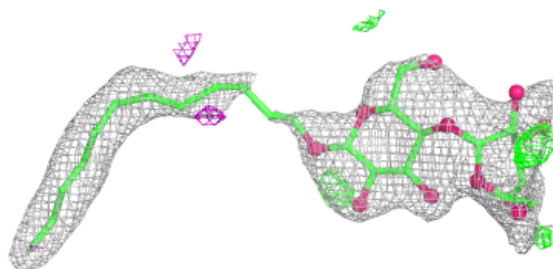
**Electron density around HTG B 632:**

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

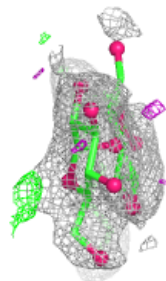
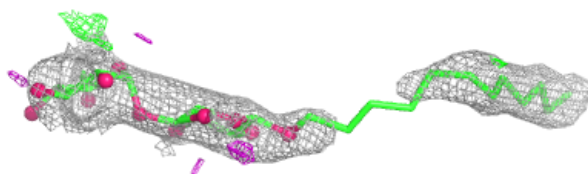
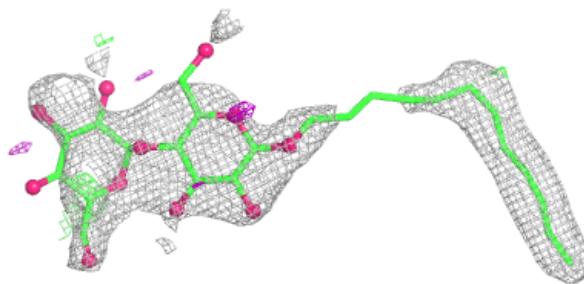


Electron density around LMT z 102:

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

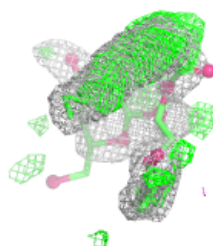
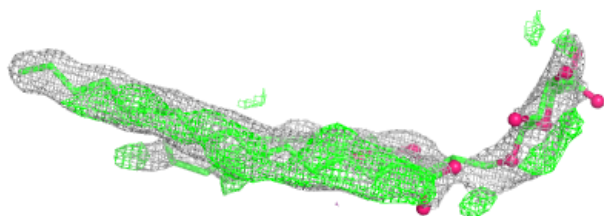
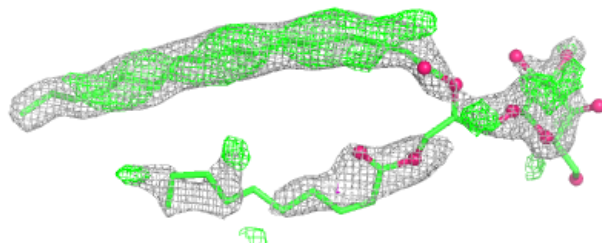
**Electron density around LMT Z 101:**

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

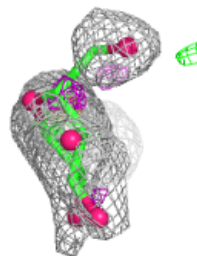
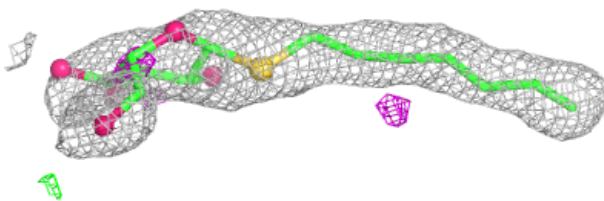
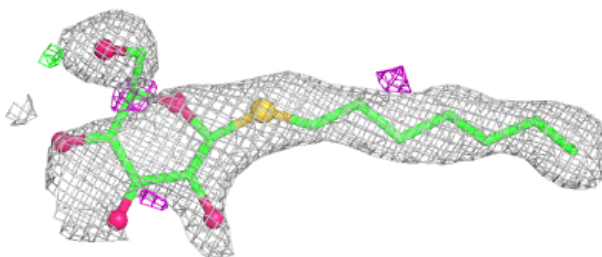


Electron density around LMG C 524:

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

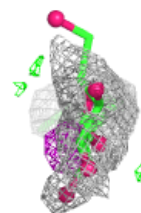
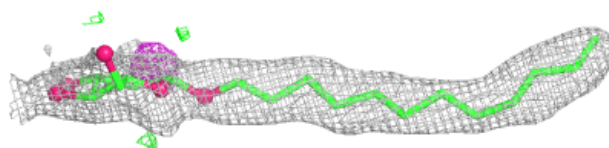
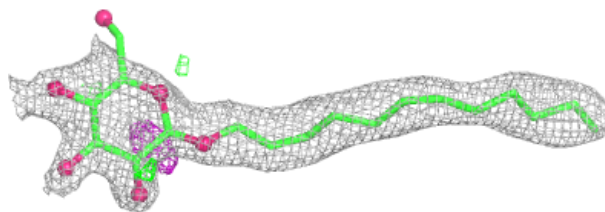
**Electron density around HTG C 521:**

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

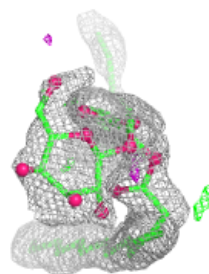
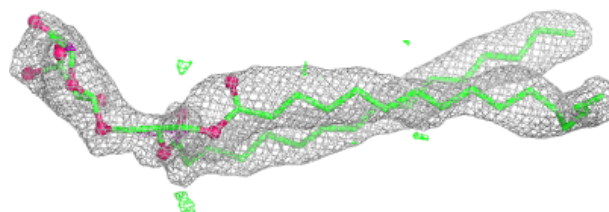
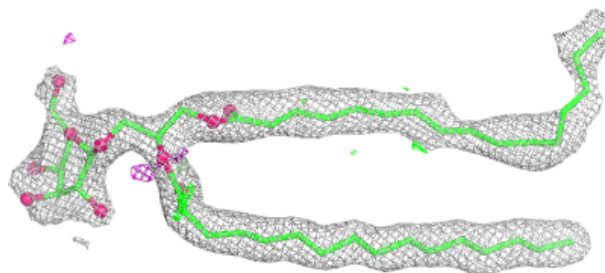


Electron density around LMT J 103:

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

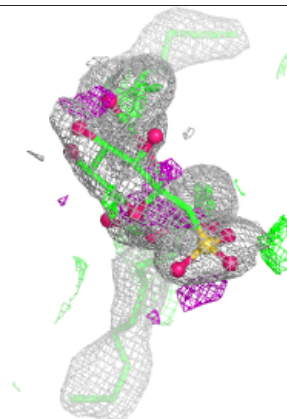
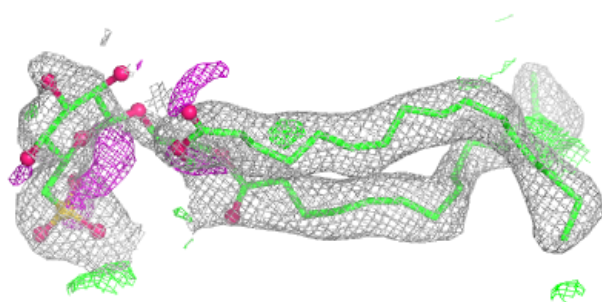
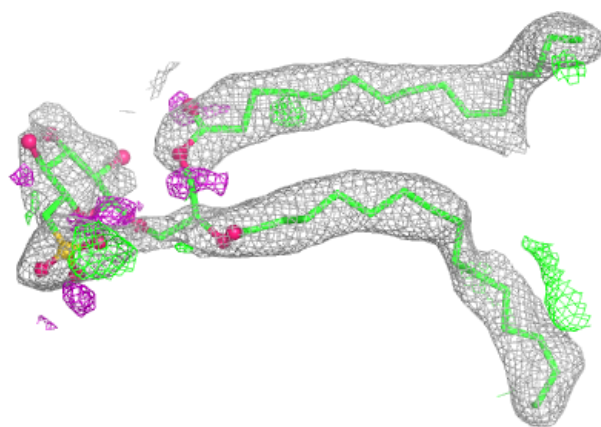
**Electron density around LMG c 518:**

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

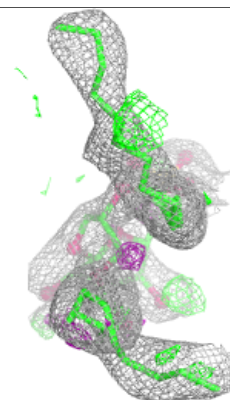
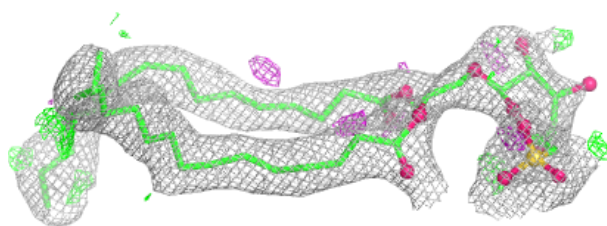
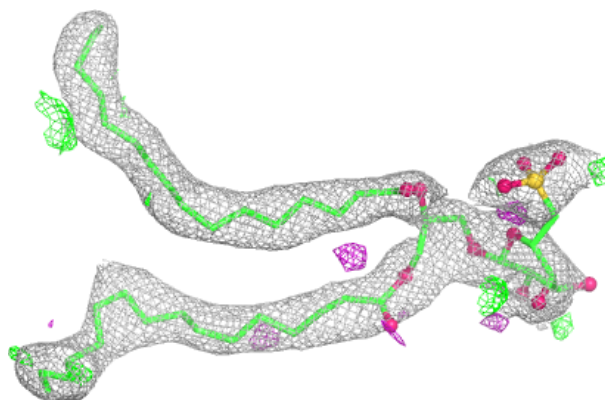


Electron density around SQD 1 101:

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

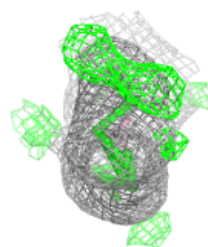
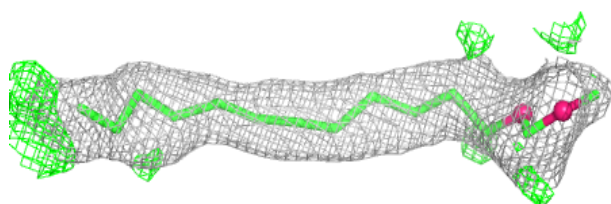
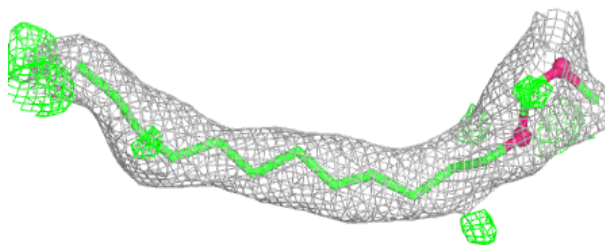
**Electron density around SQD b 622:**

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

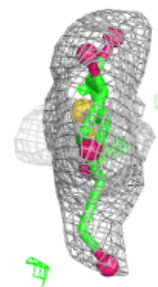
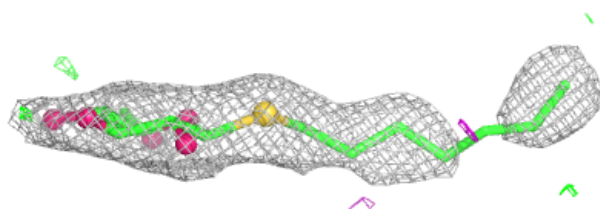
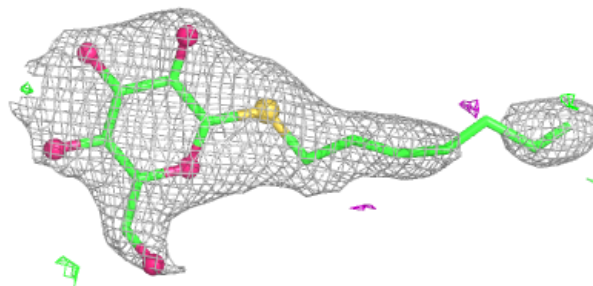


Electron density around LMT B 627:

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

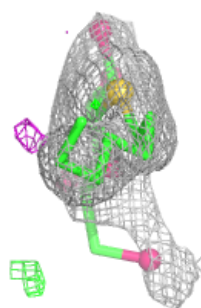
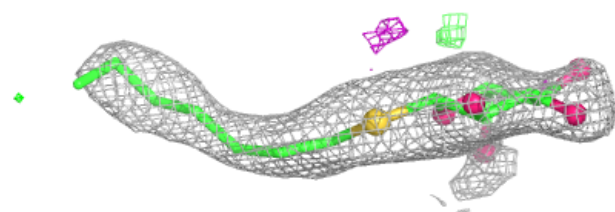
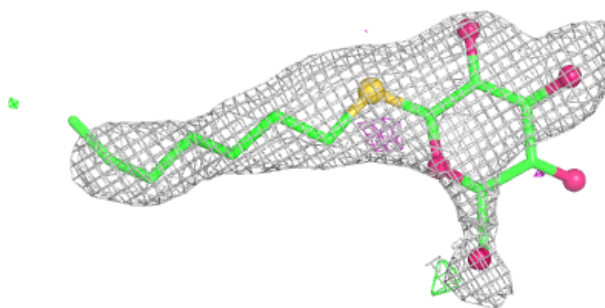
**Electron density around HTG C 520:**

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

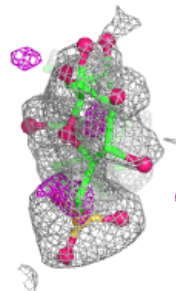
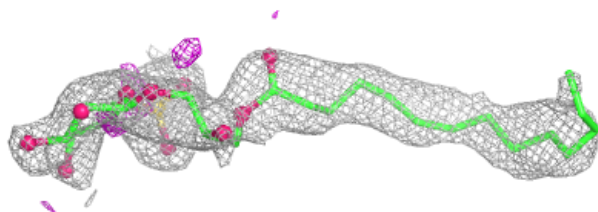
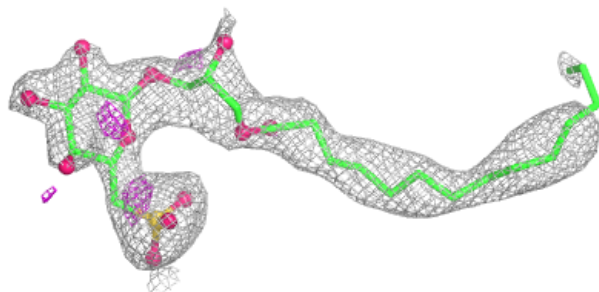


Electron density around HTG C 522:

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

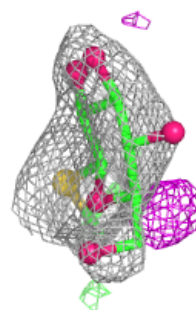
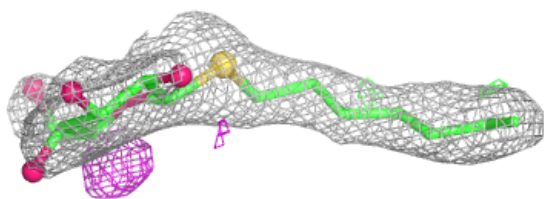
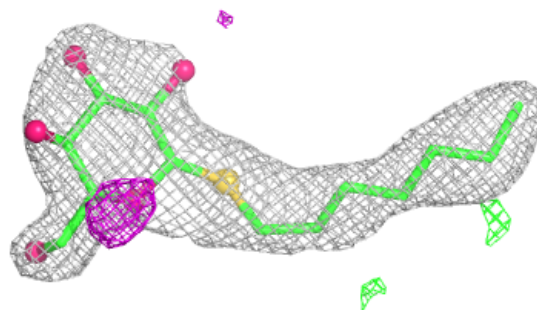
**Electron density around SQD F 101:**

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

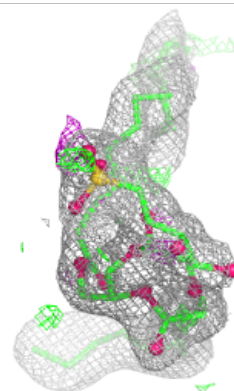
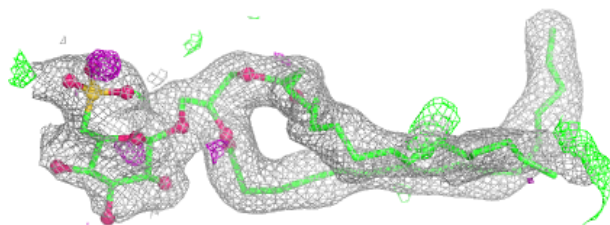
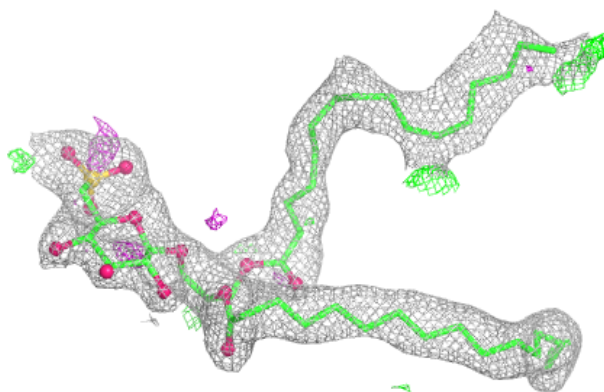


Electron density around HTG b 624:

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

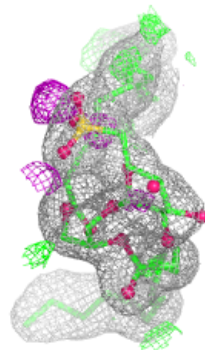
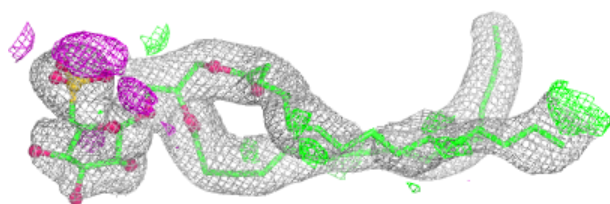
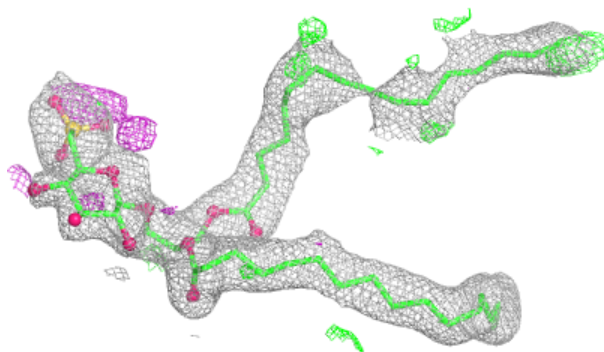
**Electron density around SQD a 401:**

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

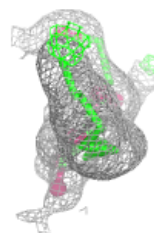
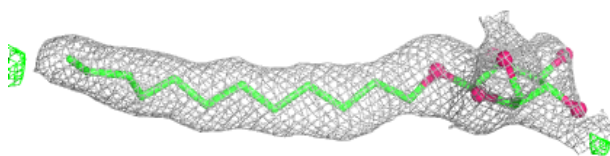
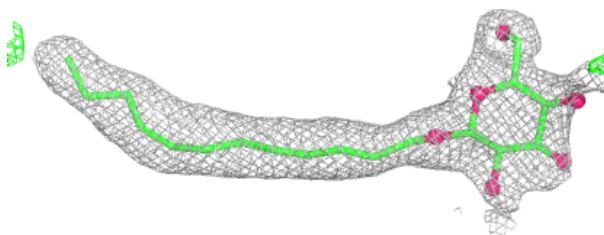


Electron density around SQD A 412:

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

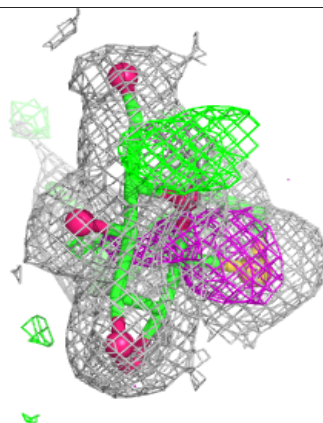
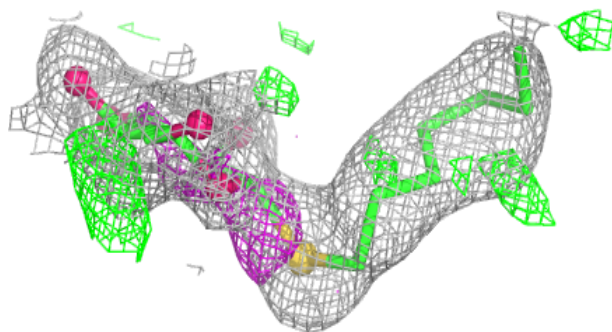
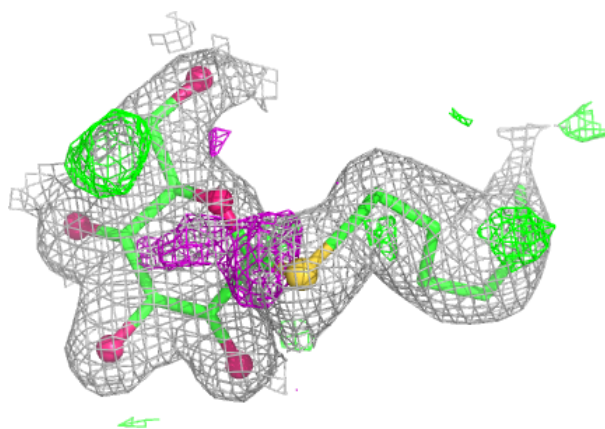
**Electron density around LMT B 625:**

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

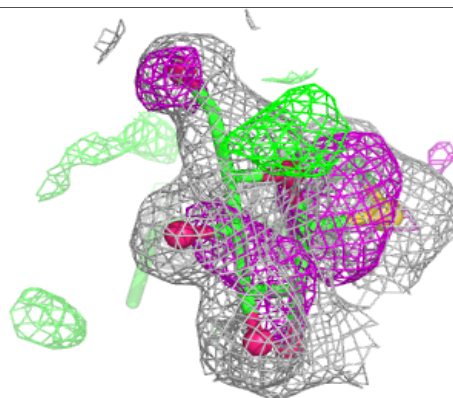
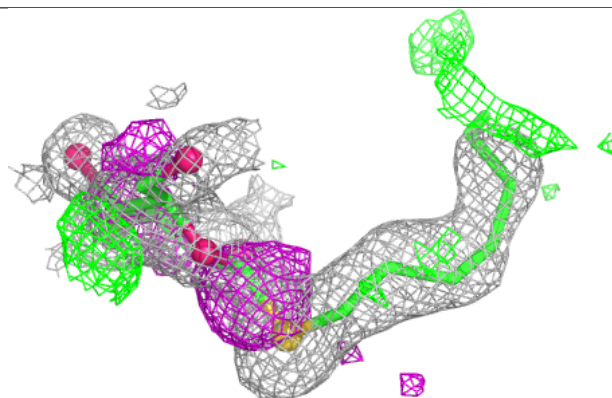
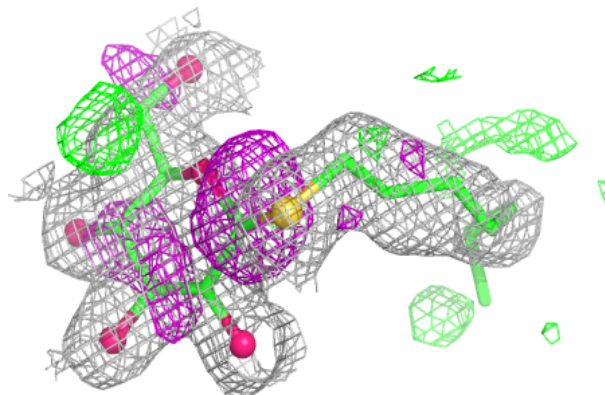


Electron density around HTG B 622:

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

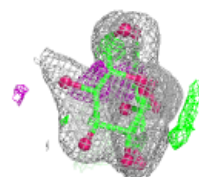
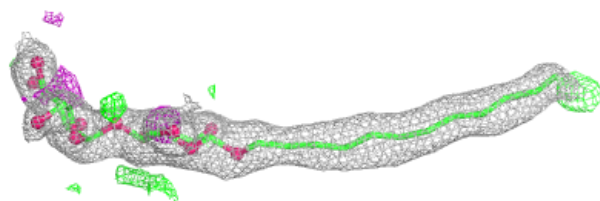
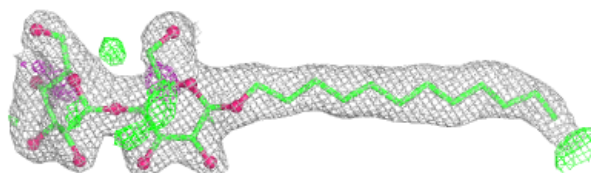
**Electron density around HTG b 625:**

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

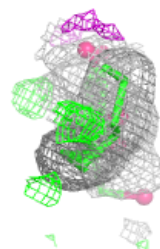
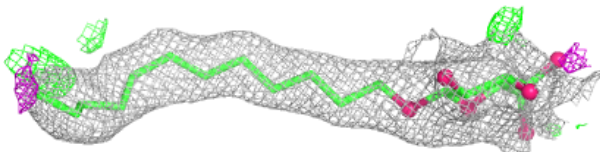
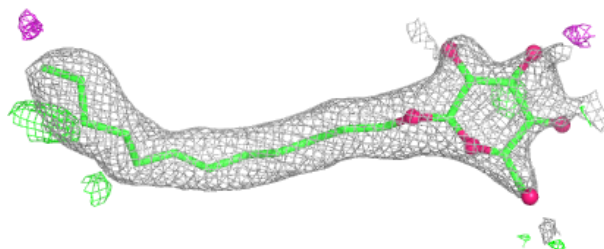


Electron density around LMT m 102:

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

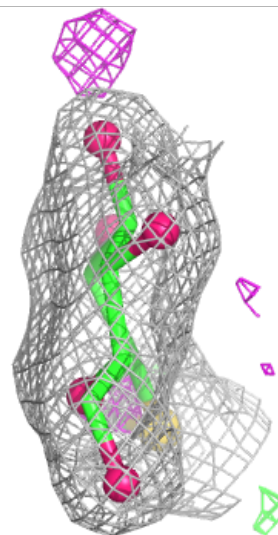
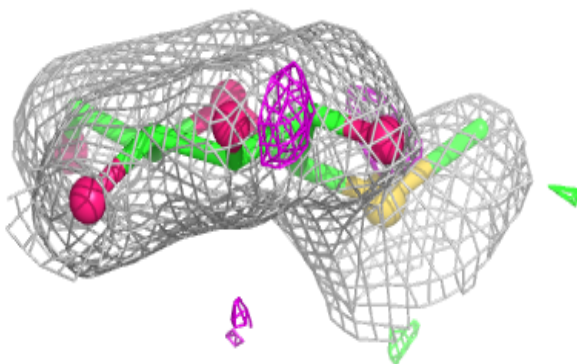
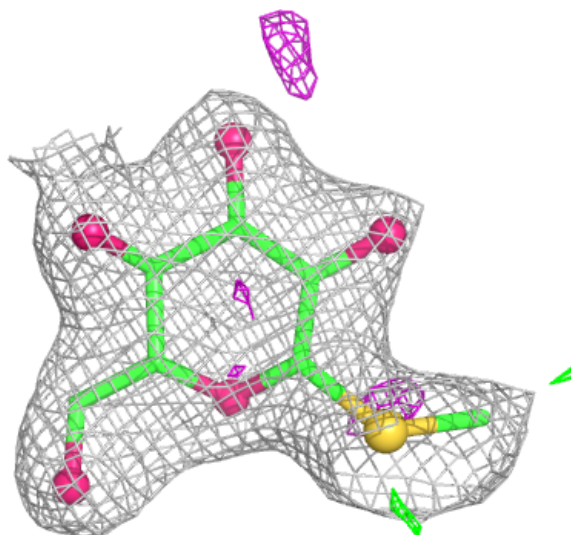
**Electron density around LMT B 626:**

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



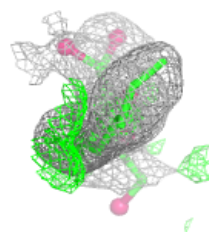
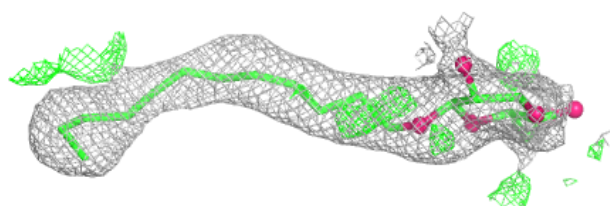
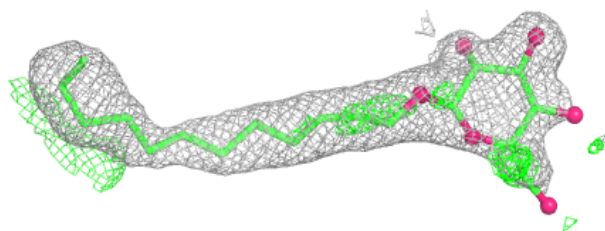
Electron density around HTG V 202:

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

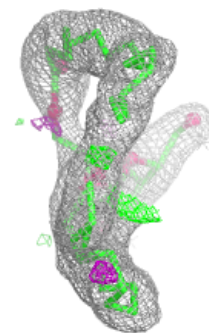
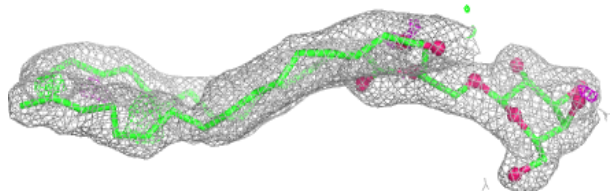
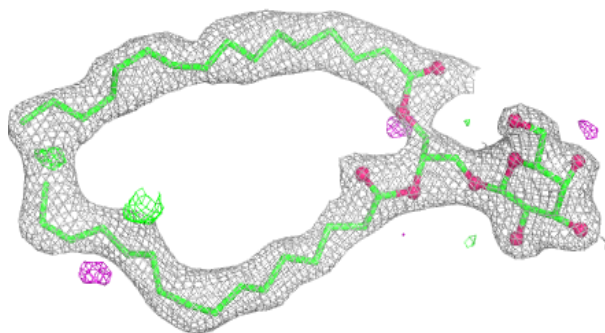


Electron density around LMT T 102:

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

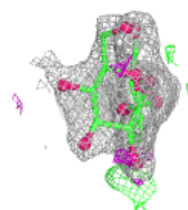
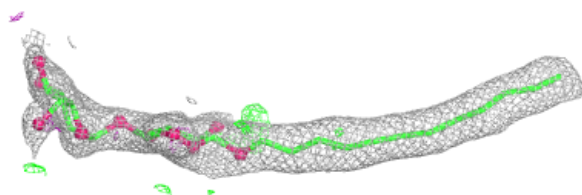
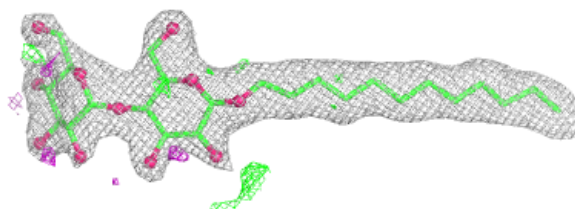
**Electron density around LMG a 410:**

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

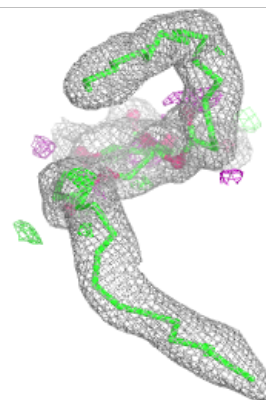
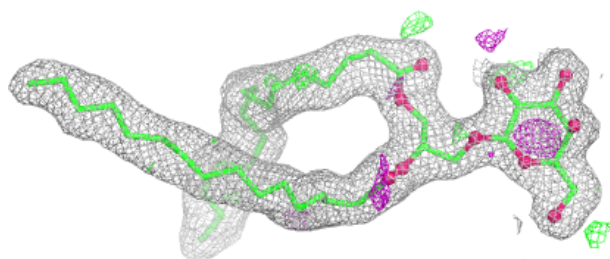
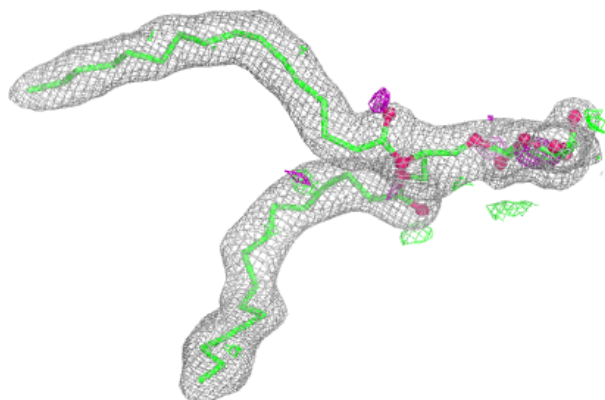


Electron density around LMT M 101:

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

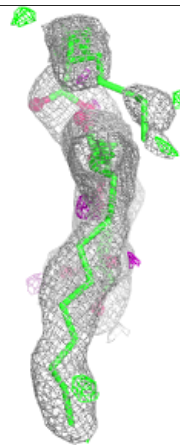
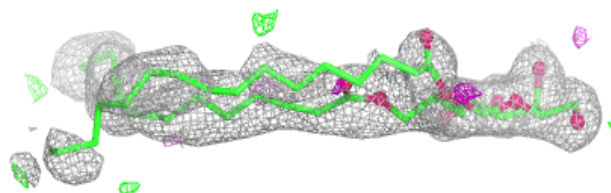
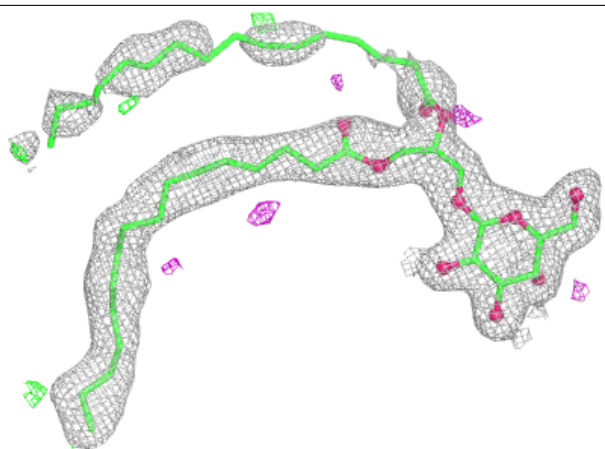
**Electron density around LMG B 620:**

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



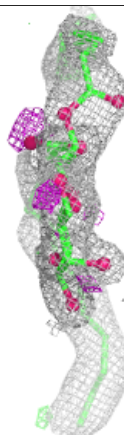
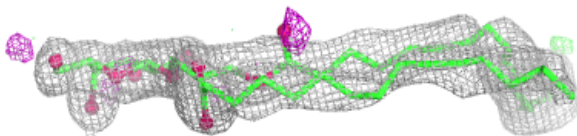
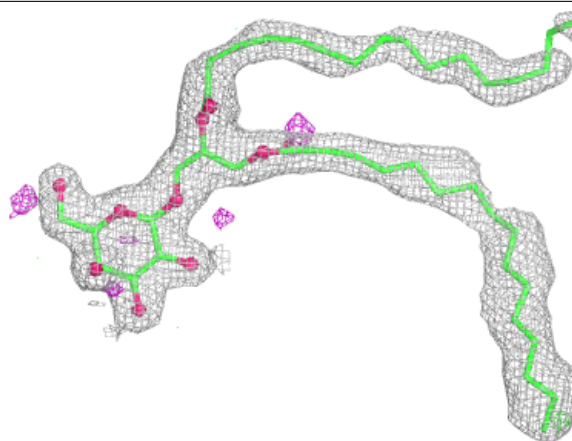
Electron density around LMG c 519:

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

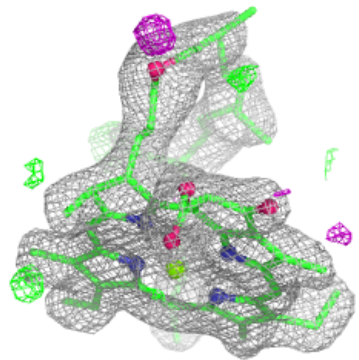
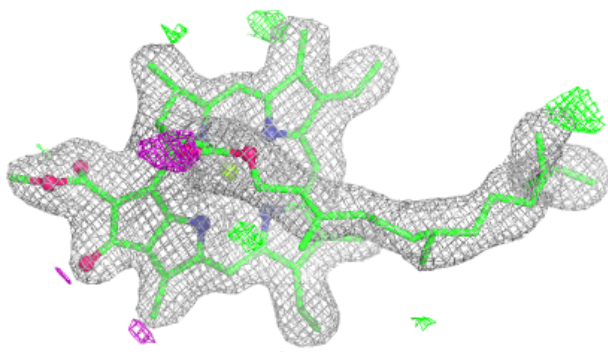
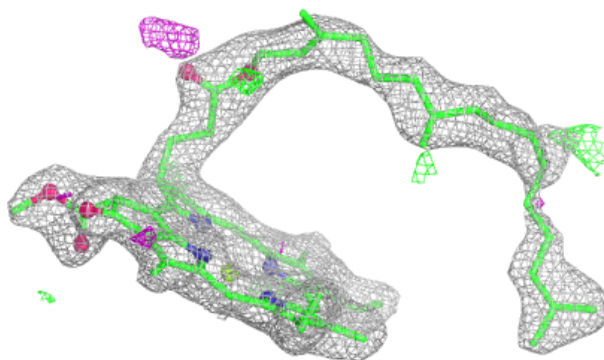


Electron density around LMG C 519:

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

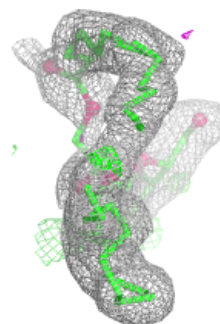
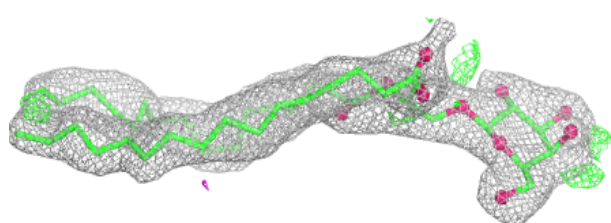
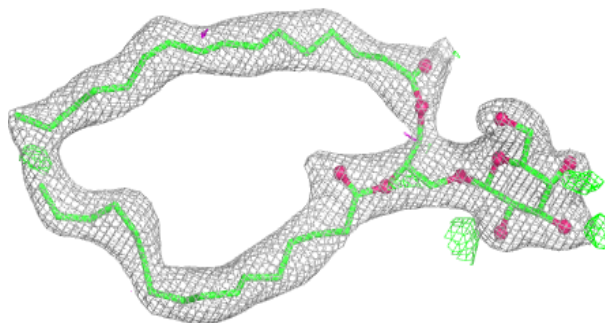
**Electron density around CLA C 513:**

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

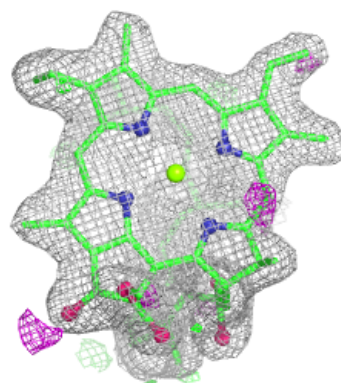
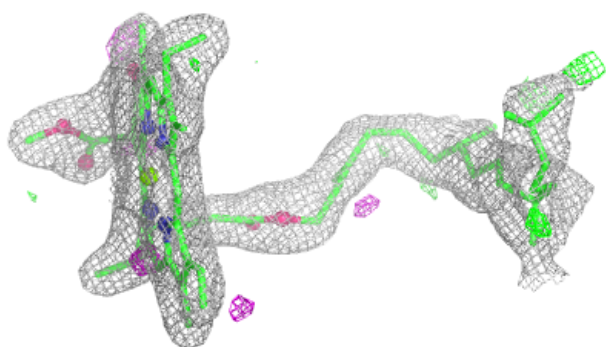
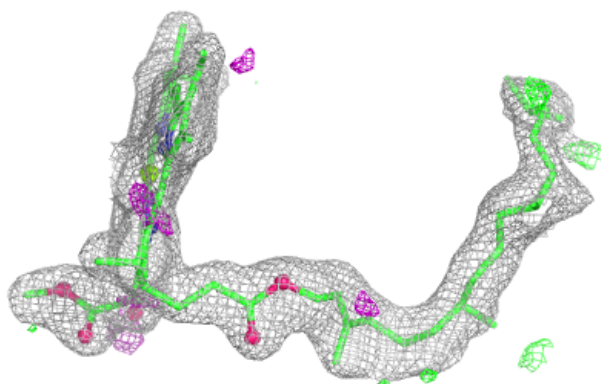


Electron density around LMG A 407:

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

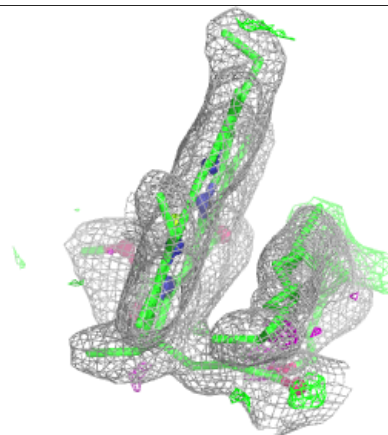
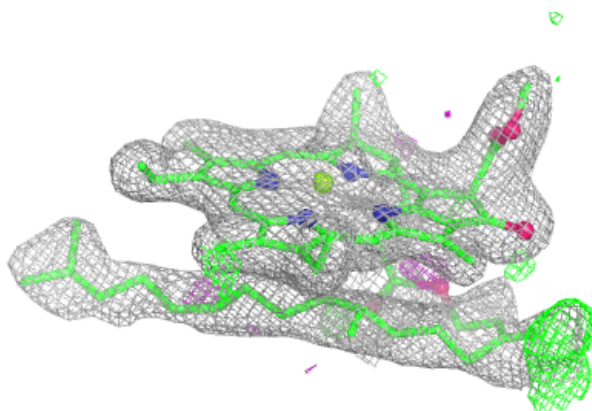
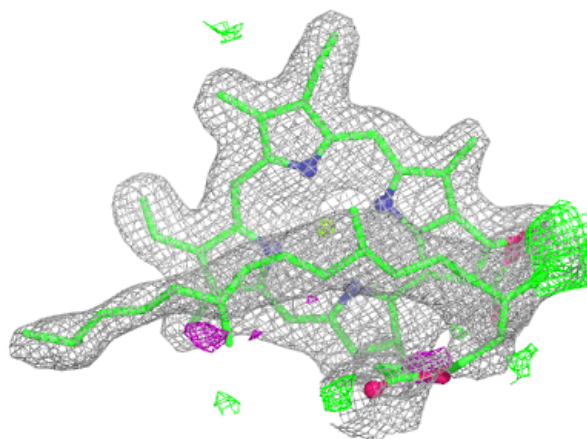
**Electron density around CLA C 506:**

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

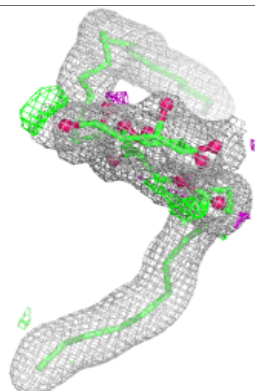
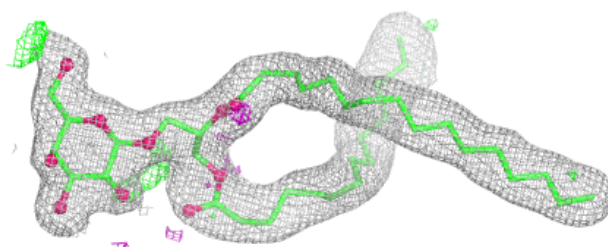
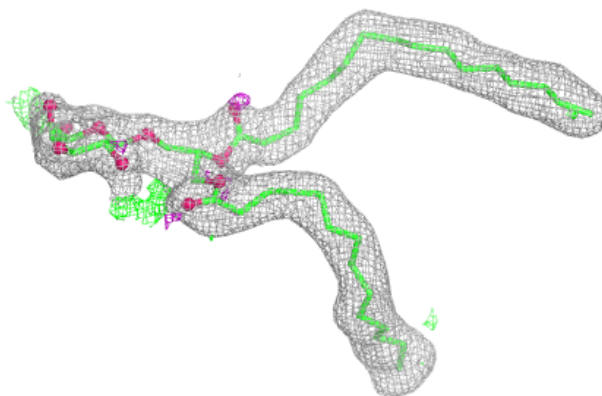


Electron density around CLA b 603:

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

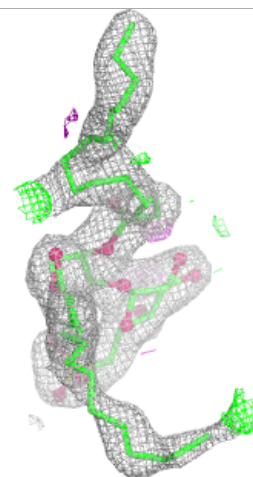
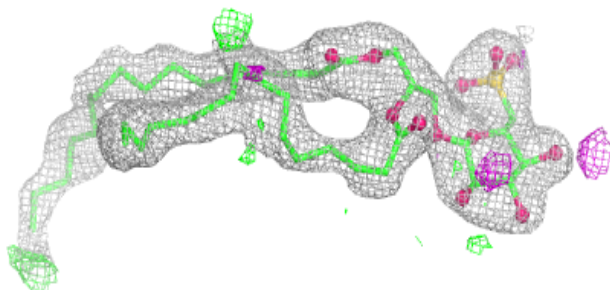
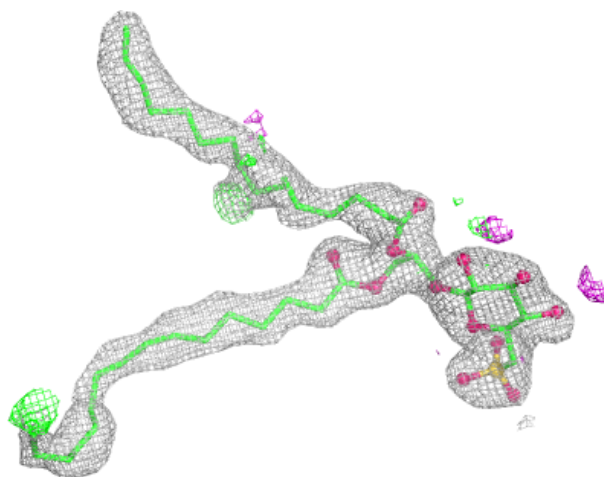
**Electron density around LMG b 623:**

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



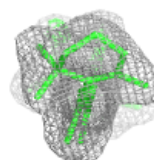
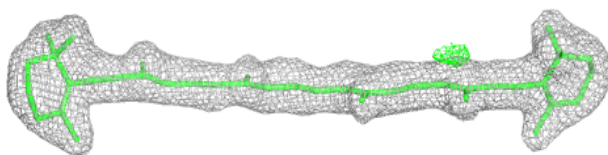
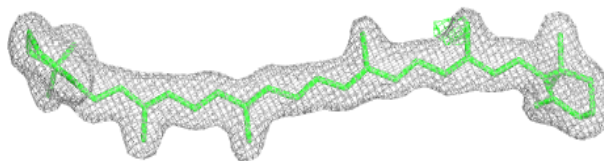
Electron density around SQD A 406:

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

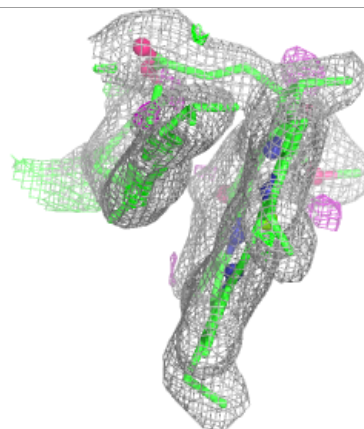
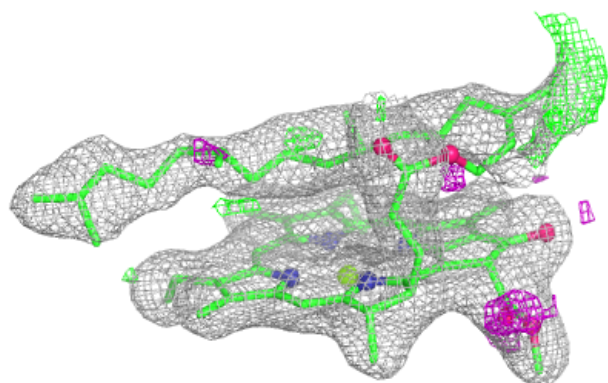
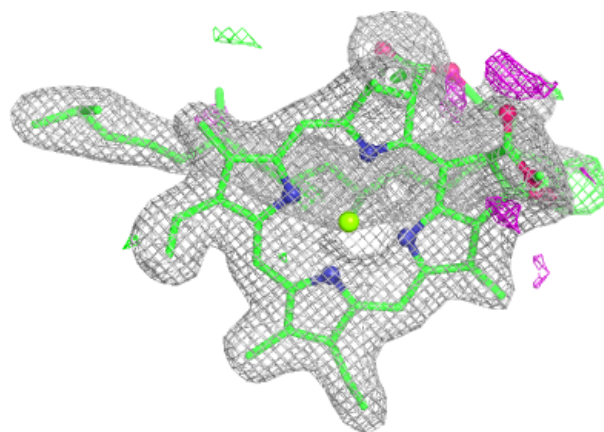


Electron density around BCR C 514:

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

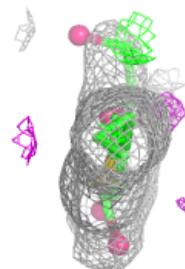
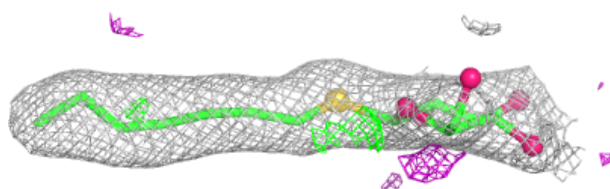
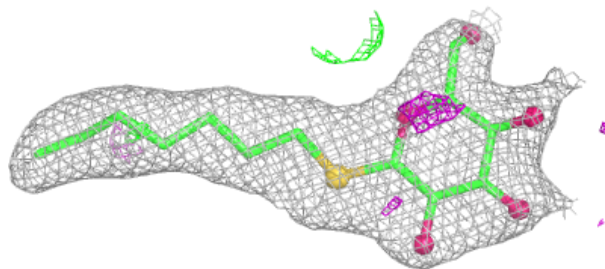
**Electron density around CLA B 602:**

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

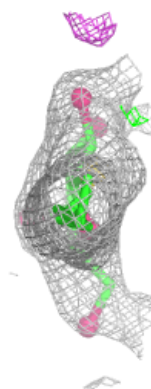
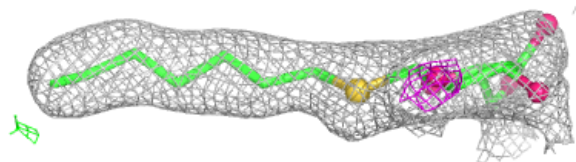
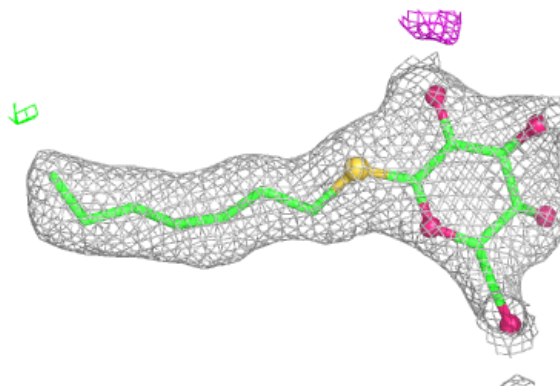


Electron density around HTG b 601:

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

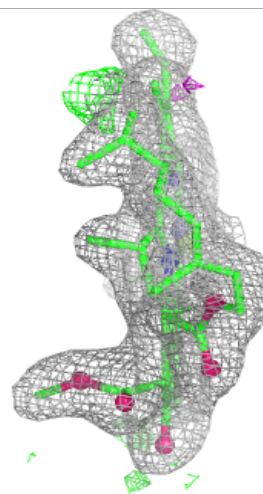
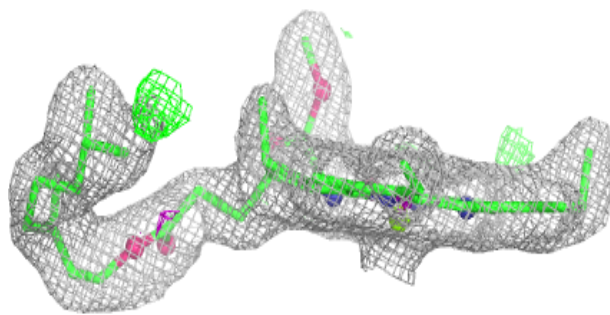
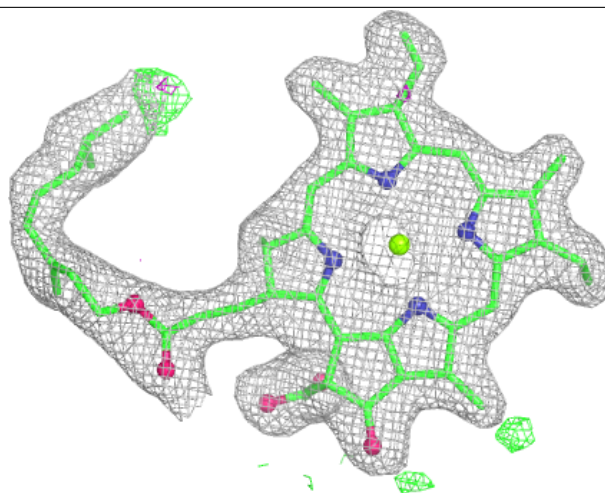
**Electron density around HTG B 631:**

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



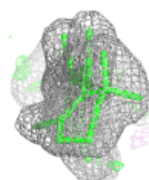
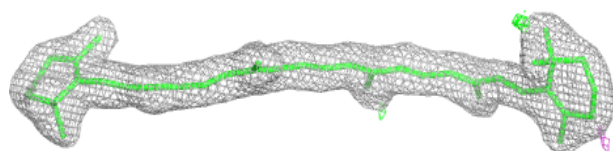
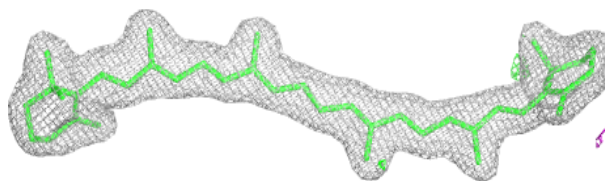
Electron density around CLA C 512:

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

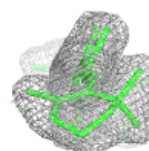
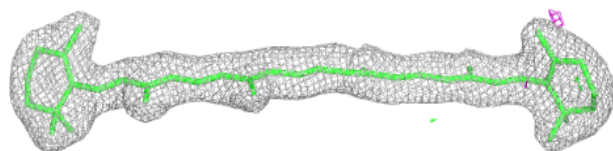
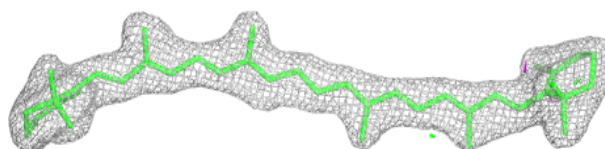


Electron density around BCR K 101:

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

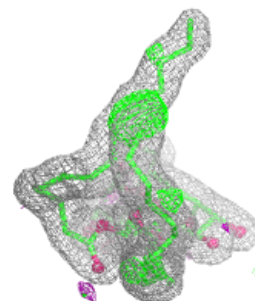
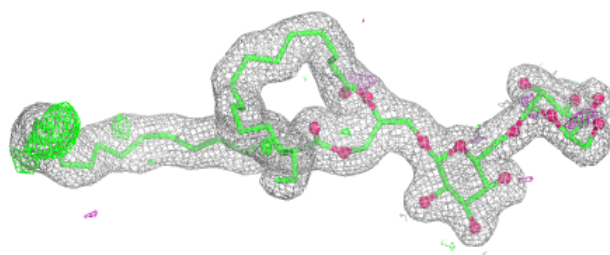
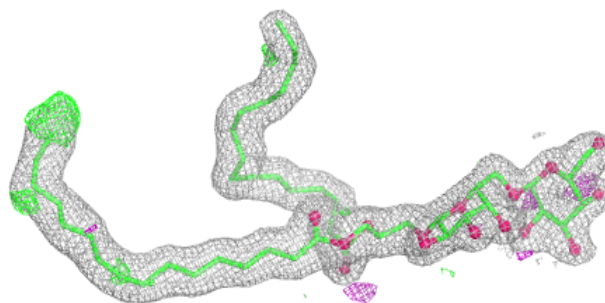
**Electron density around BCR k 102:**

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



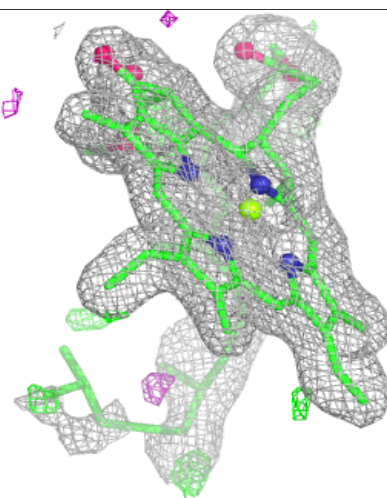
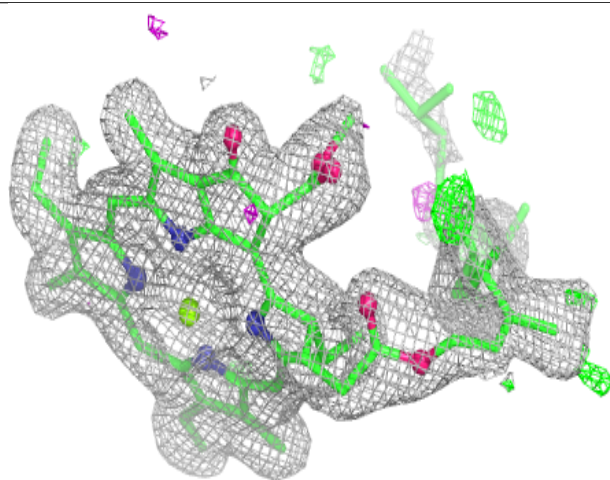
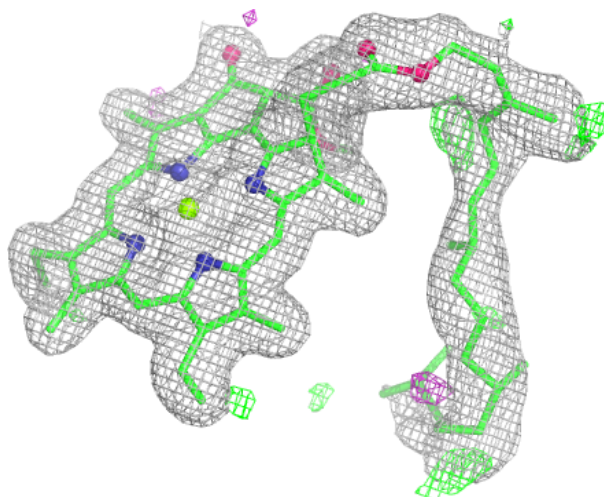
Electron density around DGD h 101:

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



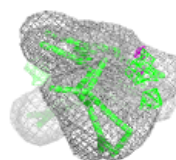
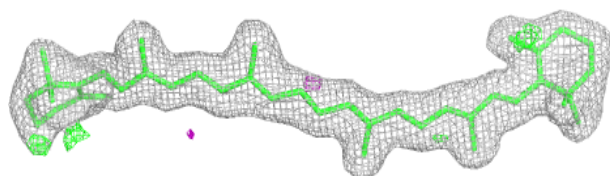
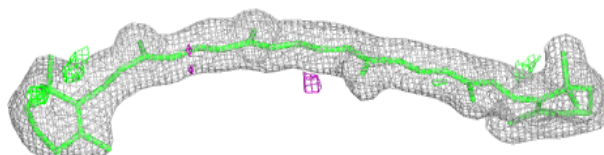
Electron density around CLA b 618:

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

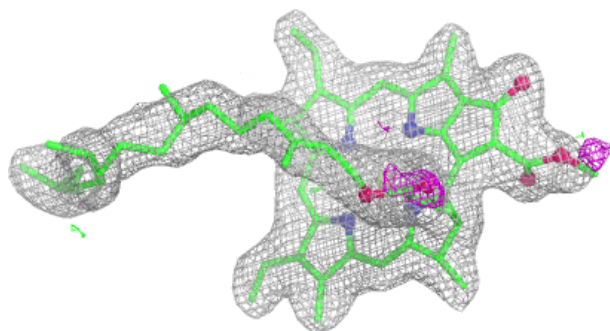
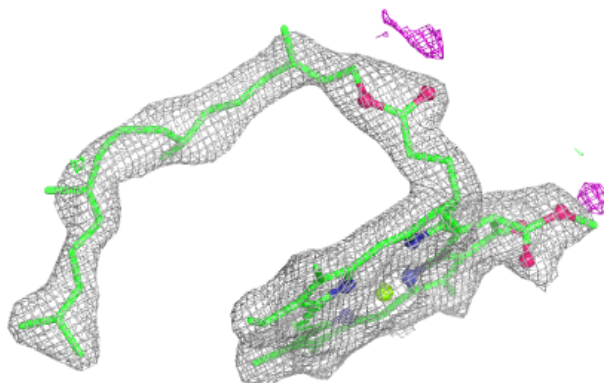


Electron density around BCR D 405:

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

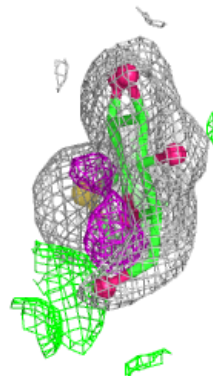
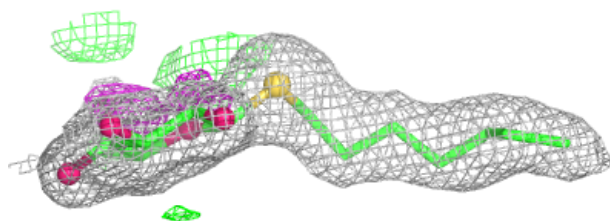
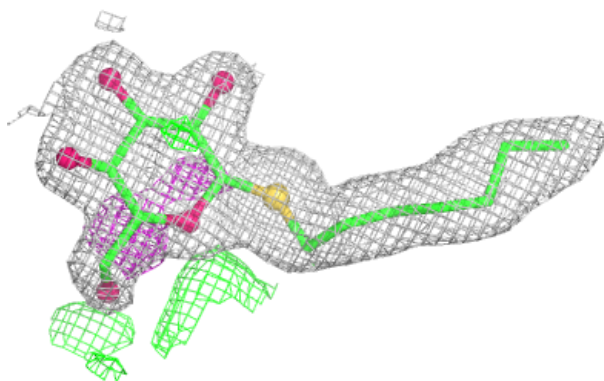
**Electron density around CLA c 513:**

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

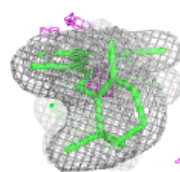
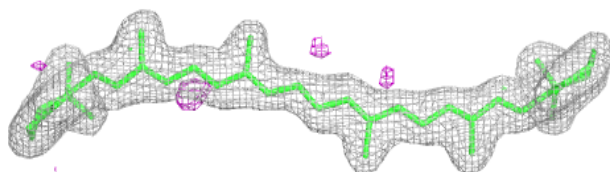
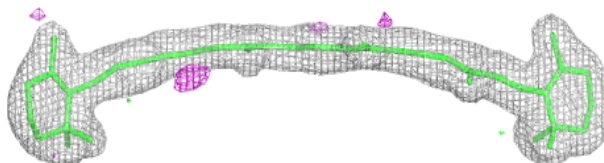


Electron density around HTG B 621:

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

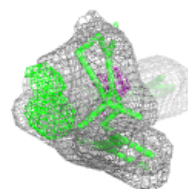
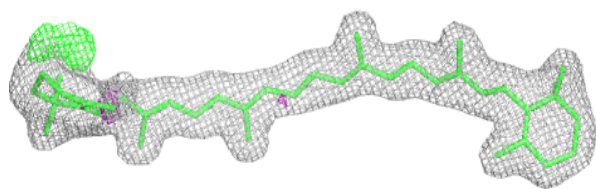
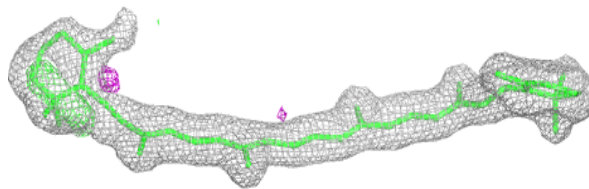
**Electron density around BCR K 102:**

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



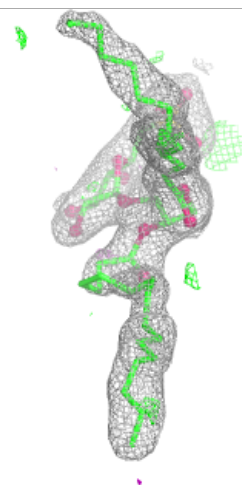
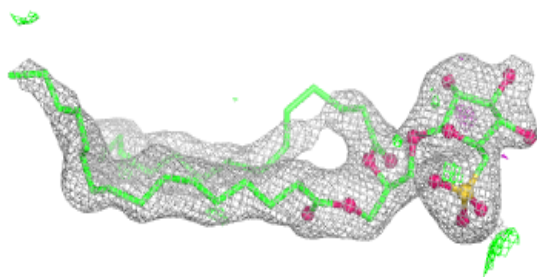
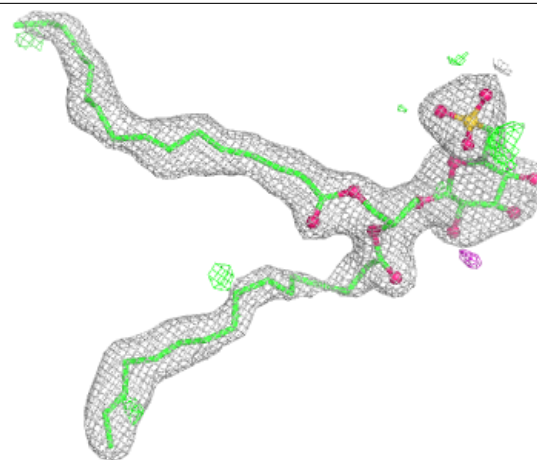
Electron density around BCR d 405:

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



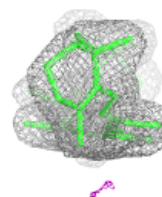
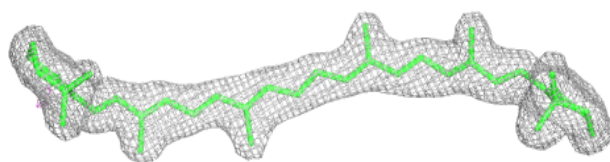
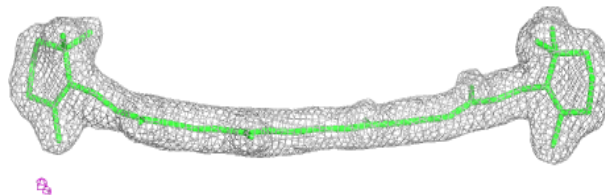
Electron density around SQD a 409:

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

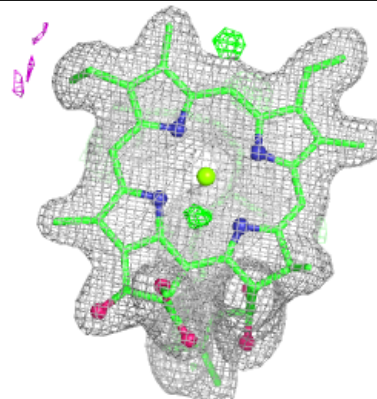
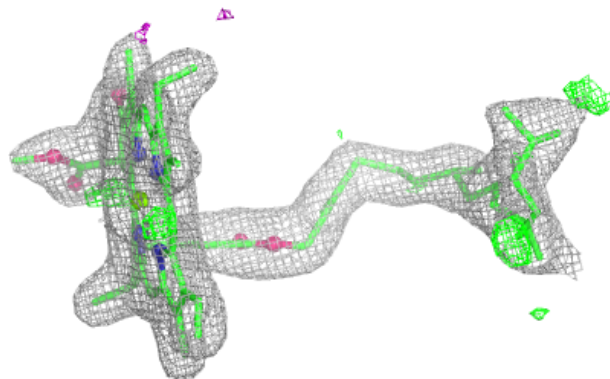
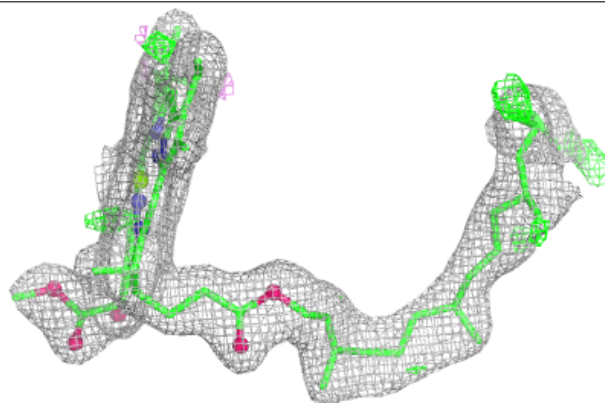


Electron density around BCR k 101:

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

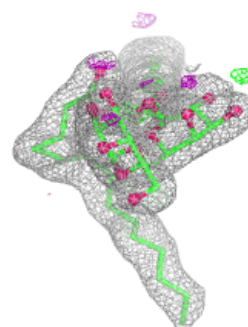
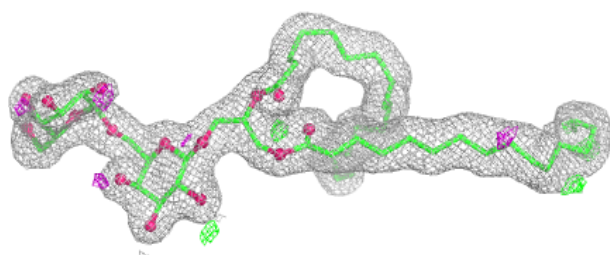
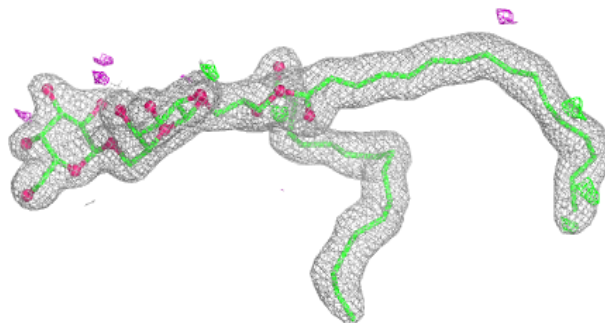
**Electron density around CLA c 506:**

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

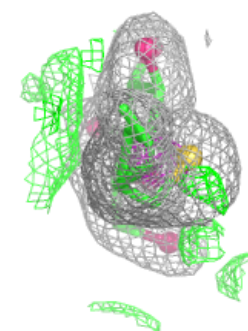
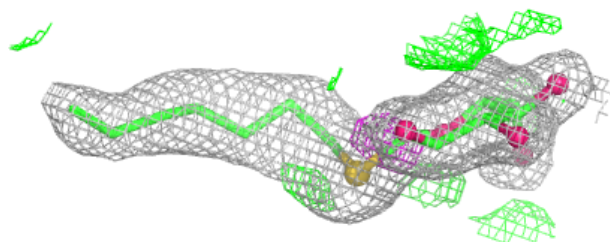
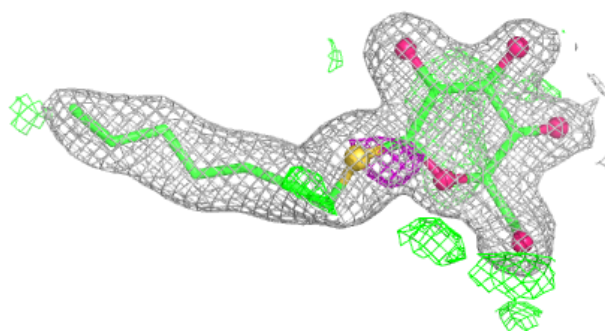


Electron density around DGD H 102:

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

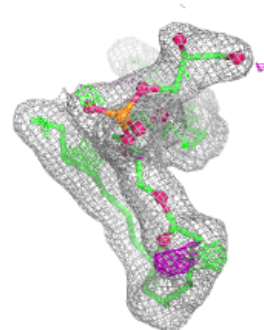
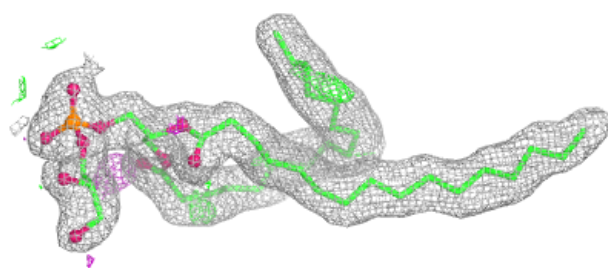
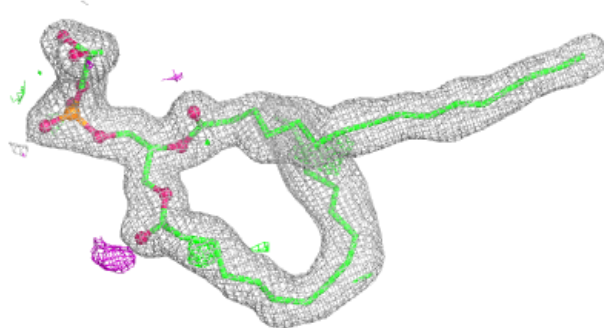
**Electron density around HTG O 302:**

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

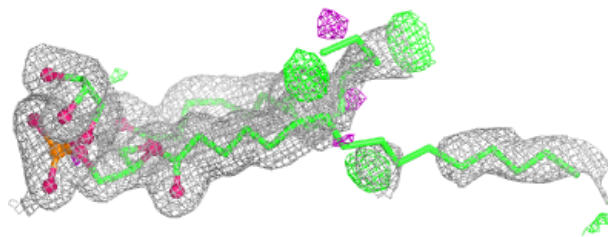
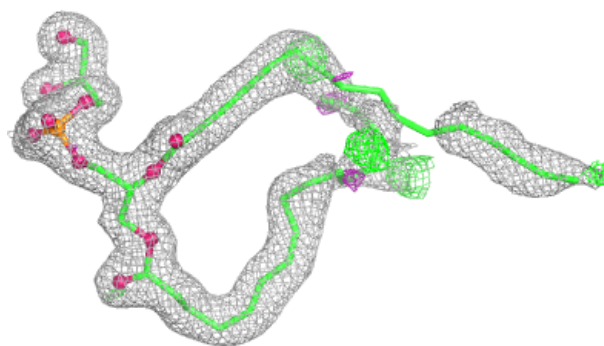


Electron density around LHG D 407:

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

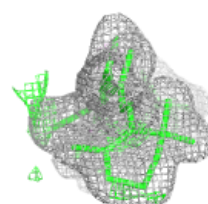
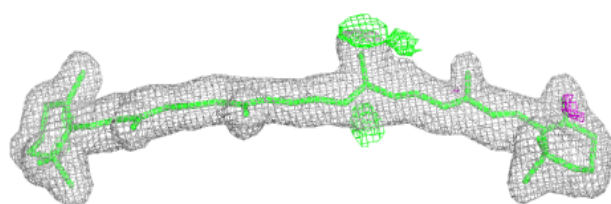
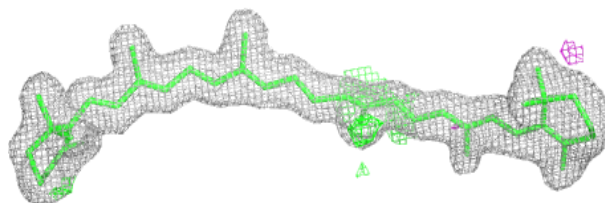
**Electron density around LHG D 409:**

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

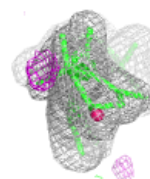
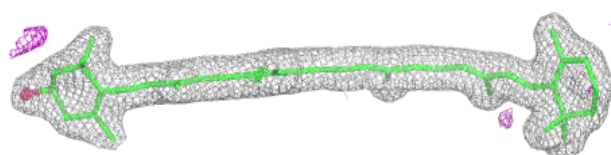
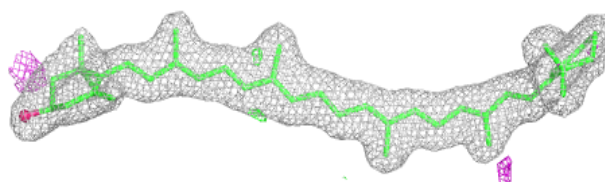


Electron density around BCR t 101:

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

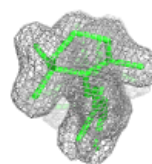
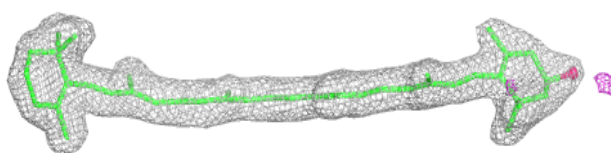
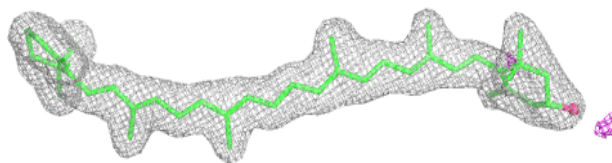
**Electron density around RRX H 101:**

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

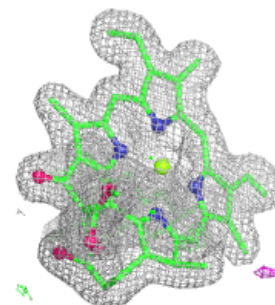
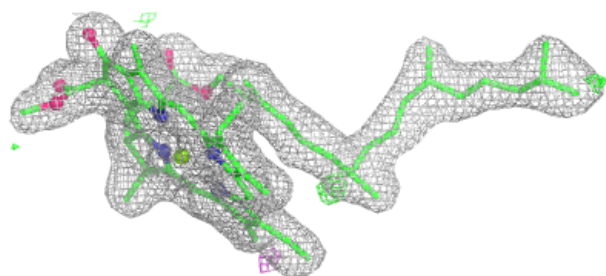
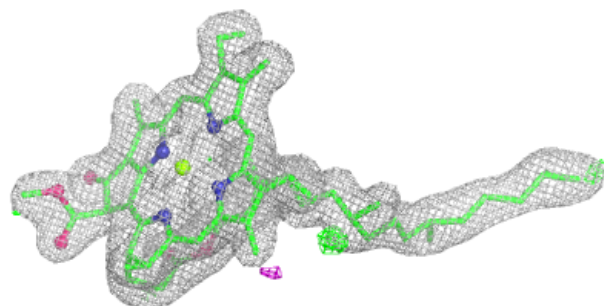


Electron density around RRX x 101:

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

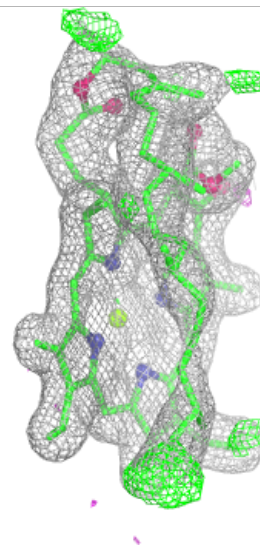
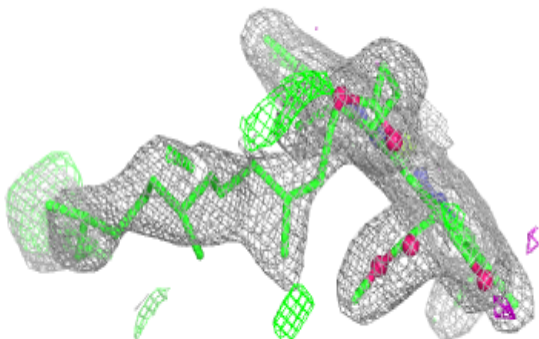
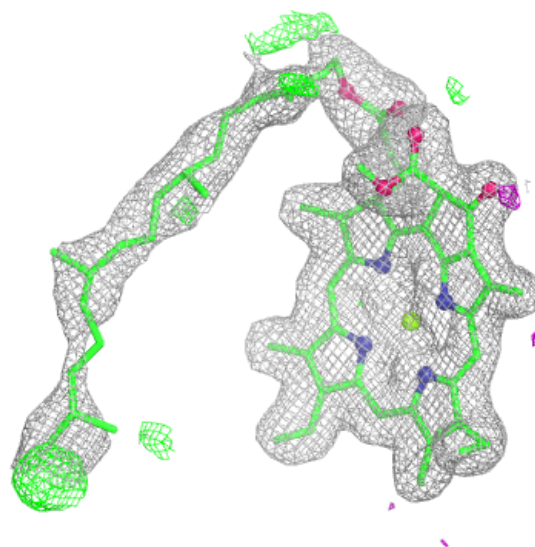
**Electron density around CLA C 505:**

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



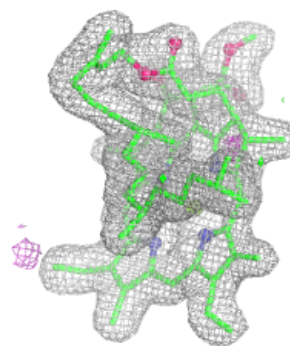
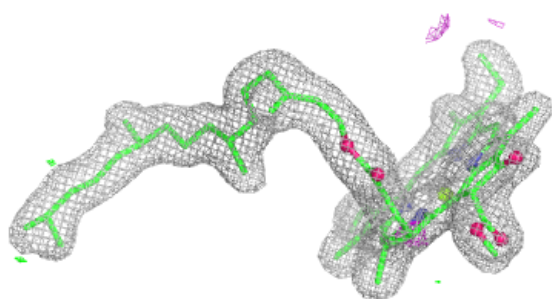
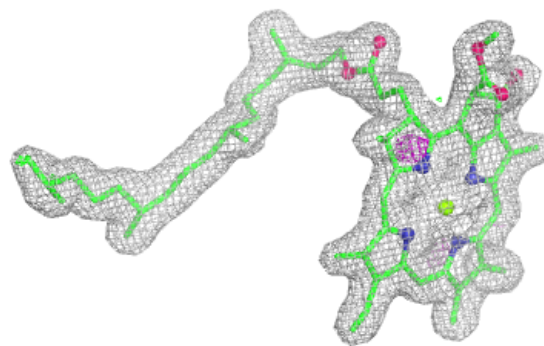
Electron density around CLA B 601:

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



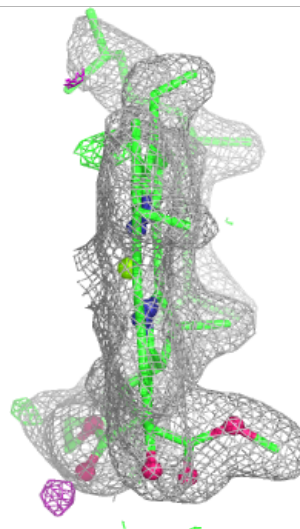
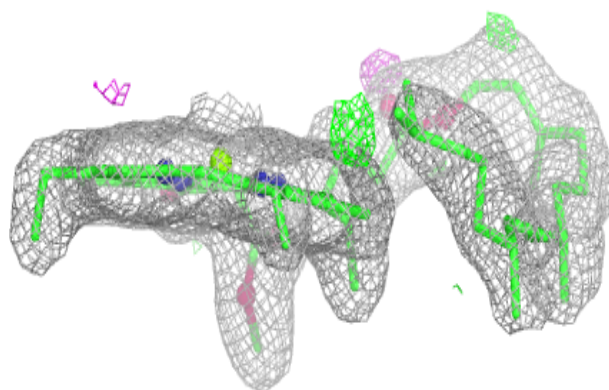
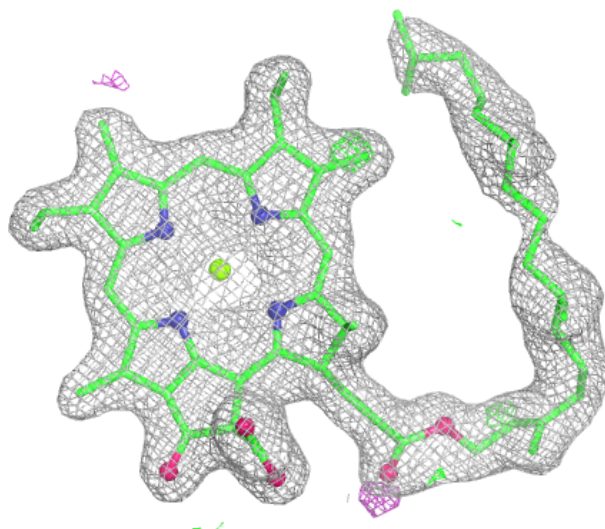
Electron density around CLA c 511:

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



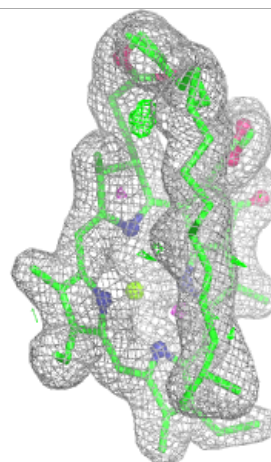
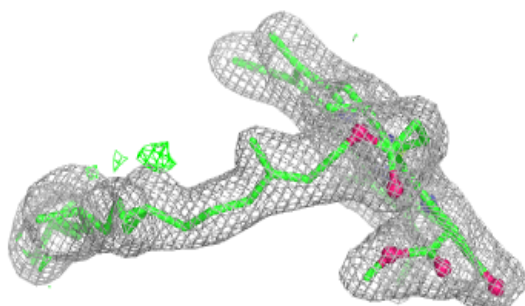
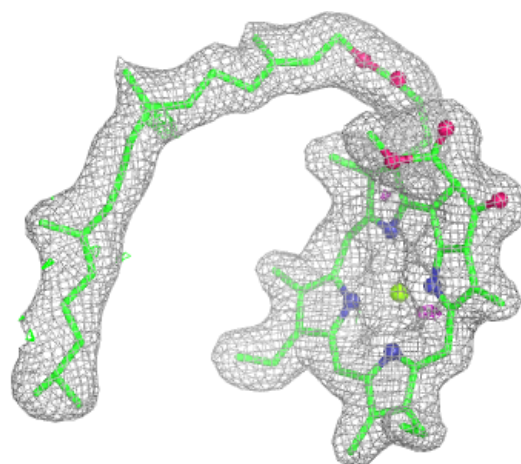
Electron density around CLA c 512:

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



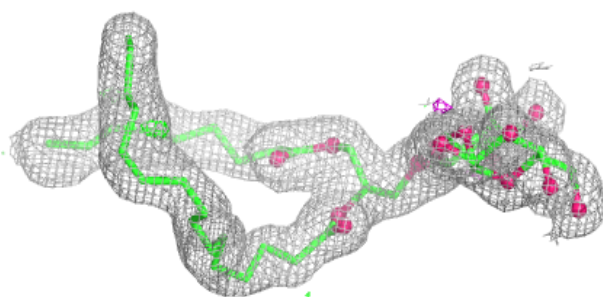
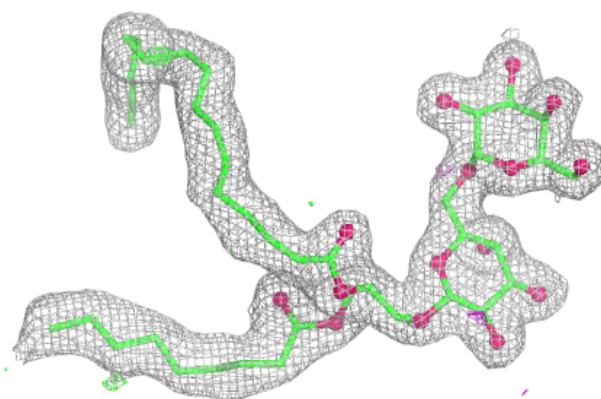
Electron density around CLA C 507:

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

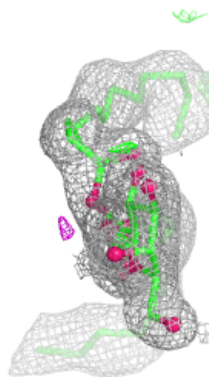
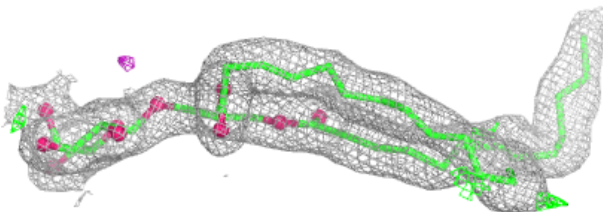
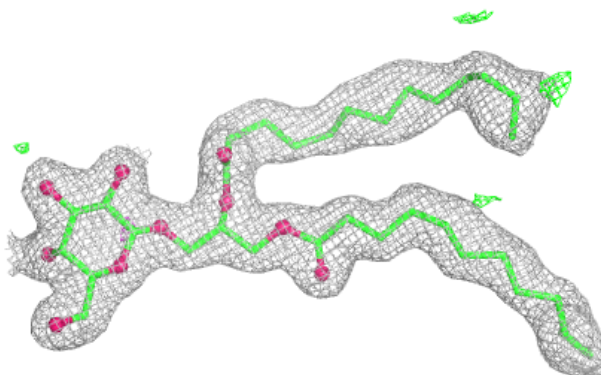


Electron density around DGD C 517:

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

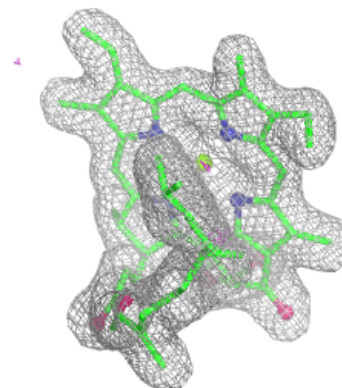
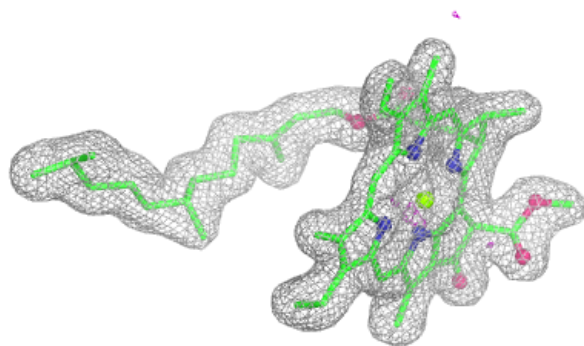
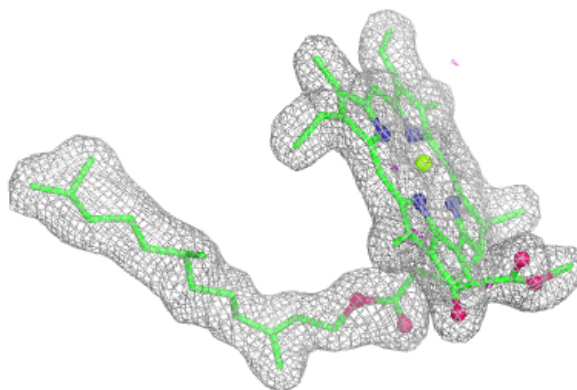
**Electron density around LMG j 101:**

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

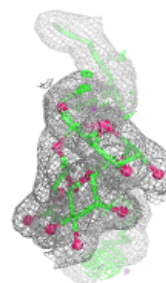
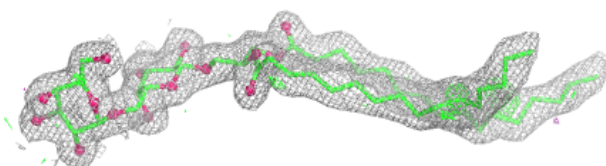
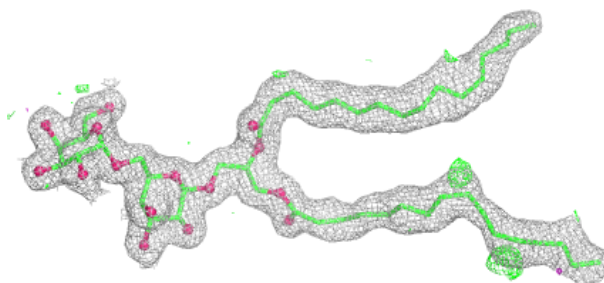


Electron density around CLA C 508:

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

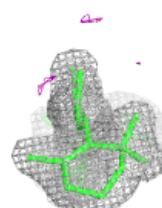
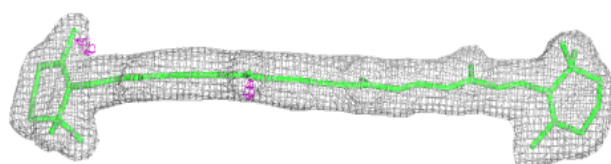
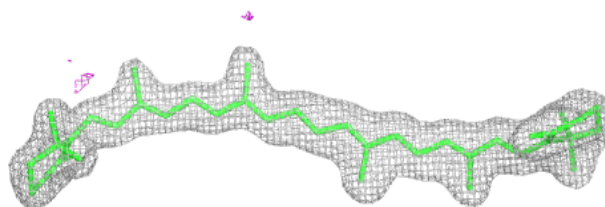
**Electron density around DGD c 517:**

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

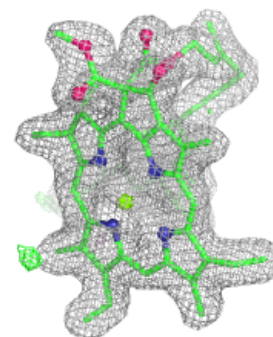
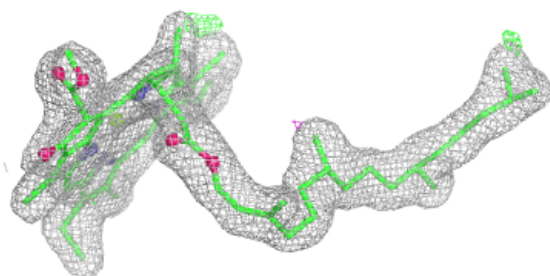
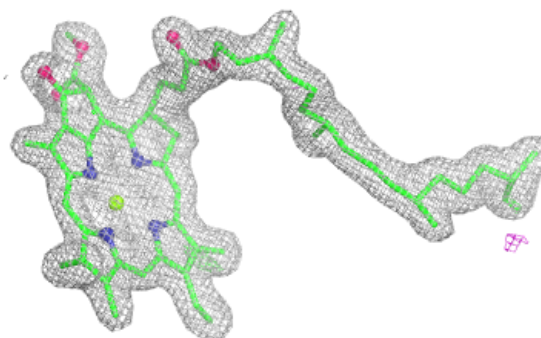


Electron density around BCR C 515:

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

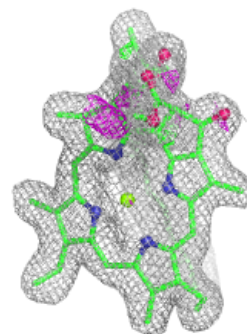
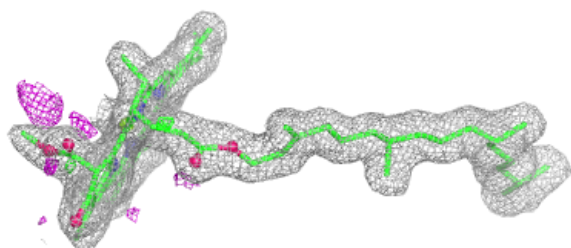
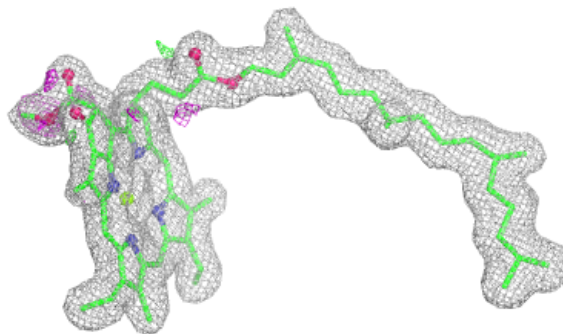
**Electron density around CLA C 511:**

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



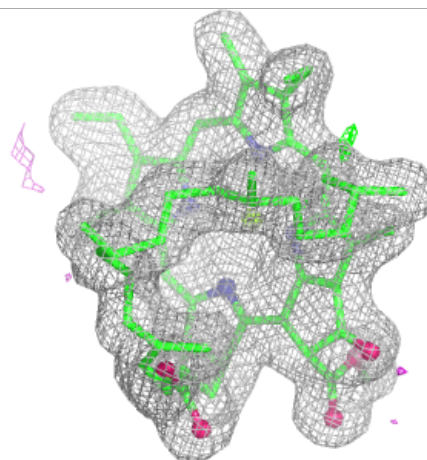
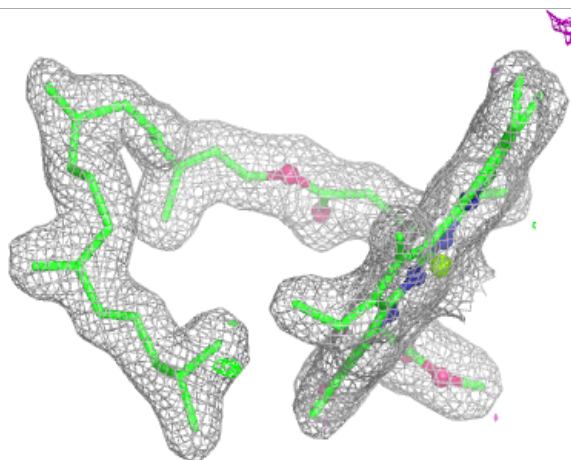
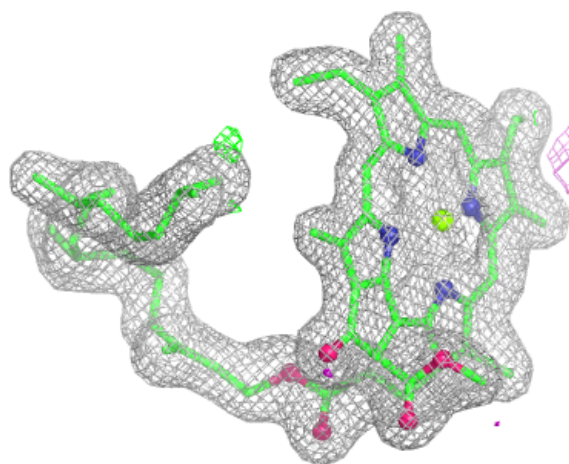
Electron density around CLA B 610:

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



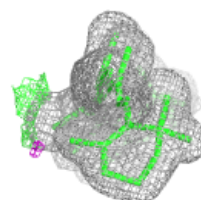
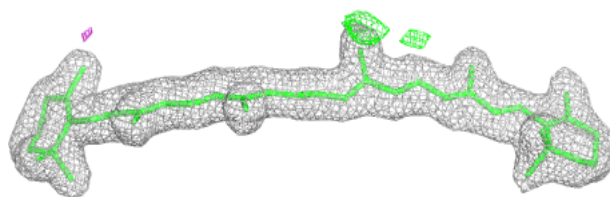
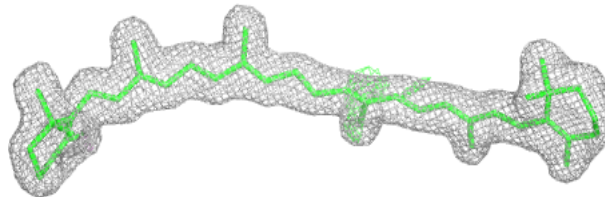
Electron density around CLA C 503:

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

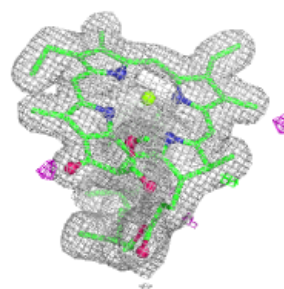
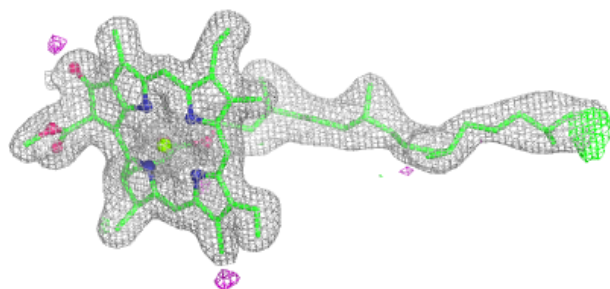
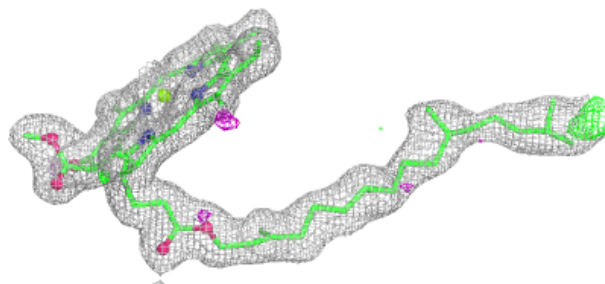


Electron density around BCR T 101:

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

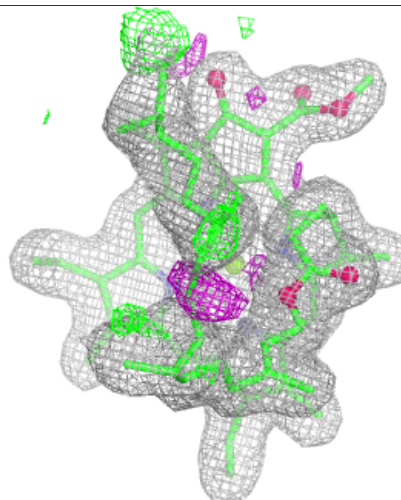
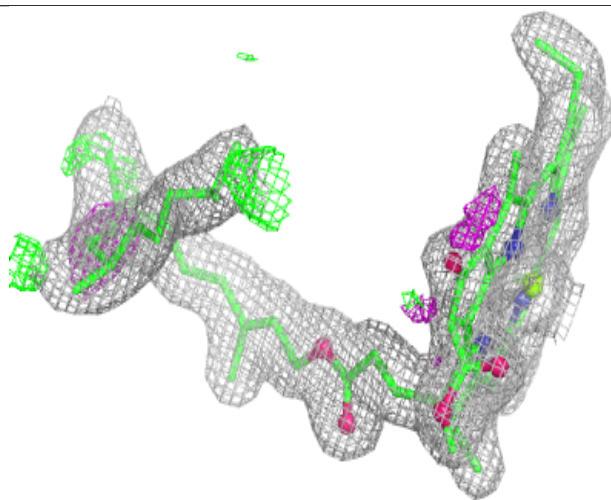
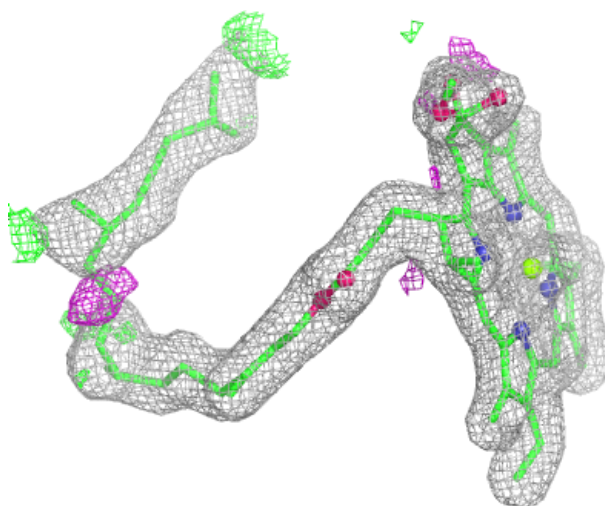
**Electron density around CLA C 504:**

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



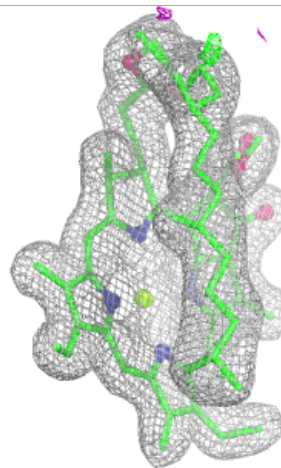
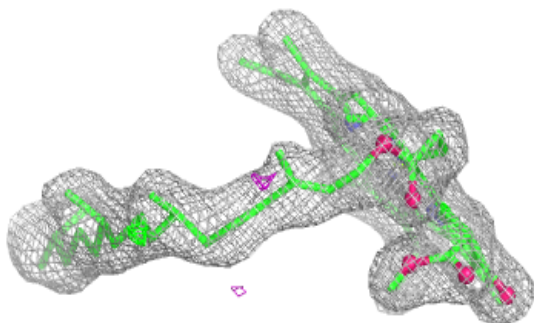
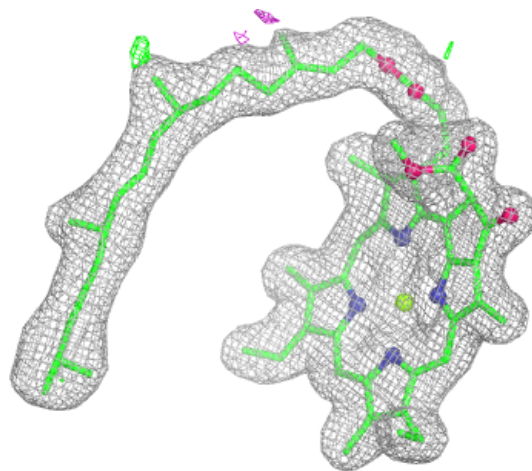
Electron density around CLA b 608:

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



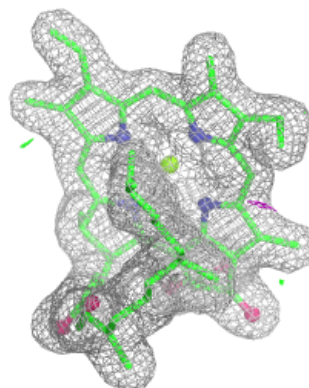
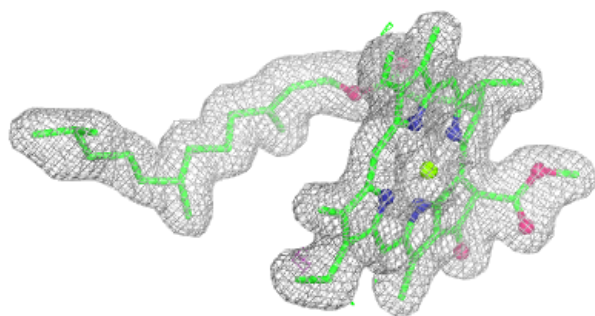
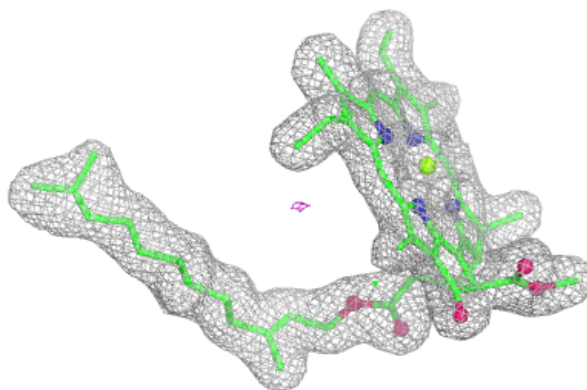
Electron density around CLA c 507:

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



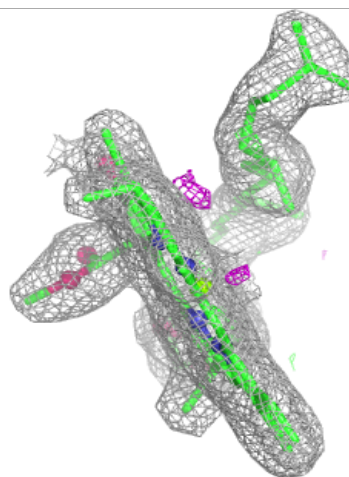
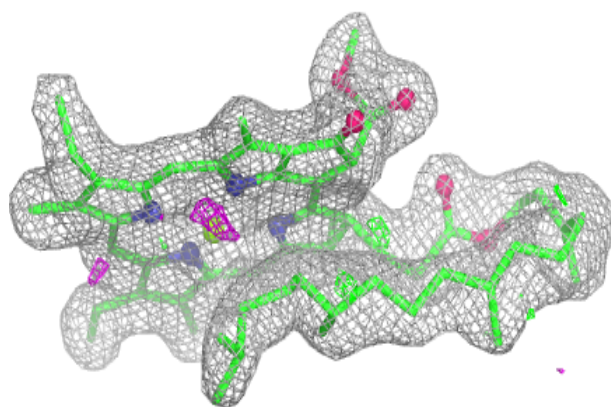
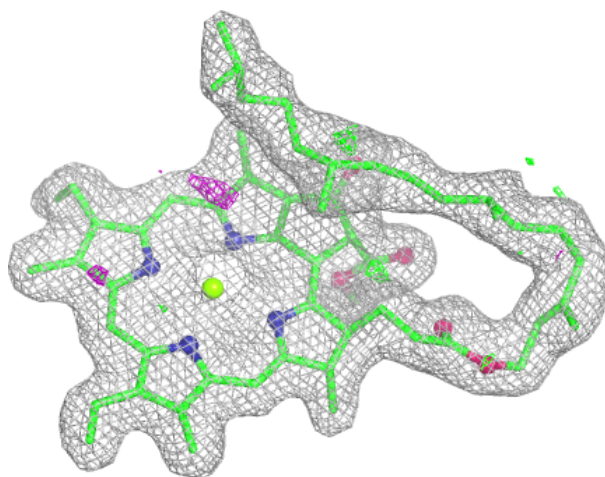
Electron density around CLA c 508:

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



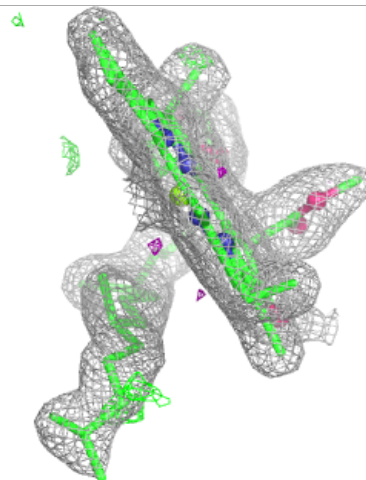
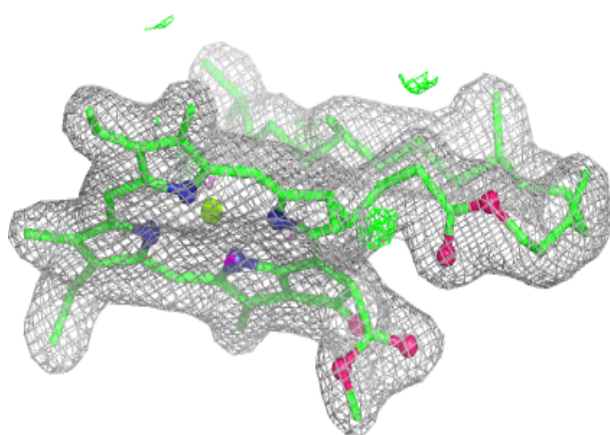
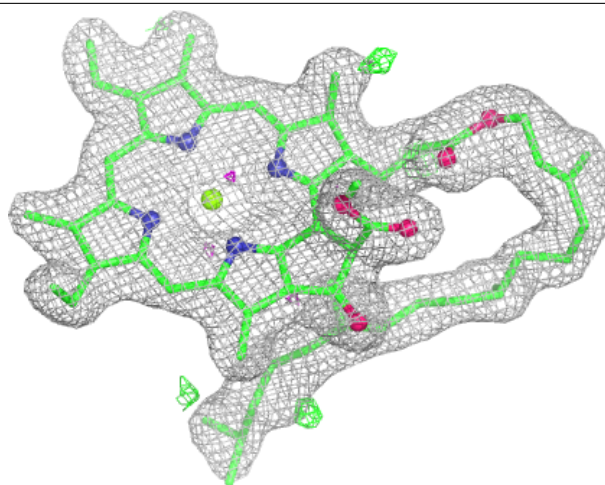
Electron density around CLA c 509:

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



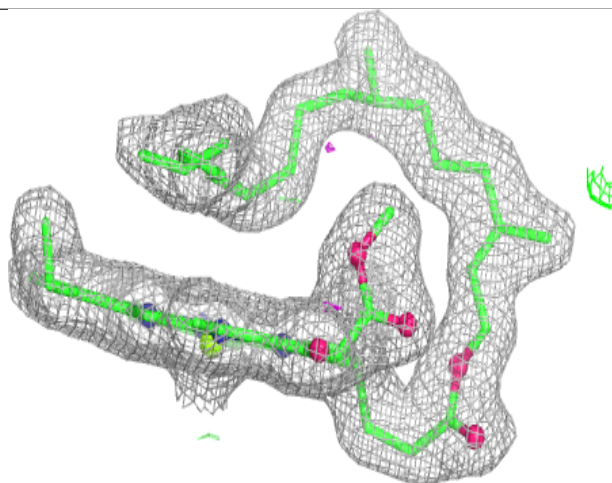
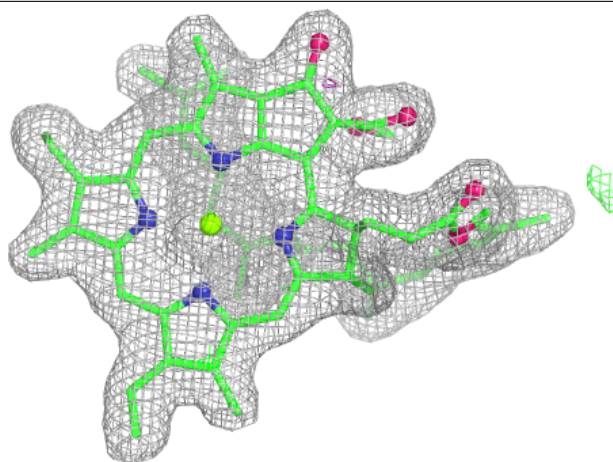
Electron density around CLA C 509:

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



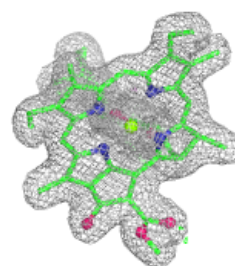
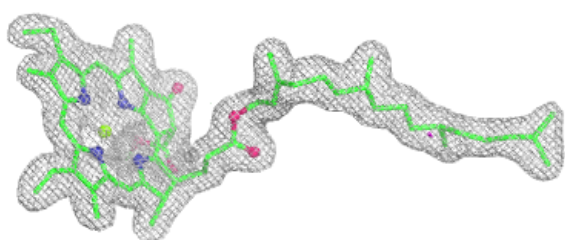
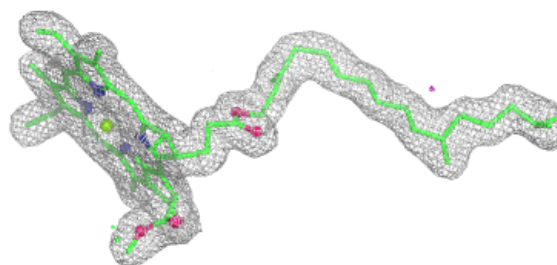
Electron density around CLA C 510:

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

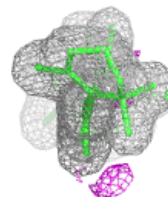
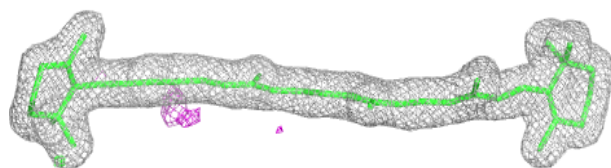
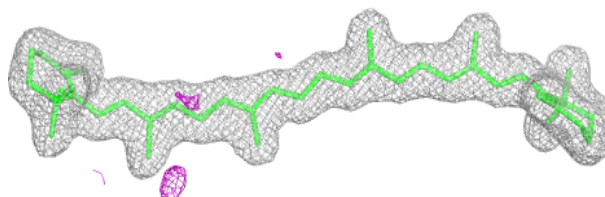


Electron density around CLA C 502:

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

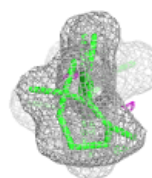
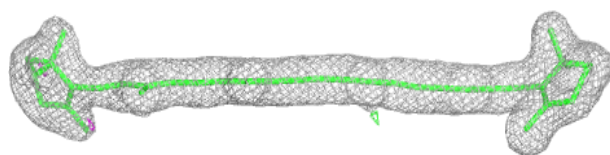
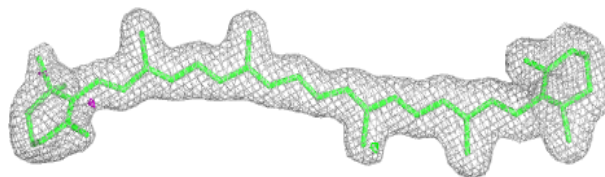
**Electron density around BCR A 405:**

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

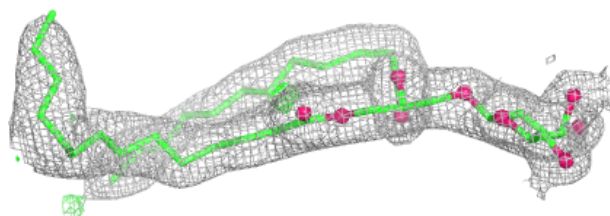
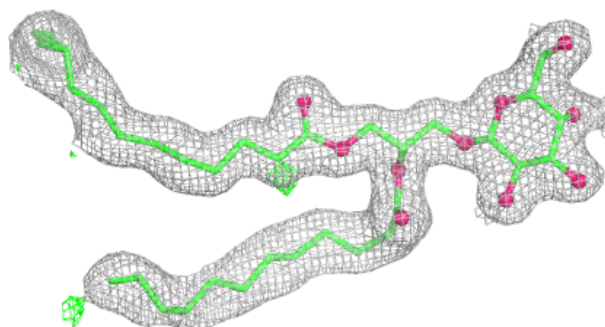


Electron density around BCR B 618:

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

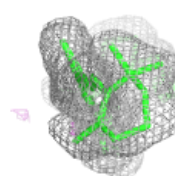
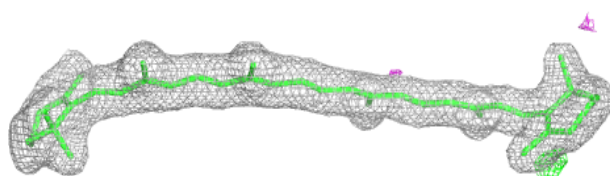
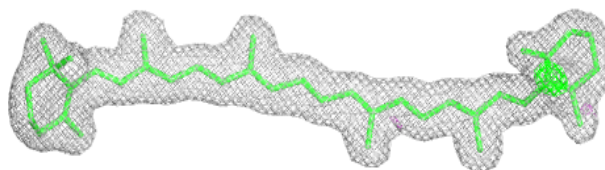
**Electron density around LMG J 101:**

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

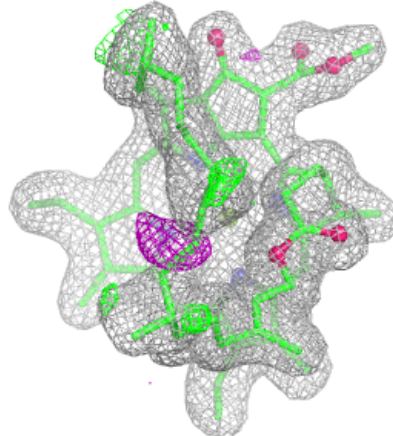
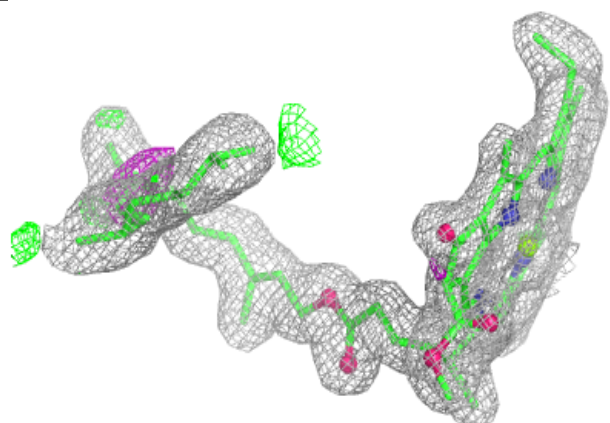
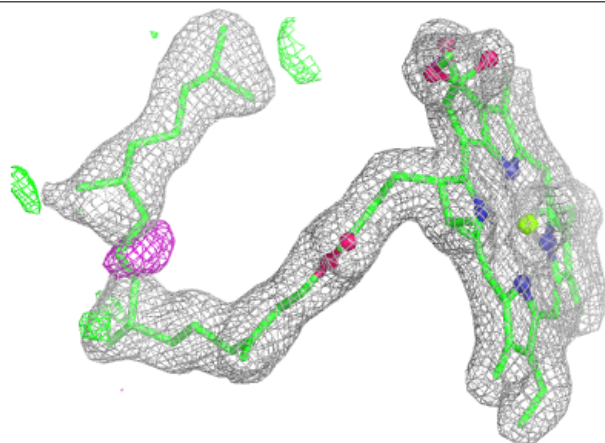


Electron density around BCR B 619:

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

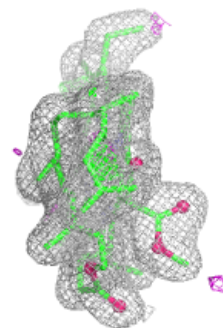
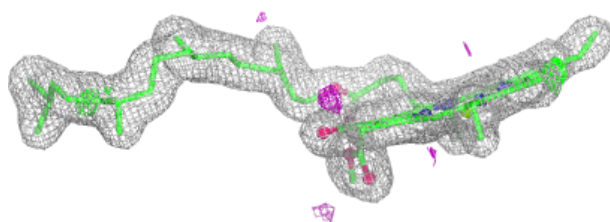
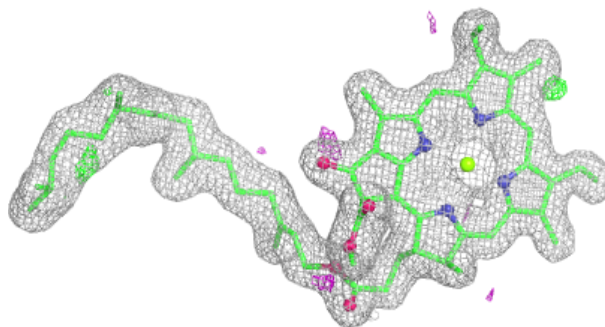
**Electron density around CLA B 607:**

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

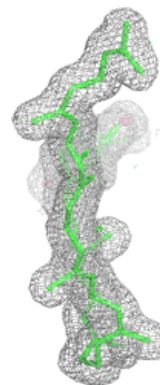
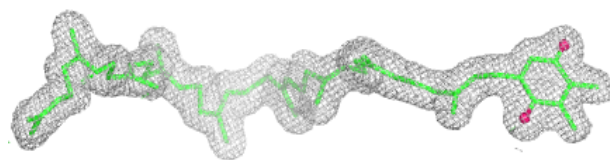
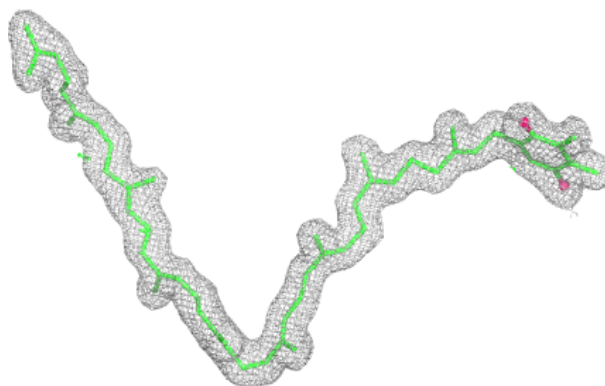


Electron density around CLA B 603:

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

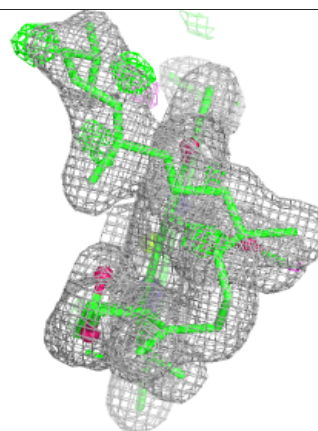
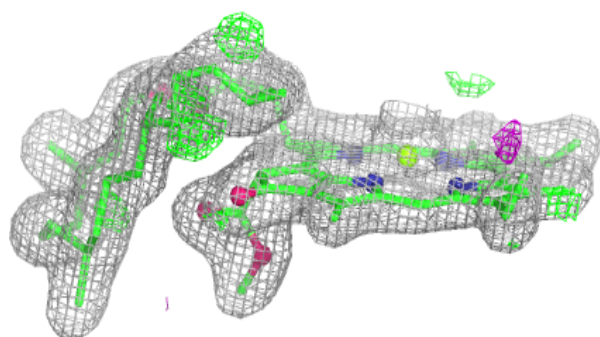
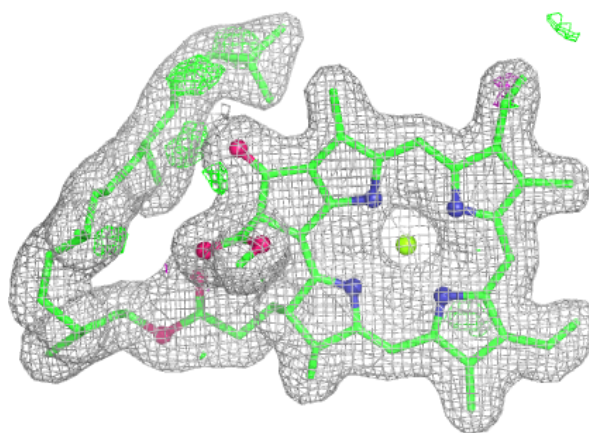
**Electron density around PL9 D 412:**

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

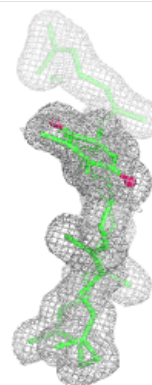
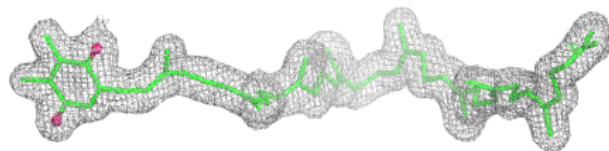
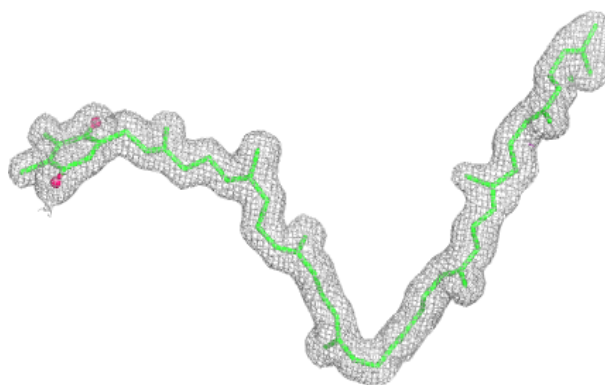


Electron density around CLA B 611:

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

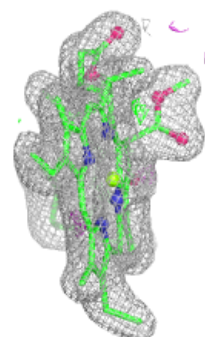
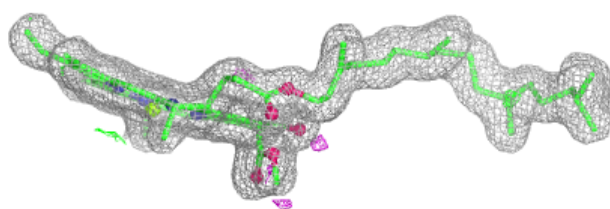
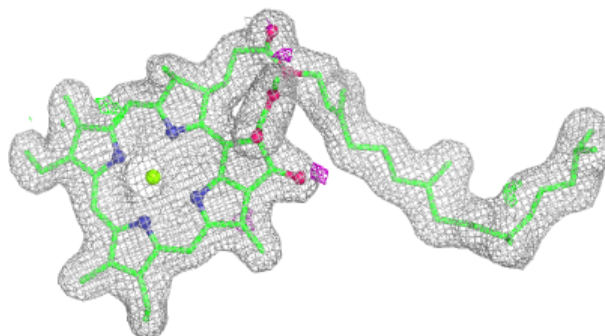
**Electron density around PL9 d 412:**

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

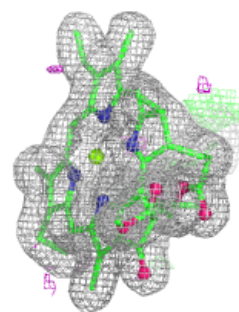
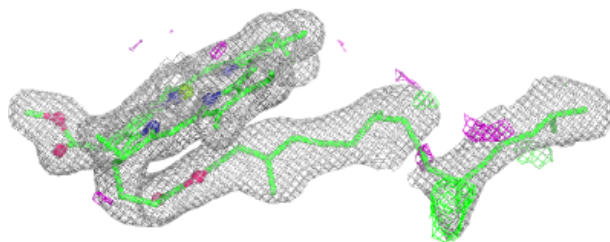
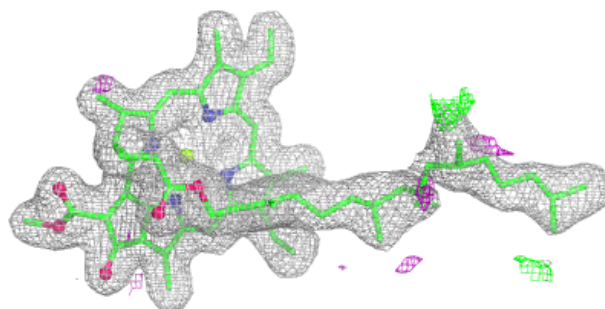


Electron density around CLA b 604:

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

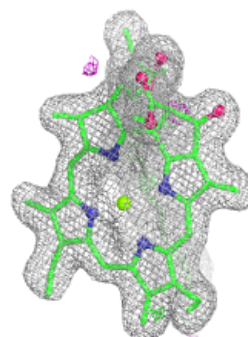
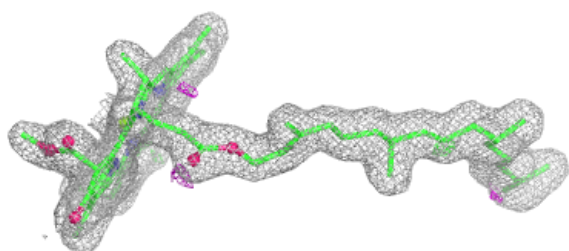
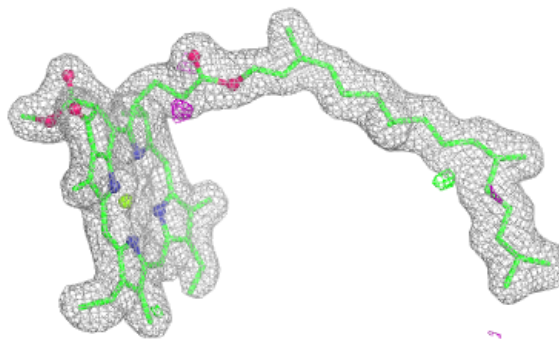
**Electron density around CLA B 615:**

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

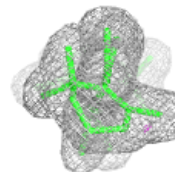
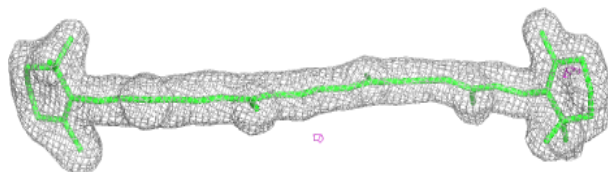
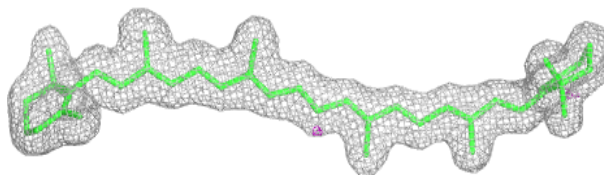


Electron density around CLA b 611:

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

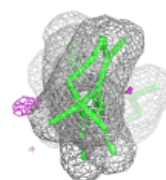
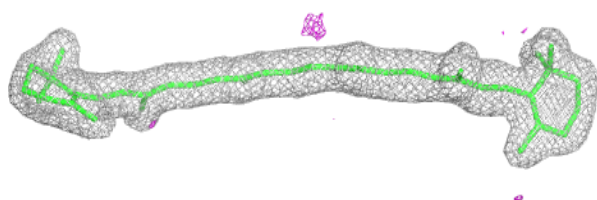
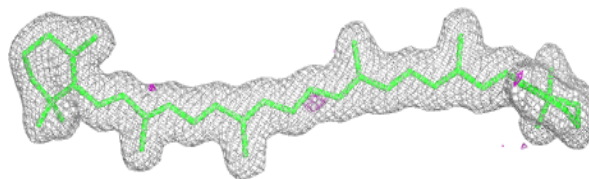
**Electron density around BCR a 408:**

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

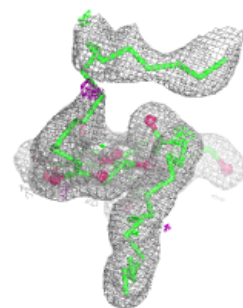
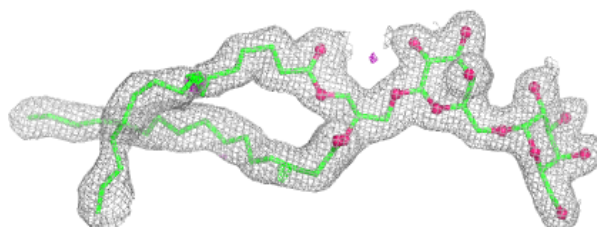
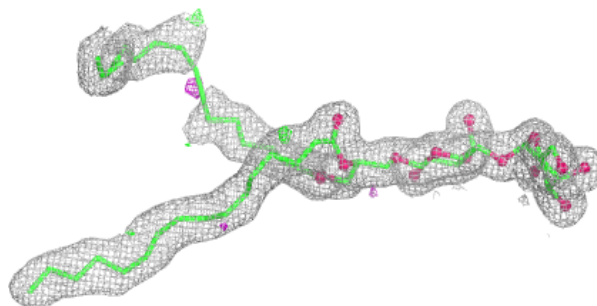


Electron density around BCR b 619:

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

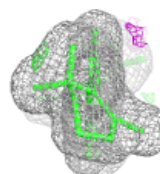
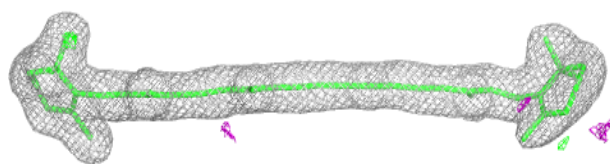
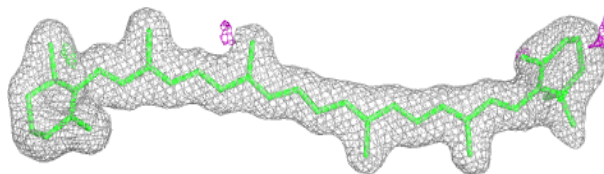
**Electron density around DGD C 516:**

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

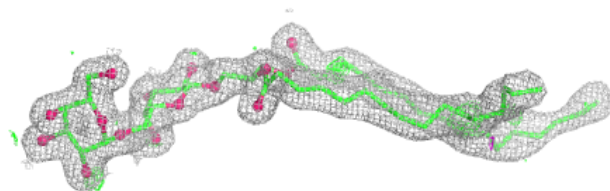
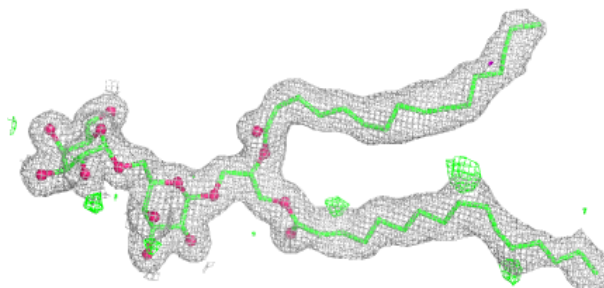


Electron density around BCR b 620:

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

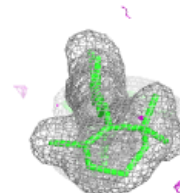
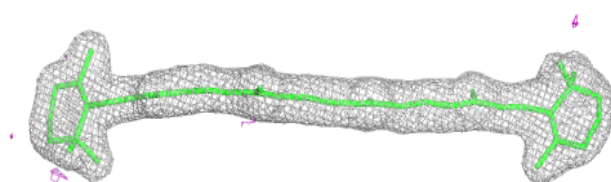
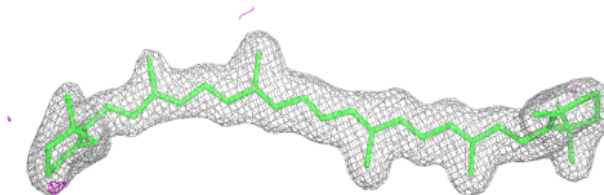
**Electron density around DGD C 518:**

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

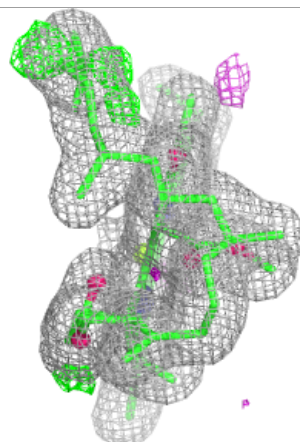
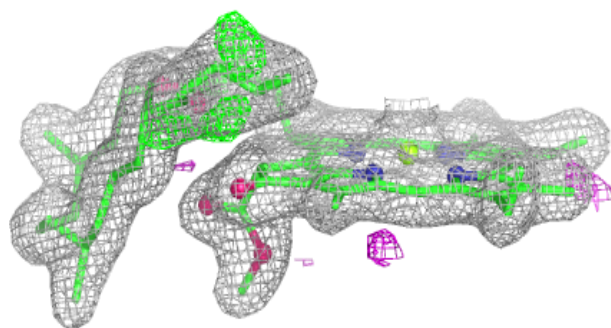
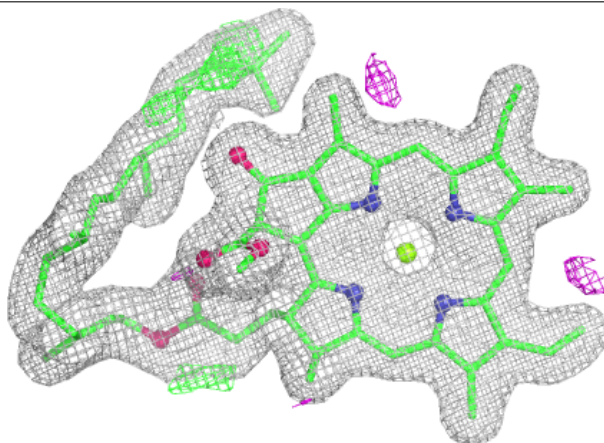


Electron density around BCR c 514:

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

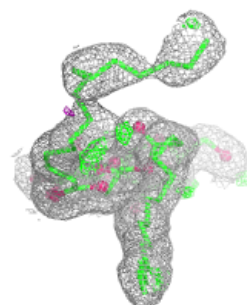
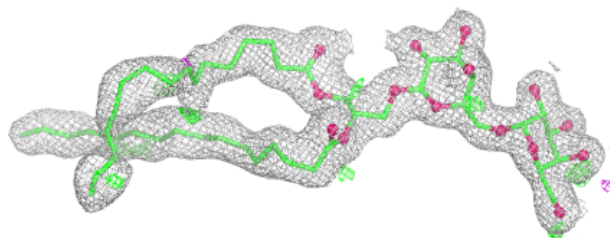
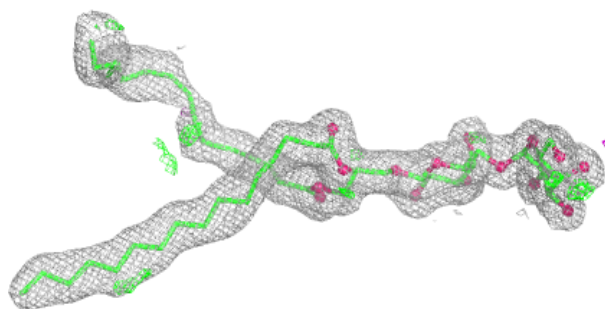
**Electron density around CLA b 612:**

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

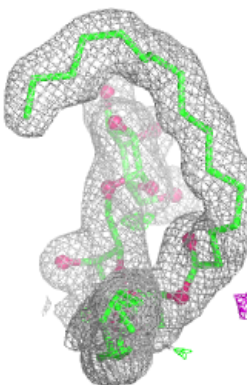
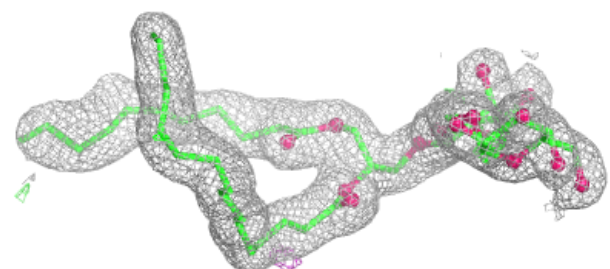
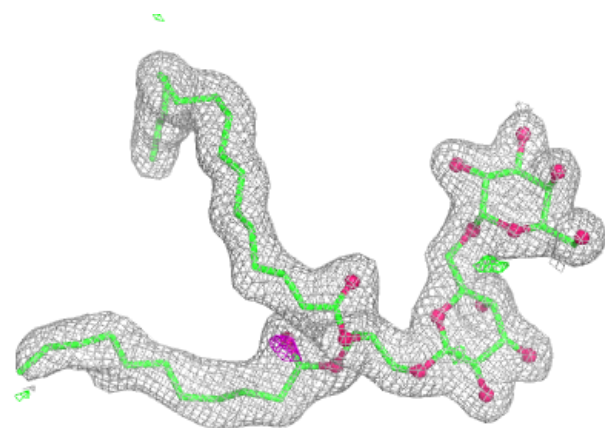


Electron density around DGD c 515:

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

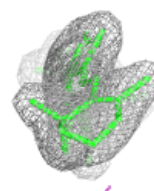
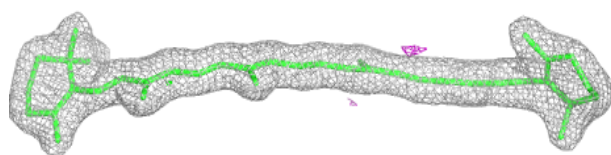
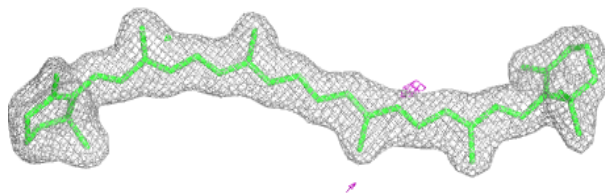
**Electron density around DGD c 516:**

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

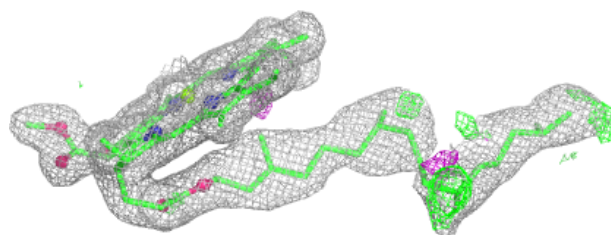
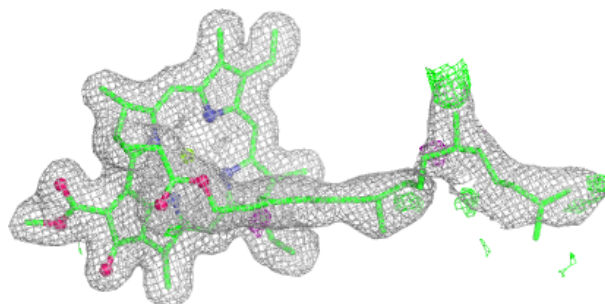


Electron density around BCR j 102:

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

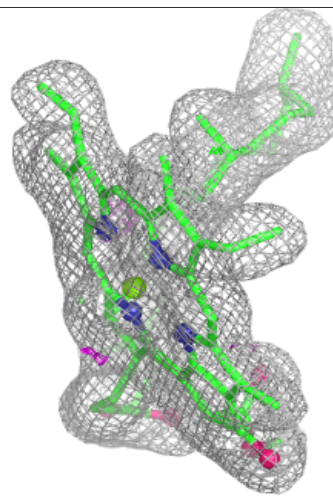
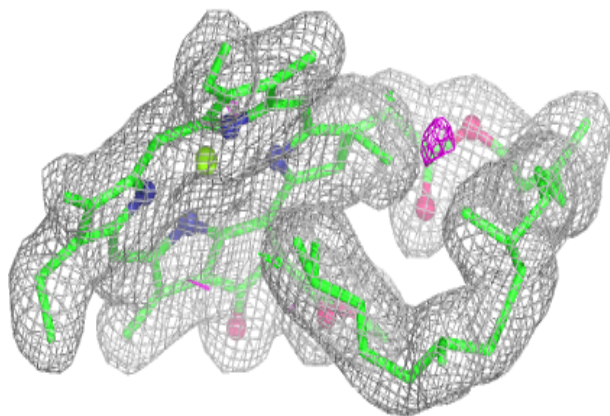
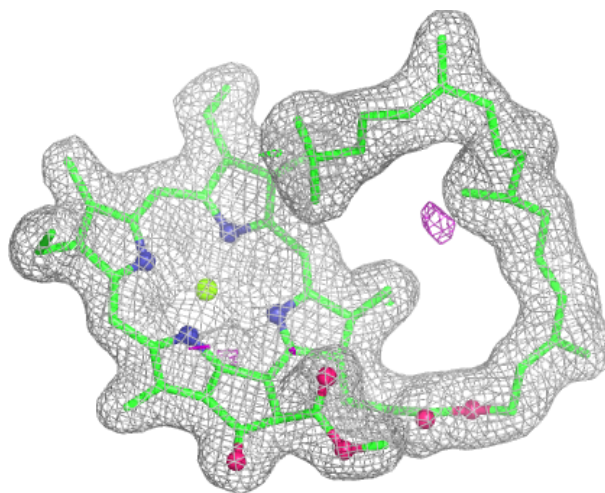
**Electron density around CLA b 616:**

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



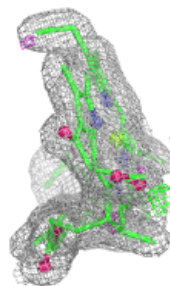
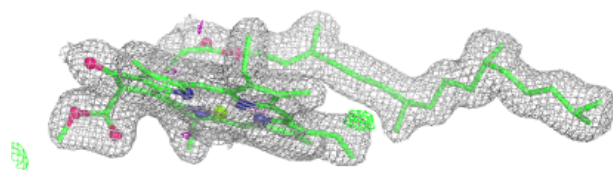
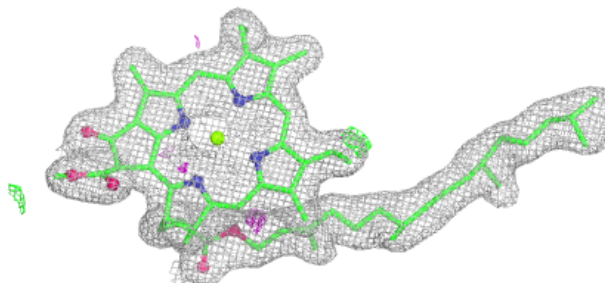
Electron density around CLA B 616:

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



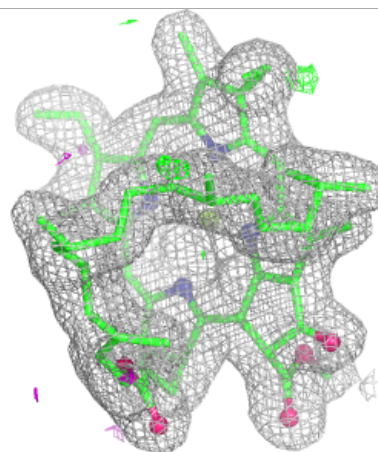
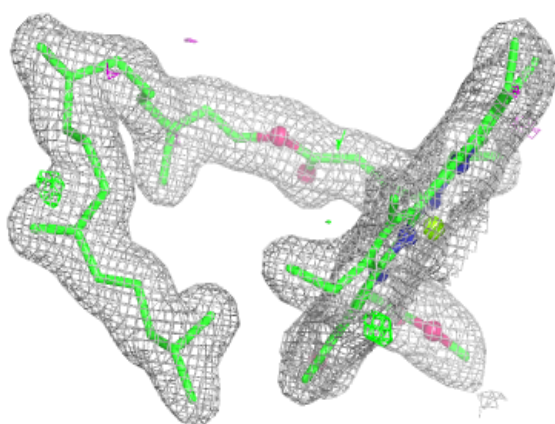
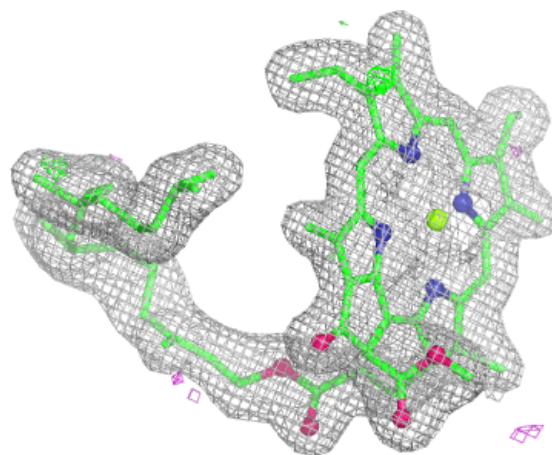
Electron density around CLA c 501:

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



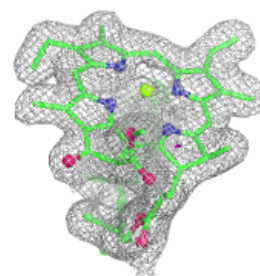
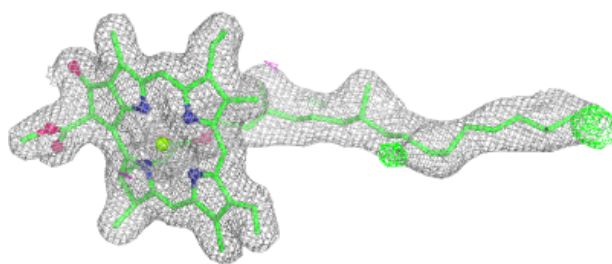
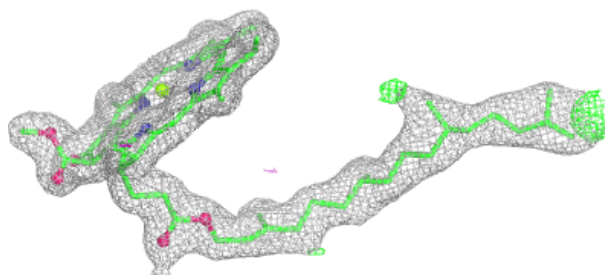
Electron density around CLA c 503:

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

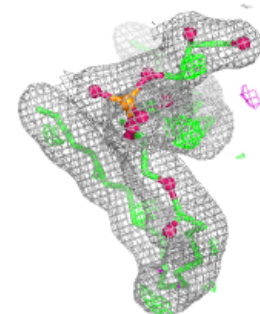
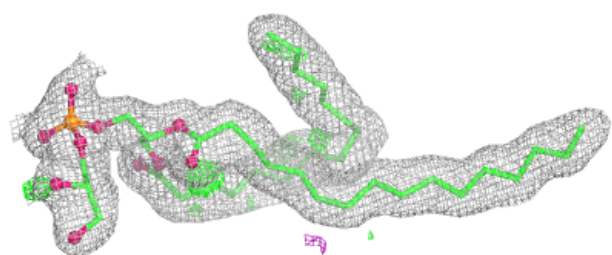
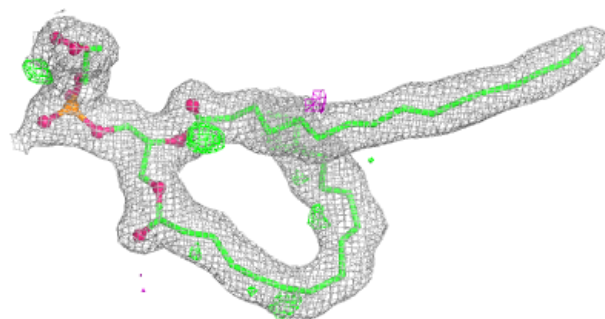


Electron density around CLA c 504:

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

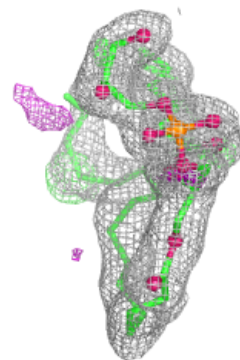
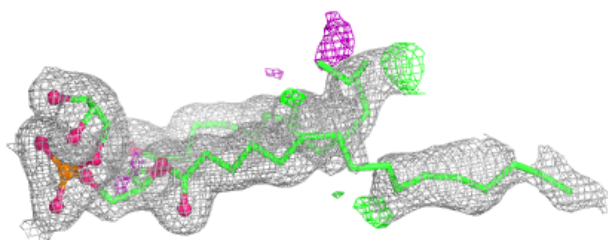
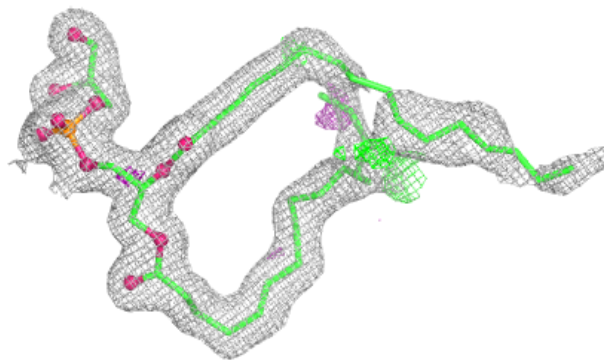
**Electron density around LHG d 406:**

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

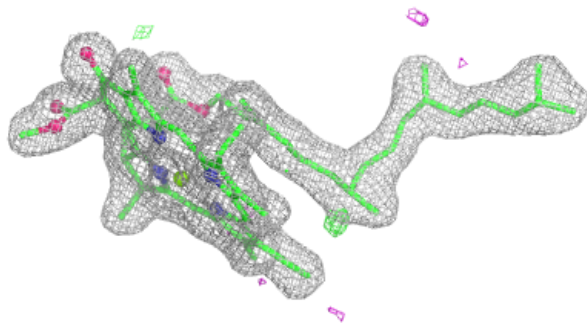
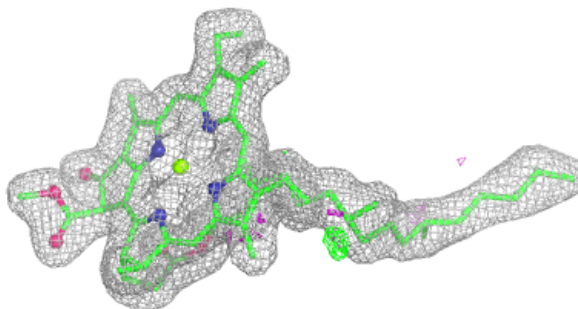


Electron density around LHG d 408:

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

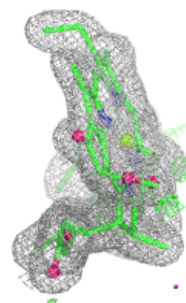
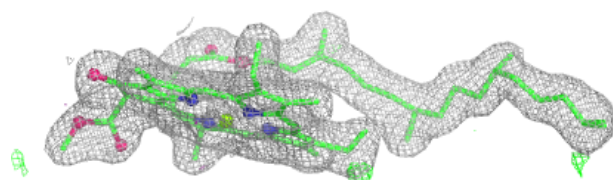
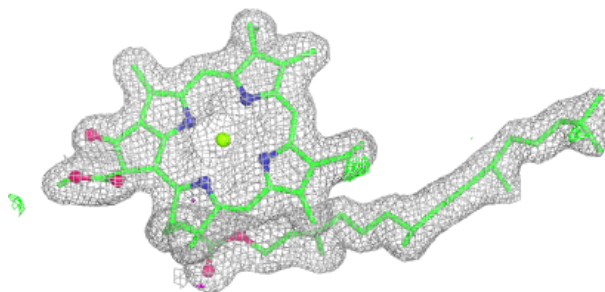
**Electron density around CLA c 505:**

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

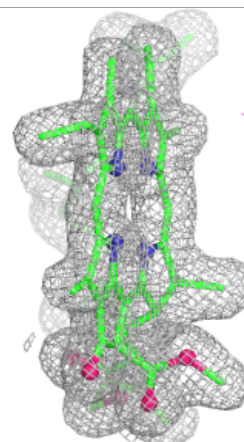
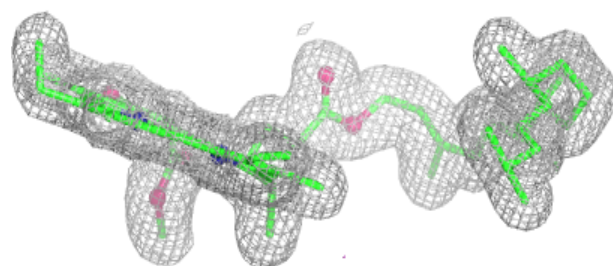
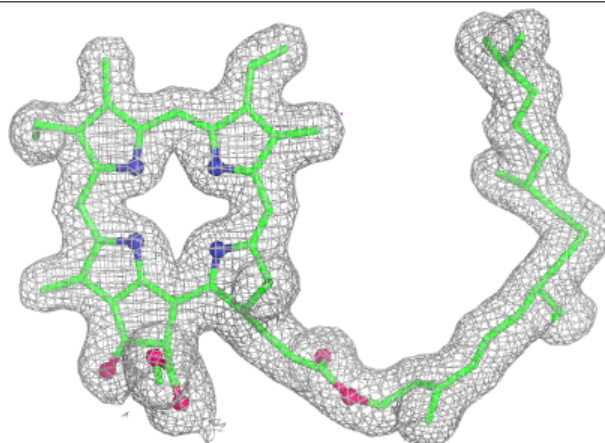


Electron density around CLA C 501:

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

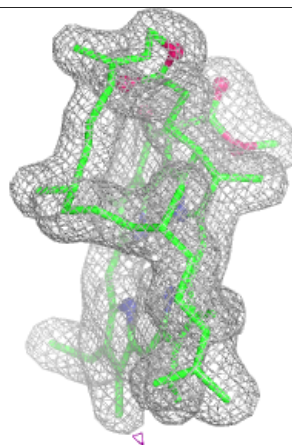
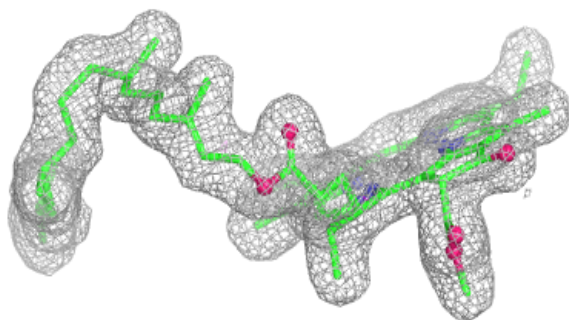
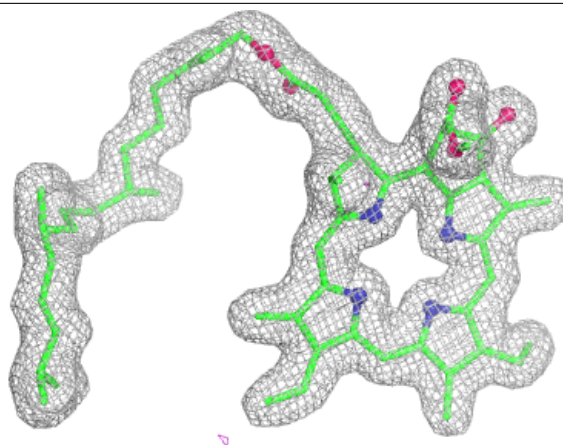
**Electron density around PHO A 403:**

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



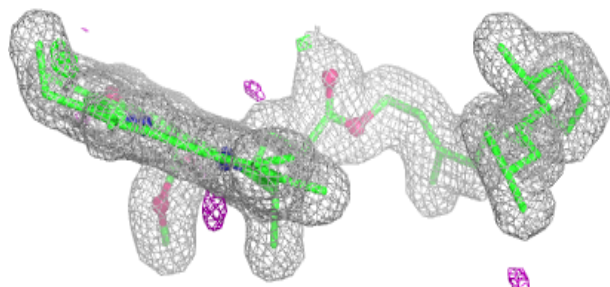
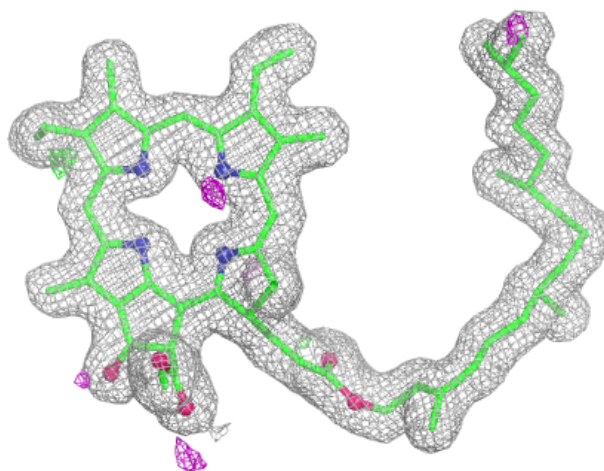
Electron density around PHO D 403:

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



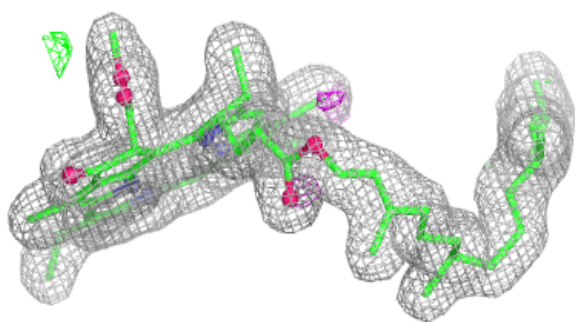
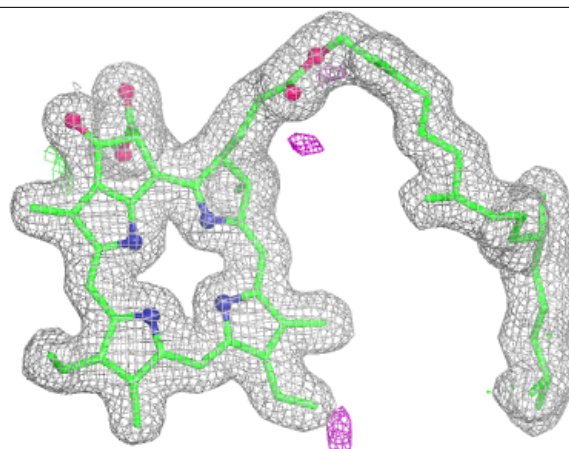
Electron density around PHO a 405:

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



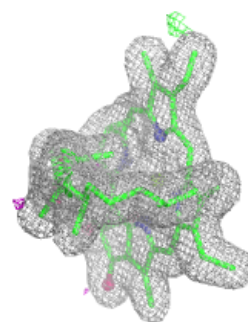
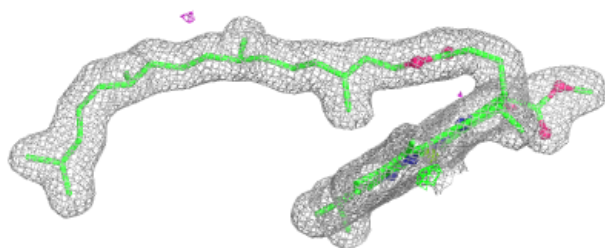
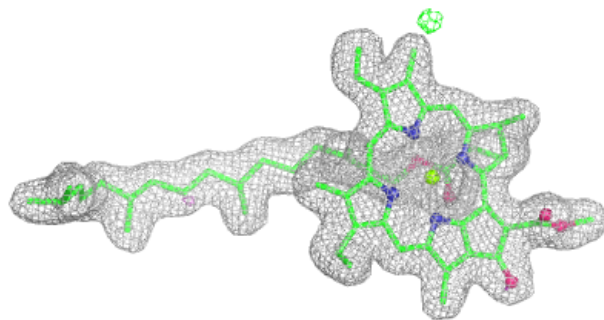
Electron density around PHO a 406:

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

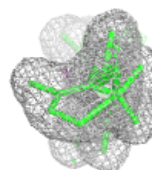
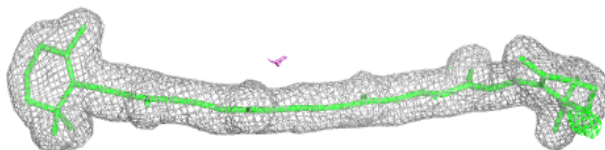
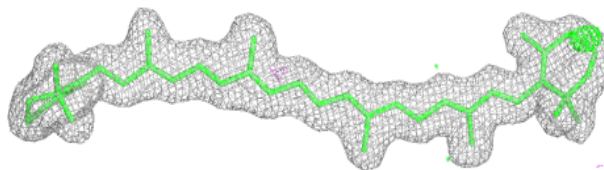


Electron density around CLA b 610:

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

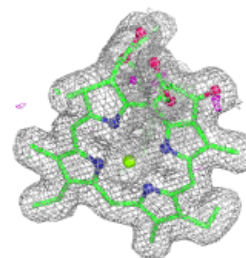
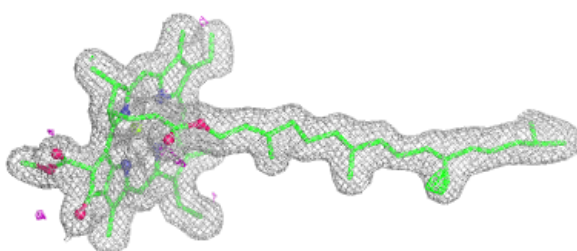
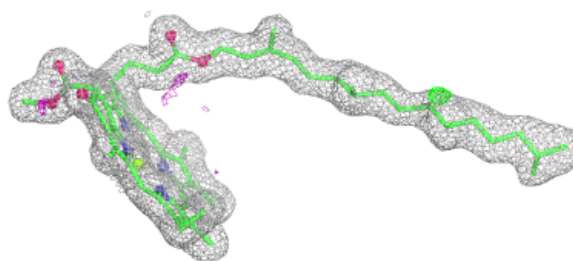
**Electron density around BCR B 617:**

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

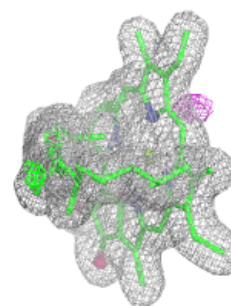
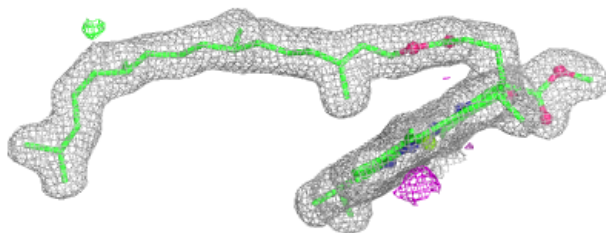
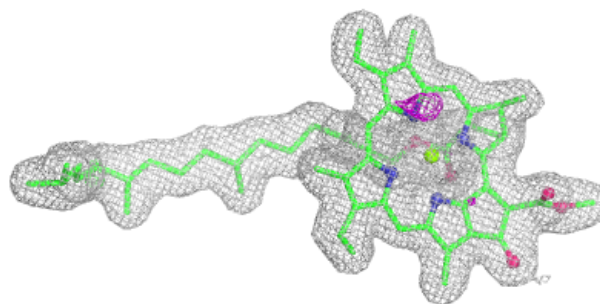


Electron density around CLA B 608:

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

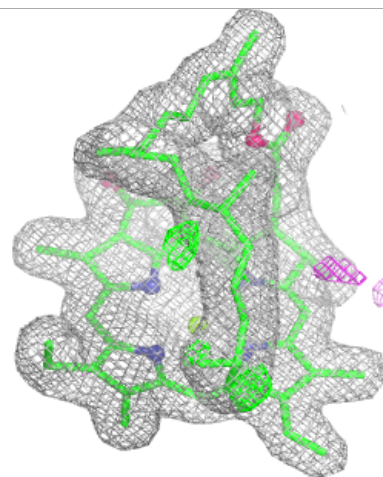
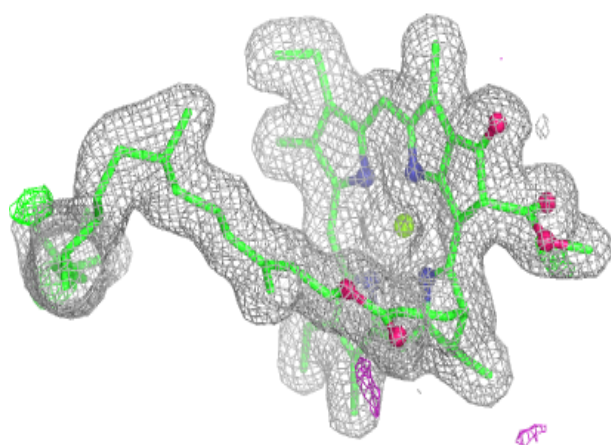
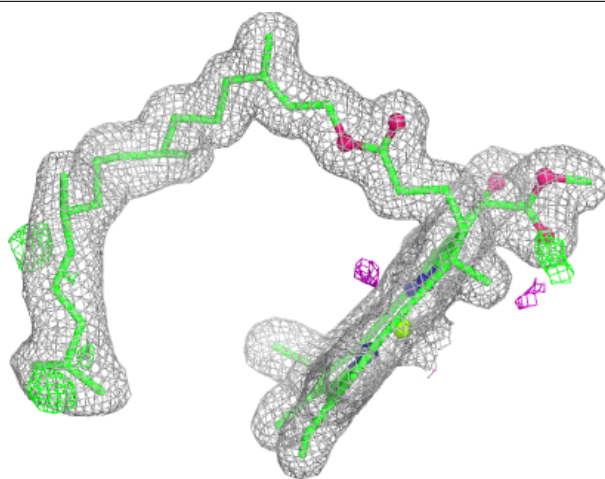
**Electron density around CLA B 609:**

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



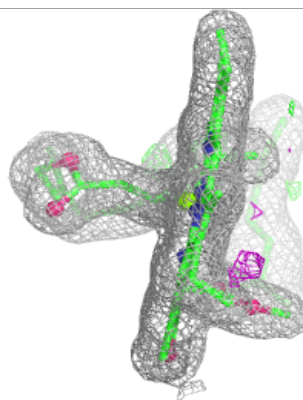
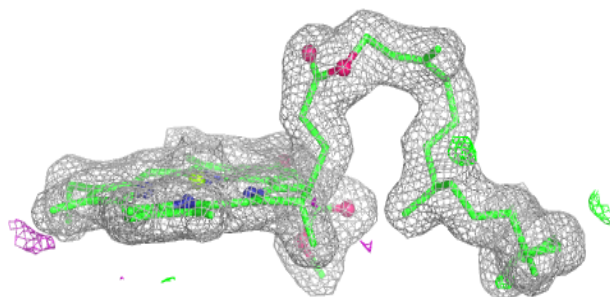
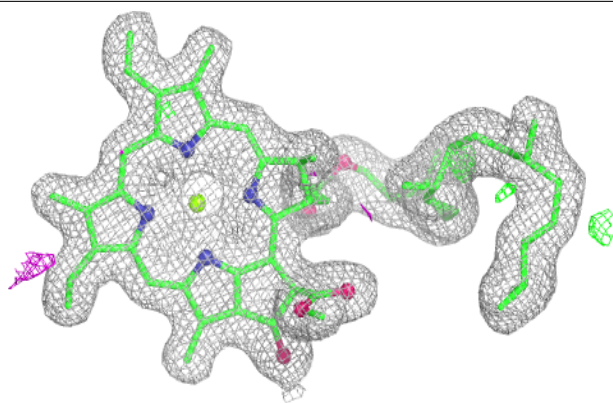
Electron density around CLA b 613:

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

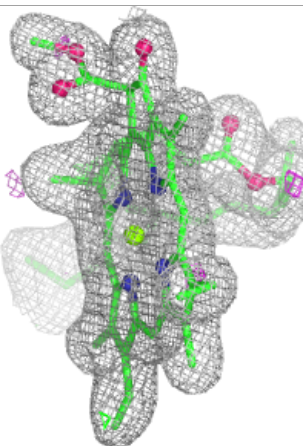
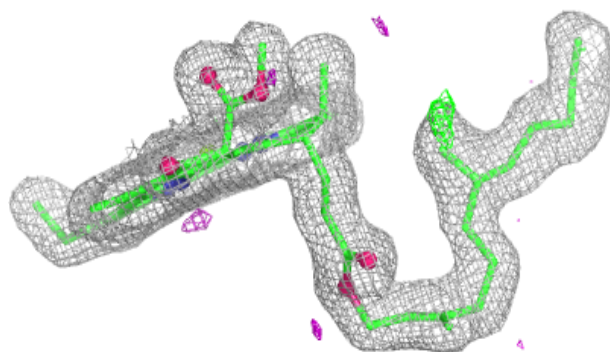
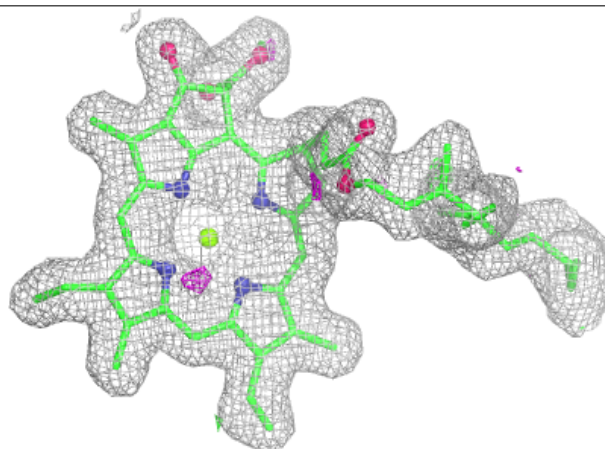


Electron density around CLA b 614:

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

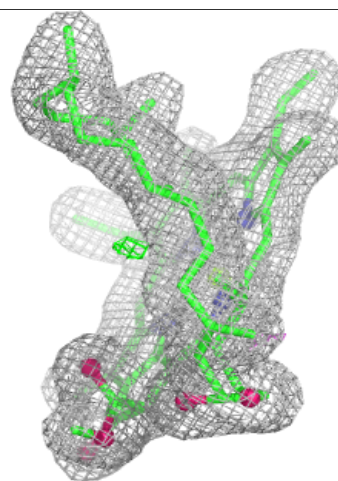
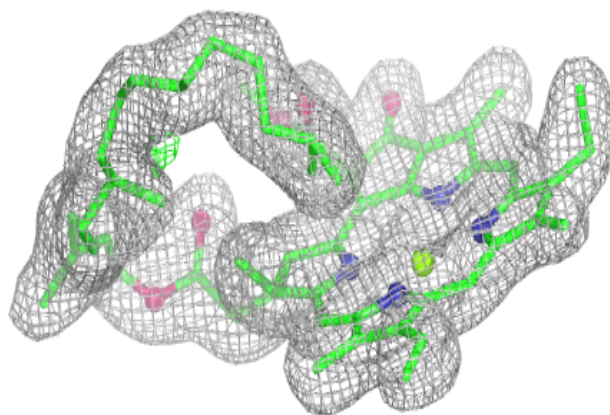
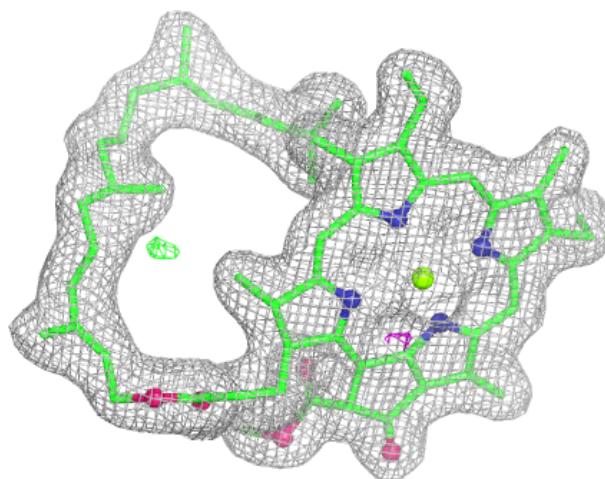
**Electron density around CLA A 402:**

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



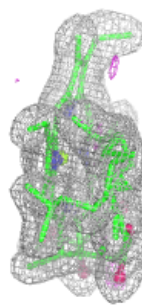
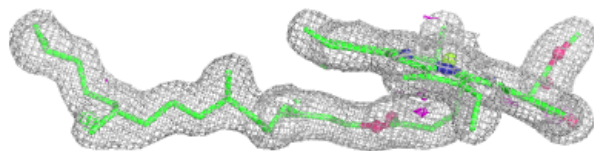
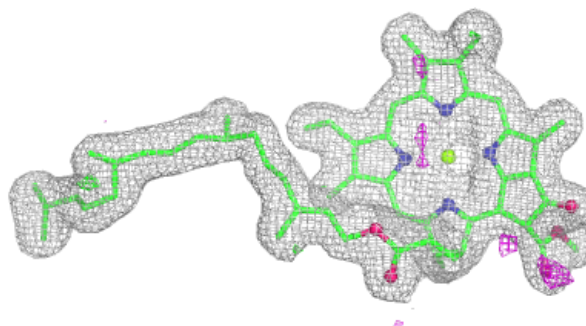
Electron density around CLA b 617:

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



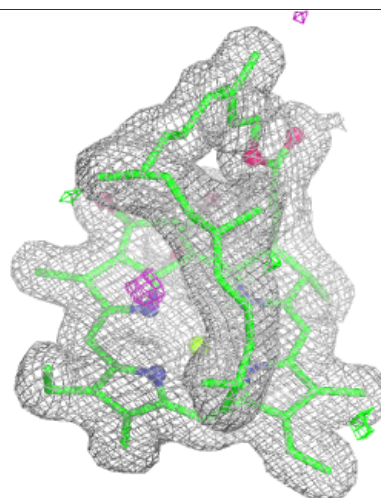
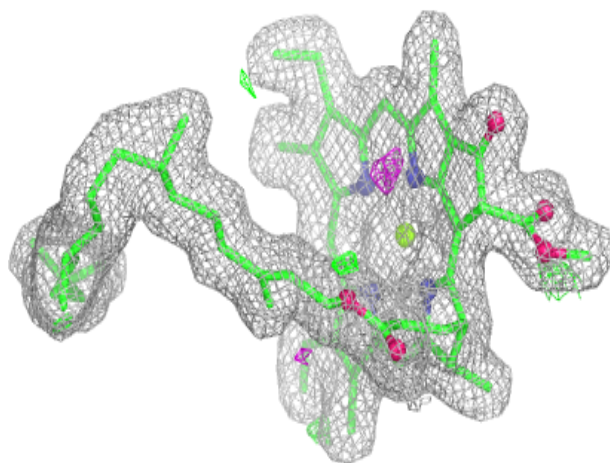
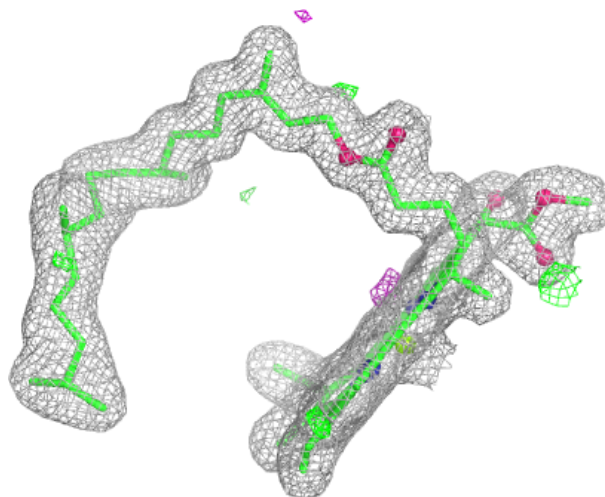
Electron density around CLA B 604:

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



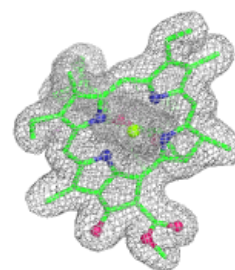
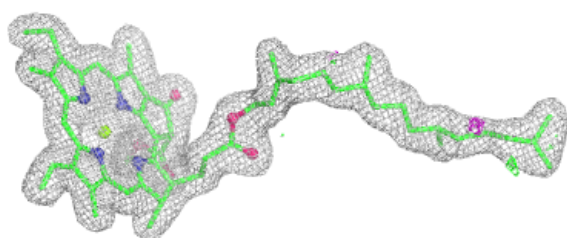
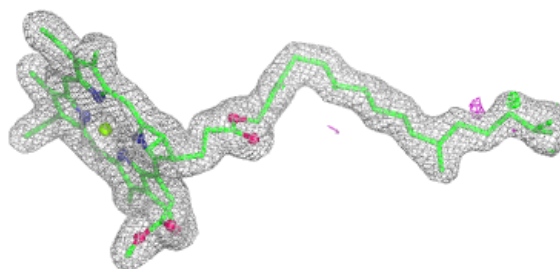
Electron density around CLA B 612:

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

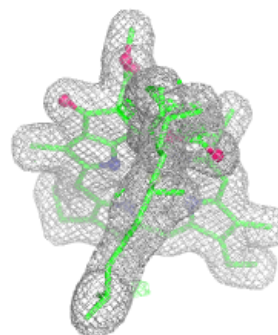
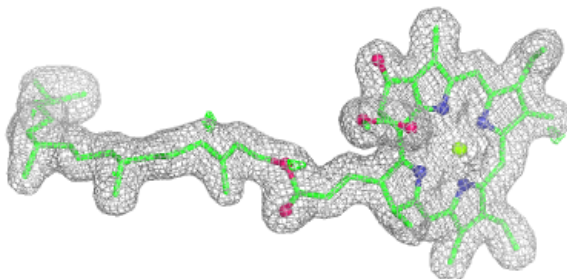
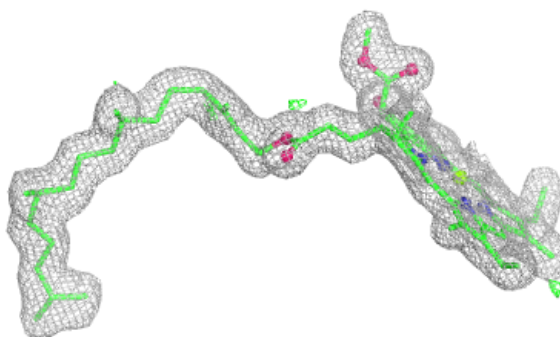


Electron density around CLA c 502:

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

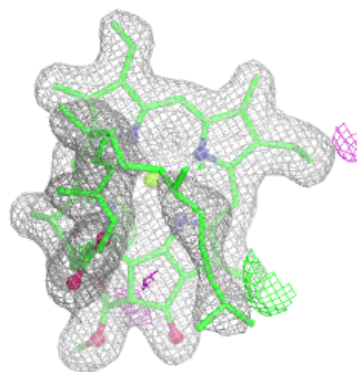
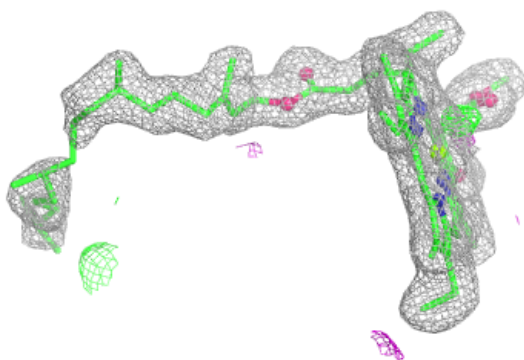
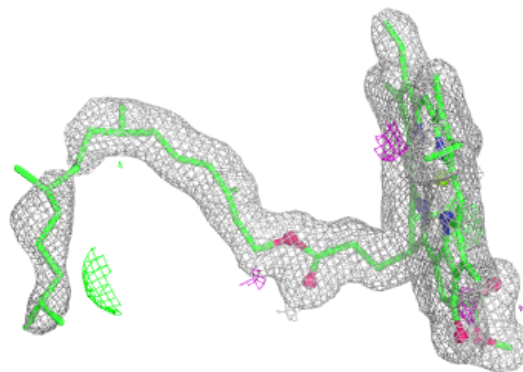
**Electron density around CLA D 401:**

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

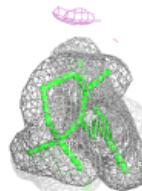
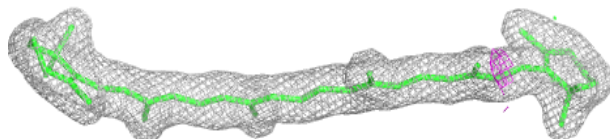
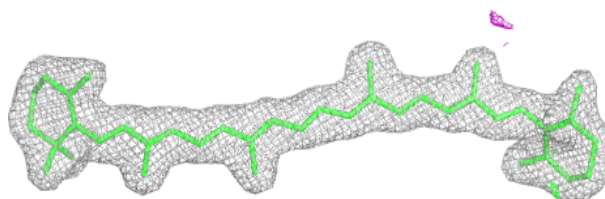


Electron density around CLA D 404:

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

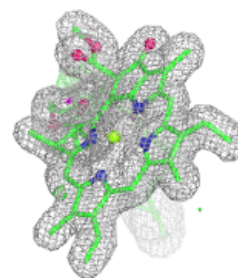
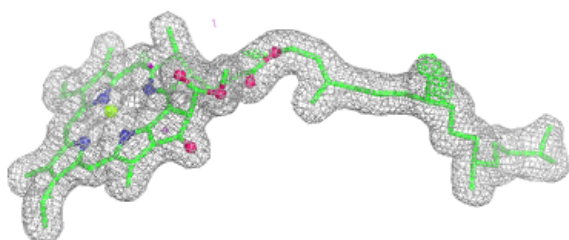
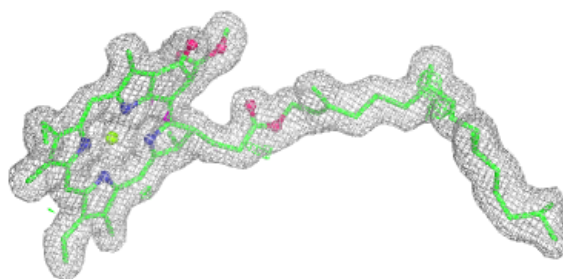
**Electron density around BCR b 621:**

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



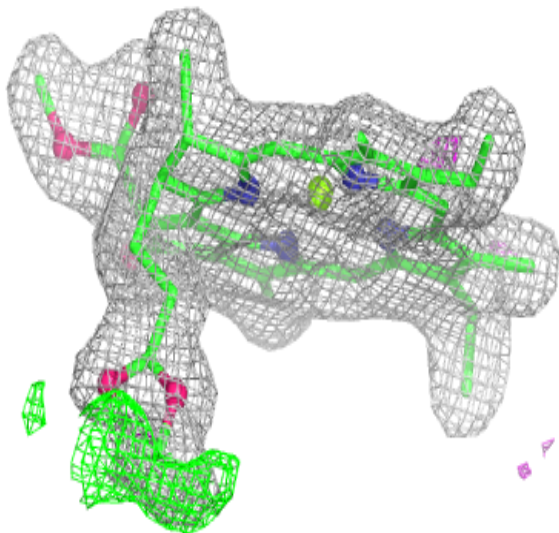
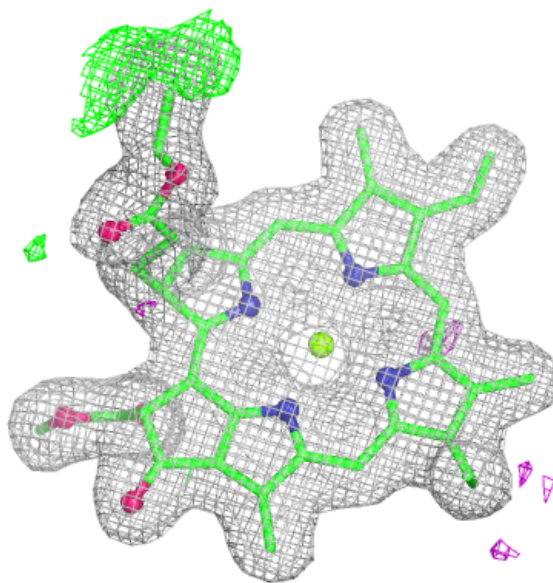
Electron density around CLA a 403:

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



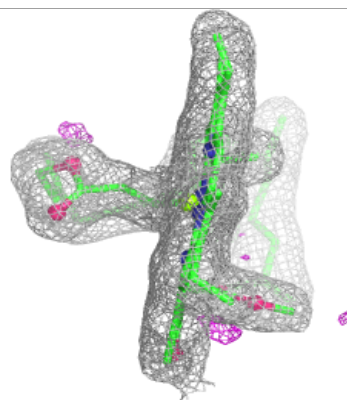
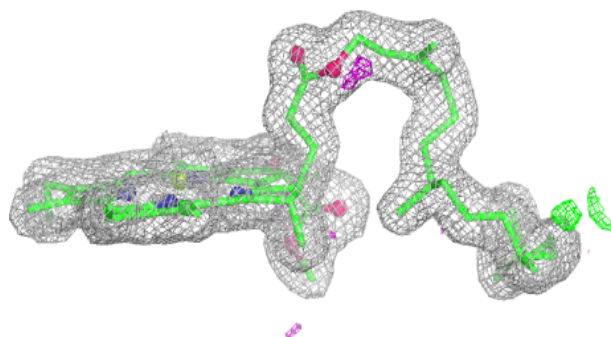
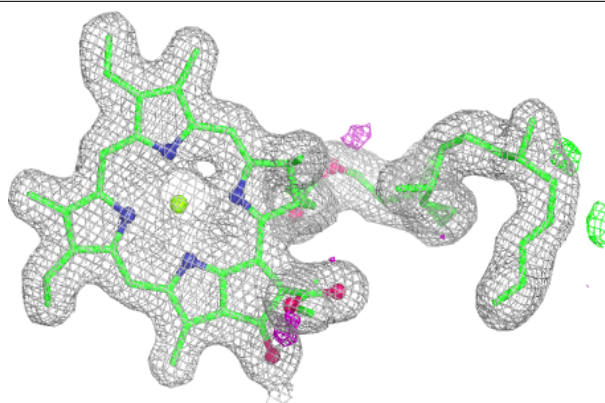
Electron density around CLA a 407:

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

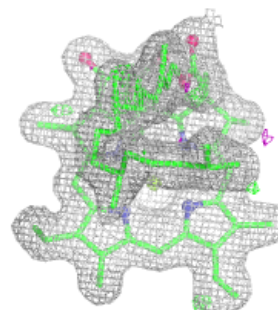
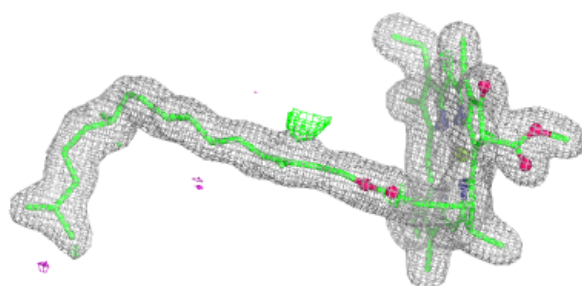
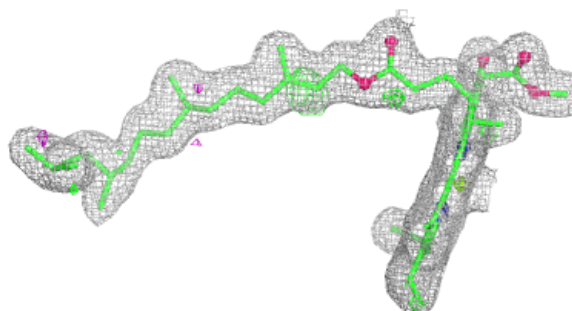


Electron density around CLA B 613:

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

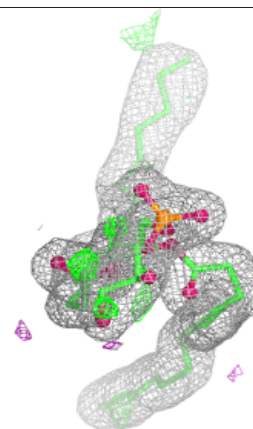
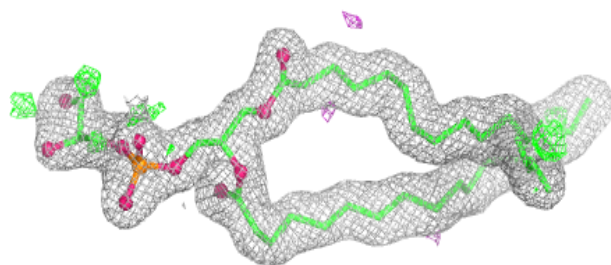
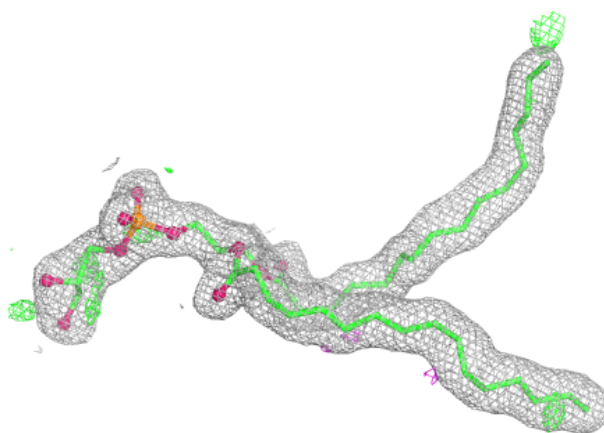
**Electron density around CLA B 606:**

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

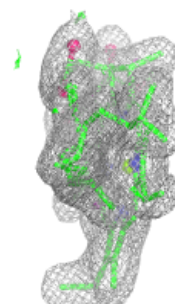
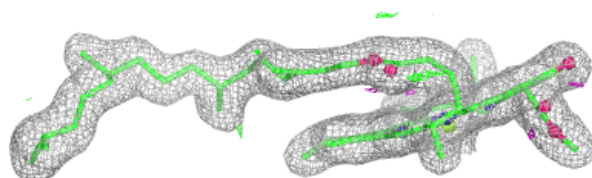
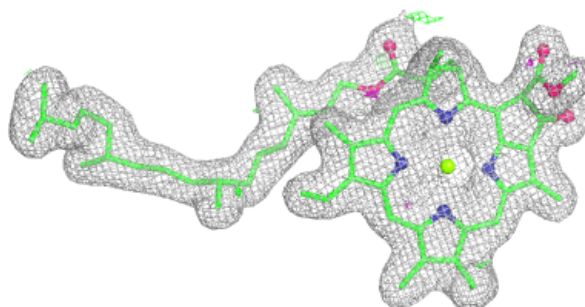


Electron density around LHG D 408:

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

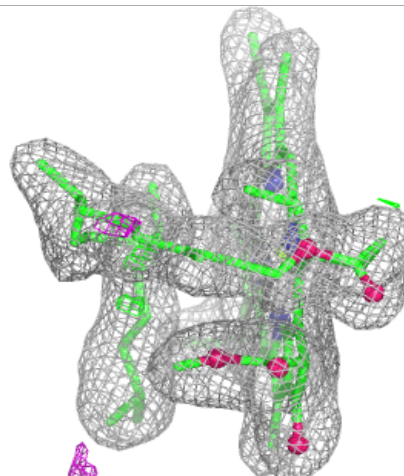
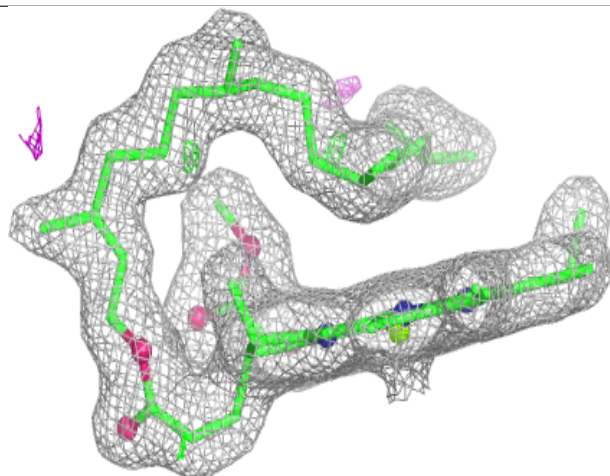
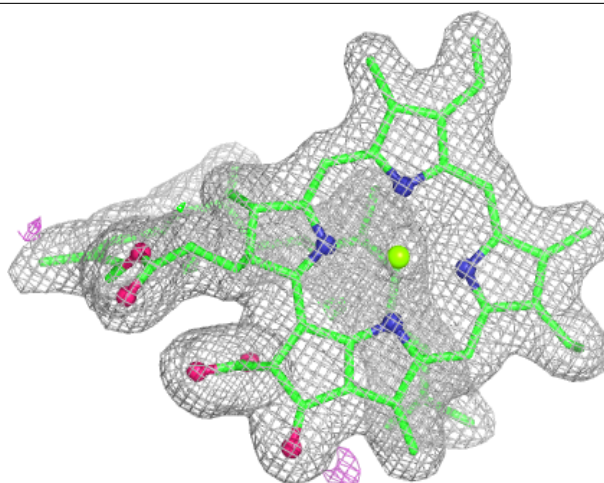
**Electron density around CLA b 605:**

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



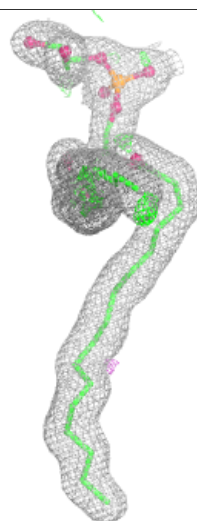
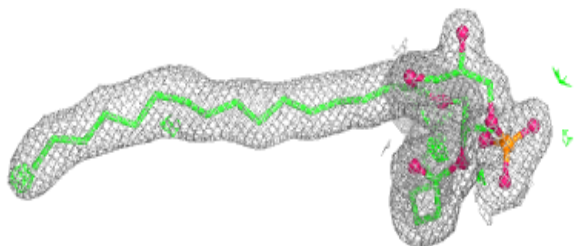
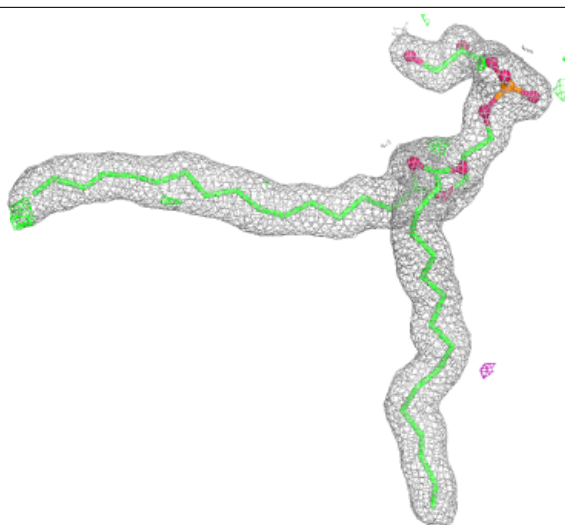
Electron density around CLA c 510:

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



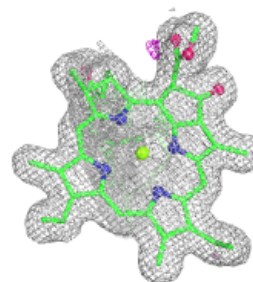
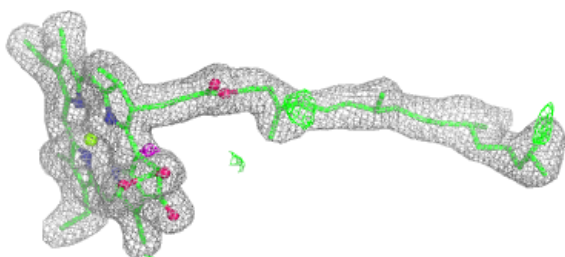
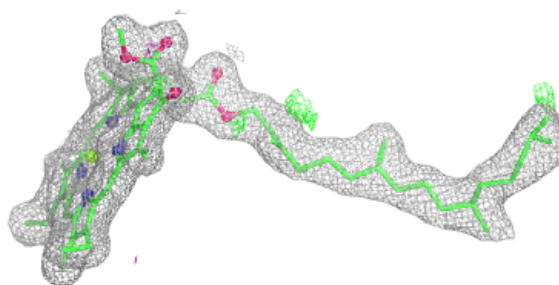
Electron density around LHG L 101:

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



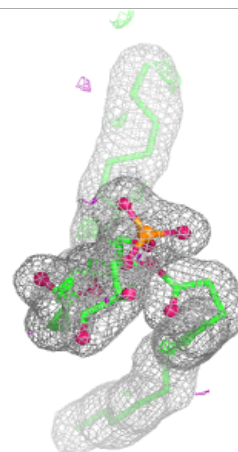
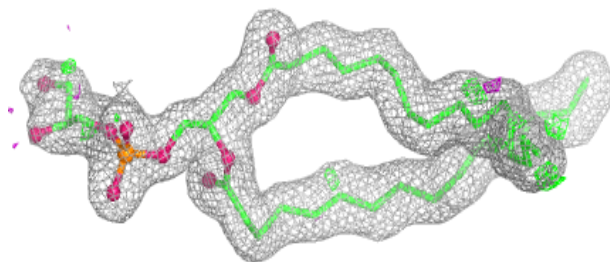
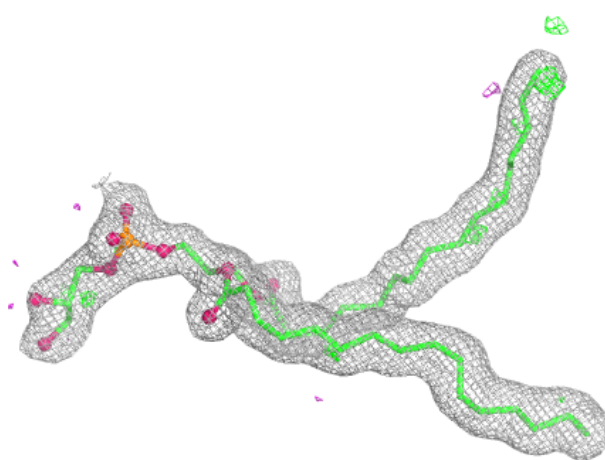
Electron density around CLA b 606:

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



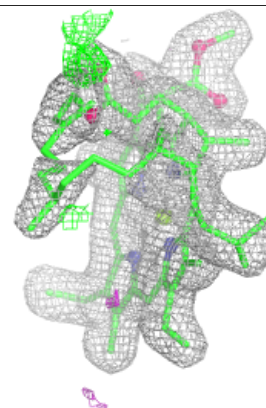
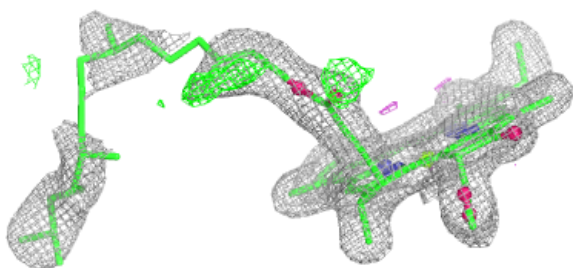
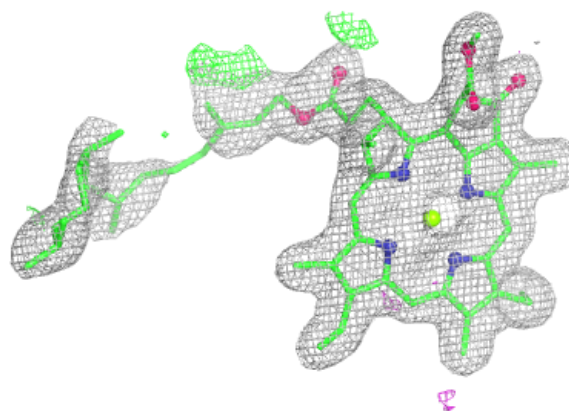
Electron density around LHG d 407:

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



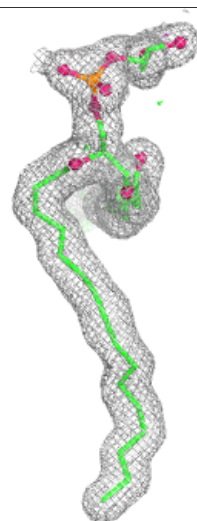
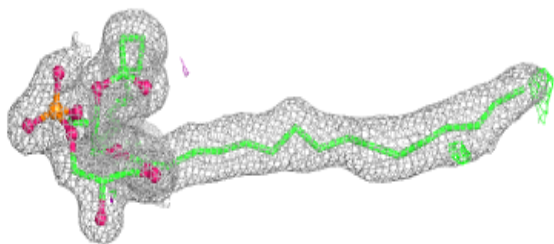
Electron density around CLA A 404:

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



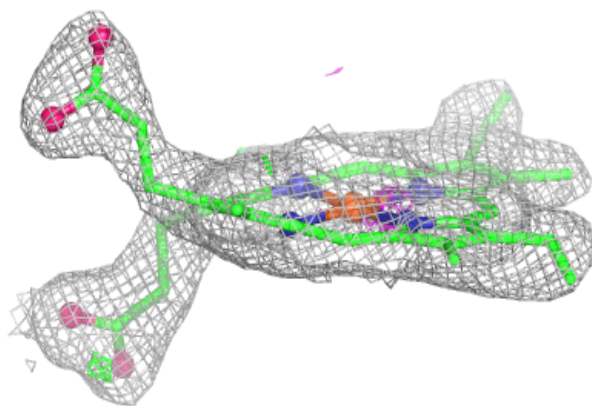
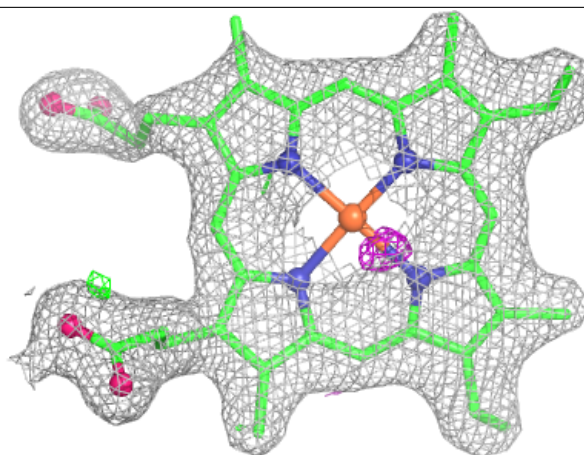
Electron density around LHG 1 102:

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



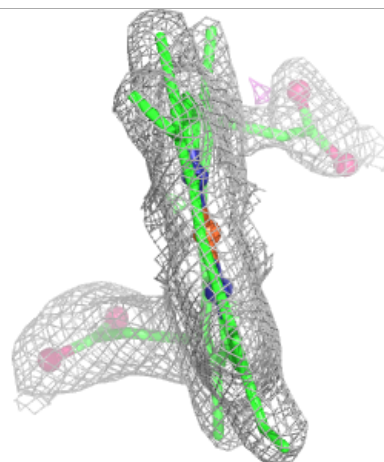
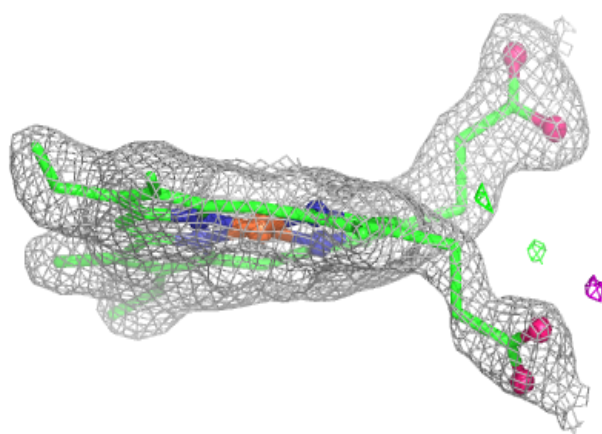
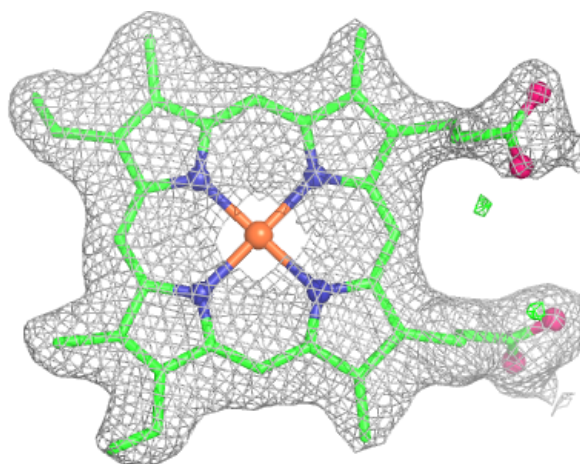
Electron density around HEM E 104:

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



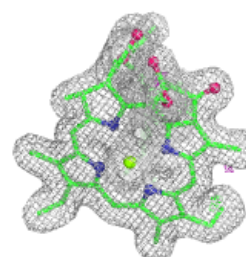
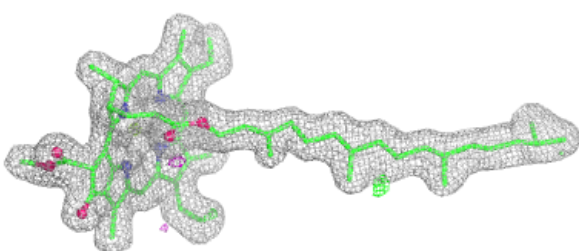
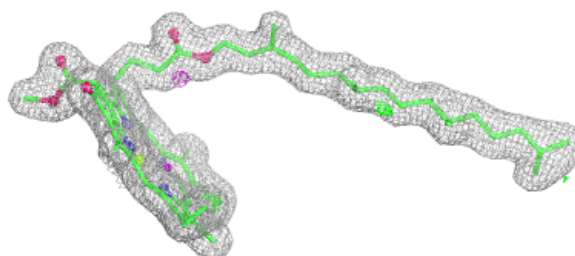
Electron density around HEM e 102:

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

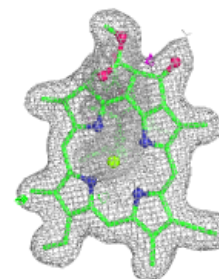
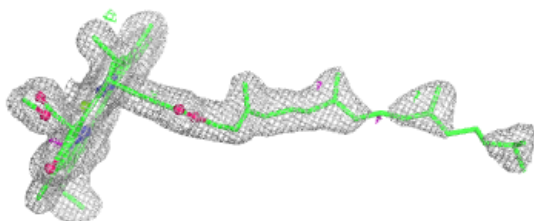
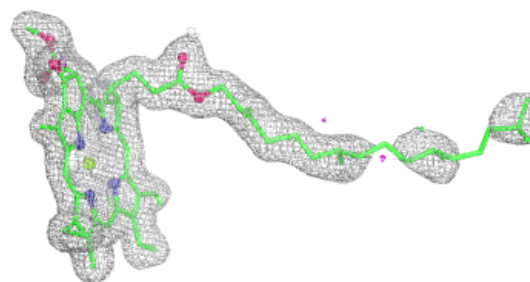


Electron density around CLA b 609:

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

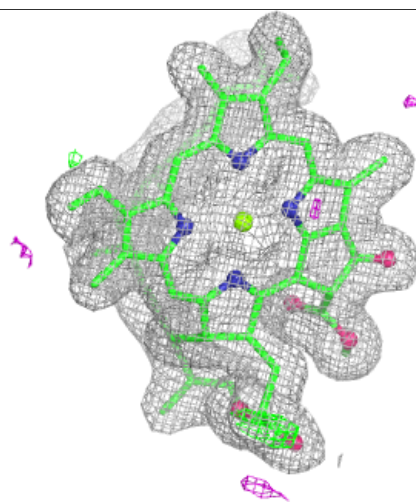
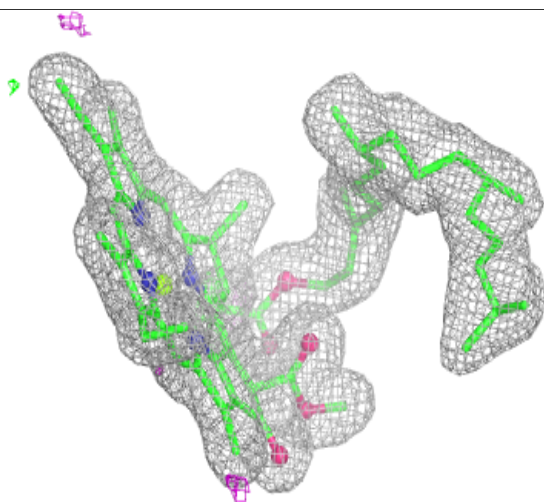
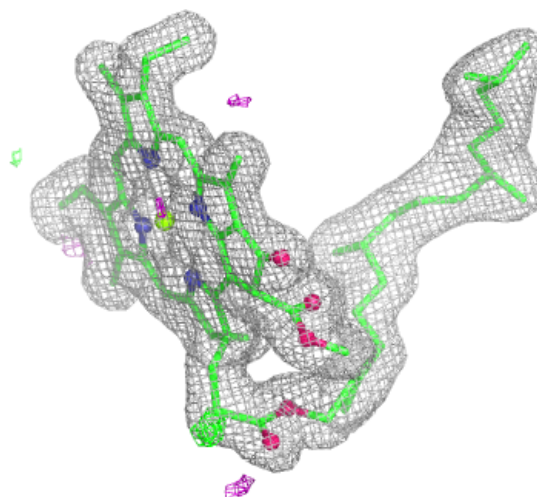
**Electron density around CLA d 404:**

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



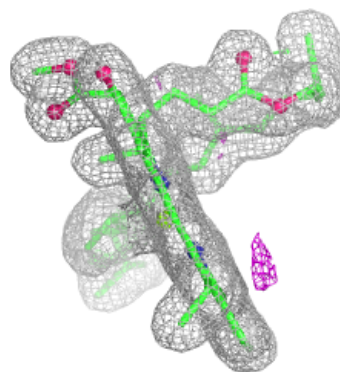
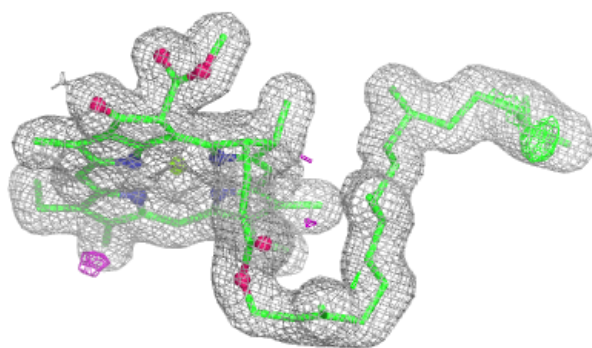
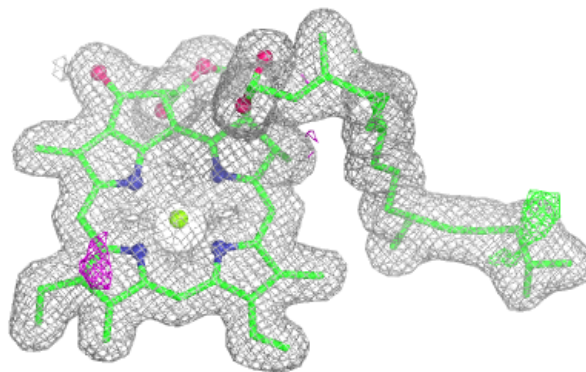
Electron density around CLA b 615:

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

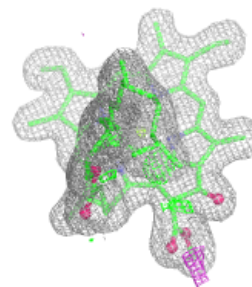
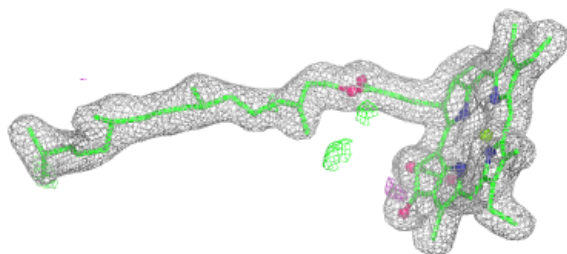
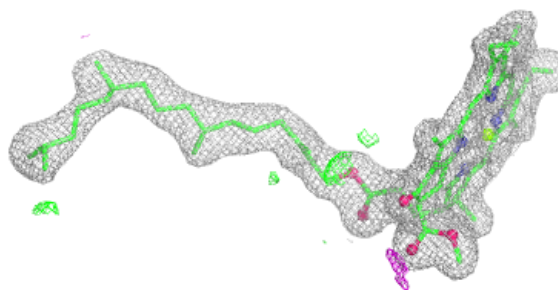


Electron density around CLA D 402:

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

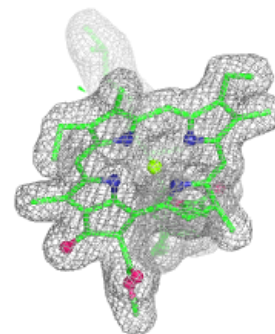
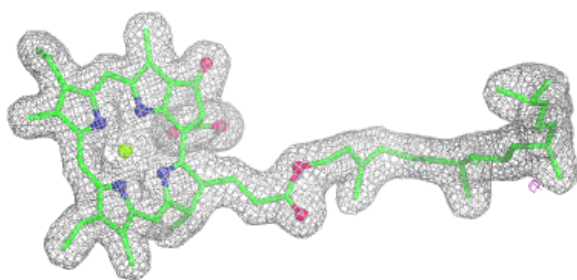
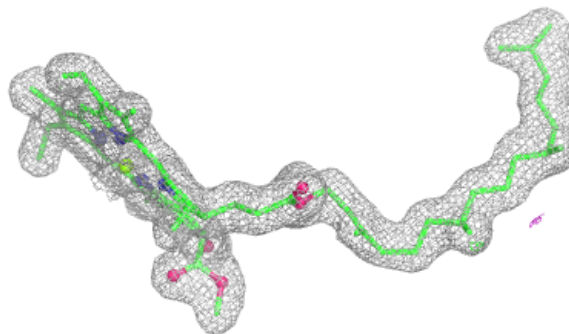
**Electron density around CLA B 605:**

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

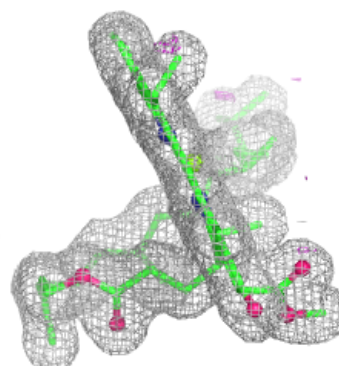
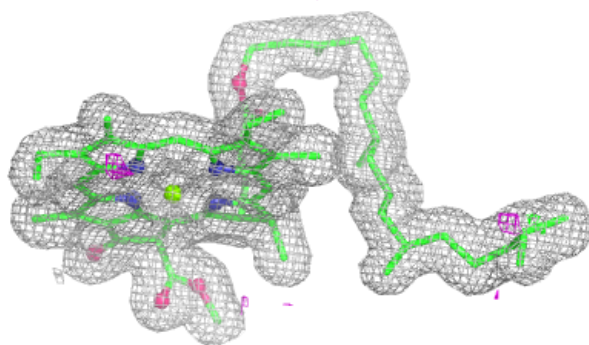
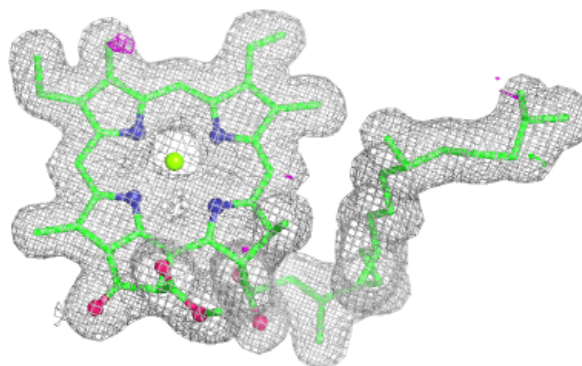


Electron density around CLA d 402:

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

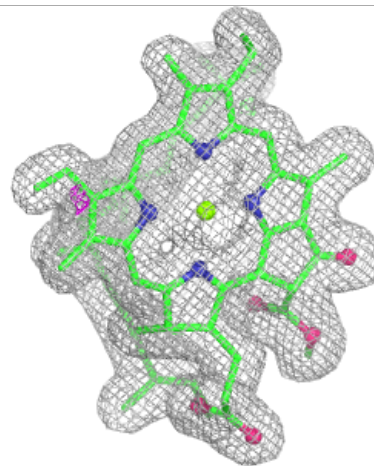
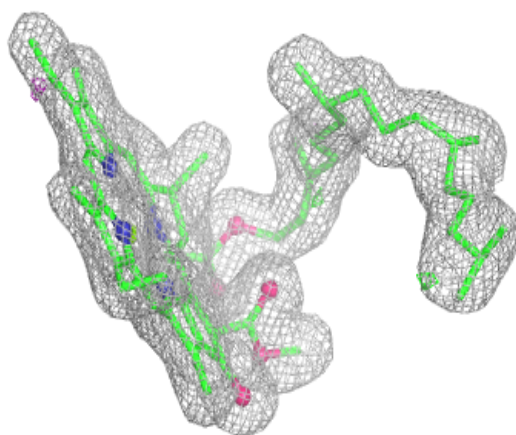
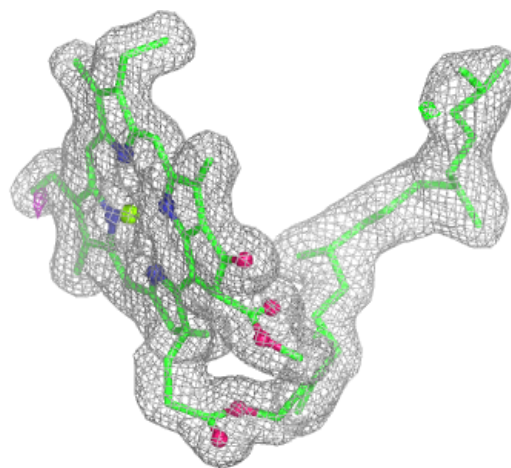
**Electron density around CLA d 403:**

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



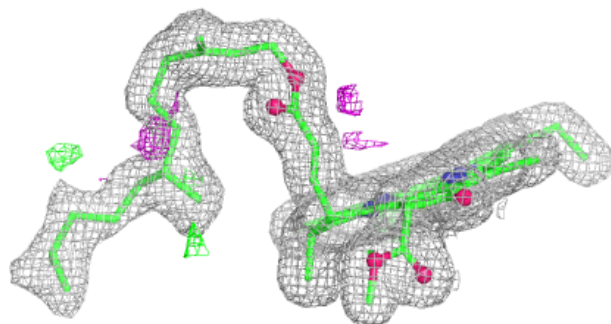
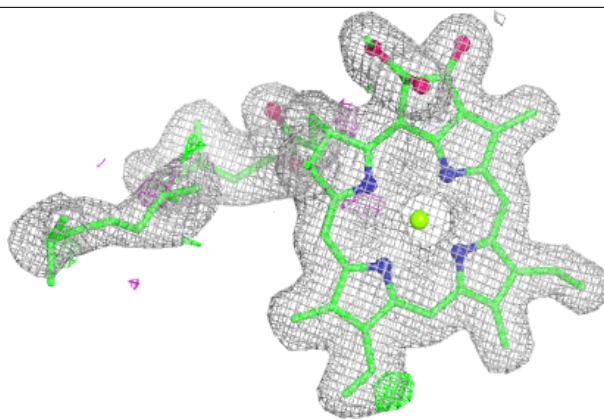
Electron density around CLA B 614:

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

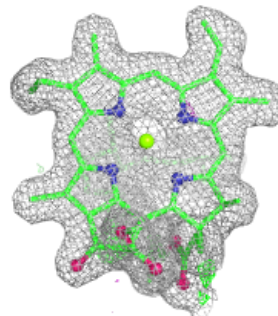
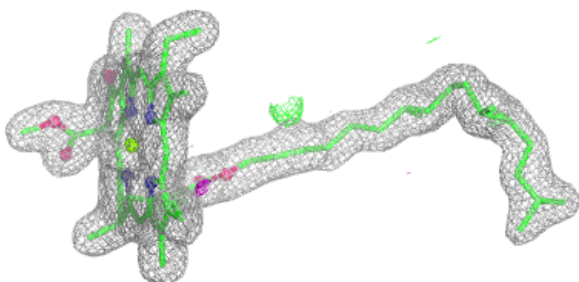
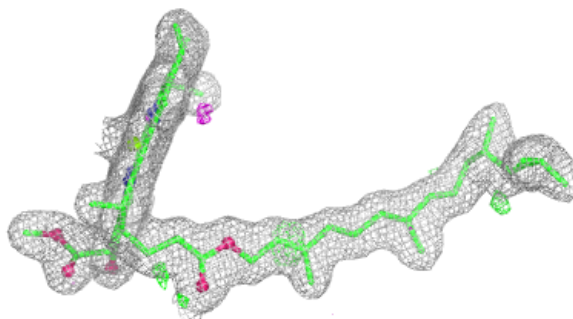


Electron density around CLA a 404:

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

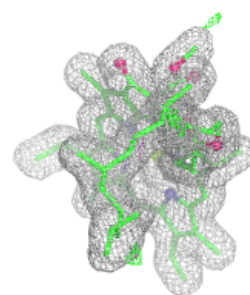
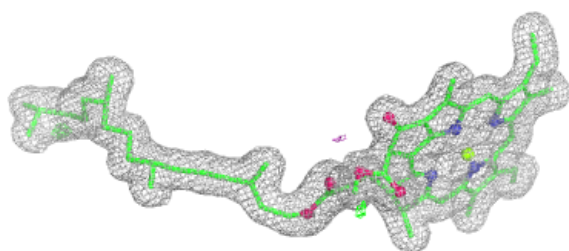
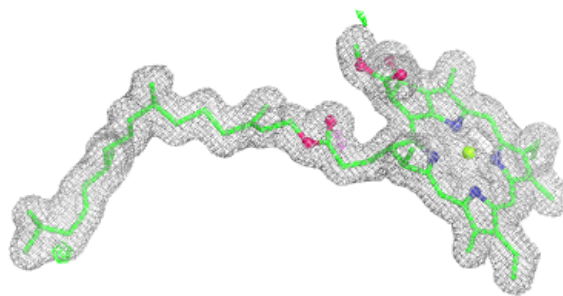
**Electron density around CLA b 607:**

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



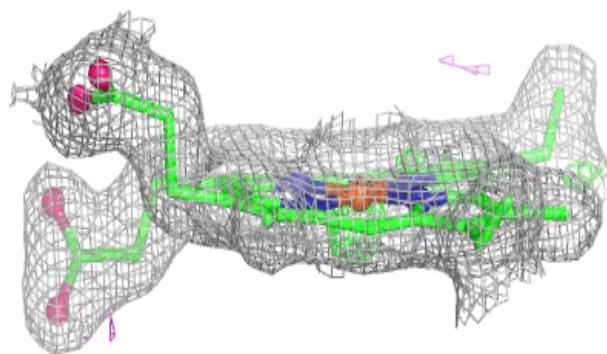
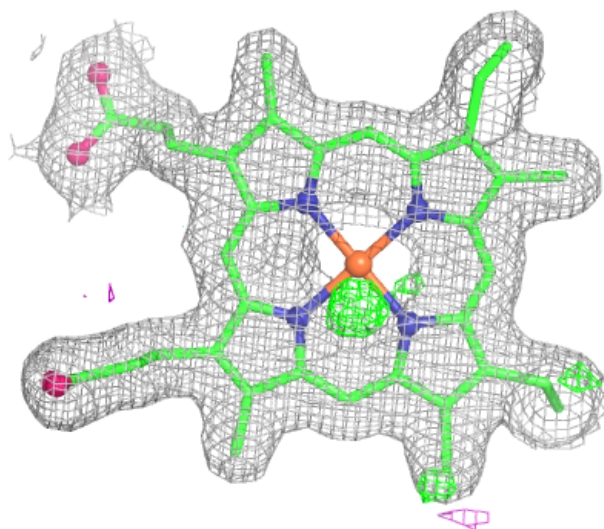
Electron density around CLA A 401:

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



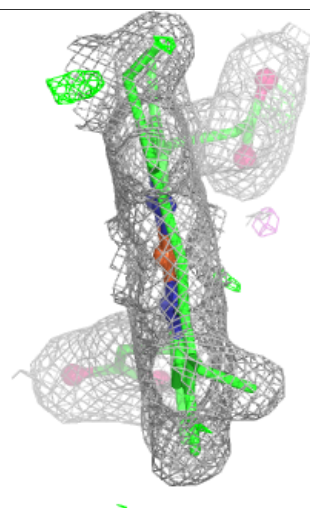
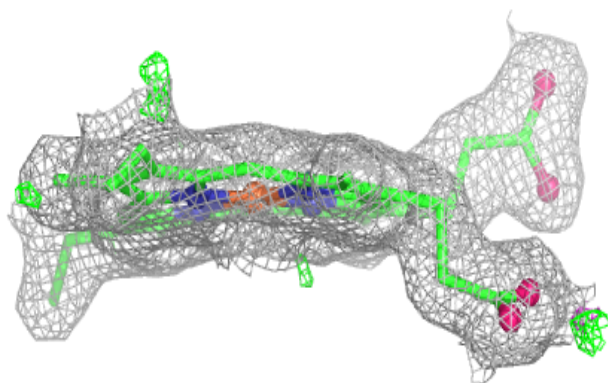
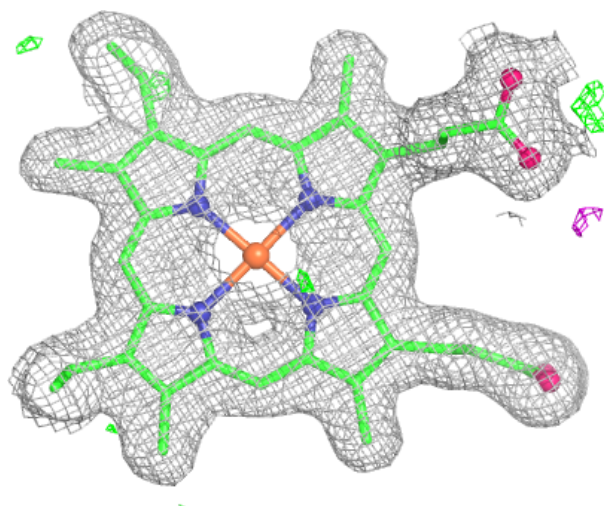
Electron density around HEC v 201:

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



Electron density around HEC V 201:

$2mF_o-DF_c$ (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.