



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:59 AM EDT

PDB ID : 7RF8 / pdb_00007rf8
Title : RT XFEL structure of the two-flash state of Photosystem II (2F, S3-rich) at 2.09 Angstrom resolution
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Deposited on : 2021-07-13
Resolution : 2.09 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	:	2022.3.0, CSD as543be (2022)
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)

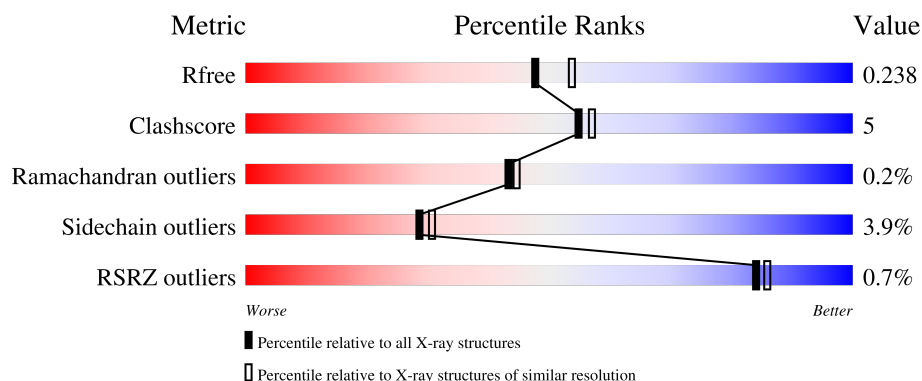
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

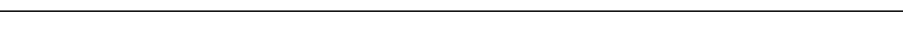
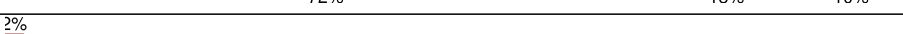
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 85% 11% ..
1	a	344	 81% 15% ..

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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

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Mol	Chain	Length	Quality of chain
2	B	510	
2	b	510	
3	C	461	
3	c	461	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	46	
10	k	46	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	272	
13	o	272	
14	R	41	

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Mol	Chain	Length	Quality of chain
14	r	41	
15	T	32	
15	t	32	
16	U	134	
16	u	134	
17	V	163	
17	v	163	
18	X	41	
18	x	41	
19	Y	46	
19	y	46	
20	Z	62	
20	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
36	HEC	V	201	X	-	-	-
36	HEC	v	201	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105937 atoms, of which 52685 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	334	Total	C	H	N	O	S	0	66	0
			6098	2030	2985	513	551	19			
1	a	334	Total	C	H	N	O	S	0	66	0
			6086	2027	2976	513	551	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7878	2631	3873	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7814	2610	3836	665	690	13			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	442	Total	C	H	N	O	S	0	14	0
			6941	2302	3432	586	607	14			
3	c	451	Total	C	H	N	O	S	0	14	0
			7086	2343	3503	602	624	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	2	0
			5368	1809	2637	446	464	12			
4	d	341	Total	C	H	N	O	S	0	3	0
			5380	1813	2643	446	466	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	82	Total	C	H	N	O	16	1	0
			1317	436	651	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1312	434	648	108	122			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			557	187	282	45	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	H	N	O	0	0	0
			1042	341	532	82	85			
7	h	63	Total	C	H	N	O	0	0	0
			1016	333	518	80	83			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			
8	i	36	Total	C	H	N	O	0	0	0
			607	200	311	46	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			
9	j	36	Total	C	H	N	O	0	0	0
			525	174	268	40	42			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	K	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	0	0	0
			620	202	316	48	53			
11	l	36	Total	C	H	N	O	0	0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	0	0	0
			525	171	269	37	47			
12	m	32	Total	C	H	N	O	0	0	0
			518	168	267	36	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	1	FME	-	initiating methionine	UNP Q8DHA7
m	1	FME	-	initiating methionine	UNP Q8DHA7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	0	1	0
			3700	1168	1830	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3720	1170	1846	317	383			

- Molecule 14 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			
14	r	28	Total	C	H	N	O	0	0	0
			459	151	238	38	32			

- Molecule 15 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	30	Total	C	H	N	O	S	0	0	0
			519	181	261	36	39	2			
15	t	30	Total	C	H	N	O	S	0	0	0
			512	180	256	36	38	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	FME	-	initiating methionine	UNP Q8DIQ0
t	1	FME	-	initiating methionine	UNP Q8DIQ0

- Molecule 16 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
16	U	97	Total	C	H	N	O		0	0	0
			1547	491	773	129	154				
16	u	97	Total	C	H	N	O		0	0	0
			1547	491	773	129	154				

- Molecule 17 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			
17	v	137	Total	C	H	N	O	S	0	0	0
			2135	675	1071	177	208	4			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
18	X	38	Total	C	H	N	O		0	0	0
			593	188	312	45	48				
18	x	39	Total	C	H	N	O		0	0	0
			602	191	316	46	49				

- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
19	Y	27	Total	C	H	N	O	S	0	0	0
			413	128	217	35	30	3			
19	y	30	Total	C	H	N	O	S	0	0	0
			459	144	241	35	36	3			

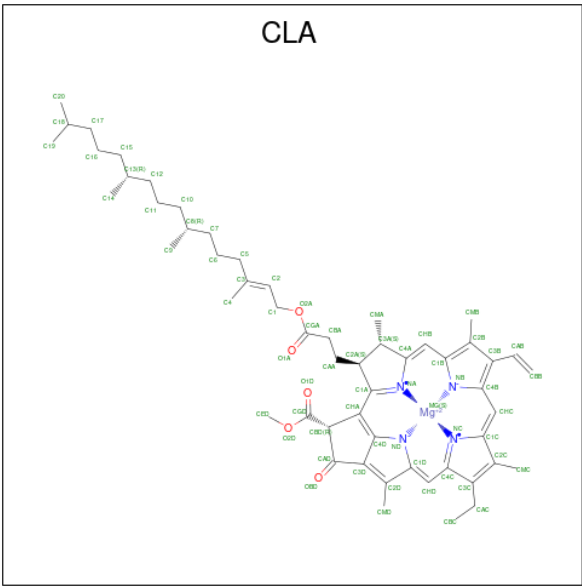
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0	0
			995	328	516	72	77	2			
20	z	62	Total	C	H	N	O	S	0	0	0
			986	326	509	72	77	2			

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
22	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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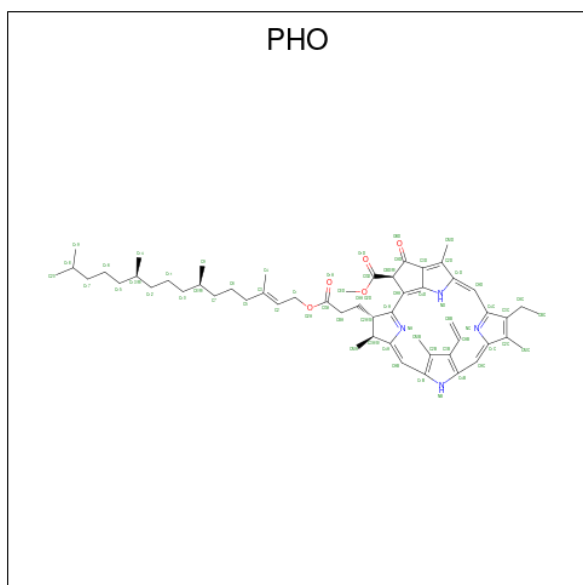
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			132	54	68	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	c	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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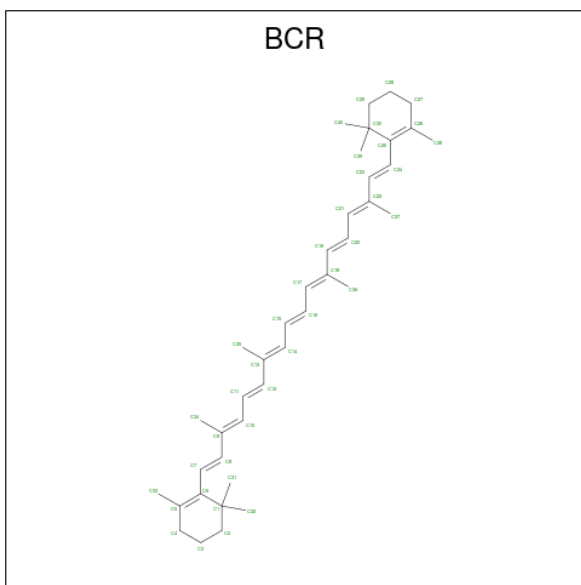
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	A	1	Total 96	C 40	H 56	0	0
24	B	1	Total 96	C 40	H 56	0	0
24	B	1	Total 96	C 40	H 56	0	0
24	B	1	Total 96	C 40	H 56	0	0
24	C	1	Total 96	C 40	H 56	0	0
24	C	1	Total 96	C 40	H 56	0	0
24	D	1	Total 96	C 40	H 56	0	0
24	H	1	Total 96	C 40	H 56	0	0
24	K	1	Total 96	C 40	H 56	0	0
24	T	1	Total 96	C 40	H 56	0	0
24	Y	1	Total 96	C 40	H 56	0	0
24	a	1	Total 96	C 40	H 56	0	0
24	b	1	Total 96	C 40	H 56	0	0
24	b	1	Total 96	C 40	H 56	0	0

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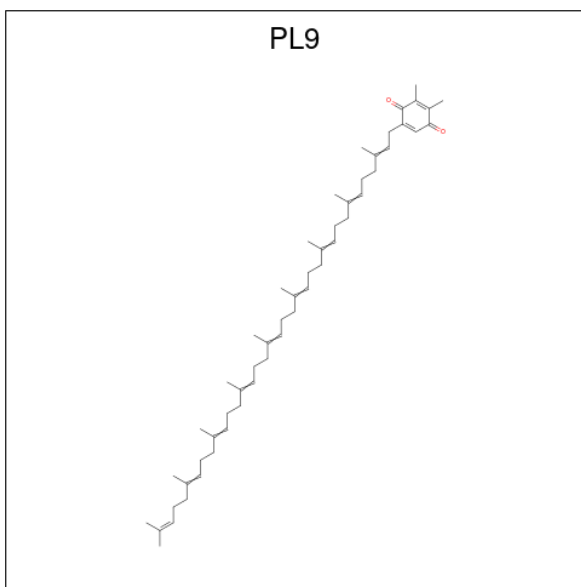
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		

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

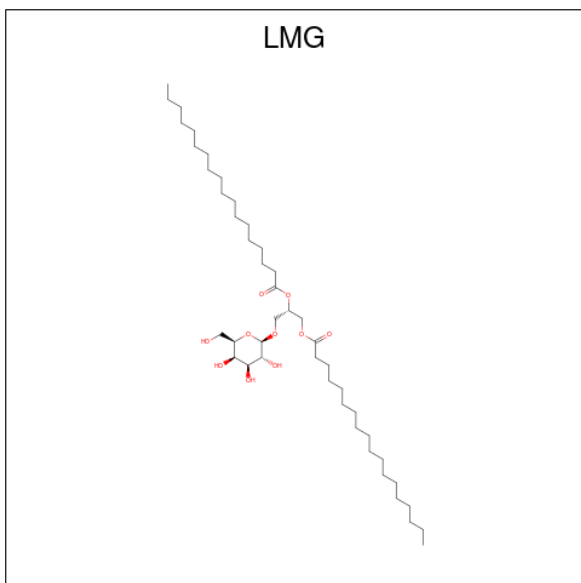
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 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).



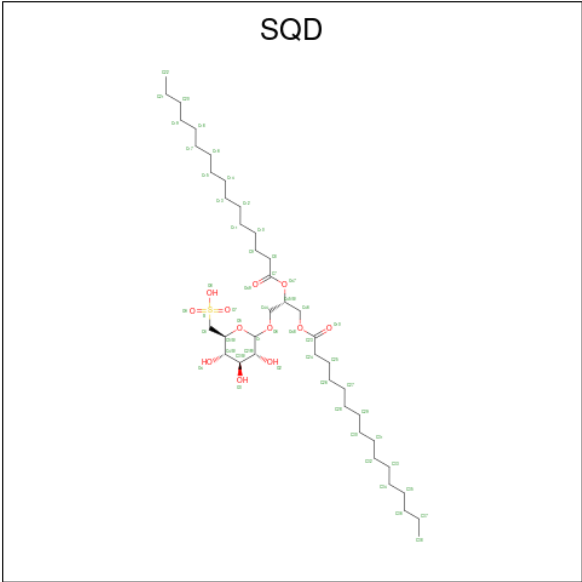
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



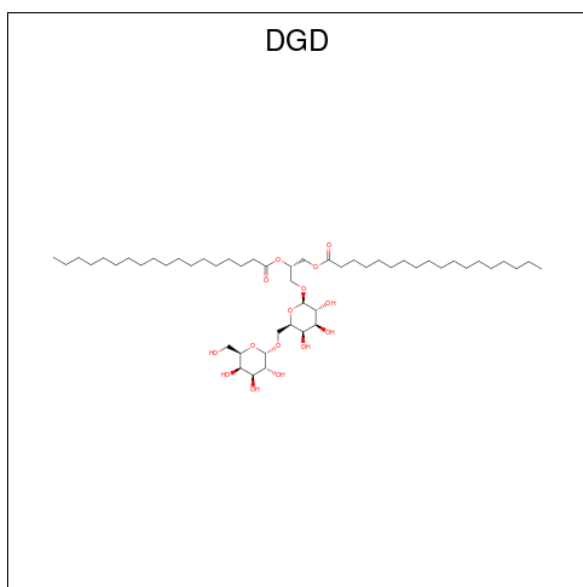
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	B	1	Total	C	H	O	0	0
			68	24	40	4		
27	C	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			123	41	72	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			57	21	34	2		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



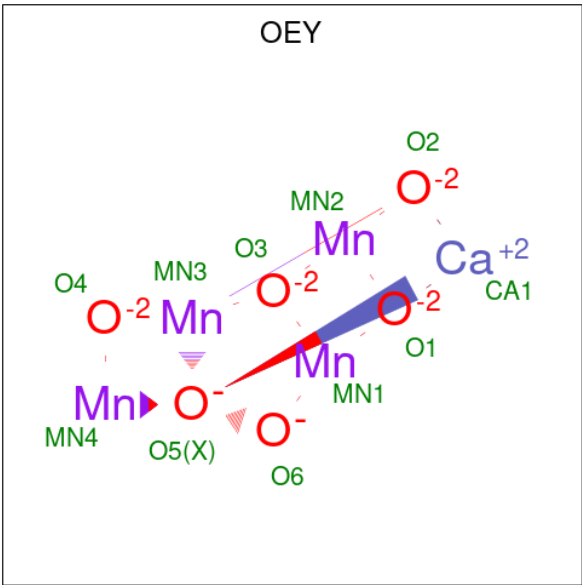
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



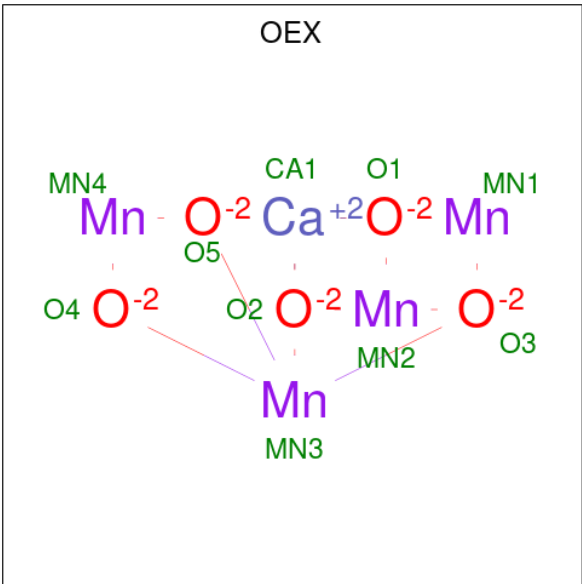
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	a	1	Total	C	H	O	0	0
			119	39	75	5		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
30	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



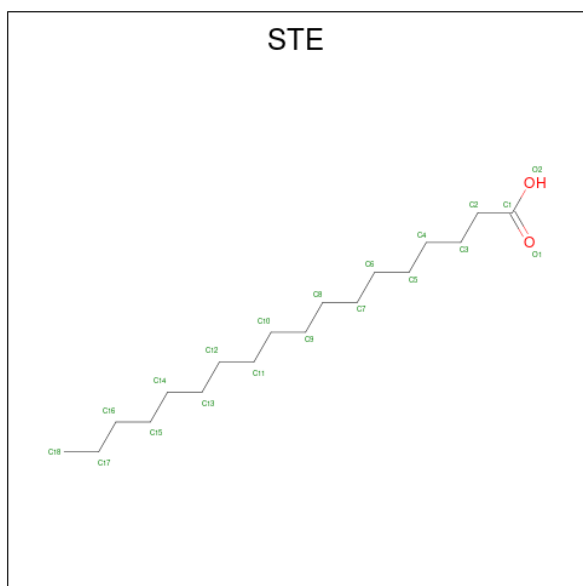
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



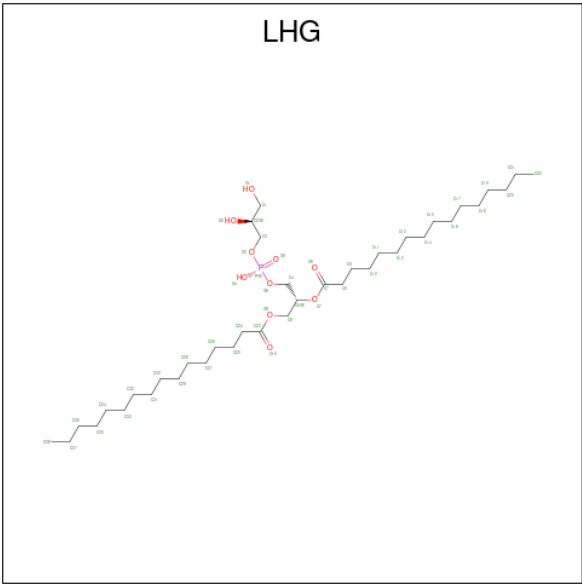
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	E	1	Total	C	H	O	0	0
			28	10	16	2		

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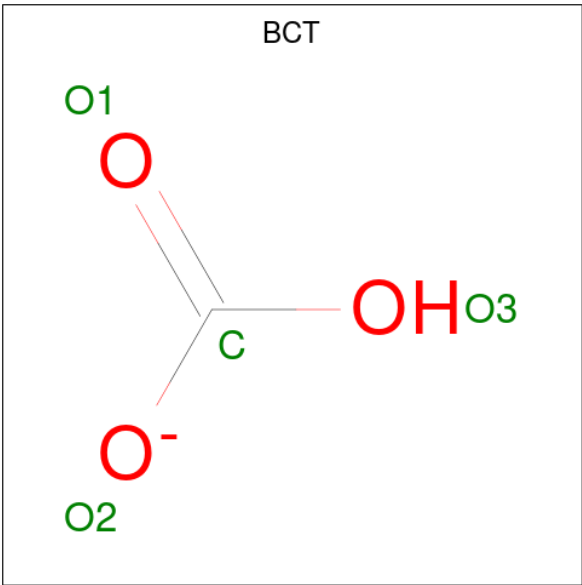
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	T	1	Total C H 47 16 31	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	m	1	Total C H O 28 10 16 2	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



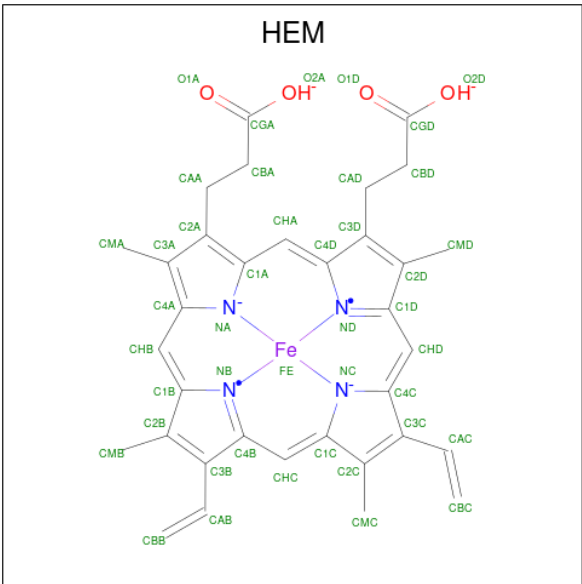
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
33	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
33	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
33	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
33	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
33	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



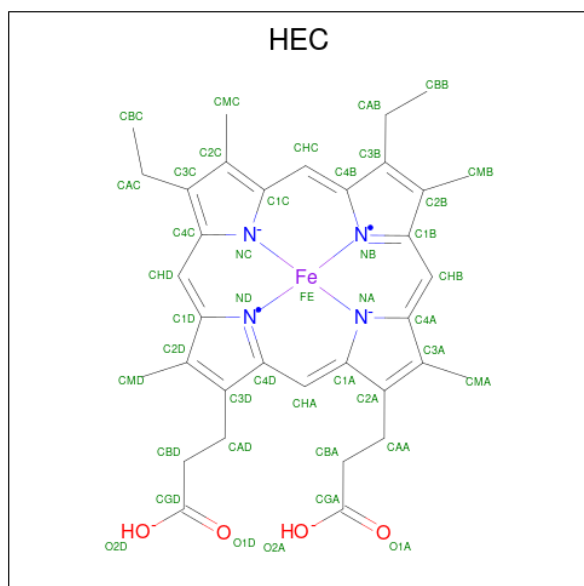
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
35	f	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 36 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	V	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
36	v	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	136	Total O 136 136	1	12
37	B	213	Total O 213 213	0	0
37	C	159	Total O 159 159	0	0
37	D	130	Total O 130 130	0	0
37	E	40	Total O 40 40	0	0
37	F	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	42	Total 42	O 42	0	0
37	I	12	Total 12	O 12	0	0
37	J	13	Total 13	O 13	0	0
37	K	4	Total 4	O 4	0	0
37	L	9	Total 9	O 9	0	0
37	M	9	Total 9	O 9	0	0
37	O	99	Total 99	O 99	0	0
37	R	4	Total 4	O 4	0	0
37	T	9	Total 9	O 9	0	0
37	U	33	Total 33	O 33	0	0
37	V	64	Total 64	O 64	0	0
37	X	14	Total 14	O 14	0	0
37	Y	4	Total 4	O 4	0	0
37	Z	3	Total 3	O 3	0	0
37	a	118	Total 118	O 118	0	8
37	b	191	Total 191	O 191	0	0
37	c	157	Total 157	O 157	0	0
37	d	105	Total 105	O 105	0	0
37	e	17	Total 17	O 17	0	0
37	f	6	Total 6	O 6	0	0
37	h	30	Total 30	O 30	0	0

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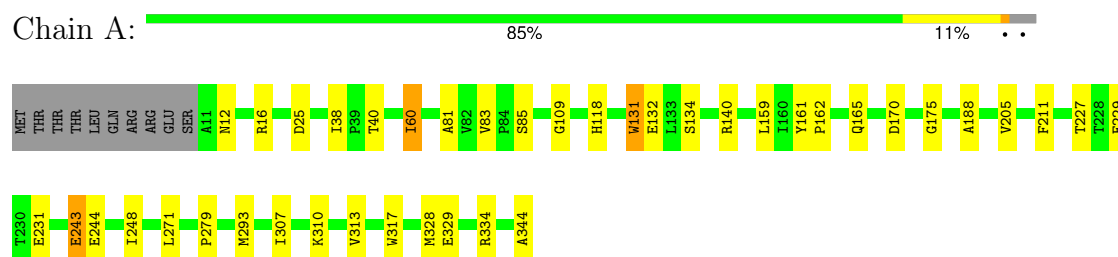
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	21	Total 21	O 21	0	0
37	j	6	Total 6	O 6	0	0
37	k	4	Total 4	O 4	0	0
37	l	12	Total 12	O 12	0	0
37	m	5	Total 5	O 5	0	0
37	o	93	Total 93	O 93	0	0
37	r	5	Total 5	O 5	0	0
37	t	8	Total 8	O 8	0	0
37	u	65	Total 65	O 65	0	0
37	v	59	Total 59	O 59	0	0
37	x	9	Total 9	O 9	0	0
37	y	4	Total 4	O 4	0	0

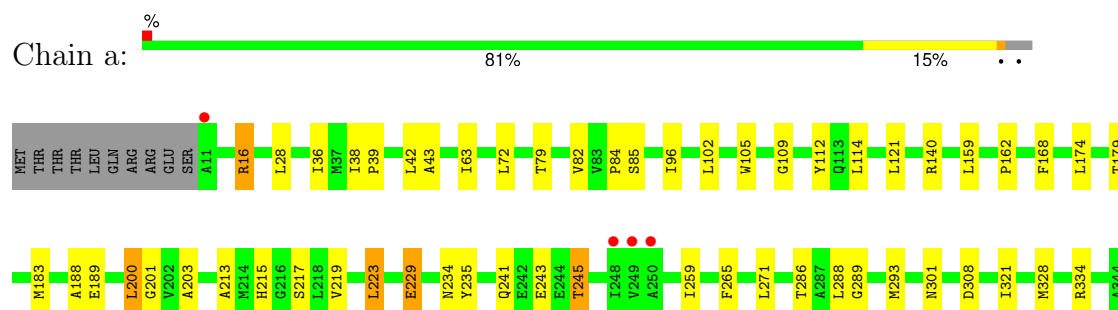
3 Residue-property plots [i](#)

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.

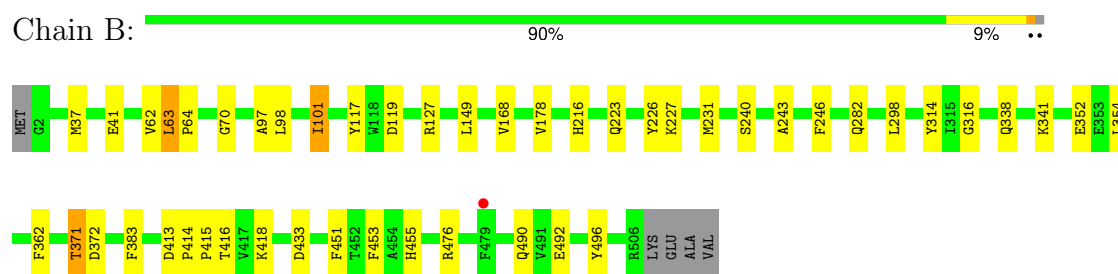
• Molecule 1: Photosystem II protein D1 1



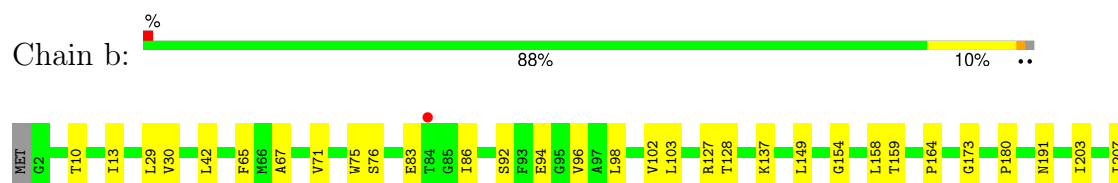
• Molecule 1: Photosystem II protein D1 1

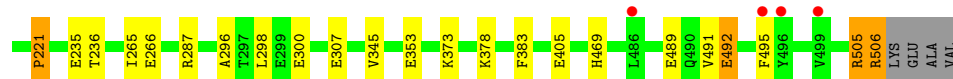


• Molecule 2: Photosystem II CP47 reaction center protein



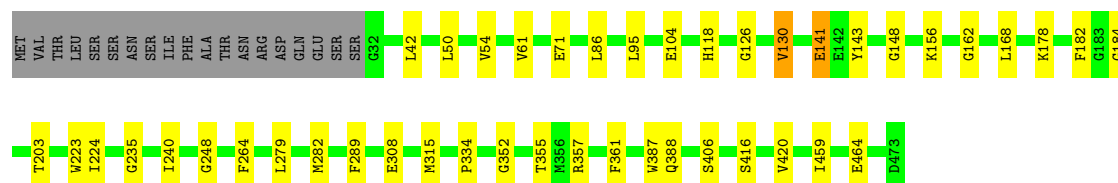
• Molecule 2: Photosystem II CP47 reaction center protein





• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 9% .



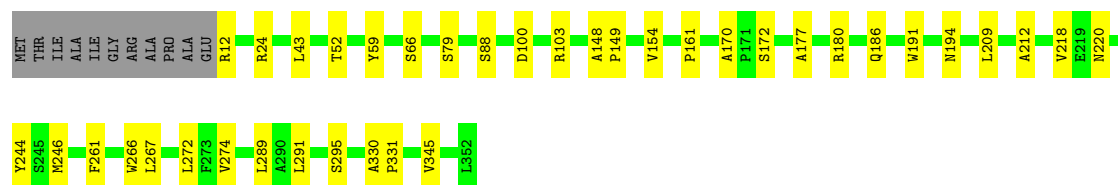
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 87% 10% .



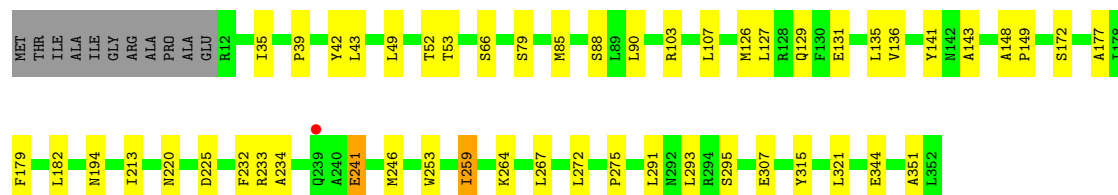
• Molecule 4: Photosystem II D2 protein

Chain D: 86% 11% .



• Molecule 4: Photosystem II D2 protein

Chain d: 82% 14% . .



• Molecule 5: Cytochrome b559 subunit alpha

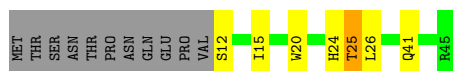
Chain E: 80% 18% .



- Molecule 5: Cytochrome b559 subunit alpha



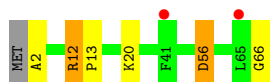
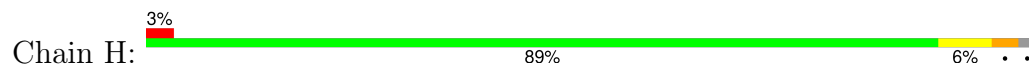
- Molecule 6: Cytochrome b559 subunit beta



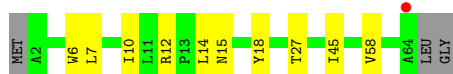
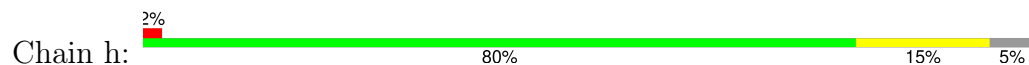
- Molecule 6: Cytochrome b559 subunit beta



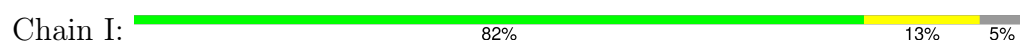
- Molecule 7: Photosystem II reaction center protein H



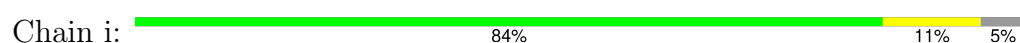
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I





• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K



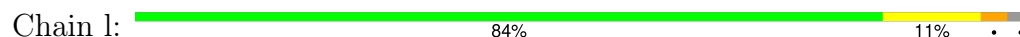
• Molecule 10: Photosystem II reaction center protein K



• Molecule 11: Photosystem II reaction center protein L

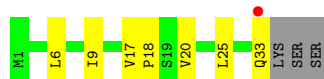


• Molecule 11: Photosystem II reaction center protein L



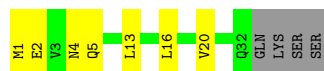
• Molecule 12: Photosystem II reaction center protein M





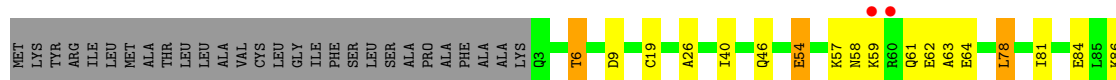
- Molecule 12: Photosystem II reaction center protein M

Chain m: 69% 19% 11%



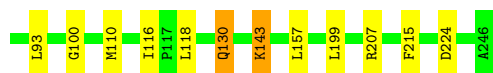
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 78% 11% 10%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 78% 10% 10%



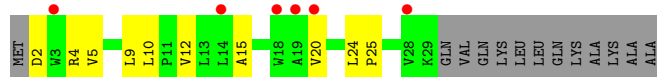
- Molecule 14: Photosystem II protein Y

Chain R: 51% 17% 32%



- Molecule 14: Photosystem II protein Y

Chain r: 15% 44% 24% 32%

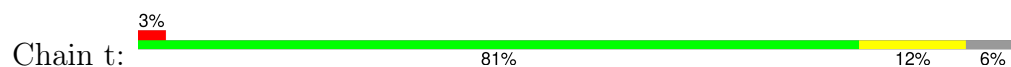


- Molecule 15: Photosystem II reaction center protein T

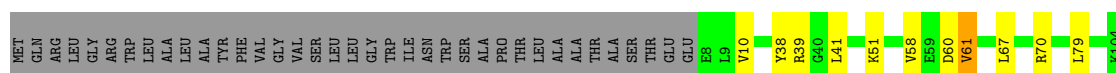
Chain T: 81% 9% 6%



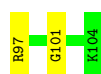
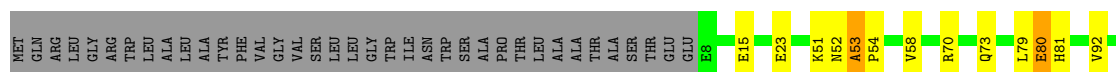
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein



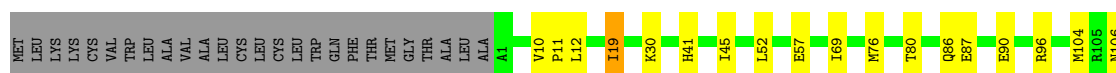
- Molecule 16: Photosystem II 12 kDa extrinsic protein



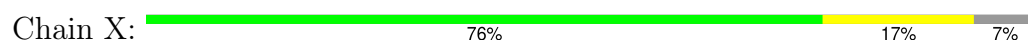
- Molecule 17: Cytochrome c-550

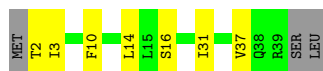


- Molecule 17: Cytochrome c-550



- Molecule 18: Photosystem II reaction center X protein

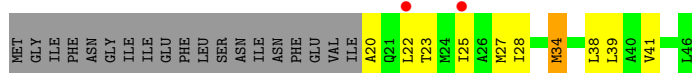




- Molecule 18: Photosystem II reaction center X protein



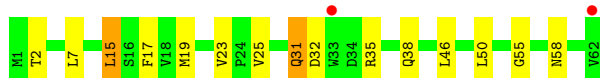
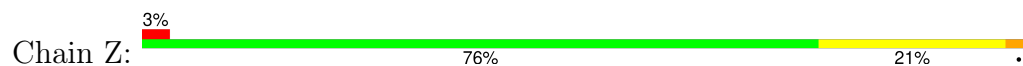
- Molecule 19: Photosystem II reaction center protein Ycf12



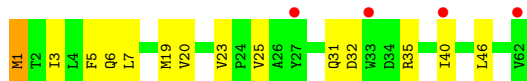
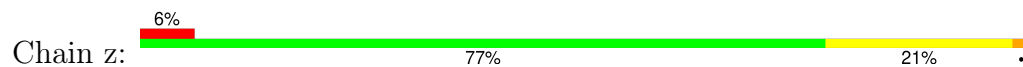
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: 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	116.96Å 221.65Å 307.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.65 – 2.09 33.65 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.65-2.09) 85.3 (33.65-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.51 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.239 0.181 , 0.238	Depositor DCC
R_{free} test set	4165 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	105937	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: SQD, FME, DGD, PHO, BCR, LHG, OEX, HEM, PL9, BCT, CL, OEY, STE, FE2, CLA, LMG, HEC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	1/3227 (0.0%)	0.62	1/4397 (0.0%)
1	a	0.50	0/3224	0.59	0/4393
2	B	0.58	0/4161	0.63	0/5669
2	b	0.56	1/4118 (0.0%)	0.62	1/5611 (0.0%)
3	C	0.54	0/3647	0.60	0/4965
3	c	0.51	0/3719	0.59	0/5061
4	D	0.60	0/2825	0.64	0/3847
4	d	0.56	0/2834	0.64	0/3859
5	E	0.52	0/688	0.58	0/940
5	e	0.46	0/683	0.56	0/932
6	F	0.54	0/284	0.57	0/387
6	f	0.50	0/284	0.66	0/387
7	H	0.64	0/523	0.68	0/713
7	h	0.58	0/511	0.64	0/697
8	I	0.64	0/293	0.66	0/396
8	i	0.69	0/293	0.64	0/396
9	J	0.52	0/263	0.63	0/356
9	j	0.49	0/263	0.60	0/356
10	K	0.50	0/303	0.61	0/416
10	k	0.44	0/303	0.58	0/416
11	L	0.72	0/311	0.71	0/422
11	l	0.65	0/303	0.70	0/412
12	M	0.71	0/249	0.71	0/341
12	m	0.68	0/244	0.74	0/334
13	O	0.63	0/1904	0.70	0/2585
13	o	0.64	0/1905	0.68	0/2583
14	R	0.40	0/227	0.53	0/313
14	r	0.36	0/227	0.49	0/313
15	T	0.69	0/257	0.68	0/349
15	t	0.66	0/255	0.68	0/346
16	U	0.55	0/785	0.64	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.61	0/785	0.68	0/1064
17	V	0.62	0/1085	0.70	0/1473
17	v	0.57	0/1085	0.63	0/1473
18	X	0.50	0/284	0.59	0/384
18	x	0.42	0/289	0.51	0/391
19	Y	0.45	0/197	0.50	0/264
19	y	0.38	0/219	0.52	0/294
20	Z	0.58	1/490 (0.2%)	0.63	0/669
20	z	0.35	0/488	0.48	0/666
All	All	0.56	3/44035 (0.0%)	0.63	2/59934 (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
17	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	221	PRO	CA-C	8.07	1.57	1.52
20	Z	23	VAL	CA-CB	7.58	1.58	1.54
1	A	38	ILE	CA-CB	-5.09	1.51	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	221	PRO	O-C-N	8.38	125.09	121.15
1	A	131	TRP	CA-CB-CG	-5.13	103.86	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	2985	2963	24	0
1	a	3110	2976	2954	38	0
2	B	4005	3873	3867	32	0
2	b	3978	3836	3836	33	0
3	C	3509	3432	3409	25	0
3	c	3583	3503	3492	26	0
4	D	2731	2637	2637	26	0
4	d	2737	2643	2643	35	0
5	E	666	651	651	11	0
5	e	664	648	648	15	0
6	F	275	282	282	6	0
6	f	275	282	282	4	0
7	H	510	532	532	5	0
7	h	498	518	518	7	0
8	I	296	311	311	2	0
8	i	296	311	311	1	0
9	J	257	268	268	11	0
9	j	257	268	268	8	0
10	K	293	305	305	4	0
10	k	293	305	305	10	0
11	L	304	316	316	3	0
11	l	296	304	304	3	0
12	M	256	269	269	5	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	21	0
13	o	1874	1846	1846	16	0
14	R	221	238	238	2	0
14	r	221	238	238	5	0
15	T	258	261	261	1	0
15	t	256	256	256	2	0
16	U	774	773	773	6	0
16	u	774	773	773	11	0
17	V	1064	1071	1073	11	0
17	v	1064	1071	1073	13	0
18	X	281	312	312	5	0
18	x	286	316	314	7	0
19	Y	196	217	217	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	6	0
20	Z	479	516	516	4	0
20	z	477	509	509	8	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	249	264	264	1	0
22	B	1035	1139	1139	22	0
22	C	839	922	922	12	0
22	D	130	144	144	3	0
22	a	195	216	216	1	0
22	b	1035	1139	1139	14	0
22	c	839	919	919	14	0
22	d	195	216	216	2	0
23	A	64	74	74	1	0
23	D	64	74	74	2	0
23	d	128	148	148	1	0
24	A	40	56	56	1	0
24	B	120	168	168	2	0
24	C	80	112	112	1	0
24	D	40	56	56	2	0
24	H	40	56	56	1	0
24	K	40	56	56	1	0
24	T	40	56	56	1	0
24	Y	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	1	0
24	c	120	168	168	3	0
24	d	40	56	56	2	0
24	h	40	56	56	0	0
24	k	40	56	56	0	0
24	t	40	56	56	2	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	3	0
26	D	55	80	80	2	0
26	a	55	80	80	5	0
26	d	55	80	80	1	0
27	A	48	66	66	0	0
27	B	28	40	40	0	0
27	C	48	66	66	1	0
27	D	84	117	116	2	0
27	M	51	72	71	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	b	106	158	158	1	0
27	c	134	181	181	1	0
27	d	67	92	92	0	0
28	A	91	136	135	0	0
28	B	54	78	78	0	0
28	F	36	46	45	1	0
28	L	49	65	64	1	0
28	a	90	134	132	4	0
28	f	41	48	47	2	0
29	A	66	96	96	5	0
29	C	186	246	243	1	0
29	H	62	82	80	0	0
29	a	44	75	75	4	0
29	c	186	246	243	2	0
29	h	62	82	81	0	0
30	A	11	0	0	2	0
30	a	11	0	0	1	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	75	117	117	1	0
32	C	40	63	63	1	0
32	D	20	35	35	2	0
32	E	12	16	16	0	0
32	H	18	35	35	2	0
32	I	15	26	26	3	0
32	J	12	16	16	0	0
32	M	25	38	38	0	0
32	T	31	60	60	1	0
32	a	22	32	32	2	0
32	b	66	110	110	1	0
32	c	32	51	51	1	0
32	d	17	26	26	2	0
32	j	12	16	16	0	0
32	l	18	35	35	1	0
32	m	12	16	16	0	0
32	t	14	20	20	1	0
32	x	20	35	35	3	0
33	B	49	74	74	1	0
33	D	96	141	141	2	0
33	E	49	74	74	1	0
33	L	49	74	74	1	0
33	d	137	199	199	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	e	42	57	57	2	0
33	l	49	74	74	2	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0
35	E	43	30	30	2	0
35	f	43	30	30	4	0
36	V	43	30	31	1	0
36	v	43	30	30	1	0
37	A	136	0	0	11	0
37	B	213	0	0	6	0
37	C	159	0	0	0	0
37	D	130	0	0	1	0
37	E	40	0	0	3	0
37	F	8	0	0	1	0
37	H	42	0	0	2	0
37	I	12	0	0	0	0
37	J	13	0	0	6	0
37	K	4	0	0	0	0
37	L	9	0	0	0	0
37	M	9	0	0	1	0
37	O	99	0	0	2	0
37	R	4	0	0	0	0
37	T	9	0	0	0	0
37	U	33	0	0	1	0
37	V	64	0	0	0	0
37	X	14	0	0	0	0
37	Y	4	0	0	0	0
37	Z	3	0	0	0	0
37	a	118	0	0	4	0
37	b	191	0	0	8	0
37	c	157	0	0	5	0
37	d	105	0	0	0	0
37	e	17	0	0	1	0
37	f	6	0	0	0	0
37	h	30	0	0	1	0
37	i	21	0	0	0	0
37	j	6	0	0	3	0
37	k	4	0	0	3	0
37	l	12	0	0	1	0
37	m	5	0	0	1	0
37	o	93	0	0	2	0
37	r	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	t	8	0	0	0	0
37	u	65	0	0	4	0
37	v	59	0	0	1	0
37	x	9	0	0	0	0
37	y	4	0	0	2	0
All	All	53252	52685	52587	498	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 5.

All (498) 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)
5:E:3:GLY:N	37:E:201:HOH:O	1.79	1.11
1:A:344[A]:ALA:O	37:A:501[A]:HOH:O	1.69	1.07
1:A:165[A]:GLN:OE1	37:A:501[A]:HOH:O	1.76	1.03
16:u:53:ALA:O	37:u:201:HOH:O	1.80	0.98
30:A:415[B]:OEY:O4	37:A:502[B]:HOH:O	1.86	0.93
16:U:60:ASP:OD2	37:U:201:HOH:O	1.85	0.93
16:u:53:ALA:O	37:u:202:HOH:O	1.84	0.92
10:k:19:ASP:OD2	37:k:201:HOH:O	1.89	0.88
2:B:223:GLN:OE1	37:B:701:HOH:O	1.92	0.87
2:B:352:GLU:OE2	37:B:702:HOH:O	1.92	0.86
32:a:414:STE:O2	37:a:501:HOH:O	1.95	0.84
37:A:502[B]:HOH:O	3:C:357[B]:ARG:NH2	2.09	0.84
1:a:229:GLU:OE2	37:a:502:HOH:O	1.96	0.83
2:b:307:GLU:OE1	37:b:701:HOH:O	1.96	0.82
16:U:70:ARG:NH2	17:V:85:GLU:OE2	2.14	0.81
13:o:28:GLY:O	37:o:301:HOH:O	2.03	0.77
9:J:19:MET:N	37:J:201:HOH:O	2.00	0.76
3:c:327[A]:ASN:ND2	37:c:601:HOH:O	2.19	0.76
5:E:53:ASP:OD1	37:E:202:HOH:O	2.02	0.76
7:H:56:ASP:OD2	18:X:2:THR:N	2.19	0.74
30:A:415[B]:OEY:O5	30:A:415[B]:OEY:O6	2.04	0.74
9:J:36:LEU:O	37:J:202:HOH:O	2.05	0.74
1:A:25:ASP:OD1	37:A:504:HOH:O	2.06	0.73
2:B:354:LEU:O	37:B:703:HOH:O	2.06	0.72
19:y:46:LEU:OXT	37:y:101:HOH:O	2.08	0.72
11:l:2:GLU:OE2	37:l:201:HOH:O	2.07	0.72
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.24	0.71
10:k:23:ASP:OD2	37:k:201:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:20:ALA:N	19:Y:23:THR:HG1	1.90	0.70
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.26	0.69
4:d:141:TYR:OH	33:d:408:LHG:O4	2.07	0.68
22:c:501:CLA:H192	22:c:507:CLA:HBB1	1.75	0.68
35:E:101:HEM:HBC2	35:E:101:HEM:HHD	1.77	0.67
2:B:490:GLN:OE1	37:B:704:HOH:O	2.11	0.66
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.61	0.65
2:b:127:ARG:NH2	7:h:18:TYR:O	2.29	0.65
3:c:78:GLU:OE1	17:v:106:ASN:ND2	2.28	0.65
9:j:36:LEU:O	37:j:201:HOH:O	2.14	0.65
9:J:15:THR:O	37:J:201:HOH:O	2.14	0.65
13:O:57:LYS:NZ	37:O:304:HOH:O	2.30	0.64
12:m:5:GLN:O	37:m:201:HOH:O	2.16	0.63
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.63
26:A:409:PL9:H361	6:F:25:THR:HG21	1.81	0.63
36:V:201:HEC:HBC3	36:V:201:HEC:HMC3	1.82	0.62
17:v:104:MET:HA	17:v:107:LEU:HD22	1.80	0.62
26:a:409:PL9:H48	4:d:39:PRO:HG3	1.81	0.62
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.33	0.62
6:f:24:HIS:O	6:f:28:VAL:HG13	1.98	0.62
16:u:52:ASN:C	37:u:202:HOH:O	2.43	0.62
6:f:21:VAL:O	6:f:25:THR:OG1	2.18	0.62
9:j:5:GLY:N	37:j:202:HOH:O	2.33	0.61
13:o:130:GLN:OE1	13:o:143:LYS:NZ	2.34	0.61
29:a:412:DGD:O1G	29:a:412:DGD:O1B	2.19	0.61
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.36	0.61
9:j:18:GLY:O	9:j:22:ILE:HD13	2.01	0.61
27:b:620:LMG:O10	12:m:4:ASN:ND2	2.35	0.59
2:B:371:THR:HG23	2:B:372:ASP:O	2.02	0.59
3:c:178:LYS:NZ	3:c:184:GLY:O	2.35	0.59
16:u:70:ARG:NH1	16:u:73:GLN:OE1	2.35	0.59
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.85	0.59
5:E:68:ASP:O	5:E:72:ALA:HB2	2.02	0.59
22:B:607:CLA:H203	33:B:622:LHG:H142	1.85	0.58
16:U:58:VAL:O	16:U:61:VAL:HG22	2.04	0.58
1:a:200:LEU:HD13	29:c:519:DGD:HAW2	1.85	0.58
16:U:39:ARG:NH2	17:V:60:ALA:O	2.36	0.57
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.40	0.57
28:L:101:SQD:H222	2:b:29:LEU:HD23	1.85	0.57
2:b:102:VAL:HG11	22:b:606:CLA:H142	1.86	0.57
13:O:58:ASN:CB	37:b:701:HOH:O	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.86	0.56
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.05	0.56
1:A:85:SER:HA	1:A:109:GLY:HA3	1.88	0.56
1:a:235:TYR:OH	11:l:11:GLU:OE2	2.22	0.56
13:o:224:ASP:OD2	37:o:302:HOH:O	2.17	0.56
22:B:604:CLA:H42	22:B:605:CLA:H42	1.87	0.56
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.41	0.55
27:D:407:LMG:H402	6:F:26:LEU:HB3	1.88	0.55
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.41	0.55
10:K:26:PRO:O	10:K:29:PRO:HD2	2.06	0.55
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.89	0.55
22:B:605:CLA:H41	22:B:612:CLA:H161	1.88	0.55
3:C:95:LEU:HD21	22:C:501:CLA:OBD	2.07	0.55
10:k:10:LYS:N	37:k:202:HOH:O	2.40	0.55
13:O:58:ASN:HB3	37:b:701:HOH:O	2.07	0.55
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.89	0.55
4:d:79:SER:HA	4:d:172:SER:HB3	1.88	0.54
7:H:12:ARG:HB3	7:H:13:PRO:HD3	1.89	0.54
4:d:241:GLU:CD	4:d:241:GLU:H	2.14	0.54
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.89	0.54
19:y:39:LEU:O	19:y:44:GLY:N	2.41	0.54
6:F:12:SER:N	37:F:201:HOH:O	2.41	0.54
28:a:410:SQD:H381	9:j:22:ILE:HD11	1.89	0.54
20:z:32:ASP:HB2	20:z:35:ARG:HB2	1.90	0.54
1:A:170[B]:ASP:HB3	37:A:607[B]:HOH:O	2.06	0.54
16:u:79:LEU:O	37:u:203:HOH:O	2.18	0.54
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.89	0.53
17:v:11:PRO:O	17:v:69:ILE:HD12	2.08	0.53
17:v:41:HIS:HA	17:v:45:ILE:O	2.08	0.53
33:d:409:LHG:H321	15:t:21:ILE:HD11	1.91	0.53
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.53
7:H:12:ARG:HB3	7:H:13:PRO:CD	2.39	0.53
18:x:16:SER:HB3	32:x:101:STE:H71	1.90	0.53
1:A:161[B]:TYR:HE2	37:A:607[B]:HOH:O	1.91	0.53
23:D:401:PHO:HBA2	22:D:403:CLA:H142	1.91	0.53
17:v:90:GLU:HB2	37:v:321:HOH:O	2.09	0.52
35:f:101:HEM:HBC2	35:f:101:HEM:HMC1	1.91	0.52
24:D:405:BCR:H23C	24:D:405:BCR:H392	1.91	0.52
1:a:189[B]:GLU:OE1	30:a:415[B]:OEY:O6	2.27	0.52
2:B:341:LYS:NZ	37:B:709:HOH:O	2.35	0.52
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334[B]:ARG:HD3	37:A:571:HOH:O	2.10	0.52
33:e:101:LHG:HC11	37:e:215:HOH:O	2.08	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.45	0.52
29:a:412:DGD:O1B	29:a:412:DGD:C1G	2.57	0.52
29:A:414:DGD:HD5	2:b:75:TRP:HB3	1.91	0.52
20:z:1:MET:SD	20:z:1:MET:N	2.77	0.52
22:b:615:CLA:H2	22:b:616:CLA:HBB2	1.91	0.51
3:c:406:SER:HA	3:c:420:VAL:HG23	1.91	0.51
17:v:10:VAL:HG23	17:v:69:ILE:HD11	1.91	0.51
3:C:148:GLY:O	3:C:156:LYS:NZ	2.42	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.46	0.51
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.92	0.51
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.91	0.51
9:J:19:MET:O	9:J:23:VAL:HG23	2.11	0.51
2:b:287:ARG:HD3	37:b:702:HOH:O	2.11	0.51
1:A:211:PHE:CD1	26:A:409:PL9:H111	2.46	0.51
37:A:597:HOH:O	13:O:107:THR:HG21	2.10	0.51
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.93	0.51
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.93	0.50
29:A:414:DGD:HB61	32:I:101:STE:H42	1.94	0.50
33:d:409:LHG:H281	15:t:17:PHE:CD1	2.46	0.50
24:t:101:BCR:H23C	24:t:101:BCR:H382	1.94	0.50
1:A:227:THR:HB	1:A:231:GLU:HG3	1.93	0.50
32:b:621:STE:O1	37:b:703:HOH:O	2.18	0.50
3:c:45:LEU:HA	3:c:139:THR:HG22	1.94	0.50
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.94	0.50
12:M:6:LEU:HD12	27:M:101:LMG:HC92	1.94	0.50
24:d:406:BCR:H331	24:d:406:BCR:C8	2.41	0.50
3:C:334:PRO:HA	13:O:153:THR:OG1	2.12	0.50
19:y:22:LEU:HA	19:y:25:ILE:HG22	1.93	0.50
13:O:184:ARG:NH2	13:O:229[A]:GLU:OE2	2.45	0.49
27:C:519:LMG:H191	10:K:27:VAL:HG11	1.95	0.49
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.94	0.49
17:v:57:GLU:CD	17:v:57:GLU:H	2.20	0.49
20:Z:15:LEU:HD22	20:Z:19:MET:HG3	1.94	0.49
3:C:406:SER:HA	3:C:420:VAL:HG23	1.94	0.49
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.95	0.49
1:A:279:PRO:HG2	4:D:212:ALA:HB2	1.93	0.49
1:A:310:LYS:NZ	37:A:516:HOH:O	2.46	0.49
29:A:414:DGD:HB61	32:I:101:STE:C5	2.43	0.49
1:a:63[A]:ILE:HB	3:c:335:THR:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:HB2	37:b:701:HOH:O	2.11	0.49
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.95	0.49
3:C:141:GLU:H	3:C:141:GLU:CD	2.20	0.49
3:C:162:GLY:HA2	3:C:248:GLY:HA2	1.94	0.49
5:E:10:PHE:HB2	33:E:102:LHG:O4	2.13	0.49
1:a:38:ILE:HB	1:a:39:PRO:HD3	1.95	0.49
5:e:36:LEU:O	5:e:40:THR:HG23	2.13	0.49
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.95	0.49
1:a:102:LEU:HD12	29:a:412:DGD:HB22	1.95	0.49
10:k:17:ILE:HD11	20:z:6:GLN:HG2	1.94	0.49
2:B:226:TYR:OH	37:B:705:HOH:O	2.20	0.48
3:c:135:ARG:NE	37:c:612:HOH:O	2.45	0.48
2:B:117:TYR:HA	11:L:1:MET:HE1	1.95	0.48
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.95	0.48
20:Z:55:GLY:HA2	20:Z:58:ASN:HB3	1.94	0.48
26:a:409:PL9:H151	33:e:101:LHG:H292	1.96	0.48
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.95	0.48
1:a:43:ALA:HA	24:a:405:BCR:C16	2.44	0.48
22:d:405:CLA:HBA2	32:x:101:STE:H21	1.95	0.48
9:j:34:ALA:O	37:j:201:HOH:O	2.20	0.48
12:M:17:VAL:HB	12:M:18:PRO:HD3	1.96	0.48
23:d:402:PHO:HHD	23:d:402:PHO:HBC2	1.96	0.48
7:h:6:TRP:NE1	7:h:10:ILE:HD11	2.29	0.48
29:A:414:DGD:HB61	32:I:101:STE:H51	1.95	0.48
32:a:414:STE:O1	37:a:503:HOH:O	2.20	0.48
4:d:259:ILE:HD12	33:d:409:LHG:H291	1.95	0.48
19:y:17:GLU:O	19:y:20:ALA:HB3	2.13	0.48
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.49	0.48
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.13	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.48
5:E:65:LEU:O	5:E:67:THR:HG23	2.13	0.48
1:a:217:SER:HA	4:d:272:LEU:HD12	1.94	0.48
16:u:92:VAL:HG12	16:u:97:ARG:HD2	1.95	0.48
3:C:50:LEU:O	3:C:54:VAL:HG23	2.14	0.47
17:v:41:HIS:CD2	36:v:201:HEC:NB	2.82	0.47
1:a:16:ARG:HH11	1:a:16:ARG:HB3	1.79	0.47
2:B:383:PHE:O	13:O:166:SER:HA	2.13	0.47
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.96	0.47
2:b:103:LEU:HB2	22:b:606:CLA:H62	1.96	0.47
2:B:119:ASP:H	11:L:1:MET:CE	2.27	0.47
5:e:30:LEU:HD11	35:f:101:HEM:CBB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:O	1:A:118:HIS:HB3	2.14	0.47
5:E:53:ASP:O	17:V:1:ALA:N	2.44	0.47
22:C:510:CLA:H193	22:C:510:CLA:HBC3	1.96	0.47
26:D:406:PL9:H412	11:L:29:LEU:HD23	1.96	0.47
12:M:33:GLN:O	37:M:201:HOH:O	2.20	0.47
2:b:159:THR:O	2:b:180:PRO:HB3	2.15	0.47
17:v:122:GLU:N	17:v:123:PRO:HD2	2.30	0.47
18:x:27:VAL:O	18:x:31:ILE:HG13	2.15	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.47
9:J:15:THR:HG22	9:J:19:MET:CE	2.45	0.47
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.31	0.47
14:r:2:ASP:HB3	14:r:5:VAL:HG23	1.97	0.47
2:B:414:PRO:N	2:B:415:PRO:HD2	2.30	0.47
9:J:19:MET:HB2	37:J:201:HOH:O	2.14	0.47
19:y:41:VAL:C	19:y:43:ARG:H	2.23	0.47
22:C:508:CLA:HBC3	22:C:510:CLA:H92	1.97	0.47
2:b:378:LYS:HE3	37:b:704:HOH:O	2.13	0.47
3:c:166:ILE:HG21	22:c:512:CLA:H202	1.97	0.47
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.98	0.46
1:A:271:LEU:HD11	26:A:409:PL9:HC71	1.97	0.46
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.98	0.46
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.04	0.46
3:c:42:LEU:HD21	22:c:511:CLA:H2A	1.97	0.46
4:d:194:ASN:HA	4:d:295:SER:OG	2.16	0.46
18:X:10:PHE:CE2	18:X:14:LEU:HD22	2.50	0.46
3:C:178:LYS:NZ	3:C:184:GLY:O	2.49	0.46
5:E:26:THR:O	5:E:30:LEU:HG	2.14	0.46
13:O:178:LYS:HG3	13:O:181:GLU:OE1	2.16	0.46
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	1.98	0.46
22:b:602:CLA:H43	7:h:45:ILE:HG22	1.97	0.46
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.81	0.46
35:f:101:HEM:HBC2	35:f:101:HEM:CMC	2.44	0.46
32:B:625:STE:H22	27:M:101:LMG:HC5	1.97	0.46
7:H:66:GLY:N	37:H:204:HOH:O	2.49	0.46
1:a:114:LEU:C	1:a:114:LEU:HD23	2.40	0.46
10:k:25:LEU:N	10:k:26:PRO:CD	2.79	0.46
7:H:2:ALA:N	37:H:203:HOH:O	2.48	0.46
24:H:101:BCR:H331	24:H:101:BCR:C8	2.44	0.46
1:a:308:ASP:OD1	1:a:308:ASP:C	2.57	0.46
4:d:39:PRO:O	4:d:43:LEU:HG	2.16	0.46
24:t:101:BCR:H321	24:t:101:BCR:HC8	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:TYR:O	5:E:65:LEU:HD12	2.15	0.46
15:T:29:ILE:HG22	15:T:30:THR:HG23	1.98	0.46
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.46	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
3:c:128:GLY:HA3	22:c:513:CLA:C3C	2.46	0.46
13:o:10:ILE:O	13:o:13:THR:HG23	2.16	0.46
18:x:12:ILE:HG21	32:x:101:STE:H141	1.98	0.46
6:F:15:ILE:HD13	14:R:23:ILE:HD11	1.98	0.45
9:J:18:GLY:HA3	24:Y:101:BCR:H371	1.98	0.45
17:V:41:HIS:HA	17:V:45:ILE:O	2.15	0.45
3:c:38:GLY:HA3	22:c:511:CLA:HMD2	1.98	0.45
4:d:246:MET:HE3	4:d:264:LYS:CG	2.47	0.45
1:A:81:ALA:HB2	1:A:175[A]:GLY:HA3	1.98	0.45
2:B:490:GLN:HG3	2:B:496:TYR:HE2	1.82	0.45
13:O:107:THR:HG22	37:O:328:HOH:O	2.15	0.45
1:a:234:ASN:OD1	33:d:408:LHG:HC11	2.16	0.45
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.97	0.45
2:B:149[B]:LEU:HD11	22:B:604:CLA:H162	1.98	0.45
22:C:503:CLA:C2B	32:C:521:STE:H151	2.45	0.45
13:O:54:GLU:O	13:O:63:ALA:HB3	2.16	0.45
1:a:82:VAL:HB	1:a:174[A]:LEU:HB2	1.98	0.45
2:b:489:GLU:OE1	2:b:505:ARG:NH1	2.50	0.45
19:Y:22:LEU:HA	19:Y:25:ILE:HG22	1.98	0.45
13:o:54:GLU:O	13:o:56:PRO:HD3	2.16	0.45
17:V:3:LEU:HD23	17:V:3:LEU:HA	1.88	0.45
22:B:603:CLA:C3D	22:B:605:CLA:H2	2.47	0.45
2:b:203:ILE:O	2:b:207:ILE:HG13	2.16	0.45
5:e:23:HIS:HA	5:e:26:THR:OG1	2.16	0.45
20:z:32:ASP:OD1	20:z:32:ASP:N	2.49	0.45
7:h:12:ARG:NH2	7:h:15:ASN:O	2.46	0.45
1:A:60[B]:ILE:HB	1:A:83:VAL:HG12	1.99	0.45
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.52	0.45
10:K:25:LEU:N	10:K:26:PRO:HD2	2.32	0.45
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.99	0.45
33:d:409:LHG:O1	33:l:101:LHG:O4	2.30	0.45
5:e:40:THR:HB	14:r:4:ARG:HD2	1.99	0.45
29:A:414:DGD:HBN1	8:I:7:THR:HG21	1.98	0.44
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.44
13:O:158:ASP:HB2	13:O:159:PRO:CD	2.47	0.44
1:a:102:LEU:H	29:a:412:DGD:HA22	1.82	0.44
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.99	0.44
2:B:149[B]:LEU:HG	22:B:604:CLA:H18	2.00	0.44
23:D:401:PHO:HBC2	23:D:401:PHO:HHD	1.99	0.44
4:D:266:TRP:CD1	33:D:408:LHG:HC31	2.52	0.44
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.50	0.44
1:a:321:ILE:HD11	4:d:179:PHE:HB2	1.99	0.44
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.99	0.44
13:o:110:MET:HE2	13:o:116:ILE:HD11	2.00	0.44
1:a:213:ALA:HB2	4:d:275:PRO:HG2	2.00	0.44
2:b:164:PRO:HG3	22:b:606:CLA:O1D	2.17	0.44
2:B:433:ASP:OD1	2:B:433:ASP:C	2.60	0.44
3:c:352:GLY:O	3:c:355[A]:THR:HG22	2.16	0.44
4:d:52:THR:O	4:d:66:SER:HA	2.17	0.44
4:d:126:MET:HE3	4:d:143:ALA:O	2.17	0.44
14:r:20:VAL:O	14:r:24:LEU:N	2.51	0.44
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.91	0.44
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.83	0.44
1:a:72:LEU:HD21	32:t:102:STE:H41	2.00	0.44
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.90	0.44
2:B:414:PRO:O	2:B:418:LYS:HG3	2.17	0.44
4:D:274:VAL:HG22	26:D:406:PL9:H222	2.00	0.44
4:d:267:LEU:C	4:d:267:LEU:HD23	2.43	0.44
2:B:37:MET:O	2:B:41:GLU:HG3	2.18	0.44
4:D:52:THR:O	4:D:66:SER:HA	2.18	0.44
4:D:330:ALA:HB3	4:D:331:PRO:HD3	2.00	0.44
1:A:329[A]:GLU:HG3	37:A:621:HOH:O	2.17	0.43
2:b:383:PHE:N	4:d:344:GLU:O	2.48	0.43
22:c:505:CLA:H193	27:c:523:LMG:H131	1.99	0.43
16:u:80:GLU:HG2	16:u:81:HIS:CD2	2.53	0.43
3:C:279:LEU:HD12	22:C:509:CLA:HED2	2.00	0.43
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.00	0.43
24:K:101:BCR:H11C	24:K:101:BCR:H341	1.87	0.43
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.99	0.43
32:D:411:STE:H91	18:X:16:SER:HB3	2.00	0.43
22:b:603:CLA:H2	22:b:605:CLA:H91	1.99	0.43
28:f:102:SQD:H312	18:x:27:VAL:HG11	2.00	0.43
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.99	0.43
22:d:405:CLA:H92	18:x:18:ALA:HB2	2.01	0.43
3:c:78:GLU:OE2	37:c:602:HOH:O	2.21	0.43
26:d:407:PL9:H201	33:l:101:LHG:H202	2.01	0.43
20:z:3:ILE:O	20:z:7:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.54	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.43
9:J:16:VAL:C	37:J:201:HOH:O	2.60	0.43
14:R:16:ALA:O	14:R:20:VAL:HG23	2.18	0.43
2:b:345:VAL:HG13	2:b:353:GLU:OE2	2.19	0.43
2:b:492:GLU:OE2	2:b:495:PHE:HE1	2.00	0.43
8:i:31:ASN:HB2	8:i:32:PRO:HD2	2.01	0.43
27:D:410:LMG:O10	27:D:410:LMG:H132	2.18	0.43
13:O:19:CYS:SG	13:O:46:GLN:HB2	2.58	0.43
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.53	0.43
22:b:607:CLA:H191	33:d:408:LHG:H141	2.01	0.43
24:c:516:BCR:H24C	24:c:516:BCR:H371	1.83	0.43
26:a:409:PL9:H513	28:f:102:SQD:H311	2.01	0.43
22:b:615:CLA:H2	22:b:616:CLA:CBB	2.49	0.43
4:d:131:GLU:O	4:d:135:LEU:HG	2.19	0.43
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.99	0.43
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.01	0.43
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.00	0.43
2:b:10:THR:HB	2:b:13:ILE:HD12	2.00	0.43
2:b:92:SER:O	2:b:96:VAL:HG23	2.19	0.43
17:v:87:GLU:CD	17:v:96:ARG:HH12	2.27	0.43
22:A:405:CLA:HMC2	24:A:406:BCR:H12C	2.00	0.43
3:C:143:TYR:CE2	22:C:513:CLA:HED3	2.54	0.43
35:E:101:HEM:HMB1	35:E:101:HEM:HBB2	2.01	0.43
17:V:63:THR:HG22	17:V:64:PRO:CD	2.48	0.43
1:a:36:ILE:HG23	22:a:404:CLA:HBB1	2.00	0.43
1:a:203:ALA:HB3	28:a:410:SQD:H221	2.00	0.43
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.00	0.42
16:u:53:ALA:HB1	16:u:54:PRO:HD2	2.00	0.42
22:B:606:CLA:H72	24:B:619:BCR:H311	2.00	0.42
22:C:509:CLA:H91	22:C:509:CLA:H112	1.75	0.42
32:T:102:STE:H82	32:T:102:STE:H51	1.79	0.42
2:b:65:PHE:HE1	22:b:604:CLA:HED2	1.83	0.42
22:c:503:CLA:H203	22:c:510:CLA:HAB	2.01	0.42
4:d:103:ARG:O	4:d:107:LEU:HG	2.19	0.42
11:l:7:ARG:HH12	32:l:102:STE:C1	2.32	0.42
22:B:614:CLA:H141	22:B:614:CLA:H161	1.86	0.42
24:B:619:BCR:H382	28:a:411:SQD:H82	2.01	0.42
4:D:272:LEU:C	4:D:272:LEU:HD23	2.44	0.42
9:J:19:MET:CB	37:J:201:HOH:O	2.68	0.42
3:c:26:ARG:NE	37:y:101:HOH:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:501:CLA:C3D	22:c:503:CLA:H2	2.49	0.42
22:c:505:CLA:C1A	22:c:505:CLA:CGA	2.98	0.42
1:A:243:GLU:H	1:A:243:GLU:CD	2.28	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.55	0.42
4:D:12:ARG:NH2	37:D:510:HOH:O	2.53	0.42
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.42
4:d:85:MET:HE1	5:e:72:ALA:HB2	2.01	0.42
13:o:57:LYS:C	13:o:59:LYS:H	2.27	0.42
23:A:404:PHO:HBC2	23:A:404:PHO:HHD	2.02	0.42
22:B:611:CLA:H71	33:L:102:LHG:H321	2.02	0.42
22:B:615:CLA:H201	22:B:615:CLA:C1B	2.49	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.20	0.42
2:b:373:LYS:HG3	37:b:789:HOH:O	2.19	0.42
22:b:606:CLA:H72	22:b:606:CLA:H111	1.84	0.42
22:c:510:CLA:H191	10:k:33:LEU:HD22	2.01	0.42
5:e:25:ILE:HD12	5:e:25:ILE:N	2.34	0.42
18:x:10:PHE:CE1	18:x:14:LEU:HD22	2.54	0.42
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.45	0.42
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.02	0.42
3:c:25:ASN:O	3:c:26:ARG:HB2	2.20	0.42
22:c:507:CLA:H92	22:c:507:CLA:H61	1.85	0.42
2:B:413:ASP:OD2	2:B:416:THR:OG1	2.35	0.42
1:a:201:GLY:HA3	1:a:286:THR:HB	2.02	0.42
1:a:334[A]:ARG:HG3	13:o:157:LEU:HB2	2.01	0.42
24:b:617:BCR:H23C	24:b:617:BCR:H382	2.01	0.42
3:c:213:LEU:HD21	24:c:515:BCR:C20	2.50	0.42
29:c:519:DGD:HAE1	29:c:519:DGD:HA82	1.81	0.42
13:o:199:LEU:HD23	13:o:215:PHE:HB3	2.01	0.42
22:C:502:CLA:H51	22:C:503:CLA:C4C	2.50	0.42
22:D:404:CLA:NB	32:D:411:STE:H151	2.35	0.42
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.08	0.41
19:Y:34:MET:O	19:Y:38:LEU:HG	2.19	0.41
3:C:126:GLY:O	3:C:130:VAL:HG13	2.20	0.41
4:D:209:LEU:HD23	4:D:209:LEU:C	2.45	0.41
24:D:405:BCR:H20C	24:D:405:BCR:H361	1.91	0.41
1:a:334[A]:ARG:NH2	37:a:515:HOH:O	2.53	0.41
2:b:30:VAL:HG12	22:b:605:CLA:HHD	2.01	0.41
17:v:12:LEU:HB2	17:v:19:ILE:HG22	2.01	0.41
22:B:601:CLA:H51	32:H:103:STE:H132	2.02	0.41
22:B:601:CLA:H51	32:H:103:STE:H151	2.01	0.41
4:D:267:LEU:C	4:D:267:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:57:ALA:HB3	5:e:60:GLN:HG2	2.02	0.41
22:B:615:CLA:H2	22:B:616:CLA:HBB2	2.02	0.41
22:C:506:CLA:H142	29:C:516:DGD:HAF1	2.01	0.41
2:b:221:PRO:HB3	22:b:609:CLA:O1D	2.21	0.41
3:c:215:LYS:NZ	37:c:616:HOH:O	2.53	0.41
5:e:13:ILE:HG22	5:e:19:TYR:CD1	2.55	0.41
5:e:26:THR:HA	14:r:15:ALA:HB1	2.02	0.41
9:j:10:LEU:O	9:j:13:VAL:HG22	2.20	0.41
13:o:62:GLU:OE2	13:o:63:ALA:N	2.53	0.41
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.55	0.41
19:Y:39:LEU:HD21	20:Z:25:VAL:HA	2.02	0.41
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.36	0.41
1:a:301:ASN:C	1:a:301:ASN:OD1	2.62	0.41
3:C:352:GLY:O	3:C:355[A]:THR:HG22	2.21	0.41
4:D:100:ASP:OD1	4:D:100:ASP:C	2.64	0.41
13:O:78:LEU:HB3	13:O:81:ILE:HD11	2.02	0.41
2:b:137:LYS:HG2	7:h:14:LEU:O	2.20	0.41
3:c:238:ILE:O	3:c:242:LEU:HG	2.21	0.41
4:d:126:MET:HA	4:d:129:GLN:OE1	2.20	0.41
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.56	0.41
22:B:601:CLA:O1D	22:B:601:CLA:H2A	2.20	0.41
28:F:101:SQD:H242	18:X:31:ILE:HD13	2.03	0.41
1:a:215:HIS:ND1	26:a:409:PL9:O1	2.43	0.41
2:b:67:ALA:HA	2:b:71:VAL:O	2.20	0.41
3:c:67:MET:HE2	37:c:688:HOH:O	2.21	0.41
4:d:49:LEU:HD13	24:d:406:BCR:C15	2.50	0.41
7:h:58:VAL:HB	37:h:211:HOH:O	2.20	0.41
14:r:24:LEU:N	14:r:25:PRO:HD2	2.36	0.41
2:B:492:GLU:HB3	37:E:201:HOH:O	2.20	0.41
4:D:79:SER:HA	4:D:172:SER:HB3	2.02	0.41
4:D:194:ASN:HA	4:D:295:SER:OG	2.20	0.41
4:D:261:PHE:CZ	33:D:408:LHG:HC81	2.56	0.41
3:c:309:ALA:HB1	3:c:399:ALA:HB2	2.02	0.41
13:o:57:LYS:HD3	13:o:59:LYS:HE3	2.03	0.41
19:y:35:ILE:HG23	20:z:25:VAL:HG23	2.02	0.41
22:B:606:CLA:H93	28:a:411:SQD:H221	2.02	0.41
3:C:168:LEU:HD21	22:C:509:CLA:H61	2.03	0.41
4:D:186:GLN:HB2	22:D:403:CLA:HBC1	2.02	0.41
9:J:15:THR:HG22	9:J:19:MET:HE2	2.03	0.41
10:K:17:ILE:HG23	10:K:18:PHE:CD2	2.56	0.41
13:O:215:PHE:CD1	13:O:215:PHE:C	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:T:101:BCR:H321	24:T:101:BCR:HC8	2.03	0.41
17:V:32:LEU:HB3	17:V:115:ILE:HD11	2.03	0.41
17:V:63:THR:HG22	17:V:64:PRO:HD2	2.01	0.41
1:a:289:GLY:O	1:a:293:MET:HE3	2.20	0.41
26:a:409:PL9:H221	26:a:409:PL9:H201	1.92	0.41
2:b:296:ALA:HB1	2:b:300:GLU:HB2	2.03	0.41
2:b:505:ARG:HG3	2:b:506:ARG:N	2.36	0.41
22:b:610:CLA:H143	22:b:610:CLA:H161	1.95	0.41
4:d:232:PHE:CE1	33:d:410:LHG:HC42	2.56	0.41
10:k:10:LYS:N	10:k:10:LYS:HD2	2.36	0.41
18:x:23:LEU:O	18:x:24:THR:C	2.64	0.41
3:C:61:VAL:HG12	3:C:118:HIS:O	2.21	0.41
22:c:506:CLA:O1A	22:c:506:CLA:C2	2.68	0.41
4:d:351[A]:ALA:HA	16:u:101:GLY:O	2.22	0.41
17:v:80:THR:HA	17:v:86:GLN:O	2.21	0.41
20:z:19:MET:O	20:z:23:VAL:HG23	2.21	0.41
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.56	0.40
2:B:63:LEU:N	2:B:64:PRO:HD2	2.36	0.40
22:B:603:CLA:H142	22:B:603:CLA:H112	1.92	0.40
22:B:614:CLA:H2A	22:B:614:CLA:O1D	2.21	0.40
3:C:264:PHE:CZ	24:C:514:BCR:H322	2.55	0.40
3:c:350:ILE:HG21	3:c:359[A]:TRP:HB2	2.02	0.40
4:d:225:ASP:HB2	4:d:234:ALA:HB1	2.02	0.40
10:k:24:VAL:O	10:k:27:VAL:HG22	2.21	0.40
2:B:97:ALA:O	2:B:101:ILE:HD12	2.21	0.40
2:B:216:HIS:HE1	22:B:609:CLA:C1A	2.35	0.40
22:B:607:CLA:H92	22:B:607:CLA:H61	1.81	0.40
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.52	0.40
17:V:99:ASP:OD1	17:V:99:ASP:N	2.54	0.40
2:b:235:GLU:OE2	2:b:469:HIS:ND1	2.31	0.40
5:e:57:ALA:H	5:e:60:GLN:HG2	1.86	0.40
22:B:603:CLA:C2D	22:B:605:CLA:H2	2.51	0.40
22:C:513:CLA:H41	22:C:513:CLA:H61	1.83	0.40
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.52	0.40
13:O:111:ALA:HA	2:b:76:SER:O	2.21	0.40
16:U:58:VAL:HG12	16:U:79:LEU:HD22	2.03	0.40
1:a:85:SER:HA	1:a:109:GLY:HA3	2.03	0.40
3:c:87:ILE:HD12	22:c:502:CLA:HMA3	2.04	0.40
4:d:35:ILE:HG22	32:d:413:STE:H131	2.03	0.40
4:d:127:LEU:HD13	32:d:413:STE:H71	2.02	0.40
22:B:616:CLA:HHC	22:B:616:CLA:HAB	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:41:HIS:O	17:V:42:VAL:C	2.65	0.40
24:c:515:BCR:H15C	24:c:515:BCR:H351	1.96	0.40
5:e:17:VAL:HG23	9:j:7:ARG:HB2	2.04	0.40
2:B:62:VAL:HB	22:B:605:CLA:HED3	2.04	0.40
2:B:338:GLN:HA	13:o:57:LYS:HE2	2.03	0.40
2:B:453:PHE:HB2	4:D:291:LEU:HD12	2.04	0.40
3:C:387:TRP:CE2	3:C:388:GLN:HG3	2.57	0.40
1:a:219:VAL:O	1:a:223:LEU:HD13	2.22	0.40
1:a:265:PHE:CD2	1:a:271:LEU:HD23	2.56	0.40
2:b:154:GLY:HA2	2:b:158:LEU:HD12	2.03	0.40
2:b:191:ASN:HB2	7:h:58:VAL:HG13	2.04	0.40
22:b:608:CLA:H141	22:b:608:CLA:H161	1.89	0.40
3:c:118:HIS:CE1	32:c:521:STE:H142	2.57	0.40
22:c:508:CLA:HBB1	22:c:508:CLA:HMB3	2.02	0.40
4:d:53:THR:O	4:d:66:SER:HB2	2.21	0.40
10:k:40:GLN:HA	10:k:43:VAL:HG22	2.04	0.40
16:u:51:LYS:HB2	16:u:51:LYS:HE2	1.95	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	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
1	a	397/344 (115%)	388 (98%)	8 (2%)	1 (0%)	36	36
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	492 (98%)	11 (2%)	0	100	100
3	C	454/461 (98%)	440 (97%)	13 (3%)	1 (0%)	43	44
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	43	44
4	D	340/352 (97%)	331 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	341/352 (97%)	332 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	3 (5%)	1 (2%)	7	4
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	227 (93%)	13 (5%)	3 (1%)	10	7
13	o	242/272 (89%)	231 (96%)	8 (3%)	3 (1%)	10	7
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	90 (95%)	4 (4%)	1 (1%)	11	8
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	15
17	v	135/163 (83%)	132 (98%)	3 (2%)	0	100	100
18	X	36/41 (88%)	34 (94%)	2 (6%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	2 (8%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5387/5700 (94%)	5225 (97%)	150 (3%)	12 (0%)	43	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
16	u	53	ALA
13	o	61	GLN
13	O	26	ALA
13	o	58	ASN
7	H	12	ARG
1	a	259	ILE
13	o	56	PRO

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	324/280 (116%)	314 (97%)	10 (3%)	35	39
1	a	323/280 (115%)	311 (96%)	12 (4%)	30	33
2	B	408/407 (100%)	397 (97%)	11 (3%)	39	45
2	b	402/407 (99%)	391 (97%)	11 (3%)	39	45
3	C	356/362 (98%)	350 (98%)	6 (2%)	53	62
3	c	364/362 (101%)	350 (96%)	14 (4%)	29	32
4	D	277/283 (98%)	273 (99%)	4 (1%)	59	67
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	28
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	28
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	34
6	f	28/39 (72%)	24 (86%)	4 (14%)	3	1
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	33
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	32
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	14
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	39
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	8
10	K	30/37 (81%)	27 (90%)	3 (10%)	7	5
10	k	30/37 (81%)	28 (93%)	2 (7%)	15	12
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	42
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	7
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	4
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	35
13	o	207/228 (91%)	198 (96%)	9 (4%)	26	27
14	R	22/33 (67%)	18 (82%)	4 (18%)	2	1
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	2
15	T	26/28 (93%)	24 (92%)	2 (8%)	12	9
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	29
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	23
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	34
17	V	117/138 (85%)	114 (97%)	3 (3%)	40	46
17	v	117/138 (85%)	112 (96%)	5 (4%)	26	27
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	38
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	13
19	Y	19/37 (51%)	16 (84%)	3 (16%)	2	1
19	y	22/37 (60%)	21 (96%)	1 (4%)	24	25
20	Z	52/52 (100%)	43 (83%)	9 (17%)	2	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	5
All	All	4451/4654 (96%)	4278 (96%)	173 (4%)	28	31

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	16	ARG
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	134	SER
1	A	205	VAL
1	A	229	GLU
1	A	243	GLU
1	A	244	GLU
1	A	248	ILE
2	B	63	LEU
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	168	VAL
2	B	227	LYS
2	B	240	SER
2	B	282	GLN
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	154	VAL
4	D	246	MET
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	81	GLU
6	F	25	THR
7	H	20	LYS

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Mol	Chain	Res	Type
7	H	56	ASP
8	I	4	LEU
8	I	6	ILE
10	K	10	LYS
10	K	13	GLU
10	K	27	VAL
11	L	10	VAL
12	M	9	ILE
12	M	25	LEU
13	O	6	THR
13	O	54	GLU
13	O	64	GLU
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	214	THR
14	R	13	LEU
14	R	21	ARG
14	R	22	ASN
14	R	29	LYS
15	T	25	GLU
15	T	30	THR
16	U	10	VAL
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	31	ARG
18	X	3	ILE
19	Y	28	ILE
19	Y	34	MET
19	Y	41	VAL
20	Z	2	THR
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	35	ARG
20	Z	38	GLN
20	Z	46	LEU
20	Z	50	LEU

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Mol	Chain	Res	Type
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	243	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	86	ILE
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	266	GLU
2	b	405	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	78	GLU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	279	LEU
3	c	315	MET
3	c	346	THR
3	c	413[A]	GLU
3	c	413[B]	GLU
4	d	90	LEU
4	d	182	LEU
4	d	233	ARG
4	d	241	GLU
4	d	259	ILE

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Mol	Chain	Res	Type
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	65	LEU
5	e	66	VAL
6	f	15	ILE
6	f	23	VAL
6	f	25	THR
6	f	28	VAL
7	h	7	LEU
7	h	27	THR
8	i	2	GLU
9	j	7	ARG
9	j	13	VAL
10	k	10	LYS
10	k	30	VAL
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	2	GLU
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS
13	o	34	SER
13	o	49	THR
13	o	60	ARG
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	143	LYS
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
15	t	25	GLU
16	u	15	GLU
16	u	23	GLU
16	u	80	GLU
17	v	19	ILE
17	v	30	LYS

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Mol	Chain	Res	Type
17	v	52	LEU
17	v	107	LEU
17	v	128	ASP
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
20	z	1	MET
20	z	20	VAL
20	z	31	GLN
20	z	40	ILE
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	374	ASN
3	C	385	GLN
3	C	415	ASN
4	D	61	HIS
7	H	59	ASN
11	L	8	GLN
12	M	5	GLN
13	O	36	GLN
13	O	88	ASN
13	O	124	ASN
13	O	132	ASN
13	O	231	HIS
14	R	22	ASN
16	U	71	GLN
16	U	78	ASN
17	V	86	GLN
2	b	179	GLN
2	b	274	GLN
2	b	409	GLN
3	c	311	GLN
3	c	322	GLN
5	e	74	GLN
13	o	61	GLN
13	o	109	GLN
13	o	124	ASN
13	o	200	ASN
18	x	33	GLN

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Mol	Chain	Res	Type
20	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	FME	T	1	15	8,9,10	1.13	1 (12%)	8,9,11	1.07	0
12	FME	M	1	12	8,9,10	0.91	0	8,9,11	0.99	0
8	FME	I	1	8	8,9,10	0.97	1 (12%)	8,9,11	1.34	1 (12%)
15	FME	t	1	15	8,9,10	1.69	1 (12%)	8,9,11	0.95	0
12	FME	m	1	12	8,9,10	1.07	1 (12%)	8,9,11	1.14	0
8	FME	i	1	8	8,9,10	1.01	1 (12%)	8,9,11	1.36	1 (12%)

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
15	FME	T	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
15	FME	t	1	15	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	i	1	8	-	4/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-4.26	1.40	1.46
12	m	1	FME	CA-N	-2.33	1.43	1.46
15	T	1	FME	CA-N	-2.28	1.43	1.46
8	I	1	FME	CA-N	-2.10	1.43	1.46
8	i	1	FME	CA-N	-2.08	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	C-CA-N	2.57	114.46	109.50
8	I	1	FME	CA-N-CN	-2.47	119.02	122.82

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 188 ligands modelled in this entry, 6 are monoatomic - leaving 182 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	$\# Z > 2$
22	CLA	A	403	37	69,73,73	1.38	7 (10%)	82,113,113	1.18	10 (12%)
22	CLA	c	509	3	69,73,73	1.38	8 (11%)	82,113,113	1.61	9 (10%)
28	SQD	f	102	-	39,41,54	1.18	4 (10%)	49,52,65	1.76	11 (22%)
22	CLA	C	512	3	69,73,73	1.55	12 (17%)	82,113,113	1.28	8 (9%)
24	BCR	C	515	-	41,41,41	1.21	5 (12%)	56,56,56	1.13	4 (7%)
22	CLA	c	507	37	69,73,73	1.24	7 (10%)	82,113,113	1.17	7 (8%)
32	STE	E	103	-	11,11,19	0.98	0	11,11,19	0.83	0
22	CLA	b	602	2	69,73,73	1.12	9 (13%)	82,113,113	1.37	9 (10%)
27	LMG	D	410	-	31,31,55	1.18	3 (9%)	33,33,63	1.11	2 (6%)
22	CLA	A	405	1	58,62,73	1.48	8 (13%)	68,99,113	1.42	10 (14%)
22	CLA	C	509	3	69,73,73	1.41	13 (18%)	82,113,113	1.37	12 (14%)
22	CLA	b	608	2	69,73,73	1.12	7 (10%)	82,113,113	1.46	11 (13%)
32	STE	x	101	-	19,19,19	0.82	0	19,19,19	0.65	0
24	BCR	c	514	-	41,41,41	1.24	2 (4%)	56,56,56	1.32	8 (14%)
33	LHG	E	102	-	48,48,48	0.88	3 (6%)	51,54,54	1.20	3 (5%)
31	OEX	A	416[A]	3,37,1	0,14,14	-	-	-	-	-
27	LMG	b	620	-	51,51,55	1.14	6 (11%)	59,59,63	1.51	11 (18%)
32	STE	J	101	-	11,11,19	0.69	0	11,11,19	1.39	1 (9%)
22	CLA	c	513	3	69,73,73	1.28	11 (15%)	82,113,113	1.28	11 (13%)
26	PL9	a	409	-	55,55,55	0.94	2 (3%)	68,69,69	1.66	16 (23%)
22	CLA	B	610	37	69,73,73	1.17	7 (10%)	82,113,113	1.41	11 (13%)
22	CLA	a	403	37	69,73,73	1.33	6 (8%)	82,113,113	1.41	11 (13%)
22	CLA	b	613	2	69,73,73	1.45	11 (15%)	82,113,113	1.43	10 (12%)
24	BCR	b	618	-	41,41,41	1.37	4 (9%)	56,56,56	1.22	5 (8%)
24	BCR	k	101	-	41,41,41	1.12	5 (12%)	56,56,56	1.13	3 (5%)
27	LMG	B	621	-	26,26,55	0.96	1 (3%)	26,26,63	1.14	1 (3%)
22	CLA	B	613	2	69,73,73	1.29	11 (15%)	82,113,113	1.41	10 (12%)
33	LHG	d	410	-	38,38,48	0.89	3 (7%)	41,44,54	1.15	3 (7%)
23	PHO	A	404	-	58,69,69	1.77	9 (15%)	55,99,99	1.67	12 (21%)
32	STE	c	524	-	11,11,19	0.75	0	11,11,19	1.20	1 (9%)
23	PHO	d	401	-	58,69,69	2.14	11 (18%)	55,99,99	1.49	11 (20%)
22	CLA	B	604	2	69,73,73	1.28	6 (8%)	82,113,113	1.66	14 (17%)
32	STE	M	102	-	14,14,19	0.84	0	14,14,19	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	402	1	69,73,73	1.38	10 (14%)	82,113,113	1.32	11 (13%)
23	PHO	d	402	-	58,69,69	2.12	9 (15%)	55,99,99	1.66	10 (18%)
36	HEC	v	201	17	50,50,50	1.73	5 (10%)	68,82,82	1.17	3 (4%)
24	BCR	Y	101	-	41,41,41	1.03	2 (4%)	56,56,56	1.21	4 (7%)
22	CLA	b	615	2	69,73,73	1.45	11 (15%)	82,113,113	1.32	10 (12%)
23	PHO	D	401	-	58,69,69	1.96	11 (18%)	55,99,99	1.54	10 (18%)
22	CLA	B	612	2	69,73,73	1.17	7 (10%)	82,113,113	1.36	10 (12%)
22	CLA	c	501	3	69,73,73	1.17	9 (13%)	82,113,113	1.40	10 (12%)
22	CLA	c	506	3	69,73,73	1.26	8 (11%)	82,113,113	1.25	8 (9%)
32	STE	D	411	-	19,19,19	0.67	1 (5%)	19,19,19	1.06	0
32	STE	B	627	-	11,11,19	1.05	1 (9%)	11,11,19	0.71	0
22	CLA	c	505	3	69,73,73	1.03	5 (7%)	82,113,113	1.34	7 (8%)
35	HEM	E	101	6,5	50,50,50	1.34	5 (10%)	67,82,82	1.16	5 (7%)
22	CLA	c	504	37	64,68,73	1.33	8 (12%)	76,107,113	1.34	6 (7%)
29	DGD	c	518	-	63,63,67	1.31	9 (14%)	77,77,81	1.52	9 (11%)
32	STE	j	101	-	11,11,19	0.84	0	11,11,19	1.65	3 (27%)
22	CLA	C	505	3	69,73,73	1.35	8 (11%)	82,113,113	1.23	6 (7%)
22	CLA	b	605	2	69,73,73	1.15	9 (13%)	82,113,113	1.42	17 (20%)
22	CLA	b	606	2	69,73,73	1.23	7 (10%)	82,113,113	1.55	9 (10%)
22	CLA	c	512	3	69,73,73	1.26	12 (17%)	82,113,113	1.39	8 (9%)
22	CLA	b	611	2	69,73,73	1.26	5 (7%)	82,113,113	1.38	6 (7%)
24	BCR	B	617	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	6 (10%)
33	LHG	L	102	-	48,48,48	1.02	2 (4%)	51,54,54	1.25	2 (3%)
22	CLA	c	503	3	69,73,73	1.26	11 (15%)	82,113,113	1.33	8 (9%)
29	DGD	a	412	-	43,43,67	1.15	3 (6%)	45,45,81	1.47	7 (15%)
26	PL9	d	407	-	55,55,55	1.44	6 (10%)	68,69,69	1.81	16 (23%)
22	CLA	b	614	2	69,73,73	1.39	11 (15%)	82,113,113	1.24	9 (10%)
32	STE	T	102	-	15,15,19	0.53	0	14,14,19	0.70	0
30	OEY	A	415[B]	3,37,1	0,16,16	-	-	-	-	-
27	LMG	A	411	-	48,48,55	0.99	3 (6%)	56,56,63	1.32	7 (12%)
22	CLA	B	614	2	69,73,73	1.36	9 (13%)	82,113,113	1.25	9 (10%)
32	STE	b	623	-	15,15,19	0.94	1 (6%)	15,15,19	0.94	1 (6%)
28	SQD	a	410	-	52,54,54	0.94	4 (7%)	62,65,65	2.02	13 (20%)
32	STE	C	521	-	15,15,19	0.57	0	14,14,19	0.51	0
32	STE	a	414	-	11,11,19	0.78	0	11,11,19	1.13	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	LHG	e	101	-	41,41,48	0.88	1 (2%)	44,47,54	1.29	4 (9%)
22	CLA	A	402	1	69,73,73	1.25	7 (10%)	82,113,113	1.33	10 (12%)
24	BCR	c	516	-	41,41,41	1.13	2 (4%)	56,56,56	1.20	7 (12%)
22	CLA	c	511	3	69,73,73	1.44	6 (8%)	82,113,113	1.49	8 (9%)
29	DGD	A	414	-	67,67,67	1.39	7 (10%)	81,81,81	1.48	11 (13%)
30	OEY	a	415[B]	3,37,1	0,16,16	-	-	-		
34	BCT	a	408	21	3,3,3	1.10	0	2,3,3	3.45	2 (100%)
22	CLA	B	606	2	69,73,73	1.33	11 (15%)	82,113,113	1.39	12 (14%)
35	HEM	f	101	6,5	50,50,50	1.47	8 (16%)	67,82,82	1.22	6 (8%)
22	CLA	D	404	4	69,73,73	1.61	10 (14%)	82,113,113	1.43	8 (9%)
29	DGD	C	516	-	63,63,67	1.36	11 (17%)	77,77,81	1.40	10 (12%)
28	SQD	B	623	-	52,54,54	1.00	2 (3%)	62,65,65	1.82	11 (17%)
22	CLA	B	608	2	69,73,73	1.25	6 (8%)	82,113,113	1.55	11 (13%)
32	STE	d	413	-	16,16,19	0.76	0	16,16,19	1.13	1 (6%)
26	PL9	D	406	-	55,55,55	1.51	5 (9%)	68,69,69	1.60	15 (22%)
22	CLA	A	410	37	69,73,73	1.17	7 (10%)	82,113,113	1.24	8 (9%)
24	BCR	T	101	-	41,41,41	1.34	4 (9%)	56,56,56	1.27	6 (10%)
24	BCR	b	619	-	41,41,41	1.21	2 (4%)	56,56,56	1.42	11 (19%)
22	CLA	C	506	3	69,73,73	1.43	9 (13%)	82,113,113	1.33	8 (9%)
22	CLA	D	403	4	69,73,73	1.32	8 (11%)	82,113,113	1.29	9 (10%)
22	CLA	B	601	37	69,73,73	1.53	11 (15%)	82,113,113	1.39	7 (8%)
32	STE	M	103	-	9,9,19	0.53	0	8,8,19	0.61	0
28	SQD	L	101	-	47,49,54	0.99	3 (6%)	57,60,65	2.25	16 (28%)
27	LMG	c	520	-	37,37,55	1.25	5 (13%)	45,45,63	1.31	6 (13%)
24	BCR	c	515	-	41,41,41	1.26	3 (7%)	56,56,56	1.41	9 (16%)
32	STE	B	626	-	15,15,19	0.49	0	14,14,19	0.73	0
32	STE	m	101	-	11,11,19	0.70	0	11,11,19	1.69	2 (18%)
22	CLA	C	511	3	69,73,73	1.37	8 (11%)	82,113,113	1.17	5 (6%)
22	CLA	c	502	3	69,73,73	1.24	9 (13%)	82,113,113	1.28	8 (9%)
32	STE	C	522	-	11,11,19	0.59	0	11,11,19	1.65	3 (27%)
22	CLA	B	616	2	64,68,73	1.31	6 (9%)	76,107,113	1.68	9 (11%)
22	CLA	b	604	2	69,73,73	1.17	9 (13%)	82,113,113	1.55	11 (13%)
24	BCR	t	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.48	9 (16%)
32	STE	I	101	-	14,14,19	0.64	0	13,13,19	0.40	0
22	CLA	C	513	3	69,73,73	1.22	8 (11%)	82,113,113	1.43	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	DGD	H	102	-	63,63,67	1.40	9 (14%)	77,77,81	1.43	8 (10%)
22	CLA	a	404	1	69,73,73	1.41	10 (14%)	82,113,113	1.19	7 (8%)
22	CLA	C	507	37	69,73,73	1.17	7 (10%)	82,113,113	1.59	8 (9%)
29	DGD	C	518	-	63,63,67	1.17	10 (15%)	77,77,81	1.36	9 (11%)
33	LHG	d	409	-	48,48,48	0.78	2 (4%)	51,54,54	1.15	3 (5%)
36	HEC	V	201	17	50,50,50	1.53	3 (6%)	68,82,82	1.26	9 (13%)
32	STE	C	520	-	11,11,19	0.74	0	11,11,19	1.54	2 (18%)
32	STE	T	103	-	14,14,19	0.44	0	13,13,19	0.89	0
22	CLA	B	609	2	69,73,73	1.13	6 (8%)	82,113,113	1.19	6 (7%)
22	CLA	C	504	37	63,67,73	1.23	8 (12%)	74,105,113	1.22	7 (9%)
24	BCR	B	618	-	41,41,41	1.27	4 (9%)	56,56,56	1.19	9 (16%)
32	STE	l	102	-	17,17,19	0.47	0	16,16,19	0.80	0
24	BCR	K	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.39	9 (16%)
32	STE	b	621	-	19,19,19	0.71	0	19,19,19	0.90	0
22	CLA	b	603	2	69,73,73	1.37	10 (14%)	82,113,113	1.39	7 (8%)
29	DGD	c	519	-	63,63,67	1.40	9 (14%)	77,77,81	1.43	12 (15%)
22	CLA	d	405	4	69,73,73	1.43	11 (15%)	82,113,113	1.18	7 (8%)
32	STE	B	620	-	16,16,19	0.71	0	16,16,19	1.05	1 (6%)
33	LHG	d	408	-	48,48,48	1.06	4 (8%)	51,54,54	1.47	8 (15%)
32	STE	t	102	-	13,13,19	0.71	0	13,13,19	1.15	1 (7%)
28	SQD	F	101	-	34,36,54	1.01	3 (8%)	42,45,65	1.84	9 (21%)
27	LMG	C	519	-	48,48,55	1.19	7 (14%)	56,56,63	1.43	7 (12%)
28	SQD	a	411	-	35,35,54	1.13	2 (5%)	37,37,65	1.19	5 (13%)
22	CLA	b	601	37	69,73,73	1.33	7 (10%)	82,113,113	1.50	6 (7%)
32	STE	c	521	-	19,19,19	0.79	1 (5%)	19,19,19	0.94	0
32	STE	a	413	-	9,9,19	0.69	0	8,8,19	0.42	0
27	LMG	d	412	-	44,44,55	1.23	6 (13%)	52,52,63	1.39	8 (15%)
22	CLA	C	502	3	69,73,73	1.18	8 (11%)	82,113,113	1.19	5 (6%)
27	LMG	c	523	-	49,49,55	1.04	3 (6%)	57,57,63	1.28	7 (12%)
24	BCR	B	619	-	41,41,41	1.13	3 (7%)	56,56,56	1.39	4 (7%)
22	CLA	b	616	2	64,68,73	1.11	4 (6%)	76,107,113	1.49	10 (13%)
22	CLA	C	508	3	69,73,73	1.37	10 (14%)	82,113,113	1.38	9 (10%)
24	BCR	H	101	-	41,41,41	1.16	1 (2%)	56,56,56	1.28	8 (14%)
32	STE	B	624	-	11,11,19	0.86	0	11,11,19	0.96	1 (9%)
24	BCR	a	405	-	41,41,41	1.17	4 (9%)	56,56,56	1.43	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	605	2	69,73,73	1.29	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	B	615	2	69,73,73	1.36	7 (10%)	82,113,113	1.45	9 (10%)
32	STE	b	625	-	9,9,19	0.64	0	8,8,19	0.48	0
28	SQD	A	412	-	50,52,54	1.02	4 (8%)	60,63,65	2.04	12 (20%)
32	STE	H	103	-	17,17,19	0.59	0	16,16,19	0.59	0
31	OEX	a	416[A]	3,37,1	0,14,14	-	-	-	-	-
33	LHG	D	409	-	46,46,48	1.13	3 (6%)	49,52,54	1.14	3 (6%)
22	CLA	b	609	2	69,73,73	1.20	8 (11%)	82,113,113	1.23	7 (8%)
27	LMG	b	622	-	55,55,55	1.04	7 (12%)	63,63,63	1.44	7 (11%)
26	PL9	A	409	-	55,55,55	1.14	5 (9%)	68,69,69	1.57	13 (19%)
24	BCR	D	405	-	41,41,41	1.22	3 (7%)	56,56,56	1.16	6 (10%)
27	LMG	D	407	-	51,51,55	1.18	4 (7%)	59,59,63	1.34	9 (15%)
22	CLA	c	508	3	68,72,73	1.25	10 (14%)	80,111,113	1.39	12 (15%)
22	CLA	b	610	37	69,73,73	1.34	9 (13%)	82,113,113	1.28	11 (13%)
22	CLA	d	403	4	69,73,73	1.24	6 (8%)	82,113,113	1.13	5 (6%)
22	CLA	B	607	37	69,73,73	1.56	9 (13%)	82,113,113	1.53	7 (8%)
22	CLA	C	503	3	69,73,73	1.60	9 (13%)	82,113,113	1.43	10 (12%)
22	CLA	C	510	3	69,73,73	1.18	8 (11%)	82,113,113	1.21	9 (10%)
22	CLA	b	607	37	69,73,73	1.37	8 (11%)	82,113,113	1.19	7 (8%)
22	CLA	B	603	2	69,73,73	1.32	12 (17%)	82,113,113	1.47	12 (14%)
24	BCR	A	406	-	41,41,41	1.19	2 (4%)	56,56,56	1.46	10 (17%)
22	CLA	d	404	37	69,73,73	1.37	5 (7%)	82,113,113	1.50	10 (12%)
32	STE	B	625	-	17,17,19	0.65	0	17,17,19	0.99	0
28	SQD	A	413	-	38,38,54	1.04	3 (7%)	40,40,65	1.45	6 (15%)
22	CLA	B	611	2	69,73,73	1.10	6 (8%)	82,113,113	1.40	15 (18%)
32	STE	b	624	-	19,19,19	0.87	0	19,19,19	0.86	1 (5%)
33	LHG	l	101	-	48,48,48	0.87	1 (2%)	51,54,54	1.16	5 (9%)
27	LMG	c	522	-	48,48,55	1.20	6 (12%)	56,56,63	1.37	8 (14%)
24	BCR	d	406	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	6 (10%)
22	CLA	B	602	2	69,73,73	1.31	10 (14%)	82,113,113	1.50	10 (12%)
22	CLA	C	501	3	69,73,73	1.31	10 (14%)	82,113,113	1.48	7 (8%)
27	LMG	d	411	-	21,21,55	0.83	0	20,20,63	1.21	1 (5%)
33	LHG	B	622	-	48,48,48	1.05	4 (8%)	51,54,54	1.42	6 (11%)
22	CLA	c	510	3	69,73,73	1.19	9 (13%)	82,113,113	1.39	8 (9%)
33	LHG	D	408	-	48,48,48	1.00	5 (10%)	51,54,54	1.29	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCT	D	402	21	3,3,3	1.02	0	2,3,3	3.66	2 (100%)
22	CLA	b	612	2	69,73,73	1.34	7 (10%)	82,113,113	1.34	10 (12%)
27	LMG	M	101	-	51,51,55	1.11	5 (9%)	59,59,63	1.41	7 (11%)
29	DGD	c	517	-	63,63,67	1.10	6 (9%)	77,77,81	1.35	7 (9%)
29	DGD	h	102	-	63,63,67	1.29	11 (17%)	77,77,81	1.54	13 (16%)
24	BCR	b	617	-	41,41,41	1.10	3 (7%)	56,56,56	1.46	11 (19%)
24	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.30	9 (16%)
29	DGD	C	517	-	63,63,67	1.40	7 (11%)	77,77,81	1.55	14 (18%)
24	BCR	C	514	-	41,41,41	1.25	4 (9%)	56,56,56	1.30	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	403	37	-	13/39/115/115	-
22	CLA	c	509	3	-	10/39/115/115	-
28	SQD	f	102	-	-	11/36/56/69	0/1/1/1
22	CLA	C	512	3	-	14/39/115/115	-
24	BCR	C	515	-	-	13/29/63/63	0/2/2/2
22	CLA	c	507	37	-	10/39/115/115	-
32	STE	E	103	-	-	6/9/9/17	-
22	CLA	b	602	2	-	11/39/115/115	-
27	LMG	D	410	-	-	17/33/33/70	-
22	CLA	A	405	1	-	3/26/102/115	-
22	CLA	C	509	3	-	14/39/115/115	-
22	CLA	b	608	2	-	9/39/115/115	-
32	STE	x	101	-	-	9/17/17/17	-
24	BCR	c	514	-	-	9/29/63/63	0/2/2/2
33	LHG	E	102	-	-	24/53/53/53	-
27	LMG	b	620	-	-	14/46/66/70	0/1/1/1
32	STE	J	101	-	-	2/9/9/17	-
22	CLA	c	513	3	-	6/39/115/115	-
26	PL9	a	409	-	-	18/53/73/73	0/1/1/1
22	CLA	B	610	37	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	403	37	-	9/39/115/115	-
22	CLA	b	613	2	-	4/39/115/115	-
24	BCR	b	618	-	-	7/29/63/63	0/2/2/2
24	BCR	k	101	-	-	9/29/63/63	0/2/2/2
27	LMG	B	621	-	-	14/22/22/70	-
22	CLA	B	613	2	-	11/39/115/115	-
33	LHG	d	410	-	-	13/43/43/53	-
23	PHO	A	404	-	-	5/37/103/103	0/5/6/6
32	STE	c	524	-	-	5/9/9/17	-
23	PHO	d	401	-	-	3/37/103/103	0/5/6/6
22	CLA	B	604	2	-	13/39/115/115	-
32	STE	M	102	-	-	4/12/12/17	-
22	CLA	a	402	1	-	6/39/115/115	-
23	PHO	d	402	-	-	7/37/103/103	0/5/6/6
36	HEC	v	201	17	1/1/7/7	5/14/54/54	-
24	BCR	Y	101	-	-	8/29/63/63	0/2/2/2
22	CLA	b	615	2	-	11/39/115/115	-
23	PHO	D	401	-	-	1/37/103/103	0/5/6/6
22	CLA	B	612	2	-	10/39/115/115	-
22	CLA	c	501	3	-	3/39/115/115	-
22	CLA	c	506	3	-	11/39/115/115	-
32	STE	D	411	-	-	12/17/17/17	-
32	STE	B	627	-	-	4/9/9/17	-
22	CLA	c	505	3	-	9/39/115/115	-
35	HEM	E	101	6,5	-	2/14/54/54	-
22	CLA	c	504	37	-	4/33/109/115	-
29	DGD	c	518	-	-	21/51/91/95	0/2/2/2
32	STE	j	101	-	-	3/9/9/17	-
22	CLA	C	505	3	-	18/39/115/115	-
22	CLA	b	605	2	-	8/39/115/115	-
22	CLA	b	606	2	-	13/39/115/115	-
22	CLA	c	512	3	-	22/39/115/115	-
22	CLA	b	611	2	-	6/39/115/115	-
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	L	102	-	-	20/53/53/53	-
22	CLA	c	503	3	-	8/39/115/115	-
29	DGD	a	412	-	-	27/45/45/95	-
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
22	CLA	b	614	2	-	15/39/115/115	-
32	STE	T	102	-	-	5/13/13/17	-
27	LMG	A	411	-	-	23/43/63/70	0/1/1/1
22	CLA	B	614	2	-	12/39/115/115	-
32	STE	b	623	-	-	6/13/13/17	-
28	SQD	a	410	-	-	20/49/69/69	0/1/1/1
32	STE	C	521	-	-	5/13/13/17	-
32	STE	a	414	-	-	7/9/9/17	-
33	LHG	e	101	-	-	22/46/46/53	-
22	CLA	A	402	1	-	5/39/115/115	-
24	BCR	c	516	-	-	4/29/63/63	0/2/2/2
22	CLA	c	511	3	-	11/39/115/115	-
29	DGD	A	414	-	-	25/55/95/95	0/2/2/2
35	HEM	f	101	6,5	-	4/14/54/54	-
22	CLA	B	606	2	-	11/39/115/115	-
22	CLA	D	404	4	-	8/39/115/115	-
29	DGD	C	516	-	-	21/51/91/95	0/2/2/2
28	SQD	B	623	-	-	24/49/69/69	0/1/1/1
22	CLA	B	608	2	-	3/39/115/115	-
32	STE	d	413	-	-	11/14/14/17	-
26	PL9	D	406	-	-	7/53/73/73	0/1/1/1
22	CLA	A	410	37	-	9/39/115/115	-
24	BCR	T	101	-	-	9/29/63/63	0/2/2/2
24	BCR	b	619	-	-	5/29/63/63	0/2/2/2
22	CLA	C	506	3	-	11/39/115/115	-
22	CLA	D	403	4	-	6/39/115/115	-
22	CLA	B	601	37	-	16/39/115/115	-
32	STE	M	103	-	-	2/7/7/17	-
28	SQD	L	101	-	-	22/44/64/69	0/1/1/1
27	LMG	c	520	-	-	8/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	c	515	-	-	3/29/63/63	0/2/2/2
32	STE	B	626	-	-	6/13/13/17	-
32	STE	m	101	-	-	5/9/9/17	-
22	CLA	C	511	3	-	6/39/115/115	-
22	CLA	c	502	3	-	9/39/115/115	-
32	STE	C	522	-	-	4/9/9/17	-
22	CLA	B	616	2	-	10/33/109/115	-
22	CLA	b	604	2	-	8/39/115/115	-
24	BCR	t	101	-	-	10/29/63/63	0/2/2/2
32	STE	I	101	-	-	8/12/12/17	-
22	CLA	C	513	3	-	16/39/115/115	-
29	DGD	H	102	-	-	22/51/91/95	0/2/2/2
22	CLA	a	404	1	-	8/39/115/115	-
22	CLA	C	507	37	-	6/39/115/115	-
29	DGD	C	518	-	-	12/51/91/95	0/2/2/2
36	HEC	V	201	17	1/1/7/7	4/14/54/54	-
33	LHG	d	409	-	-	17/53/53/53	-
32	STE	C	520	-	-	5/9/9/17	-
32	STE	T	103	-	-	7/12/12/17	-
22	CLA	B	609	2	-	4/39/115/115	-
22	CLA	C	504	37	-	6/32/108/115	-
24	BCR	B	618	-	-	5/29/63/63	0/2/2/2
32	STE	l	102	-	-	9/15/15/17	-
24	BCR	K	101	-	-	5/29/63/63	0/2/2/2
32	STE	b	621	-	-	12/17/17/17	-
22	CLA	b	603	2	-	5/39/115/115	-
29	DGD	c	519	-	-	19/51/91/95	0/2/2/2
22	CLA	d	405	4	-	10/39/115/115	-
32	STE	B	620	-	-	8/14/14/17	-
33	LHG	d	408	-	-	24/53/53/53	-
32	STE	t	102	-	-	4/11/11/17	-
28	SQD	F	101	-	-	10/28/48/69	0/1/1/1
27	LMG	C	519	-	-	19/43/63/70	0/1/1/1
28	SQD	a	411	-	-	17/37/37/69	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	b	601	37	-	15/39/115/115	-
32	STE	c	521	-	-	10/17/17/17	-
32	STE	a	413	-	-	3/7/7/17	-
27	LMG	d	412	-	-	11/39/59/70	0/1/1/1
22	CLA	C	502	3	-	10/39/115/115	-
27	LMG	c	523	-	-	23/44/64/70	0/1/1/1
24	BCR	B	619	-	-	1/29/63/63	0/2/2/2
22	CLA	b	616	2	-	6/33/109/115	-
22	CLA	C	508	3	-	7/39/115/115	-
24	BCR	H	101	-	-	7/29/63/63	0/2/2/2
32	STE	B	624	-	-	6/9/9/17	-
24	BCR	a	405	-	-	4/29/63/63	0/2/2/2
22	CLA	B	605	2	-	11/39/115/115	-
22	CLA	B	615	2	-	9/39/115/115	-
32	STE	b	625	-	-	5/7/7/17	-
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
32	STE	H	103	-	-	6/15/15/17	-
33	LHG	D	409	-	-	16/51/51/53	-
22	CLA	b	609	2	-	8/39/115/115	-
27	LMG	b	622	-	-	29/50/70/70	0/1/1/1
26	PL9	A	409	-	-	22/53/73/73	0/1/1/1
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2
27	LMG	D	407	-	-	17/46/66/70	0/1/1/1
22	CLA	c	508	3	-	5/38/114/115	-
22	CLA	b	610	37	-	3/39/115/115	-
22	CLA	d	403	4	-	11/39/115/115	-
22	CLA	B	607	37	-	11/39/115/115	-
22	CLA	C	503	3	-	8/39/115/115	-
22	CLA	C	510	3	-	10/39/115/115	-
22	CLA	b	607	37	-	15/39/115/115	-
22	CLA	B	603	2	-	11/39/115/115	-
24	BCR	A	406	-	-	3/29/63/63	0/2/2/2
22	CLA	d	404	37	-	6/39/115/115	-
32	STE	B	625	-	-	11/15/15/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	413	-	-	13/39/39/69	-
22	CLA	B	611	2	-	7/39/115/115	-
32	STE	b	624	-	-	8/17/17/17	-
33	LHG	l	101	-	-	26/53/53/53	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
24	BCR	d	406	-	-	7/29/63/63	0/2/2/2
22	CLA	B	602	2	-	9/39/115/115	-
22	CLA	C	501	3	-	4/39/115/115	-
27	LMG	d	411	-	-	10/17/17/70	-
33	LHG	B	622	-	-	18/53/53/53	-
22	CLA	c	510	3	-	14/39/115/115	-
33	LHG	D	408	-	-	26/53/53/53	-
22	CLA	b	612	2	-	6/39/115/115	-
27	LMG	M	101	-	-	24/46/66/70	0/1/1/1
29	DGD	c	517	-	-	27/51/91/95	0/2/2/2
29	DGD	h	102	-	-	15/51/91/95	0/2/2/2
24	BCR	b	617	-	-	8/29/63/63	0/2/2/2
24	BCR	h	101	-	-	10/29/63/63	0/2/2/2
29	DGD	C	517	-	-	19/51/91/95	0/2/2/2
24	BCR	C	514	-	-	6/29/63/63	0/2/2/2

All (931) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	PHO	C1B-C2B	10.16	1.50	1.39
23	d	401	PHO	C1B-C2B	9.28	1.49	1.39
23	d	401	PHO	C3B-C4B	8.71	1.50	1.41
23	D	401	PHO	C3B-C4B	8.45	1.50	1.41
22	D	404	CLA	MG-NB	-8.06	1.89	2.05
23	d	402	PHO	C3B-C4B	7.96	1.49	1.41
23	A	404	PHO	C1B-C2B	7.53	1.47	1.39
23	D	401	PHO	C1B-C2B	7.36	1.47	1.39
22	d	405	CLA	MG-NB	-7.31	1.91	2.05
36	v	201	HEC	C3D-C2D	7.07	1.52	1.36
22	B	607	CLA	MG-NB	-6.98	1.92	2.05
22	B	601	CLA	MG-NA	6.52	2.21	2.06
22	C	503	CLA	MG-NA	6.50	2.21	2.06
22	c	511	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	406	PL9	C6-C1	-6.32	1.37	1.48
22	A	405	CLA	MG-ND	-6.06	1.93	2.05
22	C	505	CLA	MG-NA	6.05	2.20	2.06
22	C	506	CLA	MG-ND	-6.02	1.93	2.05
36	V	201	HEC	C3D-C2D	5.89	1.49	1.36
22	d	404	CLA	MG-NA	5.89	2.20	2.06
22	b	612	CLA	MG-ND	-5.89	1.94	2.05
22	B	616	CLA	MG-NA	5.82	2.20	2.06
22	b	610	CLA	MG-NB	-5.79	1.94	2.05
22	b	613	CLA	MG-NA	5.73	2.19	2.06
22	C	511	CLA	MG-NA	5.62	2.19	2.06
23	A	404	PHO	C3B-C4B	5.32	1.46	1.41
22	b	615	CLA	MG-ND	-5.31	1.95	2.05
22	C	512	CLA	MG-NA	5.30	2.18	2.06
22	B	604	CLA	MG-NC	5.25	2.18	2.06
36	v	201	HEC	FE-NA	5.20	2.12	1.95
29	H	102	DGD	O5D-C1E	5.18	1.48	1.40
24	b	618	BCR	C30-C25	-5.17	1.47	1.53
22	B	615	CLA	MG-NA	5.14	2.18	2.06
22	b	611	CLA	MG-NA	5.13	2.18	2.06
22	C	512	CLA	MG-NB	5.13	2.16	2.05
22	c	506	CLA	MG-ND	-5.13	1.95	2.05
22	C	508	CLA	MG-NA	5.08	2.18	2.06
22	a	403	CLA	MG-ND	-5.06	1.95	2.05
24	B	618	BCR	C30-C25	-5.03	1.47	1.53
22	c	509	CLA	MG-ND	5.01	2.15	2.05
22	A	402	CLA	MG-NA	4.90	2.17	2.06
22	c	513	CLA	MG-ND	-4.86	1.96	2.05
22	C	503	CLA	MG-ND	4.85	2.15	2.05
22	b	607	CLA	MG-NA	4.80	2.17	2.06
29	A	414	DGD	O5D-C6D	-4.77	1.35	1.43
22	b	606	CLA	MG-NA	4.75	2.17	2.06
26	D	406	PL9	C52-C5	-4.74	1.41	1.50
22	B	603	CLA	MG-ND	4.69	2.15	2.05
22	a	404	CLA	MG-ND	-4.67	1.96	2.05
22	C	501	CLA	MG-ND	-4.63	1.96	2.05
22	c	504	CLA	MG-ND	-4.61	1.96	2.05
22	B	614	CLA	MG-ND	-4.60	1.96	2.05
36	V	201	HEC	FE-ND	4.59	2.09	1.94
29	C	517	DGD	O3G-C3G	-4.58	1.35	1.43
29	c	519	DGD	C6D-C5D	4.51	1.65	1.51
24	T	101	BCR	C1-C6	-4.47	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	603	CLA	MG-NB	-4.46	1.96	2.05
29	C	517	DGD	C4D-C3D	4.46	1.63	1.52
26	d	407	PL9	C6-C1	-4.44	1.41	1.48
22	C	503	CLA	MG-NB	-4.42	1.97	2.05
22	D	404	CLA	MG-NA	4.41	2.16	2.06
22	B	607	CLA	C1D-ND	4.40	1.43	1.37
24	C	514	BCR	C1-C6	-4.38	1.48	1.53
22	b	601	CLA	MG-NA	4.38	2.16	2.06
22	B	607	CLA	MG-NA	4.35	2.16	2.06
26	d	407	PL9	C3-C4	-4.34	1.42	1.49
24	b	619	BCR	C30-C25	-4.31	1.48	1.53
22	C	512	CLA	MG-ND	-4.31	1.97	2.05
22	b	614	CLA	C4B-NB	4.27	1.43	1.37
27	D	407	LMG	C4-C5	4.26	1.62	1.53
24	T	101	BCR	C30-C25	-4.26	1.48	1.53
29	a	412	DGD	O1G-C1A	4.21	1.45	1.33
22	B	606	CLA	MG-NB	-4.21	1.97	2.05
28	B	623	SQD	O47-C7	4.15	1.46	1.34
22	a	402	CLA	C1D-ND	4.14	1.43	1.37
29	A	414	DGD	C3E-C2E	4.14	1.63	1.52
35	f	101	HEM	FE-NA	4.14	2.08	1.95
24	c	514	BCR	C1-C6	-4.13	1.48	1.53
22	A	405	CLA	MG-NA	-4.12	1.96	2.06
27	D	410	LMG	C7-C8	4.09	1.60	1.51
22	B	615	CLA	C4B-NB	4.08	1.43	1.37
22	a	402	CLA	MG-NC	4.08	2.15	2.06
22	D	403	CLA	MG-NA	4.07	2.15	2.06
24	H	101	BCR	C30-C25	-4.07	1.48	1.53
24	A	406	BCR	C1-C6	-4.06	1.48	1.53
22	c	509	CLA	MG-NB	-4.05	1.97	2.05
22	C	506	CLA	C1B-NB	-4.03	1.32	1.37
22	C	511	CLA	MG-NC	-4.02	1.96	2.06
22	a	403	CLA	C1D-ND	4.00	1.43	1.37
22	B	608	CLA	MG-NA	3.98	2.15	2.06
24	K	101	BCR	C30-C25	-3.98	1.48	1.53
22	A	403	CLA	C1D-ND	3.97	1.43	1.37
22	C	509	CLA	MG-ND	3.97	2.13	2.05
22	c	507	CLA	MG-NB	-3.96	1.97	2.05
33	B	622	LHG	O7-C5	-3.95	1.37	1.46
24	D	405	BCR	C30-C25	-3.94	1.48	1.53
22	B	613	CLA	MG-NA	3.90	2.15	2.06
23	D	401	PHO	C4D-ND	-3.89	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	BCR	C1-C6	-3.87	1.48	1.53
22	b	607	CLA	MG-ND	-3.84	1.98	2.05
24	c	514	BCR	C30-C25	-3.84	1.48	1.53
22	b	601	CLA	C1D-ND	3.83	1.42	1.37
28	L	101	SQD	O48-C23	3.81	1.44	1.33
22	d	403	CLA	C1D-ND	3.80	1.42	1.37
22	b	609	CLA	MG-ND	-3.80	1.98	2.05
22	B	606	CLA	MG-NA	3.79	2.15	2.06
23	d	401	PHO	C1D-C2D	3.78	1.43	1.39
22	C	513	CLA	C1D-ND	3.77	1.42	1.37
22	c	502	CLA	C1D-ND	3.77	1.42	1.37
24	D	405	BCR	C1-C6	-3.74	1.49	1.53
24	B	617	BCR	C1-C6	-3.73	1.49	1.53
27	C	519	LMG	C4-C5	3.71	1.60	1.53
33	D	409	LHG	O8-C6	-3.70	1.36	1.45
27	c	523	LMG	C4-C5	3.70	1.60	1.53
29	c	519	DGD	O6D-C5D	-3.69	1.35	1.44
24	B	619	BCR	C1-C6	-3.69	1.49	1.53
22	b	615	CLA	MG-NB	3.68	2.13	2.05
29	c	519	DGD	C4E-C5E	-3.67	1.45	1.53
24	d	406	BCR	C30-C25	-3.67	1.49	1.53
24	b	618	BCR	C1-C6	-3.66	1.49	1.53
22	b	604	CLA	C4B-NB	3.65	1.42	1.37
22	b	615	CLA	MG-NA	3.62	2.14	2.06
27	c	522	LMG	O1-C1	3.62	1.46	1.40
22	b	610	CLA	C1D-ND	3.62	1.42	1.37
22	B	601	CLA	MG-ND	-3.62	1.98	2.05
28	a	411	SQD	O47-C7	3.61	1.44	1.34
22	B	610	CLA	CMB-C2B	-3.60	1.43	1.50
22	C	509	CLA	MG-NB	-3.60	1.98	2.05
26	d	407	PL9	C46-C44	-3.58	1.43	1.51
24	C	515	BCR	C30-C25	-3.57	1.49	1.53
22	d	403	CLA	MG-NA	3.55	2.14	2.06
22	b	603	CLA	C1D-ND	3.54	1.42	1.37
28	A	413	SQD	O48-C23	3.53	1.43	1.33
22	B	614	CLA	C1D-ND	3.53	1.42	1.37
22	c	508	CLA	MG-ND	3.53	2.12	2.05
29	c	518	DGD	O3E-C3E	-3.52	1.34	1.43
24	c	515	BCR	C30-C25	-3.52	1.49	1.53
29	a	412	DGD	O2G-C1B	3.51	1.44	1.34
22	C	509	CLA	MG-NA	3.51	2.14	2.06
22	C	510	CLA	MG-NA	3.51	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	602	CLA	C4B-NB	3.50	1.42	1.37
29	C	516	DGD	O2E-C2E	-3.50	1.34	1.43
22	A	403	CLA	MG-NA	3.49	2.14	2.06
23	d	402	PHO	CAC-C3C	-3.49	1.45	1.51
36	V	201	HEC	FE-NC	3.48	2.06	1.95
22	b	614	CLA	C1D-ND	3.47	1.42	1.37
24	c	516	BCR	C30-C25	-3.47	1.49	1.53
24	h	101	BCR	C30-C25	-3.47	1.49	1.53
22	b	613	CLA	MG-ND	-3.47	1.98	2.05
22	C	506	CLA	C1D-ND	3.47	1.42	1.37
29	h	102	DGD	O2G-C2G	-3.46	1.38	1.46
23	d	402	PHO	CMC-C2C	-3.46	1.45	1.50
28	f	102	SQD	O47-C7	3.45	1.44	1.34
22	b	613	CLA	C1D-ND	3.44	1.42	1.37
22	B	605	CLA	C1B-C2B	3.44	1.51	1.43
22	c	509	CLA	C1B-C2B	3.44	1.51	1.43
22	b	614	CLA	MG-ND	-3.43	1.99	2.05
22	b	612	CLA	MG-NB	3.43	2.12	2.05
29	C	516	DGD	O3E-C3E	-3.43	1.34	1.43
23	d	402	PHO	C1D-C2D	3.42	1.43	1.39
22	A	403	CLA	MG-NB	-3.42	1.99	2.05
22	A	403	CLA	MG-ND	-3.42	1.99	2.05
24	b	617	BCR	C1-C6	-3.41	1.49	1.53
28	f	102	SQD	O48-C23	3.41	1.43	1.33
29	A	414	DGD	C4E-C5E	3.41	1.60	1.53
22	B	612	CLA	MG-ND	-3.40	1.99	2.05
23	A	404	PHO	CMC-C2C	-3.39	1.45	1.50
24	B	617	BCR	C30-C25	-3.39	1.49	1.53
22	d	404	CLA	C1D-ND	3.38	1.42	1.37
22	B	603	CLA	CMC-C2C	-3.38	1.43	1.50
22	a	404	CLA	C1B-C2B	3.38	1.51	1.43
22	B	601	CLA	C1B-C2B	3.37	1.51	1.43
22	c	504	CLA	MG-NC	3.36	2.14	2.06
22	c	503	CLA	MG-NB	3.34	2.12	2.05
29	C	518	DGD	O2G-C2G	-3.34	1.38	1.46
28	a	411	SQD	O48-C23	3.34	1.43	1.33
26	D	406	PL9	C11-C9	-3.33	1.44	1.51
33	L	102	LHG	O8-C23	3.33	1.43	1.33
23	d	401	PHO	C3D-C4D	3.32	1.45	1.41
23	D	401	PHO	CMC-C2C	-3.32	1.45	1.50
27	b	620	LMG	C4-C3	3.31	1.60	1.52
22	B	612	CLA	C1D-ND	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	H	102	DGD	C4D-C5D	3.31	1.60	1.53
29	h	102	DGD	C4D-C3D	3.30	1.60	1.52
29	A	414	DGD	C6E-C5E	3.30	1.62	1.51
22	c	504	CLA	C4B-NB	3.29	1.42	1.37
22	B	601	CLA	C1D-ND	3.28	1.42	1.37
22	a	404	CLA	C1B-NB	-3.27	1.33	1.37
22	B	609	CLA	CMD-C2D	-3.27	1.44	1.50
22	D	404	CLA	C1D-ND	3.26	1.42	1.37
24	Y	101	BCR	C1-C6	-3.25	1.49	1.53
22	c	511	CLA	C4B-NB	3.25	1.42	1.37
27	d	412	LMG	O1-C7	-3.24	1.38	1.43
22	C	501	CLA	C1B-NB	-3.24	1.33	1.37
29	A	414	DGD	C4D-C5D	3.24	1.59	1.53
22	C	507	CLA	C1B-NB	-3.22	1.33	1.37
22	C	503	CLA	C4B-NB	3.22	1.42	1.37
22	a	402	CLA	MG-ND	-3.21	1.99	2.05
22	C	508	CLA	C1D-ND	3.21	1.42	1.37
22	c	510	CLA	C1D-ND	3.21	1.42	1.37
24	k	101	BCR	C30-C25	-3.21	1.49	1.53
24	b	619	BCR	C1-C6	-3.20	1.49	1.53
22	C	513	CLA	C1B-C2B	3.19	1.50	1.43
22	A	405	CLA	C1D-ND	3.19	1.42	1.37
28	L	101	SQD	O47-C7	3.19	1.43	1.34
22	B	603	CLA	C3B-C4B	3.18	1.52	1.42
22	C	505	CLA	C1B-C2B	3.18	1.50	1.43
23	d	401	PHO	O2D-CGD	3.17	1.41	1.33
22	A	410	CLA	C1D-ND	3.17	1.42	1.37
23	A	404	PHO	C4D-ND	-3.17	1.33	1.38
22	b	610	CLA	C1B-C2B	3.16	1.50	1.43
22	b	614	CLA	MG-NA	3.16	2.13	2.06
26	d	407	PL9	C53-C6	-3.15	1.44	1.50
33	d	408	LHG	O7-C5	-3.14	1.39	1.46
22	b	604	CLA	C1D-ND	3.14	1.42	1.37
27	b	620	LMG	C4-C5	3.13	1.59	1.53
24	d	406	BCR	C1-C6	-3.13	1.49	1.53
22	b	611	CLA	C1B-C2B	3.13	1.50	1.43
29	c	518	DGD	O2E-C2E	-3.13	1.35	1.43
22	D	403	CLA	CMD-C2D	-3.12	1.44	1.50
22	c	511	CLA	C1D-ND	3.12	1.42	1.37
22	B	613	CLA	MG-ND	-3.12	1.99	2.05
22	B	602	CLA	C1B-C2B	3.12	1.50	1.43
29	C	517	DGD	O3D-C3D	-3.12	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	520	LMG	O1-C1	3.12	1.45	1.40
24	b	617	BCR	C30-C25	-3.11	1.49	1.53
22	b	614	CLA	CMC-C2C	-3.11	1.44	1.50
22	d	405	CLA	C1D-ND	3.10	1.41	1.37
26	a	409	PL9	C53-C6	-3.09	1.44	1.50
22	b	601	CLA	C1B-C2B	3.09	1.50	1.43
22	b	612	CLA	C1B-NB	-3.09	1.33	1.37
27	A	411	LMG	C4-C3	3.09	1.60	1.52
22	C	501	CLA	C4B-NB	3.09	1.41	1.37
22	c	512	CLA	C1D-ND	3.09	1.41	1.37
33	D	408	LHG	P-O3	3.08	1.71	1.59
22	C	512	CLA	MG-NC	-3.08	1.99	2.06
33	D	409	LHG	P-O6	3.07	1.71	1.59
29	A	414	DGD	C1E-C2E	3.07	1.61	1.52
29	A	414	DGD	O5D-C1E	3.07	1.45	1.40
22	B	609	CLA	C1D-ND	3.07	1.41	1.37
22	c	511	CLA	C1B-C2B	3.07	1.50	1.43
22	C	503	CLA	C1D-ND	3.06	1.41	1.37
29	C	517	DGD	O5D-C6D	-3.06	1.38	1.43
22	b	615	CLA	CMD-C2D	-3.06	1.44	1.50
22	c	512	CLA	MG-NA	3.06	2.13	2.06
22	B	606	CLA	MG-ND	3.05	2.11	2.05
22	a	404	CLA	CMC-C2C	-3.05	1.44	1.50
22	B	616	CLA	C1D-ND	3.05	1.41	1.37
29	c	517	DGD	C4E-C3E	3.05	1.60	1.52
33	E	102	LHG	P-O6	3.05	1.71	1.59
22	D	404	CLA	CMC-C2C	-3.04	1.44	1.50
22	B	605	CLA	C1C-NC	-3.03	1.33	1.37
27	B	621	LMG	O7-C10	3.03	1.40	1.30
29	h	102	DGD	O2D-C2D	-3.03	1.35	1.43
22	c	507	CLA	C1D-ND	3.02	1.41	1.37
22	B	606	CLA	C1D-ND	3.01	1.41	1.37
22	c	513	CLA	C1D-ND	3.01	1.41	1.37
22	b	607	CLA	CMD-C2D	-3.01	1.44	1.50
22	C	511	CLA	C1B-C2B	3.00	1.50	1.43
22	C	509	CLA	C1D-ND	3.00	1.41	1.37
27	M	101	LMG	O7-C8	-3.00	1.39	1.46
35	E	101	HEM	CAB-C3B	3.00	1.55	1.47
22	B	615	CLA	C1B-C2B	3.00	1.50	1.43
22	B	615	CLA	C1D-ND	3.00	1.41	1.37
22	C	508	CLA	C3B-C4B	3.00	1.51	1.42
28	A	413	SQD	O47-C45	-3.00	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	MG-NA	3.00	2.13	2.06
22	C	505	CLA	C1D-ND	2.99	1.41	1.37
22	C	503	CLA	C1B-C2B	2.98	1.50	1.43
27	c	520	LMG	C4-C5	2.98	1.59	1.53
22	b	615	CLA	CMB-C2B	-2.98	1.44	1.50
29	H	102	DGD	O2D-C2D	-2.98	1.35	1.43
22	C	508	CLA	MG-ND	-2.98	1.99	2.05
22	c	511	CLA	CHC-C1C	2.98	1.44	1.38
22	B	611	CLA	CMD-C2D	-2.98	1.44	1.50
29	c	518	DGD	C1E-C2E	2.97	1.61	1.52
22	B	608	CLA	CMD-C2D	-2.97	1.44	1.50
33	d	408	LHG	C24-C23	2.97	1.59	1.50
22	a	402	CLA	MG-NA	2.97	2.13	2.06
22	c	509	CLA	C4B-NB	2.96	1.41	1.37
28	A	412	SQD	O2-C2	-2.96	1.35	1.43
22	c	501	CLA	C1D-ND	2.96	1.41	1.37
22	c	509	CLA	C1D-ND	2.96	1.41	1.37
24	K	101	BCR	C1-C6	-2.96	1.50	1.53
22	c	503	CLA	C1B-C2B	2.96	1.50	1.43
22	B	609	CLA	C1B-C2B	2.95	1.50	1.43
22	C	507	CLA	C1B-C2B	2.95	1.50	1.43
22	c	501	CLA	C1B-NB	-2.95	1.34	1.37
22	b	611	CLA	CMD-C2D	-2.95	1.44	1.50
29	c	518	DGD	C4D-C3D	2.95	1.60	1.52
28	F	101	SQD	O48-C23	2.95	1.42	1.33
22	B	604	CLA	C3B-C4B	2.95	1.51	1.42
22	c	512	CLA	C1B-C2B	2.94	1.50	1.43
27	c	522	LMG	C3-C2	2.94	1.60	1.52
28	B	623	SQD	O48-C23	2.94	1.41	1.33
22	A	403	CLA	CMD-C2D	-2.94	1.44	1.50
33	B	622	LHG	C24-C23	2.94	1.59	1.50
27	d	412	LMG	C4-C5	2.93	1.59	1.53
22	c	503	CLA	C1D-ND	2.93	1.41	1.37
22	B	605	CLA	CMC-C2C	-2.92	1.44	1.50
22	C	504	CLA	C1B-NB	-2.92	1.34	1.37
22	B	608	CLA	C1D-ND	2.92	1.41	1.37
22	B	602	CLA	C3B-C4B	2.91	1.51	1.42
24	a	405	BCR	C30-C25	-2.91	1.50	1.53
23	D	401	PHO	CMB-C2B	-2.91	1.45	1.51
22	c	510	CLA	CMB-C2B	-2.90	1.44	1.50
22	b	605	CLA	C1B-C2B	2.90	1.49	1.43
22	D	403	CLA	C1B-C2B	2.90	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	608	CLA	C1B-NB	-2.90	1.34	1.37
29	c	519	DGD	O2G-C2G	-2.89	1.39	1.46
22	C	507	CLA	MG-NA	2.89	2.13	2.06
22	B	614	CLA	C4B-NB	2.89	1.41	1.37
27	d	412	LMG	O8-C9	-2.89	1.38	1.45
22	B	607	CLA	MG-NC	2.88	2.13	2.06
26	A	409	PL9	C21-C19	2.88	1.57	1.51
28	A	413	SQD	O47-C7	2.88	1.42	1.34
29	C	516	DGD	C4D-C3D	2.87	1.59	1.52
22	B	601	CLA	C4B-NB	2.87	1.41	1.37
28	A	412	SQD	O48-C23	2.87	1.41	1.33
22	b	604	CLA	C1B-NB	-2.87	1.34	1.37
22	C	511	CLA	C3B-C4B	2.87	1.51	1.42
22	A	402	CLA	C1B-C2B	2.87	1.49	1.43
22	b	613	CLA	CAA-C2A	-2.87	1.48	1.54
22	b	609	CLA	C4B-NB	2.86	1.41	1.37
22	c	513	CLA	MG-NC	2.86	2.13	2.06
22	b	604	CLA	C1B-C2B	2.86	1.49	1.43
22	B	610	CLA	CHC-C1C	2.85	1.44	1.38
27	D	407	LMG	O2-C2	-2.85	1.35	1.43
22	B	613	CLA	CMD-C2D	-2.85	1.44	1.50
22	B	612	CLA	MG-NA	2.85	2.13	2.06
22	b	613	CLA	CMB-C2B	-2.84	1.44	1.50
22	c	502	CLA	CMD-C2D	-2.84	1.44	1.50
22	c	513	CLA	C4B-NB	2.84	1.41	1.37
22	C	501	CLA	MG-NA	2.84	2.13	2.06
27	b	620	LMG	O6-C1	2.83	1.49	1.41
22	c	502	CLA	C4B-NB	2.83	1.41	1.37
29	h	102	DGD	C4E-C5E	2.83	1.59	1.53
22	b	616	CLA	C1D-ND	2.82	1.41	1.37
29	C	516	DGD	C4E-C3E	2.81	1.59	1.52
22	C	513	CLA	CMC-C2C	-2.81	1.45	1.50
22	b	602	CLA	C1B-C2B	2.81	1.49	1.43
22	B	614	CLA	MG-NA	2.81	2.12	2.06
29	c	518	DGD	C6E-C5E	2.81	1.61	1.51
22	C	513	CLA	C4B-NB	2.80	1.41	1.37
27	C	519	LMG	O1-C7	-2.80	1.38	1.43
22	B	602	CLA	C1D-ND	2.79	1.41	1.37
22	d	404	CLA	CMB-C2B	-2.79	1.45	1.50
22	b	607	CLA	C1B-NB	-2.79	1.34	1.37
22	c	512	CLA	C4B-NB	2.79	1.41	1.37
33	L	102	LHG	P-O6	2.79	1.70	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1D-ND	2.79	1.41	1.37
24	Y	101	BCR	C30-C25	-2.78	1.50	1.53
22	b	605	CLA	C3B-C4B	2.77	1.50	1.42
22	B	611	CLA	C1D-ND	2.77	1.41	1.37
23	D	401	PHO	C1D-C2D	2.77	1.42	1.39
22	c	507	CLA	MG-NA	2.77	2.12	2.06
27	M	101	LMG	O4-C4	-2.77	1.36	1.43
35	f	101	HEM	C3B-C2B	-2.77	1.31	1.37
22	B	605	CLA	MG-ND	-2.77	2.00	2.05
22	c	502	CLA	MG-NB	-2.76	2.00	2.05
23	d	402	PHO	C4D-CHA	2.76	1.43	1.39
22	b	606	CLA	C1D-ND	2.76	1.41	1.37
23	d	402	PHO	CMD-C2D	-2.75	1.46	1.51
22	b	608	CLA	CHC-C1C	2.75	1.44	1.38
22	A	402	CLA	C1D-ND	2.75	1.41	1.37
22	b	607	CLA	C1D-ND	2.75	1.41	1.37
33	l	101	LHG	P-O6	2.75	1.70	1.59
29	c	518	DGD	O5D-C1E	2.75	1.44	1.40
22	B	612	CLA	C3B-C4B	2.75	1.50	1.42
22	B	601	CLA	CMB-C2B	-2.74	1.45	1.50
24	k	101	BCR	C1-C6	-2.74	1.50	1.53
24	t	101	BCR	C27-C26	-2.74	1.45	1.51
22	C	510	CLA	C1B-C2B	2.73	1.49	1.43
29	c	518	DGD	O3G-C1D	-2.73	1.35	1.40
22	B	611	CLA	CHC-C1C	2.73	1.44	1.38
22	C	505	CLA	CHC-C1C	2.73	1.44	1.38
22	b	612	CLA	CMB-C2B	-2.72	1.45	1.50
22	c	506	CLA	CMC-C2C	-2.72	1.45	1.50
22	a	402	CLA	CMC-C2C	-2.72	1.45	1.50
27	b	620	LMG	O7-C8	-2.72	1.40	1.46
22	a	404	CLA	C1C-NC	-2.71	1.33	1.37
22	c	508	CLA	C4B-NB	2.71	1.41	1.37
22	B	614	CLA	MG-NB	2.71	2.11	2.05
27	c	522	LMG	C4-C3	2.71	1.59	1.52
22	B	610	CLA	C1B-C2B	2.71	1.49	1.43
22	b	612	CLA	C1D-ND	2.71	1.41	1.37
33	d	410	LHG	P-O6	2.71	1.70	1.59
22	C	504	CLA	C1D-ND	2.71	1.41	1.37
22	B	610	CLA	C3B-C4B	2.71	1.50	1.42
24	C	514	BCR	C36-C18	-2.70	1.45	1.50
22	b	601	CLA	C4B-NB	2.70	1.41	1.37
22	a	402	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	C1B-C2B	2.69	1.49	1.43
28	f	102	SQD	O2-C2	-2.69	1.36	1.43
22	C	512	CLA	C1B-C2B	2.69	1.49	1.43
22	D	404	CLA	CMD-C2D	-2.69	1.45	1.50
27	c	523	LMG	O1-C7	-2.69	1.39	1.43
29	c	518	DGD	O3D-C3D	-2.69	1.36	1.43
22	D	403	CLA	CAA-C2A	-2.68	1.49	1.54
35	f	101	HEM	CAC-C3C	2.68	1.54	1.47
29	C	518	DGD	O6D-C5D	-2.68	1.37	1.44
22	b	602	CLA	CMD-C2D	-2.68	1.45	1.50
26	A	409	PL9	C7-C3	-2.68	1.47	1.51
29	c	519	DGD	O5D-C1E	2.67	1.44	1.40
23	d	401	PHO	C4D-ND	-2.67	1.34	1.38
24	t	101	BCR	C30-C25	-2.67	1.50	1.53
23	d	401	PHO	C4D-CHA	2.67	1.43	1.39
22	c	507	CLA	C1B-C2B	2.66	1.49	1.43
22	A	410	CLA	CHC-C1C	2.66	1.43	1.38
22	d	404	CLA	C1B-C2B	2.66	1.49	1.43
22	a	403	CLA	C1B-NB	-2.66	1.34	1.37
22	B	607	CLA	CAC-C3C	-2.65	1.44	1.51
22	B	607	CLA	C3B-C4B	2.65	1.50	1.42
24	c	516	BCR	C1-C6	-2.65	1.50	1.53
24	B	617	BCR	C33-C5	-2.65	1.46	1.50
22	C	512	CLA	C1D-ND	2.65	1.41	1.37
27	c	520	LMG	C3-C2	2.65	1.59	1.52
22	A	405	CLA	CMD-C2D	-2.64	1.45	1.50
23	A	404	PHO	CMD-C2D	-2.64	1.46	1.51
22	C	506	CLA	CMC-C2C	-2.64	1.45	1.50
22	B	609	CLA	C1B-NB	-2.64	1.34	1.37
22	C	511	CLA	CMB-C2B	-2.64	1.45	1.50
22	d	404	CLA	C4B-NB	2.64	1.41	1.37
22	B	615	CLA	CMB-C2B	-2.64	1.45	1.50
22	a	403	CLA	CMC-C2C	-2.63	1.45	1.50
22	d	403	CLA	CMB-C2B	-2.63	1.45	1.50
22	C	502	CLA	C3B-C4B	2.63	1.50	1.42
22	c	508	CLA	CMC-C2C	-2.63	1.45	1.50
22	b	603	CLA	MG-NA	2.63	2.12	2.06
24	A	406	BCR	C33-C5	-2.62	1.46	1.50
22	D	403	CLA	C1C-NC	-2.62	1.33	1.37
28	a	410	SQD	O48-C23	2.62	1.41	1.33
27	D	407	LMG	O1-C1	2.62	1.44	1.40
22	b	608	CLA	CMB-C2B	-2.62	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	509	CLA	MG-NC	2.61	2.12	2.06
22	c	510	CLA	CMD-C2D	-2.61	1.45	1.50
22	c	504	CLA	CMD-C2D	-2.61	1.45	1.50
22	c	501	CLA	C1B-C2B	2.61	1.49	1.43
24	B	619	BCR	C30-C25	-2.60	1.50	1.53
22	c	506	CLA	CMD-C2D	-2.60	1.45	1.50
22	B	602	CLA	CMD-C2D	-2.60	1.45	1.50
22	c	513	CLA	C3B-C4B	2.60	1.50	1.42
24	a	405	BCR	C1-C6	-2.60	1.50	1.53
35	E	101	HEM	FE-NC	2.60	2.03	1.95
24	T	101	BCR	C38-C26	-2.60	1.46	1.50
22	B	605	CLA	C3B-C4B	2.60	1.50	1.42
22	C	507	CLA	C3B-C4B	2.59	1.50	1.42
22	C	509	CLA	MG-NC	-2.59	2.00	2.06
23	D	401	PHO	CHA-CBD	-2.59	1.48	1.51
28	F	101	SQD	O2-C2	-2.59	1.36	1.43
22	C	508	CLA	C1B-C2B	2.58	1.49	1.43
27	b	622	LMG	C7-C8	2.58	1.58	1.50
22	c	505	CLA	C3B-C4B	2.58	1.50	1.42
28	a	410	SQD	O2-C2	-2.58	1.36	1.43
22	C	506	CLA	MG-NA	2.58	2.12	2.06
24	C	515	BCR	C27-C26	-2.58	1.46	1.51
22	C	509	CLA	CMD-C2D	-2.58	1.45	1.50
22	B	612	CLA	CMC-C2C	-2.58	1.45	1.50
22	A	405	CLA	C1B-NB	-2.58	1.34	1.37
27	M	101	LMG	C4-C5	2.58	1.58	1.53
22	C	502	CLA	MG-NA	2.57	2.12	2.06
22	b	615	CLA	C4B-NB	2.57	1.41	1.37
22	D	404	CLA	C3B-C4B	2.57	1.50	1.42
22	b	605	CLA	CMD-C2D	-2.57	1.45	1.50
28	a	410	SQD	O47-C7	2.57	1.41	1.34
27	C	519	LMG	O8-C9	-2.57	1.39	1.45
24	C	514	BCR	C33-C5	-2.57	1.46	1.50
22	c	510	CLA	MG-ND	-2.57	2.00	2.05
22	b	613	CLA	CMD-C2D	-2.56	1.45	1.50
22	c	510	CLA	MG-NC	2.56	2.12	2.06
22	B	605	CLA	CMD-C2D	-2.56	1.45	1.50
22	B	616	CLA	C1B-C2B	2.56	1.49	1.43
29	C	516	DGD	C2B-C1B	-2.56	1.43	1.50
22	c	506	CLA	C1D-ND	2.56	1.41	1.37
22	C	505	CLA	MG-NC	-2.55	2.00	2.06
22	c	508	CLA	CMD-C2D	-2.55	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	404	CLA	CHC-C4B	-2.55	1.33	1.39
22	C	512	CLA	CHC-C1C	2.55	1.43	1.38
33	e	101	LHG	P-O6	2.55	1.69	1.59
33	B	622	LHG	P-O6	2.55	1.69	1.59
22	b	613	CLA	C1B-C2B	2.55	1.49	1.43
27	c	520	LMG	O7-C10	2.55	1.40	1.35
22	C	513	CLA	MG-NA	2.54	2.12	2.06
22	b	613	CLA	CMC-C2C	-2.53	1.45	1.50
22	b	604	CLA	CHC-C1C	2.53	1.43	1.38
22	B	608	CLA	C1B-C2B	2.53	1.49	1.43
22	B	605	CLA	O2D-CED	-2.53	1.39	1.45
22	a	402	CLA	CMB-C2B	-2.53	1.45	1.50
27	c	522	LMG	C9-C8	2.52	1.58	1.50
22	c	513	CLA	C1B-C2B	2.52	1.49	1.43
29	C	516	DGD	O2G-C2G	-2.52	1.40	1.46
24	b	617	BCR	C33-C5	-2.52	1.46	1.50
22	C	504	CLA	C4B-NB	2.52	1.41	1.37
22	b	609	CLA	CMD-C2D	-2.51	1.45	1.50
22	C	509	CLA	C1B-C2B	2.51	1.49	1.43
28	A	412	SQD	O47-C7	2.51	1.41	1.34
22	B	613	CLA	C1B-NB	-2.51	1.34	1.37
23	d	401	PHO	C3B-C2B	-2.51	1.37	1.40
22	b	608	CLA	C3B-C4B	2.51	1.50	1.42
29	c	519	DGD	C1D-C2D	2.51	1.59	1.52
22	C	501	CLA	C1D-ND	2.51	1.41	1.37
23	A	404	PHO	C3D-C4D	2.51	1.44	1.41
22	b	605	CLA	MG-ND	2.51	2.10	2.05
22	b	604	CLA	CMC-C2C	-2.50	1.45	1.50
22	B	611	CLA	C1B-NB	-2.50	1.34	1.37
29	H	102	DGD	C3E-C2E	2.50	1.58	1.52
29	c	517	DGD	O2G-C2G	-2.50	1.40	1.46
22	B	602	CLA	CMB-C2B	-2.50	1.45	1.50
22	a	404	CLA	CMB-C2B	-2.50	1.45	1.50
22	b	601	CLA	O2A-CGA	2.50	1.40	1.33
22	C	509	CLA	C3B-C4B	2.50	1.50	1.42
22	b	609	CLA	C1D-ND	2.50	1.41	1.37
29	C	517	DGD	O2G-C2G	-2.49	1.40	1.46
22	a	404	CLA	CMD-C2D	-2.49	1.45	1.50
22	c	502	CLA	CHC-C4B	-2.49	1.33	1.39
35	f	101	HEM	FE-NB	2.49	2.02	1.94
22	c	508	CLA	C1D-ND	2.48	1.41	1.37
22	C	507	CLA	C1D-ND	2.48	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	518	DGD	O1G-C1G	-2.48	1.39	1.45
22	B	607	CLA	CMC-C2C	-2.48	1.45	1.50
22	c	501	CLA	C4B-NB	2.48	1.41	1.37
22	C	510	CLA	C4B-NB	2.47	1.41	1.37
35	f	101	HEM	C2A-C3A	-2.47	1.32	1.38
22	D	404	CLA	CMB-C2B	-2.47	1.45	1.50
22	B	613	CLA	C4B-NB	2.47	1.41	1.37
22	c	505	CLA	C1B-C2B	2.47	1.48	1.43
22	C	510	CLA	C3B-C4B	2.47	1.49	1.42
22	A	410	CLA	C4B-NB	2.47	1.41	1.37
27	b	622	LMG	C3-C2	2.47	1.58	1.52
22	b	602	CLA	C1D-ND	2.46	1.41	1.37
22	c	504	CLA	C1B-NB	-2.46	1.34	1.37
22	d	405	CLA	MG-ND	-2.46	2.00	2.05
22	b	615	CLA	C3B-C4B	2.46	1.49	1.42
22	C	504	CLA	C3B-C4B	2.45	1.49	1.42
22	B	603	CLA	CMA-C3A	-2.45	1.48	1.53
22	b	610	CLA	CMD-C2D	-2.45	1.45	1.50
22	B	613	CLA	MG-NB	-2.45	2.00	2.05
22	A	402	CLA	C3B-C4B	2.45	1.49	1.42
22	C	502	CLA	MG-ND	-2.45	2.00	2.05
22	b	606	CLA	MG-ND	2.45	2.10	2.05
22	b	612	CLA	CMC-C2C	-2.45	1.45	1.50
22	b	614	CLA	MG-NB	-2.45	2.00	2.05
22	C	506	CLA	C1B-C2B	2.44	1.48	1.43
27	d	412	LMG	O7-C8	-2.44	1.40	1.46
33	D	409	LHG	C3-C2	2.44	1.59	1.51
22	c	509	CLA	C3B-C4B	2.44	1.49	1.42
22	B	616	CLA	CMD-C2D	-2.44	1.45	1.50
27	b	620	LMG	O1-C7	-2.44	1.39	1.43
22	B	606	CLA	C4B-NB	2.44	1.41	1.37
23	D	401	PHO	CAC-C3C	-2.44	1.47	1.51
22	C	508	CLA	C4B-NB	2.44	1.41	1.37
29	H	102	DGD	C1E-C2E	2.44	1.59	1.52
23	D	401	PHO	CMD-C2D	-2.44	1.46	1.51
29	c	517	DGD	C4D-C3D	2.43	1.58	1.52
22	B	604	CLA	C1D-ND	2.43	1.41	1.37
22	b	602	CLA	C4B-NB	2.43	1.41	1.37
22	B	610	CLA	C4B-NB	2.43	1.41	1.37
29	C	517	DGD	C4D-C5D	2.43	1.58	1.53
27	M	101	LMG	C9-C8	2.43	1.58	1.50
22	B	606	CLA	C1B-NB	-2.43	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	516	DGD	C2A-C1A	-2.43	1.43	1.50
22	C	513	CLA	C3B-C4B	2.43	1.49	1.42
22	d	405	CLA	CMB-C2B	-2.43	1.45	1.50
22	d	403	CLA	C1B-C2B	2.43	1.48	1.43
22	B	601	CLA	C3B-C4B	2.43	1.49	1.42
29	C	516	DGD	O1G-C1G	-2.43	1.39	1.45
22	C	512	CLA	C3B-C4B	2.43	1.49	1.42
22	B	614	CLA	CMB-C2B	-2.42	1.45	1.50
22	c	508	CLA	C1B-C2B	2.42	1.48	1.43
22	D	403	CLA	C4B-NB	2.42	1.41	1.37
22	B	603	CLA	MG-NC	-2.42	2.00	2.06
22	c	502	CLA	CMC-C2C	-2.42	1.45	1.50
22	b	615	CLA	C1B-C2B	2.42	1.48	1.43
22	c	501	CLA	CMB-C2B	-2.42	1.45	1.50
22	a	404	CLA	O1D-CGD	2.41	1.27	1.21
24	t	101	BCR	C1-C6	-2.41	1.50	1.53
22	C	505	CLA	C4B-NB	2.41	1.41	1.37
22	b	605	CLA	C4B-NB	2.41	1.41	1.37
22	b	602	CLA	C3B-C4B	2.41	1.49	1.42
22	b	601	CLA	CHC-C1C	2.41	1.43	1.38
22	B	603	CLA	MG-NA	2.41	2.12	2.06
26	d	407	PL9	C41-C39	-2.41	1.46	1.51
29	c	519	DGD	C2A-C1A	-2.41	1.43	1.50
24	c	515	BCR	C33-C5	-2.40	1.47	1.50
22	C	512	CLA	CMD-C2D	-2.40	1.45	1.50
29	C	518	DGD	O3G-C3G	-2.40	1.39	1.43
22	b	602	CLA	MG-NC	-2.40	2.00	2.06
22	B	602	CLA	CMC-C2C	-2.40	1.45	1.50
22	A	405	CLA	C4B-NB	2.40	1.41	1.37
24	C	515	BCR	C1-C6	-2.40	1.50	1.53
22	B	603	CLA	CHC-C1C	2.39	1.43	1.38
22	C	501	CLA	CMC-C2C	-2.39	1.45	1.50
22	C	502	CLA	C1B-C2B	2.39	1.48	1.43
22	c	501	CLA	CMC-C2C	-2.39	1.45	1.50
22	d	405	CLA	C4B-NB	2.39	1.41	1.37
29	h	102	DGD	C2A-C1A	-2.39	1.43	1.50
22	C	510	CLA	C1D-ND	2.38	1.41	1.37
24	B	618	BCR	C33-C5	-2.38	1.47	1.50
22	c	508	CLA	CMB-C2B	-2.38	1.45	1.50
22	B	615	CLA	CAC-C3C	-2.38	1.45	1.51
33	D	408	LHG	O8-C6	-2.38	1.39	1.45
33	D	408	LHG	P-O4	-2.38	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	611	CLA	MG-NC	-2.37	2.00	2.06
29	a	412	DGD	C1G-C2G	2.37	1.58	1.50
23	d	401	PHO	CBD-CGD	-2.37	1.49	1.52
22	A	410	CLA	C1B-C2B	2.37	1.48	1.43
22	A	402	CLA	CHC-C1C	2.37	1.43	1.38
22	B	602	CLA	MG-NA	2.37	2.11	2.06
24	B	618	BCR	C1-C6	-2.37	1.50	1.53
22	C	504	CLA	C1B-C2B	2.37	1.48	1.43
22	b	604	CLA	C3B-C4B	2.37	1.49	1.42
28	a	410	SQD	O4-C4	-2.37	1.37	1.43
35	f	101	HEM	CAB-C3B	2.37	1.53	1.47
29	h	102	DGD	O5D-C6D	-2.37	1.39	1.43
24	T	101	BCR	C27-C26	-2.37	1.46	1.51
22	b	611	CLA	CMC-C2C	-2.37	1.45	1.50
22	b	601	CLA	C3B-C4B	2.36	1.49	1.42
22	c	508	CLA	C3B-C4B	2.36	1.49	1.42
28	L	101	SQD	O2-C2	-2.36	1.37	1.43
22	c	512	CLA	C3B-C4B	2.36	1.49	1.42
22	C	502	CLA	MG-NB	-2.36	2.01	2.05
22	B	603	CLA	C1B-C2B	2.36	1.48	1.43
22	B	603	CLA	CMD-C2D	-2.35	1.45	1.50
22	B	612	CLA	C1B-C2B	2.35	1.48	1.43
22	c	512	CLA	C1B-NB	-2.35	1.34	1.37
27	D	410	LMG	C9-C8	2.35	1.58	1.50
22	c	506	CLA	C1B-NB	-2.35	1.34	1.37
32	b	623	STE	C2-C1	2.35	1.56	1.50
22	C	503	CLA	CMB-C2B	-2.35	1.46	1.50
22	a	403	CLA	CMB-C2B	-2.35	1.46	1.50
22	d	403	CLA	CMD-C2D	-2.35	1.46	1.50
22	c	502	CLA	CMB-C2B	-2.34	1.46	1.50
22	B	606	CLA	CHC-C1C	2.34	1.43	1.38
29	H	102	DGD	C6D-C5D	2.34	1.58	1.51
22	b	613	CLA	C3B-C4B	2.34	1.49	1.42
27	b	622	LMG	O1-C7	-2.34	1.39	1.43
32	B	627	STE	O1-C1	2.34	1.29	1.22
24	b	618	BCR	C33-C5	-2.34	1.47	1.50
22	B	602	CLA	CHC-C1C	2.34	1.43	1.38
22	c	512	CLA	CMB-C2B	-2.33	1.46	1.50
29	H	102	DGD	C1G-C2G	2.33	1.58	1.50
22	c	512	CLA	CMC-C2C	-2.33	1.46	1.50
29	h	102	DGD	C1E-C2E	2.33	1.59	1.52
24	C	514	BCR	C30-C25	-2.33	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	405	CLA	C3B-C4B	2.33	1.49	1.42
22	C	509	CLA	CMB-C2B	-2.33	1.46	1.50
22	B	616	CLA	CMC-C2C	-2.33	1.46	1.50
22	b	614	CLA	C1B-C2B	2.32	1.48	1.43
22	C	506	CLA	C3B-C4B	2.32	1.49	1.42
22	D	404	CLA	C1B-C2B	2.32	1.48	1.43
22	b	603	CLA	CHC-C4B	-2.32	1.34	1.39
22	C	501	CLA	CMD-C2D	-2.32	1.46	1.50
23	d	401	PHO	CMB-C2B	-2.32	1.47	1.51
29	C	516	DGD	O5D-C6D	-2.32	1.39	1.43
22	a	402	CLA	C3B-C4B	2.32	1.49	1.42
22	c	505	CLA	CHC-C1C	2.32	1.43	1.38
22	b	607	CLA	CMC-C2C	-2.32	1.46	1.50
22	C	513	CLA	MG-NB	2.32	2.10	2.05
22	C	511	CLA	C4B-NB	2.32	1.40	1.37
22	b	615	CLA	CMC-C2C	-2.31	1.46	1.50
22	c	510	CLA	CMC-C2C	-2.31	1.46	1.50
22	c	503	CLA	CMC-C2C	-2.31	1.46	1.50
22	c	505	CLA	CMC-C2C	-2.31	1.46	1.50
22	b	603	CLA	C1B-NB	-2.31	1.34	1.37
28	f	102	SQD	O3-C3	-2.31	1.37	1.43
27	d	412	LMG	O3-C3	-2.31	1.37	1.43
22	c	502	CLA	C1B-C2B	2.30	1.48	1.43
22	c	507	CLA	CMC-C2C	-2.30	1.46	1.50
29	h	102	DGD	C4E-C3E	2.30	1.58	1.52
22	b	603	CLA	CMB-C2B	-2.30	1.46	1.50
22	b	609	CLA	C3B-C4B	2.30	1.49	1.42
22	B	609	CLA	CHC-C4B	-2.30	1.34	1.39
22	b	613	CLA	C4B-NB	2.30	1.40	1.37
22	B	601	CLA	CMC-C2C	-2.29	1.46	1.50
22	B	613	CLA	C1B-C2B	2.29	1.48	1.43
22	b	605	CLA	CHC-C1C	2.29	1.43	1.38
24	B	618	BCR	C36-C18	-2.29	1.46	1.50
22	b	607	CLA	CMB-C2B	-2.29	1.46	1.50
22	c	507	CLA	C1B-NB	-2.29	1.34	1.37
22	A	403	CLA	CAA-C2A	-2.28	1.49	1.54
22	b	609	CLA	CMB-C2B	-2.28	1.46	1.50
29	c	517	DGD	O3G-C3G	-2.28	1.39	1.43
22	B	607	CLA	CMD-C2D	-2.28	1.46	1.50
33	D	408	LHG	P-O6	2.28	1.68	1.59
22	B	615	CLA	CHC-C1C	2.28	1.43	1.38
22	c	506	CLA	CAC-C3C	-2.28	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	411	LMG	C4-C5	2.28	1.57	1.53
22	c	503	CLA	O2D-CGD	2.28	1.38	1.33
22	C	501	CLA	C1C-NC	-2.27	1.34	1.37
36	v	201	HEC	FE-ND	2.27	2.01	1.94
22	b	602	CLA	CHC-C4B	-2.27	1.34	1.39
22	c	513	CLA	CMB-C2B	-2.27	1.46	1.50
29	c	518	DGD	O6D-C5D	-2.27	1.38	1.44
22	d	405	CLA	O2D-CGD	2.27	1.38	1.33
33	E	102	LHG	O8-C23	2.27	1.40	1.33
22	c	503	CLA	CMB-C2B	-2.26	1.46	1.50
26	D	406	PL9	C21-C19	-2.26	1.46	1.51
22	b	615	CLA	C1D-ND	2.26	1.40	1.37
28	F	101	SQD	O3-C3	-2.26	1.37	1.43
22	B	606	CLA	CMB-C2B	-2.26	1.46	1.50
27	C	519	LMG	O1-C1	2.26	1.44	1.40
22	B	613	CLA	C1D-ND	2.25	1.40	1.37
22	c	504	CLA	CHC-C1C	2.25	1.43	1.38
29	c	519	DGD	O4E-C4E	-2.25	1.37	1.43
22	b	602	CLA	CAC-C3C	-2.25	1.45	1.51
24	k	101	BCR	C36-C18	-2.25	1.46	1.50
22	c	507	CLA	CMB-C2B	-2.25	1.46	1.50
22	b	603	CLA	C1B-C2B	2.25	1.48	1.43
33	d	410	LHG	O8-C23	2.24	1.39	1.33
22	c	506	CLA	CHC-C4B	-2.24	1.34	1.39
29	C	518	DGD	O4D-C4D	-2.24	1.37	1.43
27	b	622	LMG	C1-C2	2.24	1.59	1.52
24	t	101	BCR	C38-C26	-2.23	1.47	1.50
22	B	602	CLA	MG-ND	-2.23	2.01	2.05
33	D	408	LHG	C8-C7	-2.23	1.44	1.50
22	b	614	CLA	O2D-CED	-2.23	1.40	1.45
22	B	611	CLA	MG-NA	2.23	2.11	2.06
22	B	614	CLA	CHC-C1C	2.23	1.43	1.38
23	A	404	PHO	CAC-C3C	-2.23	1.47	1.51
22	b	606	CLA	MG-NB	2.22	2.10	2.05
29	h	102	DGD	O4D-C4D	-2.22	1.37	1.43
29	C	517	DGD	C1E-C2E	2.22	1.59	1.52
22	b	605	CLA	MG-NA	2.22	2.11	2.06
24	a	405	BCR	C35-C13	-2.22	1.46	1.50
22	c	504	CLA	C1B-C2B	2.22	1.48	1.43
22	b	614	CLA	CMB-C2B	-2.22	1.46	1.50
22	C	511	CLA	CHC-C4B	-2.21	1.34	1.39
27	C	519	LMG	O7-C8	-2.21	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	501	CLA	MG-NB	-2.21	2.01	2.05
22	c	512	CLA	C1D-C2D	2.21	1.49	1.45
22	a	403	CLA	C4B-NB	2.21	1.40	1.37
22	D	404	CLA	C1C-NC	-2.21	1.34	1.37
22	d	405	CLA	CMD-C2D	-2.21	1.46	1.50
22	B	609	CLA	MG-NB	-2.21	2.01	2.05
35	E	101	HEM	C3C-C2C	-2.20	1.32	1.37
22	B	608	CLA	CMB-C2B	-2.20	1.46	1.50
23	D	401	PHO	C3B-C2B	-2.20	1.37	1.40
22	b	614	CLA	C3B-C4B	2.20	1.49	1.42
22	b	616	CLA	O2D-CED	-2.20	1.40	1.45
22	C	504	CLA	MG-ND	-2.20	2.01	2.05
24	a	405	BCR	C38-C26	-2.20	1.47	1.50
22	C	510	CLA	CMD-C2D	-2.20	1.46	1.50
22	C	510	CLA	CHC-C1C	2.20	1.42	1.38
27	c	522	LMG	C1-C2	2.19	1.58	1.52
22	C	502	CLA	C1D-ND	2.19	1.40	1.37
22	C	507	CLA	CHC-C1C	2.19	1.42	1.38
22	c	511	CLA	CMC-C2C	-2.19	1.46	1.50
22	C	505	CLA	C3B-C4B	2.19	1.49	1.42
22	c	506	CLA	C3B-C4B	2.19	1.49	1.42
22	B	601	CLA	CMD-C2D	-2.19	1.46	1.50
22	c	502	CLA	C1B-NB	-2.19	1.35	1.37
22	c	509	CLA	CMB-C2B	-2.19	1.46	1.50
23	d	402	PHO	C4D-ND	-2.19	1.35	1.38
22	b	610	CLA	C3D-C4D	2.18	1.49	1.44
22	A	403	CLA	C1B-C2B	2.18	1.48	1.43
22	C	512	CLA	CMB-C2B	-2.18	1.46	1.50
24	C	515	BCR	C38-C26	-2.18	1.47	1.50
22	B	605	CLA	C1B-NB	-2.18	1.35	1.37
29	c	519	DGD	O3G-C1D	2.18	1.43	1.40
27	c	520	LMG	C1-C2	2.18	1.58	1.52
35	f	101	HEM	CMA-C3A	2.18	1.55	1.50
27	C	519	LMG	C6-C5	2.17	1.59	1.51
22	B	613	CLA	C5-C3	-2.17	1.46	1.51
22	C	503	CLA	C3B-C4B	2.17	1.49	1.42
22	b	604	CLA	CMB-C2B	-2.17	1.46	1.50
23	d	401	PHO	CMD-C2D	-2.17	1.47	1.51
22	C	509	CLA	C4B-NB	2.17	1.40	1.37
22	c	503	CLA	C4B-NB	2.17	1.40	1.37
22	c	513	CLA	CMD-C2D	-2.16	1.46	1.50
27	d	412	LMG	C7-C8	2.16	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	CMD-C2D	-2.16	1.46	1.50
22	b	613	CLA	C1B-NB	-2.16	1.35	1.37
27	b	620	LMG	C1-C2	2.16	1.58	1.52
26	d	407	PL9	C43-C44	-2.16	1.28	1.33
22	C	504	CLA	CAC-C3C	-2.16	1.45	1.51
22	b	603	CLA	CMD-C2D	-2.16	1.46	1.50
22	C	508	CLA	C1D-C2D	2.16	1.49	1.45
22	C	506	CLA	C3D-C4D	2.15	1.49	1.44
29	h	102	DGD	O2G-C1B	2.15	1.40	1.34
22	C	502	CLA	C4B-NB	2.15	1.40	1.37
22	C	509	CLA	O2D-CED	-2.15	1.40	1.45
22	B	612	CLA	CHC-C4B	-2.15	1.34	1.39
22	a	402	CLA	C4B-NB	2.15	1.40	1.37
23	d	402	PHO	CAA-C2A	-2.15	1.49	1.54
22	c	508	CLA	CHC-C1C	2.15	1.42	1.38
22	c	513	CLA	CHC-C1C	2.15	1.42	1.38
23	A	404	PHO	CMB-C2B	-2.15	1.47	1.51
22	c	501	CLA	CMD-C2D	-2.14	1.46	1.50
22	C	509	CLA	O2A-CGA	2.14	1.39	1.33
22	C	508	CLA	CHC-C1C	2.14	1.42	1.38
22	b	606	CLA	CHC-C1C	2.14	1.42	1.38
22	C	507	CLA	CMB-C2B	-2.14	1.46	1.50
22	B	601	CLA	CHC-C1C	2.14	1.42	1.38
22	A	402	CLA	C4B-NB	2.14	1.40	1.37
22	b	610	CLA	CMC-C2C	-2.14	1.46	1.50
22	C	505	CLA	MG-NB	-2.14	2.01	2.05
22	C	502	CLA	CMB-C2B	-2.13	1.46	1.50
29	H	102	DGD	O1G-C1G	-2.13	1.40	1.45
29	h	102	DGD	O2E-C2E	-2.13	1.37	1.43
26	D	406	PL9	C3-C4	-2.13	1.46	1.49
22	A	402	CLA	CMD-C2D	-2.13	1.46	1.50
27	M	101	LMG	C4-C3	2.13	1.57	1.52
22	b	616	CLA	C3B-C4B	2.13	1.48	1.42
29	C	516	DGD	O5D-C1E	2.13	1.43	1.40
26	a	409	PL9	C25-C24	-2.13	1.45	1.50
22	b	609	CLA	C1B-NB	-2.13	1.35	1.37
22	B	611	CLA	CMB-C2B	-2.13	1.46	1.50
22	B	616	CLA	C3B-C4B	2.13	1.48	1.42
22	b	605	CLA	C1B-NB	-2.13	1.35	1.37
22	C	509	CLA	O2D-CGD	2.13	1.38	1.33
22	c	501	CLA	CHC-C4B	-2.13	1.34	1.39
22	B	606	CLA	C1B-C2B	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	C1B-NB	-2.12	1.35	1.37
33	E	102	LHG	C24-C23	2.12	1.56	1.50
22	A	410	CLA	CMC-C2C	-2.12	1.46	1.50
27	b	622	LMG	O6-C1	2.12	1.47	1.41
22	c	503	CLA	CMD-C2D	-2.12	1.46	1.50
22	C	510	CLA	CMC-C2C	-2.12	1.46	1.50
29	C	518	DGD	C2A-C1A	-2.12	1.44	1.50
22	b	602	CLA	C1A-CHA	-2.12	1.34	1.43
22	c	510	CLA	C1B-C2B	2.12	1.48	1.43
33	d	409	LHG	O7-C5	-2.12	1.41	1.46
27	c	523	LMG	O6-C5	-2.12	1.39	1.44
22	b	608	CLA	C3C-C2C	2.12	1.41	1.36
28	A	412	SQD	O47-C45	-2.11	1.41	1.46
22	B	603	CLA	CMB-C2B	-2.11	1.46	1.50
35	E	101	HEM	CAC-C3C	2.11	1.53	1.47
27	b	622	LMG	O1-C1	2.11	1.43	1.40
24	h	101	BCR	C1-C6	-2.11	1.51	1.53
36	v	201	HEC	CAC-C3C	2.11	1.56	1.51
22	B	605	CLA	CHC-C1C	2.11	1.42	1.38
22	b	608	CLA	C4B-NB	2.11	1.40	1.37
22	b	612	CLA	CMD-C2D	-2.11	1.46	1.50
22	b	610	CLA	C3B-C4B	2.11	1.48	1.42
22	b	603	CLA	MG-NC	-2.11	2.01	2.06
22	B	610	CLA	C1A-CHA	-2.10	1.34	1.43
22	c	505	CLA	C1D-ND	2.10	1.40	1.37
22	d	403	CLA	C1B-NB	-2.10	1.35	1.37
22	b	608	CLA	C1B-NB	-2.10	1.35	1.37
22	c	503	CLA	C1B-NB	-2.10	1.35	1.37
22	c	508	CLA	C1B-NB	-2.10	1.35	1.37
22	b	608	CLA	MG-NA	2.10	2.11	2.06
29	H	102	DGD	O2G-C2G	-2.10	1.41	1.46
36	v	201	HEC	O1D-CGD	2.10	1.29	1.22
29	C	518	DGD	O5D-C6D	-2.10	1.40	1.43
22	C	512	CLA	C5-C3	-2.10	1.47	1.51
29	C	518	DGD	O5D-C1E	2.09	1.43	1.40
22	d	405	CLA	C1B-C2B	2.09	1.48	1.43
29	c	517	DGD	O5D-C1E	2.09	1.43	1.40
22	C	508	CLA	C3D-C4D	2.09	1.48	1.44
26	A	409	PL9	C37-C38	2.09	1.56	1.50
24	B	619	BCR	C31-C1	-2.09	1.49	1.53
24	D	405	BCR	C27-C26	-2.09	1.47	1.51
33	B	622	LHG	P-O4	-2.09	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	614	CLA	CAB-C3B	-2.09	1.41	1.47
22	b	610	CLA	CHC-C4B	-2.09	1.34	1.39
27	C	519	LMG	C1-C2	2.09	1.58	1.52
29	C	518	DGD	C3B-C2B	-2.09	1.44	1.52
22	a	402	CLA	C1B-NB	-2.09	1.35	1.37
22	c	504	CLA	C3B-C4B	2.09	1.48	1.42
22	b	615	CLA	MG-NC	-2.08	2.01	2.06
22	C	506	CLA	C4B-NB	2.08	1.40	1.37
24	b	618	BCR	C36-C18	-2.08	1.46	1.50
22	B	613	CLA	C3B-C4B	2.08	1.48	1.42
22	C	504	CLA	CHC-C1C	2.08	1.42	1.38
22	C	513	CLA	CMB-C2B	-2.08	1.46	1.50
22	a	404	CLA	C4B-NB	2.08	1.40	1.37
32	D	411	STE	O1-C1	2.08	1.28	1.22
22	B	610	CLA	C3B-C2B	-2.08	1.34	1.41
22	A	410	CLA	C1D-C2D	2.08	1.49	1.45
22	c	510	CLA	CAA-C2A	-2.07	1.50	1.54
22	C	503	CLA	CHC-C1C	2.07	1.42	1.38
22	b	603	CLA	C3D-C4D	2.07	1.48	1.44
22	B	601	CLA	C1B-NB	-2.07	1.35	1.37
22	c	512	CLA	CHC-C1C	2.07	1.42	1.38
22	c	512	CLA	CMD-C2D	-2.07	1.46	1.50
27	c	522	LMG	O1-C7	-2.07	1.40	1.43
35	f	101	HEM	CMC-C2C	2.07	1.55	1.50
22	B	603	CLA	C1A-CHA	-2.06	1.34	1.43
22	B	604	CLA	CHC-C1C	2.06	1.42	1.38
29	C	518	DGD	C6D-C5D	2.06	1.57	1.51
22	C	511	CLA	CMC-C2C	-2.06	1.46	1.50
33	d	408	LHG	O6-C4	-2.06	1.36	1.44
22	b	616	CLA	CMD-C2D	-2.06	1.46	1.50
33	d	409	LHG	O6-C4	-2.06	1.36	1.44
22	B	613	CLA	CMC-C2C	-2.06	1.46	1.50
22	A	405	CLA	CHC-C4B	-2.06	1.34	1.39
23	D	401	PHO	C3D-CAD	-2.06	1.43	1.47
22	C	508	CLA	CAC-C3C	-2.05	1.45	1.51
24	k	101	BCR	C33-C5	-2.05	1.47	1.50
27	b	622	LMG	C4-C5	2.05	1.57	1.53
22	B	606	CLA	CAB-C3B	-2.05	1.41	1.47
22	C	512	CLA	C1D-C2D	2.04	1.49	1.45
23	A	404	PHO	CBD-CGD	-2.04	1.49	1.52
22	B	606	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	604	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	k	101	BCR	C38-C26	-2.04	1.47	1.50
22	B	607	CLA	C1B-C2B	2.04	1.47	1.43
27	A	411	LMG	C1-C2	2.03	1.58	1.52
27	D	410	LMG	O8-C28	2.03	1.39	1.33
32	c	521	STE	C2-C1	2.03	1.55	1.50
22	b	604	CLA	CMD-C2D	-2.03	1.46	1.50
22	d	405	CLA	O1D-CGD	2.03	1.26	1.21
22	d	405	CLA	CMC-C2C	-2.03	1.46	1.50
26	A	409	PL9	C41-C39	2.03	1.55	1.51
22	C	501	CLA	C3B-C4B	2.03	1.48	1.42
22	B	614	CLA	C1A-CHA	-2.03	1.34	1.43
35	E	101	HEM	C3D-C2D	-2.03	1.32	1.36
29	c	517	DGD	O3E-C3E	-2.03	1.37	1.43
22	c	510	CLA	C5-C3	-2.03	1.47	1.51
22	b	606	CLA	C1B-C2B	2.02	1.47	1.43
22	b	607	CLA	C4B-NB	2.02	1.40	1.37
22	A	410	CLA	O2D-CED	-2.02	1.40	1.45
33	d	410	LHG	C6-C5	2.02	1.57	1.50
22	c	513	CLA	CMC-C2C	-2.02	1.46	1.50
22	D	403	CLA	C3B-C4B	2.01	1.48	1.42
22	c	503	CLA	C3B-C4B	2.01	1.48	1.42
22	D	404	CLA	CHC-C4B	-2.01	1.34	1.39
26	A	409	PL9	C25-C24	-2.01	1.45	1.50
22	c	512	CLA	C3D-C4D	2.01	1.48	1.44
22	b	605	CLA	MG-NC	-2.01	2.01	2.06
22	b	609	CLA	C1A-CHA	-2.01	1.34	1.43
29	C	516	DGD	C3E-C2E	2.01	1.57	1.52
24	C	515	BCR	C33-C5	-2.01	1.47	1.50
27	D	407	LMG	C7-C8	2.01	1.57	1.50
22	B	603	CLA	O2D-CGD	2.00	1.38	1.33
33	d	408	LHG	P-O6	2.00	1.67	1.59
22	b	610	CLA	CMB-C2B	-2.00	1.46	1.50
22	A	405	CLA	CAC-C3C	-2.00	1.46	1.51
22	C	501	CLA	C1B-C2B	2.00	1.47	1.43
22	b	614	CLA	C1A-CHA	-2.00	1.34	1.43

All (1238) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C4A-NA-C1A	9.84	111.17	106.68
28	L	101	SQD	O6-C1-C2	9.53	122.74	108.27
22	c	511	CLA	C4A-NA-C1A	9.36	110.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	C4A-NA-C1A	9.28	110.91	106.68
22	C	507	CLA	C4A-NA-C1A	9.25	110.90	106.68
22	B	607	CLA	C4A-NA-C1A	8.80	110.69	106.68
22	C	501	CLA	C4A-NA-C1A	8.69	110.64	106.68
28	a	410	SQD	O6-C1-C2	8.62	121.37	108.27
22	B	601	CLA	C4A-NA-C1A	8.45	110.53	106.68
22	b	601	CLA	C4A-NA-C1A	8.37	110.50	106.68
28	A	412	SQD	O6-C1-C2	8.29	120.86	108.27
22	B	604	CLA	C4A-NA-C1A	8.27	110.45	106.68
22	B	615	CLA	C4A-NA-C1A	7.71	110.20	106.68
22	b	606	CLA	C4A-NA-C1A	7.49	110.09	106.68
22	C	506	CLA	C4A-NA-C1A	7.08	109.91	106.68
22	c	503	CLA	C4A-NA-C1A	7.08	109.91	106.68
22	b	604	CLA	C4A-NA-C1A	6.96	109.85	106.68
28	B	623	SQD	O6-C1-C2	6.95	118.82	108.27
22	C	513	CLA	C4A-NA-C1A	6.73	109.75	106.68
22	d	404	CLA	C4A-NA-C1A	6.32	109.56	106.68
22	c	508	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	c	512	CLA	C4A-NA-C1A	6.29	109.55	106.68
22	D	404	CLA	C4A-NA-C1A	6.28	109.54	106.68
26	D	406	PL9	C7-C3-C4	6.23	122.04	116.91
22	C	508	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	C	503	CLA	C4A-NA-C1A	6.22	109.52	106.68
22	B	602	CLA	C4A-NA-C1A	6.12	109.47	106.68
22	c	501	CLA	C4A-NA-C1A	5.82	109.33	106.68
22	B	608	CLA	O2D-CGD-O1D	-5.74	112.67	123.85
22	c	504	CLA	C4A-NA-C1A	5.55	109.21	106.68
22	b	613	CLA	C4A-NA-C1A	5.54	109.21	106.68
22	A	402	CLA	C4A-NA-C1A	5.53	109.20	106.68
28	L	101	SQD	O7-S-C6	5.43	114.86	106.76
22	C	511	CLA	C4A-NA-C1A	5.32	109.11	106.68
22	c	510	CLA	C4A-NA-C1A	5.32	109.10	106.68
22	B	608	CLA	C4A-NA-C1A	5.30	109.10	106.68
26	d	407	PL9	C7-C3-C4	5.26	121.24	116.91
22	c	505	CLA	C4A-NA-C1A	5.21	109.06	106.68
22	c	501	CLA	O2D-CGD-O1D	-5.16	113.80	123.85
22	b	615	CLA	C4A-NA-C1A	5.16	109.03	106.68
22	b	603	CLA	C4A-NA-C1A	5.14	109.02	106.68
22	b	608	CLA	C3B-C4B-NB	-5.13	105.95	110.53
26	d	407	PL9	C40-C39-C41	5.09	124.06	115.23
22	C	509	CLA	C4A-NA-C1A	5.08	109.00	106.68
22	a	403	CLA	C4A-NA-C1A	5.06	108.99	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	C4A-NA-C1A	5.05	108.98	106.68
26	a	409	PL9	C7-C3-C4	5.05	121.07	116.91
22	B	610	CLA	O2D-CGD-O1D	-5.04	114.04	123.85
28	a	410	SQD	C1-O5-C5	-5.03	103.90	113.72
22	C	505	CLA	C4A-NA-C1A	5.00	108.96	106.68
22	c	506	CLA	C4A-NA-C1A	4.98	108.95	106.68
22	B	612	CLA	C4A-NA-C1A	4.95	108.94	106.68
22	a	402	CLA	C4A-NA-C1A	4.91	108.92	106.68
28	A	412	SQD	O8-S-C6	4.90	115.43	105.97
22	b	611	CLA	C4A-NA-C1A	4.85	108.89	106.68
26	A	409	PL9	C7-C3-C4	4.81	120.87	116.91
22	D	404	CLA	O2D-CGD-O1D	-4.77	114.56	123.85
22	c	502	CLA	C4A-NA-C1A	4.73	108.84	106.68
33	L	102	LHG	O4-P-O5	4.70	134.32	112.44
23	A	404	PHO	O2D-CGD-CBD	4.70	116.11	110.95
28	F	101	SQD	O6-C1-C2	4.69	115.40	108.27
22	B	605	CLA	C4A-NA-C1A	4.64	108.80	106.68
22	b	616	CLA	CMB-C2B-C1B	-4.64	118.36	125.42
34	D	402	BCT	O2-C-O1	4.63	131.53	119.68
28	F	101	SQD	O9-S-C6	4.61	113.65	106.76
22	c	513	CLA	C4A-NA-C1A	4.58	108.77	106.68
22	C	510	CLA	C4A-NA-C1A	4.57	108.77	106.68
29	H	102	DGD	O3G-C3G-C2G	-4.56	99.72	110.82
28	A	412	SQD	O7-S-C6	4.55	113.55	106.76
22	B	602	CLA	O2D-CGD-CBD	4.55	119.19	111.23
29	A	414	DGD	C4E-C3E-C2E	-4.55	102.85	110.83
26	A	409	PL9	C20-C19-C21	4.54	123.12	115.23
22	b	602	CLA	C4A-NA-C1A	4.53	108.75	106.68
22	c	505	CLA	C3B-C4B-NB	-4.51	106.50	110.53
33	e	101	LHG	O4-P-O5	4.48	133.31	112.44
22	c	512	CLA	C1-C2-C3	-4.47	118.87	126.20
27	b	622	LMG	C1-O6-C5	-4.47	105.00	113.72
22	b	608	CLA	C4A-NA-C1A	4.46	108.71	106.68
22	B	603	CLA	C3B-C4B-NB	-4.45	106.56	110.53
24	b	617	BCR	C2-C1-C6	4.44	116.89	110.44
22	D	403	CLA	C4A-NA-C1A	4.44	108.70	106.68
22	b	614	CLA	C4A-NA-C1A	4.43	108.70	106.68
28	B	623	SQD	O47-C7-C8	4.43	121.07	111.48
22	c	510	CLA	O2D-CGD-O1D	-4.41	115.26	123.85
29	a	412	DGD	O3G-C3G-C2G	-4.40	100.46	111.77
22	C	513	CLA	C4-C3-C5	4.37	122.82	115.23
22	B	614	CLA	C3B-C4B-NB	-4.36	106.63	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C2-C1-C6	4.36	116.77	110.44
22	b	616	CLA	C4A-NA-C1A	4.36	108.67	106.68
23	d	402	PHO	O1D-CGD-CBD	4.35	131.32	124.72
28	B	623	SQD	O7-S-C6	4.35	113.25	106.76
33	d	408	LHG	O8-C23-O10	-4.34	112.77	123.63
28	f	102	SQD	O7-S-C6	4.33	113.22	106.76
29	h	102	DGD	O3G-C3G-C2G	-4.32	100.31	110.82
33	E	102	LHG	O4-P-O5	4.31	132.50	112.44
28	A	412	SQD	C1-C2-C3	-4.31	100.95	110.01
33	B	622	LHG	O4-P-O5	4.30	132.43	112.44
22	B	608	CLA	O2D-CGD-CBD	4.29	118.74	111.23
33	d	408	LHG	O4-P-O5	4.27	132.31	112.44
32	m	101	STE	O2-C1-C2	4.27	127.49	114.00
22	B	609	CLA	C4A-NA-C1A	4.26	108.62	106.68
22	C	507	CLA	O2D-CGD-O1D	-4.26	115.55	123.85
23	d	402	PHO	O2D-CGD-O1D	-4.26	115.56	123.85
33	d	410	LHG	O4-P-O5	4.25	132.22	112.44
22	B	613	CLA	C1-C2-C3	-4.24	119.25	126.20
22	b	611	CLA	O2D-CGD-O1D	-4.24	115.60	123.85
23	d	402	PHO	C2B-C1B-NB	-4.19	106.40	109.43
22	A	410	CLA	C3B-C4B-NB	-4.19	106.79	110.53
26	d	407	PL9	C42-C43-C44	-4.16	118.09	127.62
23	A	404	PHO	C2B-C1B-NB	-4.16	106.42	109.43
22	b	606	CLA	O2D-CGD-O1D	-4.16	115.76	123.85
28	F	101	SQD	O8-S-C6	4.16	114.00	105.97
29	C	517	DGD	O3G-C3G-C2G	-4.15	100.72	110.82
22	B	610	CLA	C4A-NA-C1A	4.15	108.57	106.68
22	B	605	CLA	O1D-CGD-CBD	4.13	132.66	124.52
22	A	410	CLA	C4A-NA-C1A	4.12	108.56	106.68
22	A	405	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
33	D	408	LHG	O4-P-O5	4.07	131.37	112.44
22	b	616	CLA	CMB-C2B-C3B	4.06	136.09	126.55
22	C	512	CLA	C4A-NA-C1A	4.06	108.53	106.68
28	L	101	SQD	O48-C23-C24	4.06	124.20	111.83
22	c	509	CLA	O2A-CGA-O1A	-4.05	113.49	123.63
23	A	404	PHO	CMB-C2B-C3B	4.05	132.78	124.68
34	a	408	BCT	O2-C-O1	4.04	130.02	119.68
22	d	404	CLA	O2D-CGD-CBD	4.04	118.29	111.23
26	a	409	PL9	C7-C3-C2	-4.04	118.63	123.39
22	D	404	CLA	CMB-C2B-C1B	-4.03	119.28	125.42
28	A	412	SQD	O9-S-O7	-4.03	100.73	113.82
22	B	611	CLA	O2D-CGD-O1D	-4.02	116.03	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	519	DGD	O3G-C3G-C2G	-4.00	101.08	110.82
36	v	201	HEC	C1D-ND-C4D	4.00	109.95	105.21
33	d	409	LHG	O4-P-O5	3.99	131.00	112.44
32	j	101	STE	O2-C1-C2	3.98	126.58	114.00
22	b	604	CLA	CHB-C4A-NA	3.97	130.12	124.40
24	T	101	BCR	C27-C26-C25	3.96	128.06	122.70
22	b	612	CLA	CMB-C2B-C1B	-3.95	119.41	125.42
22	b	604	CLA	C1-C2-C3	-3.95	119.73	126.20
23	D	401	PHO	C2B-C1B-NB	-3.94	106.58	109.43
28	f	102	SQD	O6-C1-C2	3.93	114.25	108.27
28	f	102	SQD	O9-S-O7	-3.92	101.07	113.82
22	b	607	CLA	C4A-NA-C1A	3.92	108.47	106.68
28	A	412	SQD	O47-C7-O49	-3.92	114.54	123.70
22	B	604	CLA	O2D-CGD-O1D	-3.91	116.24	123.85
22	b	601	CLA	CHB-C4A-NA	3.90	130.03	124.40
24	C	514	BCR	C36-C18-C17	-3.90	116.50	122.82
28	a	410	SQD	C1-C2-C3	-3.89	101.83	110.01
29	c	518	DGD	O3G-C3G-C2G	-3.88	101.39	110.82
22	b	612	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
22	b	605	CLA	C4-C3-C5	3.87	121.94	115.23
22	c	502	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
22	B	607	CLA	C3B-C4B-NB	-3.87	107.08	110.53
22	C	502	CLA	C4A-NA-C1A	3.86	108.44	106.68
33	D	409	LHG	O4-P-O5	3.86	130.39	112.44
23	A	404	PHO	C4D-CHA-CBD	-3.86	106.61	108.45
29	C	518	DGD	O3G-C3G-C2G	-3.85	101.45	110.82
27	d	411	LMG	O7-C10-O9	-3.84	113.46	123.33
29	C	517	DGD	O5D-C6D-C5D	-3.84	100.77	109.42
23	d	402	PHO	C4D-CHA-CBD	-3.83	106.62	108.45
28	A	413	SQD	O48-C23-C24	3.82	123.48	111.83
22	B	613	CLA	C4A-NA-C1A	3.79	108.41	106.68
24	b	618	BCR	C36-C18-C17	-3.79	116.68	122.82
33	l	101	LHG	O4-P-O5	3.78	130.04	112.44
33	B	622	LHG	O8-C23-C24	3.77	123.33	111.83
28	a	410	SQD	O9-S-O7	-3.77	101.57	113.82
22	b	610	CLA	CAC-C3C-C4C	3.77	129.69	124.79
23	D	401	PHO	C4D-CHA-CBD	-3.76	106.65	108.45
28	a	410	SQD	O7-S-C6	3.76	112.36	106.76
22	b	602	CLA	CHB-C4A-NA	3.75	129.82	124.40
24	B	617	BCR	C2-C1-C6	3.75	115.88	110.44
22	B	610	CLA	CHB-C4A-NA	3.74	129.81	124.40
22	B	602	CLA	CMB-C2B-C1B	-3.72	119.75	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	616	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
29	h	102	DGD	O3E-C3E-C2E	-3.70	101.65	110.38
22	B	605	CLA	O2D-CGD-O1D	-3.69	116.67	123.85
29	C	516	DGD	O3G-C3G-C2G	-3.68	101.87	110.82
29	C	518	DGD	O3G-C1D-C2D	-3.68	102.69	108.27
29	C	516	DGD	O1G-C1A-C2A	-3.65	100.71	111.83
28	f	102	SQD	O5-C5-C4	3.62	116.22	109.70
24	a	405	BCR	C39-C30-C25	-3.62	104.57	110.24
22	b	604	CLA	C3B-C4B-NB	-3.61	107.30	110.53
22	b	603	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
22	C	509	CLA	CMB-C2B-C1B	-3.60	119.94	125.42
26	a	409	PL9	C35-C34-C36	3.60	121.47	115.23
28	B	623	SQD	O9-S-O7	-3.59	102.13	113.82
22	b	613	CLA	C1-C2-C3	-3.59	120.31	126.20
29	C	517	DGD	O2D-C2D-C1D	-3.59	101.51	110.08
33	d	408	LHG	O8-C23-C24	3.59	122.77	111.83
28	A	413	SQD	C45-O47-C7	3.58	122.95	117.78
22	D	403	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
22	c	501	CLA	O2D-CGD-CBD	3.58	117.48	111.23
22	B	606	CLA	C3B-C4B-NB	-3.58	107.34	110.53
23	D	401	PHO	O1D-CGD-CBD	3.57	130.13	124.72
22	D	403	CLA	C3B-C4B-NB	-3.56	107.36	110.53
23	D	401	PHO	CMB-C2B-C3B	3.56	131.79	124.68
24	c	515	BCR	C2-C1-C6	3.55	115.59	110.44
22	B	602	CLA	O2D-CGD-O1D	-3.55	116.95	123.85
24	d	406	BCR	C38-C26-C25	-3.54	120.62	124.48
22	b	602	CLA	O2D-CGD-CBD	3.54	117.42	111.23
28	B	623	SQD	O48-C23-C24	3.54	122.63	111.83
24	T	101	BCR	C7-C8-C9	-3.53	121.02	126.23
28	L	101	SQD	O9-S-C6	3.53	112.02	106.76
22	B	610	CLA	O2D-CGD-CBD	3.52	117.38	111.23
27	b	620	LMG	O1-C1-C2	-3.51	102.94	108.27
22	d	404	CLA	C3B-C4B-NB	-3.50	107.41	110.53
22	b	608	CLA	CMB-C2B-C1B	-3.49	120.10	125.42
29	A	414	DGD	O3G-C3G-C2G	-3.49	102.32	110.82
28	L	101	SQD	O5-C1-C2	-3.49	103.19	110.37
22	a	403	CLA	CMB-C2B-C1B	-3.49	120.11	125.42
22	a	404	CLA	C4A-NA-C1A	3.49	108.27	106.68
26	d	407	PL9	C37-C38-C39	-3.49	119.64	127.62
22	A	402	CLA	CHB-C4A-NA	3.48	129.42	124.40
23	d	401	PHO	C4D-CHA-CBD	-3.48	106.79	108.45
27	C	519	LMG	O2-C2-C1	-3.47	101.81	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	611	CLA	C3B-C4B-NB	-3.46	107.44	110.53
24	K	101	BCR	C15-C16-C17	-3.46	116.44	123.52
28	B	623	SQD	C3-C4-C5	3.45	116.50	110.23
22	c	508	CLA	CHB-C4A-NA	3.45	129.38	124.40
22	C	504	CLA	C4-C3-C5	3.45	121.21	115.23
22	B	604	CLA	CHB-C4A-NA	3.44	129.37	124.40
22	b	603	CLA	CHD-C1D-ND	-3.44	119.97	124.80
27	C	519	LMG	O1-C1-C2	-3.43	103.06	108.27
28	A	413	SQD	O47-C7-C8	3.43	118.90	111.48
22	d	404	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
28	a	410	SQD	O48-C23-C24	3.42	122.26	111.83
28	A	412	SQD	C1-O5-C5	-3.42	107.05	113.72
29	c	517	DGD	O3G-C1D-C2D	-3.42	103.08	108.27
23	d	402	PHO	C1-C2-C3	-3.42	120.60	126.20
22	c	513	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
22	C	512	CLA	CHB-C4A-NA	3.41	129.32	124.40
22	B	603	CLA	C4-C3-C5	3.41	121.14	115.23
22	c	512	CLA	O2D-CGD-O1D	-3.40	117.22	123.85
26	A	409	PL9	C36-C34-C33	-3.40	113.53	121.17
29	c	518	DGD	O2D-C2D-C1D	-3.40	101.97	110.08
28	a	410	SQD	C3-C4-C5	3.40	116.39	110.23
24	C	514	BCR	C2-C1-C6	3.40	115.37	110.44
22	B	612	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
24	d	406	BCR	C27-C26-C25	3.37	127.26	122.70
28	L	101	SQD	C1-C2-C3	-3.37	102.93	110.01
29	c	517	DGD	O3G-C3G-C2G	-3.36	102.65	110.82
27	d	412	LMG	O2-C2-C1	-3.36	102.08	110.08
28	L	101	SQD	O9-S-O7	-3.34	102.94	113.82
24	a	405	BCR	C2-C1-C6	3.33	115.27	110.44
29	H	102	DGD	C3E-C4E-C5E	-3.33	104.20	110.23
29	C	517	DGD	O4D-C4D-C3D	3.33	118.21	110.38
22	b	604	CLA	C11-C12-C13	-3.32	104.91	115.97
26	d	407	PL9	C36-C34-C33	-3.32	113.71	121.17
22	d	403	CLA	C4A-NA-C1A	3.32	108.19	106.68
24	b	617	BCR	C38-C26-C25	-3.32	120.86	124.48
35	f	101	HEM	C3B-C2B-C1B	3.32	108.90	106.41
24	a	405	BCR	C40-C30-C25	3.32	115.44	110.24
22	B	612	CLA	CMB-C2B-C3B	3.32	134.35	126.55
22	B	613	CLA	CAC-C3C-C4C	3.31	129.10	124.79
22	B	606	CLA	C6-C5-C3	-3.30	105.42	113.47
29	C	517	DGD	C3D-C4D-C5D	-3.30	104.24	110.23
27	b	620	LMG	O1-C7-C8	-3.30	102.79	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	C3B-C4B-NB	-3.29	107.59	110.53
22	B	616	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
32	C	520	STE	C3-C2-C1	-3.29	105.92	114.51
29	c	518	DGD	C3D-C4D-C5D	-3.28	104.28	110.23
22	b	612	CLA	O1D-CGD-CBD	3.27	130.97	124.52
22	b	611	CLA	O2D-CGD-CBD	3.27	116.95	111.23
36	v	201	HEC	CHB-C1B-NB	3.27	127.94	124.42
27	b	620	LMG	O3-C3-C2	-3.26	102.70	110.38
27	c	523	LMG	C1-O6-C5	-3.25	107.37	113.72
22	B	615	CLA	CHB-C4A-NA	3.25	129.09	124.40
27	M	101	LMG	C1-O6-C5	-3.25	107.38	113.72
26	d	407	PL9	C22-C23-C24	-3.25	120.19	127.62
26	A	409	PL9	C40-C39-C38	-3.24	115.30	123.63
24	D	405	BCR	C2-C1-C6	3.24	115.14	110.44
22	a	404	CLA	CHB-C4A-NA	3.24	129.07	124.40
22	B	611	CLA	O2D-CGD-CBD	3.23	116.88	111.23
22	D	404	CLA	O2D-CGD-CBD	3.23	116.87	111.23
22	B	610	CLA	O2A-CGA-O1A	-3.23	115.56	123.63
23	d	401	PHO	CMB-C2B-C3B	3.23	131.13	124.68
22	b	608	CLA	CHB-C4A-NA	3.22	129.05	124.40
29	C	516	DGD	O3E-C3E-C2E	-3.22	102.78	110.38
26	a	409	PL9	C40-C39-C41	3.22	120.82	115.23
24	b	619	BCR	C12-C13-C14	-3.22	113.95	119.01
24	K	101	BCR	C11-C10-C9	-3.22	122.77	127.28
22	d	405	CLA	CMB-C2B-C1B	-3.22	120.52	125.42
22	c	507	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
24	c	515	BCR	C15-C16-C17	-3.21	116.95	123.52
26	A	409	PL9	C22-C23-C24	-3.20	120.29	127.62
22	c	504	CLA	CMB-C2B-C1B	-3.20	120.54	125.42
22	C	507	CLA	CHB-C4A-NA	3.20	129.02	124.40
22	C	513	CLA	O2A-CGA-O1A	-3.20	115.63	123.63
22	A	405	CLA	O2D-CGD-CBD	3.20	116.82	111.23
27	D	407	LMG	C3-C4-C5	-3.19	104.44	110.23
22	c	513	CLA	CMB-C2B-C1B	-3.18	120.57	125.42
22	A	410	CLA	CHB-C4A-NA	3.18	128.99	124.40
22	B	614	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
28	L	101	SQD	C3-C4-C5	3.17	115.97	110.23
27	b	622	LMG	O2-C2-C1	-3.16	102.54	110.08
24	t	101	BCR	C1-C6-C5	-3.15	118.33	122.64
22	B	612	CLA	C11-C12-C13	-3.14	105.52	115.97
22	B	602	CLA	CHB-C4A-NA	3.14	128.93	124.40
22	B	608	CLA	CMB-C2B-C1B	-3.14	120.64	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	403	CLA	CHB-C4A-NA	3.14	128.93	124.40
22	B	615	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
22	a	403	CLA	CAC-C3C-C4C	3.13	128.87	124.79
22	B	613	CLA	CMB-C2B-C1B	-3.13	120.65	125.42
24	c	515	BCR	C27-C26-C25	3.13	126.94	122.70
22	C	508	CLA	O2D-CGD-O1D	-3.13	117.75	123.85
27	M	101	LMG	C1-C2-C3	-3.13	103.43	110.01
26	D	406	PL9	C7-C3-C2	-3.13	119.70	123.39
27	b	622	LMG	C3-C4-C5	-3.13	104.56	110.23
22	b	616	CLA	CHB-C4A-NA	3.12	128.91	124.40
22	b	606	CLA	CMB-C2B-C1B	-3.12	120.67	125.42
28	F	101	SQD	O48-C23-O10	-3.12	115.82	123.63
22	b	602	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
22	C	502	CLA	C3B-C4B-NB	-3.12	107.75	110.53
24	d	406	BCR	C16-C15-C14	-3.12	117.14	123.52
22	D	403	CLA	O2D-CGD-CBD	3.12	116.68	111.23
28	L	101	SQD	O5-C5-C4	3.12	115.31	109.70
22	B	603	CLA	CHD-C4C-NC	3.11	129.06	124.23
24	b	619	BCR	C36-C18-C17	-3.11	117.77	122.82
22	B	611	CLA	C1-C2-C3	-3.11	121.10	126.20
26	D	406	PL9	C12-C13-C14	-3.11	120.51	127.62
22	C	506	CLA	C3B-C4B-NB	-3.11	107.76	110.53
22	C	509	CLA	CHB-C4A-NA	3.10	128.88	124.40
29	C	517	DGD	O5D-C1E-C2E	3.10	112.98	108.27
22	B	607	CLA	CHB-C1B-NB	3.10	128.69	124.05
22	b	613	CLA	O2D-CGD-CBD	3.10	116.64	111.23
23	D	401	PHO	C3B-C4B-NB	-3.09	105.45	107.46
26	a	409	PL9	C22-C23-C24	-3.09	120.55	127.62
28	f	102	SQD	C45-O47-C7	3.09	125.19	117.80
22	C	509	CLA	CMB-C2B-C3B	3.09	133.82	126.55
22	B	616	CLA	CAA-CBA-CGA	-3.08	104.45	113.21
28	A	412	SQD	O47-C7-C8	3.08	118.15	111.48
24	b	618	BCR	C8-C7-C6	-3.08	118.76	127.00
22	b	615	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
22	b	601	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
35	f	101	HEM	CBD-CAD-C3D	-3.07	104.05	112.53
22	C	513	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
22	b	610	CLA	CHB-C4A-NA	3.06	128.82	124.40
22	A	402	CLA	O1D-CGD-CBD	3.06	130.55	124.52
22	C	510	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
23	d	401	PHO	OBD-CAD-CBD	-3.05	121.35	125.82
27	d	412	LMG	C3-C4-C5	-3.04	104.72	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	CMB-C2B-C1B	-3.04	120.79	125.42
26	A	409	PL9	C7-C3-C2	-3.04	119.81	123.39
32	C	522	STE	C4-C3-C2	-3.04	101.97	113.13
22	B	601	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
22	b	605	CLA	C3B-C4B-NB	-3.03	107.82	110.53
33	E	102	LHG	O8-C23-C24	3.03	121.06	111.83
22	C	506	CLA	O1D-CGD-CBD	3.02	130.48	124.52
26	a	409	PL9	C36-C34-C33	-3.02	114.39	121.17
28	a	410	SQD	O47-C7-O49	-3.02	116.65	123.70
22	B	613	CLA	O2A-CGA-O1A	-3.02	116.08	123.63
22	c	512	CLA	CHB-C4A-NA	3.02	128.76	124.40
22	b	602	CLA	C1-C2-C3	-3.02	121.26	126.20
28	F	101	SQD	O48-C23-C24	3.01	121.03	111.83
22	c	513	CLA	C3B-C4B-NB	-3.01	107.84	110.53
27	b	622	LMG	O7-C10-O9	-3.01	116.66	123.70
33	D	408	LHG	O8-C23-O10	-3.01	116.10	123.63
28	A	412	SQD	O48-C23-O10	-3.01	116.11	123.63
22	B	602	CLA	C16-C15-C13	-3.01	105.97	115.97
22	c	510	CLA	C3B-C4B-NB	-3.00	107.85	110.53
28	L	101	SQD	O2-C2-C1	3.00	117.23	110.08
28	F	101	SQD	C44-O6-C1	3.00	118.81	113.68
24	B	619	BCR	C29-C30-C25	3.00	114.80	110.44
22	d	405	CLA	CMB-C2B-C3B	3.00	133.60	126.55
35	E	101	HEM	CBD-CAD-C3D	-3.00	104.25	112.53
24	A	406	BCR	C37-C22-C21	-3.00	117.96	122.82
26	d	407	PL9	C7-C3-C2	-3.00	119.86	123.39
24	c	516	BCR	C2-C1-C6	3.00	114.79	110.44
24	B	618	BCR	C2-C1-C6	2.99	114.79	110.44
24	k	101	BCR	C27-C26-C25	2.99	126.75	122.70
22	b	609	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
22	c	505	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
27	c	522	LMG	O1-C1-C2	-2.99	103.74	108.27
23	d	401	PHO	C2B-C1B-NB	-2.99	107.27	109.43
28	a	411	SQD	O48-C23-O10	-2.98	116.17	123.63
22	B	613	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	Y	101	BCR	C27-C26-C25	2.98	126.73	122.70
24	C	514	BCR	C15-C16-C17	-2.98	117.42	123.52
22	B	604	CLA	C3B-C4B-NB	-2.98	107.87	110.53
24	A	406	BCR	C27-C26-C25	2.98	126.73	122.70
33	D	408	LHG	C18-C17-C16	-2.98	99.32	114.37
22	a	402	CLA	CMB-C2B-C1B	-2.98	120.89	125.42
29	C	518	DGD	CDB-CCB-CBB	-2.97	99.35	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	V	201	HEC	C1D-ND-C4D	2.97	108.72	105.21
22	B	602	CLA	CMB-C2B-C3B	2.97	133.54	126.55
24	D	405	BCR	C27-C26-C25	2.97	126.72	122.70
22	c	510	CLA	O1D-CGD-CBD	2.97	130.37	124.52
22	D	404	CLA	CMB-C2B-C3B	2.97	133.53	126.55
28	f	102	SQD	C1-C2-C3	-2.96	103.77	110.01
29	h	102	DGD	O2D-C2D-C1D	-2.96	103.02	110.08
22	C	504	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
22	b	606	CLA	CHB-C4A-NA	2.95	128.65	124.40
22	B	607	CLA	C4-C3-C5	2.94	120.34	115.23
22	b	604	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
29	h	102	DGD	C4D-C3D-C2D	-2.94	105.67	110.83
26	a	409	PL9	C20-C19-C21	2.93	120.32	115.23
27	C	519	LMG	O1-C7-C8	-2.93	103.68	110.82
22	C	501	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
22	C	503	CLA	CHD-C1D-ND	-2.93	120.68	124.80
22	c	508	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
27	b	622	LMG	O8-C28-O10	-2.93	116.30	123.63
29	a	412	DGD	C5B-C4B-C3B	-2.93	99.56	114.37
24	h	101	BCR	C15-C16-C17	-2.93	117.53	123.52
22	c	511	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
22	c	509	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	B	615	CLA	C3B-C4B-NB	-2.92	107.92	110.53
27	d	412	LMG	O6-C1-O1	-2.92	103.15	110.04
22	a	402	CLA	O1D-CGD-CBD	2.91	130.27	124.52
22	C	509	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	C	507	CLA	O1D-CGD-CBD	2.91	130.26	124.52
24	H	101	BCR	C16-C15-C14	-2.91	117.56	123.52
22	C	509	CLA	C1-C2-C3	-2.91	121.43	126.20
22	d	405	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	c	507	CLA	C4A-NA-C1A	2.90	108.00	106.68
29	c	518	DGD	O4D-C4D-C3D	2.90	117.20	110.38
22	B	604	CLA	CMB-C2B-C1B	-2.90	121.01	125.42
22	b	616	CLA	CHD-C1D-ND	-2.90	120.73	124.80
22	C	508	CLA	CHD-C1D-ND	-2.89	120.73	124.80
23	D	401	PHO	C1-C2-C3	-2.89	121.46	126.20
24	K	101	BCR	C38-C26-C25	-2.89	121.33	124.48
33	d	410	LHG	O8-C23-C24	2.89	120.63	111.83
28	L	101	SQD	O8-S-O7	-2.89	104.18	111.40
22	b	612	CLA	C1-C2-C3	-2.88	121.47	126.20
22	b	615	CLA	C3B-C4B-NB	-2.88	107.96	110.53
29	H	102	DGD	C1D-C2D-C3D	-2.86	103.99	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	101	STE	C3-C2-C1	-2.86	107.04	114.51
22	C	512	CLA	C1-C2-C3	-2.86	121.51	126.20
22	b	608	CLA	O2D-CGD-CBD	2.85	116.22	111.23
22	B	612	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
22	B	604	CLA	C2D-C1D-ND	-2.85	107.30	110.13
22	A	402	CLA	C7-C6-C5	-2.85	105.66	113.26
29	H	102	DGD	O2D-C2D-C1D	-2.85	103.28	110.08
22	c	505	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	C	508	CLA	CMB-C2B-C1B	-2.85	121.09	125.42
27	c	522	LMG	O7-C10-O9	-2.84	117.06	123.70
24	c	514	BCR	C2-C1-C6	2.84	114.57	110.44
22	C	502	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
22	b	610	CLA	C1-C2-C3	-2.84	121.54	126.20
22	C	508	CLA	O2D-CGD-CBD	2.84	116.19	111.23
22	a	402	CLA	C3B-C4B-NB	-2.84	108.00	110.53
29	a	412	DGD	C1G-C2G-C3G	-2.84	105.25	111.80
26	D	406	PL9	C22-C23-C24	-2.83	121.14	127.62
26	D	406	PL9	C7-C8-C9	-2.83	121.95	126.83
24	b	619	BCR	C38-C26-C25	-2.83	121.40	124.48
23	A	404	PHO	C3B-C4B-NB	-2.82	105.62	107.46
22	c	502	CLA	CHD-C1D-ND	-2.82	120.83	124.80
22	b	609	CLA	C3B-C4B-NB	-2.82	108.01	110.53
27	c	520	LMG	C9-C8-C7	-2.82	105.22	111.78
22	b	610	CLA	CAA-CBA-CGA	-2.82	105.21	113.21
22	c	506	CLA	CHB-C4A-NA	2.81	128.46	124.40
22	b	602	CLA	C11-C12-C13	-2.81	106.63	115.97
22	c	509	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
22	B	601	CLA	C4-C3-C5	2.81	120.10	115.23
22	B	605	CLA	C3B-C4B-NB	-2.81	108.03	110.53
32	d	413	STE	O2-C1-C2	2.81	122.87	114.00
27	b	620	LMG	O7-C10-O9	-2.80	117.15	123.70
24	A	406	BCR	C15-C16-C17	-2.80	117.79	123.52
22	b	609	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
24	H	101	BCR	C2-C1-C6	2.79	114.50	110.44
22	b	609	CLA	O1D-CGD-CBD	2.79	130.03	124.52
29	A	414	DGD	O5D-C6D-C5D	-2.79	103.12	109.42
22	b	608	CLA	CMB-C2B-C3B	2.79	133.11	126.55
24	t	101	BCR	C36-C18-C19	2.79	122.35	118.09
22	B	614	CLA	C4-C3-C5	2.78	120.06	115.23
32	m	101	STE	O1-C1-C2	-2.78	114.27	123.09
22	B	604	CLA	C1D-ND-C4D	2.78	108.26	106.31
22	B	603	CLA	C4A-NA-C1A	2.77	107.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	402	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
29	H	102	DGD	C1E-O6E-C5E	2.77	119.13	113.72
22	b	609	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	c	515	BCR	C38-C26-C25	-2.77	121.46	124.48
22	b	605	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
22	B	610	CLA	C3B-C4B-NB	-2.76	108.06	110.53
28	L	101	SQD	O10-C23-C24	-2.76	112.97	123.78
22	b	608	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
28	B	623	SQD	O8-S-C6	2.76	111.31	105.97
29	c	518	DGD	O6D-C1D-O3G	-2.76	103.52	110.04
22	b	613	CLA	CHB-C4A-NA	2.76	128.38	124.40
22	b	615	CLA	CMB-C2B-C1B	-2.76	121.22	125.42
22	C	513	CLA	CHB-C4A-NA	2.75	128.37	124.40
28	a	411	SQD	O49-C7-C8	-2.75	113.03	123.78
24	c	514	BCR	C15-C14-C13	-2.75	123.43	127.28
27	d	412	LMG	O1-C1-C2	-2.75	104.10	108.27
22	D	403	CLA	CHB-C4A-NA	2.74	128.36	124.40
22	B	613	CLA	C4-C3-C5	2.74	119.99	115.23
22	B	613	CLA	CMB-C2B-C3B	2.74	132.99	126.55
28	A	412	SQD	O5-C1-O6	2.74	116.52	110.04
24	c	514	BCR	C15-C16-C17	-2.74	117.92	123.52
22	A	405	CLA	CHD-C1D-ND	-2.73	120.96	124.80
26	a	409	PL9	O2-C1-C2	-2.73	115.61	121.83
22	B	614	CLA	CHC-C4B-NB	2.73	128.15	124.05
22	B	611	CLA	C4A-NA-C1A	2.73	107.92	106.68
29	C	516	DGD	O6D-C1D-O3G	-2.73	103.60	110.04
27	c	523	LMG	O6-C1-O1	-2.72	103.61	110.04
34	a	408	BCT	O3-C-O1	-2.72	112.71	119.68
22	A	403	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
22	c	508	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
22	c	510	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
22	b	614	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
22	d	404	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	c	504	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
28	a	410	SQD	O9-S-C6	2.71	110.81	106.76
23	d	402	PHO	CMB-C2B-C3B	2.71	130.11	124.68
22	b	615	CLA	CHB-C4A-NA	2.71	128.31	124.40
26	d	407	PL9	C8-C7-C3	2.71	119.04	112.03
22	c	505	CLA	O2D-CGD-CBD	2.71	115.97	111.23
22	c	507	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
22	C	508	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	c	502	CLA	O1D-CGD-CBD	2.71	129.86	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	501	CLA	O2A-CGA-O1A	-2.71	116.86	123.63
22	B	615	CLA	O2D-CGD-CBD	2.71	115.96	111.23
26	D	406	PL9	C20-C19-C21	2.70	119.92	115.23
24	c	516	BCR	C27-C26-C25	2.70	126.36	122.70
24	a	405	BCR	C37-C22-C23	2.70	122.22	118.09
27	b	620	LMG	C38-C37-C36	-2.70	100.72	114.37
22	b	612	CLA	CMB-C2B-C3B	2.69	132.88	126.55
24	Y	101	BCR	C37-C22-C21	-2.69	118.45	122.82
27	M	101	LMG	C38-C37-C36	-2.69	100.77	114.37
22	b	601	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	B	614	CLA	CHB-C4A-NA	2.69	128.28	124.40
22	C	503	CLA	C7-C6-C5	-2.69	106.10	113.26
22	c	513	CLA	CHB-C4A-NA	2.68	128.27	124.40
24	b	619	BCR	C2-C1-C6	2.68	114.33	110.44
26	a	409	PL9	C37-C38-C39	-2.68	121.49	127.62
22	c	504	CLA	C3B-C4B-NB	-2.68	108.14	110.53
22	B	603	CLA	C5-C3-C2	-2.68	115.16	121.17
22	B	610	CLA	CMA-C3A-C4A	-2.68	104.58	111.77
33	l	101	LHG	O8-C23-O10	-2.68	116.94	123.63
22	b	605	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
32	C	520	STE	O2-C1-C2	2.67	122.45	114.00
24	B	618	BCR	C3-C4-C5	-2.67	109.29	114.06
36	V	201	HEC	CMC-C2C-C1C	-2.67	121.35	125.42
22	b	612	CLA	CHB-C4A-NA	2.67	128.25	124.40
33	B	622	LHG	O8-C23-O10	-2.67	116.96	123.63
22	C	503	CLA	CHB-C1B-NB	2.67	128.05	124.05
29	A	414	DGD	C3E-C4E-C5E	-2.67	105.40	110.23
22	C	503	CLA	C4D-CHA-C1A	2.67	124.42	121.24
22	b	602	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
27	D	407	LMG	O6-C1-O1	-2.66	103.75	110.04
22	A	410	CLA	CMB-C2B-C3B	2.66	132.82	126.55
27	D	407	LMG	O3-C3-C2	-2.66	104.10	110.38
29	C	517	DGD	C1D-O6D-C5D	-2.66	108.52	113.72
22	B	611	CLA	CHD-C4C-NC	2.66	128.35	124.23
33	e	101	LHG	O8-C23-C24	2.66	119.94	111.83
22	c	511	CLA	O2D-CGD-CBD	2.66	115.88	111.23
29	h	102	DGD	O2E-C2E-C3E	-2.66	104.11	110.38
22	b	614	CLA	CAC-C3C-C4C	2.66	128.25	124.79
22	b	605	CLA	O1D-CGD-CBD	2.66	129.75	124.52
24	c	515	BCR	C36-C18-C17	-2.65	118.52	122.82
22	c	501	CLA	CHB-C4A-NA	2.65	128.22	124.40
22	B	608	CLA	CMB-C2B-C3B	2.65	132.78	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	404	CLA	C3D-C4D-ND	2.65	114.29	109.99
22	b	605	CLA	C4A-NA-C1A	2.65	107.89	106.68
36	V	201	HEC	CBD-CAD-C3D	-2.65	105.22	112.53
26	D	406	PL9	C30-C29-C31	-2.64	110.64	115.23
24	k	101	BCR	C38-C26-C25	-2.64	121.60	124.48
22	A	405	CLA	C2C-C1C-NC	2.64	112.75	109.98
24	K	101	BCR	C7-C8-C9	-2.64	122.33	126.23
22	B	602	CLA	C3B-C4B-NB	-2.64	108.18	110.53
27	b	620	LMG	O6-C1-O1	-2.63	103.82	110.04
27	b	622	LMG	O6-C5-C6	2.63	112.97	106.44
24	b	618	BCR	C27-C26-C25	2.63	126.26	122.70
24	h	101	BCR	C27-C26-C25	2.63	126.26	122.70
22	C	511	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
29	A	414	DGD	CDB-CCB-CBB	-2.63	101.08	114.37
33	d	410	LHG	C26-C25-C24	2.63	122.79	113.13
22	b	613	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
33	D	408	LHG	C20-C19-C18	-2.62	101.12	114.37
22	a	403	CLA	CED-O2D-CGD	-2.62	109.98	115.92
22	A	405	CLA	CMB-C2B-C3B	2.61	132.70	126.55
32	b	624	STE	C3-C2-C1	-2.61	107.69	114.51
22	b	616	CLA	C3B-C4B-NB	-2.61	108.20	110.53
22	B	603	CLA	CHD-C1D-ND	-2.61	121.13	124.80
26	d	407	PL9	C7-C8-C9	-2.61	122.34	126.83
22	b	608	CLA	C11-C10-C8	-2.60	107.32	115.97
22	d	404	CLA	CMC-C2C-C1C	2.60	129.09	125.03
28	A	412	SQD	O5-C1-C2	-2.60	105.03	110.37
22	c	507	CLA	C3B-C4B-NB	-2.60	108.21	110.53
22	A	402	CLA	CMB-C2B-C1B	-2.59	121.47	125.42
22	b	602	CLA	CMB-C2B-C3B	2.59	132.64	126.55
23	D	401	PHO	O2D-CGD-O1D	-2.59	118.81	123.85
24	b	617	BCR	C29-C30-C25	2.59	114.20	110.44
22	c	504	CLA	CMB-C2B-C3B	2.59	132.64	126.55
22	a	403	CLA	CMB-C2B-C3B	2.59	132.64	126.55
28	F	101	SQD	C1-C2-C3	-2.59	104.57	110.01
22	B	612	CLA	O1D-CGD-CBD	2.59	129.62	124.52
22	C	508	CLA	CHB-C1B-NB	2.59	127.93	124.05
22	B	604	CLA	CGD-CBD-CAD	-2.58	102.48	110.85
35	f	101	HEM	CBA-CAA-C2A	-2.58	105.39	112.53
28	a	411	SQD	O48-C23-C24	2.58	119.70	111.83
22	d	404	CLA	CHC-C4B-NB	2.58	127.91	124.05
22	a	402	CLA	CHB-C4A-NA	2.57	128.11	124.40
22	c	513	CLA	CAC-C3C-C4C	2.57	128.14	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	512	CLA	CHD-C1D-ND	-2.57	121.18	124.80
27	D	407	LMG	O4-C4-C5	2.57	115.65	109.32
29	C	516	DGD	C3G-C2G-C1G	-2.57	105.80	111.78
26	A	409	PL9	O1-C4-C3	-2.56	118.03	120.73
22	C	510	CLA	C3B-C4B-NB	-2.56	108.24	110.53
22	c	501	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
27	M	101	LMG	O8-C28-O10	-2.56	117.22	123.63
22	c	508	CLA	C1-C2-C3	-2.56	122.00	126.20
22	A	402	CLA	C3B-C4B-NB	-2.56	108.24	110.53
22	C	501	CLA	O2D-CGD-CBD	2.56	115.70	111.23
23	D	401	PHO	C1A-C2A-C3A	-2.56	100.41	102.84
29	c	519	DGD	O6D-C1D-O3G	-2.55	104.01	110.04
23	A	404	PHO	CMA-C3A-C2A	-2.55	104.28	114.13
26	a	409	PL9	C27-C28-C29	-2.55	121.79	127.62
22	c	503	CLA	C4-C3-C5	2.55	119.65	115.23
26	d	407	PL9	C50-C49-C48	-2.55	115.00	122.66
22	b	606	CLA	CMB-C2B-C3B	2.55	132.55	126.55
24	d	406	BCR	C24-C23-C22	-2.54	122.47	126.23
28	B	623	SQD	O5-C5-C4	2.54	114.28	109.70
22	b	611	CLA	CHD-C1D-ND	-2.54	121.22	124.80
24	a	405	BCR	C29-C30-C25	2.54	114.13	110.44
22	B	603	CLA	CHD-C1D-C2D	2.54	130.78	125.49
22	c	508	CLA	CMB-C2B-C3B	2.54	132.53	126.55
24	C	514	BCR	C37-C22-C21	-2.54	118.70	122.82
27	D	407	LMG	C38-C37-C36	-2.54	101.53	114.37
24	b	617	BCR	C27-C26-C25	2.54	126.14	122.70
22	B	613	CLA	CHB-C4A-NA	2.54	128.06	124.40
26	d	407	PL9	C20-C19-C21	2.54	119.63	115.23
28	A	413	SQD	O48-C46-C45	2.54	115.57	108.35
22	B	611	CLA	CHB-C4A-NA	2.53	128.06	124.40
22	B	604	CLA	C11-C10-C8	-2.53	107.55	115.97
22	c	506	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
29	c	518	DGD	C1D-C2D-C3D	-2.53	104.69	110.01
22	D	404	CLA	CHB-C1B-NB	2.53	127.84	124.05
28	f	102	SQD	O48-C23-C24	2.53	119.54	111.83
33	D	409	LHG	O8-C6-C5	-2.53	101.11	108.40
22	C	511	CLA	CHB-C4A-NA	2.53	128.04	124.40
27	c	522	LMG	C9-C8-C7	-2.52	105.91	111.78
26	D	406	PL9	C42-C43-C44	-2.52	121.86	127.62
22	a	402	CLA	CMB-C2B-C3B	2.52	132.47	126.55
22	B	606	CLA	CHD-C4C-NC	2.51	128.13	124.23
22	B	609	CLA	O2A-CGA-O1A	-2.51	117.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	CMB-C2B-C3B	2.51	132.46	126.55
22	b	615	CLA	CHC-C1C-NC	2.51	128.09	124.31
27	M	101	LMG	O7-C10-O9	-2.51	117.84	123.70
29	A	414	DGD	C5B-C4B-C3B	-2.51	101.70	114.37
29	h	102	DGD	C1D-O6D-C5D	-2.51	108.83	113.72
22	b	605	CLA	CHB-C1B-NB	2.51	127.81	124.05
22	B	611	CLA	C14-C13-C15	-2.50	102.35	111.27
22	a	403	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
23	A	404	PHO	C1A-C2A-C3A	-2.50	100.46	102.84
35	E	101	HEM	O2D-CGD-CBD	2.50	121.91	114.00
29	A	414	DGD	C1D-C2D-C3D	-2.50	104.75	110.01
22	C	510	CLA	CMB-C2B-C3B	2.50	132.44	126.55
23	A	404	PHO	C4B-NB-C1B	2.50	112.46	108.82
22	b	613	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
23	A	404	PHO	C1-C2-C3	-2.50	122.10	126.20
36	V	201	HEC	CHB-C4A-NA	2.50	127.17	124.45
28	a	410	SQD	O47-C7-C8	2.50	116.88	111.48
22	B	606	CLA	C4-C3-C5	2.50	119.56	115.23
22	c	509	CLA	CHD-C1D-ND	-2.49	121.29	124.80
24	b	619	BCR	C36-C18-C19	2.49	121.90	118.09
33	d	409	LHG	O8-C23-C24	2.49	119.43	111.83
22	d	403	CLA	CMB-C2B-C1B	-2.49	121.62	125.42
22	d	403	CLA	CMB-C2B-C3B	2.49	132.41	126.55
22	A	402	CLA	CMB-C2B-C3B	2.49	132.41	126.55
22	b	613	CLA	CHA-C1A-NA	-2.49	120.75	126.39
23	A	404	PHO	C16-C17-C18	-2.49	104.84	115.94
24	A	406	BCR	C16-C15-C14	-2.49	118.43	123.52
22	b	612	CLA	C11-C12-C13	-2.48	107.71	115.97
22	B	612	CLA	O2A-CGA-O1A	-2.48	117.41	123.63
24	t	101	BCR	C4-C5-C6	2.48	126.06	122.70
22	B	612	CLA	CHB-C4A-NA	2.48	127.98	124.40
26	A	409	PL9	C12-C13-C14	-2.48	121.94	127.62
24	B	618	BCR	C15-C16-C17	-2.48	118.45	123.52
22	b	610	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
29	C	517	DGD	CDB-CCB-CBB	-2.47	101.87	114.37
29	C	518	DGD	C3G-C2G-C1G	-2.47	106.02	111.78
33	d	409	LHG	C18-C17-C16	-2.47	101.87	114.37
28	A	413	SQD	O47-C45-C44	2.47	113.50	107.96
22	b	608	CLA	CHB-C1B-NB	2.47	127.75	124.05
22	A	410	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
22	c	510	CLA	C1-C2-C3	-2.47	122.15	126.20
22	b	614	CLA	O2A-CGA-O1A	-2.47	117.46	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	102	DGD	C4E-C3E-C2E	-2.46	106.51	110.83
23	d	402	PHO	O2A-CGA-O1A	-2.46	117.47	123.63
22	c	510	CLA	CMB-C2B-C3B	2.46	132.34	126.55
24	c	516	BCR	C24-C23-C22	-2.46	122.59	126.23
22	A	403	CLA	CHB-C1B-NB	2.46	127.74	124.05
22	B	614	CLA	O1D-CGD-CBD	2.46	129.37	124.52
22	B	610	CLA	CHD-C1D-ND	-2.46	121.34	124.80
22	B	609	CLA	C2C-C1C-NC	2.46	112.56	109.98
22	b	603	CLA	CHD-C1D-C2D	2.46	130.59	125.49
28	f	102	SQD	O5-C1-O6	2.45	115.84	110.04
22	c	513	CLA	C11-C12-C13	-2.45	107.81	115.97
28	B	623	SQD	O48-C23-O10	-2.45	117.49	123.63
24	B	619	BCR	C1-C6-C5	-2.45	119.29	122.64
27	c	522	LMG	O2-C2-C1	-2.45	104.23	110.08
27	A	411	LMG	O1-C7-C8	-2.45	104.86	110.82
27	c	523	LMG	C9-C8-C7	-2.45	106.07	111.78
22	a	403	CLA	O2D-CGD-CBD	2.45	115.51	111.23
35	E	101	HEM	CHC-C4B-NB	2.45	127.06	124.42
22	B	614	CLA	C4A-NA-C1A	2.45	107.80	106.68
24	B	617	BCR	C38-C26-C25	-2.45	121.81	124.48
22	C	511	CLA	CMB-C2B-C1B	-2.45	121.69	125.42
22	B	604	CLA	O2D-CGD-CBD	2.45	115.50	111.23
22	B	604	CLA	CMB-C2B-C3B	2.44	132.30	126.55
22	d	403	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
24	t	101	BCR	C19-C18-C17	-2.44	115.17	119.01
24	c	514	BCR	C20-C21-C22	-2.44	123.85	127.28
22	B	608	CLA	CHB-C1B-NB	2.44	127.71	124.05
23	d	401	PHO	C1-C2-C3	-2.44	122.20	126.20
28	f	102	SQD	O5-C1-C2	-2.44	105.36	110.37
24	c	515	BCR	C7-C8-C9	-2.44	122.63	126.23
22	C	509	CLA	CED-O2D-CGD	2.43	121.44	115.92
22	B	616	CLA	CMB-C2B-C3B	2.43	132.27	126.55
22	A	403	CLA	C4A-NA-C1A	2.43	107.79	106.68
24	H	101	BCR	C27-C26-C25	2.43	125.99	122.70
22	A	403	CLA	CED-O2D-CGD	-2.43	110.41	115.92
22	C	510	CLA	CMB-C2B-C1B	-2.43	121.72	125.42
24	h	101	BCR	C2-C1-C6	2.43	113.97	110.44
24	A	406	BCR	C11-C10-C9	-2.43	123.88	127.28
22	B	615	CLA	CHC-C4B-NB	2.43	127.69	124.05
22	B	603	CLA	CHB-C4A-NA	2.42	127.90	124.40
27	c	522	LMG	O3-C3-C2	-2.42	104.66	110.38
22	A	402	CLA	C6-C5-C3	2.42	119.36	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	620	LMG	C1-O6-C5	-2.42	109.00	113.72
22	B	616	CLA	O1D-CGD-CBD	2.42	129.29	124.52
22	b	604	CLA	O1D-CGD-CBD	2.42	129.28	124.52
23	d	402	PHO	C3D-C4D-ND	2.41	110.80	107.71
27	b	620	LMG	C9-C8-C7	-2.41	106.16	111.78
22	c	504	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
24	c	516	BCR	C38-C26-C25	-2.41	121.85	124.48
22	B	613	CLA	CHA-C1A-NA	-2.41	120.93	126.39
28	L	101	SQD	O47-C45-C46	2.41	116.98	108.34
24	H	101	BCR	C29-C30-C25	2.41	113.94	110.44
22	c	511	CLA	C2B-C1B-NB	-2.41	107.83	110.33
24	a	405	BCR	C27-C26-C25	2.41	125.96	122.70
22	C	512	CLA	CAA-CBA-CGA	-2.41	106.38	113.21
24	T	101	BCR	C4-C5-C6	2.41	125.95	122.70
22	a	404	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
23	d	401	PHO	C3D-C4D-ND	2.40	110.78	107.71
22	d	405	CLA	CHB-C1B-NB	2.40	127.65	124.05
33	L	102	LHG	O8-C23-O10	-2.40	117.63	123.63
22	D	403	CLA	C1-C2-C3	-2.40	122.27	126.20
24	C	515	BCR	C27-C26-C25	2.40	125.94	122.70
22	b	605	CLA	C1-C2-C3	-2.40	122.27	126.20
29	c	519	DGD	CDB-CCB-CBB	-2.40	102.26	114.37
24	t	101	BCR	C28-C27-C26	-2.40	109.78	114.06
29	a	412	DGD	C7B-C6B-C5B	-2.39	102.26	114.37
22	c	506	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
27	A	411	LMG	O3-C3-C2	-2.39	104.74	110.38
22	c	508	CLA	CHD-C1D-ND	-2.39	121.44	124.80
22	c	510	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	a	402	CLA	CAC-C3C-C4C	2.39	127.90	124.79
22	B	609	CLA	CAC-C3C-C4C	2.39	127.90	124.79
24	B	617	BCR	C3-C4-C5	-2.39	109.80	114.06
32	b	623	STE	O2-C1-C2	2.39	121.54	114.00
22	b	603	CLA	C3B-C4B-NB	-2.38	108.40	110.53
22	b	614	CLA	CHB-C4A-NA	2.38	127.84	124.40
29	H	102	DGD	C3G-C2G-C1G	-2.38	106.23	111.78
33	B	622	LHG	C18-C17-C16	-2.38	102.34	114.37
22	C	503	CLA	C3B-C4B-NB	-2.38	108.41	110.53
28	a	410	SQD	O8-S-O9	-2.38	105.45	111.40
33	l	101	LHG	O10-C23-C24	-2.38	114.49	123.78
22	c	508	CLA	CHD-C1D-C2D	2.37	130.43	125.49
22	A	402	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
24	h	101	BCR	C37-C22-C23	2.37	121.71	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	611	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
27	c	523	LMG	O8-C28-O10	-2.37	117.70	123.63
22	c	506	CLA	C1-O2A-CGA	2.37	122.39	116.65
26	D	406	PL9	C32-C33-C34	-2.37	122.20	127.62
29	H	102	DGD	CAB-C9B-C8B	-2.37	102.39	114.37
23	d	401	PHO	C3B-C4B-NB	-2.37	105.92	107.46
22	c	509	CLA	C11-C10-C8	-2.37	108.09	115.97
29	c	518	DGD	CDB-CCB-CBB	-2.37	102.39	114.37
22	C	507	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
24	t	101	BCR	C15-C16-C17	-2.37	118.68	123.52
24	t	101	BCR	C27-C26-C25	2.37	125.90	122.70
22	b	606	CLA	O1D-CGD-CBD	2.36	129.18	124.52
24	b	617	BCR	C23-C22-C21	-2.36	115.29	119.01
27	C	519	LMG	C38-C37-C36	-2.36	102.42	114.37
28	a	410	SQD	O8-S-C6	2.36	110.53	105.97
27	c	523	LMG	O1-C7-C8	-2.36	105.07	110.82
24	a	405	BCR	C37-C22-C21	-2.36	118.99	122.82
24	K	101	BCR	C2-C1-C6	2.36	113.87	110.44
22	B	603	CLA	OBD-CAD-C3D	2.36	133.94	128.42
24	c	515	BCR	C37-C22-C23	2.36	121.69	118.09
22	C	510	CLA	O2D-CGD-CBD	2.36	115.36	111.23
22	B	602	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
24	D	405	BCR	C7-C8-C9	-2.36	122.74	126.23
26	D	406	PL9	C35-C34-C36	2.36	119.32	115.23
22	b	607	CLA	C3B-C4B-NB	-2.36	108.42	110.53
24	t	101	BCR	C16-C17-C18	-2.35	123.98	127.28
26	a	409	PL9	O2-C1-C6	2.35	124.22	120.48
22	b	606	CLA	C3B-C4B-NB	-2.35	108.43	110.53
22	C	512	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
26	a	409	PL9	C40-C39-C38	-2.35	117.59	123.63
24	A	406	BCR	C38-C26-C25	-2.35	121.92	124.48
22	b	613	CLA	C16-C15-C13	-2.35	108.16	115.97
29	c	519	DGD	C6B-C5B-C4B	-2.34	102.52	114.37
22	b	616	CLA	CGD-CBD-CAD	-2.34	103.26	110.85
29	A	414	DGD	O6D-C1D-O3G	-2.34	104.51	110.04
22	b	615	CLA	CHB-C1B-NB	2.34	127.56	124.05
22	C	506	CLA	C1-C2-C3	-2.34	122.36	126.20
22	b	614	CLA	O2D-CGD-CBD	2.34	115.32	111.23
29	C	518	DGD	C4D-C3D-C2D	-2.34	106.72	110.83
22	b	603	CLA	O2D-CGD-CBD	2.34	115.32	111.23
22	A	405	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	c	512	CLA	C3B-C4B-NB	-2.34	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	CMB-C2B-C3B	2.34	132.05	126.55
22	c	509	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
22	c	502	CLA	C1-C2-C3	-2.34	122.37	126.20
22	b	614	CLA	CHD-C1D-ND	-2.33	121.52	124.80
29	c	519	DGD	C6D-O5D-C1E	2.33	118.80	113.80
26	a	409	PL9	O1-C4-C3	-2.33	118.27	120.73
24	b	619	BCR	C27-C26-C25	2.33	125.86	122.70
22	C	505	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
22	b	610	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
33	d	408	LHG	C5-O7-C7	-2.33	112.22	117.80
22	b	605	CLA	CHD-C4C-NC	2.33	127.84	124.23
22	C	504	CLA	CHA-C1A-NA	-2.32	121.13	126.39
22	c	513	CLA	O1D-CGD-CBD	2.32	129.10	124.52
33	l	101	LHG	C20-C19-C18	-2.32	102.62	114.37
22	C	513	CLA	CHD-C1D-ND	-2.32	121.53	124.80
26	D	406	PL9	C36-C34-C33	-2.32	115.95	121.17
23	d	401	PHO	CMA-C3A-C4A	-2.32	109.61	114.61
22	b	607	CLA	CED-O2D-CGD	2.32	121.18	115.92
28	F	101	SQD	O9-S-O7	-2.32	106.28	113.82
24	b	619	BCR	C29-C30-C25	2.32	113.81	110.44
28	a	411	SQD	O47-C7-C8	2.32	116.50	111.48
24	B	619	BCR	C15-C16-C17	-2.32	118.77	123.52
22	B	612	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	c	514	BCR	C27-C26-C25	2.32	125.84	122.70
29	A	414	DGD	C3G-C2G-C1G	-2.32	106.38	111.78
22	C	512	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
22	b	608	CLA	C1-C2-C3	-2.32	122.40	126.20
28	a	411	SQD	O6-C44-C45	-2.32	105.82	111.77
22	B	606	CLA	O2D-CGD-CBD	2.31	115.28	111.23
29	C	517	DGD	C6D-O5D-C1E	2.31	118.76	113.80
29	C	517	DGD	CAB-C9B-C8B	-2.31	102.68	114.37
22	b	612	CLA	CAC-C3C-C4C	2.31	127.80	124.79
22	c	513	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
22	c	511	CLA	CHB-C4A-NA	2.31	127.73	124.40
22	B	607	CLA	C2A-C1A-CHA	2.31	127.88	123.87
24	b	619	BCR	C16-C15-C14	-2.31	118.79	123.52
35	f	101	HEM	CHB-C1B-NB	2.31	127.22	124.37
22	B	611	CLA	CMB-C2B-C3B	2.31	131.98	126.55
32	C	522	STE	O1-C1-C2	-2.31	115.78	123.09
22	B	604	CLA	C6-C7-C8	-2.31	108.30	115.97
29	C	517	DGD	C1D-C2D-C3D	-2.31	105.16	110.01
29	c	519	DGD	O5D-C1E-C2E	2.31	111.77	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	502	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
22	b	613	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
22	B	611	CLA	C9-C8-C10	-2.30	103.06	111.27
29	h	102	DGD	CDB-CCB-CBB	-2.30	102.72	114.37
27	c	522	LMG	C6-C5-C4	-2.30	107.36	113.02
28	B	623	SQD	C1-C2-C3	-2.30	105.17	110.01
34	D	402	BCT	O3-C-O1	-2.30	113.79	119.68
22	b	615	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
22	A	402	CLA	CAA-CBA-CGA	-2.30	106.67	113.21
24	b	619	BCR	C37-C22-C21	-2.30	119.09	122.82
23	d	402	PHO	C3B-C4B-NB	-2.30	105.97	107.46
22	B	606	CLA	CGD-CBD-CAD	-2.30	103.41	110.85
22	B	610	CLA	C11-C10-C8	-2.29	108.34	115.97
29	C	517	DGD	C7B-C6B-C5B	-2.29	102.79	114.37
29	C	516	DGD	C4E-C3E-C2E	-2.29	106.81	110.83
26	a	409	PL9	C25-C24-C26	2.29	119.20	115.23
22	C	501	CLA	OBD-CAD-C3D	2.29	133.76	128.42
22	B	603	CLA	O2A-CGA-O1A	-2.28	117.91	123.63
26	D	406	PL9	C37-C38-C39	-2.28	122.40	127.62
27	A	411	LMG	C12-C11-C10	-2.28	105.33	113.69
22	b	612	CLA	C4A-NA-C1A	2.28	107.72	106.68
22	c	507	CLA	CHA-C1A-NA	-2.28	121.23	126.39
22	D	403	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
24	b	619	BCR	C15-C16-C17	-2.28	118.86	123.52
23	A	404	PHO	O2D-CGD-O1D	-2.28	119.41	123.85
27	C	519	LMG	C6-C5-C4	-2.28	107.43	113.02
22	b	604	CLA	C4D-C3D-CAD	-2.28	105.63	108.11
33	d	408	LHG	C11-C10-C9	-2.28	102.86	114.37
29	a	412	DGD	CFB-CEB-CDB	-2.28	102.87	114.37
29	c	519	DGD	O1G-C1G-C2G	-2.27	101.84	108.40
35	f	101	HEM	CHD-C4C-NC	2.27	126.93	124.45
22	B	602	CLA	C11-C12-C13	-2.27	108.40	115.97
32	j	101	STE	O1-C1-C2	-2.27	115.88	123.09
22	b	611	CLA	CHB-C4A-NA	2.27	127.68	124.40
29	c	519	DGD	O2D-C2D-C1D	-2.27	104.66	110.08
22	a	402	CLA	C4-C3-C5	2.27	119.17	115.23
22	b	607	CLA	CHB-C4A-NA	2.27	127.68	124.40
22	d	403	CLA	C1C-C2C-C3C	-2.27	104.59	106.98
24	A	406	BCR	C2-C1-C6	2.27	113.73	110.44
22	A	405	CLA	C4A-NA-C1A	2.27	107.71	106.68
29	C	516	DGD	C9B-C8B-C7B	-2.27	102.90	114.37
29	H	102	DGD	CDB-CCB-CBB	-2.27	102.90	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	612	CLA	CED-O2D-CGD	-2.27	110.77	115.92
28	A	413	SQD	O48-C23-O10	-2.27	117.96	123.63
22	C	509	CLA	C2A-C3A-C4A	2.27	105.53	101.87
22	c	503	CLA	C5-C3-C2	-2.26	116.08	121.17
22	b	605	CLA	CHD-C1D-C2D	2.26	130.19	125.49
22	c	507	CLA	O1D-CGD-CBD	2.26	128.98	124.52
22	C	508	CLA	CHD-C4C-NC	2.26	127.74	124.23
22	B	616	CLA	CHA-C4D-ND	2.26	137.21	132.55
22	B	614	CLA	C1-C2-C3	-2.26	122.49	126.20
22	b	606	CLA	CHD-C4C-NC	2.26	127.73	124.23
22	b	605	CLA	CHA-C1A-NA	-2.26	121.28	126.39
28	L	101	SQD	O8-S-C6	2.26	110.33	105.97
24	Y	101	BCR	C15-C16-C17	-2.25	118.91	123.52
29	h	102	DGD	C7B-C6B-C5B	-2.25	102.97	114.37
24	c	515	BCR	C8-C9-C10	2.25	122.55	119.01
29	C	518	DGD	CBB-CAB-C9B	-2.25	102.98	114.37
26	d	407	PL9	C27-C28-C29	-2.25	122.47	127.62
32	j	101	STE	O2-C1-O1	-2.25	117.54	123.33
23	d	401	PHO	CBC-CAC-C3C	-2.25	109.65	112.87
22	B	606	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	T	101	BCR	C1-C6-C5	-2.25	119.56	122.64
26	d	407	PL9	C12-C13-C14	-2.25	122.48	127.62
28	a	410	SQD	O48-C23-O10	-2.25	118.01	123.63
26	a	409	PL9	C7-C8-C9	-2.25	122.96	126.83
22	C	505	CLA	C3B-C4B-NB	-2.24	108.53	110.53
24	H	101	BCR	C37-C22-C21	-2.24	119.18	122.82
22	B	610	CLA	C1-C2-C3	-2.24	122.52	126.20
22	B	614	CLA	CHD-C4C-NC	2.24	127.71	124.23
22	C	504	CLA	C3B-C4B-NB	-2.24	108.53	110.53
23	D	401	PHO	C4B-NB-C1B	2.24	112.08	108.82
22	C	501	CLA	CHB-C1B-NB	2.24	127.41	124.05
27	D	407	LMG	O1-C1-C2	-2.24	104.87	108.27
24	B	618	BCR	C38-C26-C25	-2.24	122.04	124.48
26	A	409	PL9	C20-C19-C18	-2.24	117.88	123.63
24	B	617	BCR	C29-C30-C25	2.24	113.69	110.44
22	c	502	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	B	609	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
24	c	516	BCR	C15-C16-C17	-2.23	118.95	123.52
33	e	101	LHG	C11-C10-C9	-2.23	103.08	114.37
24	b	617	BCR	C24-C23-C22	-2.23	122.93	126.23
24	B	618	BCR	C27-C26-C25	2.23	125.72	122.70
22	b	611	CLA	CHD-C1D-C2D	2.23	130.12	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	412	DGD	CDB-CCB-CBB	-2.23	103.10	114.37
22	C	507	CLA	C4-C3-C5	2.23	119.09	115.23
22	d	404	CLA	C1C-C2C-C3C	-2.23	104.64	106.98
29	h	102	DGD	O3E-C3E-C4E	2.23	115.63	110.38
24	b	617	BCR	C37-C22-C21	-2.23	119.21	122.82
22	c	508	CLA	C3B-C4B-NB	-2.23	108.54	110.53
22	C	508	CLA	CMB-C2B-C3B	2.23	131.78	126.55
27	c	522	LMG	O6-C1-O1	-2.22	104.79	110.04
24	b	617	BCR	C8-C7-C6	-2.22	121.06	127.00
23	d	401	PHO	OBD-CAD-C3D	2.22	131.36	127.89
36	v	201	HEC	CHA-C4D-ND	2.22	126.81	124.42
22	C	503	CLA	CHD-C4C-NC	2.22	127.68	124.23
33	B	622	LHG	C20-C19-C18	-2.22	103.14	114.37
28	f	102	SQD	O47-C7-O49	-2.22	118.51	123.70
29	c	517	DGD	C4E-C3E-C2E	-2.22	106.94	110.83
24	A	406	BCR	C34-C9-C8	-2.22	114.70	118.09
24	C	515	BCR	C37-C22-C21	-2.22	119.22	122.82
22	B	615	CLA	C2A-C3A-C4A	2.22	105.45	101.87
22	B	604	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	d	406	BCR	C2-C1-C6	2.22	113.66	110.44
24	B	617	BCR	C37-C22-C23	2.22	121.47	118.09
24	T	101	BCR	C38-C26-C27	-2.22	108.87	113.60
22	a	403	CLA	CMA-C3A-C4A	-2.22	105.82	111.77
22	B	611	CLA	C5-C3-C2	2.22	126.14	121.17
22	C	504	CLA	CHD-C1D-ND	-2.22	121.69	124.80
26	d	407	PL9	C32-C33-C34	-2.21	122.56	127.62
22	c	507	CLA	CHC-C4B-NB	2.21	127.37	124.05
22	b	610	CLA	O1D-CGD-CBD	2.21	128.88	124.52
33	l	101	LHG	O8-C23-C24	2.21	118.57	111.83
22	B	608	CLA	CHB-C4A-NA	2.21	127.58	124.40
27	b	620	LMG	O8-C28-O10	-2.21	118.11	123.63
22	b	608	CLA	C4-C3-C5	2.21	119.06	115.23
29	c	519	DGD	C8B-C7B-C6B	-2.20	103.23	114.37
27	d	412	LMG	C40-C39-C38	-2.20	103.23	114.37
22	C	513	CLA	O1D-CGD-CBD	2.20	128.86	124.52
27	M	101	LMG	O3-C3-C2	-2.20	105.18	110.38
22	a	404	CLA	C1-O2A-CGA	-2.20	111.32	116.65
32	C	522	STE	C6-C5-C4	-2.20	103.24	114.37
33	E	102	LHG	C18-C17-C16	-2.20	103.25	114.37
22	c	512	CLA	CHD-C1D-ND	-2.20	121.71	124.80
22	B	612	CLA	C3B-C2B-C1B	-2.20	104.58	107.17
22	c	503	CLA	C3B-C4B-NB	-2.20	108.57	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	h	101	BCR	C36-C18-C19	2.20	121.45	118.09
22	b	613	CLA	C2A-C1A-CHA	2.20	127.68	123.87
22	A	410	CLA	CHD-C1D-ND	-2.20	121.71	124.80
22	B	608	CLA	C11-C12-C13	-2.20	108.67	115.97
22	C	511	CLA	CHD-C1D-ND	-2.20	121.71	124.80
22	C	506	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	c	514	BCR	C33-C5-C6	-2.20	122.09	124.48
22	b	605	CLA	C16-C15-C13	-2.20	108.67	115.97
22	D	403	CLA	C4-C3-C5	2.19	119.04	115.23
24	K	101	BCR	C31-C1-C6	2.19	113.69	110.24
29	c	517	DGD	O2G-C1B-C2B	-2.19	106.74	111.48
29	h	102	DGD	O6E-C1E-O5D	-2.19	104.86	110.04
27	c	520	LMG	O6-C1-O1	-2.19	104.86	110.04
22	C	507	CLA	C1-C2-C3	-2.19	122.61	126.20
29	A	414	DGD	C8B-C7B-C6B	-2.19	103.29	114.37
22	A	410	CLA	CMB-C2B-C1B	-2.19	122.08	125.42
22	C	501	CLA	C3B-C4B-NB	-2.19	108.57	110.53
29	C	517	DGD	O6D-C1D-O3G	-2.19	104.87	110.04
27	C	519	LMG	O7-C10-O9	-2.19	118.58	123.70
22	c	503	CLA	C11-C12-C13	-2.19	108.69	115.97
22	b	609	CLA	CHA-C1A-NA	-2.19	121.43	126.39
27	c	520	LMG	C40-C39-C38	-2.19	103.30	114.37
33	e	101	LHG	O8-C23-O10	-2.19	118.16	123.63
22	b	614	CLA	C4-C3-C5	2.19	119.03	115.23
28	L	101	SQD	O47-C7-C8	2.19	116.21	111.48
24	b	617	BCR	C36-C18-C17	-2.18	119.28	122.82
22	A	405	CLA	C1C-C2C-C3C	-2.18	104.68	106.98
22	B	601	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
22	C	512	CLA	C3B-C4B-NB	-2.18	108.58	110.53
22	A	403	CLA	C1-C2-C3	-2.18	122.63	126.20
22	D	404	CLA	CHB-C1B-C2B	-2.18	121.11	127.43
28	L	101	SQD	C45-O47-C7	2.18	123.01	117.80
35	f	101	HEM	CAB-C3B-C2B	-2.18	121.36	128.43
29	C	518	DGD	C7B-C6B-C5B	-2.18	103.37	114.37
22	c	506	CLA	CMB-C2B-C3B	2.18	131.67	126.55
24	c	514	BCR	C36-C18-C17	-2.17	119.30	122.82
22	C	502	CLA	CHB-C1B-NB	2.17	127.31	124.05
22	b	605	CLA	C2D-C1D-ND	-2.17	107.98	110.13
23	d	401	PHO	O2A-CGA-O1A	-2.17	118.20	123.63
22	b	610	CLA	C11-C12-C13	-2.17	108.75	115.97
22	A	403	CLA	CHB-C1B-C2B	-2.17	121.13	127.43
22	c	506	CLA	C4-C3-C2	-2.17	118.06	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	509	CLA	CHD-C4C-NC	2.17	127.59	124.23
22	B	611	CLA	C7-C6-C5	-2.17	107.49	113.26
22	B	609	CLA	CAA-CBA-CGA	-2.16	107.06	113.21
22	c	513	CLA	C1-C2-C3	-2.16	122.65	126.20
22	c	503	CLA	CHB-C4A-NA	2.16	127.52	124.40
22	b	602	CLA	CHC-C1C-NC	2.16	127.57	124.31
22	B	616	CLA	C3B-C4B-NB	-2.16	108.60	110.53
22	a	403	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
22	b	616	CLA	O1D-CGD-CBD	2.16	128.78	124.52
22	B	607	CLA	CHA-C1A-NA	-2.16	121.50	126.39
22	b	601	CLA	CHD-C1D-ND	-2.16	121.77	124.80
24	h	101	BCR	C7-C8-C9	-2.16	123.04	126.23
29	c	517	DGD	C4A-C3A-C2A	-2.16	105.20	113.13
22	c	512	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	c	503	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
24	D	405	BCR	C3-C4-C5	-2.16	110.21	114.06
32	B	624	STE	C4-C3-C2	-2.15	105.21	113.13
29	A	414	DGD	C6E-C5E-C4E	2.15	118.31	113.02
24	H	101	BCR	C16-C17-C18	-2.15	124.26	127.28
22	b	615	CLA	O2D-CGD-CBD	2.15	115.00	111.23
29	C	516	DGD	CDB-CCB-CBB	-2.15	103.48	114.37
22	C	510	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	B	606	CLA	CHB-C1B-NB	2.15	127.28	124.05
27	A	411	LMG	O6-C1-O1	-2.15	104.96	110.04
24	t	101	BCR	C7-C8-C9	-2.15	123.06	126.23
24	b	619	BCR	C11-C10-C9	-2.15	124.27	127.28
22	B	604	CLA	C2A-C3A-C4A	2.15	105.34	101.87
24	B	618	BCR	C7-C8-C9	-2.15	123.06	126.23
24	b	617	BCR	C11-C10-C9	-2.15	124.27	127.28
32	c	524	STE	O2-C1-C2	2.14	120.78	114.00
22	a	402	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
22	C	502	CLA	CHA-C1A-NA	-2.14	121.54	126.39
29	h	102	DGD	C1D-C2D-C3D	-2.14	105.50	110.01
22	c	509	CLA	CMB-C2B-C3B	2.14	131.59	126.55
22	C	509	CLA	CHD-C1D-ND	-2.14	121.79	124.80
22	b	607	CLA	O1A-CGA-CBA	2.14	132.16	123.78
22	b	610	CLA	CBC-CAC-C3C	2.14	118.22	112.42
22	b	610	CLA	CHD-C1D-ND	-2.14	121.79	124.80
22	d	404	CLA	C2B-C1B-NB	-2.14	108.11	110.33
22	B	606	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
22	B	603	CLA	C2D-C1D-ND	-2.14	108.01	110.13
29	c	518	DGD	O5D-C1E-C2E	2.14	111.52	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	t	102	STE	O2-C1-C2	2.14	120.75	114.00
22	b	606	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
29	C	518	DGD	O3E-C3E-C2E	-2.13	105.34	110.38
24	B	618	BCR	C37-C22-C21	-2.13	119.36	122.82
22	c	505	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
22	B	608	CLA	C1C-C2C-C3C	-2.13	104.74	106.98
22	A	403	CLA	C1-O2A-CGA	2.13	121.80	116.65
22	C	509	CLA	C1-O2A-CGA	2.13	121.80	116.65
33	d	408	LHG	O8-C6-C5	-2.13	102.27	108.40
24	B	617	BCR	C15-C16-C17	-2.12	119.17	123.52
22	b	610	CLA	CHC-C1C-C2C	-2.12	120.92	126.95
33	B	622	LHG	C11-C10-C9	-2.12	103.64	114.37
29	c	519	DGD	O5D-C6D-C5D	-2.12	104.64	109.42
29	C	517	DGD	O6E-C1E-O5D	-2.12	105.03	110.04
29	c	519	DGD	O1G-C1A-O1A	-2.12	118.32	123.63
22	B	615	CLA	C6-C7-C8	-2.12	108.92	115.97
22	c	511	CLA	O1A-CGA-CBA	2.12	132.07	123.78
22	b	605	CLA	CHD-C1D-ND	-2.12	121.82	124.80
24	C	514	BCR	C27-C26-C25	2.12	125.56	122.70
27	c	520	LMG	C6-C5-C4	-2.11	107.83	113.02
27	b	620	LMG	C22-C21-C20	-2.11	103.69	114.37
24	h	101	BCR	C36-C18-C17	-2.11	119.39	122.82
32	a	414	STE	C3-C2-C1	-2.11	109.00	114.51
26	d	407	PL9	O1-C4-C3	-2.11	118.50	120.73
22	C	503	CLA	C1-C2-C3	2.11	129.66	126.20
22	c	501	CLA	O1D-CGD-CBD	2.11	128.68	124.52
22	c	502	CLA	CHD-C1D-C2D	2.11	129.88	125.49
27	D	407	LMG	O1-C7-C8	-2.11	105.68	110.82
24	H	101	BCR	C38-C26-C25	-2.11	122.18	124.48
26	a	409	PL9	C32-C33-C34	-2.11	122.79	127.62
22	b	616	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
36	V	201	HEC	CMC-C2C-C3C	2.11	130.10	125.62
22	d	405	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
22	C	505	CLA	C6-C7-C8	-2.11	108.96	115.97
29	c	517	DGD	CDB-CCB-CBB	-2.11	103.71	114.37
27	d	412	LMG	O3-C3-C2	-2.11	105.41	110.38
24	K	101	BCR	C27-C26-C25	2.11	125.55	122.70
22	a	404	CLA	CHA-C1A-NA	-2.11	121.62	126.39
23	d	402	PHO	C4B-NB-C1B	2.11	111.89	108.82
22	D	403	CLA	C2B-C1B-NB	-2.10	108.14	110.33
27	c	520	LMG	O2-C2-C1	-2.10	105.06	110.08
22	A	410	CLA	CED-O2D-CGD	-2.10	111.14	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	BCR	C24-C23-C22	-2.10	123.12	126.23
22	c	501	CLA	C1-C2-C3	-2.10	122.75	126.20
22	C	503	CLA	C3A-C2A-C1A	2.10	104.49	101.34
22	d	405	CLA	CHA-C1A-NA	-2.10	121.64	126.39
24	h	101	BCR	C37-C22-C21	-2.10	119.42	122.82
22	A	403	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
24	B	618	BCR	C29-C30-C25	2.10	113.48	110.44
22	b	615	CLA	CHC-C1C-C2C	-2.09	121.00	126.95
22	C	505	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
24	C	515	BCR	C3-C4-C5	-2.09	110.32	114.06
27	B	621	LMG	O7-C10-O9	-2.09	117.95	123.33
22	B	606	CLA	CHB-C4A-NA	2.09	127.42	124.40
27	D	410	LMG	O8-C28-O10	-2.09	118.39	123.63
22	B	603	CLA	CHD-C4C-C3C	-2.09	121.72	124.77
22	C	507	CLA	C2A-C1A-CHA	2.09	127.50	123.87
22	a	403	CLA	CHA-C1A-NA	-2.09	121.66	126.39
22	B	605	CLA	CHC-C4B-NB	2.09	127.19	124.05
22	C	509	CLA	C11-C12-C13	-2.09	109.02	115.97
22	b	605	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
22	c	512	CLA	O1D-CGD-CBD	2.09	128.64	124.52
33	d	408	LHG	C18-C17-C16	-2.09	103.81	114.37
28	B	623	SQD	C25-C24-C23	-2.09	106.04	113.69
36	V	201	HEC	CAC-C3C-C4C	-2.09	122.04	124.91
27	D	410	LMG	C38-C37-C36	-2.09	103.81	114.37
29	c	517	DGD	O6D-C1D-O3G	-2.09	105.11	110.04
35	E	101	HEM	CHB-C1B-NB	2.09	126.95	124.37
24	C	514	BCR	C7-C8-C9	-2.08	123.15	126.23
23	D	401	PHO	C3D-C4D-ND	2.08	110.38	107.71
33	d	408	LHG	C20-C19-C18	-2.08	103.84	114.37
24	T	101	BCR	C37-C22-C21	-2.08	119.44	122.82
33	D	409	LHG	O8-C23-O10	-2.08	118.42	123.63
22	c	501	CLA	CHD-C1D-ND	-2.08	121.88	124.80
22	b	604	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	b	607	CLA	C1-O2A-CGA	2.08	121.68	116.65
27	D	407	LMG	O2-C2-C1	-2.08	105.13	110.08
22	b	603	CLA	C11-C12-C13	-2.08	109.06	115.97
22	C	503	CLA	CHA-C1A-NA	-2.07	121.69	126.39
24	Y	101	BCR	C16-C15-C14	-2.07	119.28	123.52
22	A	405	CLA	C4-C3-C5	2.07	118.82	115.23
22	d	405	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
28	A	412	SQD	C3-C4-C5	2.07	113.98	110.23
22	B	608	CLA	CHA-C1A-NA	-2.07	121.71	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	601	CLA	O2D-CGD-CBD	2.07	114.84	111.23
29	a	412	DGD	CBB-CAB-C9B	-2.07	103.92	114.37
22	C	506	CLA	O2D-CGD-O1D	-2.06	119.83	123.85
28	f	102	SQD	O47-C7-C8	2.06	118.51	110.93
26	A	409	PL9	O2-C1-C2	-2.06	117.14	121.83
22	a	402	CLA	CHA-C4D-ND	2.06	136.80	132.55
22	c	509	CLA	C1-O2A-CGA	-2.06	111.66	116.65
22	c	511	CLA	C11-C12-C13	-2.06	109.12	115.97
22	a	404	CLA	CAC-C3C-C4C	2.06	127.47	124.79
22	C	504	CLA	CHB-C1B-NB	2.06	127.14	124.05
24	d	406	BCR	C30-C25-C26	-2.06	119.82	122.64
24	b	618	BCR	C15-C16-C17	-2.06	119.31	123.52
22	B	611	CLA	C4-C3-C2	-2.06	118.34	123.63
27	C	519	LMG	C40-C39-C38	-2.06	103.97	114.37
26	d	407	PL9	C41-C39-C38	-2.06	116.55	121.17
27	A	411	LMG	C9-C8-C7	-2.06	106.99	111.78
22	b	605	CLA	O1A-CGA-CBA	2.05	131.82	123.78
27	c	522	LMG	C3-C4-C5	-2.05	106.51	110.23
24	b	618	BCR	C30-C25-C26	-2.05	119.83	122.64
22	A	403	CLA	CHA-C1A-NA	-2.05	121.74	126.39
36	V	201	HEC	CMD-C2D-C1D	2.05	128.24	125.03
22	b	604	CLA	CHC-C1C-NC	2.05	127.40	124.31
27	c	520	LMG	O8-C28-O10	-2.05	118.50	123.63
22	b	607	CLA	CHA-C1A-NA	-2.05	121.75	126.39
24	A	406	BCR	C7-C8-C9	-2.05	123.20	126.23
22	D	404	CLA	O1D-CGD-CBD	2.05	128.56	124.52
29	C	516	DGD	O5D-C6D-C5D	-2.05	104.80	109.42
22	B	601	CLA	CHA-C4D-ND	2.05	136.78	132.55
27	M	101	LMG	C22-C21-C20	-2.05	104.01	114.37
22	C	510	CLA	CHD-C1D-ND	-2.05	121.92	124.80
27	b	622	LMG	C40-C39-C38	-2.05	104.03	114.37
35	E	101	HEM	CHD-C1D-ND	2.04	126.62	124.42
22	c	508	CLA	CHD-C4C-NC	2.04	127.40	124.23
22	c	503	CLA	CHD-C1D-ND	-2.04	121.93	124.80
36	V	201	HEC	CAC-C3C-C2C	2.04	130.12	126.89
22	c	501	CLA	C3D-C4D-ND	2.04	113.31	109.99
24	B	618	BCR	C24-C23-C22	-2.04	123.21	126.23
24	c	516	BCR	C21-C20-C19	-2.04	117.28	123.20
24	b	617	BCR	C34-C9-C8	-2.04	114.97	118.09
24	c	516	BCR	C16-C15-C14	-2.04	119.35	123.52
22	C	513	CLA	C6-C5-C3	2.04	118.43	113.47
22	C	505	CLA	CMB-C2B-C3B	2.04	131.34	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	615	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	c	519	DGD	O3G-C1D-C2D	-2.04	105.18	108.27
26	D	406	PL9	C50-C49-C48	-2.04	116.54	122.66
22	C	510	CLA	C7-C6-C5	-2.04	107.83	113.26
36	V	201	HEC	C1D-C2D-C3D	-2.04	104.84	106.98
22	B	610	CLA	O1D-CGD-CBD	2.03	128.53	124.52
22	c	508	CLA	C7-C6-C5	-2.03	107.84	113.26
27	A	411	LMG	C1-O6-C5	-2.03	109.75	113.72
22	c	501	CLA	CHC-C1C-NC	2.03	127.37	124.31
22	B	616	CLA	C2C-C1C-NC	2.03	112.12	109.98
33	D	408	LHG	C11-C10-C9	-2.03	104.10	114.37
22	A	403	CLA	O1D-CGD-CBD	2.03	128.53	124.52
27	d	412	LMG	C7-O1-C1	-2.03	109.44	113.80
24	c	515	BCR	C1-C6-C5	-2.03	119.86	122.64
26	D	406	PL9	C27-C28-C29	-2.03	122.98	127.62
27	b	620	LMG	C33-C32-C31	-2.03	104.11	114.37
22	C	506	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	D	407	LMG	O2-C2-C3	-2.03	105.60	110.38
22	c	505	CLA	C4D-C3D-CAD	-2.03	105.90	108.11
22	B	606	CLA	CHD-C4C-C3C	-2.03	121.82	124.77
22	b	604	CLA	C6-C7-C8	-2.03	109.23	115.97
24	a	405	BCR	C21-C20-C19	-2.02	117.33	123.20
24	D	405	BCR	C30-C25-C26	-2.02	119.87	122.64
28	F	101	SQD	O8-S-O9	-2.02	106.33	111.40
29	c	518	DGD	CCB-CBB-CAB	-2.02	104.14	114.37
22	B	608	CLA	O1D-CGD-CBD	2.02	128.51	124.52
24	h	101	BCR	C15-C14-C13	-2.02	124.44	127.28
22	C	506	CLA	CMB-C2B-C3B	2.02	131.31	126.55
29	C	516	DGD	CAB-C9B-C8B	-2.02	104.15	114.37
27	d	412	LMG	C1-C2-C3	-2.02	105.76	110.01
26	A	409	PL9	C41-C39-C38	-2.02	116.63	121.17
29	C	518	DGD	O6D-C1D-O3G	-2.02	105.27	110.04
22	b	605	CLA	C4-C3-C2	-2.02	118.44	123.63
26	A	409	PL9	C42-C43-C44	-2.02	123.00	127.62
22	c	508	CLA	C2D-C1D-ND	-2.02	108.13	110.13
22	B	616	CLA	CMB-C2B-C1B	-2.02	122.35	125.42
27	c	523	LMG	C12-C11-C10	-2.01	106.31	113.69
22	C	504	CLA	C11-C10-C8	-2.01	109.27	115.97
22	B	611	CLA	CHD-C1D-ND	-2.01	121.97	124.80
29	h	102	DGD	C3E-C4E-C5E	-2.01	106.58	110.23
22	b	614	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
32	B	620	STE	O2-C1-C2	2.01	120.35	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	515	BCR	C2-C1-C6	2.01	113.36	110.44
22	c	506	CLA	C3B-C4B-NB	-2.01	108.73	110.53
24	K	101	BCR	C15-C14-C13	-2.01	124.46	127.28
26	A	409	PL9	C27-C28-C29	-2.01	123.02	127.62
22	d	404	CLA	CGD-CBD-CAD	-2.01	104.34	110.85
26	D	406	PL9	O2-C1-C2	-2.01	117.26	121.83
24	k	101	BCR	C30-C25-C26	-2.01	119.89	122.64
27	c	523	LMG	O2-C2-C1	-2.01	105.30	110.08
24	c	514	BCR	C38-C26-C25	-2.01	122.30	124.48
27	A	411	LMG	C38-C37-C36	-2.00	104.24	114.37
24	A	406	BCR	C8-C7-C6	-2.00	121.65	127.00
22	B	601	CLA	C3B-C4B-NB	-2.00	108.74	110.53
23	A	404	PHO	OBD-CAD-CBD	-2.00	122.89	125.82
24	H	101	BCR	C1-C6-C5	-2.00	119.90	122.64
22	B	607	CLA	CHB-C1B-C2B	-2.00	121.62	127.43
24	K	101	BCR	C36-C18-C17	-2.00	119.57	122.82
22	b	601	CLA	O1D-CGD-CBD	2.00	128.46	124.52

All (2) chirality outliers are listed below:

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

All (1850) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C2B-C3B-CAB-CBB
22	A	403	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	605	CLA	C4B-C3B-CAB-CBB
22	B	607	CLA	C14-C13-C15-C16
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	B	615	CLA	C2B-C3B-CAB-CBB
22	B	615	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	508	CLA	C12-C13-C15-C16
22	C	509	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C6-C7-C8-C9
22	b	601	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	614	CLA	C2-C3-C5-C6
22	b	616	CLA	CHA-CBD-CGD-O1D
22	b	616	CLA	CHA-CBD-CGD-O2D
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	509	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C12-C13-C14
24	A	406	BCR	C17-C18-C19-C20
24	B	618	BCR	C20-C21-C22-C37
24	C	514	BCR	C20-C21-C22-C37
24	C	515	BCR	C17-C18-C19-C20
24	D	405	BCR	C22-C23-C24-C25
24	D	405	BCR	C23-C24-C25-C26
24	D	405	BCR	C23-C24-C25-C30
24	K	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C36-C18-C19-C20
24	T	101	BCR	C20-C21-C22-C37
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	Y	101	BCR	C21-C22-C23-C24
24	b	617	BCR	C20-C21-C22-C37
24	c	514	BCR	C35-C13-C14-C15
24	c	514	BCR	C16-C17-C18-C36
24	d	406	BCR	C21-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C10
24	k	101	BCR	C7-C8-C9-C34
24	k	101	BCR	C17-C18-C19-C20
24	t	101	BCR	C11-C10-C9-C34
24	t	101	BCR	C36-C18-C19-C20
24	t	101	BCR	C20-C21-C22-C37
26	A	409	PL9	C12-C13-C14-C15
26	A	409	PL9	C12-C13-C14-C16
26	A	409	PL9	C22-C23-C24-C25
26	A	409	PL9	C22-C23-C24-C26
26	A	409	PL9	C37-C38-C39-C40
26	D	406	PL9	C32-C33-C34-C36

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Mol	Chain	Res	Type	Atoms
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C32-C33-C34-C36
26	a	409	PL9	C42-C43-C44-C46
26	d	407	PL9	C42-C43-C44-C45
27	A	411	LMG	O6-C1-O1-C7
27	A	411	LMG	O1-C7-C8-O7
27	A	411	LMG	O9-C10-O7-C8
27	c	522	LMG	O7-C8-C9-O8
27	c	522	LMG	O9-C10-O7-C8
27	c	523	LMG	O6-C1-O1-C7
28	B	623	SQD	O5-C1-O6-C44
28	B	623	SQD	O49-C7-O47-C45
28	L	101	SQD	C8-C7-O47-C45
28	L	101	SQD	O10-C23-O48-C46
28	L	101	SQD	C24-C23-O48-C46
28	a	411	SQD	C8-C7-O47-C45
28	f	102	SQD	C2-C1-O6-C44
28	f	102	SQD	O5-C1-O6-C44
29	A	414	DGD	O1B-C1B-O2G-C2G
29	C	517	DGD	C2E-C1E-O5D-C6D
33	B	622	LHG	O1-C1-C2-C3
33	B	622	LHG	C3-O3-P-O5
33	B	622	LHG	C3-O3-P-O6
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	C3-O3-P-O5
33	D	408	LHG	C3-O3-P-O6
33	D	408	LHG	C4-O6-P-O4
33	D	409	LHG	C4-O6-P-O4
33	E	102	LHG	C3-O3-P-O5
33	L	102	LHG	C3-O3-P-O4
33	L	102	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C3-O3-P-O6
33	d	408	LHG	C4-O6-P-O5
33	d	409	LHG	O1-C1-C2-C3
33	d	409	LHG	C3-O3-P-O4
33	d	409	LHG	C3-O3-P-O6
33	d	409	LHG	C4-O6-P-O4
33	e	101	LHG	O1-C1-C2-O2
33	e	101	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
33	e	101	LHG	C3-O3-P-O4
33	e	101	LHG	C3-O3-P-O6
33	e	101	LHG	O10-C23-O8-C6
33	l	101	LHG	C3-O3-P-O4
33	l	101	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O4
36	V	201	HEC	C2C-C3C-CAC-CBC
22	b	614	CLA	O1D-CGD-O2D-CED
22	D	404	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
23	d	402	PHO	CBD-CGD-O2D-CED
22	B	601	CLA	O1A-CGA-O2A-C1
28	f	102	SQD	O10-C23-O48-C46
33	E	102	LHG	O10-C23-O8-C6
36	V	201	HEC	C4C-C3C-CAC-CBC
26	d	407	PL9	C47-C48-C49-C50
22	B	601	CLA	CBA-CGA-O2A-C1
33	e	101	LHG	C24-C23-O8-C6
27	M	101	LMG	O10-C28-O8-C9
28	F	101	SQD	O10-C23-O48-C46
28	a	411	SQD	O10-C23-O48-C46
27	b	622	LMG	O9-C10-O7-C8
28	f	102	SQD	O49-C7-O47-C45
26	d	407	PL9	C47-C48-C49-C51
22	b	614	CLA	C3-C5-C6-C7
28	a	411	SQD	C24-C23-O48-C46
22	c	511	CLA	CBD-CGD-O2D-CED
22	c	512	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
27	A	411	LMG	C11-C10-O7-C8
27	C	519	LMG	C11-C10-O7-C8
27	D	410	LMG	C11-C10-O7-C8
28	B	623	SQD	C8-C7-O47-C45
29	A	414	DGD	C2B-C1B-O2G-C2G
22	A	405	CLA	C4-C3-C5-C6
22	B	603	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
26	A	409	PL9	C20-C19-C21-C22
26	a	409	PL9	C20-C19-C21-C22
26	d	407	PL9	C40-C39-C41-C42
22	C	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C43-C44-C46-C47
22	c	509	CLA	CBD-CGD-O2D-CED
22	D	404	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
22	b	606	CLA	C3-C5-C6-C7
22	c	510	CLA	C3-C5-C6-C7
27	c	523	LMG	C29-C28-O8-C9
28	B	623	SQD	C24-C23-O48-C46
28	f	102	SQD	C24-C23-O48-C46
33	E	102	LHG	C24-C23-O8-C6
26	A	409	PL9	C32-C33-C34-C36
26	A	409	PL9	C37-C38-C39-C41
27	A	411	LMG	O6-C5-C6-O5
26	D	406	PL9	C47-C48-C49-C51
22	B	605	CLA	C3-C5-C6-C7
22	b	601	CLA	CBD-CGD-O2D-CED
33	D	408	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
22	a	404	CLA	CBA-CGA-O2A-C1
28	F	101	SQD	C24-C23-O48-C46
29	c	519	DGD	O1A-C1A-O1G-C1G
23	d	402	PHO	O1D-CGD-O2D-CED
28	f	102	SQD	C8-C7-O47-C45
22	c	510	CLA	CBD-CGD-O2D-CED
27	A	411	LMG	C4-C5-C6-O5
26	a	409	PL9	C35-C34-C36-C37
22	A	405	CLA	C2-C3-C5-C6
26	A	409	PL9	C18-C19-C21-C22
26	A	409	PL9	C38-C39-C41-C42
26	a	409	PL9	C33-C34-C36-C37
26	d	407	PL9	C38-C39-C41-C42
27	c	523	LMG	O10-C28-O8-C9
27	D	410	LMG	O9-C10-O7-C8
26	A	409	PL9	C19-C21-C22-C23
26	A	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C44-C46-C47-C48
26	d	407	PL9	C44-C46-C47-C48
28	B	623	SQD	O10-C23-O48-C46
29	C	517	DGD	O6E-C1E-O5D-C6D
22	D	403	CLA	CBD-CGD-O2D-CED
33	l	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	A	409	PL9	C32-C33-C34-C35
26	D	406	PL9	C37-C38-C39-C40
22	a	404	CLA	O1A-CGA-O2A-C1
26	d	407	PL9	C42-C43-C44-C46
22	B	603	CLA	CBD-CGD-O2D-CED
22	B	610	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
27	b	622	LMG	C11-C10-O7-C8
33	d	408	LHG	C1-C2-C3-O3
22	C	513	CLA	CBA-CGA-O2A-C1
27	C	519	LMG	C29-C28-O8-C9
27	M	101	LMG	C29-C28-O8-C9
32	b	625	STE	C3-C4-C5-C6
27	c	522	LMG	C4-C5-C6-O5
22	C	513	CLA	C4-C3-C5-C6
26	A	409	PL9	C45-C44-C46-C47
22	B	603	CLA	C2-C3-C5-C6
22	C	513	CLA	C2-C3-C5-C6
26	a	409	PL9	C38-C39-C41-C42
22	B	604	CLA	C3-C5-C6-C7
22	B	606	CLA	C11-C10-C8-C9
22	B	611	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	B	616	CLA	C11-C10-C8-C9
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	601	CLA	C14-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	502	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C9
29	H	102	DGD	C4E-C5E-C6E-O5E
33	d	408	LHG	O2-C2-C3-O3
28	F	101	SQD	C44-C45-C46-O48
32	B	624	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	C	515	BCR	C36-C18-C19-C20
24	C	515	BCR	C37-C22-C23-C24
24	D	405	BCR	C37-C22-C23-C24
24	H	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C37-C22-C23-C24
24	a	405	BCR	C36-C18-C19-C20
24	b	617	BCR	C7-C8-C9-C34
24	b	618	BCR	C36-C18-C19-C20
24	b	619	BCR	C11-C12-C13-C35
24	b	619	BCR	C37-C22-C23-C24
24	d	406	BCR	C7-C8-C9-C34
24	d	406	BCR	C37-C22-C23-C24
24	t	101	BCR	C7-C8-C9-C34
29	c	518	DGD	C1A-C2A-C3A-C4A
32	D	411	STE	C1-C2-C3-C4
28	L	101	SQD	O49-C7-O47-C45
28	a	411	SQD	O49-C7-O47-C45
27	c	522	LMG	O6-C5-C6-O5
29	H	102	DGD	O6E-C5E-C6E-O5E
28	a	410	SQD	O6-C44-C45-O47
22	C	509	CLA	C5-C6-C7-C8
22	b	603	CLA	C5-C6-C7-C8
22	b	615	CLA	C5-C6-C7-C8
22	c	506	CLA	C2-C1-O2A-CGA
22	c	512	CLA	O1D-CGD-O2D-CED
26	a	409	PL9	C47-C48-C49-C51
28	A	413	SQD	C7-C8-C9-C10
33	e	101	LHG	C23-C24-C25-C26
22	c	511	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C7
22	b	615	CLA	C11-C12-C13-C15
28	a	410	SQD	C11-C12-C13-C14
22	B	603	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
22	c	505	CLA	C5-C6-C7-C8
27	c	520	LMG	C4-C5-C6-O5
28	L	101	SQD	C23-C24-C25-C26
32	d	413	STE	C1-C2-C3-C4
26	A	409	PL9	C34-C36-C37-C38
27	c	523	LMG	C4-C5-C6-O5
22	C	509	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	C10-C11-C12-C13
22	C	505	CLA	C2C-C3C-CAC-CBC
27	d	412	LMG	C28-C29-C30-C31
33	d	408	LHG	C7-C8-C9-C10
22	C	509	CLA	CBD-CGD-O2D-CED
22	A	410	CLA	C13-C15-C16-C17
22	B	603	CLA	C15-C16-C17-C18
22	C	509	CLA	C8-C10-C11-C12
22	C	510	CLA	C13-C15-C16-C17
22	C	513	CLA	C8-C10-C11-C12
22	b	602	CLA	C13-C15-C16-C17
22	B	606	CLA	C2A-CAA-CBA-CGA
24	C	514	BCR	C18-C19-C20-C21
24	t	101	BCR	C10-C11-C12-C13
22	A	410	CLA	C15-C16-C17-C18
22	C	513	CLA	C5-C6-C7-C8
22	a	404	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
26	D	406	PL9	C47-C48-C49-C50
26	a	409	PL9	C47-C48-C49-C50
29	A	414	DGD	O6E-C5E-C6E-O5E
28	a	410	SQD	C23-C24-C25-C26
29	C	516	DGD	C1B-C2B-C3B-C4B
29	H	102	DGD	C1A-C2A-C3A-C4A
29	a	412	DGD	C1A-C2A-C3A-C4A
32	B	620	STE	C1-C2-C3-C4
22	c	513	CLA	O1D-CGD-O2D-CED
22	C	513	CLA	O1A-CGA-O2A-C1
27	b	622	LMG	O10-C28-O8-C9
29	C	518	DGD	O1A-C1A-O1G-C1G
29	a	412	DGD	O1A-C1A-O1G-C1G
29	A	414	DGD	C4E-C5E-C6E-O5E
22	B	601	CLA	C5-C6-C7-C8
22	B	607	CLA	C5-C6-C7-C8
22	B	614	CLA	C13-C15-C16-C17
22	C	503	CLA	C5-C6-C7-C8
22	C	506	CLA	C8-C10-C11-C12
22	b	603	CLA	C13-C15-C16-C17
22	b	611	CLA	C8-C10-C11-C12
22	c	503	CLA	C5-C6-C7-C8
22	c	503	CLA	C8-C10-C11-C12
22	c	506	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	509	CLA	C10-C11-C12-C13
33	B	622	LHG	C28-C29-C30-C31
33	B	622	LHG	O2-C2-C3-O3
23	d	401	PHO	CBD-CGD-O2D-CED
33	d	408	LHG	C23-C24-C25-C26
22	b	605	CLA	C10-C11-C12-C13
22	b	615	CLA	C10-C11-C12-C13
22	b	616	CLA	C5-C6-C7-C8
22	b	602	CLA	C3-C5-C6-C7
22	c	509	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	C10-C11-C12-C13
22	b	601	CLA	O1D-CGD-O2D-CED
22	b	608	CLA	C5-C6-C7-C8
22	c	510	CLA	C15-C16-C17-C18
22	c	506	CLA	CBA-CGA-O2A-C1
27	c	522	LMG	C29-C28-O8-C9
22	c	506	CLA	O1A-CGA-O2A-C1
32	T	102	STE	C5-C6-C7-C8
22	B	601	CLA	C15-C16-C17-C18
33	B	622	LHG	C1-C2-C3-O3
33	E	102	LHG	C1-C2-C3-O3
33	e	101	LHG	C1-C2-C3-O3
22	B	604	CLA	C13-C15-C16-C17
22	B	607	CLA	C10-C11-C12-C13
22	B	607	CLA	C13-C15-C16-C17
22	B	611	CLA	C8-C10-C11-C12
22	B	613	CLA	C8-C10-C11-C12
22	B	615	CLA	C5-C6-C7-C8
22	C	513	CLA	C13-C15-C16-C17
22	C	513	CLA	C15-C16-C17-C18
22	D	404	CLA	C10-C11-C12-C13
22	b	607	CLA	C8-C10-C11-C12
22	b	613	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
22	B	605	CLA	C13-C15-C16-C17
22	b	601	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
22	c	512	CLA	C13-C15-C16-C17
36	v	201	HEC	C4C-C3C-CAC-CBC
22	c	506	CLA	C13-C15-C16-C17
29	c	519	DGD	C1A-C2A-C3A-C4A
22	b	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C3-C5-C6-C7
22	b	614	CLA	C6-C7-C8-C9
27	C	519	LMG	C2-C1-O1-C7
28	B	623	SQD	C2-C1-O6-C44
28	F	101	SQD	C2-C1-O6-C44
29	c	518	DGD	C2E-C1E-O5D-C6D
22	d	405	CLA	C5-C6-C7-C8
27	b	620	LMG	C29-C28-O8-C9
29	c	519	DGD	C2A-C1A-O1G-C1G
24	C	515	BCR	C20-C21-C22-C37
24	K	101	BCR	C16-C17-C18-C36
24	T	101	BCR	C11-C10-C9-C34
24	T	101	BCR	C35-C13-C14-C15
24	Y	101	BCR	C16-C17-C18-C36
24	a	405	BCR	C35-C13-C14-C15
24	b	618	BCR	C20-C21-C22-C37
24	b	619	BCR	C35-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C37
24	c	515	BCR	C16-C17-C18-C36
24	h	101	BCR	C35-C13-C14-C15
24	h	101	BCR	C20-C21-C22-C37
24	k	101	BCR	C35-C13-C14-C15
24	k	101	BCR	C16-C17-C18-C36
24	t	101	BCR	C35-C13-C14-C15
22	b	607	CLA	C10-C11-C12-C13
22	c	510	CLA	C8-C10-C11-C12
24	C	514	BCR	C36-C18-C19-C20
27	c	520	LMG	O6-C5-C6-O5
33	D	408	LHG	O1-C1-C2-C3
33	d	410	LHG	O1-C1-C2-C3
28	L	101	SQD	C46-C45-O47-C7
33	d	410	LHG	C24-C25-C26-C27
22	a	403	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C19
22	b	607	CLA	C16-C17-C18-C20
22	B	601	CLA	C10-C11-C12-C13
24	C	514	BCR	C16-C17-C18-C19
24	C	514	BCR	C20-C21-C22-C23
24	C	515	BCR	C12-C13-C14-C15
24	K	101	BCR	C16-C17-C18-C19
24	b	617	BCR	C12-C13-C14-C15
24	b	618	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	b	618	BCR	C20-C21-C22-C23
24	c	514	BCR	C12-C13-C14-C15
24	c	514	BCR	C16-C17-C18-C19
24	d	406	BCR	C20-C21-C22-C23
24	h	101	BCR	C11-C10-C9-C8
24	h	101	BCR	C16-C17-C18-C19
24	h	101	BCR	C20-C21-C22-C23
27	C	519	LMG	O6-C1-O1-C7
27	M	101	LMG	O6-C1-O1-C7
28	F	101	SQD	O5-C1-O6-C44
28	L	101	SQD	O5-C1-O6-C44
29	c	518	DGD	O6E-C1E-O5D-C6D
27	b	622	LMG	C28-C29-C30-C31
22	C	512	CLA	C13-C15-C16-C17
26	a	409	PL9	C18-C19-C21-C22
26	d	407	PL9	C33-C34-C36-C37
22	D	403	CLA	O1D-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	512	CLA	CBA-CGA-O2A-C1
29	a	412	DGD	C2A-C1A-O1G-C1G
22	c	509	CLA	C8-C10-C11-C12
27	M	101	LMG	C28-C29-C30-C31
22	B	602	CLA	C16-C17-C18-C19
22	B	602	CLA	C16-C17-C18-C20
22	B	604	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C20
24	K	101	BCR	C14-C15-C16-C17
24	k	101	BCR	C14-C15-C16-C17
27	B	621	LMG	C33-C34-C35-C36
27	D	410	LMG	C14-C15-C16-C17
27	M	101	LMG	C38-C39-C40-C41
27	b	620	LMG	C39-C40-C41-C42
27	c	522	LMG	C30-C31-C32-C33
28	A	413	SQD	C12-C13-C14-C15
28	a	411	SQD	C18-C19-C20-C21
32	B	626	STE	C5-C6-C7-C8
32	l	102	STE	C3-C4-C5-C6
33	D	409	LHG	C34-C35-C36-C37
33	d	408	LHG	C32-C33-C34-C35
33	d	409	LHG	C12-C13-C14-C15
33	d	409	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	e	101	LHG	C27-C28-C29-C30
33	l	101	LHG	C28-C29-C30-C31
22	B	616	CLA	C5-C6-C7-C8
22	D	404	CLA	C13-C15-C16-C17
22	b	601	CLA	C13-C15-C16-C17
27	c	523	LMG	C12-C13-C14-C15
29	C	516	DGD	C5B-C6B-C7B-C8B
32	x	101	STE	C2-C3-C4-C5
29	A	414	DGD	C2A-C1A-O1G-C1G
27	B	621	LMG	C32-C33-C34-C35
27	b	622	LMG	C16-C17-C18-C19
27	b	622	LMG	C23-C24-C25-C26
28	A	412	SQD	C16-C17-C18-C19
28	a	411	SQD	C10-C11-C12-C13
29	C	518	DGD	C2B-C3B-C4B-C5B
29	a	412	DGD	C3A-C4A-C5A-C6A
29	c	517	DGD	C7A-C8A-C9A-CAA
29	c	518	DGD	CCA-CDA-CEA-CFA
29	c	519	DGD	CCA-CDA-CEA-CFA
32	H	103	STE	C5-C6-C7-C8
32	T	103	STE	C5-C6-C7-C8
33	L	102	LHG	C27-C28-C29-C30
33	l	101	LHG	C24-C25-C26-C27
33	B	622	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
33	d	409	LHG	O1-C1-C2-O2
27	M	101	LMG	C12-C13-C14-C15
27	M	101	LMG	C15-C16-C17-C18
27	c	522	LMG	C36-C37-C38-C39
28	a	410	SQD	C17-C18-C19-C20
28	a	411	SQD	C11-C10-C9-C8
29	a	412	DGD	C6A-C7A-C8A-C9A
29	c	518	DGD	C8A-C9A-CAA-CBA
32	I	101	STE	C4-C5-C6-C7
32	I	101	STE	C10-C11-C12-C13
32	a	414	STE	C5-C6-C7-C8
32	x	101	STE	C3-C4-C5-C6
22	C	502	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
27	C	519	LMG	C17-C18-C19-C20
27	d	411	LMG	C34-C35-C36-C37
29	H	102	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
32	H	103	STE	C11-C12-C13-C14
32	x	101	STE	C12-C13-C14-C15
22	a	403	CLA	C16-C17-C18-C19
22	b	606	CLA	C2A-CAA-CBA-CGA
27	c	522	LMG	C33-C34-C35-C36
28	B	623	SQD	C11-C12-C13-C14
29	C	517	DGD	C6B-C7B-C8B-C9B
33	d	410	LHG	C33-C34-C35-C36
22	b	604	CLA	C15-C16-C17-C18
22	b	615	CLA	C15-C16-C17-C18
29	a	412	DGD	C2B-C1B-O2G-C2G
22	B	611	CLA	C12-C13-C15-C16
27	D	407	LMG	C31-C32-C33-C34
27	M	101	LMG	C14-C15-C16-C17
27	b	622	LMG	C11-C12-C13-C14
27	c	523	LMG	C34-C35-C36-C37
28	a	410	SQD	C34-C35-C36-C37
29	h	102	DGD	C6B-C7B-C8B-C9B
32	B	625	STE	C5-C6-C7-C8
32	B	627	STE	C5-C6-C7-C8
27	D	407	LMG	C10-C11-C12-C13
32	x	101	STE	C1-C2-C3-C4
22	b	615	CLA	C13-C15-C16-C17
22	c	507	CLA	C5-C6-C7-C8
29	C	517	DGD	C9A-CAA-CBA-CCA
32	B	620	STE	C6-C7-C8-C9
22	B	607	CLA	C4-C3-C5-C6
22	c	512	CLA	C3A-C2A-CAA-CBA
23	d	402	PHO	C3A-C2A-CAA-CBA
33	d	409	LHG	C32-C33-C34-C35
33	e	101	LHG	C14-C15-C16-C17
27	d	411	LMG	C35-C36-C37-C38
29	c	517	DGD	C4B-C5B-C6B-C7B
22	b	615	CLA	C16-C17-C18-C20
29	C	518	DGD	C8A-C9A-CAA-CBA
32	B	624	STE	C2-C3-C4-C5
33	L	102	LHG	C12-C13-C14-C15
27	M	101	LMG	C37-C38-C39-C40
27	c	522	LMG	C16-C17-C18-C19
28	A	412	SQD	C10-C11-C12-C13
28	F	101	SQD	C25-C26-C27-C28
29	C	516	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
32	T	102	STE	C7-C8-C9-C10
32	c	521	STE	C9-C10-C11-C12
33	D	408	LHG	C10-C11-C12-C13
33	E	102	LHG	C17-C18-C19-C20
28	A	412	SQD	O6-C44-C45-C46
27	D	407	LMG	C14-C15-C16-C17
27	D	410	LMG	C34-C35-C36-C37
27	b	620	LMG	C17-C18-C19-C20
28	a	411	SQD	C11-C12-C13-C14
32	J	101	STE	C3-C4-C5-C6
32	M	102	STE	C9-C10-C11-C12
32	c	524	STE	C5-C6-C7-C8
33	e	101	LHG	C16-C17-C18-C19
22	d	405	CLA	C10-C11-C12-C13
27	A	411	LMG	C31-C32-C33-C34
27	D	407	LMG	C17-C18-C19-C20
27	c	523	LMG	C35-C36-C37-C38
27	d	411	LMG	C31-C32-C33-C34
28	A	413	SQD	C28-C29-C30-C31
28	a	410	SQD	C13-C14-C15-C16
29	A	414	DGD	C2B-C3B-C4B-C5B
29	A	414	DGD	C8B-C9B-CAB-CBB
32	B	620	STE	C9-C10-C11-C12
32	a	414	STE	C4-C5-C6-C7
32	m	101	STE	C5-C6-C7-C8
33	B	622	LHG	C26-C27-C28-C29
33	E	102	LHG	C27-C28-C29-C30
33	E	102	LHG	C32-C33-C34-C35
33	l	101	LHG	C16-C17-C18-C19
28	B	623	SQD	C16-C17-C18-C19
29	c	519	DGD	C8B-C9B-CAB-CBB
29	h	102	DGD	C5B-C6B-C7B-C8B
28	a	410	SQD	C29-C30-C31-C32
29	c	517	DGD	C3B-C4B-C5B-C6B
33	d	410	LHG	C27-C28-C29-C30
28	A	413	SQD	C18-C19-C20-C21
29	C	517	DGD	C5A-C6A-C7A-C8A
22	A	410	CLA	C16-C17-C18-C20
22	B	605	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C16-C17-C18-C19
22	c	512	CLA	O1A-CGA-O2A-C1
22	B	605	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C2B-C3B-CAB-CBB
24	H	101	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C30
24	T	101	BCR	C5-C6-C7-C8
24	b	617	BCR	C1-C6-C7-C8
24	k	101	BCR	C1-C6-C7-C8
24	t	101	BCR	C1-C6-C7-C8
27	d	411	LMG	C32-C33-C34-C35
29	h	102	DGD	C3B-C4B-C5B-C6B
32	E	103	STE	C3-C4-C5-C6
33	E	102	LHG	C33-C34-C35-C36
22	d	404	CLA	CBD-CGD-O2D-CED
22	a	402	CLA	C15-C16-C17-C18
22	c	503	CLA	C15-C16-C17-C18
27	C	519	LMG	C13-C14-C15-C16
29	c	519	DGD	C9A-CAA-CBA-CCA
32	c	521	STE	C2-C3-C4-C5
33	e	101	LHG	C11-C10-C9-C8
32	b	623	STE	C6-C7-C8-C9
27	c	522	LMG	C10-C11-C12-C13
29	C	516	DGD	C1A-C2A-C3A-C4A
29	c	518	DGD	C1B-C2B-C3B-C4B
29	H	102	DGD	C6B-C7B-C8B-C9B
29	c	517	DGD	CBB-CCB-CDB-CEB
29	c	518	DGD	C4A-C5A-C6A-C7A
33	d	409	LHG	C34-C35-C36-C37
26	A	409	PL9	C4-C3-C7-C8
27	c	523	LMG	C18-C19-C20-C21
28	L	101	SQD	C11-C10-C9-C8
32	C	521	STE	C7-C8-C9-C10
33	D	409	LHG	C29-C30-C31-C32
33	d	408	LHG	C11-C10-C9-C8
33	l	101	LHG	C10-C11-C12-C13
22	B	614	CLA	C4-C3-C5-C6
27	c	522	LMG	C40-C41-C42-C43
27	d	411	LMG	C36-C37-C38-C39
32	C	520	STE	C3-C4-C5-C6
32	b	621	STE	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	E	102	LHG	C29-C30-C31-C32
24	C	515	BCR	C18-C19-C20-C21
24	H	101	BCR	C10-C11-C12-C13
24	c	514	BCR	C18-C19-C20-C21
24	d	406	BCR	C10-C11-C12-C13
22	C	509	CLA	C13-C15-C16-C17
22	B	605	CLA	C2-C3-C5-C6
22	B	607	CLA	C2-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
27	b	622	LMG	C12-C13-C14-C15
27	c	522	LMG	C31-C32-C33-C34
29	c	517	DGD	C9B-CAB-CBB-CCB
33	E	102	LHG	C25-C26-C27-C28
33	L	102	LHG	C18-C19-C20-C21
33	l	101	LHG	C23-C24-C25-C26
22	A	403	CLA	C14-C13-C15-C16
27	C	519	LMG	C31-C32-C33-C34
27	c	522	LMG	C15-C16-C17-C18
28	F	101	SQD	C26-C27-C28-C29
28	f	102	SQD	C29-C30-C31-C32
29	c	517	DGD	C4A-C5A-C6A-C7A
29	c	517	DGD	CCB-CDB-CEB-CFB
32	b	624	STE	C4-C5-C6-C7
27	A	411	LMG	C14-C15-C16-C17
29	c	517	DGD	O6E-C1E-O5D-C6D
27	B	621	LMG	C34-C35-C36-C37
27	D	407	LMG	C15-C16-C17-C18
27	d	411	LMG	C38-C39-C40-C41
28	A	413	SQD	C30-C31-C32-C33
28	a	410	SQD	C27-C28-C29-C30
29	H	102	DGD	C6A-C7A-C8A-C9A
32	D	411	STE	C4-C5-C6-C7
32	d	413	STE	C10-C11-C12-C13
33	E	102	LHG	C11-C10-C9-C8
27	c	523	LMG	O6-C5-C6-O5
27	c	523	LMG	C2-C1-O1-C7
22	c	507	CLA	C8-C10-C11-C12
29	a	412	DGD	C8B-C9B-CAB-CBB
29	c	517	DGD	C8A-C9A-CAA-CBA
29	C	516	DGD	O6E-C5E-C6E-O5E
27	c	520	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
28	B	623	SQD	C33-C34-C35-C36
29	C	516	DGD	C3B-C4B-C5B-C6B
29	c	517	DGD	C6B-C7B-C8B-C9B
32	I	101	STE	C2-C3-C4-C5
32	x	101	STE	C7-C8-C9-C10
27	D	407	LMG	C38-C39-C40-C41
27	c	522	LMG	C13-C14-C15-C16
29	H	102	DGD	CAB-CBB-CCB-CDB
32	b	621	STE	C3-C4-C5-C6
32	t	102	STE	C11-C10-C9-C8
33	d	410	LHG	C26-C27-C28-C29
22	B	606	CLA	C15-C16-C17-C18
28	f	102	SQD	C24-C25-C26-C27
27	c	522	LMG	C11-C10-O7-C8
28	L	101	SQD	C7-C8-C9-C10
33	d	410	LHG	C23-C24-C25-C26
22	b	616	CLA	C10-C11-C12-C13
29	c	517	DGD	O1B-C1B-O2G-C2G
27	b	622	LMG	C13-C14-C15-C16
32	x	101	STE	C5-C6-C7-C8
27	d	411	LMG	C37-C38-C39-C40
22	B	607	CLA	C8-C10-C11-C12
27	D	407	LMG	C32-C33-C34-C35
29	a	412	DGD	CEB-CFB-CGB-CHB
26	D	406	PL9	C32-C33-C34-C35
32	b	621	STE	C14-C15-C16-C17
33	l	101	LHG	C33-C34-C35-C36
29	C	517	DGD	CBA-CCA-CDA-CEA
33	E	102	LHG	C24-C25-C26-C27
22	B	605	CLA	C16-C17-C18-C19
22	B	612	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
27	c	522	LMG	C32-C33-C34-C35
29	A	414	DGD	C2A-C3A-C4A-C5A
32	C	522	STE	C6-C7-C8-C9
32	d	413	STE	C4-C5-C6-C7
33	D	408	LHG	C30-C31-C32-C33
26	D	406	PL9	C30-C29-C31-C32
29	C	517	DGD	C4B-C5B-C6B-C7B
29	c	517	DGD	CCA-CDA-CEA-CFA
29	c	519	DGD	CBA-CCA-CDA-CEA
32	d	413	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	x	101	STE	C4-C5-C6-C7
33	d	410	LHG	C31-C32-C33-C34
27	M	101	LMG	C13-C14-C15-C16
33	E	102	LHG	C34-C35-C36-C37
22	B	606	CLA	C13-C15-C16-C17
22	C	505	CLA	C5-C6-C7-C8
33	D	409	LHG	C13-C14-C15-C16
33	L	102	LHG	C17-C18-C19-C20
29	a	412	DGD	O1B-C1B-O2G-C2G
33	L	102	LHG	C30-C31-C32-C33
22	B	603	CLA	C10-C11-C12-C13
22	B	606	CLA	C5-C6-C7-C8
22	C	509	CLA	C10-C11-C12-C13
22	B	604	CLA	C16-C17-C18-C19
27	B	621	LMG	C11-C12-C13-C14
33	D	409	LHG	C33-C34-C35-C36
27	D	410	LMG	O10-C28-O8-C9
27	M	101	LMG	C33-C34-C35-C36
29	H	102	DGD	C8A-C9A-CAA-CBA
29	c	517	DGD	C5B-C6B-C7B-C8B
29	h	102	DGD	C9A-CAA-CBA-CCA
33	B	622	LHG	C12-C13-C14-C15
28	A	412	SQD	C7-C8-C9-C10
32	E	103	STE	C1-C2-C3-C4
22	D	403	CLA	C15-C16-C17-C18
22	b	602	CLA	C15-C16-C17-C18
29	C	518	DGD	C4B-C5B-C6B-C7B
29	c	518	DGD	C2A-C3A-C4A-C5A
27	d	412	LMG	O6-C5-C6-O5
22	C	512	CLA	C3-C5-C6-C7
28	A	412	SQD	O6-C44-C45-O47
28	a	410	SQD	O47-C45-C46-O48
27	A	411	LMG	C29-C30-C31-C32
27	b	622	LMG	C18-C19-C20-C21
27	A	411	LMG	C37-C38-C39-C40
22	c	502	CLA	C13-C15-C16-C17
27	c	522	LMG	C38-C39-C40-C41
29	c	519	DGD	C2A-C3A-C4A-C5A
29	c	519	DGD	C6A-C7A-C8A-C9A
33	D	409	LHG	C9-C10-C11-C12
27	D	407	LMG	C36-C37-C38-C39
29	a	412	DGD	C8A-C9A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
32	a	413	STE	C5-C6-C7-C8
32	c	521	STE	C11-C12-C13-C14
32	j	101	STE	C4-C5-C6-C7
22	A	403	CLA	C10-C11-C12-C13
22	B	615	CLA	C13-C15-C16-C17
22	C	505	CLA	C10-C11-C12-C13
32	T	103	STE	C11-C12-C13-C14
32	l	102	STE	C7-C8-C9-C10
33	D	409	LHG	C27-C28-C29-C30
32	B	625	STE	C2-C3-C4-C5
29	c	517	DGD	O6D-C5D-C6D-O5D
22	C	510	CLA	C3-C5-C6-C7
28	B	623	SQD	C18-C19-C20-C21
29	C	516	DGD	C9B-CAB-CBB-CCB
29	h	102	DGD	C2B-C3B-C4B-C5B
33	D	409	LHG	C11-C12-C13-C14
33	L	102	LHG	C11-C12-C13-C14
28	A	412	SQD	C11-C10-C9-C8
29	a	412	DGD	C3B-C4B-C5B-C6B
33	D	409	LHG	C25-C26-C27-C28
33	L	102	LHG	C32-C33-C34-C35
28	B	623	SQD	C45-C46-O48-C23
27	c	522	LMG	C11-C12-C13-C14
32	B	620	STE	C11-C12-C13-C14
32	l	102	STE	C13-C14-C15-C16
33	l	101	LHG	C11-C12-C13-C14
27	c	520	LMG	C31-C32-C33-C34
32	T	103	STE	C6-C7-C8-C9
33	D	408	LHG	C29-C30-C31-C32
33	E	102	LHG	C13-C14-C15-C16
33	d	410	LHG	O1-C1-C2-O2
29	A	414	DGD	CCA-CDA-CEA-CFA
22	B	604	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C8-C10-C11-C12
28	f	102	SQD	C28-C29-C30-C31
32	B	620	STE	C7-C8-C9-C10
22	C	505	CLA	C4C-C3C-CAC-CBC
27	D	410	LMG	C16-C17-C18-C19
32	B	625	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C15-C16-C17-C18
22	b	609	CLA	C13-C15-C16-C17
33	e	101	LHG	O6-C4-C5-C6
27	C	519	LMG	O9-C10-O7-C8
33	e	101	LHG	O9-C7-O7-C5
27	D	407	LMG	C12-C13-C14-C15
29	A	414	DGD	CEA-CFA-CGA-CHA
32	a	413	STE	C2-C3-C4-C5
22	b	604	CLA	C3-C5-C6-C7
22	A	403	CLA	C6-C7-C8-C10
22	B	602	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C15
22	C	503	CLA	C12-C13-C15-C16
22	C	505	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	b	604	CLA	C12-C13-C15-C16
22	b	606	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	b	608	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C10-C8-C7
22	c	504	CLA	C11-C10-C8-C7
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	509	CLA	C6-C7-C8-C10
29	c	517	DGD	C8B-C9B-CAB-CBB
32	M	102	STE	C11-C10-C9-C8
27	C	519	LMG	O10-C28-O8-C9
28	L	101	SQD	C29-C30-C31-C32
29	H	102	DGD	CCB-CDB-CEB-CFB
29	a	412	DGD	C4B-C5B-C6B-C7B
28	F	101	SQD	C30-C31-C32-C33
32	I	101	STE	C7-C8-C9-C10
27	c	523	LMG	C15-C16-C17-C18
32	l	102	STE	C4-C5-C6-C7
22	B	601	CLA	C8-C10-C11-C12
22	C	511	CLA	O1D-CGD-O2D-CED
22	B	604	CLA	C11-C12-C13-C14
22	B	605	CLA	C11-C12-C13-C14
22	B	607	CLA	C6-C7-C8-C9
22	B	608	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C6-C7-C8-C9
22	C	507	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9
22	D	404	CLA	C6-C7-C8-C9
22	b	602	CLA	C6-C7-C8-C9
22	b	607	CLA	C6-C7-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C9
29	A	414	DGD	CBB-CCB-CDB-CEB
29	C	517	DGD	C4A-C5A-C6A-C7A
22	c	506	CLA	C16-C17-C18-C20
32	D	411	STE	C6-C7-C8-C9
28	a	410	SQD	C24-C25-C26-C27
33	L	102	LHG	C31-C32-C33-C34
27	M	101	LMG	C2-C1-O1-C7
27	A	411	LMG	O1-C7-C8-C9
27	M	101	LMG	C7-C8-C9-O8
27	c	522	LMG	C7-C8-C9-O8
27	c	523	LMG	C7-C8-C9-O8
28	B	623	SQD	O6-C44-C45-C46
28	a	410	SQD	C44-C45-C46-O48
28	a	411	SQD	C44-C45-C46-O48
33	E	102	LHG	C4-C5-C6-O8
27	C	519	LMG	C30-C31-C32-C33
32	T	103	STE	C9-C10-C11-C12
33	e	101	LHG	C17-C18-C19-C20
22	B	605	CLA	C8-C10-C11-C12
22	B	614	CLA	C15-C16-C17-C18
22	b	601	CLA	C15-C16-C17-C18
28	B	623	SQD	C32-C33-C34-C35
29	c	519	DGD	C8A-C9A-CAA-CBA
32	c	524	STE	C6-C7-C8-C9
27	b	622	LMG	O6-C5-C6-O5
27	C	519	LMG	C14-C15-C16-C17
27	c	522	LMG	C34-C35-C36-C37
29	H	102	DGD	CBA-CCA-CDA-CEA
29	h	102	DGD	CAB-CBB-CCB-CDB
22	C	509	CLA	O1D-CGD-O2D-CED
29	c	517	DGD	O6E-C5E-C6E-O5E
33	l	101	LHG	C25-C26-C27-C28
24	b	619	BCR	C16-C17-C18-C36
27	A	411	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C4-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
29	c	517	DGD	C4D-C5D-C6D-O5D
27	d	411	LMG	C30-C31-C32-C33
28	B	623	SQD	C12-C13-C14-C15
33	L	102	LHG	C13-C14-C15-C16
27	D	407	LMG	O6-C5-C6-O5
22	b	606	CLA	C10-C11-C12-C13
22	b	606	CLA	C15-C16-C17-C18
28	a	410	SQD	C25-C26-C27-C28
29	H	102	DGD	C5A-C6A-C7A-C8A
29	h	102	DGD	O6E-C5E-C6E-O5E
27	A	411	LMG	C16-C17-C18-C19
32	b	621	STE	C5-C6-C7-C8
22	b	601	CLA	O2A-C1-C2-C3
27	D	410	LMG	C9-C8-O7-C10
29	a	412	DGD	C1G-C2G-O2G-C1B
27	b	622	LMG	C40-C41-C42-C43
29	A	414	DGD	C5B-C6B-C7B-C8B
32	d	413	STE	C9-C10-C11-C12
32	l	102	STE	C10-C11-C12-C13
29	a	412	DGD	CBA-CCA-CDA-CEA
32	B	625	STE	C3-C4-C5-C6
32	B	626	STE	C6-C7-C8-C9
32	D	411	STE	C14-C15-C16-C17
22	a	402	CLA	CBD-CGD-O2D-CED
24	b	618	BCR	C16-C17-C18-C19
33	e	101	LHG	O6-C4-C5-O7
27	b	622	LMG	C37-C38-C39-C40
28	A	412	SQD	C12-C13-C14-C15
28	A	413	SQD	C32-C33-C34-C35
29	C	518	DGD	C8B-C9B-CAB-CBB
22	B	604	CLA	CBA-CGA-O2A-C1
32	b	625	STE	C7-C8-C9-C10
32	b	621	STE	C1-C2-C3-C4
32	b	623	STE	C3-C4-C5-C6
27	b	622	LMG	C38-C39-C40-C41
32	D	411	STE	C7-C8-C9-C10
27	c	523	LMG	C20-C21-C22-C23
32	M	103	STE	C1-C2-C3-C4
28	a	411	SQD	C15-C16-C17-C18
29	C	517	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
33	D	409	LHG	C30-C31-C32-C33
22	B	614	CLA	C16-C17-C18-C19
27	B	621	LMG	C31-C32-C33-C34
27	M	101	LMG	C35-C36-C37-C38
27	b	620	LMG	C37-C38-C39-C40
27	b	622	LMG	C33-C34-C35-C36
27	c	520	LMG	C39-C40-C41-C42
29	a	412	DGD	C4A-C5A-C6A-C7A
32	a	414	STE	C2-C3-C4-C5
32	b	624	STE	C12-C13-C14-C15
32	c	521	STE	C10-C11-C12-C13
33	l	101	LHG	C14-C15-C16-C17
28	f	102	SQD	C35-C36-C37-C38
27	B	621	LMG	C16-C17-C18-C19
27	d	412	LMG	C30-C31-C32-C33
28	B	623	SQD	C9-C10-C11-C12
32	x	101	STE	C9-C10-C11-C12
27	M	101	LMG	O7-C8-C9-O8
28	B	623	SQD	O6-C44-C45-O47
29	A	414	DGD	O2G-C2G-C3G-O3G
29	c	519	DGD	CDA-CEA-CFA-CGA
27	d	412	LMG	C36-C37-C38-C39
32	t	102	STE	C6-C7-C8-C9
28	A	412	SQD	C17-C18-C19-C20
29	A	414	DGD	CFA-CGA-CHA-CIA
32	D	411	STE	C15-C16-C17-C18
32	C	520	STE	C6-C7-C8-C9
32	t	102	STE	C2-C3-C4-C5
33	D	408	LHG	C11-C12-C13-C14
29	H	102	DGD	O2G-C1B-C2B-C3B
27	M	101	LMG	C17-C18-C19-C20
28	B	623	SQD	C31-C32-C33-C34
32	b	621	STE	C13-C14-C15-C16
29	c	518	DGD	CBA-CCA-CDA-CEA
33	d	408	LHG	C16-C17-C18-C19
22	a	404	CLA	C10-C11-C12-C13
22	b	606	CLA	C8-C10-C11-C12
27	D	410	LMG	C15-C16-C17-C18
29	c	519	DGD	C5B-C6B-C7B-C8B
32	C	521	STE	C5-C6-C7-C8
28	A	412	SQD	C8-C7-O47-C45
28	A	412	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	D	408	LHG	C18-C19-C20-C21
33	d	409	LHG	C14-C15-C16-C17
22	b	608	CLA	C13-C15-C16-C17
23	d	401	PHO	O1D-CGD-O2D-CED
29	A	414	DGD	CFB-CGB-CHB-CIB
33	d	409	LHG	C35-C36-C37-C38
32	E	103	STE	C4-C5-C6-C7
22	B	610	CLA	O1D-CGD-O2D-CED
22	b	605	CLA	C4-C3-C5-C6
26	a	409	PL9	C15-C14-C16-C17
23	A	404	PHO	C2-C3-C5-C6
26	d	407	PL9	C13-C14-C16-C17
27	c	520	LMG	C29-C28-O8-C9
23	d	402	PHO	C2C-C3C-CAC-CBC
27	b	620	LMG	C15-C16-C17-C18
33	B	622	LHG	O9-C7-O7-C5
22	A	403	CLA	C6-C7-C8-C9
22	A	403	CLA	C11-C12-C13-C14
22	B	602	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	C	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	b	604	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C10-C8-C9
22	b	615	CLA	C11-C12-C13-C14
22	c	505	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
33	L	102	LHG	C15-C16-C17-C18
22	b	613	CLA	C10-C11-C12-C13
22	c	507	CLA	C4B-C3B-CAB-CBB
22	d	403	CLA	C4B-C3B-CAB-CBB
28	L	101	SQD	C16-C17-C18-C19
29	c	518	DGD	C7B-C8B-C9B-CAB
32	B	625	STE	C10-C11-C12-C13
32	T	102	STE	C12-C13-C14-C15
27	D	410	LMG	C35-C36-C37-C38
27	d	412	LMG	C37-C38-C39-C40
29	a	412	DGD	CDA-CEA-CFA-CGA
29	a	412	DGD	CEA-CFA-CGA-CHA
29	C	517	DGD	C3A-C4A-C5A-C6A

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Mol	Chain	Res	Type	Atoms
32	b	621	STE	C7-C8-C9-C10
33	d	408	LHG	C17-C18-C19-C20
29	a	412	DGD	C7B-C8B-C9B-CAB
22	A	403	CLA	C11-C10-C8-C7
22	A	403	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	608	CLA	C6-C7-C8-C10
22	B	613	CLA	C12-C13-C15-C16
22	B	614	CLA	C12-C13-C15-C16
22	C	512	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	C	513	CLA	C6-C7-C8-C10
22	D	404	CLA	C6-C7-C8-C10
22	b	601	CLA	C12-C13-C15-C16
22	b	602	CLA	C6-C7-C8-C10
22	b	609	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	509	CLA	C11-C12-C13-C15
22	c	511	CLA	C12-C13-C15-C16
22	b	612	CLA	C13-C15-C16-C17
22	b	614	CLA	C13-C15-C16-C17
32	m	101	STE	C1-C2-C3-C4
27	b	622	LMG	C24-C25-C26-C27
29	C	517	DGD	CDA-CEA-CFA-CGA
33	l	101	LHG	C31-C32-C33-C34
22	c	503	CLA	C16-C17-C18-C19
27	c	520	LMG	C35-C36-C37-C38
29	C	518	DGD	CDA-CEA-CFA-CGA
22	C	510	CLA	C4-C3-C5-C6
22	c	505	CLA	C4-C3-C5-C6
32	H	103	STE	C15-C16-C17-C18
29	C	517	DGD	CCB-CDB-CEB-CFB
29	a	412	DGD	CFA-CGA-CHA-CIA
28	B	623	SQD	C14-C15-C16-C17
28	L	101	SQD	C12-C13-C14-C15
28	L	101	SQD	C18-C19-C20-C21
32	b	624	STE	C14-C15-C16-C17
33	L	102	LHG	O10-C23-O8-C6
32	T	102	STE	C15-C16-C17-C18
22	B	616	CLA	CBA-CGA-O2A-C1
27	D	410	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
27	c	523	LMG	C31-C32-C33-C34
33	d	408	LHG	C29-C30-C31-C32
24	h	101	BCR	C15-C16-C17-C18
22	b	607	CLA	C13-C15-C16-C17
27	d	412	LMG	C14-C15-C16-C17
22	B	616	CLA	O1A-CGA-O2A-C1
27	A	411	LMG	C30-C31-C32-C33
28	f	102	SQD	C34-C35-C36-C37
32	a	413	STE	C4-C5-C6-C7
27	d	412	LMG	C39-C40-C41-C42
28	a	411	SQD	C14-C15-C16-C17
29	a	412	DGD	C5A-C6A-C7A-C8A
29	c	518	DGD	CBB-CCB-CDB-CEB
22	c	512	CLA	C2A-CAA-CBA-CGA
32	B	625	STE	C13-C14-C15-C16
22	B	612	CLA	CBA-CGA-O2A-C1
27	b	620	LMG	C31-C32-C33-C34
29	a	412	DGD	C9A-CAA-CBA-CCA
33	d	409	LHG	C11-C12-C13-C14
27	C	519	LMG	O1-C7-C8-C9
27	M	101	LMG	O1-C7-C8-C9
28	a	410	SQD	O6-C44-C45-C46
29	A	414	DGD	C1G-C2G-C3G-O3G
27	c	523	LMG	C29-C30-C31-C32
27	c	523	LMG	C38-C39-C40-C41
33	d	408	LHG	C15-C16-C17-C18
32	c	521	STE	C1-C2-C3-C4
33	D	408	LHG	C15-C16-C17-C18
27	D	410	LMG	C33-C34-C35-C36
27	b	622	LMG	C31-C32-C33-C34
29	a	412	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	C5A-C6A-C7A-C8A
32	b	621	STE	C12-C13-C14-C15
22	b	609	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
28	A	413	SQD	C10-C11-C12-C13
29	A	414	DGD	C7B-C8B-C9B-CAB
29	C	517	DGD	C8B-C9B-CAB-CBB
33	D	408	LHG	C32-C33-C34-C35
22	b	609	CLA	C2-C3-C5-C6
27	c	522	LMG	O10-C28-O8-C9
28	a	411	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	a	403	CLA	CBD-CGD-O2D-CED
22	a	402	CLA	C16-C17-C18-C20
22	A	402	CLA	C15-C16-C17-C18
29	c	517	DGD	CAB-CBB-CCB-CDB
24	C	515	BCR	C1-C6-C7-C8
24	d	406	BCR	C23-C24-C25-C30
27	b	620	LMG	C11-C10-O7-C8
27	b	620	LMG	C20-C21-C22-C23
29	C	518	DGD	CBB-CCB-CDB-CEB
33	D	408	LHG	C12-C13-C14-C15
36	v	201	HEC	C2C-C3C-CAC-CBC
32	b	621	STE	C2-C3-C4-C5
32	t	102	STE	C3-C4-C5-C6
29	H	102	DGD	CDB-CEB-CFB-CGB
27	C	519	LMG	C32-C33-C34-C35
33	d	409	LHG	C33-C34-C35-C36
22	B	612	CLA	C16-C17-C18-C19
22	b	604	CLA	C13-C15-C16-C17
27	c	523	LMG	O7-C8-C9-O8
33	d	410	LHG	C35-C36-C37-C38
32	x	101	STE	C11-C10-C9-C8
29	h	102	DGD	CDB-CEB-CFB-CGB
32	E	103	STE	C7-C8-C9-C10
33	e	101	LHG	C28-C29-C30-C31
27	c	522	LMG	C41-C42-C43-C44
32	H	103	STE	C13-C14-C15-C16
33	e	101	LHG	C11-C12-C13-C14
27	c	523	LMG	C28-C29-C30-C31
32	B	627	STE	C1-C2-C3-C4
32	d	413	STE	C12-C13-C14-C15
22	b	602	CLA	CBD-CGD-O2D-CED
24	T	101	BCR	C18-C19-C20-C21
22	C	510	CLA	C2-C3-C5-C6
22	c	505	CLA	C2-C3-C5-C6
26	d	407	PL9	C43-C44-C46-C47
27	D	407	LMG	C22-C23-C24-C25
27	A	411	LMG	C12-C13-C14-C15
33	d	408	LHG	C14-C15-C16-C17
22	A	410	CLA	C16-C17-C18-C19
22	B	609	CLA	C16-C17-C18-C19
27	A	411	LMG	C35-C36-C37-C38
28	a	411	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	D	411	STE	C12-C13-C14-C15
32	j	101	STE	C5-C6-C7-C8
28	A	413	SQD	C23-C24-C25-C26
28	a	410	SQD	C15-C16-C17-C18
29	C	516	DGD	O6D-C5D-C6D-O5D
22	B	613	CLA	C14-C13-C15-C16
22	C	503	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	a	403	CLA	C14-C13-C15-C16
28	A	413	SQD	C14-C15-C16-C17
22	B	614	CLA	C16-C17-C18-C20
22	B	603	CLA	O1D-CGD-O2D-CED
29	a	412	DGD	C6B-C7B-C8B-C9B
27	M	101	LMG	C39-C40-C41-C42
27	A	411	LMG	C11-C12-C13-C14
28	L	101	SQD	C24-C25-C26-C27
29	H	102	DGD	C3B-C4B-C5B-C6B
32	M	102	STE	C10-C11-C12-C13
33	E	102	LHG	O2-C2-C3-O3
22	B	612	CLA	C10-C11-C12-C13
33	D	408	LHG	O1-C1-C2-O2
22	c	502	CLA	CBA-CGA-O2A-C1
22	c	506	CLA	C16-C17-C18-C19
32	j	101	STE	C7-C8-C9-C10
27	C	519	LMG	C18-C19-C20-C21
33	E	102	LHG	C10-C11-C12-C13
29	h	102	DGD	C7A-C8A-C9A-CAA
22	c	513	CLA	C5-C6-C7-C8
22	C	505	CLA	CBD-CGD-O2D-CED
33	l	101	LHG	C17-C18-C19-C20
24	B	617	BCR	C35-C13-C14-C15
24	B	617	BCR	C20-C21-C22-C37
24	C	515	BCR	C35-C13-C14-C15
24	C	515	BCR	C16-C17-C18-C36
24	H	101	BCR	C11-C10-C9-C34
24	H	101	BCR	C20-C21-C22-C37
24	Y	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C11-C10-C9-C34
24	b	617	BCR	C35-C13-C14-C15
24	c	515	BCR	C20-C21-C22-C37
24	h	101	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	C3-C5-C6-C7
29	c	519	DGD	C5A-C6A-C7A-C8A
22	B	611	CLA	C13-C15-C16-C17
33	B	622	LHG	C9-C10-C11-C12
32	B	626	STE	C4-C5-C6-C7
33	l	101	LHG	C30-C31-C32-C33
22	B	616	CLA	C6-C7-C8-C10
22	C	502	CLA	C11-C12-C13-C15
22	C	503	CLA	C11-C10-C8-C7
22	C	508	CLA	C11-C10-C8-C7
22	C	509	CLA	C11-C10-C8-C7
22	C	510	CLA	C11-C10-C8-C7
22	a	404	CLA	C12-C13-C15-C16
22	b	605	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C15
22	c	510	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C12-C13-C15
27	B	621	LMG	C15-C16-C17-C18
29	A	414	DGD	CDB-CEB-CFB-CGB
33	D	409	LHG	C11-C10-C9-C8
22	C	502	CLA	C3-C5-C6-C7
22	b	609	CLA	C15-C16-C17-C18
24	D	405	BCR	C21-C22-C23-C24
24	H	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C17-C18-C19-C20
33	D	409	LHG	O10-C23-O8-C6
29	C	517	DGD	C2G-C3G-O3G-C1D
27	D	407	LMG	C30-C31-C32-C33
27	b	622	LMG	C10-C11-C12-C13
28	B	623	SQD	C23-C24-C25-C26
28	L	101	SQD	C19-C20-C21-C22
29	A	414	DGD	C8A-C9A-CAA-CBA
33	L	102	LHG	O9-C7-O7-C5
22	c	512	CLA	C4-C3-C5-C6
26	d	407	PL9	C15-C14-C16-C17
22	c	502	CLA	O1A-CGA-O2A-C1
32	m	101	STE	C3-C4-C5-C6
32	B	625	STE	C4-C5-C6-C7
22	C	501	CLA	CBD-CGD-O2D-CED
29	H	102	DGD	C4B-C5B-C6B-C7B
22	c	508	CLA	C8-C10-C11-C12
22	B	604	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	T	103	STE	C13-C14-C15-C16
22	B	613	CLA	C5-C6-C7-C8
22	c	509	CLA	C13-C15-C16-C17
24	k	101	BCR	C19-C20-C21-C22
32	b	624	STE	C5-C6-C7-C8
22	b	612	CLA	C16-C17-C18-C20
27	D	407	LMG	C39-C40-C41-C42
33	d	409	LHG	C15-C16-C17-C18
24	t	101	BCR	C20-C21-C22-C23
28	L	101	SQD	C26-C27-C28-C29
29	a	412	DGD	C9B-CAB-CBB-CCB
32	C	520	STE	C4-C5-C6-C7
29	c	518	DGD	O6D-C1D-O3G-C3G
29	a	412	DGD	C5B-C6B-C7B-C8B
32	T	102	STE	C6-C7-C8-C9
32	c	524	STE	C7-C8-C9-C10
32	b	623	STE	C1-C2-C3-C4
22	c	510	CLA	C5-C6-C7-C8
22	b	609	CLA	C16-C17-C18-C20
29	c	519	DGD	CAB-CBB-CCB-CDB
33	d	408	LHG	C27-C28-C29-C30
22	B	612	CLA	O1A-CGA-O2A-C1
29	C	516	DGD	C4D-C5D-C6D-O5D
27	c	523	LMG	C13-C14-C15-C16
32	C	520	STE	C5-C6-C7-C8
22	C	506	CLA	C4-C3-C5-C6
32	I	101	STE	C12-C13-C14-C15
28	A	412	SQD	C14-C15-C16-C17
27	C	519	LMG	O1-C7-C8-O7
27	M	101	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
29	C	516	DGD	O1G-C1G-C2G-O2G
22	B	614	CLA	C6-C7-C8-C9
29	c	519	DGD	C4A-C5A-C6A-C7A
29	c	519	DGD	C7B-C8B-C9B-CAB
28	L	101	SQD	C11-C12-C13-C14
22	C	508	CLA	C5-C6-C7-C8
22	c	506	CLA	C5-C6-C7-C8
32	a	414	STE	C6-C7-C8-C9
32	b	625	STE	C1-C2-C3-C4
22	C	505	CLA	O1A-CGA-O2A-C1
27	C	519	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	A	411	LMG	C2-C1-O1-C7
29	c	517	DGD	C2E-C1E-O5D-C6D
22	D	404	CLA	C16-C17-C18-C19
22	b	604	CLA	C16-C17-C18-C19
27	A	411	LMG	C17-C18-C19-C20
32	C	521	STE	C4-C5-C6-C7
26	a	409	PL9	C25-C24-C26-C27
33	E	102	LHG	O9-C7-O7-C5
22	b	610	CLA	C2A-CAA-CBA-CGA
22	c	503	CLA	CBA-CGA-O2A-C1
32	c	524	STE	C2-C3-C4-C5
22	a	402	CLA	C16-C17-C18-C19
22	c	505	CLA	C16-C17-C18-C20
22	d	404	CLA	C16-C17-C18-C19
33	D	408	LHG	C17-C18-C19-C20
27	c	522	LMG	C42-C43-C44-C45
33	L	102	LHG	C19-C20-C21-C22
32	B	625	STE	C7-C8-C9-C10
32	d	413	STE	C6-C7-C8-C9
33	E	102	LHG	C28-C29-C30-C31
22	B	606	CLA	C10-C11-C12-C13
22	D	403	CLA	C2C-C3C-CAC-CBC
32	B	626	STE	C3-C4-C5-C6
22	C	505	CLA	CBA-CGA-O2A-C1
33	l	101	LHG	C24-C23-O8-C6
32	B	620	STE	C11-C10-C9-C8
22	c	502	CLA	O1D-CGD-O2D-CED
28	F	101	SQD	C45-C44-O6-C1
27	b	620	LMG	C14-C15-C16-C17
22	B	601	CLA	C1A-C2A-CAA-CBA
24	K	101	BCR	C6-C7-C8-C9
22	c	512	CLA	C2-C3-C5-C6
28	a	410	SQD	C19-C20-C21-C22
24	t	101	BCR	C17-C18-C19-C20
28	A	412	SQD	C29-C30-C31-C32
32	M	102	STE	C4-C5-C6-C7
33	d	410	LHG	C30-C31-C32-C33
27	b	622	LMG	C19-C20-C21-C22
29	C	518	DGD	C3A-C4A-C5A-C6A
22	B	602	CLA	C12-C13-C15-C16
22	B	603	CLA	C12-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	616	CLA	C11-C10-C8-C7
22	C	505	CLA	C6-C7-C8-C10
22	C	506	CLA	C12-C13-C15-C16
22	C	509	CLA	C12-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C15
22	b	603	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C12-C13-C15
22	c	505	CLA	C6-C7-C8-C10
22	c	512	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
32	I	101	STE	C11-C12-C13-C14
22	b	604	CLA	C16-C17-C18-C20
22	b	608	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C20
22	b	612	CLA	C16-C17-C18-C19
22	d	404	CLA	C16-C17-C18-C20
29	H	102	DGD	CDA-CEA-CFA-CGA
32	B	620	STE	C4-C5-C6-C7
32	b	624	STE	C6-C7-C8-C9
33	d	408	LHG	C18-C19-C20-C21
22	C	504	CLA	C11-C12-C13-C14
33	d	409	LHG	C17-C18-C19-C20
32	l	102	STE	C1-C2-C3-C4
29	C	516	DGD	CCB-CDB-CEB-CFB
32	B	620	STE	C10-C11-C12-C13
33	D	408	LHG	C25-C26-C27-C28
22	B	601	CLA	C3A-C2A-CAA-CBA
22	B	610	CLA	C16-C17-C18-C19
22	a	402	CLA	O1D-CGD-O2D-CED
33	L	102	LHG	C10-C11-C12-C13
27	A	411	LMG	C40-C41-C42-C43
22	B	613	CLA	C6-C7-C8-C9
22	a	404	CLA	C14-C13-C15-C16
22	b	601	CLA	C6-C7-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C14
22	c	507	CLA	C11-C10-C8-C9
22	d	405	CLA	C11-C12-C13-C14
27	c	523	LMG	C39-C40-C41-C42
29	c	518	DGD	CCB-CDB-CEB-CFB
22	B	601	CLA	C16-C17-C18-C20
32	H	103	STE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	B	605	CLA	C10-C11-C12-C13
27	C	519	LMG	C16-C17-C18-C19
32	a	414	STE	C1-C2-C3-C4
28	L	101	SQD	O47-C45-C46-O48
32	J	101	STE	C2-C3-C4-C5
33	B	622	LHG	C4-C5-C6-O8
29	c	518	DGD	C5B-C6B-C7B-C8B
22	A	405	CLA	C6-C7-C8-C9
29	A	414	DGD	CBA-CCA-CDA-CEA
33	l	101	LHG	C32-C33-C34-C35
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
29	c	517	DGD	CDB-CEB-CFB-CGB
22	C	501	CLA	C16-C17-C18-C20
22	C	506	CLA	C16-C17-C18-C20
23	A	404	PHO	C2C-C3C-CAC-CBC
27	b	622	LMG	C39-C40-C41-C42
29	A	414	DGD	O1A-C1A-O1G-C1G
27	c	522	LMG	C29-C30-C31-C32
29	a	412	DGD	CFB-CGB-CHB-CIB
29	C	518	DGD	C6A-C7A-C8A-C9A
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	b	607	CLA	CAD-CBD-CGD-O1D
22	c	504	CLA	CAD-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
24	a	405	BCR	C19-C20-C21-C22
28	A	413	SQD	C46-C45-O47-C7
33	D	408	LHG	C3-O3-P-O4
33	D	408	LHG	C4-O6-P-O3
33	L	102	LHG	C3-O3-P-O6
33	d	408	LHG	C3-O3-P-O5
33	d	409	LHG	C4-O6-P-O3
33	l	101	LHG	C3-O3-P-O6
33	l	101	LHG	C4-O6-P-O5
22	c	502	CLA	CBD-CGD-O2D-CED
27	b	622	LMG	C34-C35-C36-C37
32	E	103	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	502	CLA	C2B-C3B-CAB-CBB
22	d	403	CLA	C2B-C3B-CAB-CBB
24	C	514	BCR	C23-C24-C25-C30
33	l	101	LHG	C27-C28-C29-C30
22	C	506	CLA	C2-C3-C5-C6
26	D	406	PL9	C38-C39-C41-C42
32	b	623	STE	C11-C10-C9-C8
32	B	624	STE	C7-C8-C9-C10
27	B	621	LMG	C29-C30-C31-C32
28	B	623	SQD	C27-C28-C29-C30
32	b	623	STE	C7-C8-C9-C10
22	c	509	CLA	CAA-CBA-CGA-O2A
32	B	625	STE	C6-C7-C8-C9
33	d	409	LHG	C31-C32-C33-C34
27	C	519	LMG	C37-C38-C39-C40
29	h	102	DGD	CBA-CCA-CDA-CEA
26	a	409	PL9	C4-C3-C7-C8
28	a	410	SQD	C12-C13-C14-C15
33	D	409	LHG	O1-C1-C2-C3
27	A	411	LMG	C9-C8-O7-C10
27	b	622	LMG	C9-C8-O7-C10
28	B	623	SQD	C46-C45-O47-C7
29	C	516	DGD	O1G-C1A-C2A-C3A
29	c	517	DGD	C6A-C7A-C8A-C9A
27	c	523	LMG	C40-C41-C42-C43
32	H	103	STE	C7-C8-C9-C10
22	b	614	CLA	C16-C17-C18-C20
22	A	403	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	C	502	CLA	C11-C12-C13-C14
22	b	602	CLA	C11-C12-C13-C14
22	c	510	CLA	C6-C7-C8-C9
22	c	512	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C11-C10-C8-C7
22	a	403	CLA	C12-C13-C15-C16
22	c	512	CLA	C11-C10-C8-C7
24	B	619	BCR	C11-C10-C9-C8
27	d	412	LMG	C11-C12-C13-C14
33	L	102	LHG	C14-C15-C16-C17
27	A	411	LMG	C13-C14-C15-C16
33	l	101	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	D	410	LMG	C31-C32-C33-C34
32	l	102	STE	C12-C13-C14-C15
33	l	101	LHG	C26-C27-C28-C29
27	d	412	LMG	C10-C11-C12-C13
33	d	408	LHG	C25-C26-C27-C28
22	b	608	CLA	C2C-C3C-CAC-CBC
32	T	103	STE	C10-C11-C12-C13
26	a	409	PL9	C13-C14-C16-C17
29	H	102	DGD	C9B-CAB-CBB-CCB
33	E	102	LHG	O7-C5-C6-O8
22	c	503	CLA	O1A-CGA-O2A-C1
29	H	102	DGD	C3A-C4A-C5A-C6A
29	C	518	DGD	C2A-C1A-O1G-C1G
33	d	410	LHG	C7-C8-C9-C10
33	B	622	LHG	C19-C20-C21-C22
32	l	102	STE	C15-C16-C17-C18
22	B	603	CLA	C2A-CAA-CBA-CGA
22	c	501	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C13-C15-C16-C17
22	C	509	CLA	C2-C1-O2A-CGA
22	d	405	CLA	C4-C3-C5-C6
22	A	403	CLA	C16-C17-C18-C20
27	D	407	LMG	C34-C35-C36-C37
27	b	620	LMG	C12-C13-C14-C15
27	c	523	LMG	C11-C12-C13-C14
32	m	101	STE	C6-C7-C8-C9
32	b	625	STE	C4-C5-C6-C7
27	D	410	LMG	C32-C33-C34-C35
32	C	522	STE	C3-C4-C5-C6
24	c	514	BCR	C17-C18-C19-C20
22	C	511	CLA	CBA-CGA-O2A-C1
22	C	505	CLA	C15-C16-C17-C18
29	C	516	DGD	C5D-C6D-O5D-C1E
29	c	518	DGD	C5D-C6D-O5D-C1E
22	A	402	CLA	C4C-C3C-CAC-CBC
22	D	404	CLA	C16-C17-C18-C20
33	d	410	LHG	C25-C26-C27-C28
28	a	411	SQD	C30-C31-C32-C33
29	h	102	DGD	C7B-C8B-C9B-CAB
32	D	411	STE	C2-C3-C4-C5
22	B	616	CLA	C4-C3-C5-C6
29	c	518	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
32	d	413	STE	C5-C6-C7-C8
29	C	516	DGD	CDA-CEA-CFA-CGA
22	B	615	CLA	C16-C17-C18-C19
22	c	505	CLA	C16-C17-C18-C19
22	B	602	CLA	C14-C13-C15-C16
22	C	505	CLA	C6-C7-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	c	505	CLA	C6-C7-C8-C9
33	D	409	LHG	C2-C3-O3-P
33	d	410	LHG	C2-C3-O3-P
33	l	101	LHG	C11-C10-C9-C8
22	B	606	CLA	C4B-C3B-CAB-CBB
22	C	503	CLA	C4B-C3B-CAB-CBB
33	d	408	LHG	C33-C34-C35-C36
22	b	609	CLA	C16-C17-C18-C19
26	A	409	PL9	C15-C14-C16-C17
29	C	518	DGD	CBA-CCA-CDA-CEA
26	A	409	PL9	C13-C14-C16-C17
32	c	521	STE	C7-C8-C9-C10
29	c	518	DGD	C3B-C4B-C5B-C6B
29	h	102	DGD	C5A-C6A-C7A-C8A
29	c	518	DGD	C8B-C9B-CAB-CBB
32	b	623	STE	C9-C10-C11-C12
22	A	410	CLA	C11-C12-C13-C15
22	C	512	CLA	C6-C7-C8-C10
22	b	606	CLA	C6-C7-C8-C10
22	d	405	CLA	C12-C13-C15-C16
22	C	511	CLA	O1A-CGA-O2A-C1
32	T	103	STE	C12-C13-C14-C15
27	D	410	LMG	C29-C30-C31-C32
29	C	516	DGD	C2A-C3A-C4A-C5A
22	a	403	CLA	O1D-CGD-O2D-CED
22	C	508	CLA	C16-C17-C18-C19
22	A	402	CLA	C2C-C3C-CAC-CBC
32	b	625	STE	C5-C6-C7-C8
26	d	407	PL9	C32-C33-C34-C36
28	B	623	SQD	C28-C29-C30-C31
29	H	102	DGD	C2B-C3B-C4B-C5B
24	C	515	BCR	C11-C10-C9-C34
24	b	617	BCR	C6-C7-C8-C9
29	A	414	DGD	O6D-C1D-O3G-C3G
27	b	620	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
36	v	201	HEC	CAD-CBD-CGD-O1D
24	B	618	BCR	C19-C20-C21-C22
22	c	511	CLA	C8-C10-C11-C12
24	B	618	BCR	C37-C22-C23-C24
24	c	515	BCR	C7-C8-C9-C34
33	E	102	LHG	C19-C20-C21-C22
22	c	512	CLA	C5-C6-C7-C8
32	M	103	STE	C4-C5-C6-C7
35	f	101	HEM	C2A-CAA-CBA-CGA
33	E	102	LHG	C30-C31-C32-C33
29	h	102	DGD	O2G-C1B-C2B-C3B
22	C	502	CLA	C16-C17-C18-C20
22	b	611	CLA	C16-C17-C18-C19
22	b	601	CLA	C2A-CAA-CBA-CGA
22	C	503	CLA	C15-C16-C17-C18
27	b	622	LMG	O1-C7-C8-C9
32	m	101	STE	C4-C5-C6-C7
22	B	604	CLA	C11-C10-C8-C9
22	C	501	CLA	C14-C13-C15-C16
22	C	505	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	b	606	CLA	C6-C7-C8-C9
22	c	510	CLA	C14-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C9
22	d	405	CLA	C14-C13-C15-C16
27	d	412	LMG	C15-C16-C17-C18
32	C	521	STE	C14-C15-C16-C17
32	D	411	STE	C11-C12-C13-C14
32	c	521	STE	C3-C4-C5-C6
27	c	523	LMG	C7-C8-O7-C10
22	b	614	CLA	C10-C11-C12-C13
23	d	402	PHO	C1A-C2A-CAA-CBA
24	c	514	BCR	C15-C16-C17-C18
32	d	413	STE	O2-C1-C2-C3
27	b	622	LMG	C29-C30-C31-C32
22	B	614	CLA	C2A-CAA-CBA-CGA
22	B	602	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C23-C24-C25-C30
24	C	515	BCR	C5-C6-C7-C8
24	b	617	BCR	C5-C6-C7-C8
24	d	406	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C30
24	k	101	BCR	C5-C6-C7-C8
32	d	413	STE	O1-C1-C2-C3
29	c	518	DGD	CDA-CEA-CFA-CGA
23	D	401	PHO	C2C-C3C-CAC-CBC
27	b	622	LMG	C29-C28-O8-C9
32	C	521	STE	C9-C10-C11-C12
33	D	408	LHG	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
27	d	411	LMG	O7-C10-C11-C12
32	c	521	STE	O1-C1-C2-C3
36	V	201	HEC	CAD-CBD-CGD-O2D
36	v	201	HEC	CAD-CBD-CGD-O2D
22	B	605	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
27	A	411	LMG	C28-C29-C30-C31
27	B	621	LMG	O9-C10-C11-C12
32	b	621	STE	O1-C1-C2-C3
35	f	101	HEM	CAD-CBD-CGD-O1D
22	A	410	CLA	C6-C7-C8-C10
22	B	613	CLA	C11-C12-C13-C15
22	C	505	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	b	616	CLA	C11-C10-C8-C7
22	c	502	CLA	C6-C7-C8-C10
22	c	512	CLA	C11-C12-C13-C15
22	B	601	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
33	B	622	LHG	O7-C5-C6-O8
32	D	411	STE	C13-C14-C15-C16
32	b	624	STE	O1-C1-C2-C3
29	A	414	DGD	O6D-C5D-C6D-O5D
29	C	517	DGD	C8A-C9A-CAA-CBA
24	h	101	BCR	C7-C8-C9-C34
22	c	506	CLA	C4-C3-C5-C6
27	B	621	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C5-C6-C7-C8
32	B	625	STE	O2-C1-C2-C3
28	A	412	SQD	C34-C35-C36-C37
33	D	409	LHG	C17-C18-C19-C20
27	B	621	LMG	C28-C29-C30-C31
32	E	103	STE	C6-C7-C8-C9
33	D	408	LHG	C11-C10-C9-C8
33	B	622	LHG	C29-C30-C31-C32
22	C	502	CLA	C4-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
22	d	403	CLA	C4-C3-C5-C6
22	B	612	CLA	C13-C15-C16-C17
22	C	510	CLA	C8-C10-C11-C12
35	f	101	HEM	CAD-CBD-CGD-O2D
36	V	201	HEC	CAD-CBD-CGD-O1D
26	a	409	PL9	C23-C24-C26-C27
22	b	604	CLA	C8-C10-C11-C12
22	B	602	CLA	C15-C16-C17-C18
29	H	102	DGD	O1A-C1A-O1G-C1G
29	C	518	DGD	C9A-CAA-CBA-CCA
33	d	408	LHG	C31-C32-C33-C34
27	D	410	LMG	C7-C8-C9-O8
29	C	516	DGD	O1G-C1G-C2G-C3G
27	B	621	LMG	O7-C10-C11-C12
32	b	621	STE	O2-C1-C2-C3
32	b	624	STE	O2-C1-C2-C3
32	c	521	STE	O2-C1-C2-C3
33	D	409	LHG	C12-C13-C14-C15
29	C	516	DGD	C8A-C9A-CAA-CBA
28	A	413	SQD	C16-C17-C18-C19
32	a	414	STE	C7-C8-C9-C10
22	c	510	CLA	C4-C3-C5-C6
24	C	515	BCR	C15-C16-C17-C18
24	c	516	BCR	C13-C14-C15-C16
32	c	521	STE	C4-C5-C6-C7
22	d	404	CLA	O1D-CGD-O2D-CED
22	C	506	CLA	C16-C17-C18-C19
22	d	404	CLA	C2C-C3C-CAC-CBC
24	a	405	BCR	C11-C10-C9-C34
22	b	608	CLA	C4C-C3C-CAC-CBC
22	b	610	CLA	C10-C11-C12-C13
32	B	624	STE	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	B	625	STE	O1-C1-C2-C3
22	B	610	CLA	C16-C17-C18-C20
22	B	611	CLA	C16-C17-C18-C20
22	B	609	CLA	C4-C3-C5-C6
27	b	622	LMG	O1-C7-C8-O7
28	L	101	SQD	O6-C44-C45-O47
29	c	517	DGD	O1G-C1G-C2G-O2G
35	E	101	HEM	CAD-CBD-CGD-O1D
22	c	510	CLA	C2-C3-C5-C6
32	B	626	STE	C11-C12-C13-C14
22	b	607	CLA	C5-C6-C7-C8
22	c	501	CLA	C11-C12-C13-C15
32	B	627	STE	C2-C3-C4-C5
32	C	522	STE	C7-C8-C9-C10
32	B	624	STE	O1-C1-C2-C3
36	v	201	HEC	C2B-C3B-CAB-CBB
26	A	409	PL9	C44-C46-C47-C48
22	A	410	CLA	C11-C12-C13-C14
22	B	603	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C14
27	b	620	LMG	C18-C19-C20-C21
27	b	622	LMG	C14-C15-C16-C17
22	C	501	CLA	C2A-CAA-CBA-CGA
22	d	405	CLA	C16-C17-C18-C19
33	D	408	LHG	C35-C36-C37-C38
29	H	102	DGD	C7B-C8B-C9B-CAB
22	C	512	CLA	C3A-C2A-CAA-CBA
28	B	623	SQD	C19-C20-C21-C22
22	c	507	CLA	C2-C3-C5-C6
22	d	405	CLA	C8-C10-C11-C12
32	b	624	STE	C1-C2-C3-C4
27	M	101	LMG	C9-C8-O7-C10
32	b	621	STE	C4-C5-C6-C7
22	a	403	CLA	C13-C15-C16-C17
27	D	410	LMG	C11-C12-C13-C14
24	c	516	BCR	C11-C10-C9-C8
22	B	607	CLA	C15-C16-C17-C18
32	d	413	STE	C11-C10-C9-C8
29	c	519	DGD	C1B-C2B-C3B-C4B
33	B	622	LHG	C24-C23-O8-C6
32	D	411	STE	O2-C1-C2-C3
28	L	101	SQD	C44-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
29	c	517	DGD	C1G-C2G-C3G-O3G
35	f	101	HEM	C4B-C3B-CAB-CBB
27	d	411	LMG	O9-C10-C11-C12
27	b	620	LMG	C32-C33-C34-C35
22	C	505	CLA	O1D-CGD-O2D-CED
22	d	405	CLA	C2-C3-C5-C6
22	A	403	CLA	C16-C17-C18-C19
28	a	410	SQD	C14-C15-C16-C17
27	M	101	LMG	C36-C37-C38-C39
33	E	102	LHG	C16-C17-C18-C19
22	b	613	CLA	CAA-CBA-CGA-O2A
33	D	408	LHG	C33-C34-C35-C36
33	E	102	LHG	C35-C36-C37-C38
28	A	413	SQD	C17-C18-C19-C20
22	B	601	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	C	506	CLA	C14-C13-C15-C16
22	C	510	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C10-C8-C9
22	b	607	CLA	C14-C13-C15-C16
33	l	101	LHG	O7-C7-C8-C9
27	D	407	LMG	C13-C14-C15-C16
22	C	507	CLA	C5-C6-C7-C8
29	c	517	DGD	O1G-C1A-C2A-C3A
22	C	502	CLA	C2-C3-C5-C6
22	A	403	CLA	C12-C13-C15-C16
22	B	601	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	B	612	CLA	C11-C10-C8-C7
22	B	615	CLA	C12-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C7
22	b	605	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7
22	b	611	CLA	C12-C13-C15-C16
22	b	614	CLA	C11-C12-C13-C15
22	c	508	CLA	C11-C10-C8-C7
22	c	510	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
29	C	517	DGD	C3B-C4B-C5B-C6B
22	B	606	CLA	C2B-C3B-CAB-CBB
22	C	503	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	D	403	CLA	C2B-C3B-CAB-CBB
22	c	507	CLA	C2B-C3B-CAB-CBB
24	A	406	BCR	C1-C6-C7-C8
24	A	406	BCR	C5-C6-C7-C8
24	B	618	BCR	C23-C24-C25-C26
24	C	515	BCR	C23-C24-C25-C30
24	Y	101	BCR	C23-C24-C25-C30
24	b	618	BCR	C23-C24-C25-C26
24	b	618	BCR	C23-C24-C25-C30
24	c	514	BCR	C1-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	c	516	BCR	C23-C24-C25-C26
24	c	516	BCR	C23-C24-C25-C30
24	t	101	BCR	C5-C6-C7-C8
27	d	412	LMG	C32-C33-C34-C35
32	B	626	STE	C11-C10-C9-C8
22	A	402	CLA	C2-C1-O2A-CGA
22	B	613	CLA	C2-C1-O2A-CGA
22	a	402	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
33	L	102	LHG	C9-C10-C11-C12
26	A	409	PL9	C9-C11-C12-C13
22	B	613	CLA	C16-C17-C18-C19
22	a	404	CLA	C4-C3-C5-C6
28	F	101	SQD	C23-C24-C25-C26
22	B	612	CLA	CAA-CBA-CGA-O2A
22	b	612	CLA	CAA-CBA-CGA-O2A
22	B	609	CLA	C2-C3-C5-C6
35	E	101	HEM	CAD-CBD-CGD-O2D
22	C	512	CLA	C2A-CAA-CBA-CGA
22	b	602	CLA	C2A-CAA-CBA-CGA
22	C	508	CLA	C8-C10-C11-C12
27	b	620	LMG	O8-C28-C29-C30
22	c	508	CLA	O1D-CGD-O2D-CED
27	M	101	LMG	C40-C41-C42-C43
32	c	524	STE	C3-C4-C5-C6
22	b	601	CLA	CAA-CBA-CGA-O2A
22	B	616	CLA	C2-C3-C5-C6
32	C	522	STE	C4-C5-C6-C7
29	c	518	DGD	CAB-CBB-CCB-CDB
29	c	517	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
22	b	612	CLA	C8-C10-C11-C12
29	a	412	DGD	C7A-C8A-C9A-CAA
22	A	410	CLA	C6-C7-C8-C9
22	B	610	CLA	C14-C13-C15-C16
22	c	501	CLA	C11-C12-C13-C14
22	c	508	CLA	C11-C10-C8-C9
27	D	407	LMG	C37-C38-C39-C40
32	C	520	STE	C1-C2-C3-C4
28	A	412	SQD	O47-C7-C8-C9
33	L	102	LHG	O7-C7-C8-C9
27	c	520	LMG	C36-C37-C38-C39
27	D	407	LMG	O10-C28-O8-C9
29	C	516	DGD	C1G-C2G-C3G-O3G
22	B	601	CLA	C4B-C3B-CAB-CBB
22	b	603	CLA	C4B-C3B-CAB-CBB
29	C	516	DGD	O6E-C1E-O5D-C6D
29	C	517	DGD	O6D-C1D-O3G-C3G
29	A	414	DGD	O2G-C1B-C2B-C3B
33	e	101	LHG	C12-C13-C14-C15
27	M	101	LMG	O6-C5-C6-O5
32	l	102	STE	C9-C10-C11-C12
28	a	411	SQD	C29-C30-C31-C32
28	a	410	SQD	O47-C7-C8-C9
27	b	622	LMG	C32-C33-C34-C35
28	L	101	SQD	C25-C26-C27-C28
32	B	624	STE	C3-C4-C5-C6
23	A	404	PHO	C16-C17-C18-C20
22	B	613	CLA	CAA-CBA-CGA-O2A
22	b	602	CLA	C8-C10-C11-C12
32	B	627	STE	C4-C5-C6-C7
22	d	403	CLA	C2C-C3C-CAC-CBC
28	a	410	SQD	C5-C6-S-O7
33	d	408	LHG	C35-C36-C37-C38
22	C	506	CLA	C2-C1-O2A-CGA
22	b	608	CLA	C2-C1-O2A-CGA
29	c	519	DGD	C4B-C5B-C6B-C7B
22	B	606	CLA	C11-C12-C13-C15
22	B	611	CLA	C11-C12-C13-C15
22	C	504	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	a	403	CLA	C11-C10-C8-C7
22	b	614	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	d	403	CLA	C11-C12-C13-C15
22	b	615	CLA	C8-C10-C11-C12
32	D	411	STE	O1-C1-C2-C3
22	C	505	CLA	C16-C17-C18-C19
29	h	102	DGD	CCA-CDA-CEA-CFA
33	D	408	LHG	C13-C14-C15-C16
22	c	512	CLA	C15-C16-C17-C18
28	L	101	SQD	C14-C15-C16-C17
29	h	102	DGD	O1B-C1B-C2B-C3B
22	c	502	CLA	C16-C17-C18-C19
29	c	519	DGD	C2B-C3B-C4B-C5B
27	B	621	LMG	O10-C28-C29-C30
22	c	510	CLA	CAA-CBA-CGA-O2A
33	D	408	LHG	O10-C23-O8-C6
22	b	611	CLA	C10-C11-C12-C13
22	c	503	CLA	C10-C11-C12-C13
22	B	602	CLA	C3A-C2A-CAA-CBA
32	I	101	STE	C6-C7-C8-C9
27	C	519	LMG	C36-C37-C38-C39
22	B	612	CLA	CAA-CBA-CGA-O1A
29	c	518	DGD	O1A-C1A-C2A-C3A
33	e	101	LHG	O10-C23-C24-C25
22	B	611	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	B	615	CLA	C14-C13-C15-C16
22	C	508	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C10-C8-C9
22	c	512	CLA	C14-C13-C15-C16
29	C	516	DGD	CAA-CBA-CCA-CDA
33	B	622	LHG	O10-C23-O8-C6
22	b	602	CLA	O1D-CGD-O2D-CED
32	I	101	STE	C5-C6-C7-C8
28	a	410	SQD	C35-C36-C37-C38
22	B	603	CLA	C13-C15-C16-C17
28	B	623	SQD	O5-C5-C6-S
29	A	414	DGD	O1B-C1B-C2B-C3B
22	a	404	CLA	C15-C16-C17-C18
22	b	613	CLA	CAA-CBA-CGA-O1A
29	c	517	DGD	O1B-C1B-C2B-C3B
33	l	101	LHG	O9-C7-C8-C9
33	B	622	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
28	A	412	SQD	C23-C24-C25-C26
23	d	402	PHO	C5-C6-C7-C8
27	M	101	LMG	C8-C7-O1-C1
27	B	621	LMG	O8-C28-C29-C30
28	A	413	SQD	O10-C23-C24-C25
33	d	408	LHG	O8-C23-C24-C25
29	H	102	DGD	C5B-C6B-C7B-C8B
27	b	622	LMG	O10-C28-C29-C30
28	a	411	SQD	O10-C23-C24-C25
22	d	404	CLA	C4C-C3C-CAC-CBC
22	B	610	CLA	C10-C11-C12-C13
24	Y	101	BCR	C13-C14-C15-C16
22	b	601	CLA	CAA-CBA-CGA-O1A
22	b	612	CLA	CAA-CBA-CGA-O1A
22	A	410	CLA	C4C-C3C-CAC-CBC
22	B	607	CLA	CAD-CBD-CGD-O2D
22	c	513	CLA	CAD-CBD-CGD-O2D
23	A	404	PHO	CAD-CBD-CGD-O2D
23	d	401	PHO	CAD-CBD-CGD-O2D
29	C	516	DGD	O1B-C1B-C2B-C3B
33	d	408	LHG	C10-C11-C12-C13
32	a	414	STE	O2-C1-C2-C3
22	b	611	CLA	C13-C15-C16-C17
33	e	101	LHG	O8-C23-C24-C25
33	D	408	LHG	C28-C29-C30-C31
26	A	409	PL9	C2-C3-C7-C8
29	C	517	DGD	C9B-CAB-CBB-CCB
22	b	610	CLA	C13-C15-C16-C17
29	C	517	DGD	C2B-C3B-C4B-C5B

There are no ring outliers.

112 monomers are involved in 157 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	f	102	SQD	2	0
22	c	507	CLA	2	0
22	b	602	CLA	1	0
27	D	410	LMG	1	0
22	A	405	CLA	1	0
22	C	509	CLA	3	0
22	b	608	CLA	1	0
32	x	101	STE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	E	102	LHG	1	0
27	b	620	LMG	1	0
22	c	513	CLA	1	0
26	a	409	PL9	5	0
33	d	410	LHG	1	0
23	A	404	PHO	1	0
22	B	604	CLA	3	0
23	d	402	PHO	1	0
36	v	201	HEC	1	0
24	Y	101	BCR	2	0
22	b	615	CLA	2	0
23	D	401	PHO	2	0
22	B	612	CLA	1	0
22	c	501	CLA	2	0
22	c	506	CLA	1	0
32	D	411	STE	2	0
22	c	505	CLA	2	0
35	E	101	HEM	2	0
22	b	605	CLA	2	0
22	b	606	CLA	4	0
22	c	512	CLA	1	0
33	L	102	LHG	1	0
22	c	503	CLA	2	0
29	a	412	DGD	4	0
26	d	407	PL9	1	0
32	T	102	STE	1	0
30	A	415[B]	OEY	2	0
22	B	614	CLA	2	0
28	a	410	SQD	2	0
32	C	521	STE	1	0
32	a	414	STE	2	0
33	e	101	LHG	2	0
24	c	516	BCR	1	0
22	c	511	CLA	2	0
29	A	414	DGD	5	0
30	a	415[B]	OEY	1	0
22	B	606	CLA	2	0
35	f	101	HEM	4	0
22	D	404	CLA	1	0
29	C	516	DGD	1	0
32	d	413	STE	2	0
26	D	406	PL9	2	0

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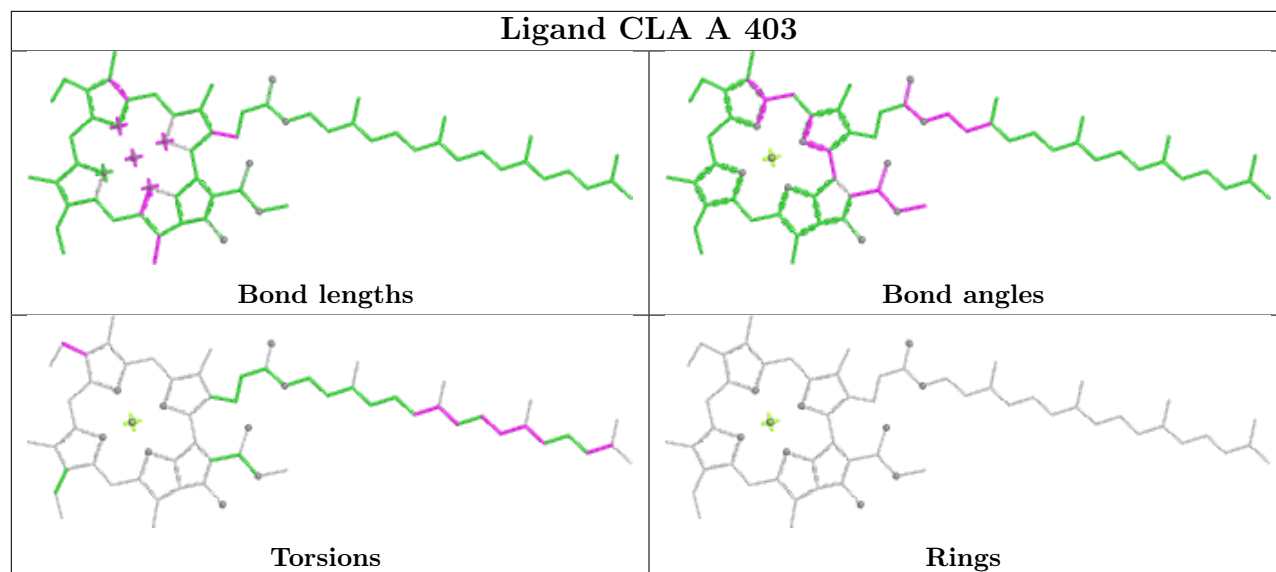
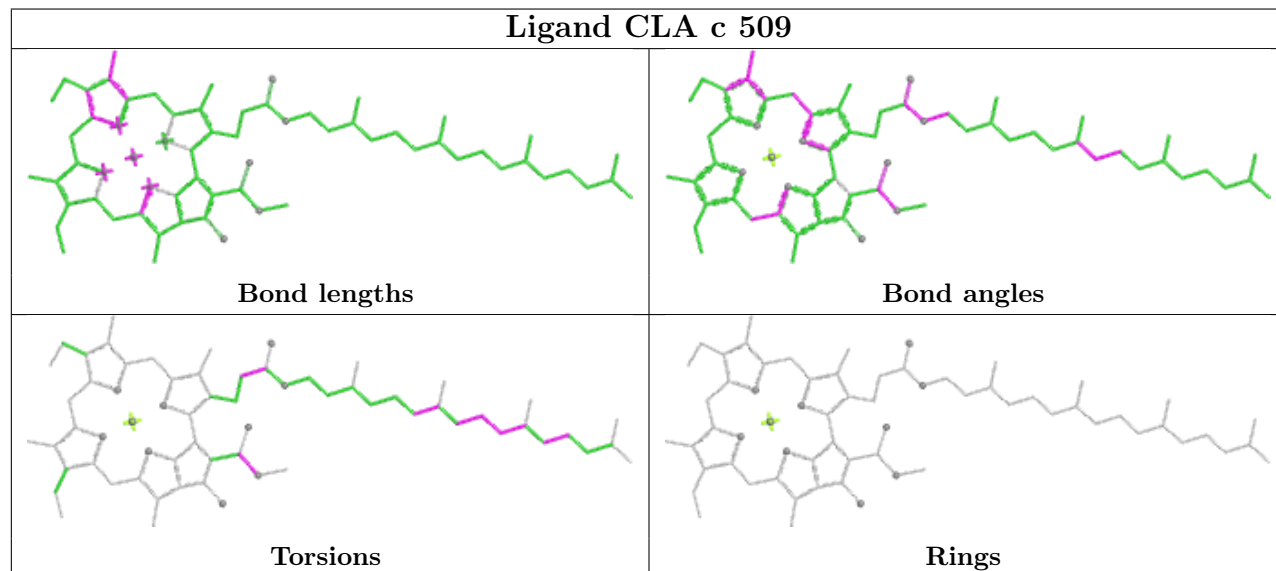
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	T	101	BCR	1	0
22	C	506	CLA	1	0
22	D	403	CLA	2	0
22	B	601	CLA	3	0
28	L	101	SQD	1	0
24	c	515	BCR	2	0
22	C	511	CLA	1	0
22	c	502	CLA	1	0
22	B	616	CLA	2	0
22	b	604	CLA	1	0
24	t	101	BCR	2	0
32	I	101	STE	3	0
22	C	513	CLA	2	0
22	a	404	CLA	1	0
33	d	409	LHG	4	0
36	V	201	HEC	1	0
22	B	609	CLA	1	0
32	l	102	STE	1	0
24	K	101	BCR	1	0
32	b	621	STE	1	0
22	b	603	CLA	1	0
29	c	519	DGD	2	0
22	d	405	CLA	2	0
33	d	408	LHG	3	0
32	t	102	STE	1	0
28	F	101	SQD	1	0
27	C	519	LMG	1	0
28	a	411	SQD	2	0
32	c	521	STE	1	0
22	C	502	CLA	1	0
27	c	523	LMG	1	0
24	B	619	BCR	2	0
22	b	616	CLA	2	0
22	C	508	CLA	1	0
24	H	101	BCR	1	0
24	a	405	BCR	1	0
22	B	605	CLA	5	0
22	B	615	CLA	2	0
32	H	103	STE	2	0
22	b	609	CLA	1	0
26	A	409	PL9	3	0
24	D	405	BCR	2	0

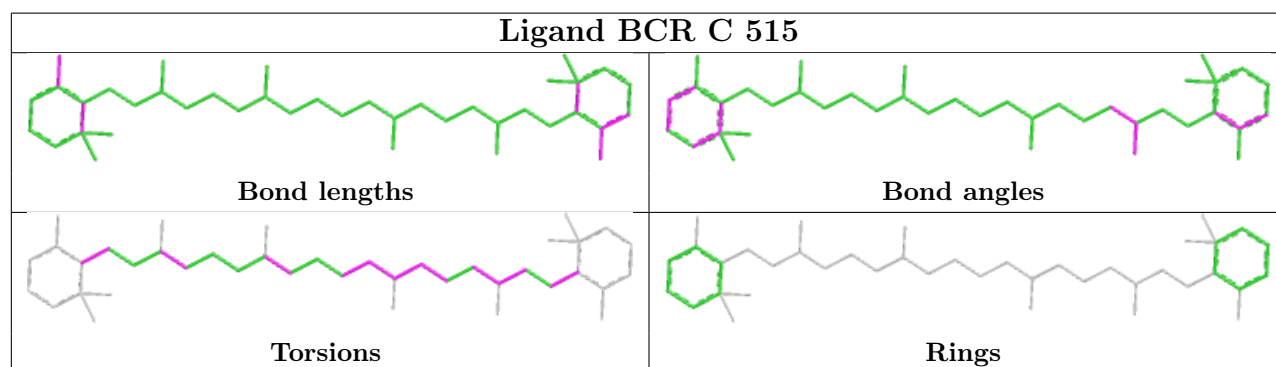
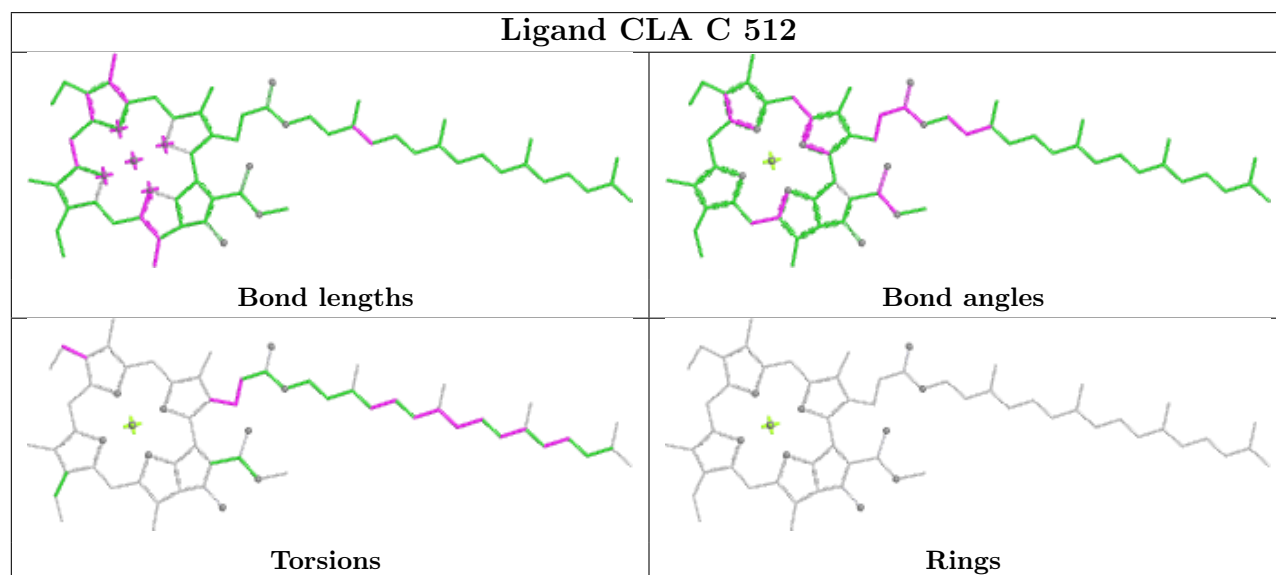
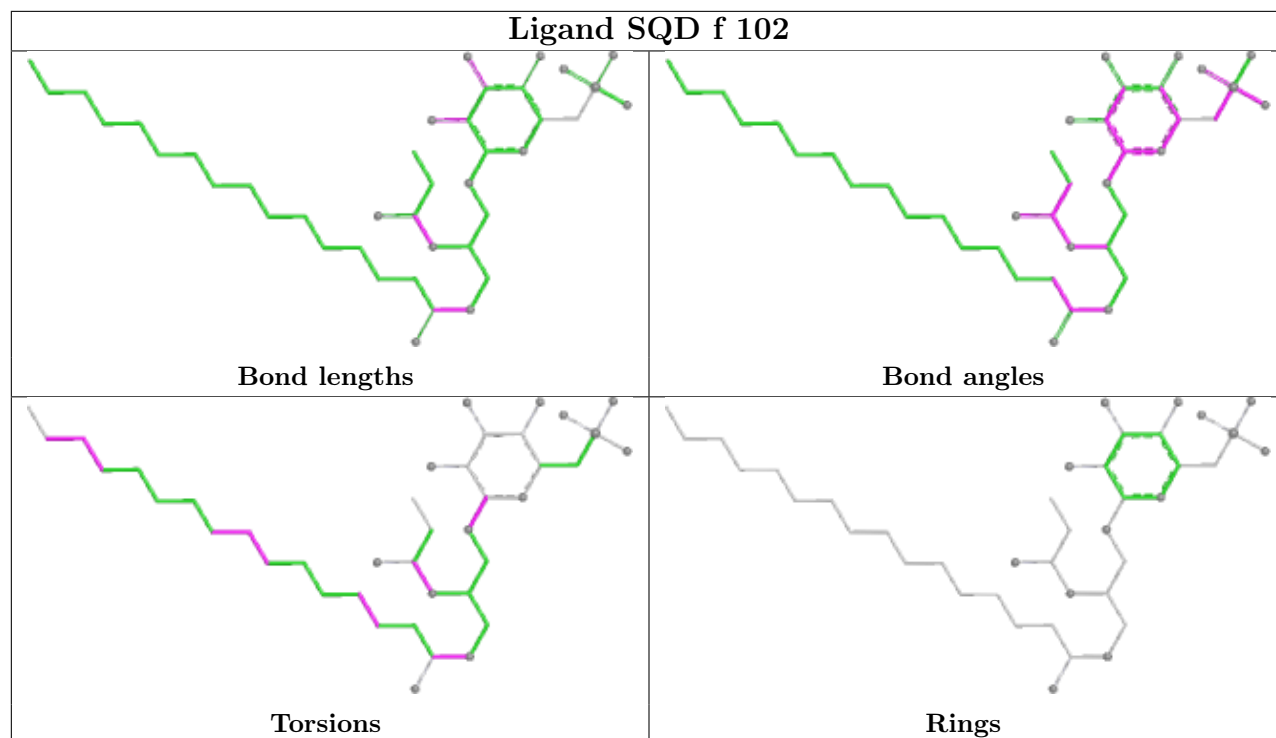
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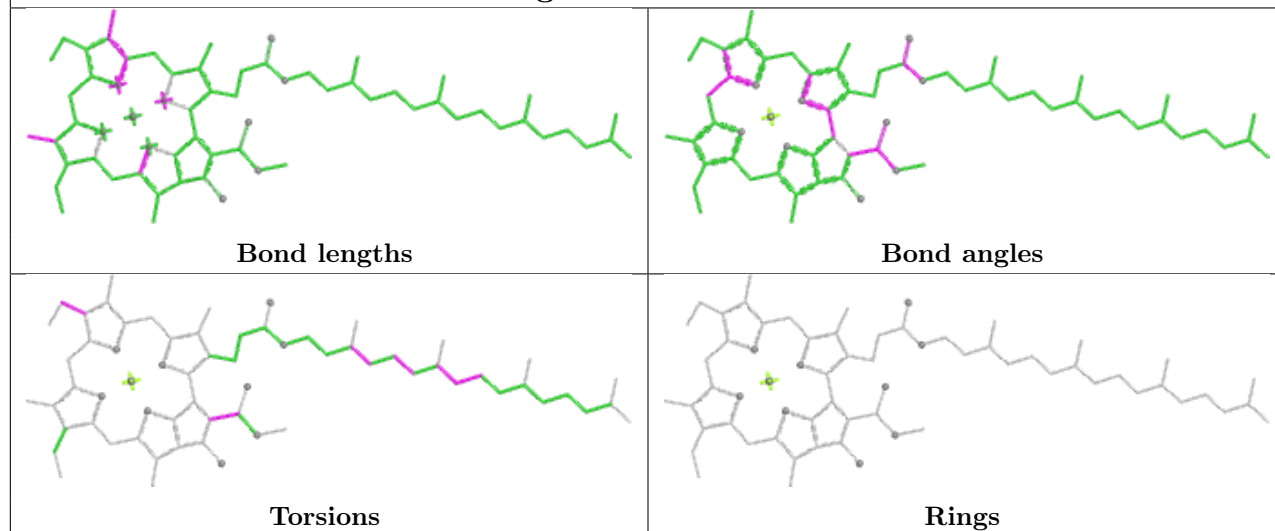
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	407	LMG	1	0
22	c	508	CLA	1	0
22	b	610	CLA	1	0
22	B	607	CLA	2	0
22	C	503	CLA	2	0
22	C	510	CLA	2	0
22	b	607	CLA	1	0
22	B	603	CLA	3	0
24	A	406	BCR	1	0
32	B	625	STE	1	0
22	B	611	CLA	1	0
33	l	101	LHG	2	0
24	d	406	BCR	2	0
22	C	501	CLA	1	0
33	B	622	LHG	1	0
22	c	510	CLA	2	0
33	D	408	LHG	2	0
27	M	101	LMG	2	0
24	b	617	BCR	1	0
24	C	514	BCR	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.

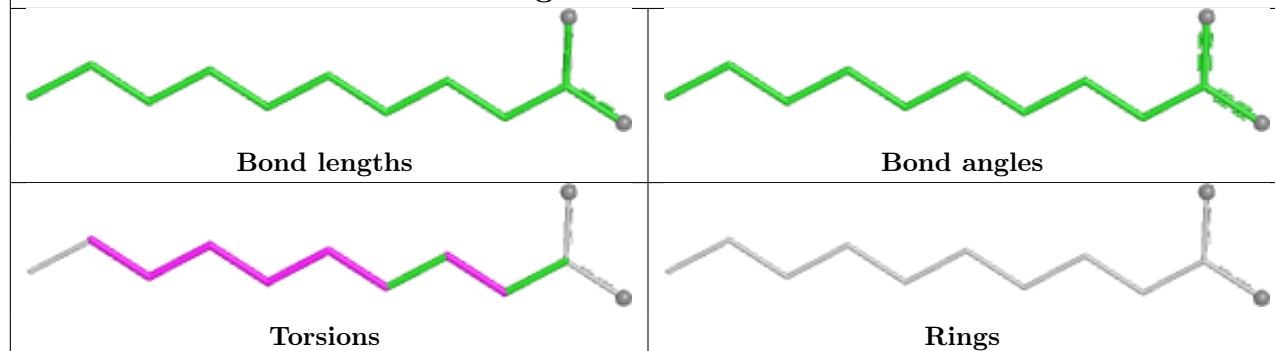
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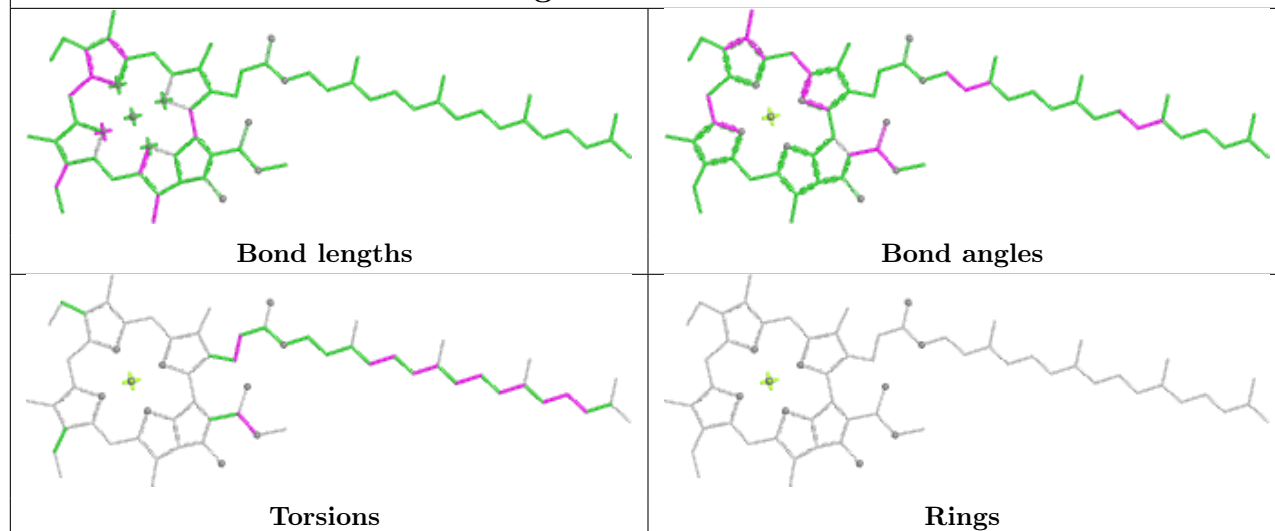
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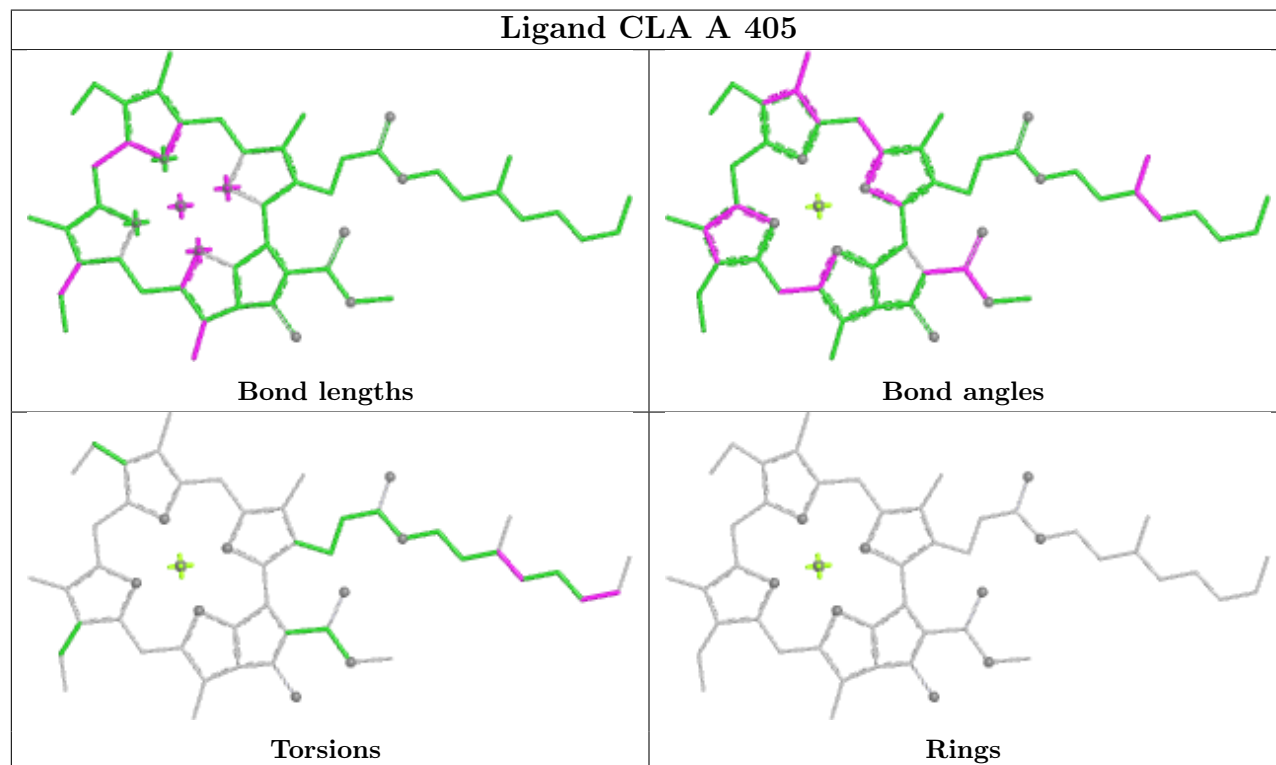
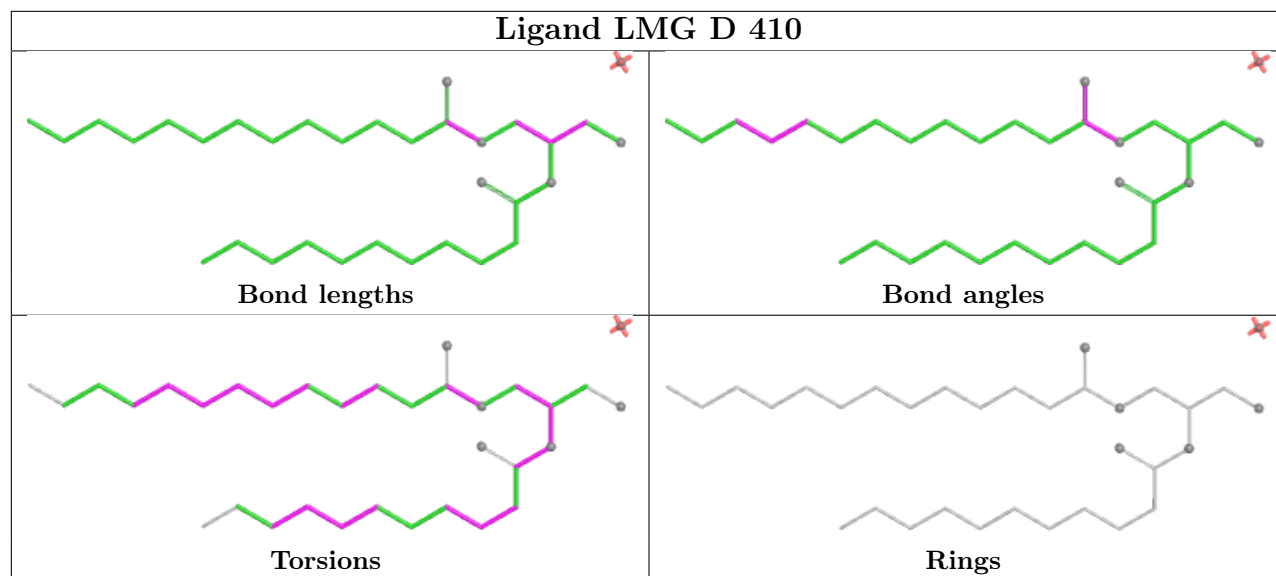


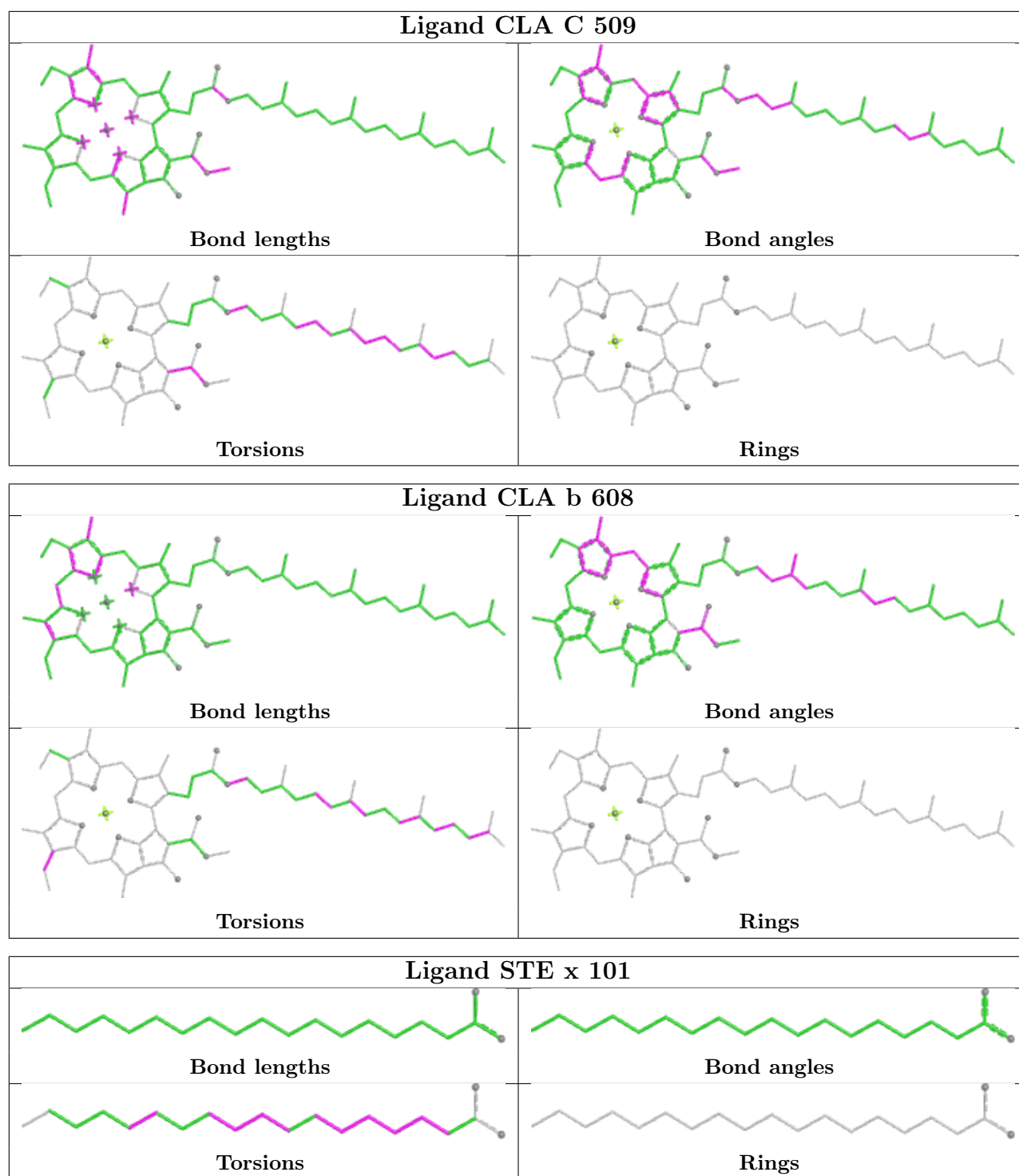
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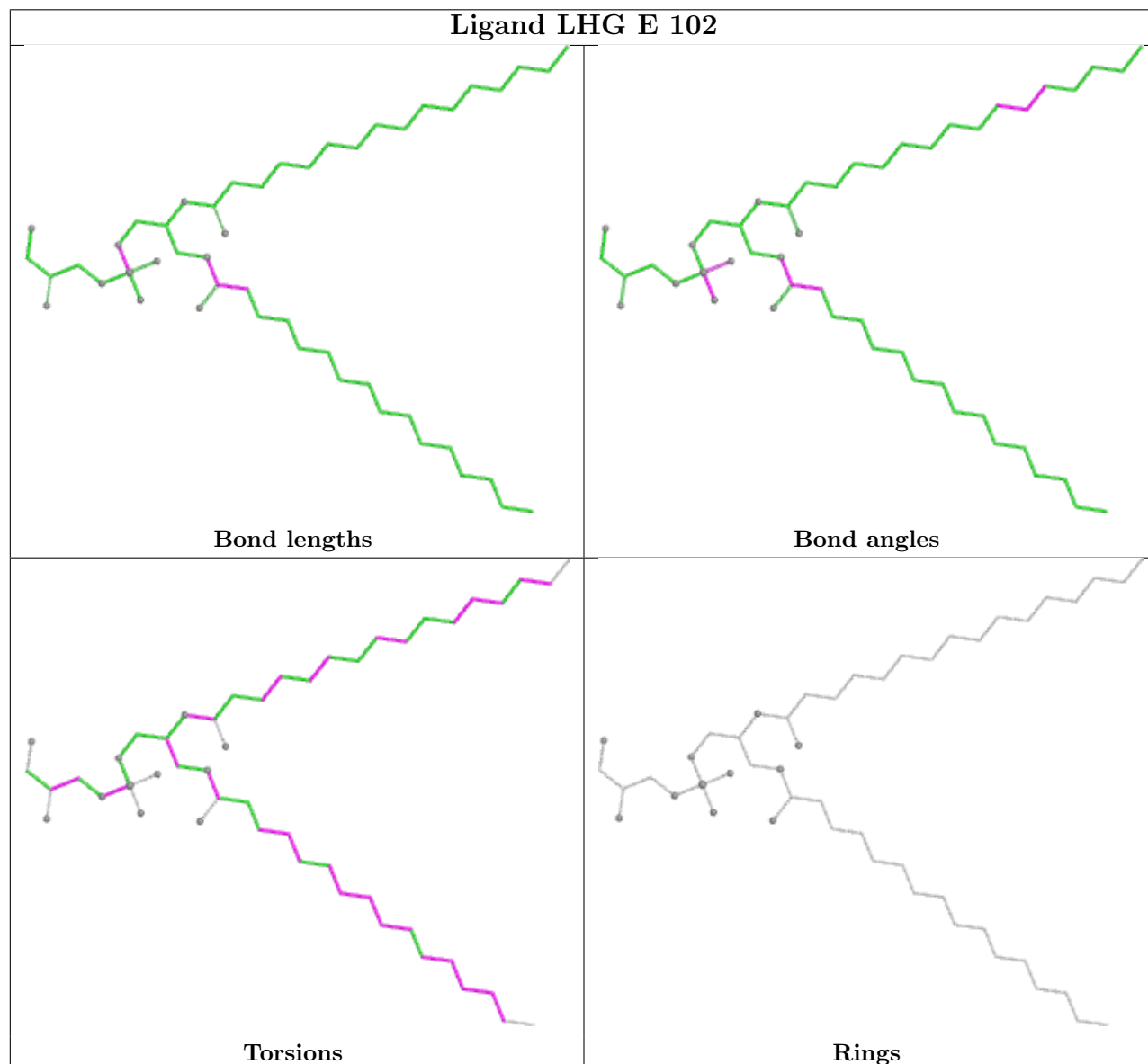
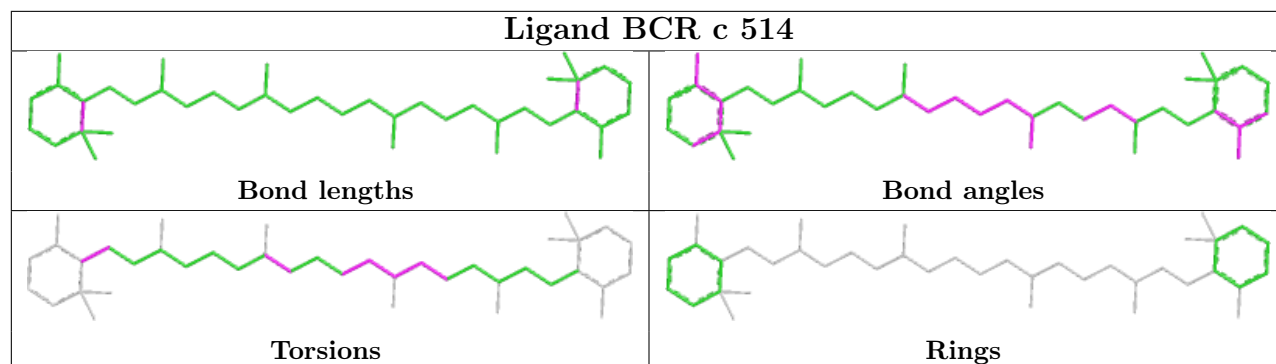


Ligand CLA b 602

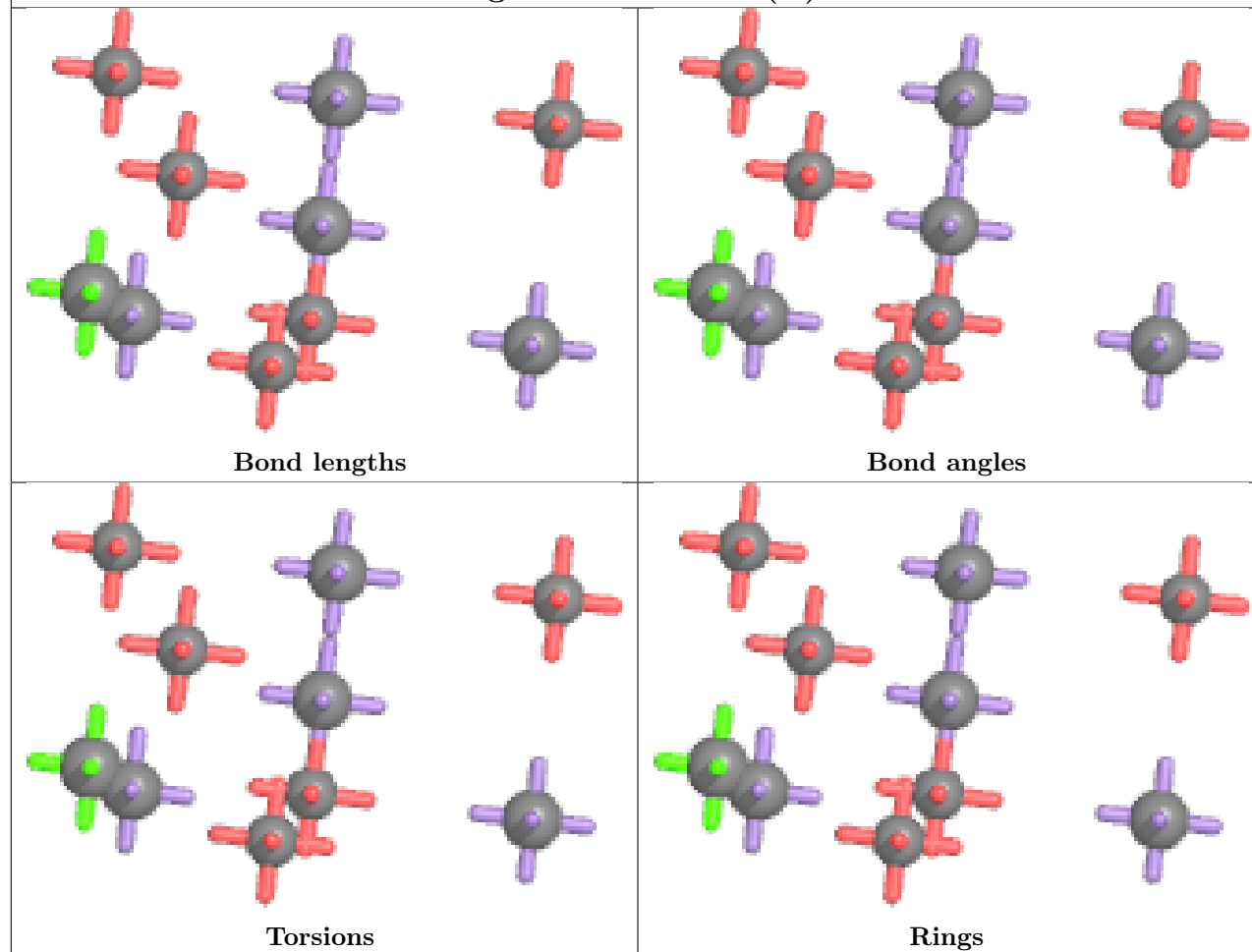




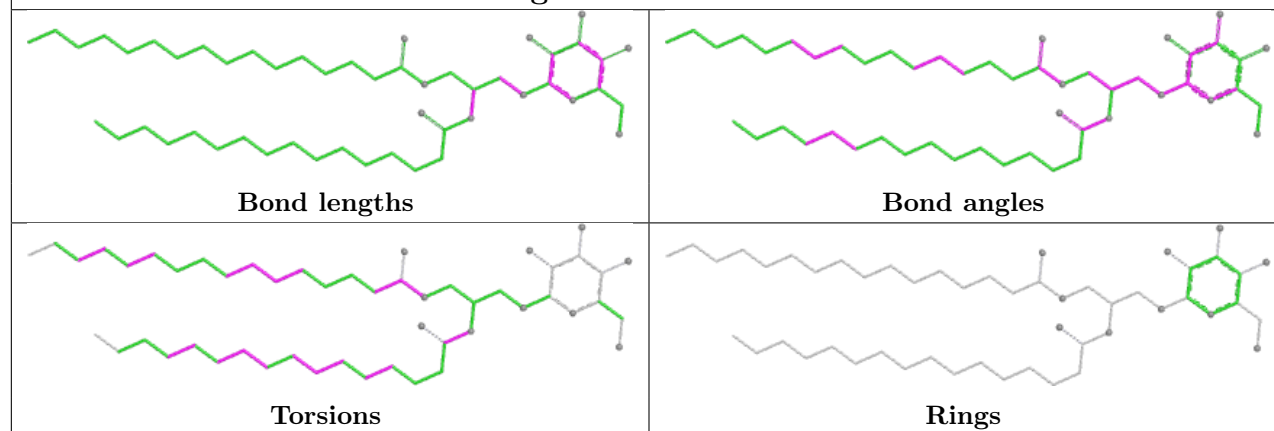


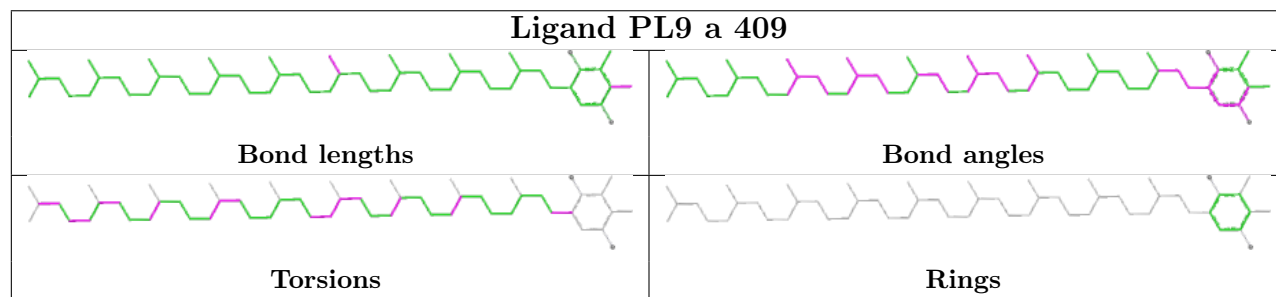
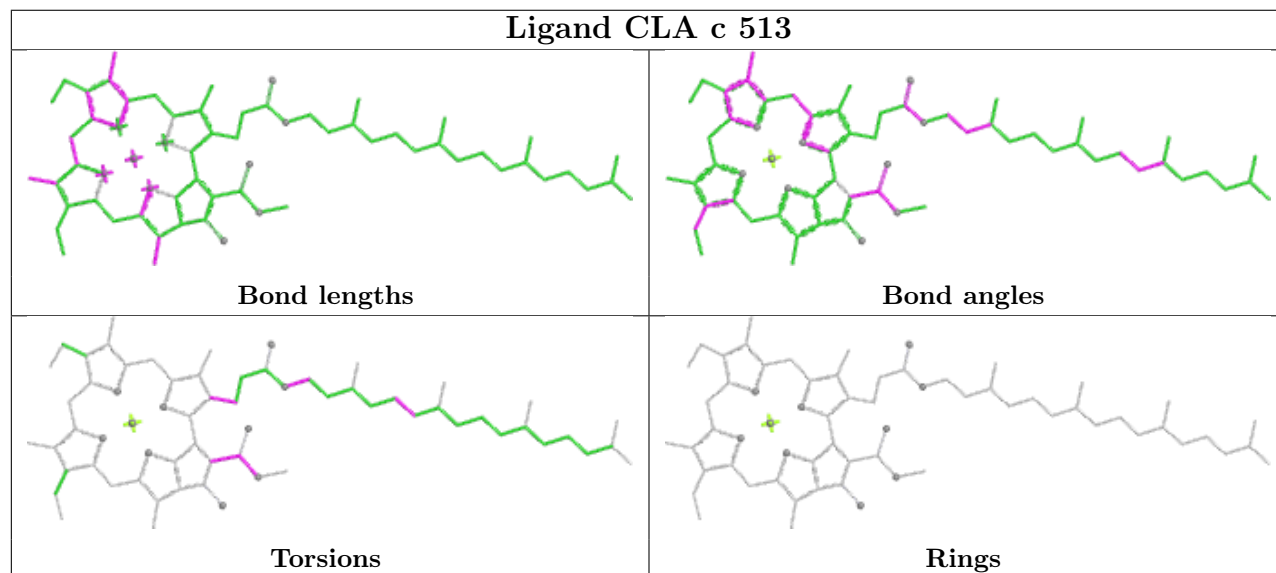
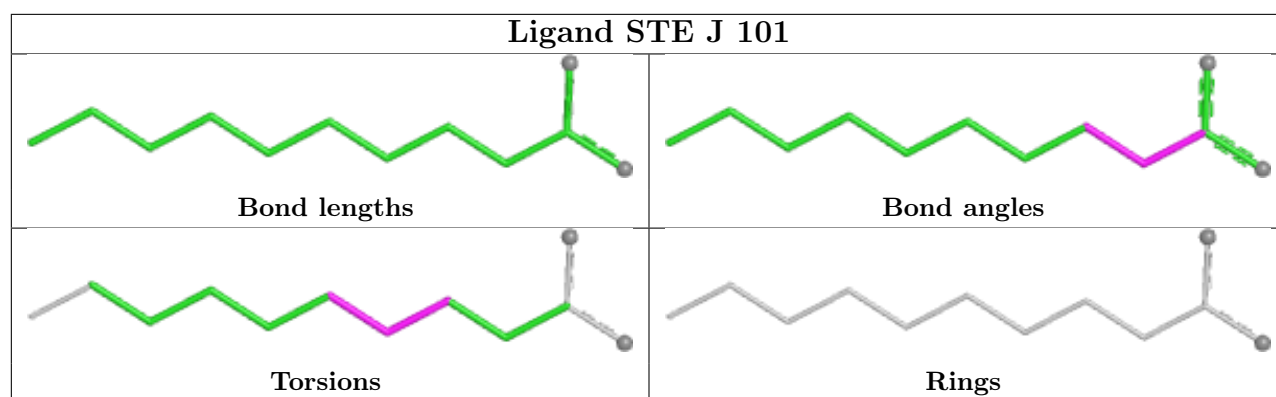


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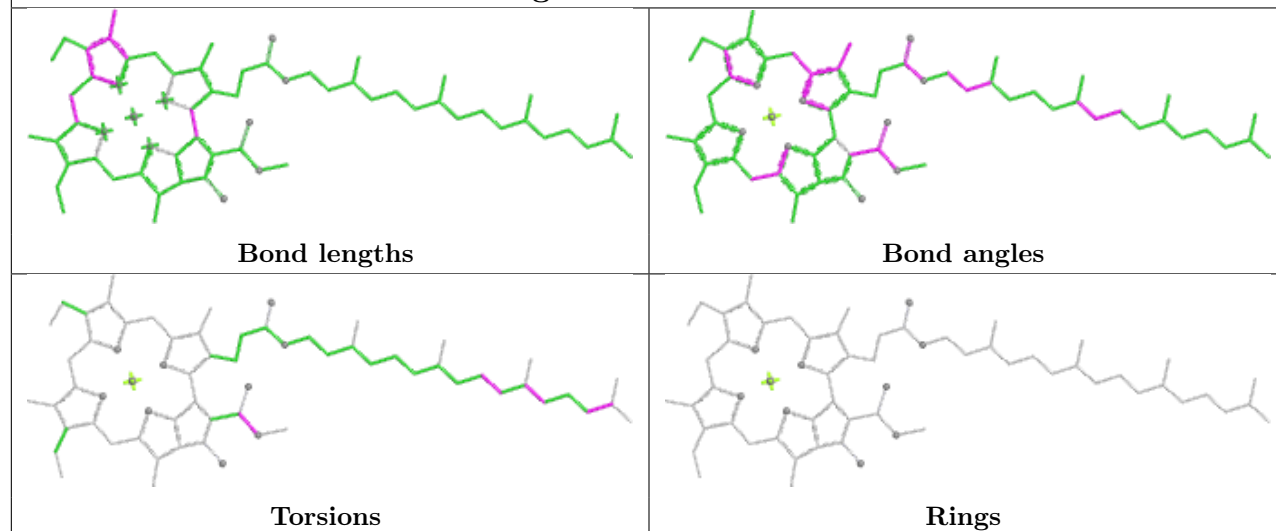


Ligand LMG b 620

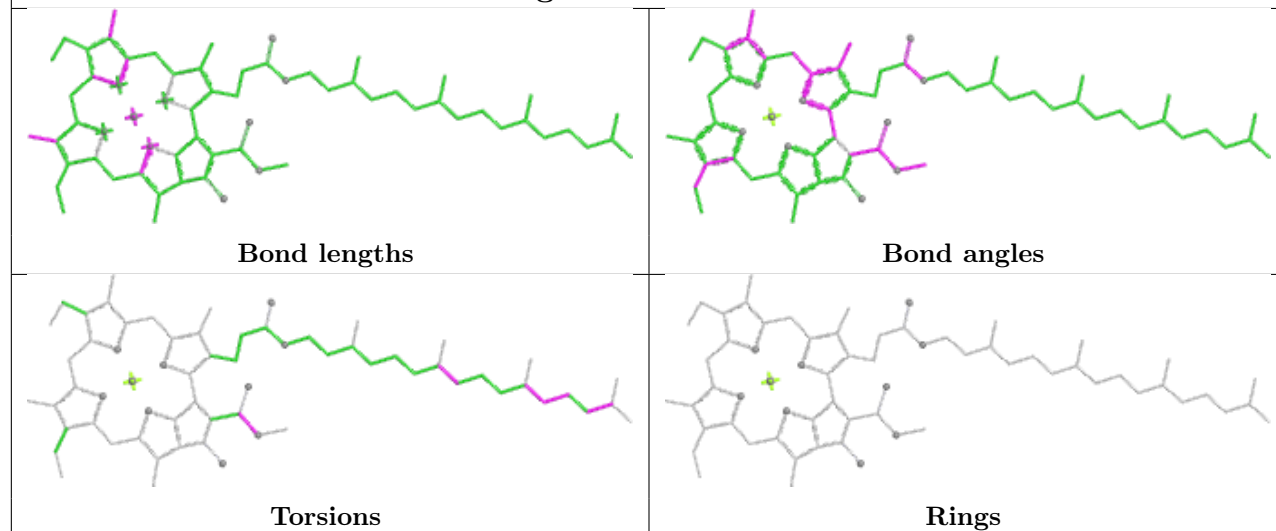




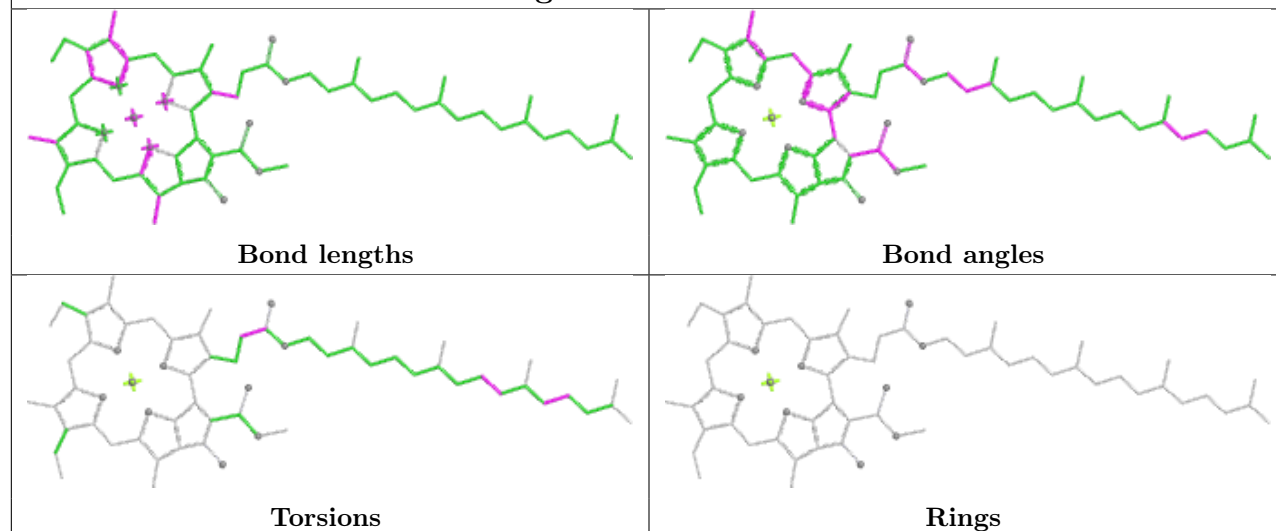
Ligand CLA B 610

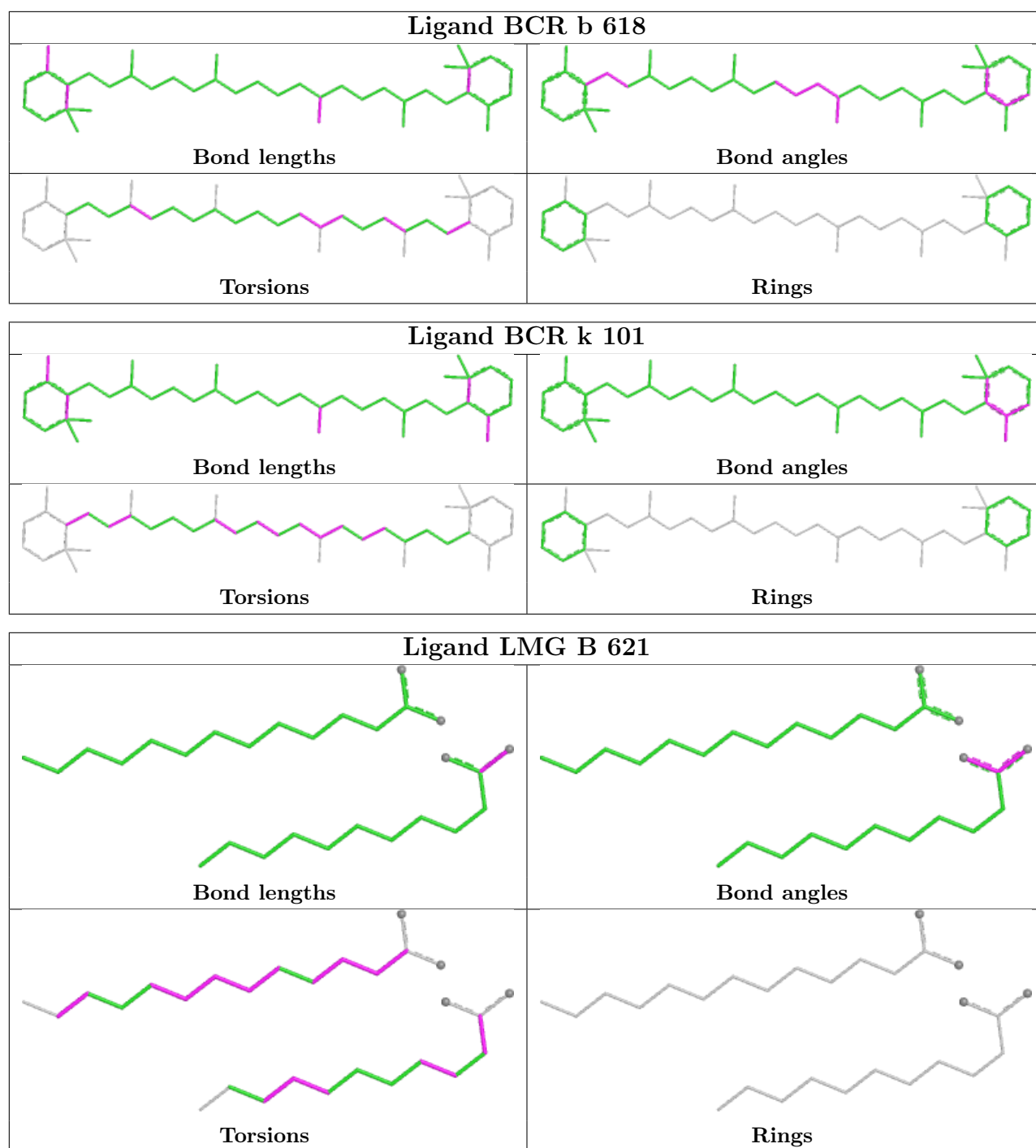


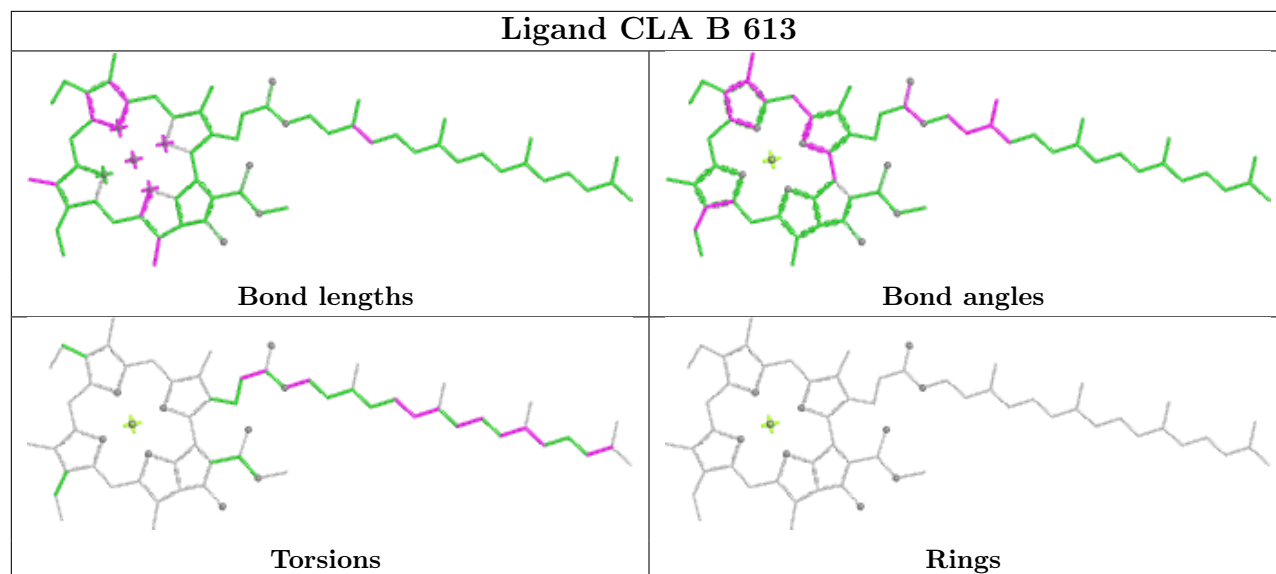
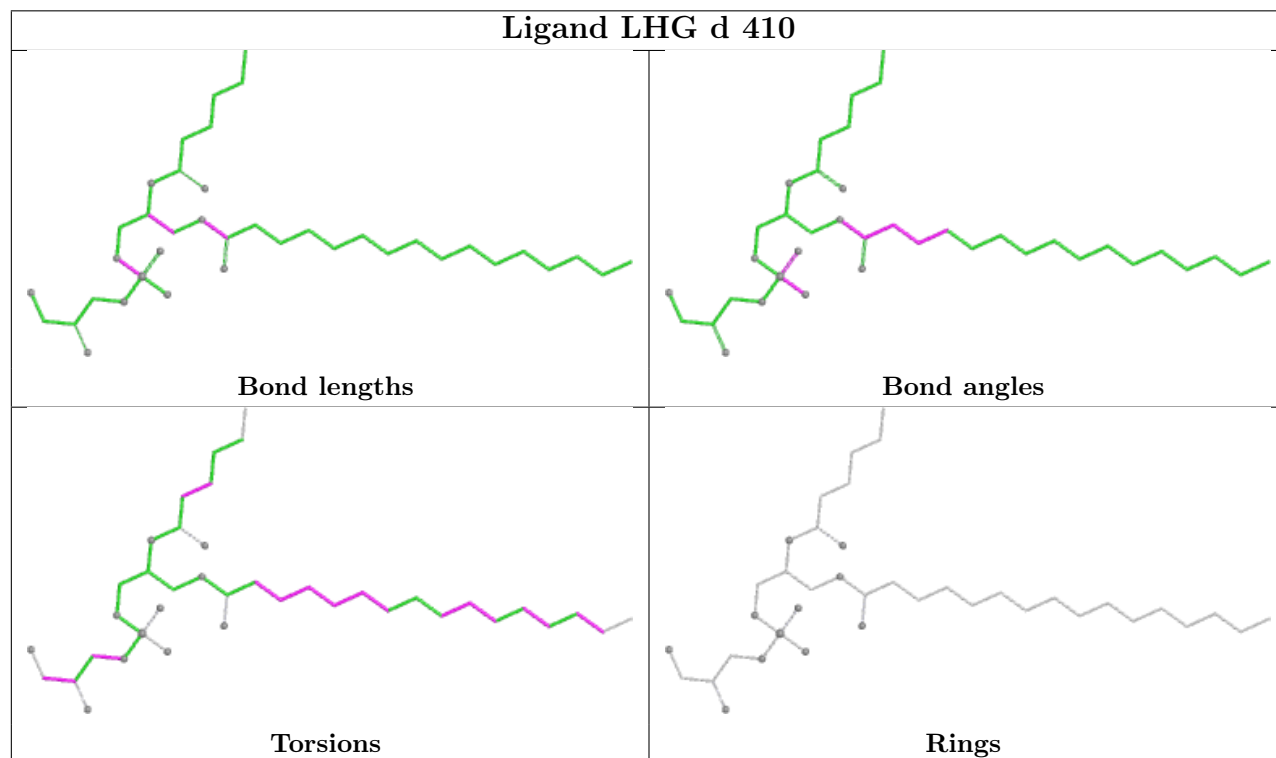
Ligand CLA a 403

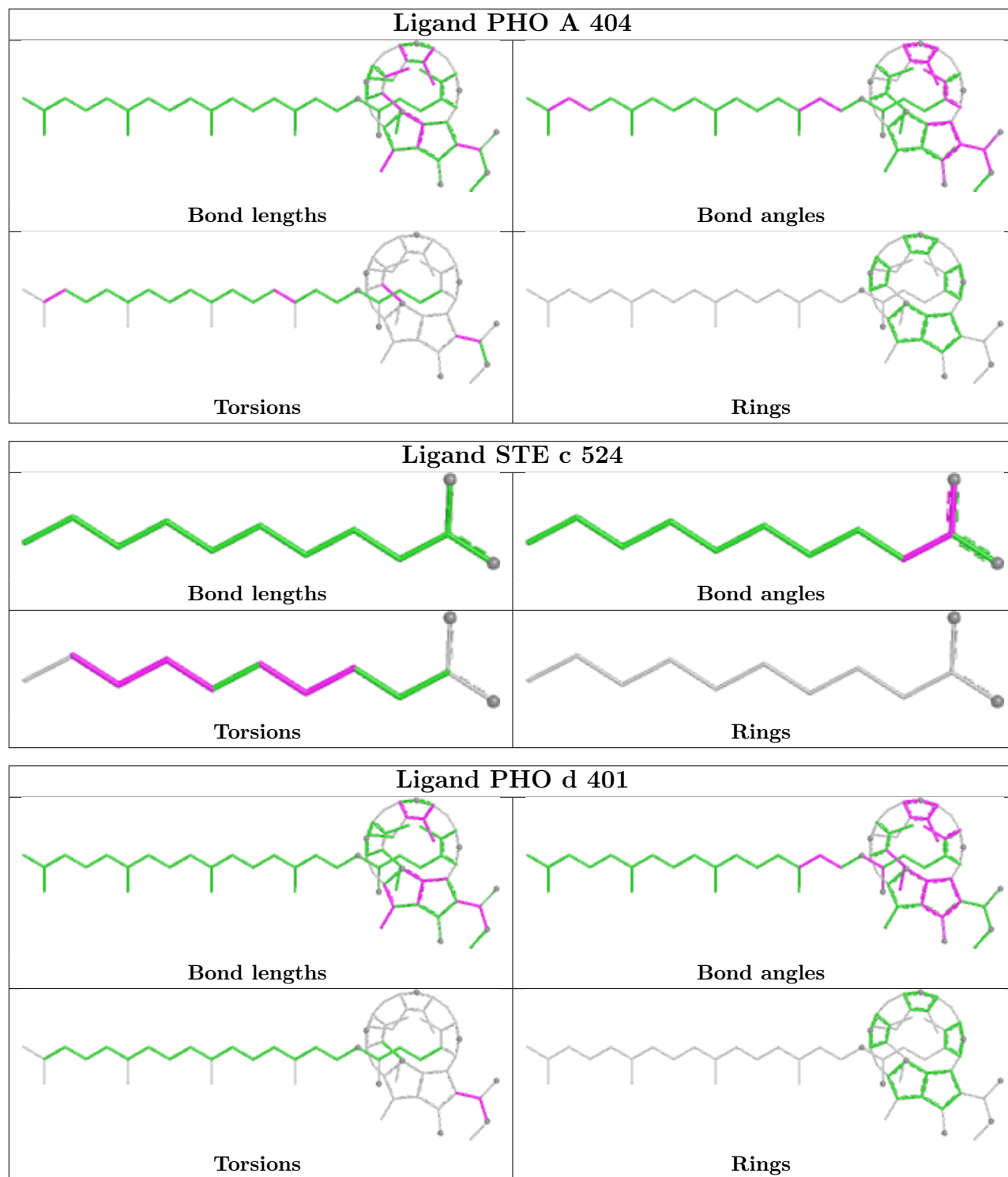


Ligand CLA b 613

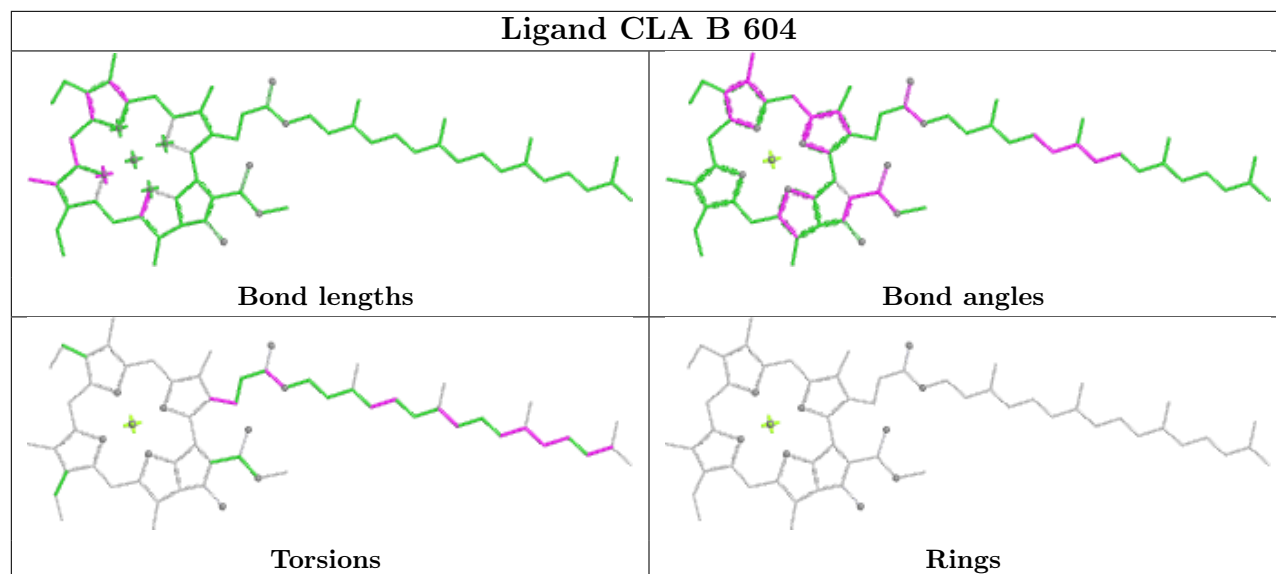




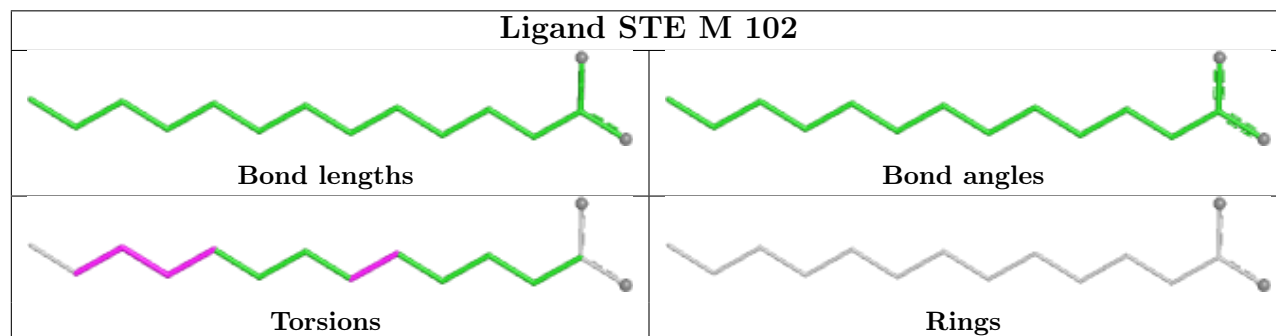
Ligand CLA B 613**Ligand LHG d 410**



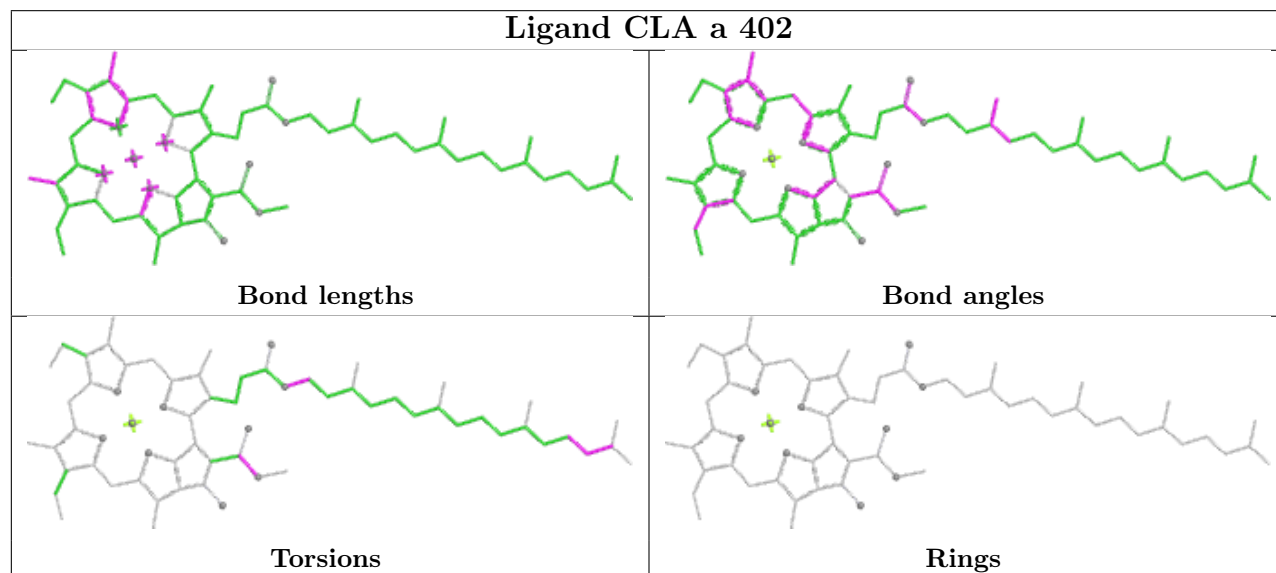
Ligand CLA B 604



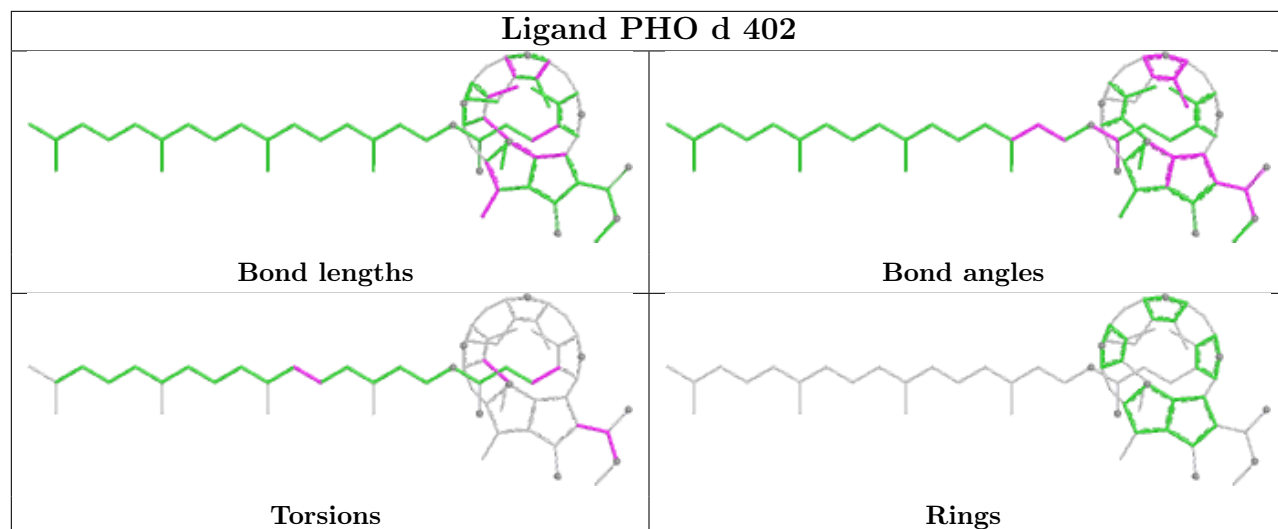
Ligand STE M 102



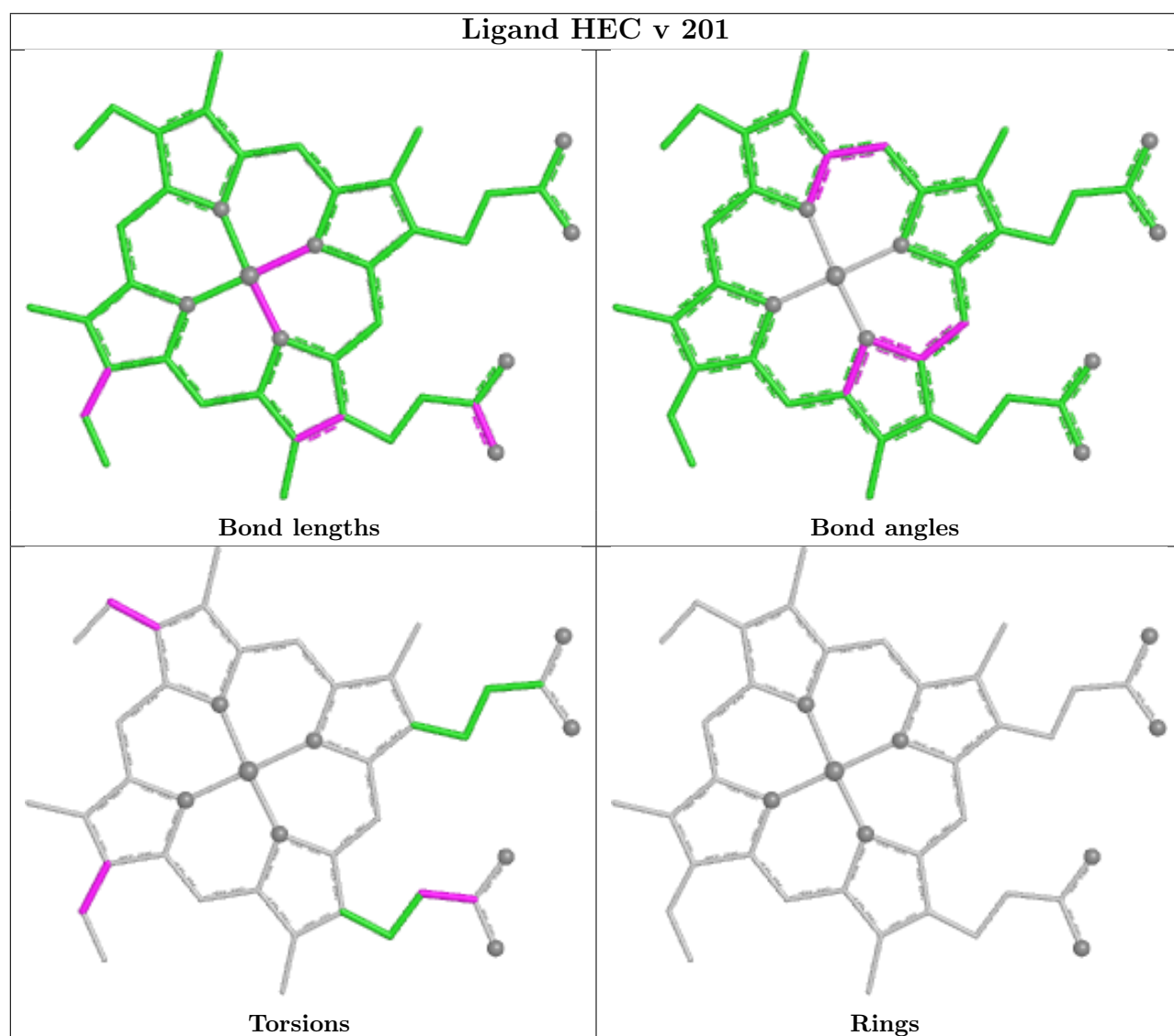
Ligand CLA a 402



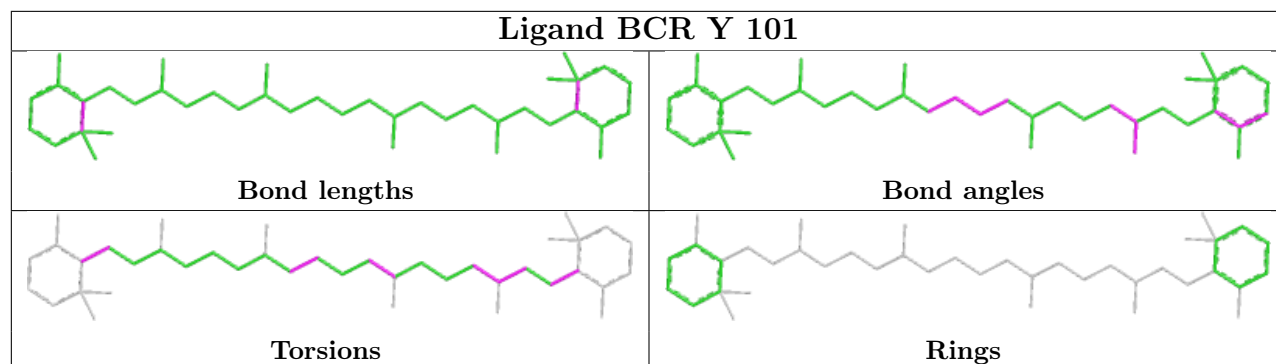
Ligand PHO d 402



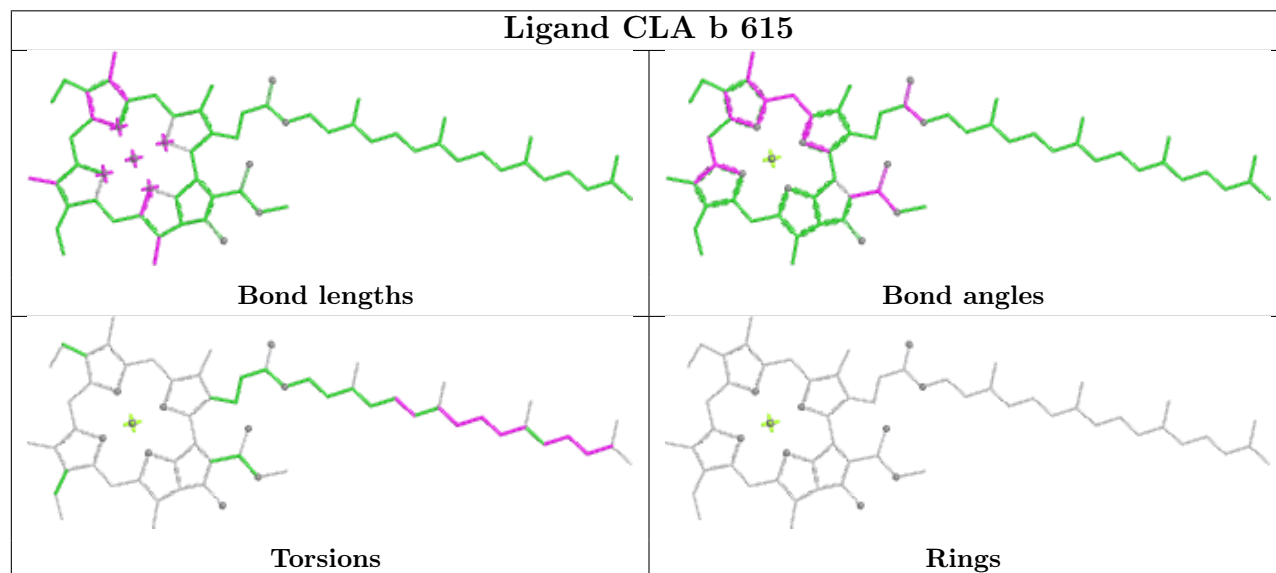
Ligand HEC v 201



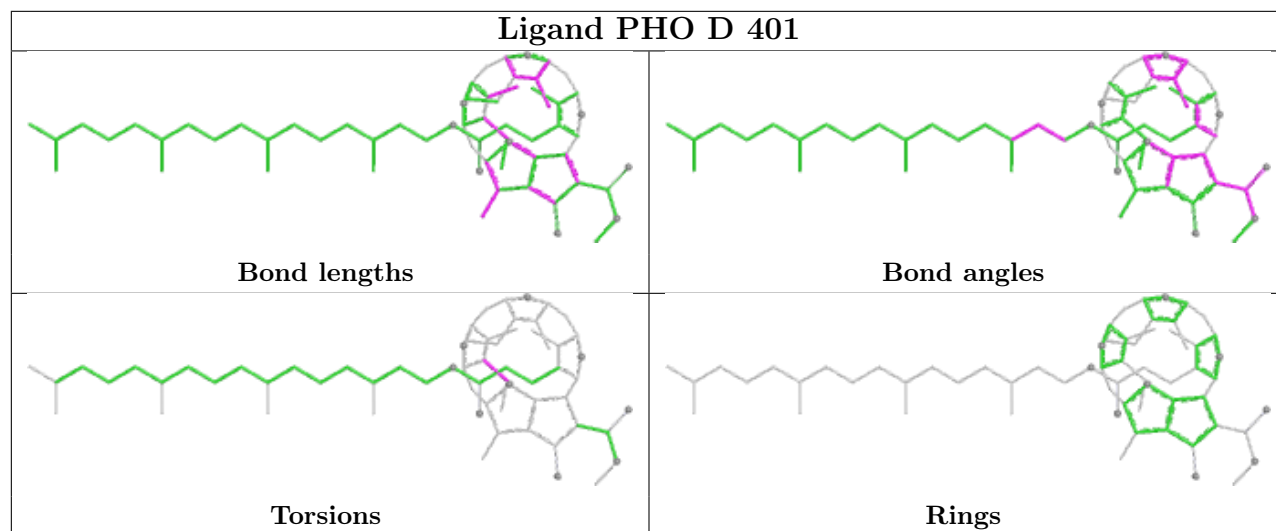
Ligand BCR Y 101



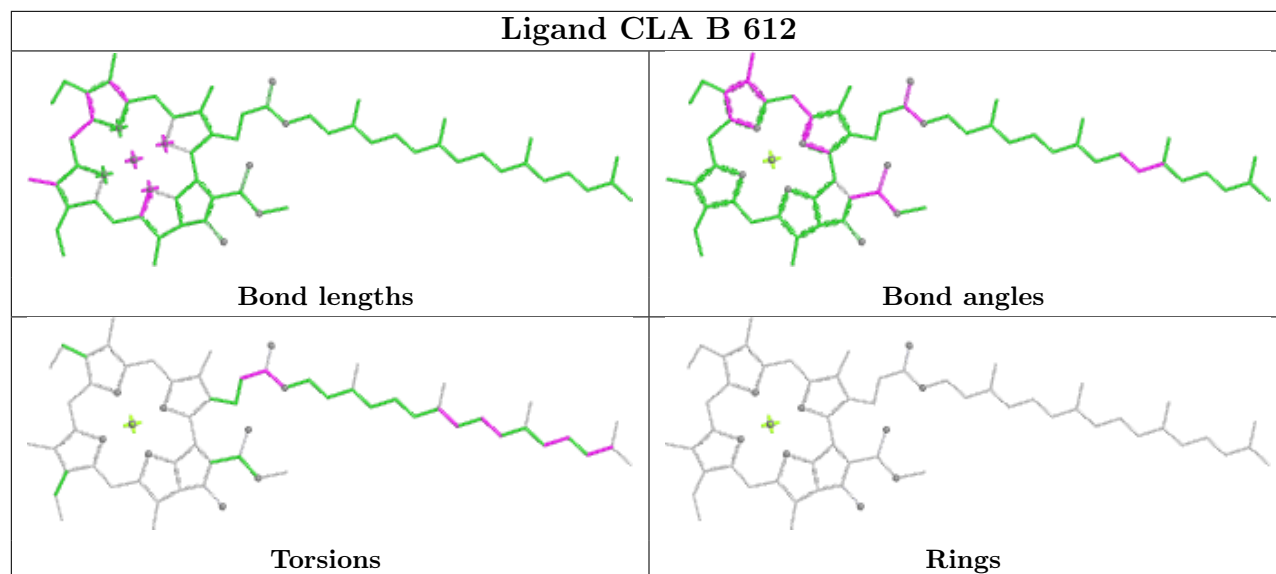
Ligand CLA b 615



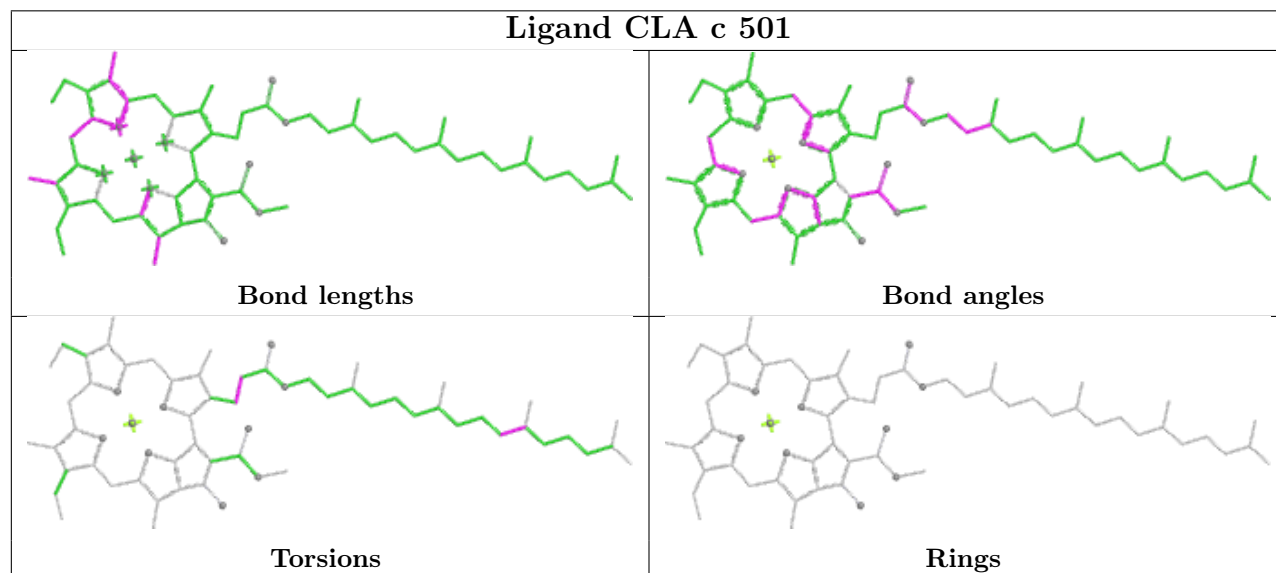
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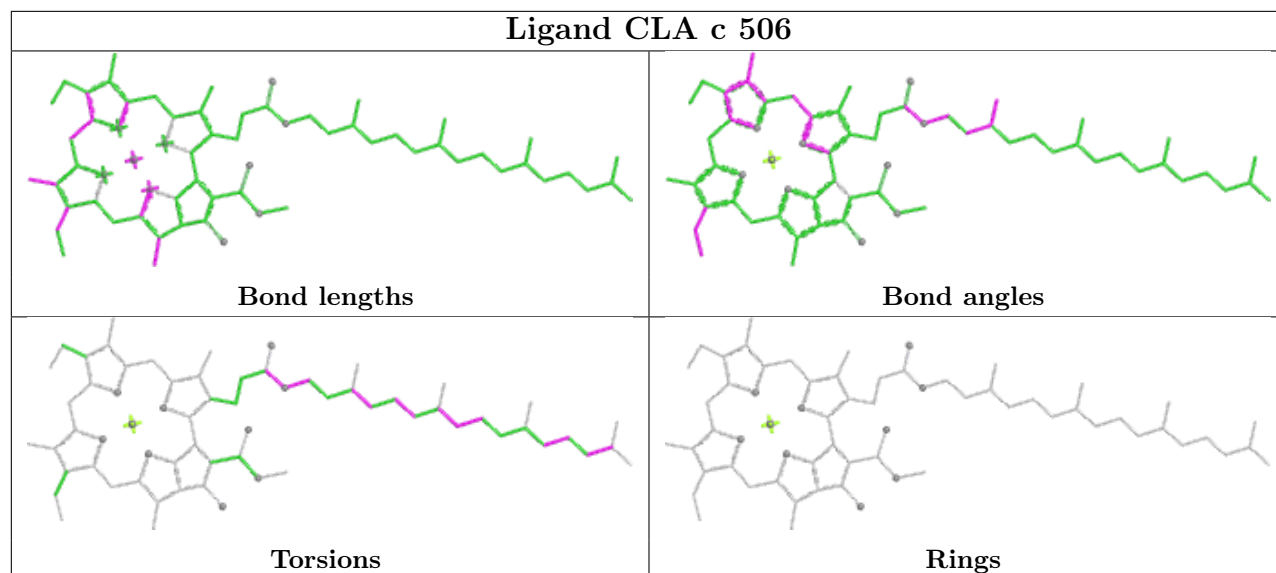
Ligand CLA B 612

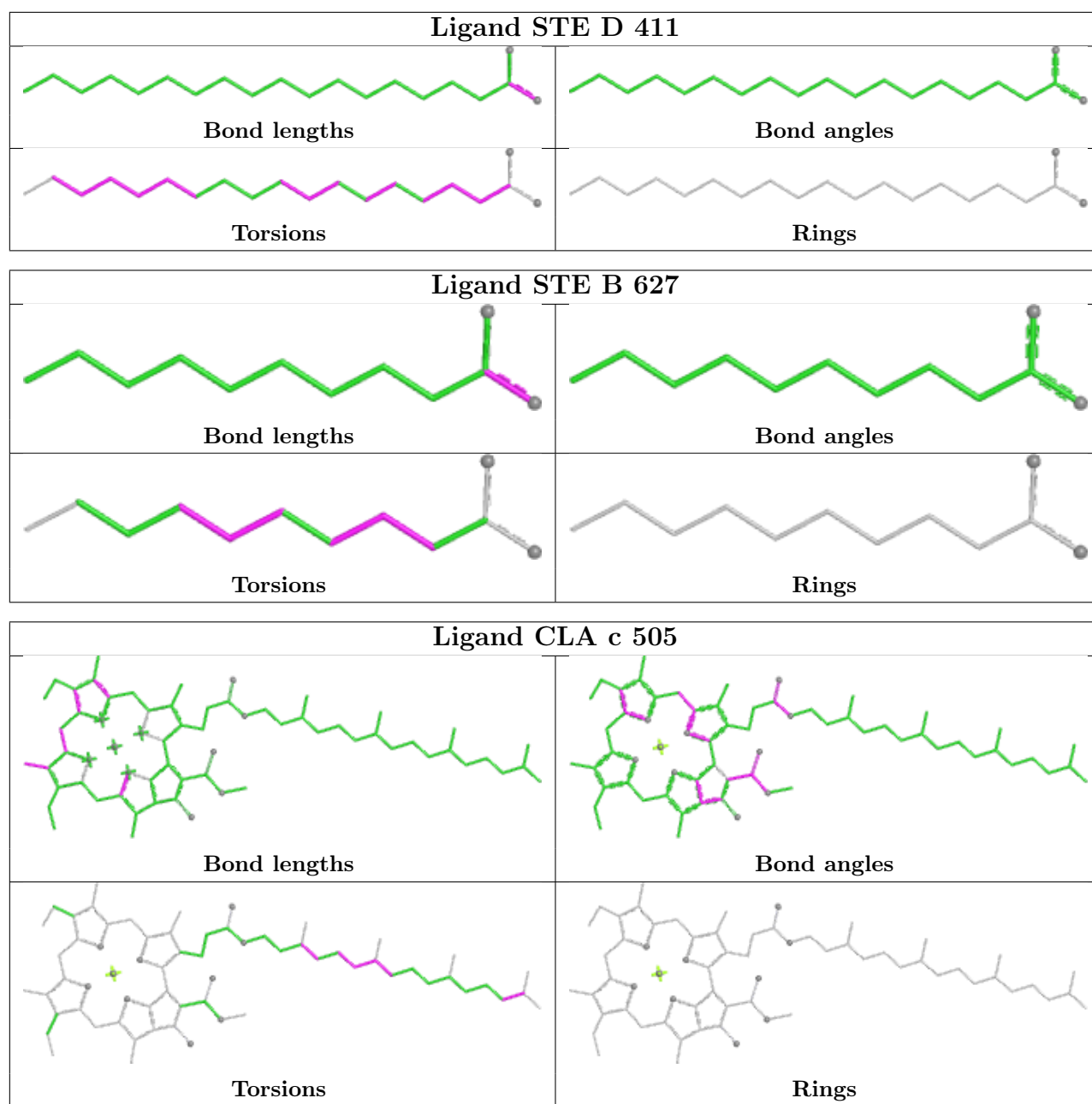


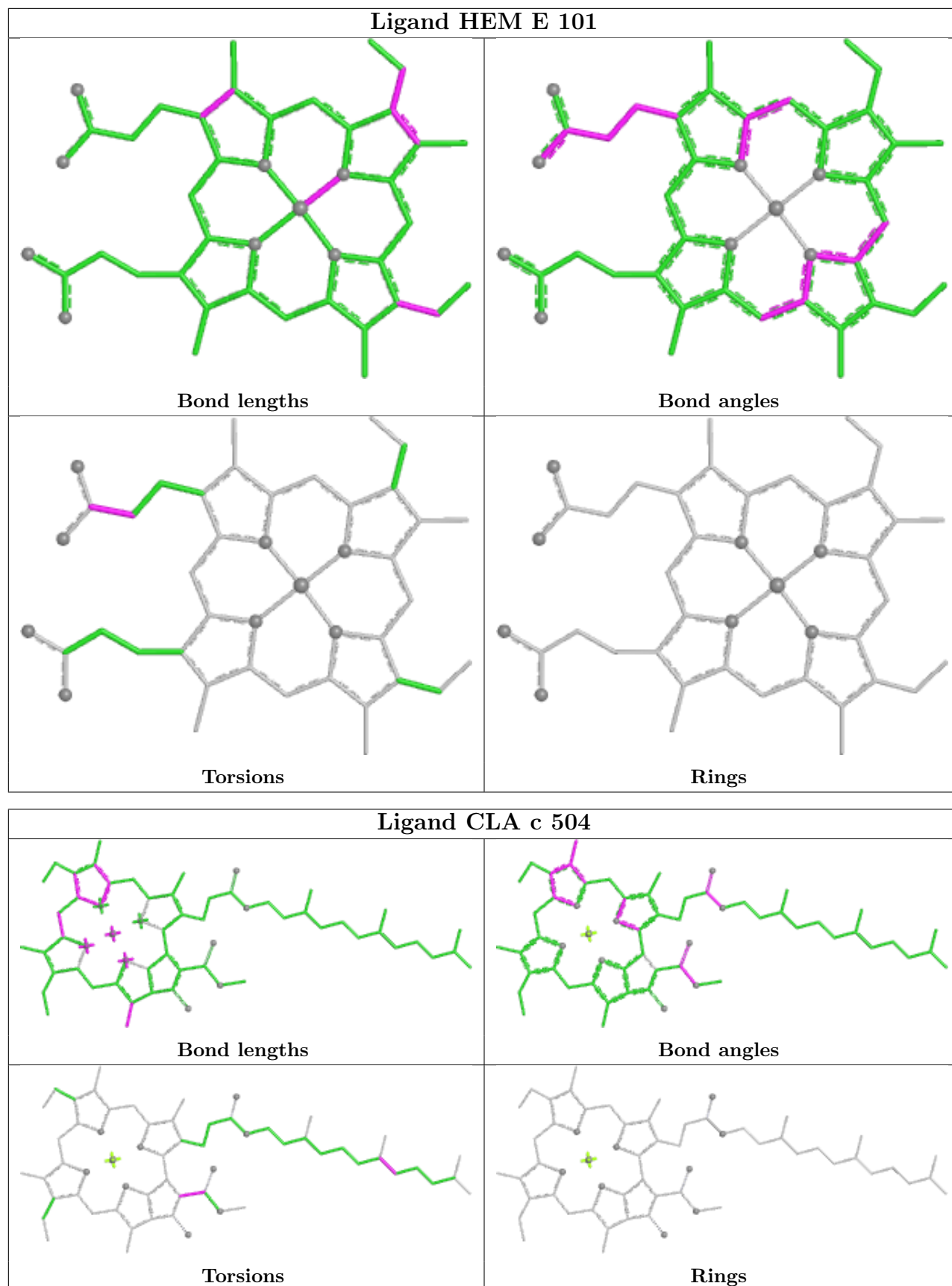
Ligand CLA c 501

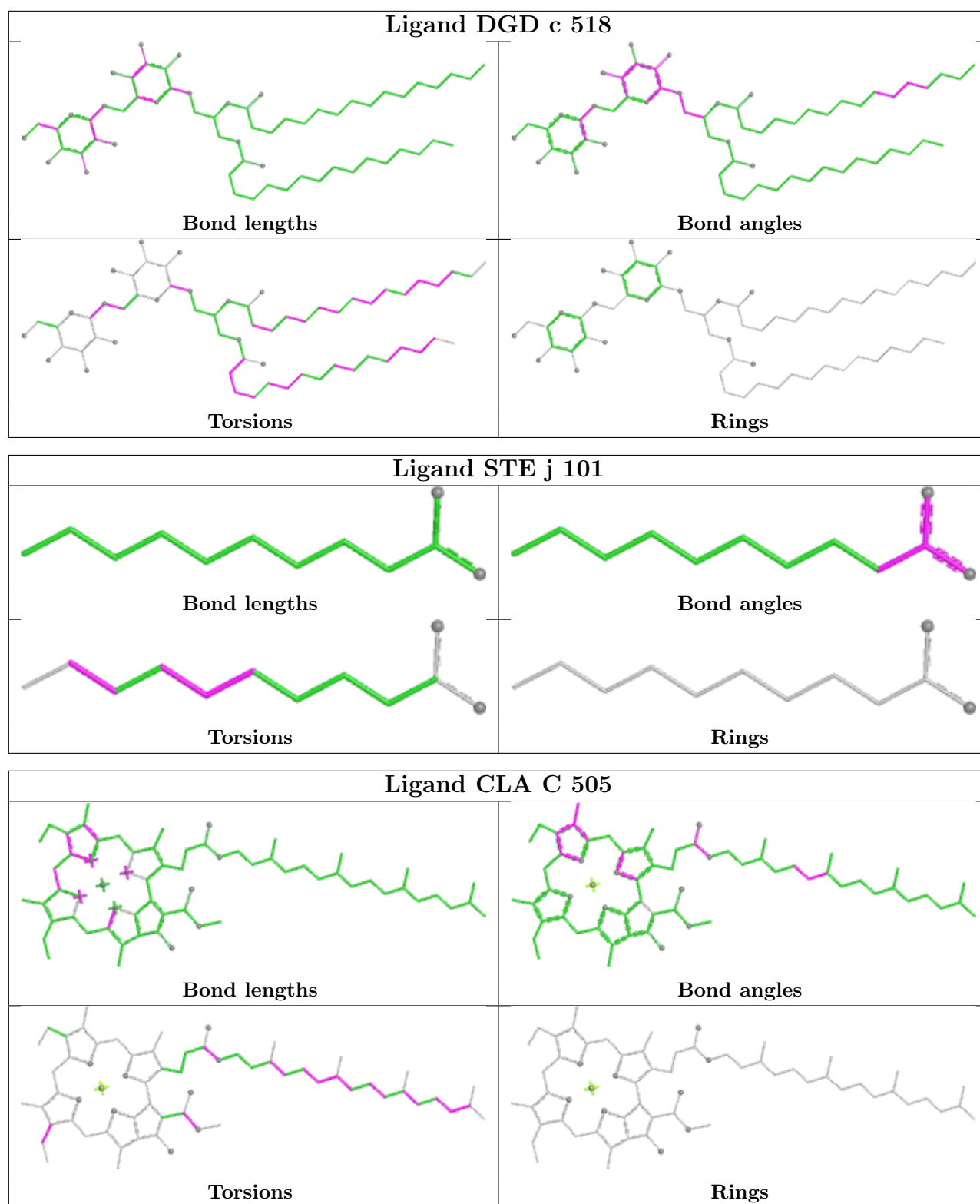


Ligand CLA c 506

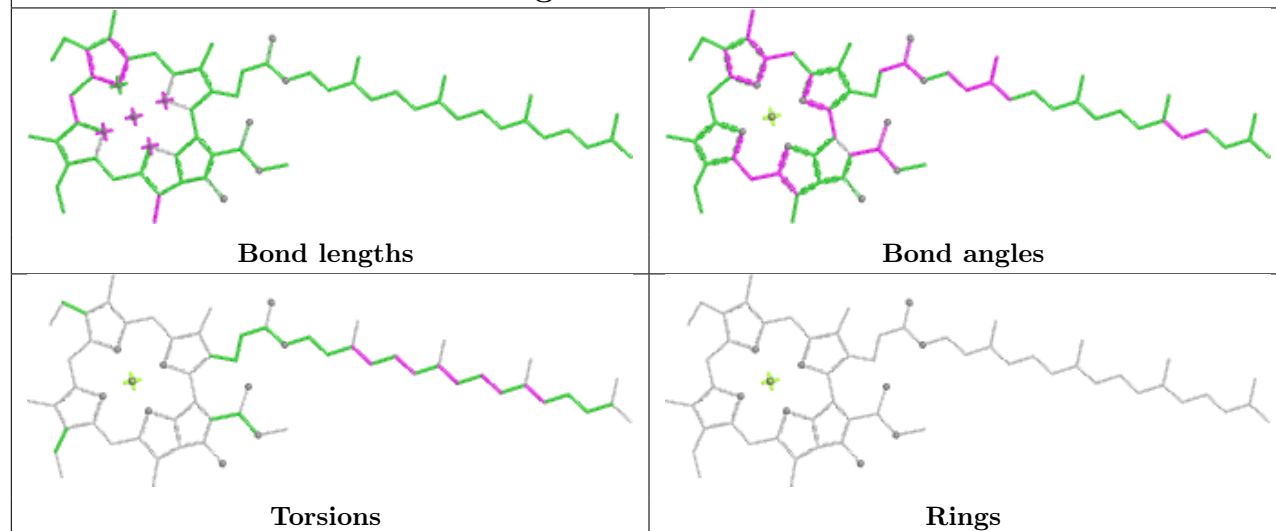




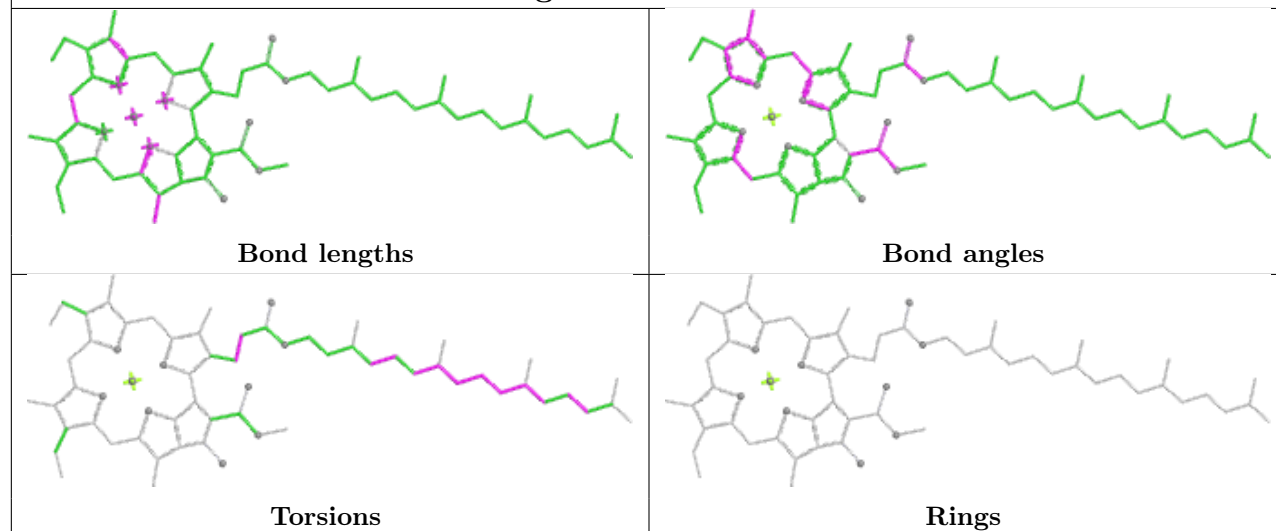




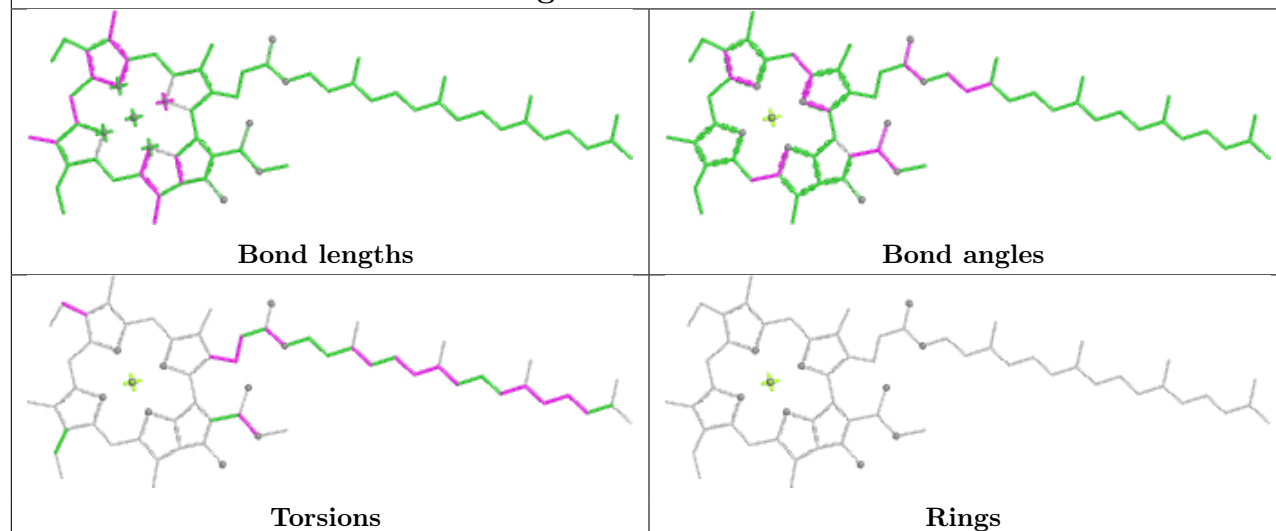
Ligand CLA b 605

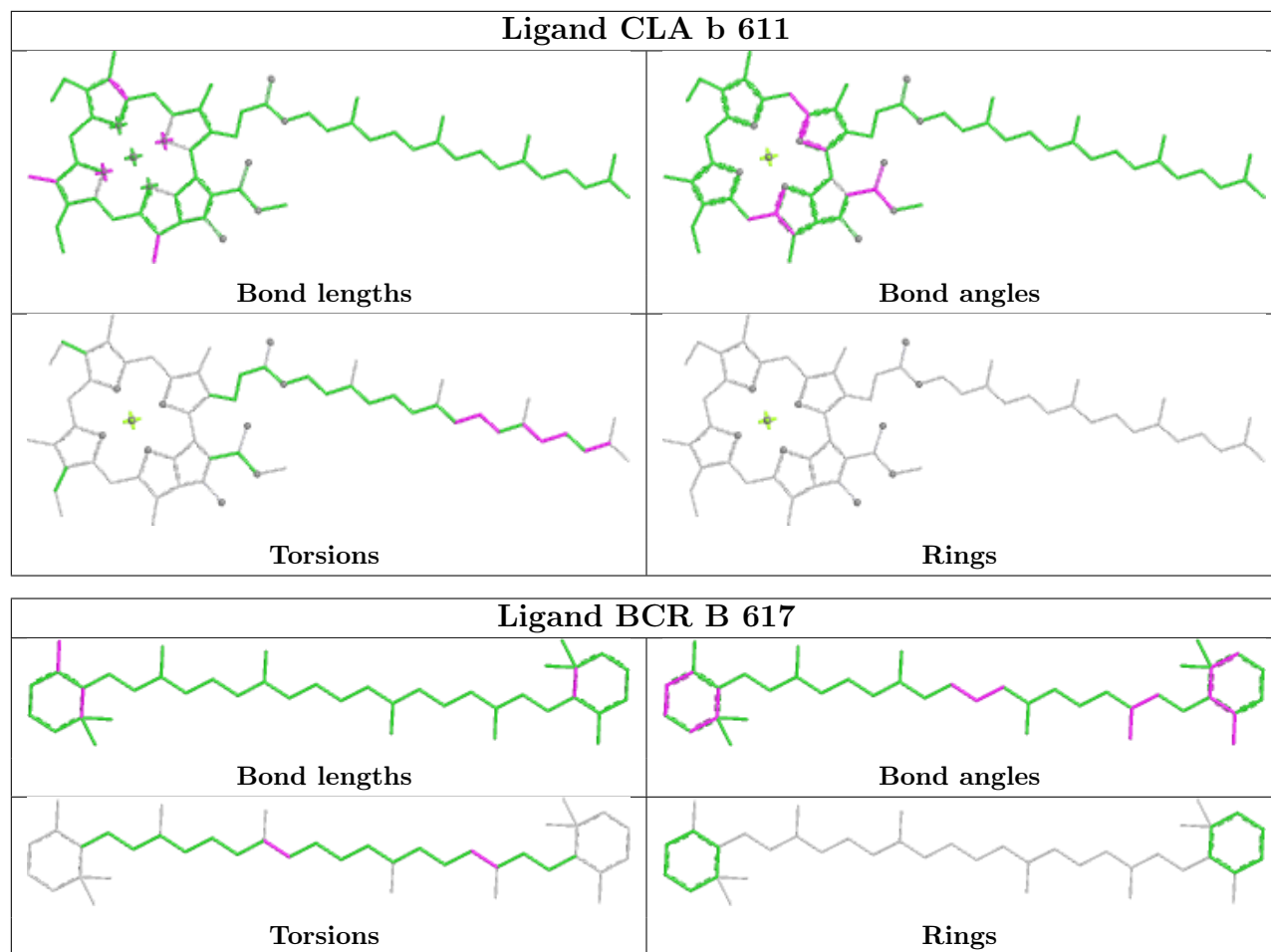


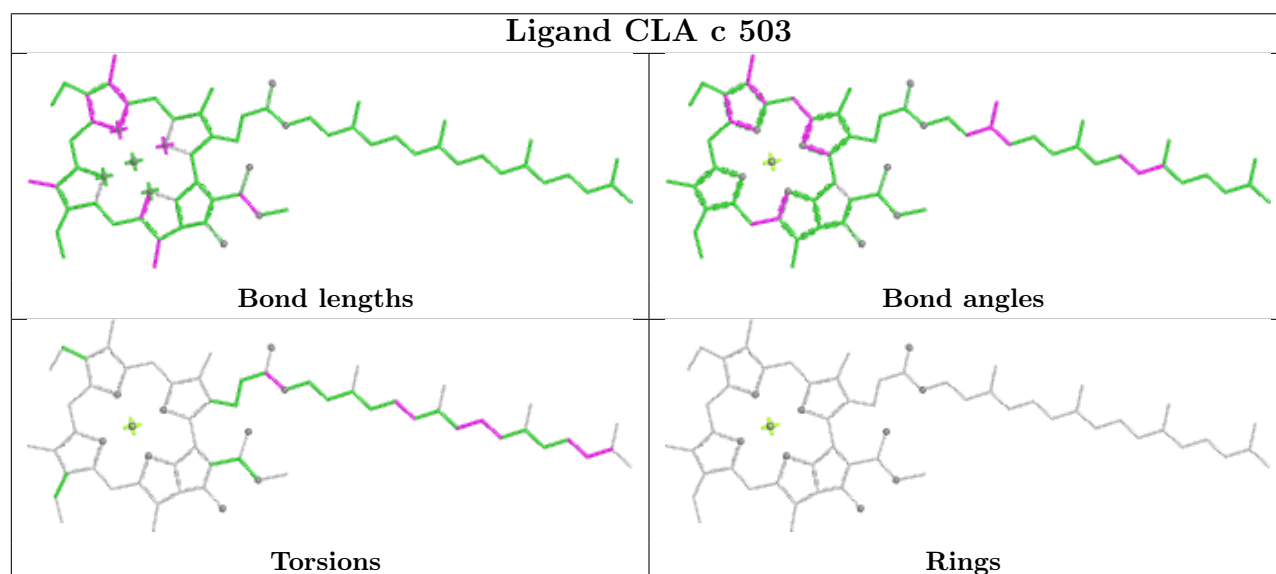
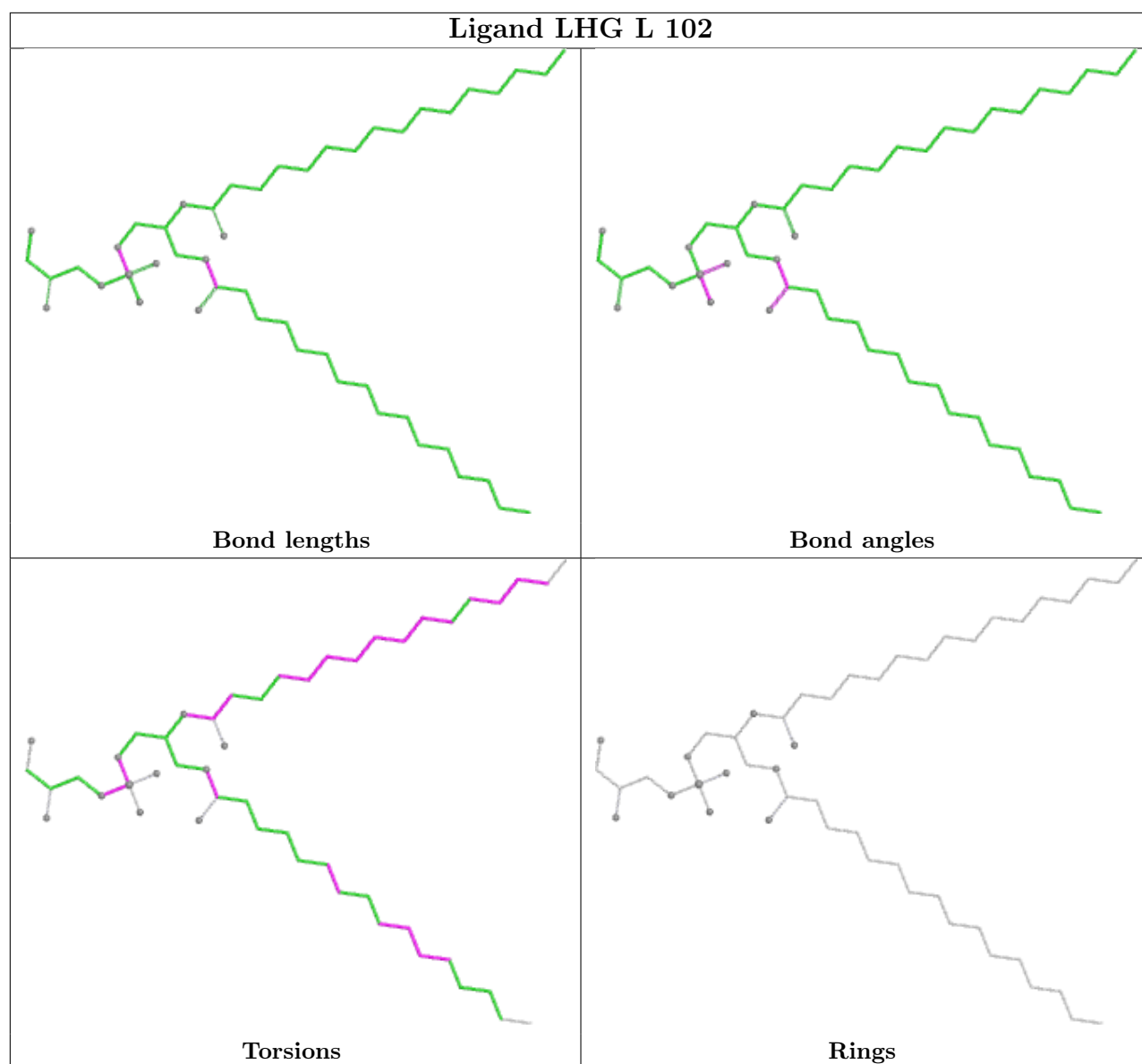
Ligand CLA b 606

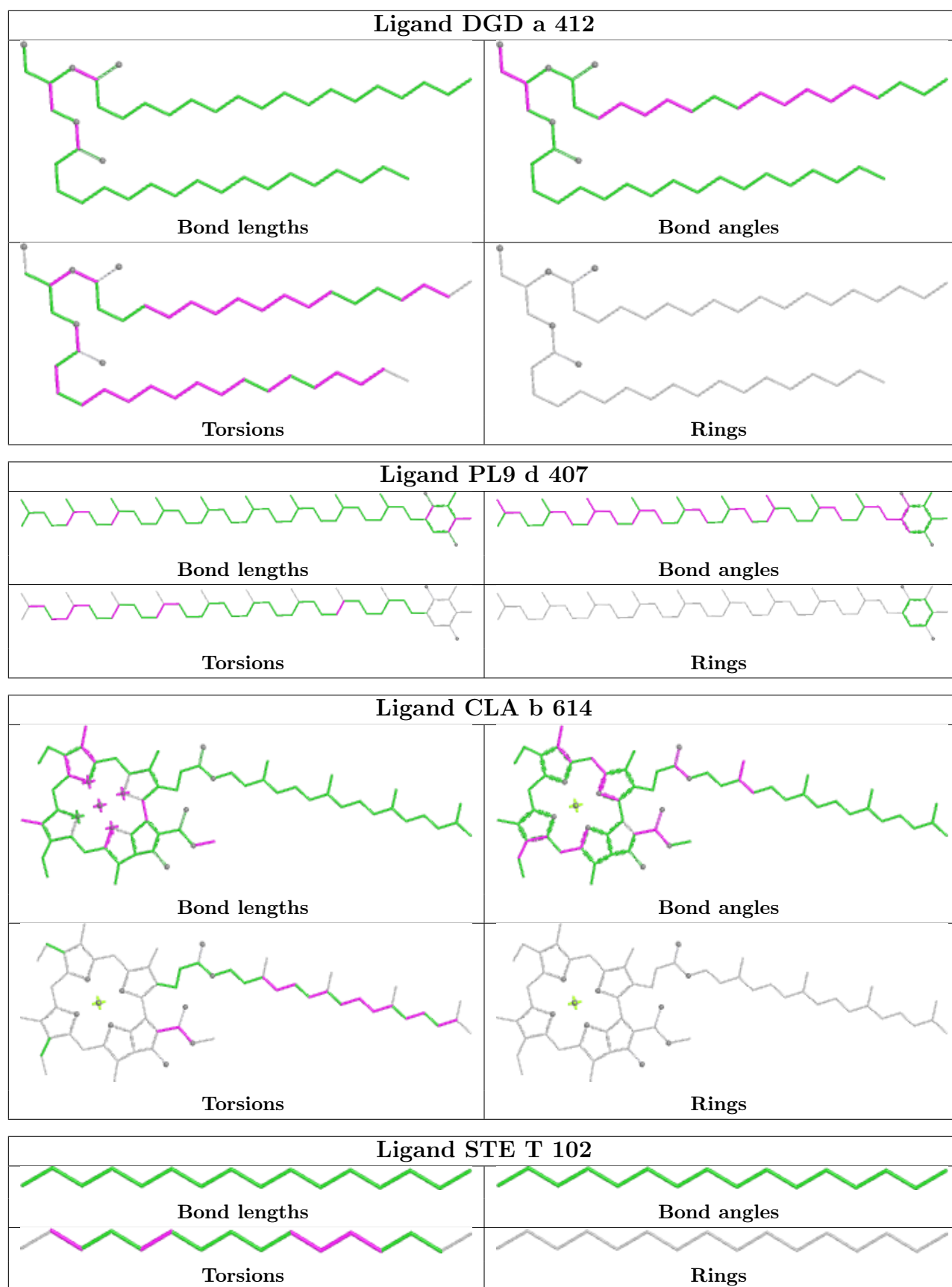


Ligand CLA c 512

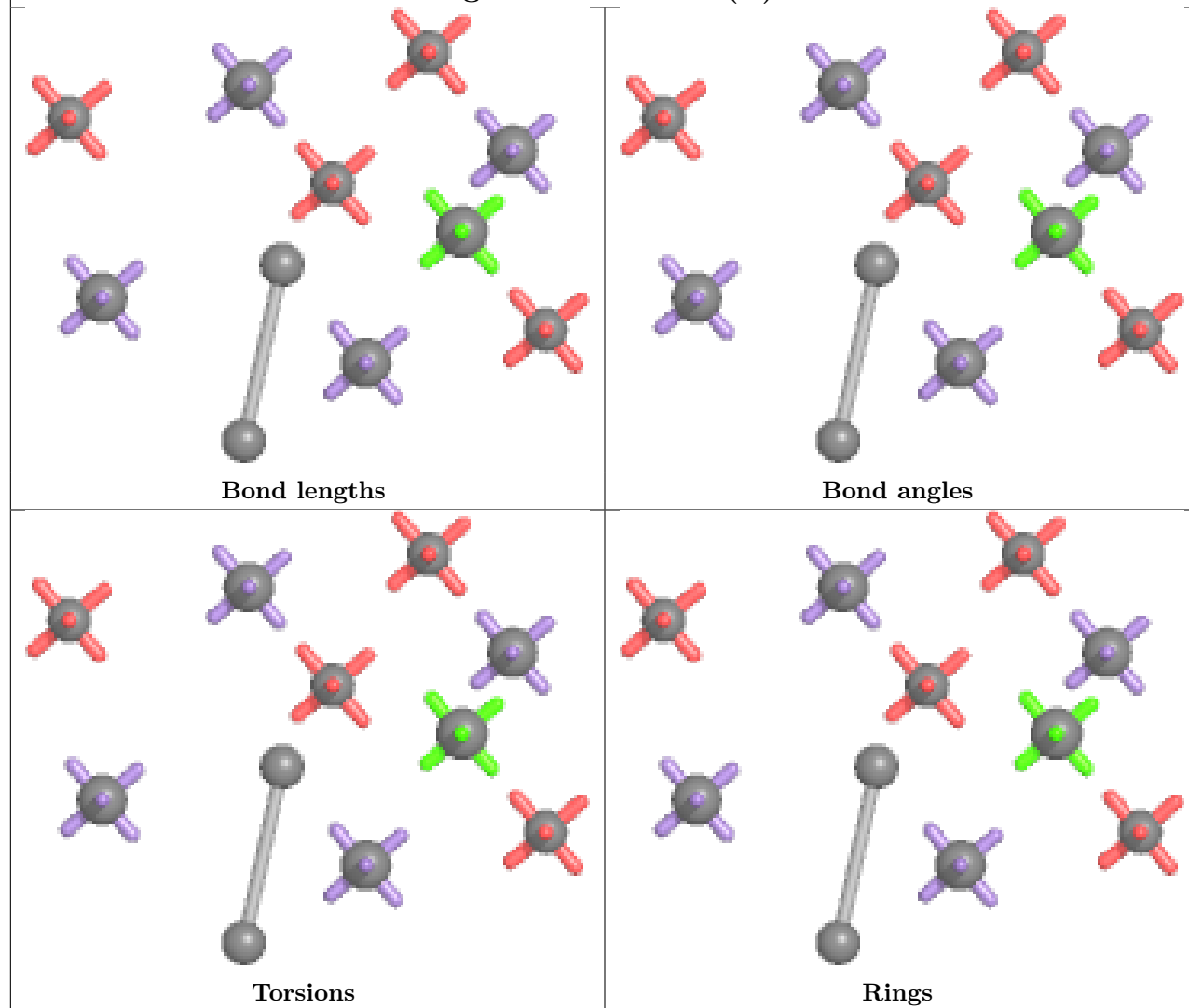




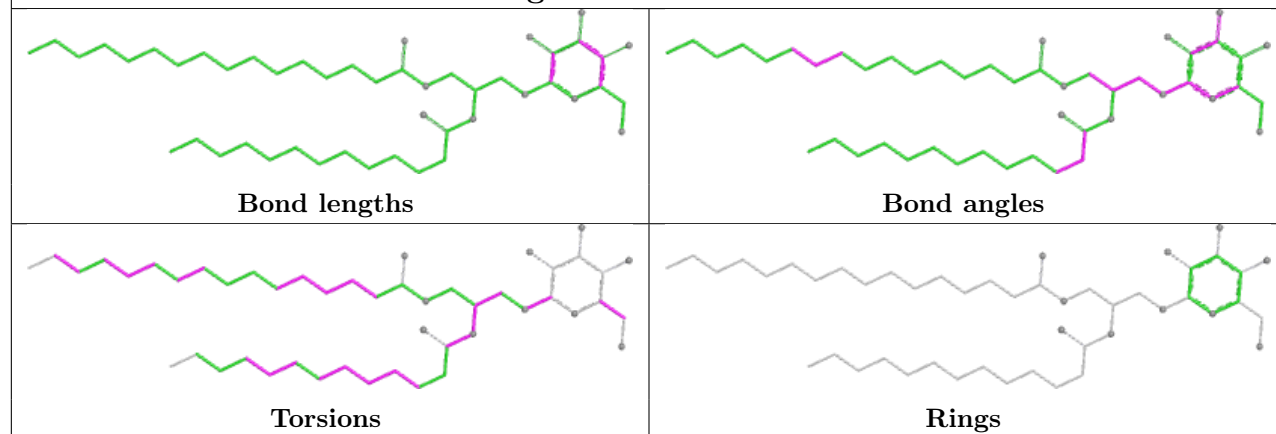


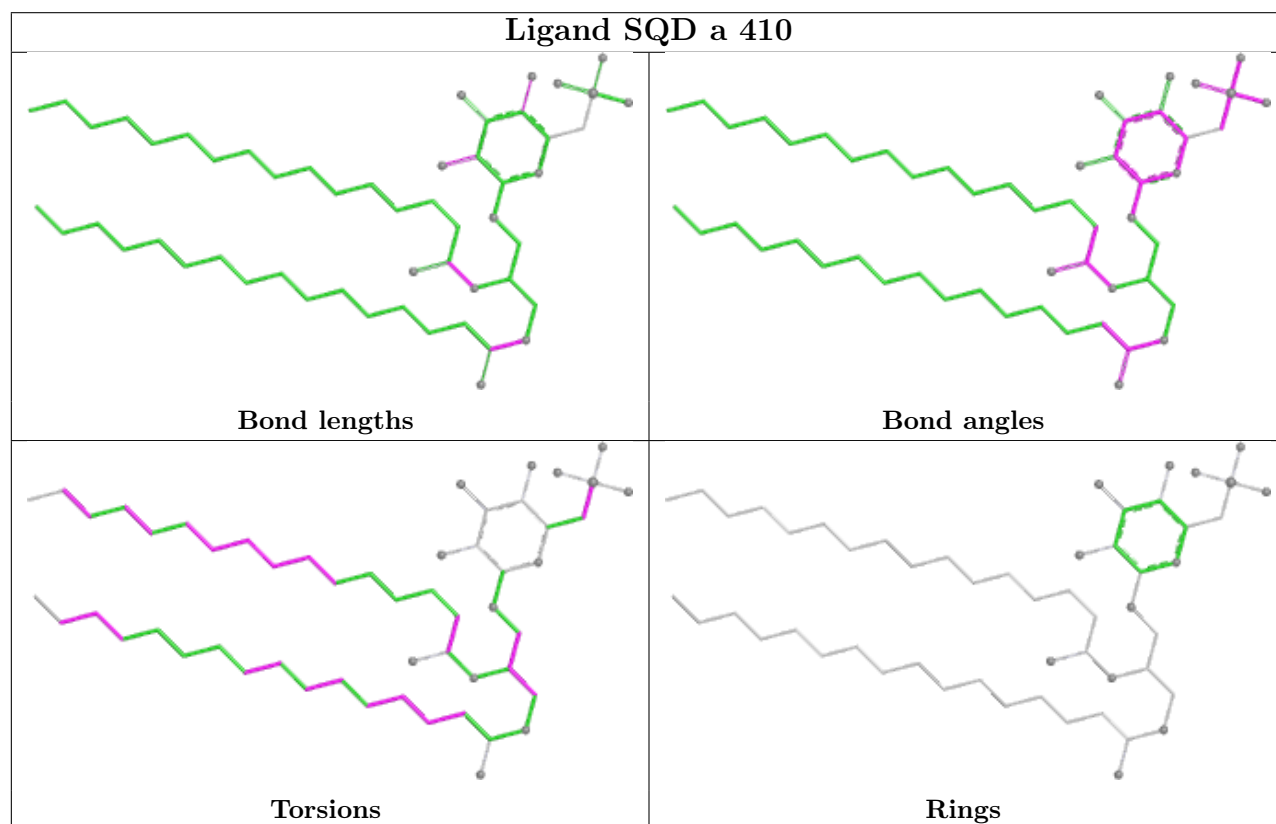
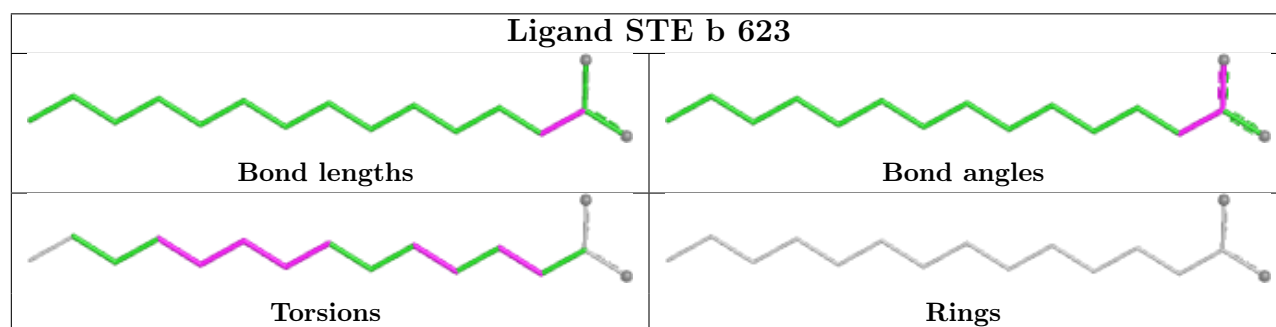
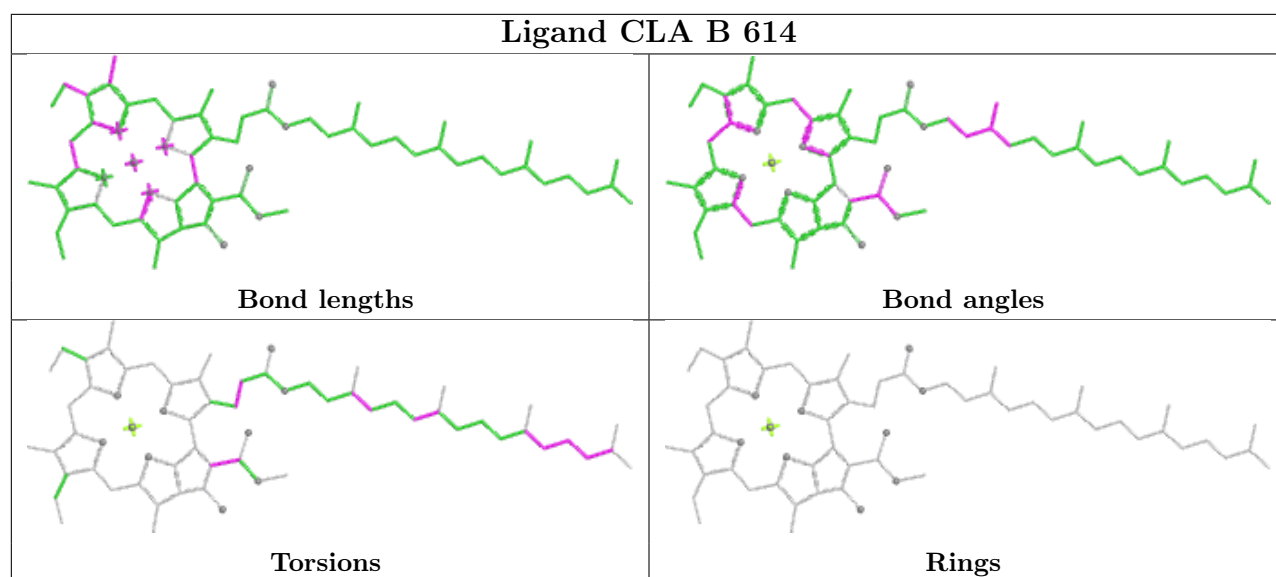


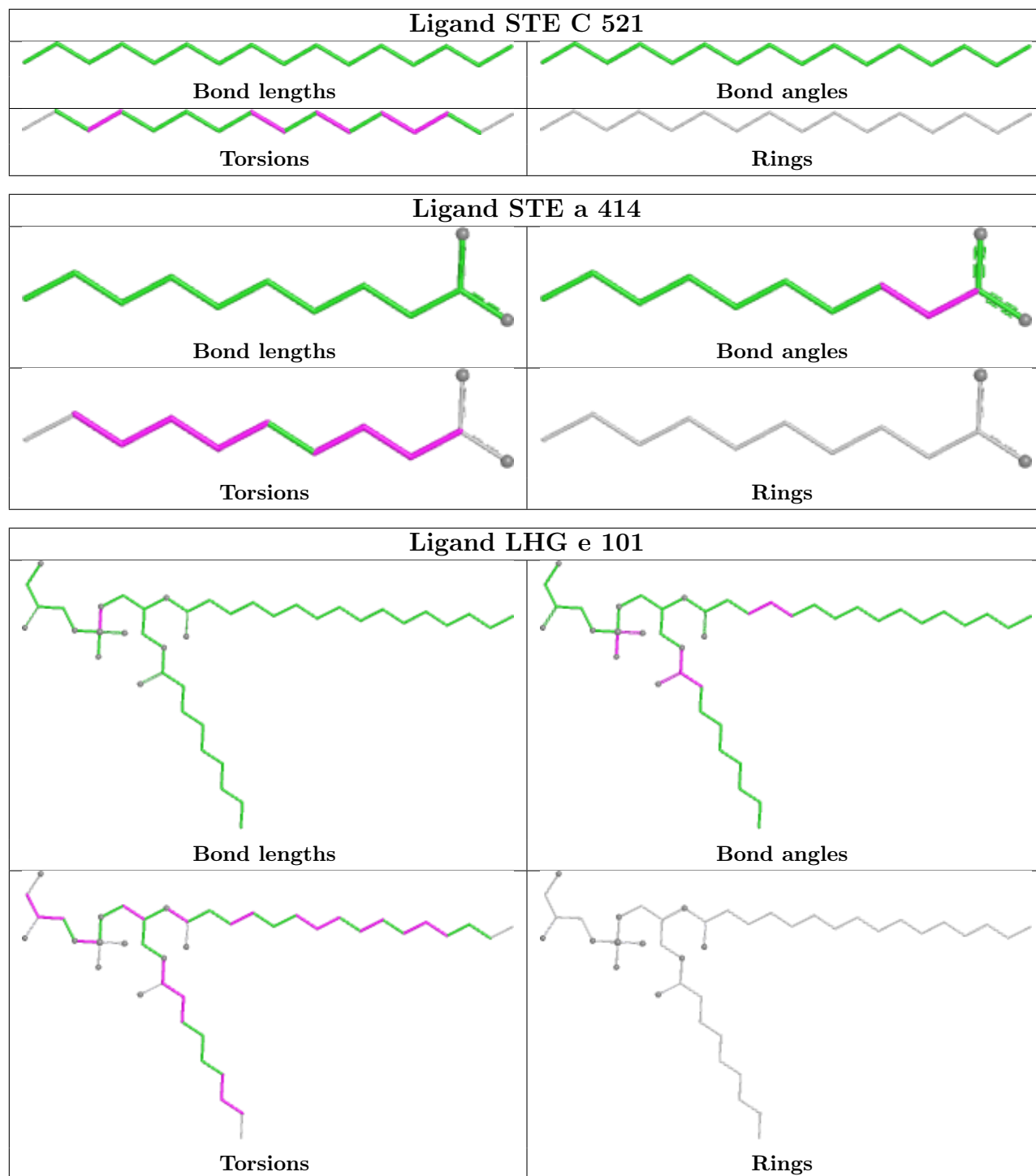
Ligand OEY A 415 (B)

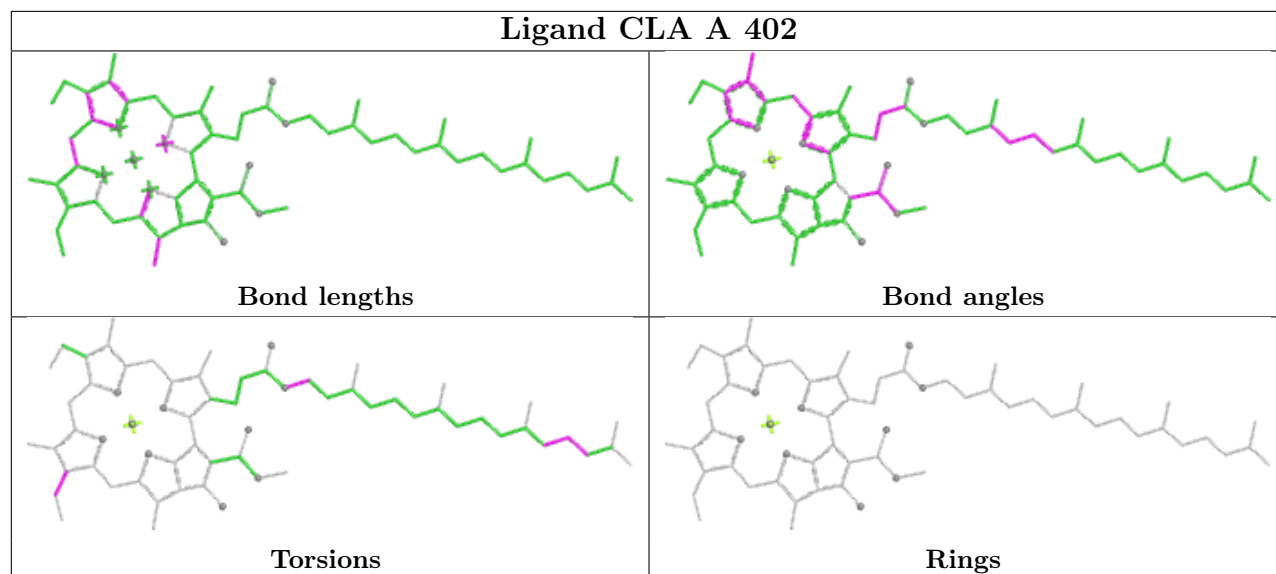
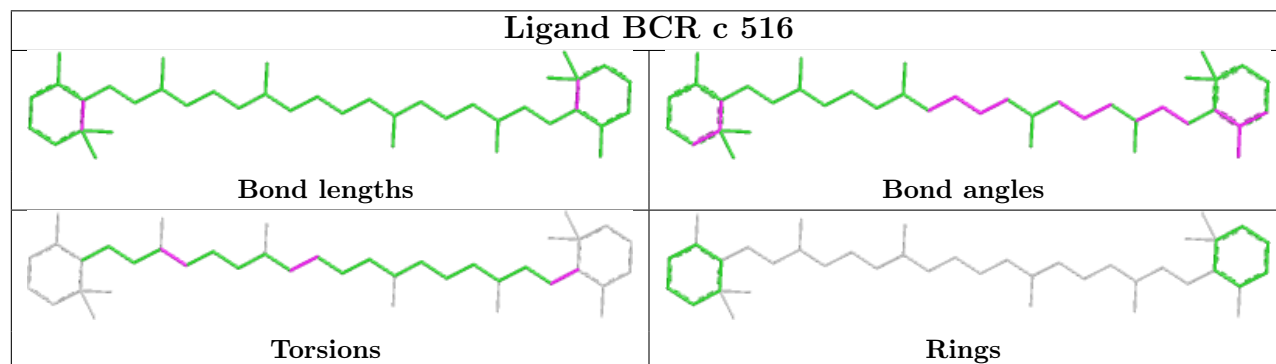
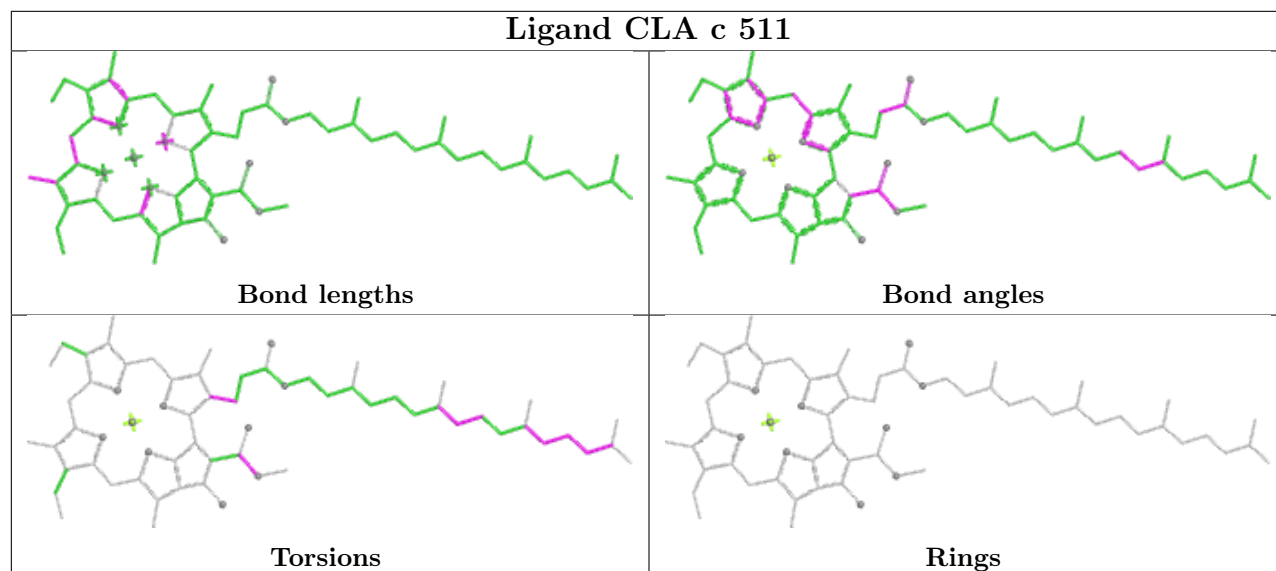


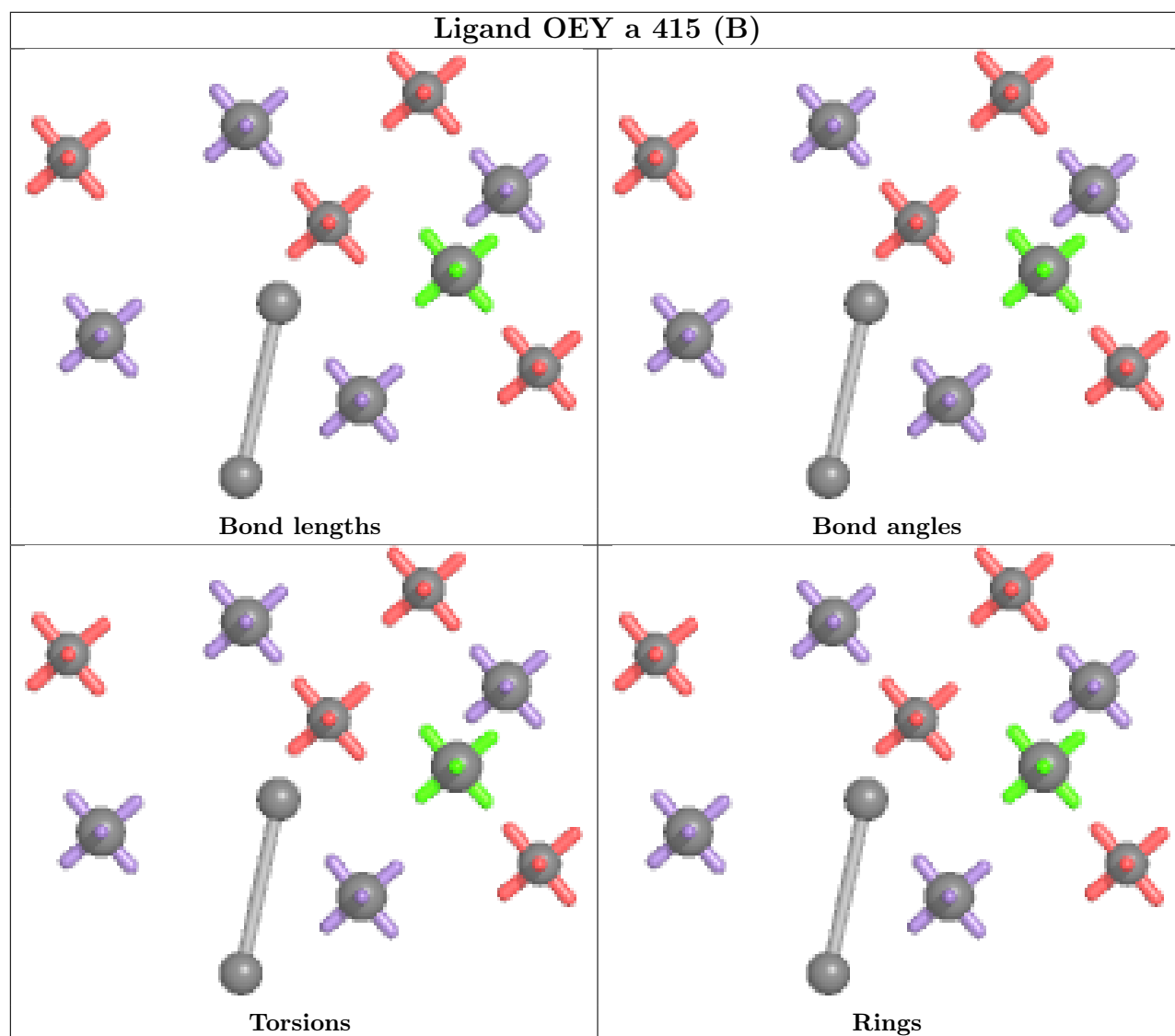
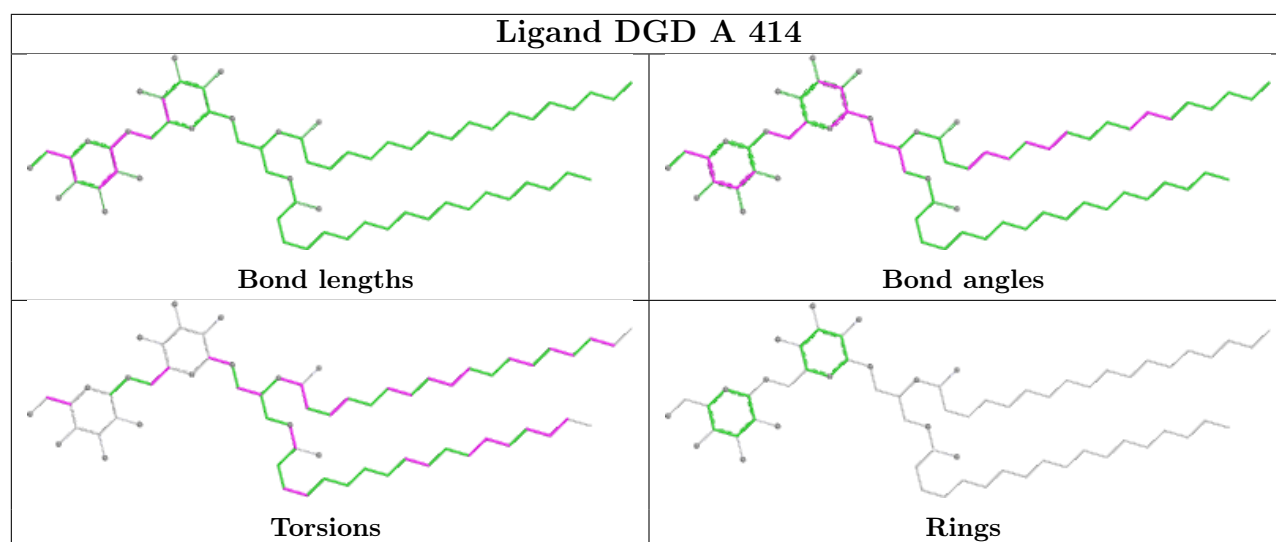
Ligand LMG A 411



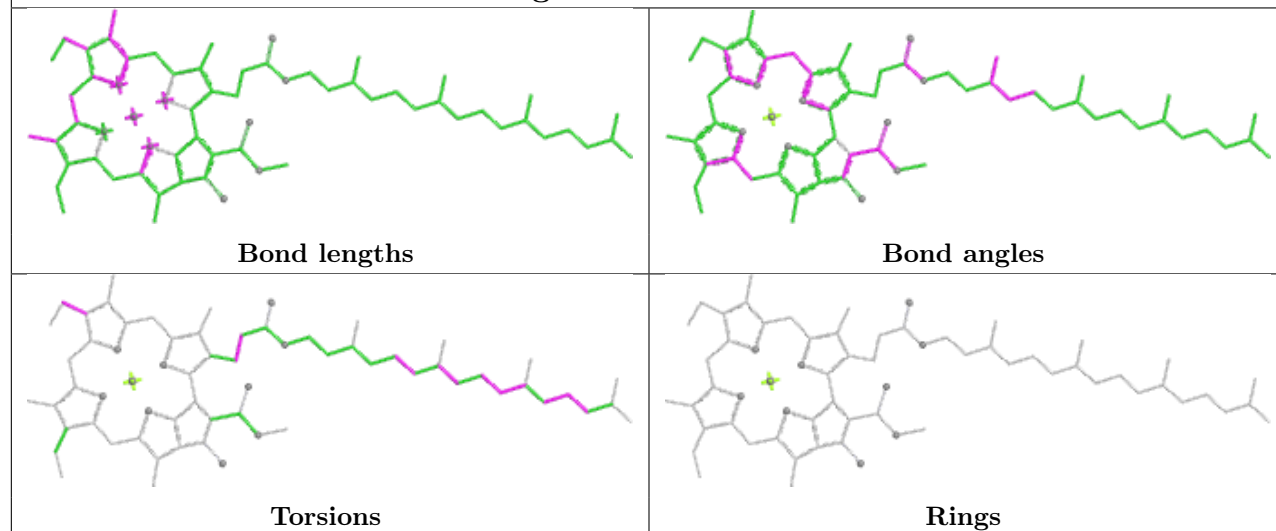




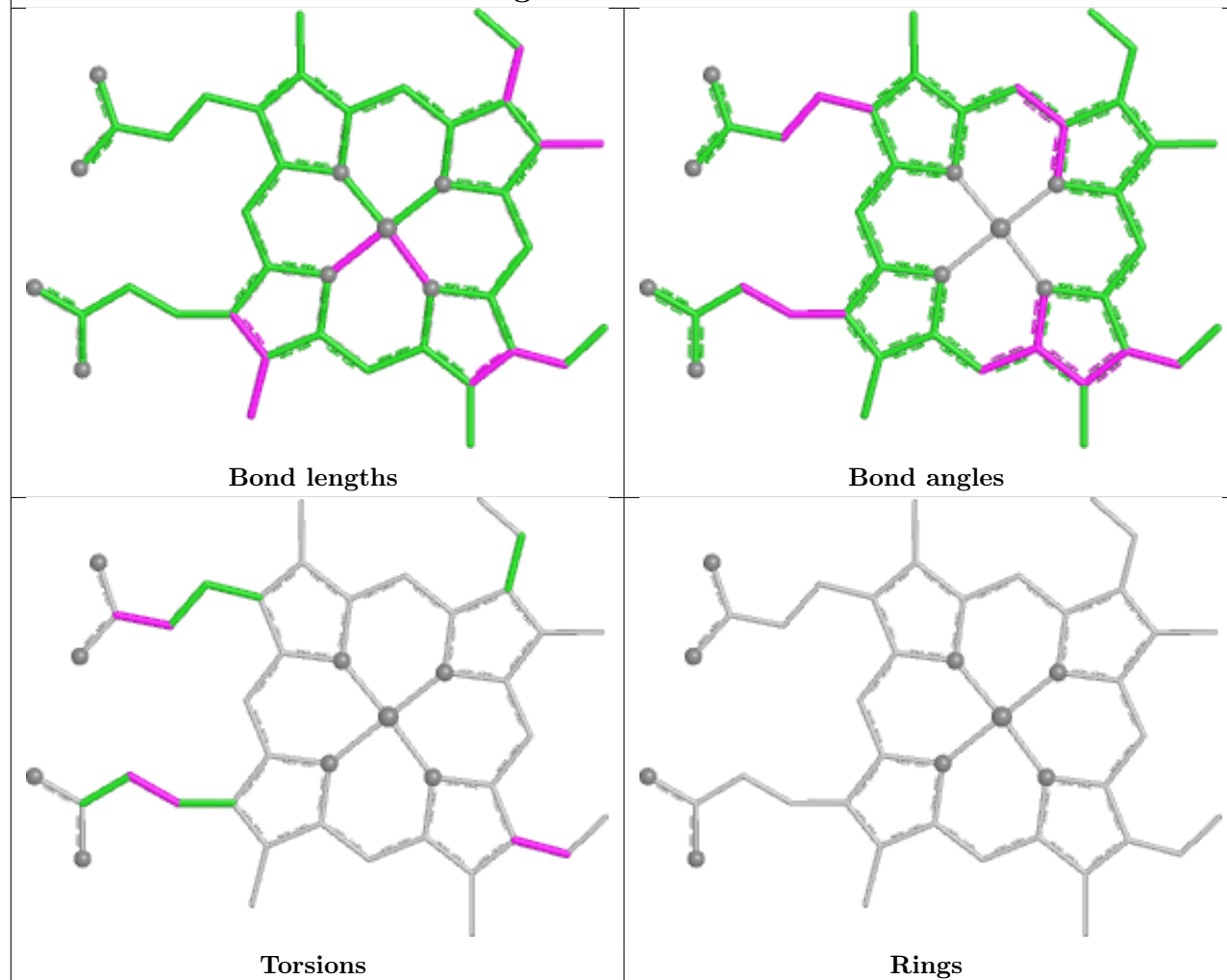
Ligand CLA A 402**Ligand BCR c 516****Ligand CLA c 511**



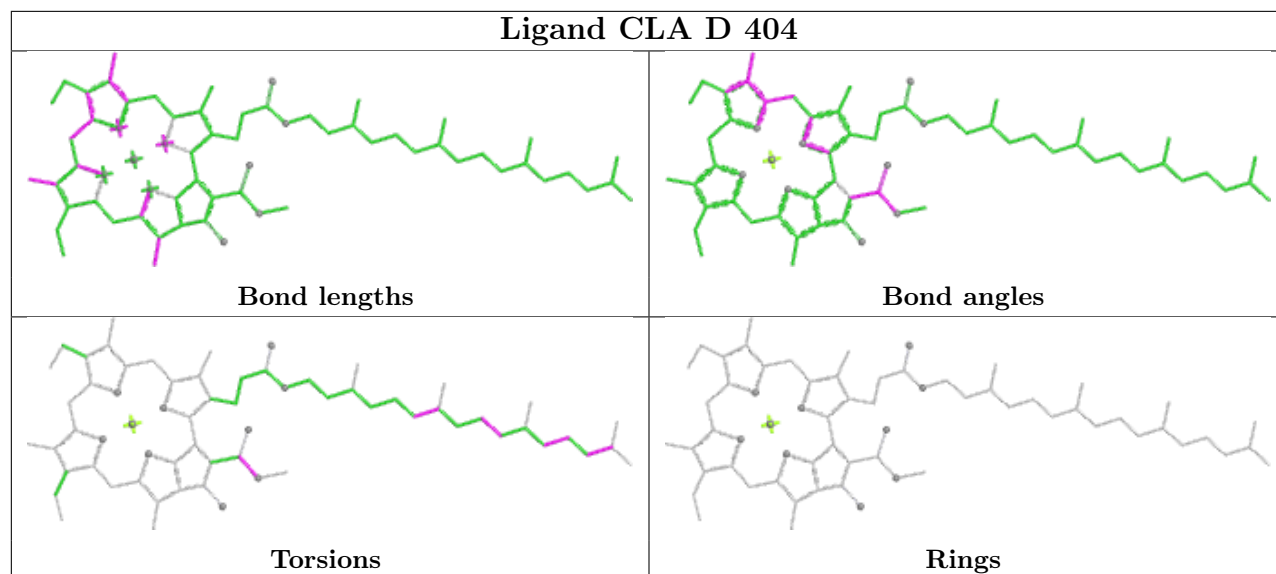
Ligand CLA B 606



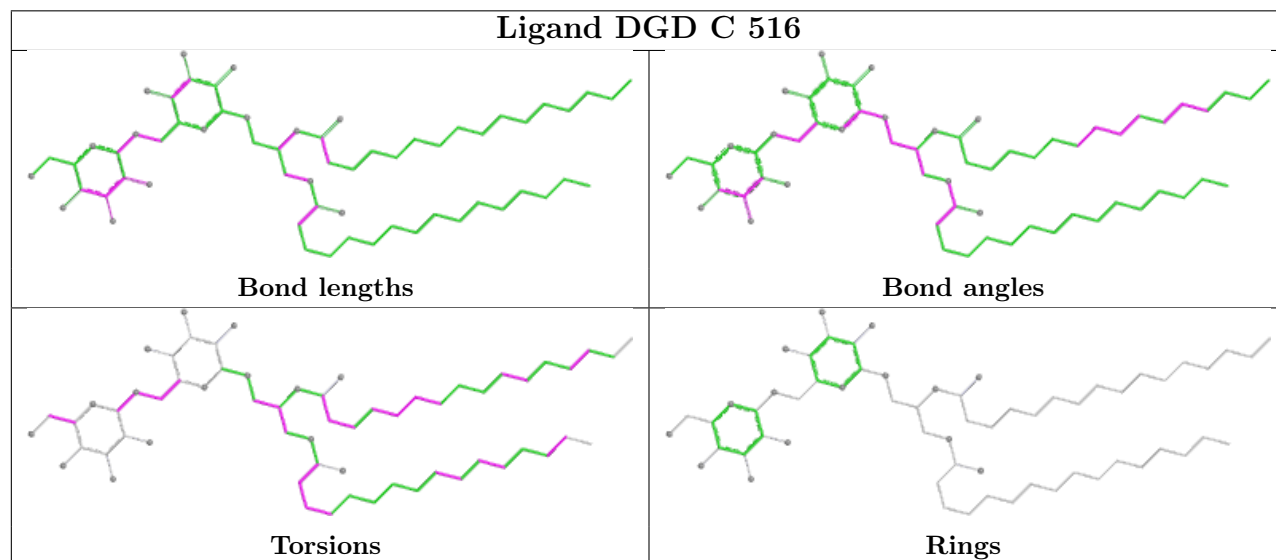
Ligand HEM f 101

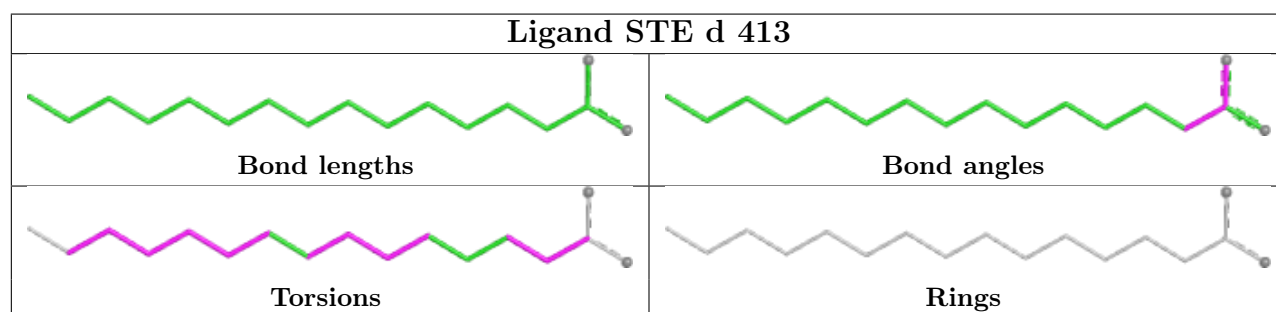
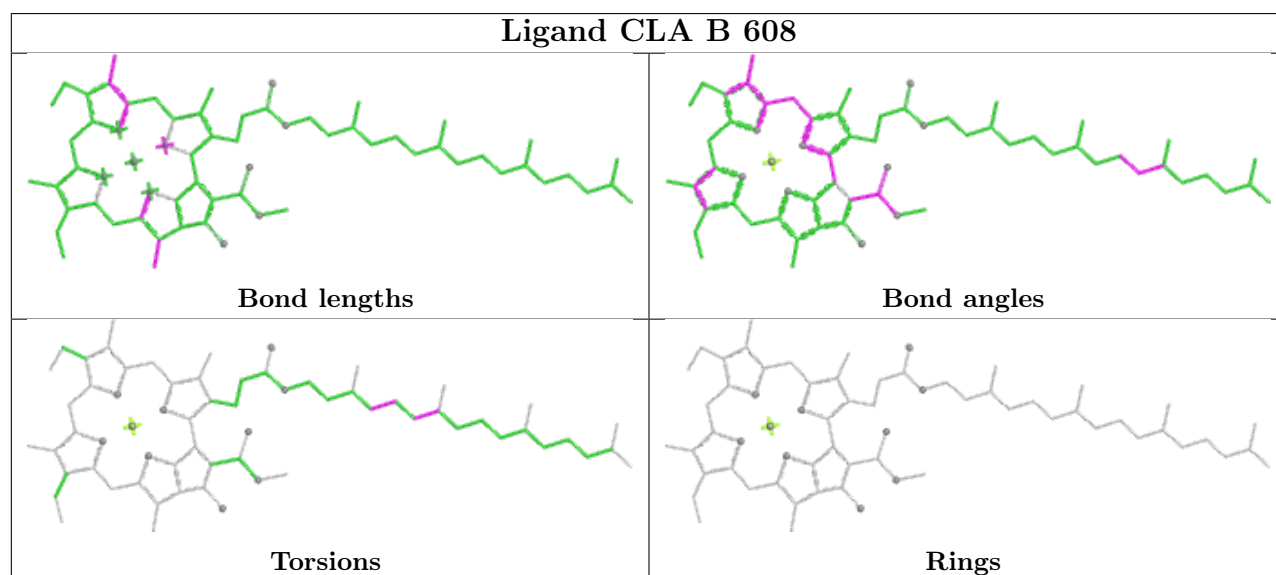
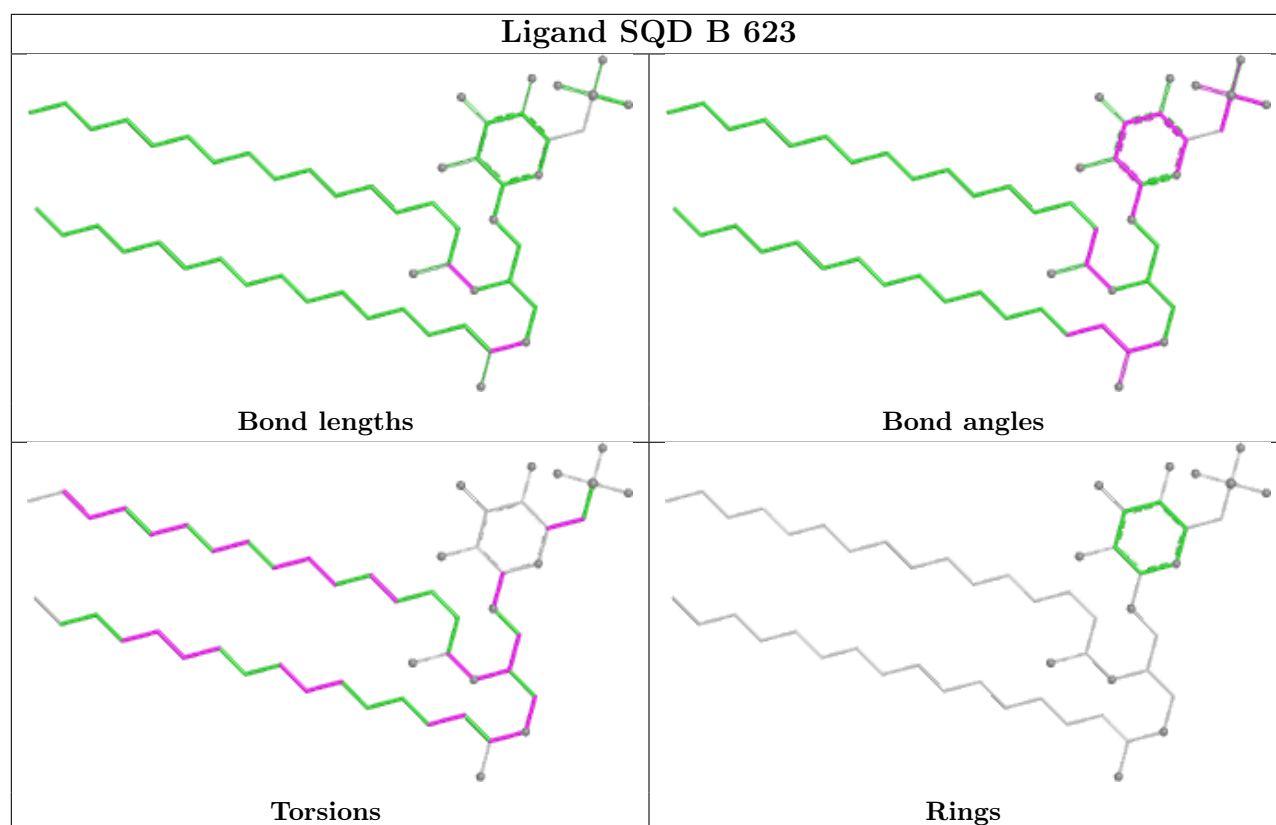


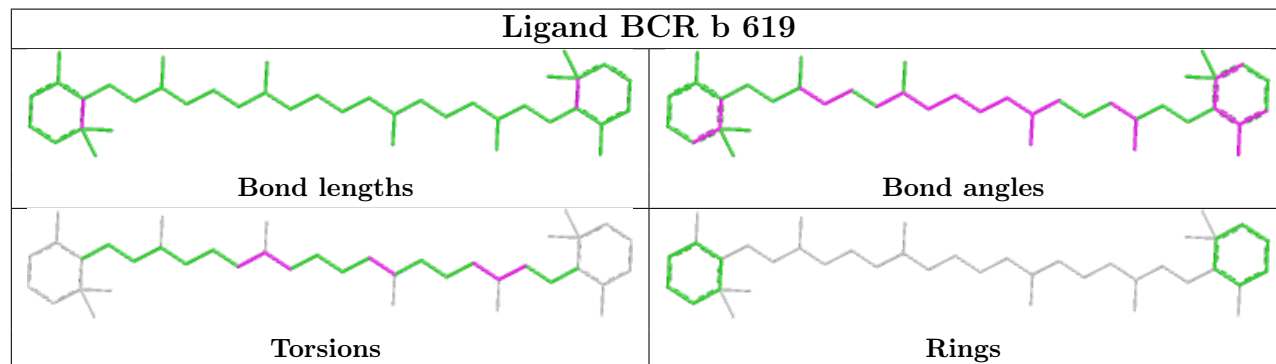
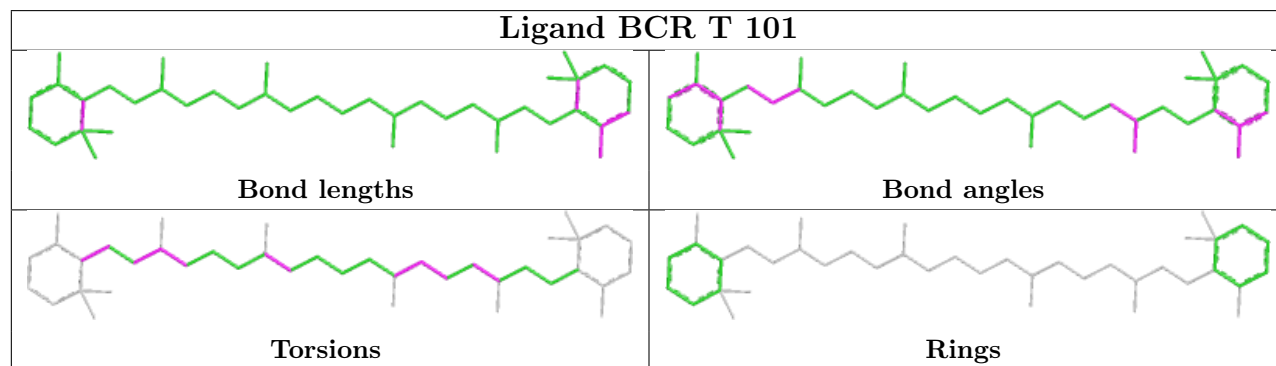
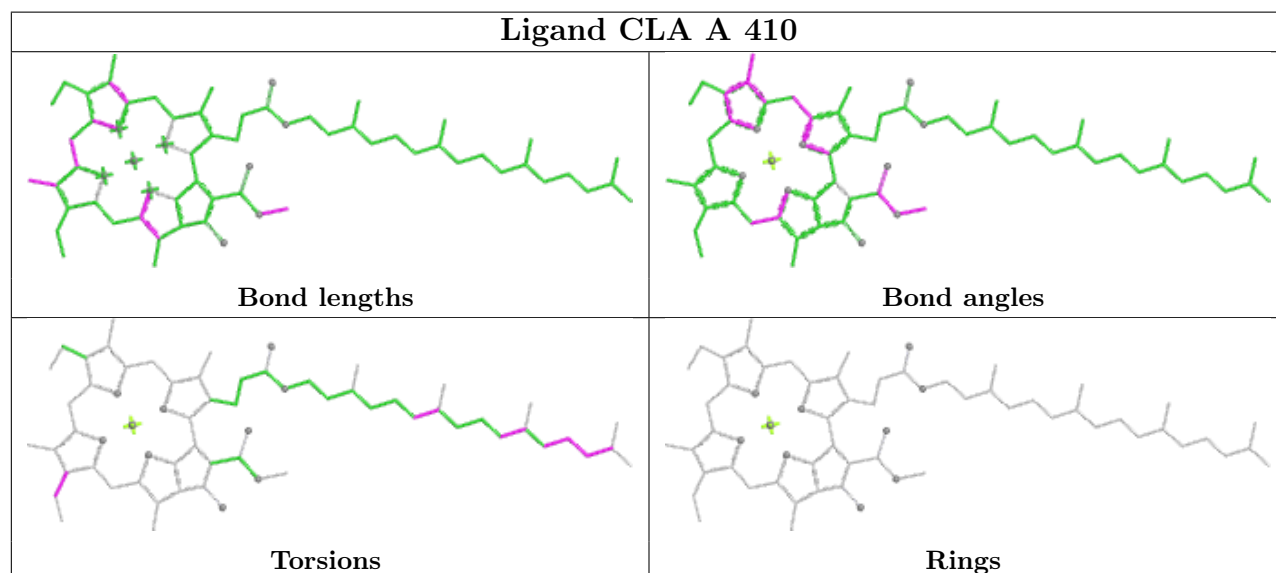
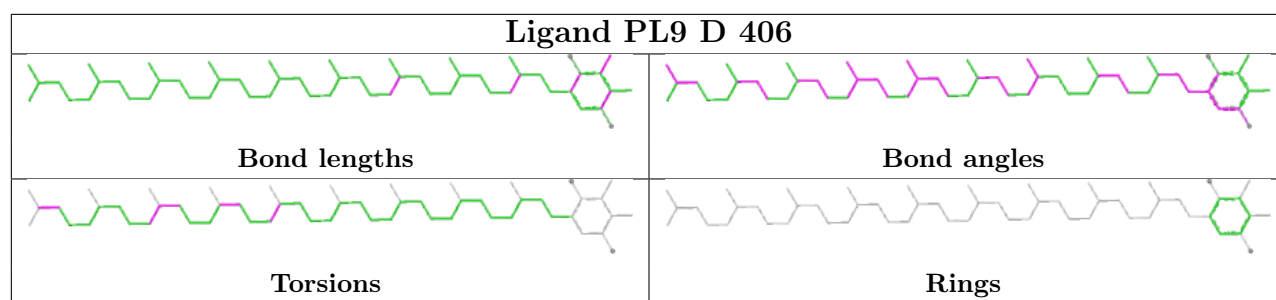
Ligand CLA D 404



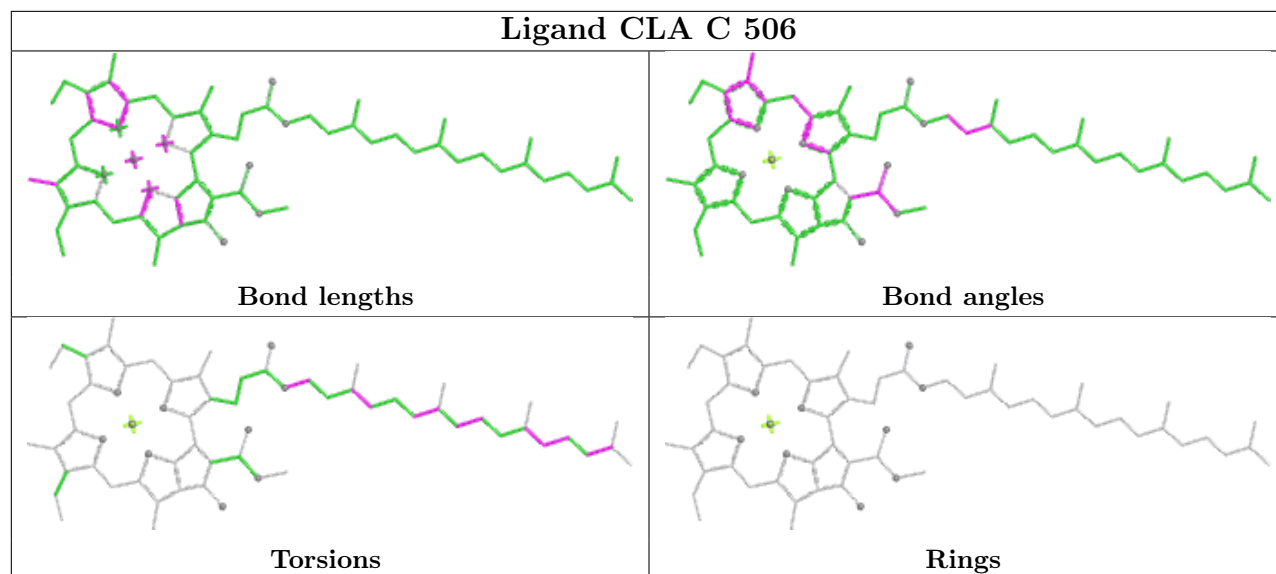
Ligand DGD C 516



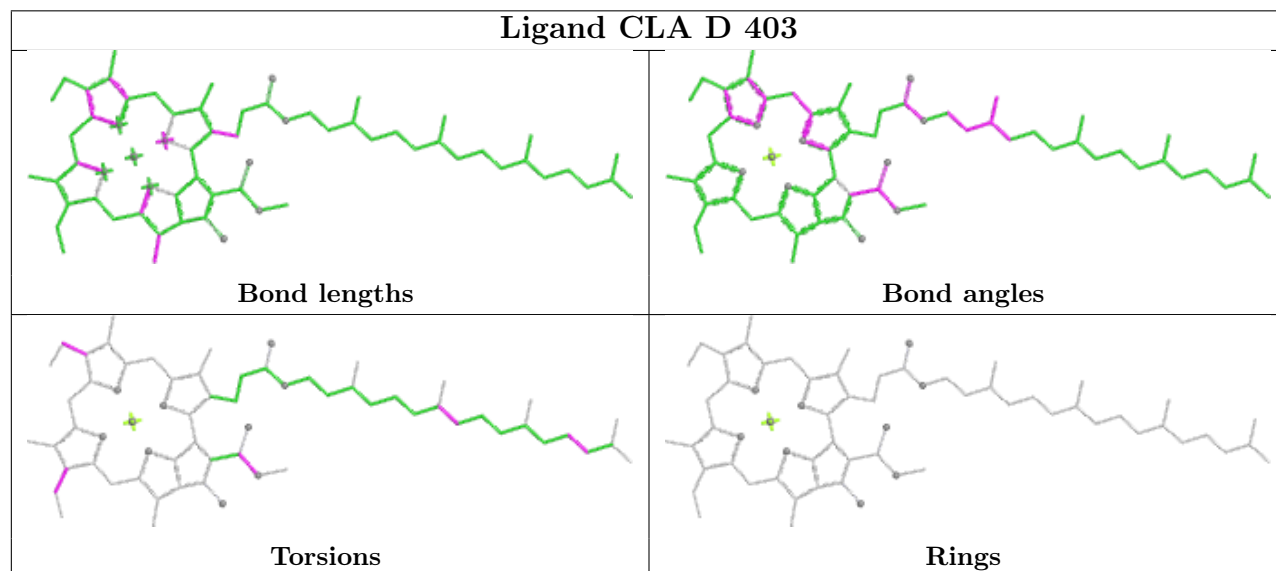




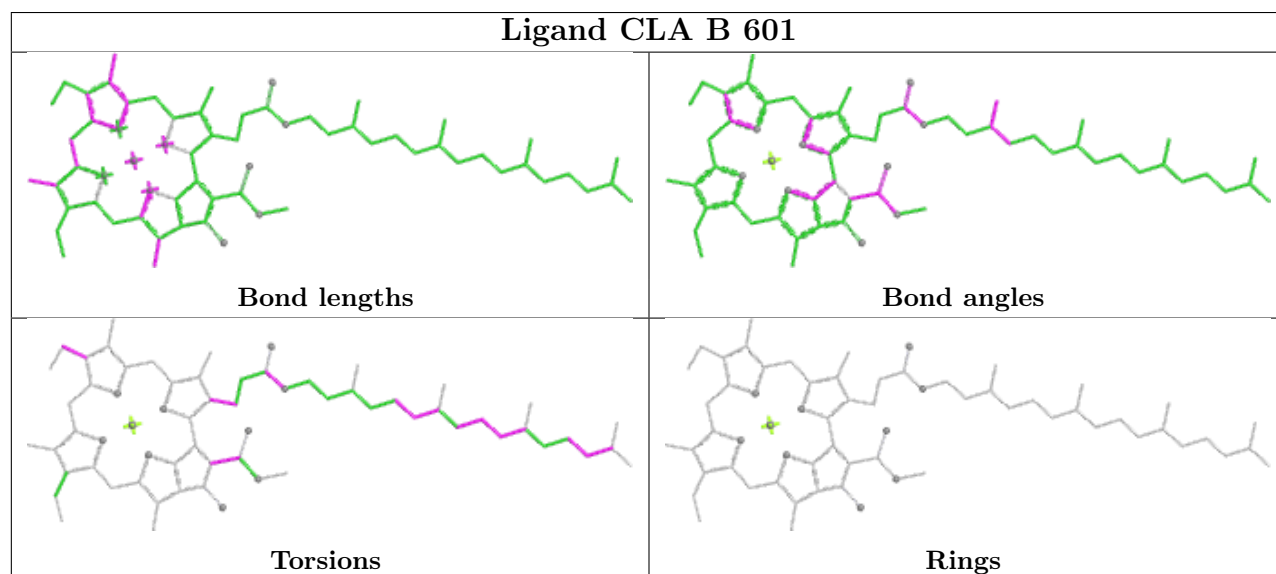
Ligand CLA C 506

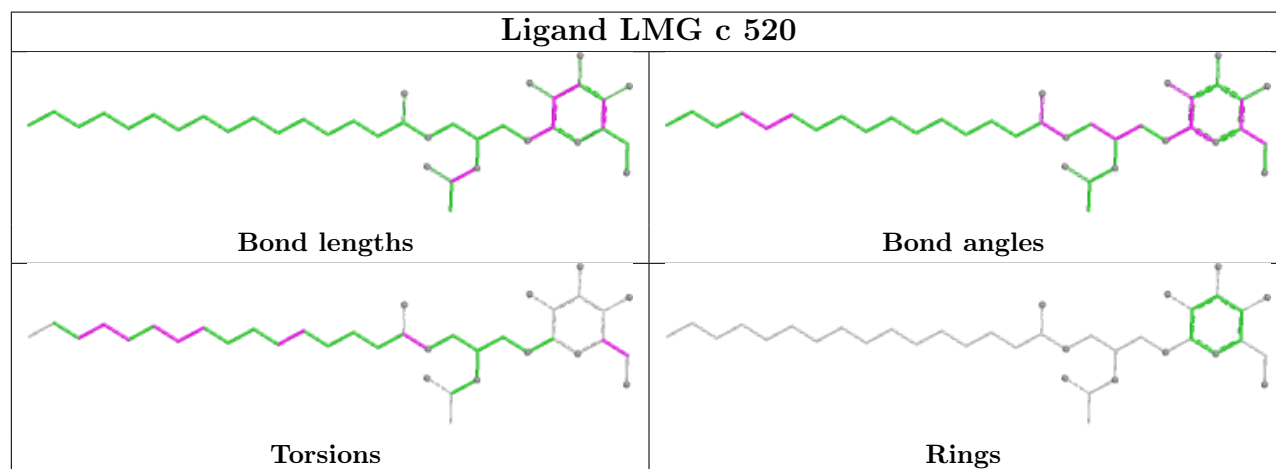
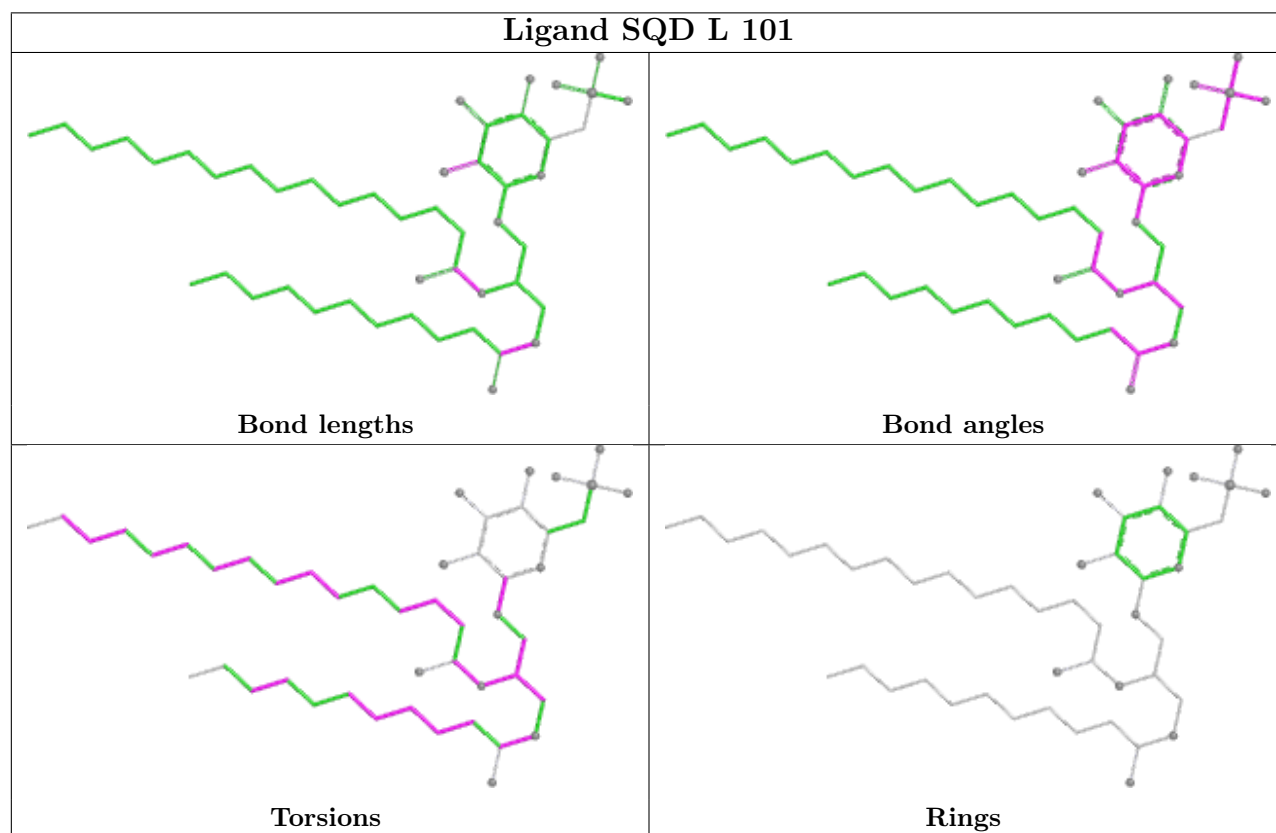
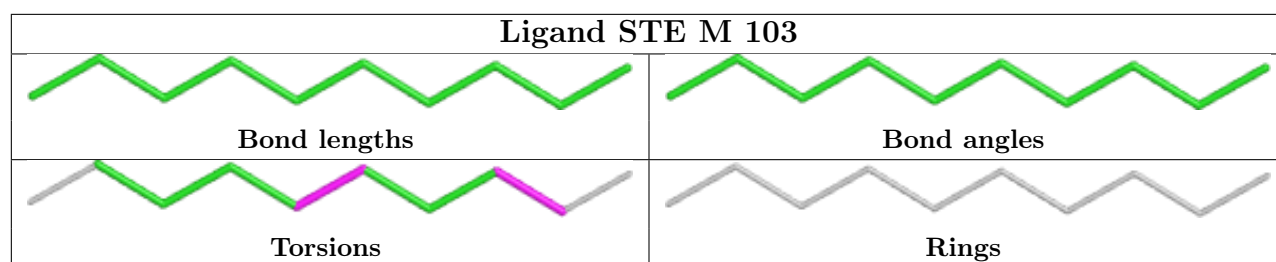


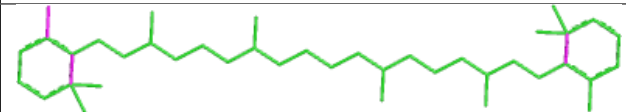
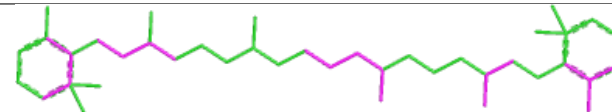
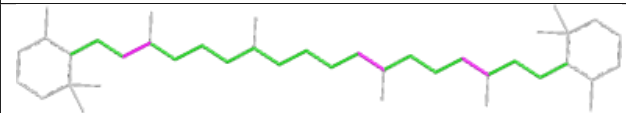
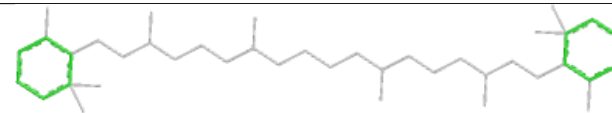
Ligand CLA D 403

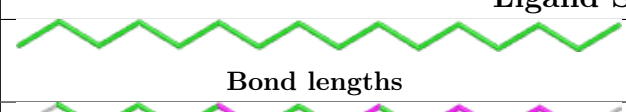
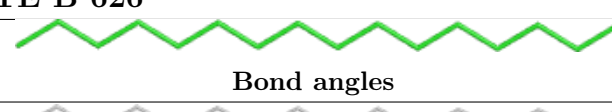
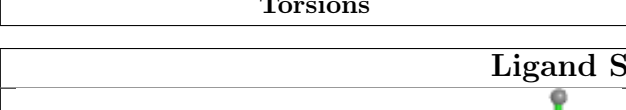


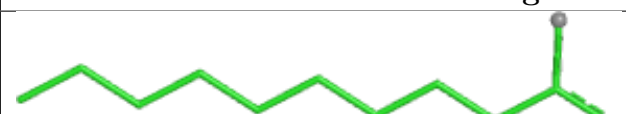
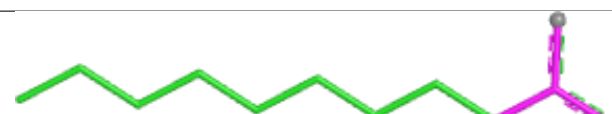
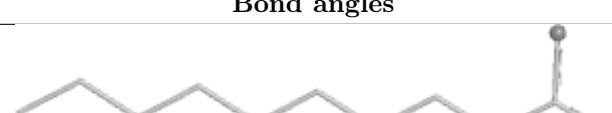
Ligand CLA B 601

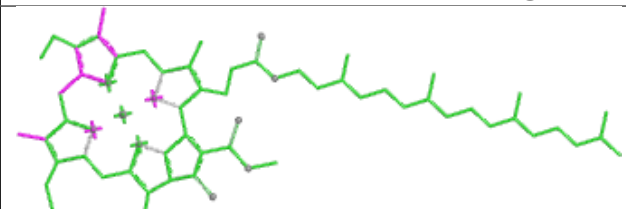
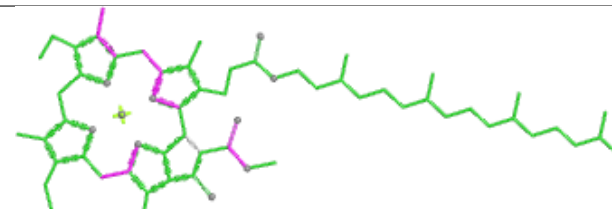
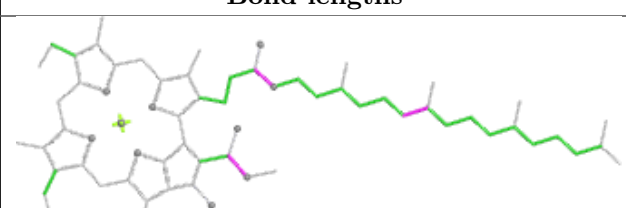
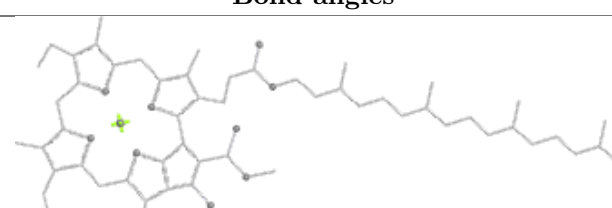




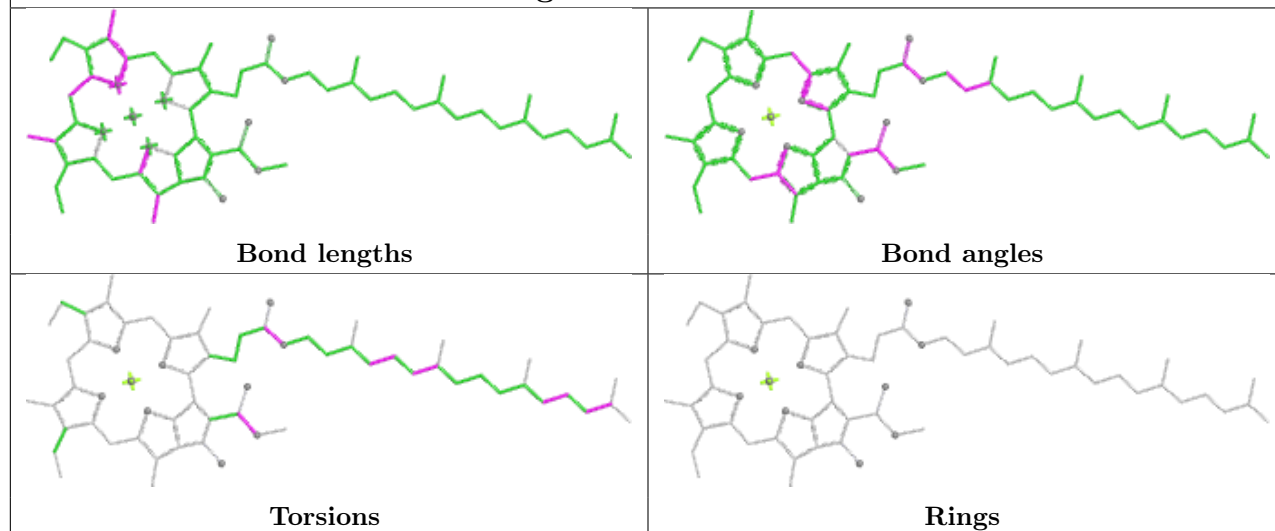
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE B 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

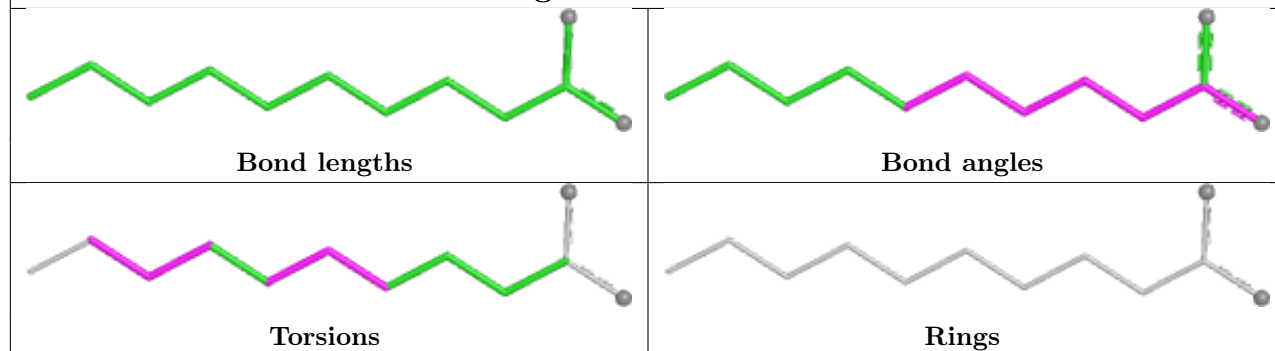
Ligand STE m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

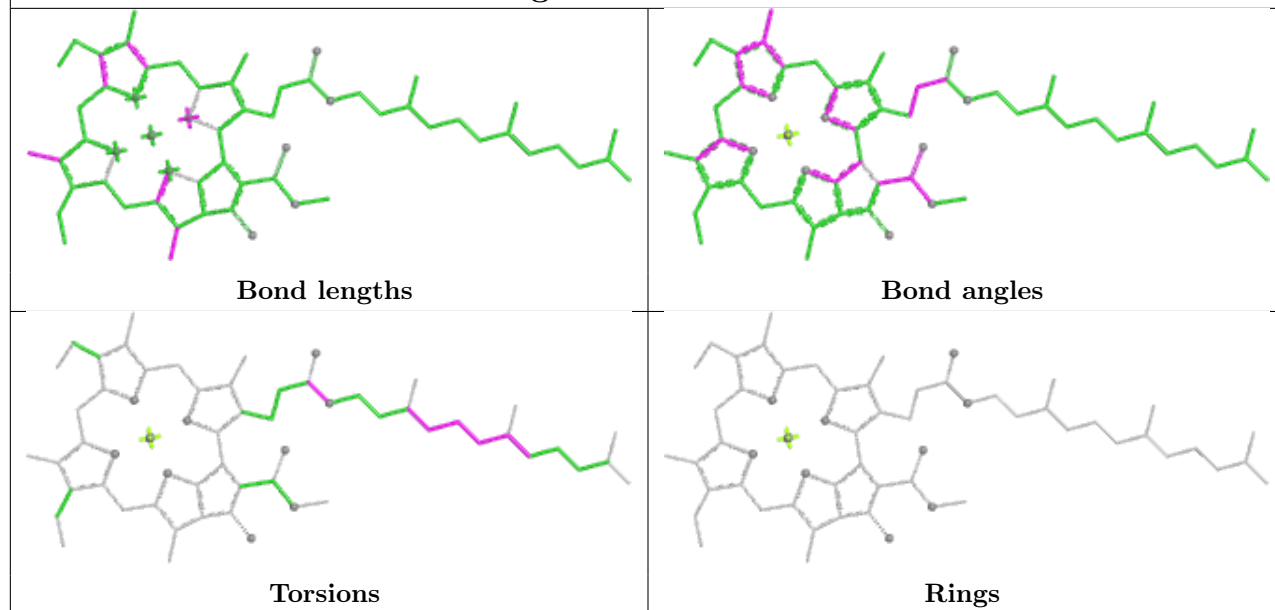
Ligand CLA c 502

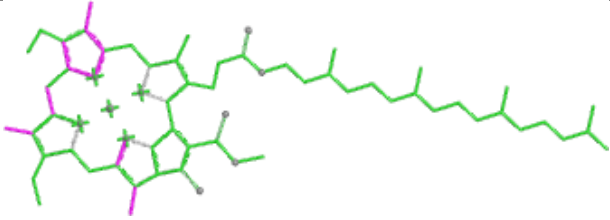
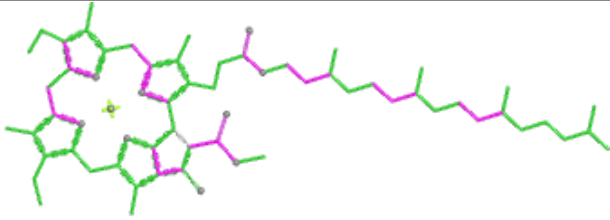
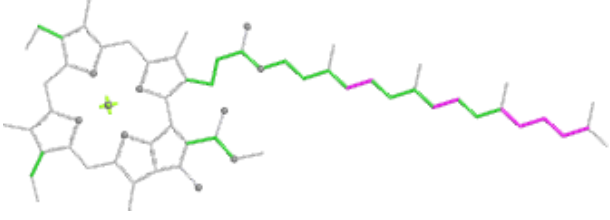
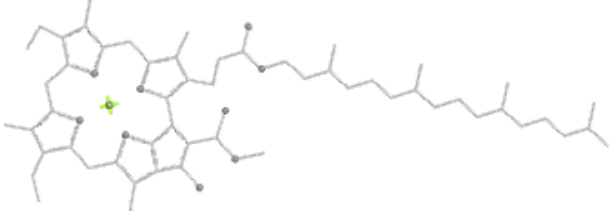
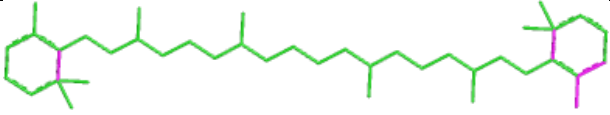
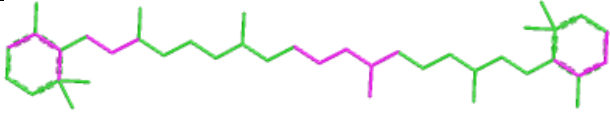
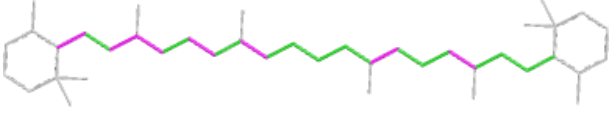
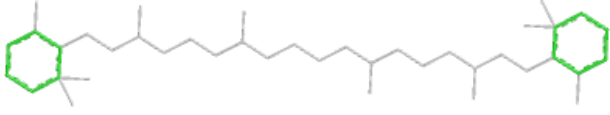
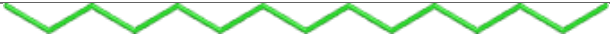
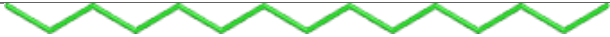
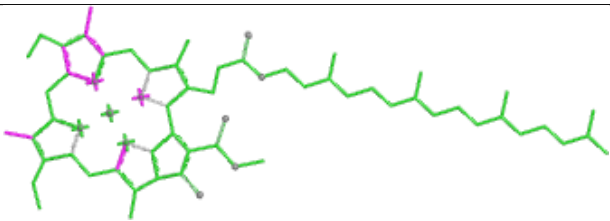
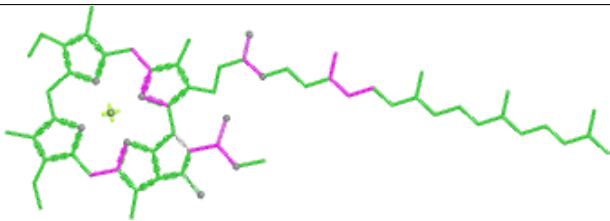
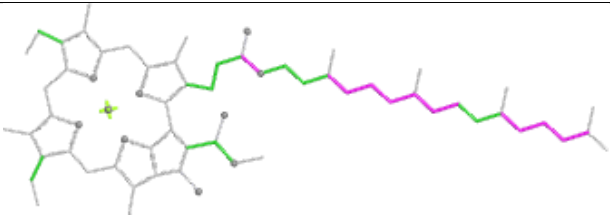
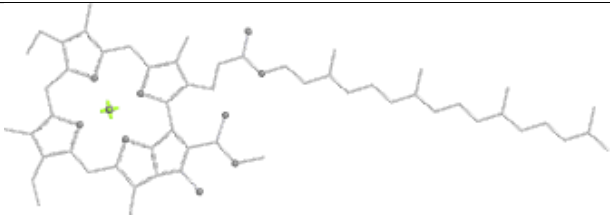


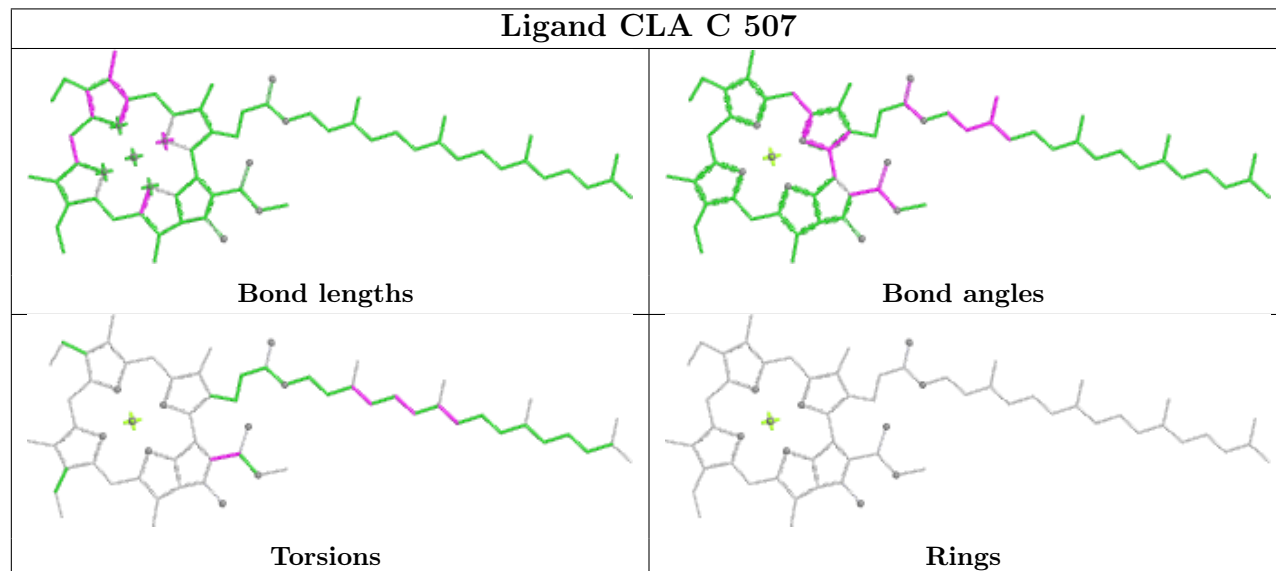
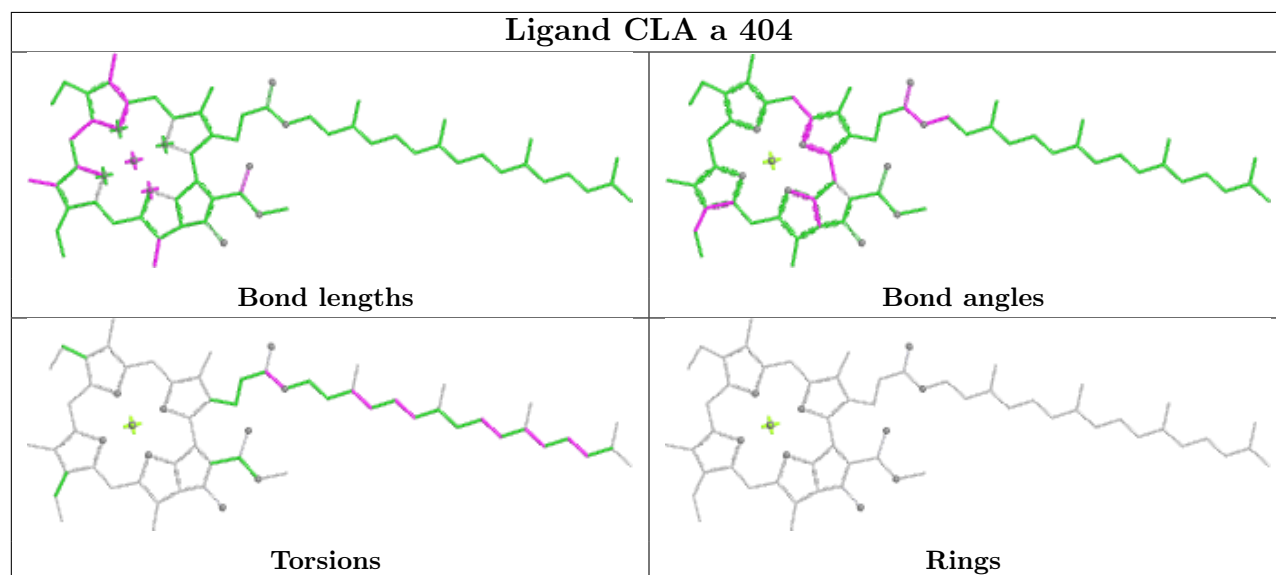
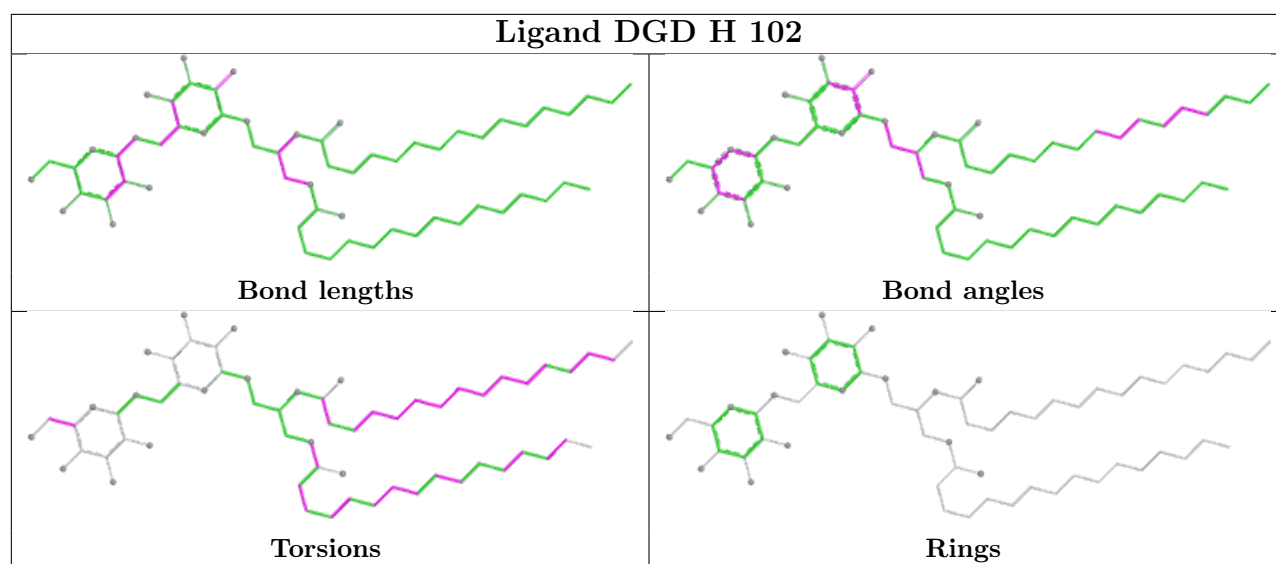
Ligand STE C 522

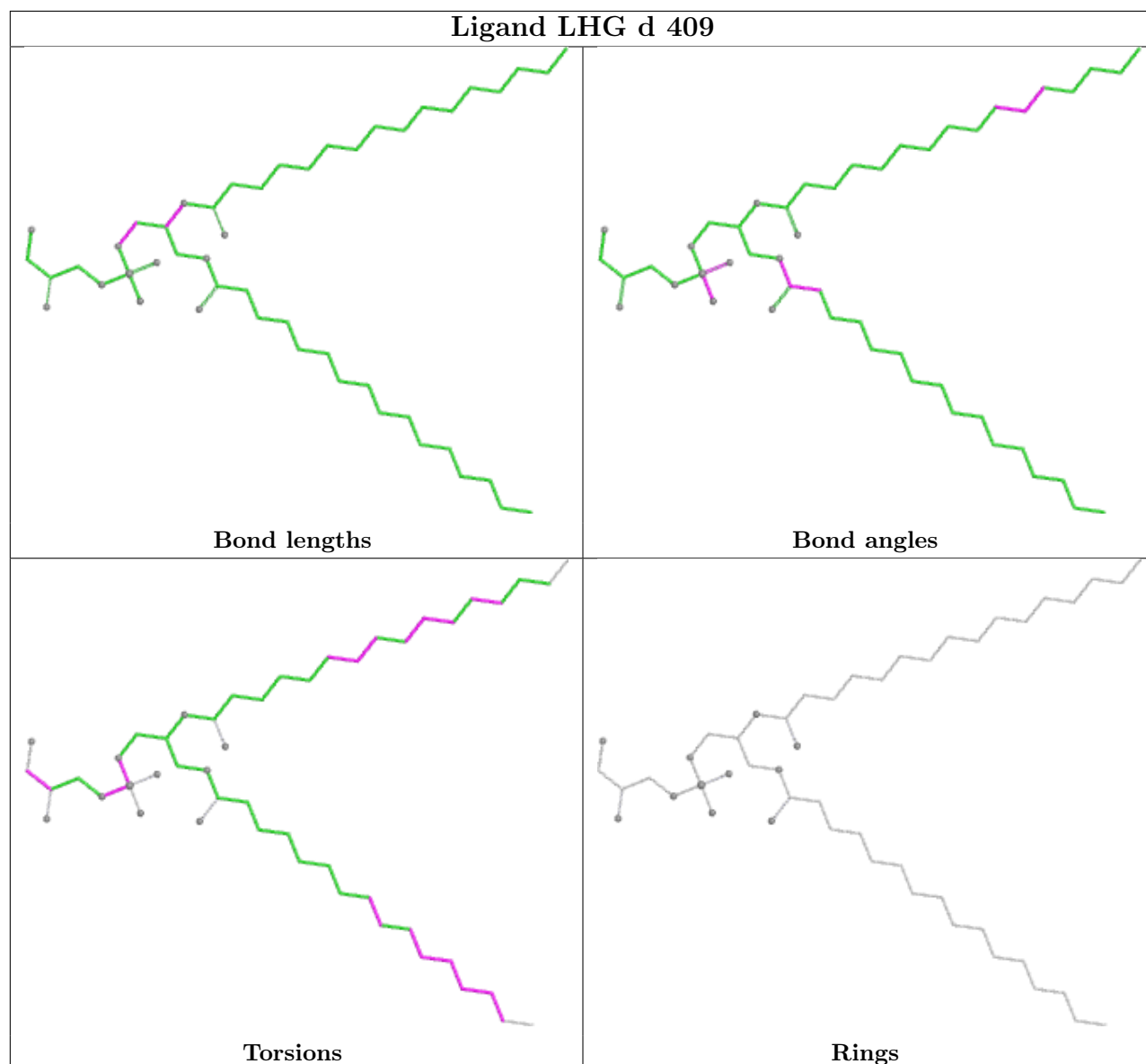
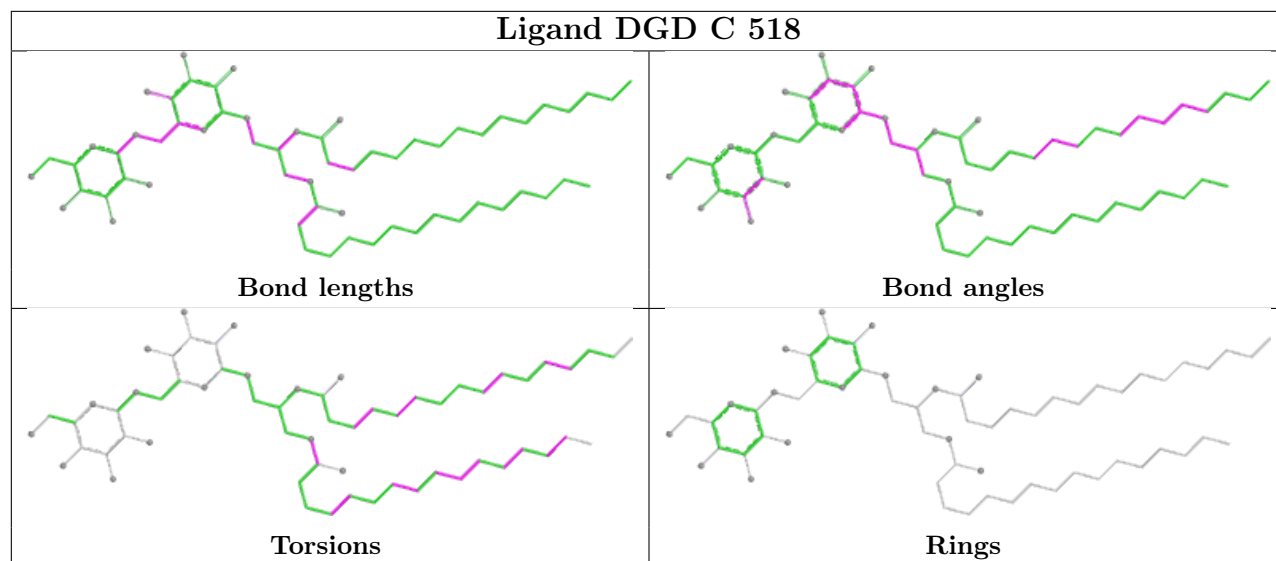


Ligand CLA B 616

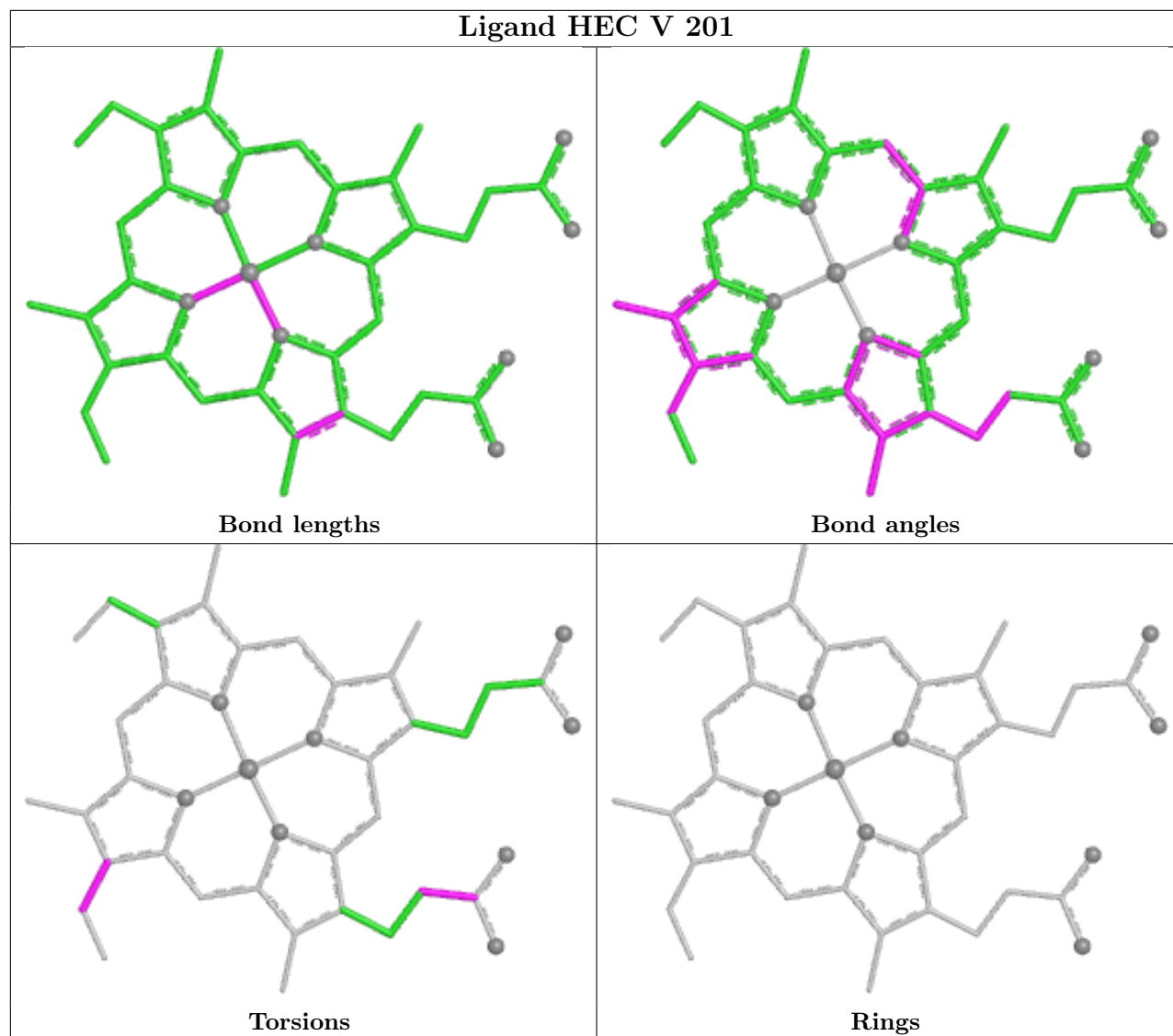


Ligand CLA b 604	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR t 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings

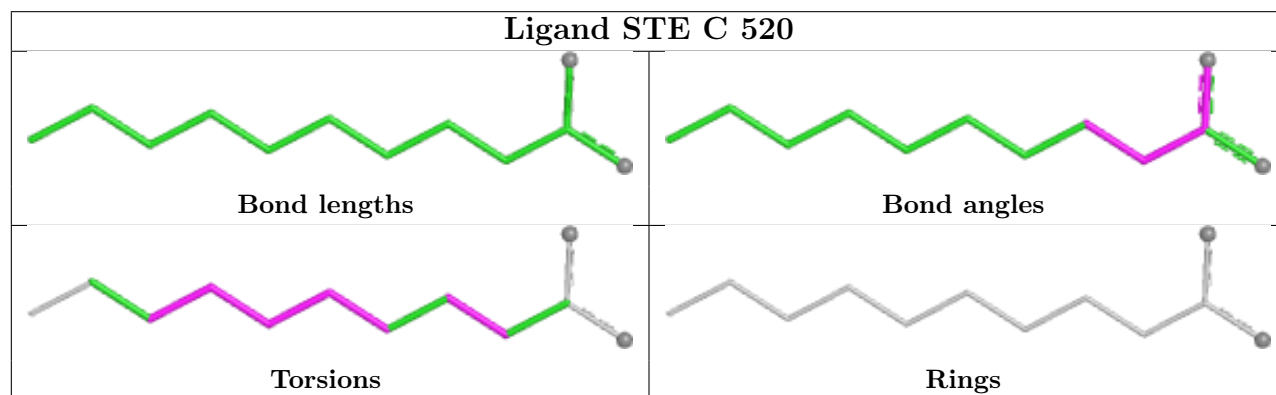




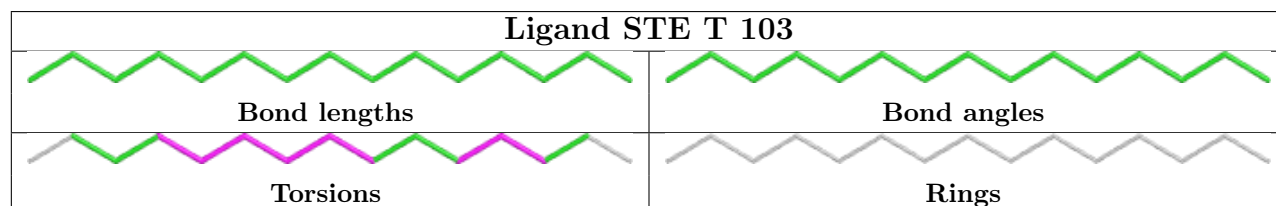
Ligand HEC V 201



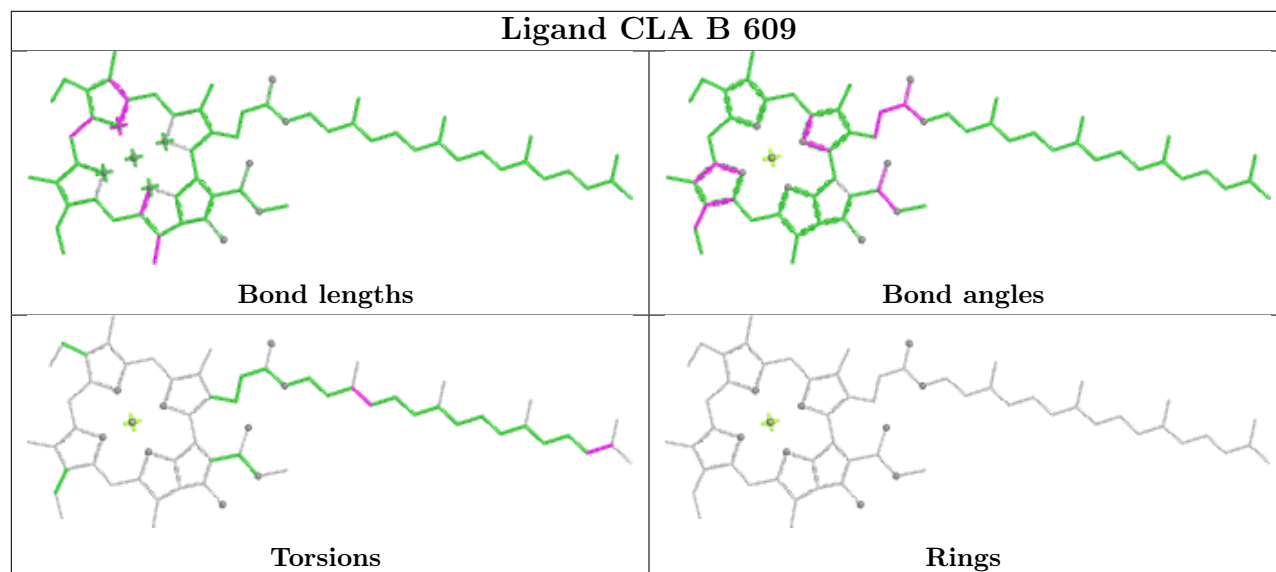
Ligand STE C 520



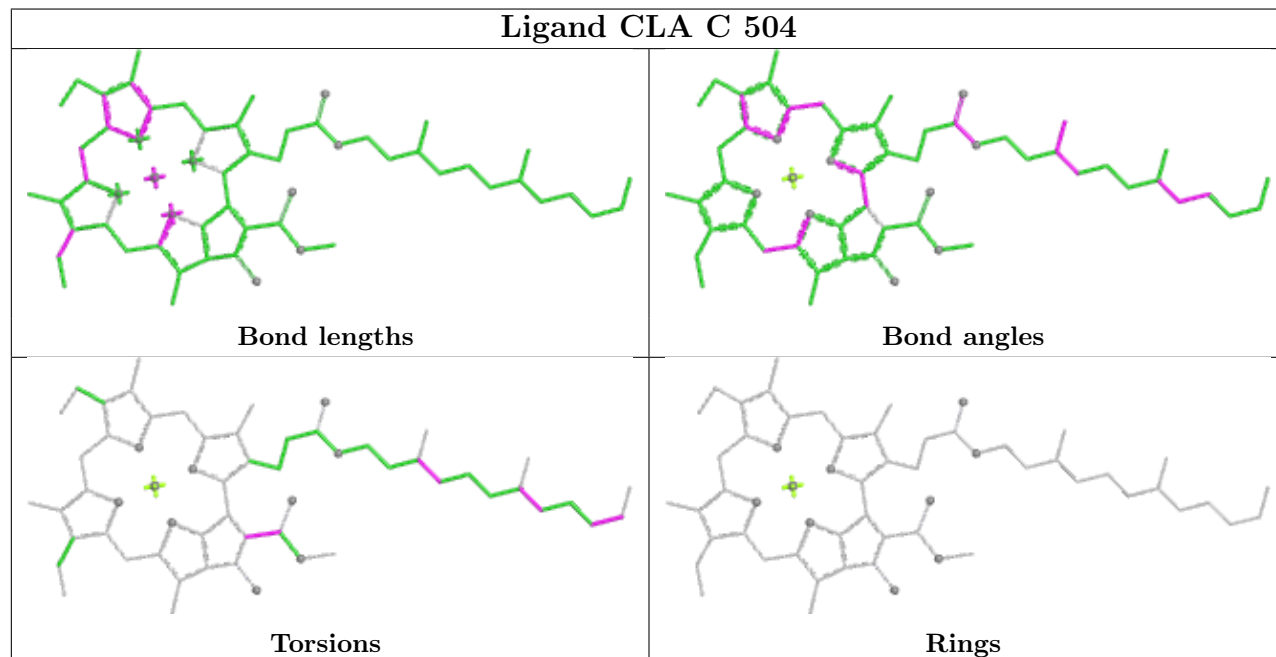
Ligand STE T 103



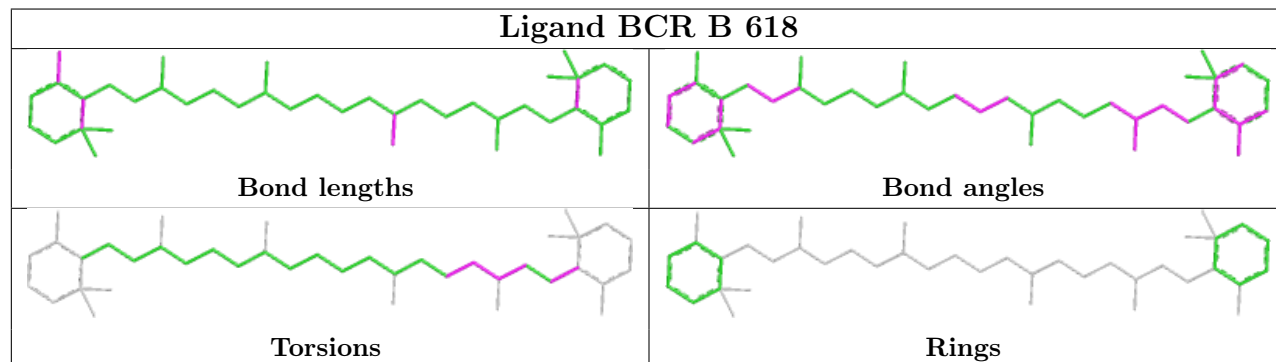
Ligand CLA B 609



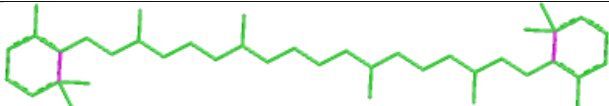
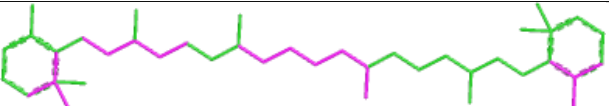
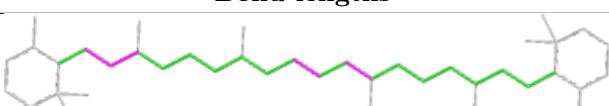
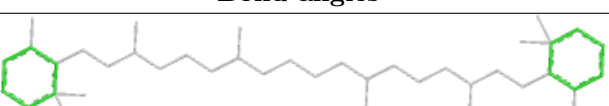
Ligand CLA C 504

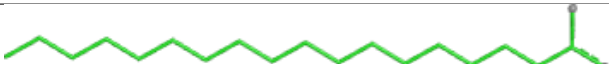
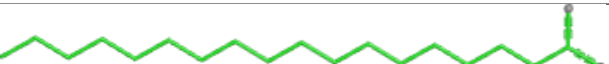
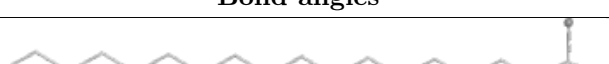


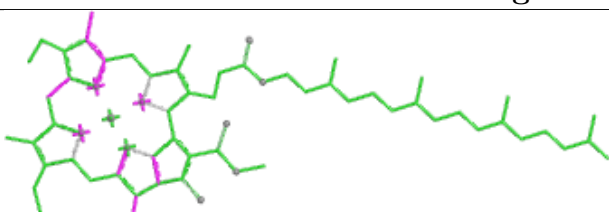
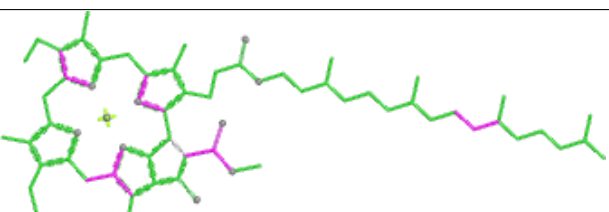
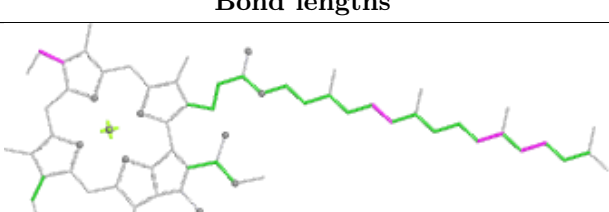
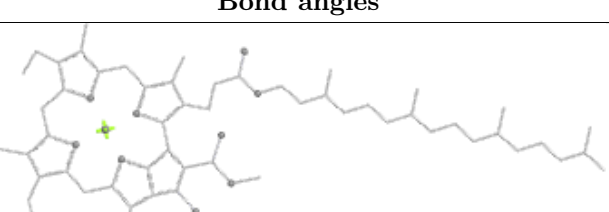
Ligand BCR B 618

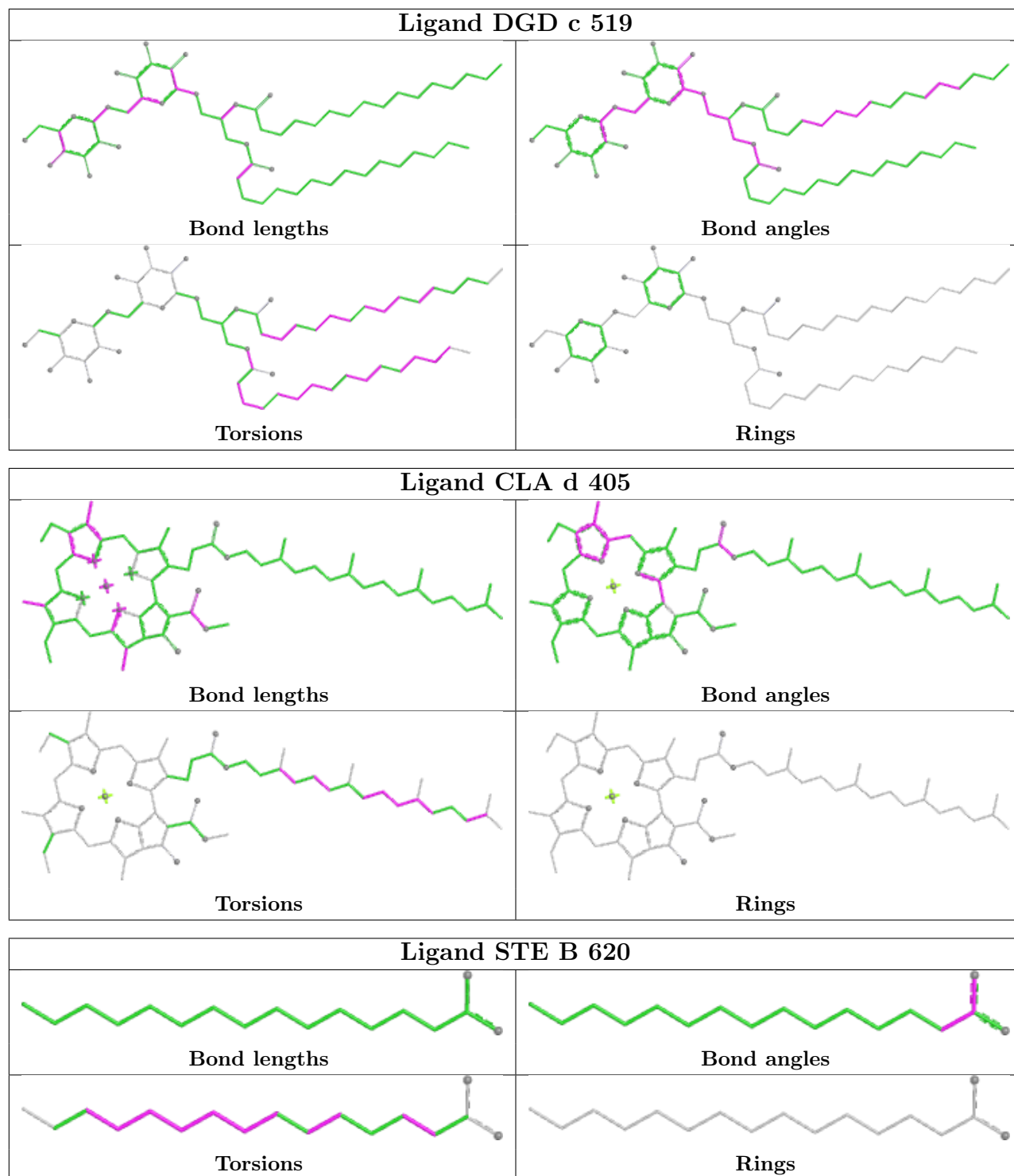


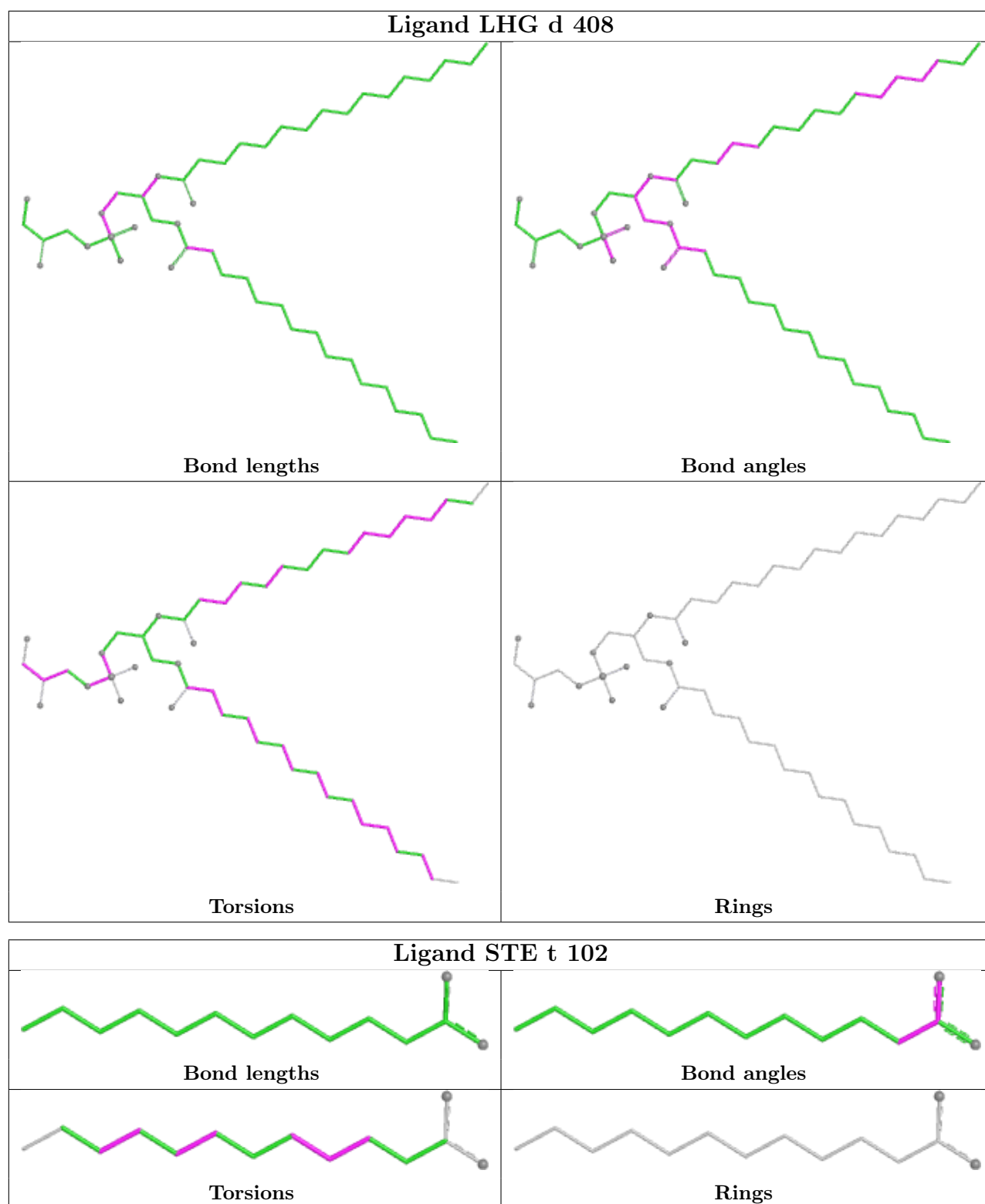
Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

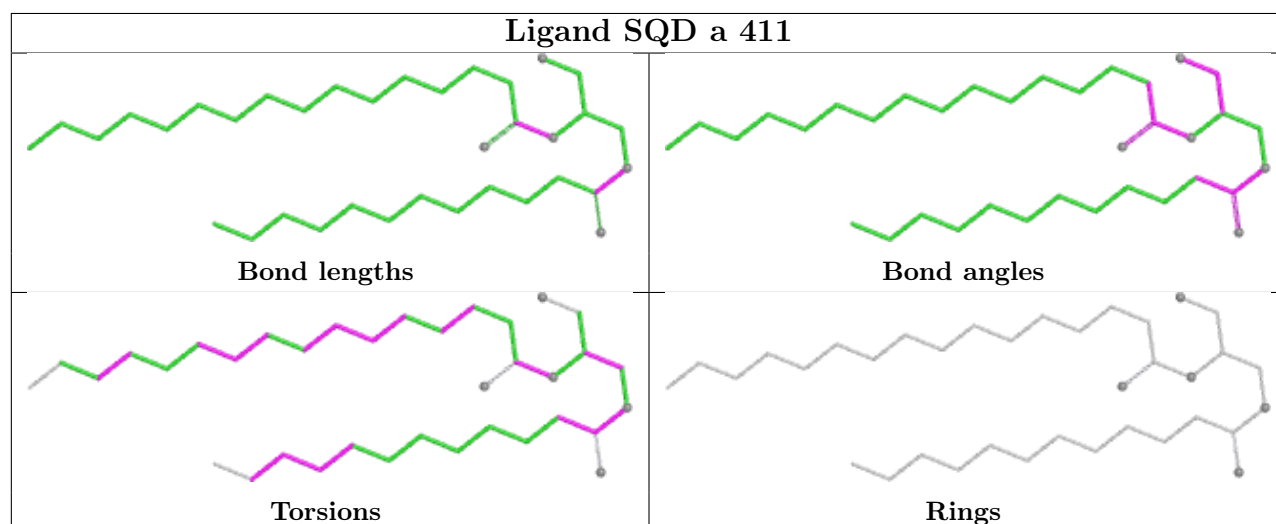
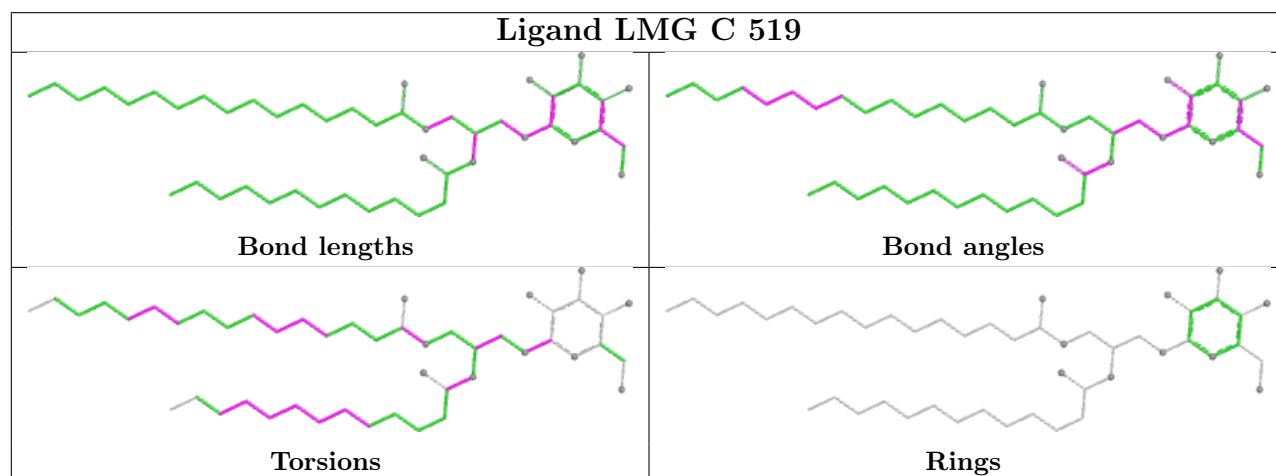
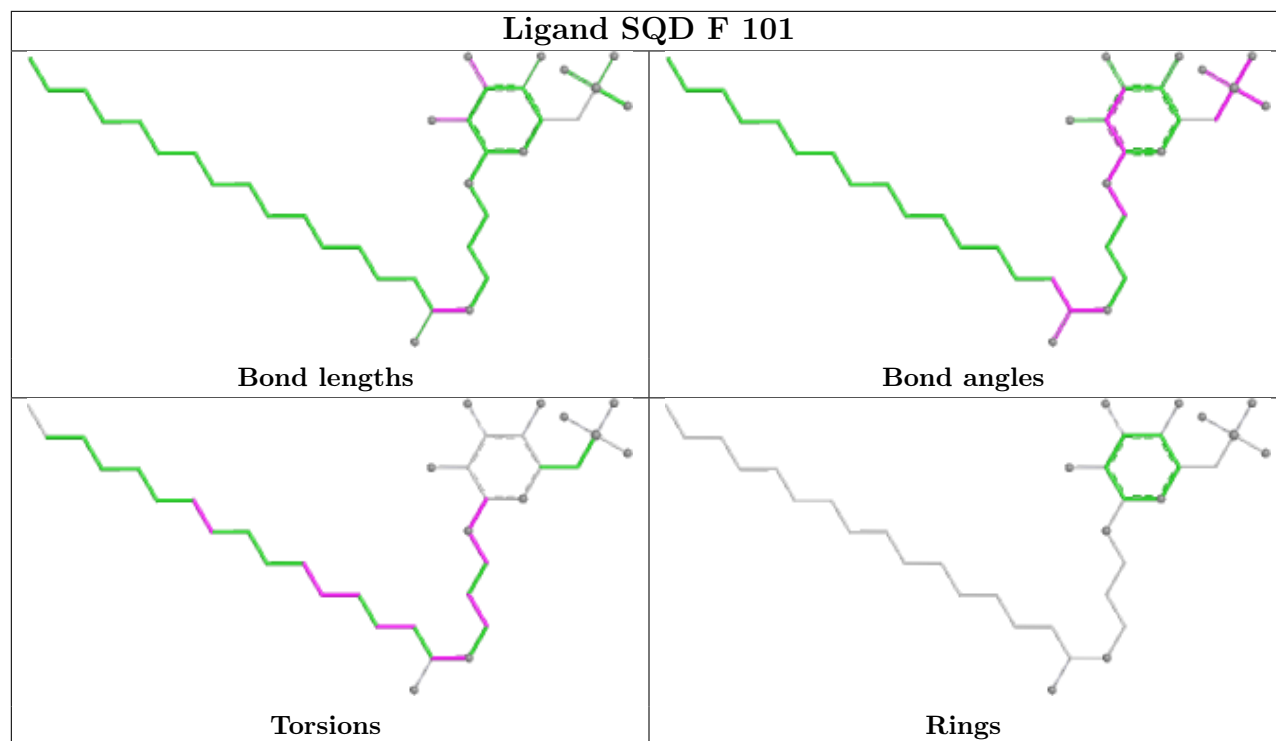
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

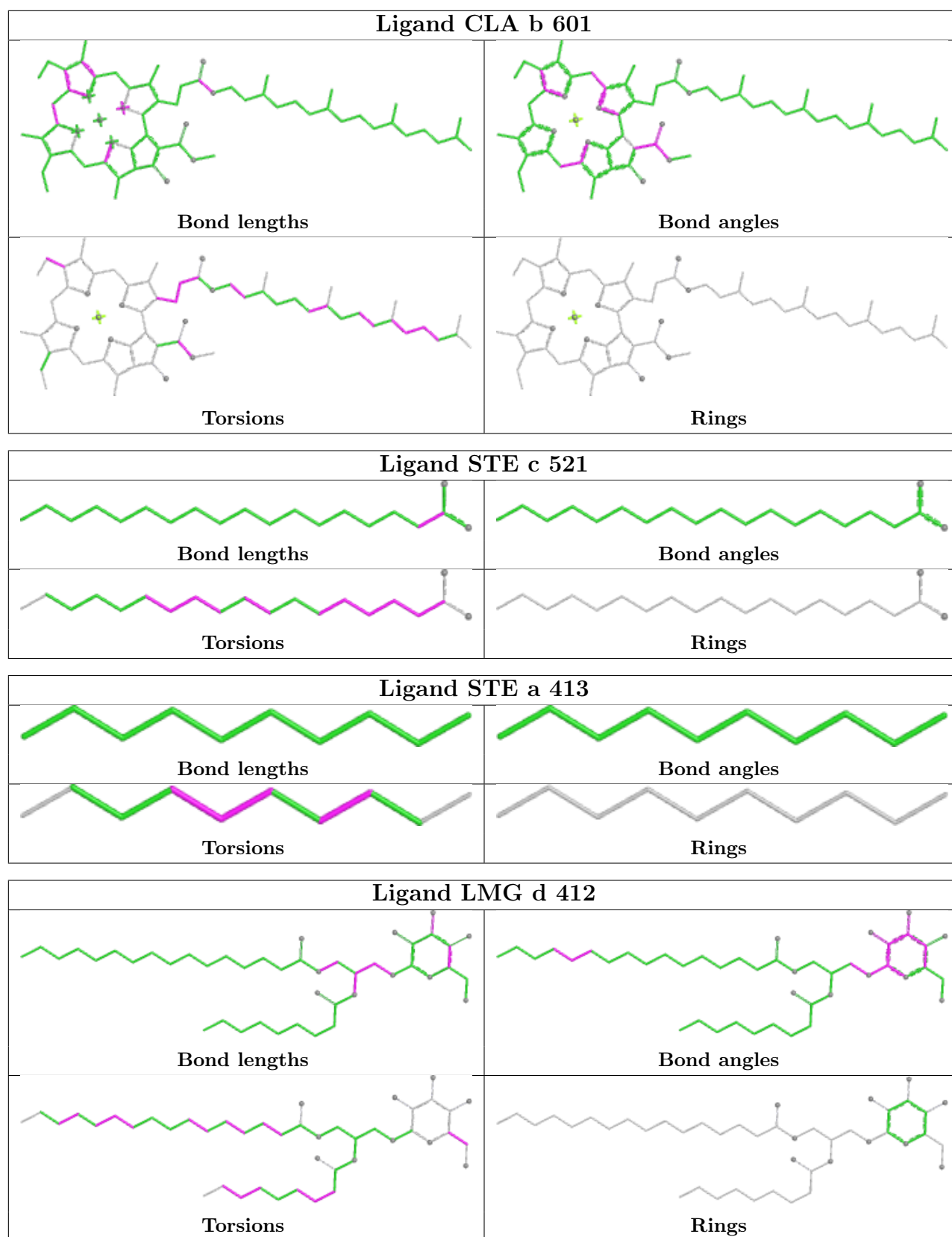
Ligand STE b 621	
 Bond lengths	 Bond angles
 Torsions	 Rings

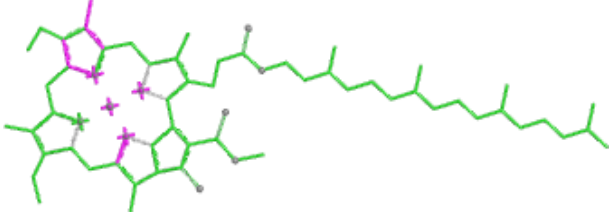
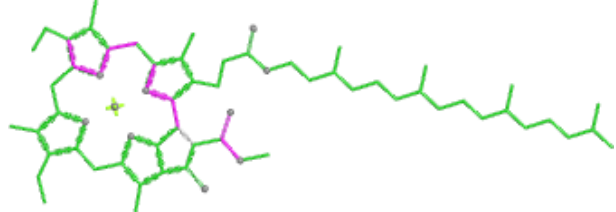
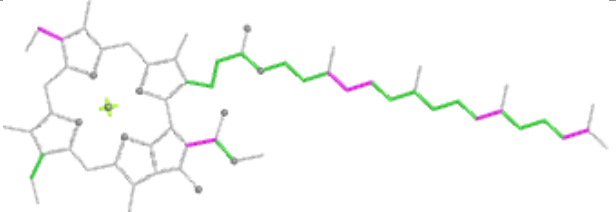
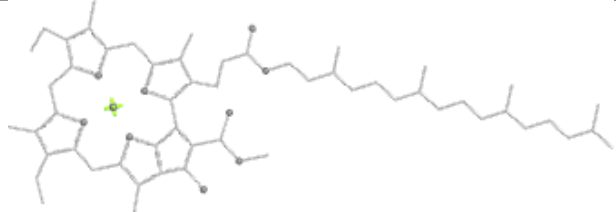
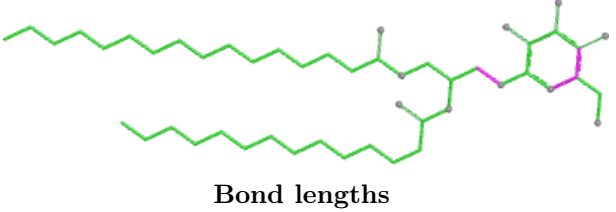
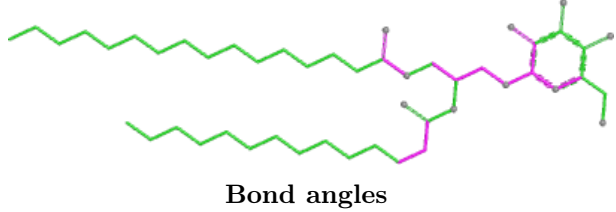
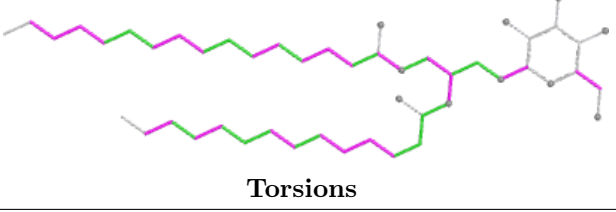
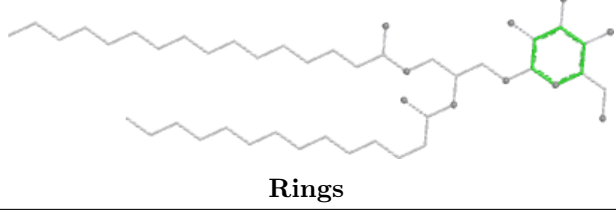
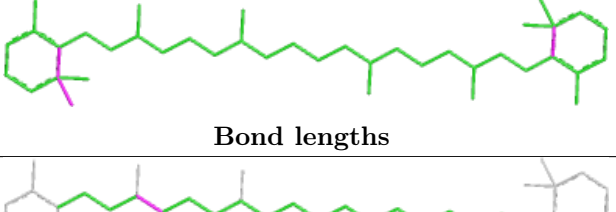
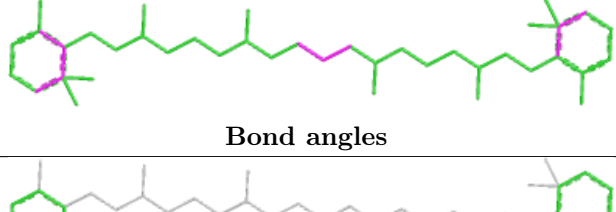
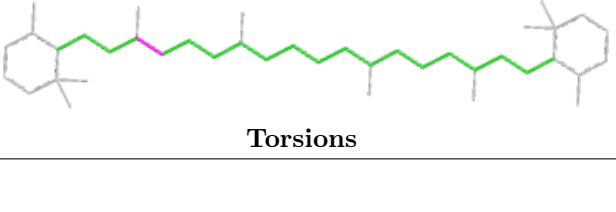
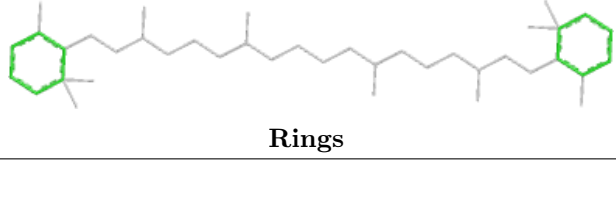
Ligand CLA b 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

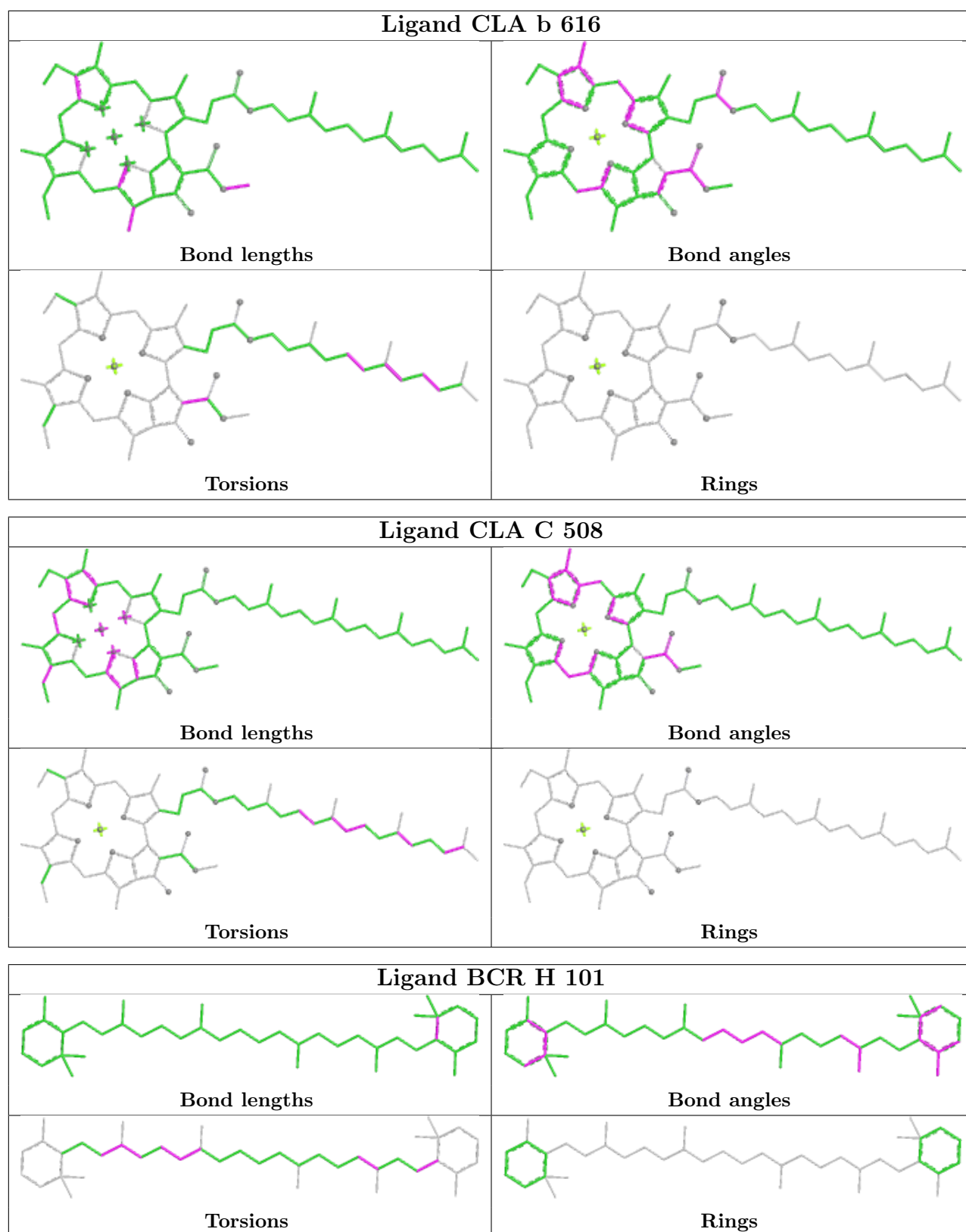


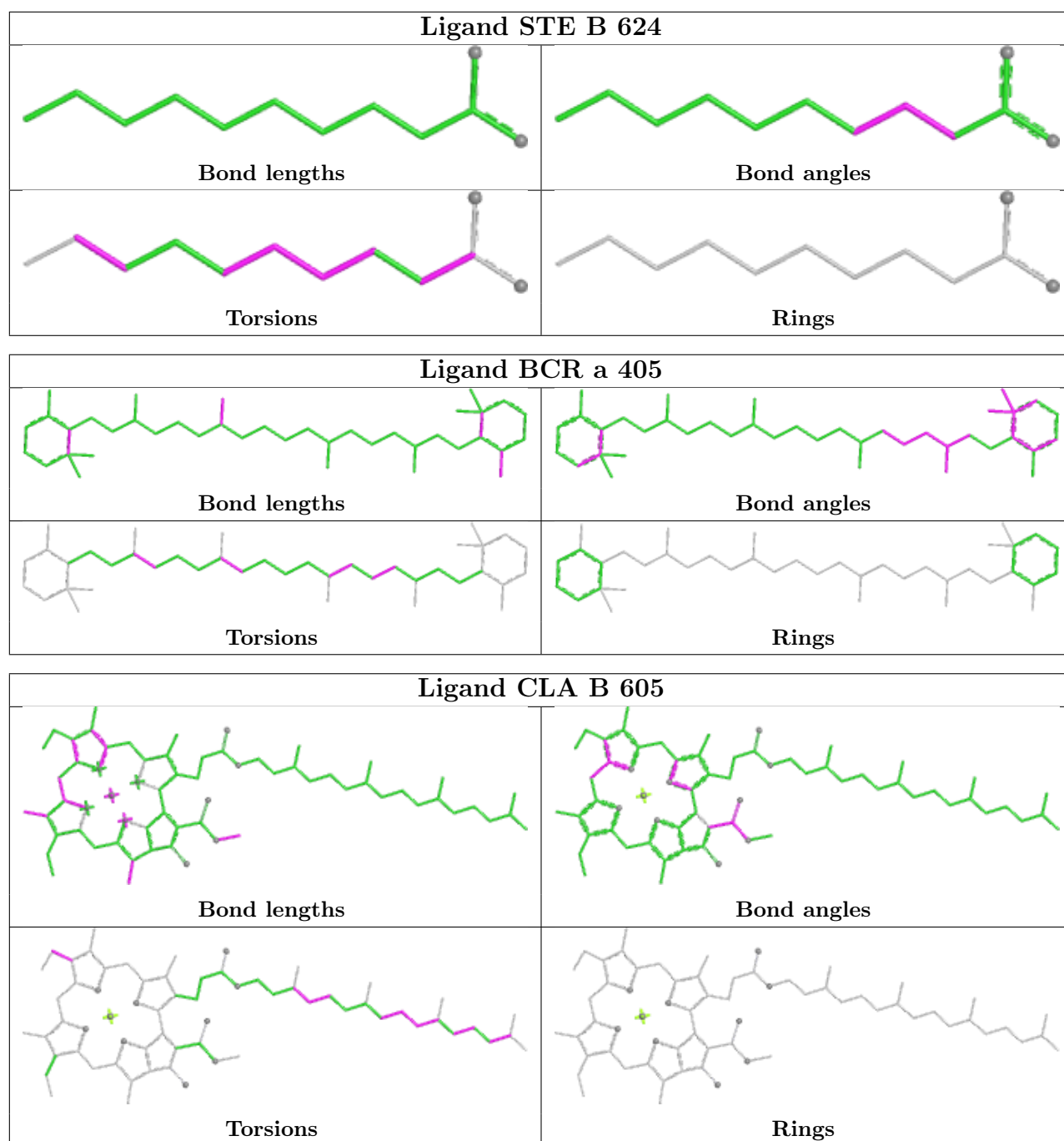




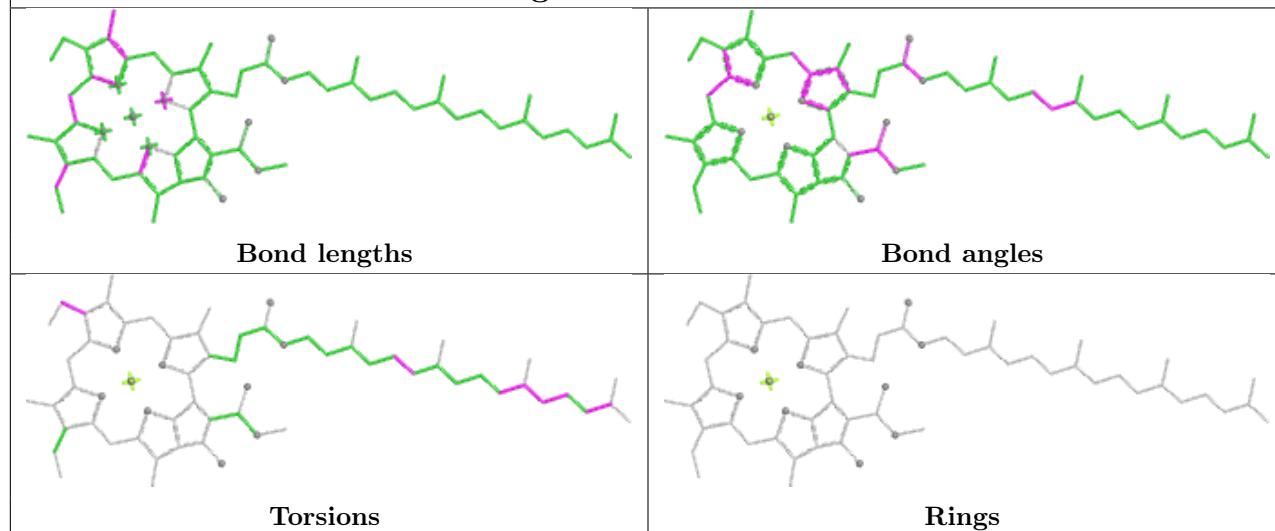


Ligand CLA C 502	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG c 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

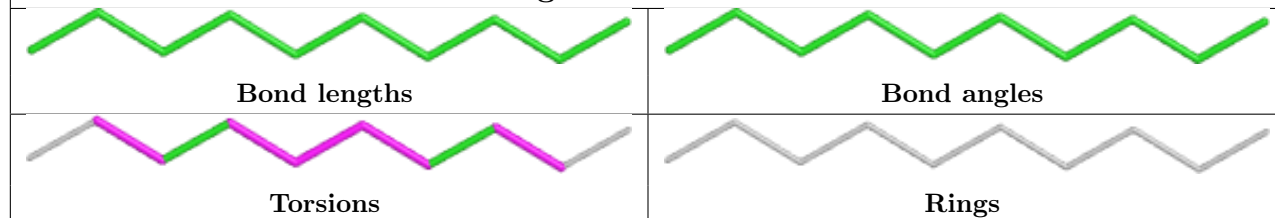




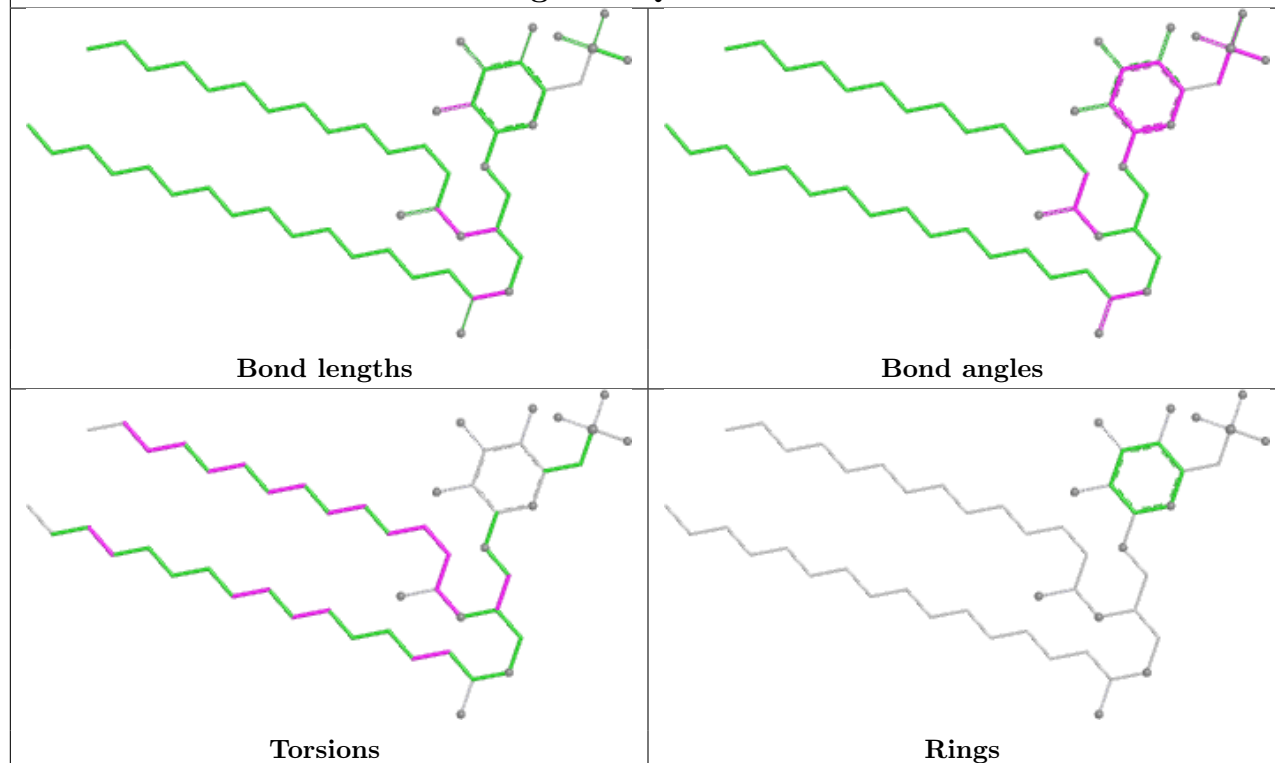
Ligand CLA B 615



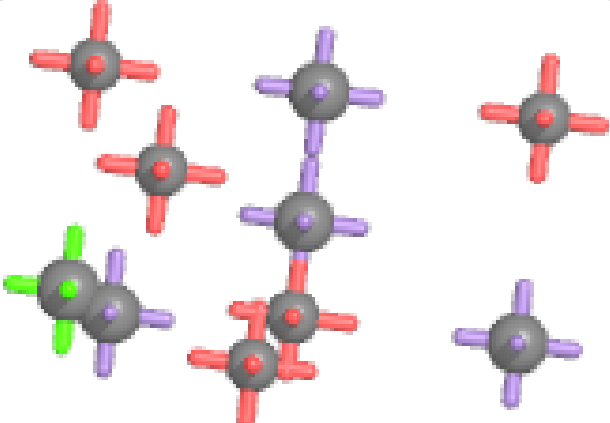
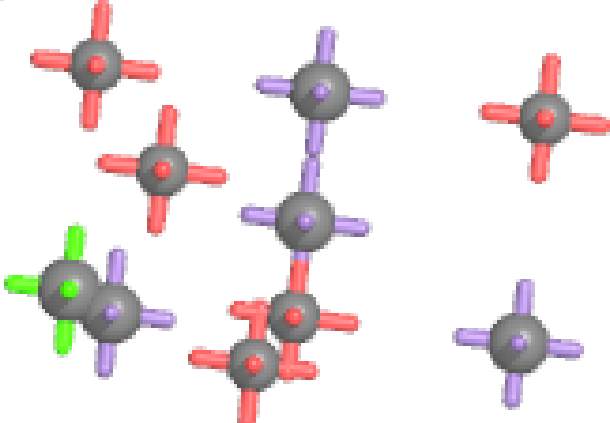
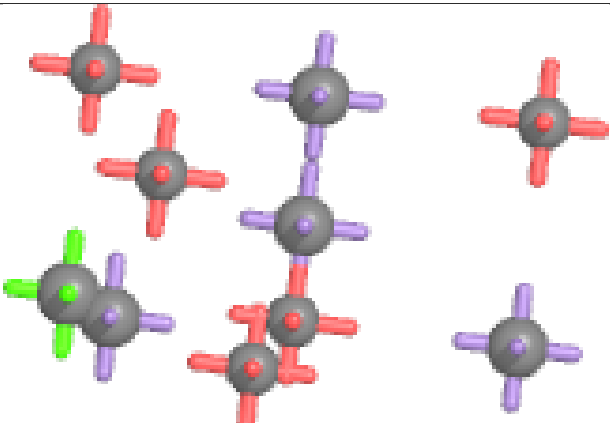
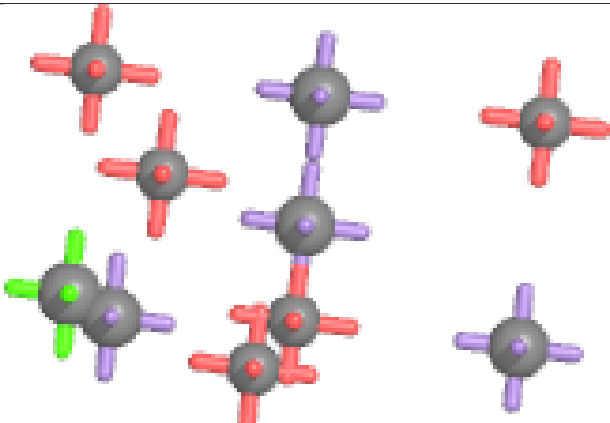
Ligand STE b 625

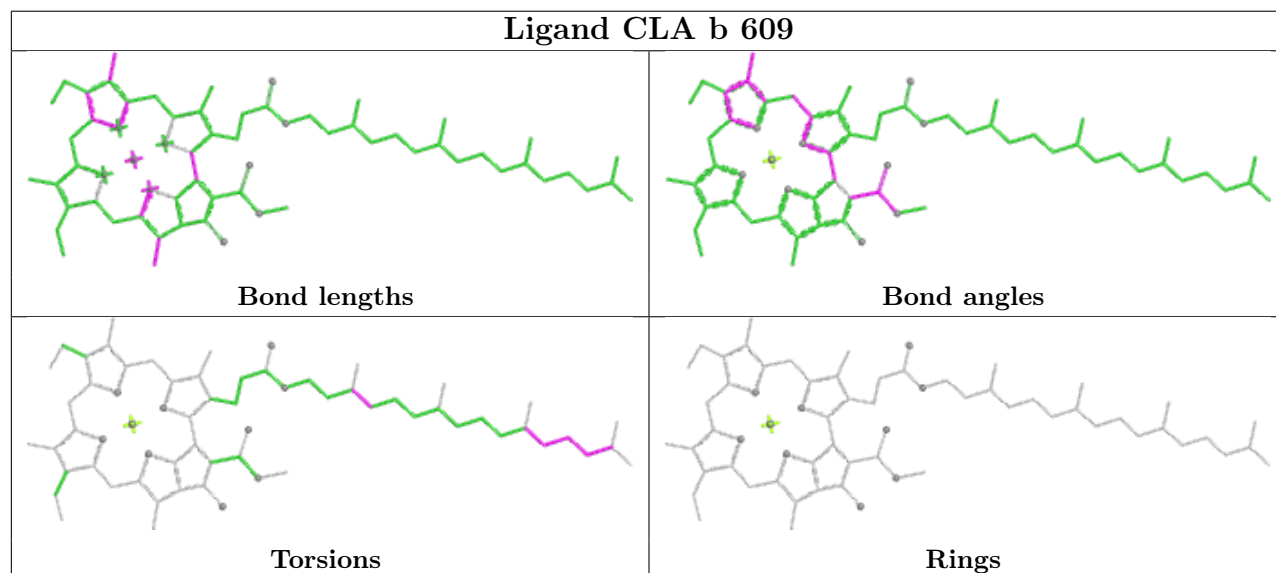
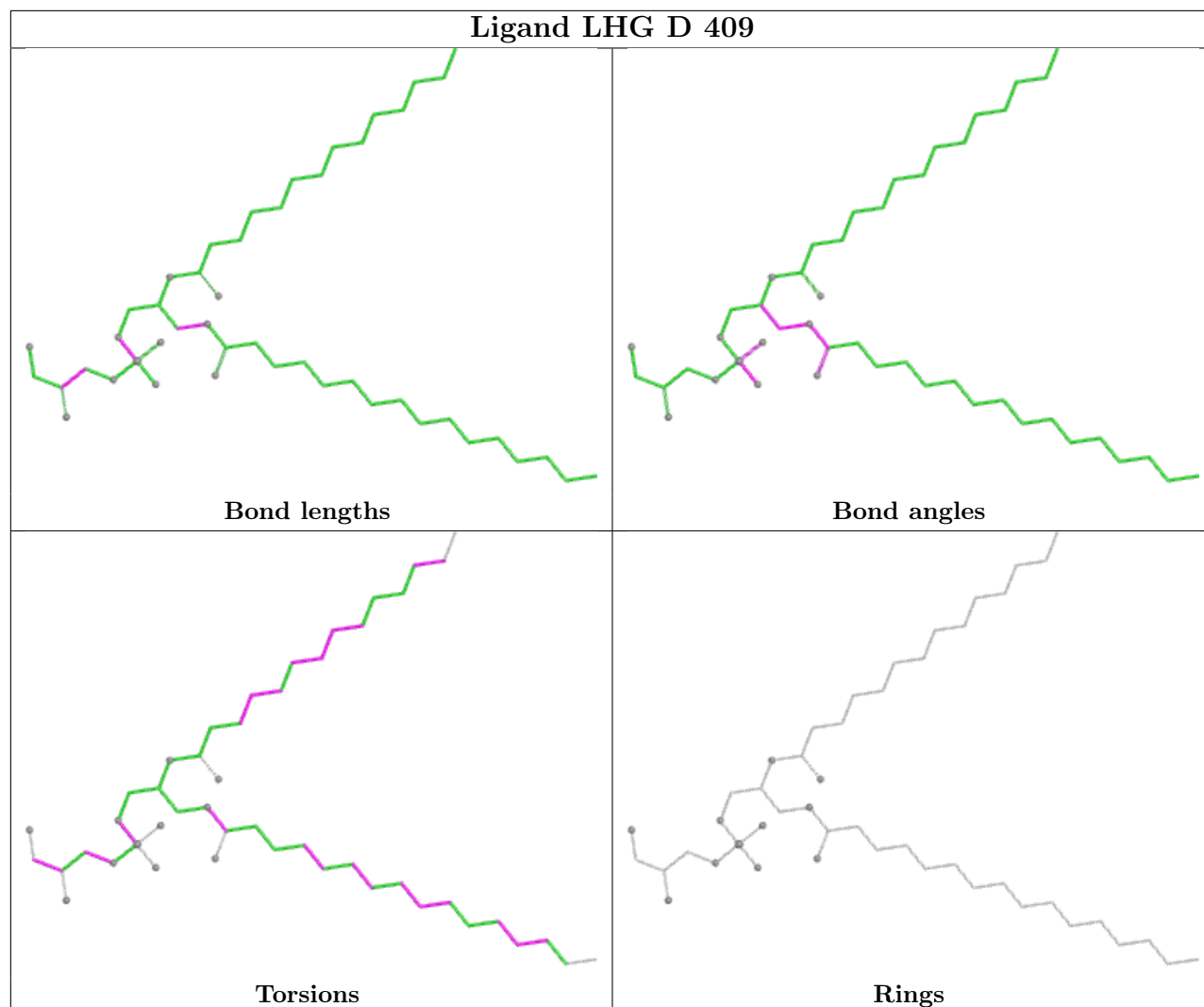


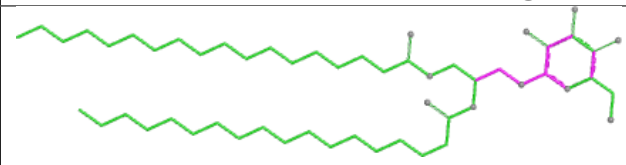
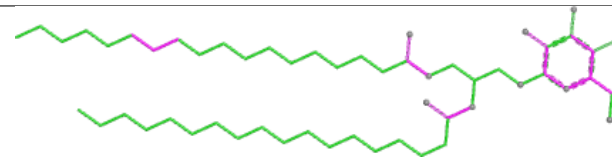
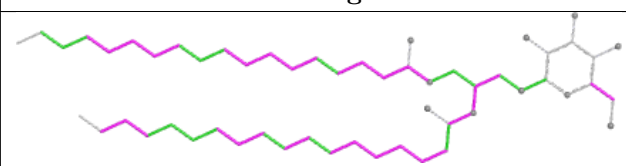
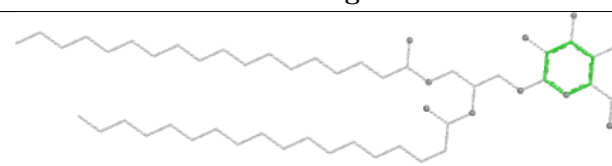
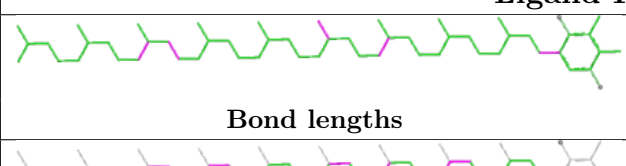
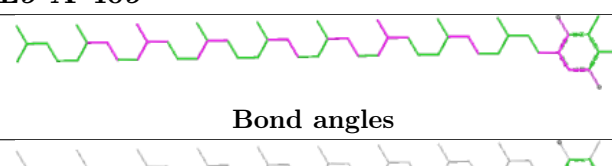
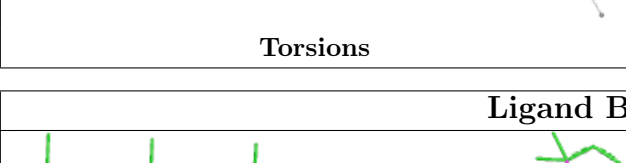
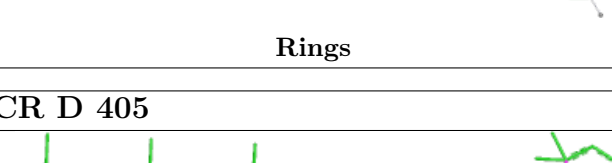
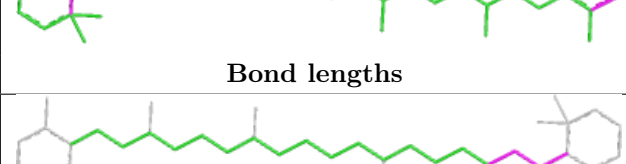
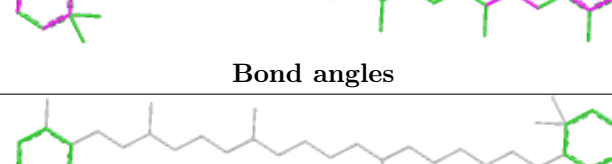
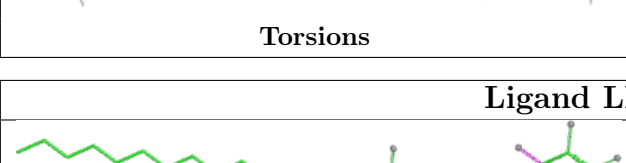
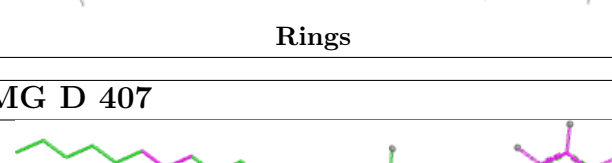
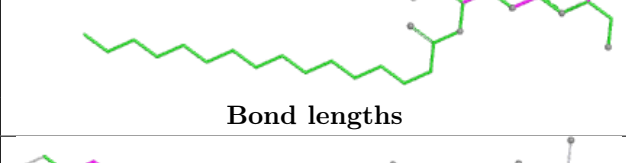
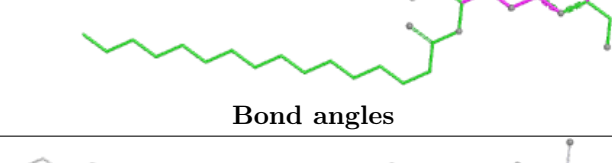
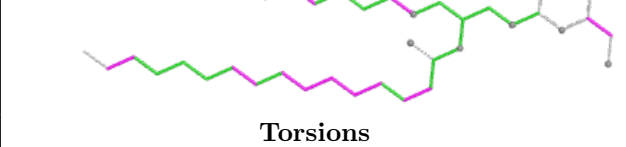
Ligand SQD A 412

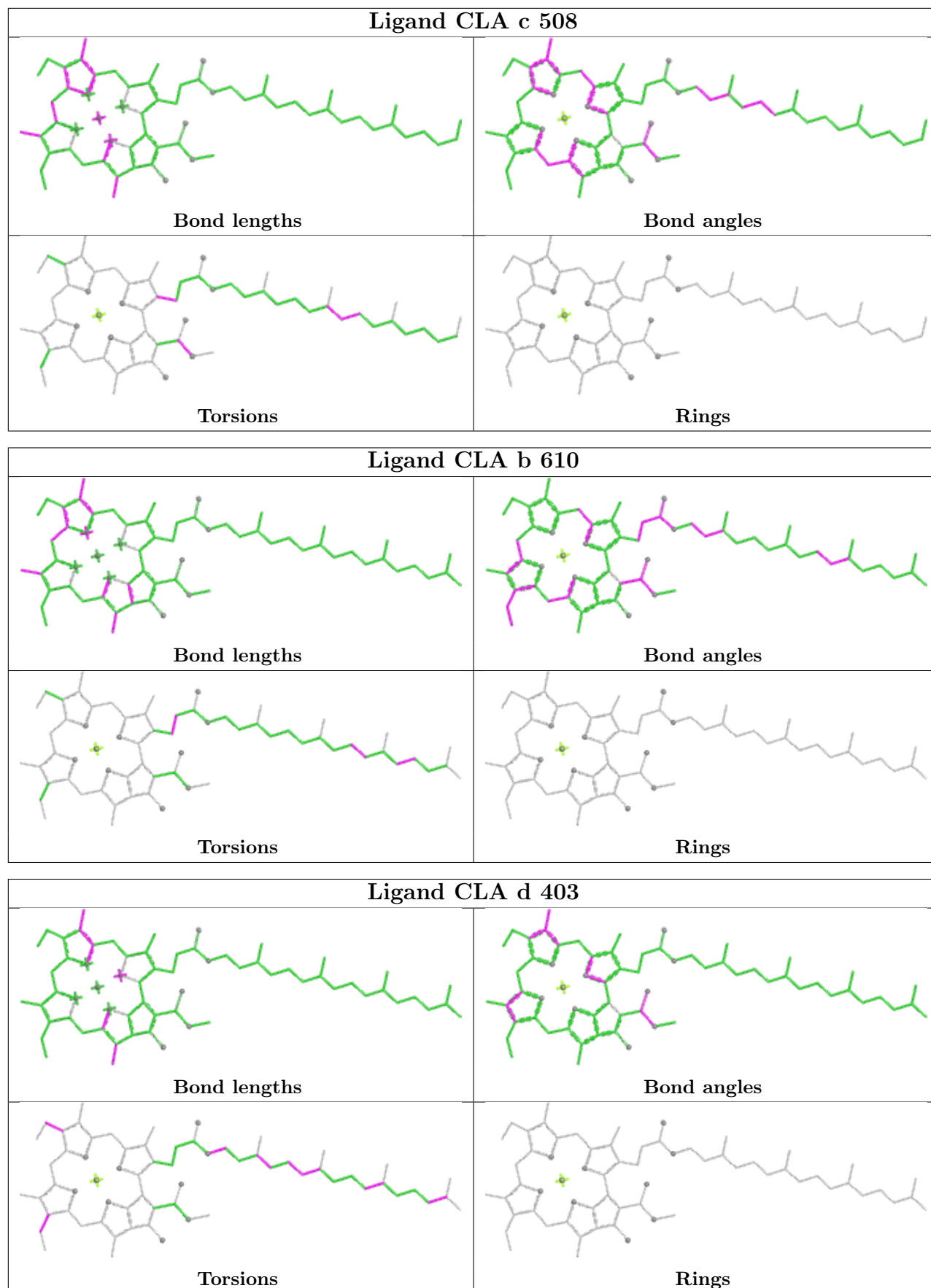


Ligand STE H 103	
 Bond lengths	 Bond angles
 Torsions	 Rings

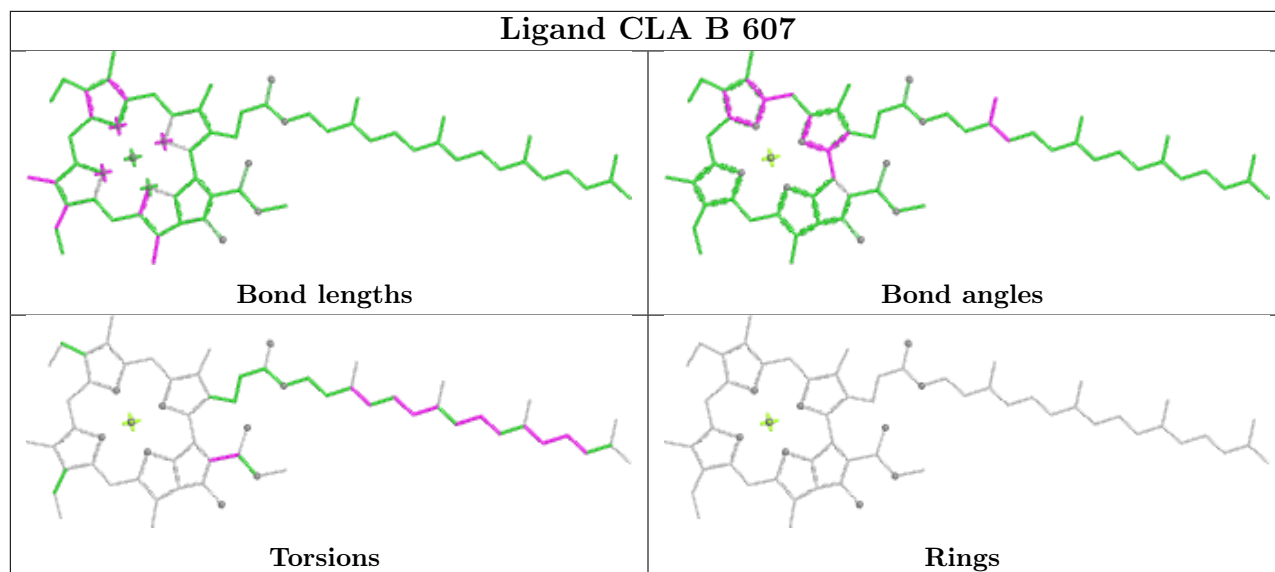
Ligand OEX a 416 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings



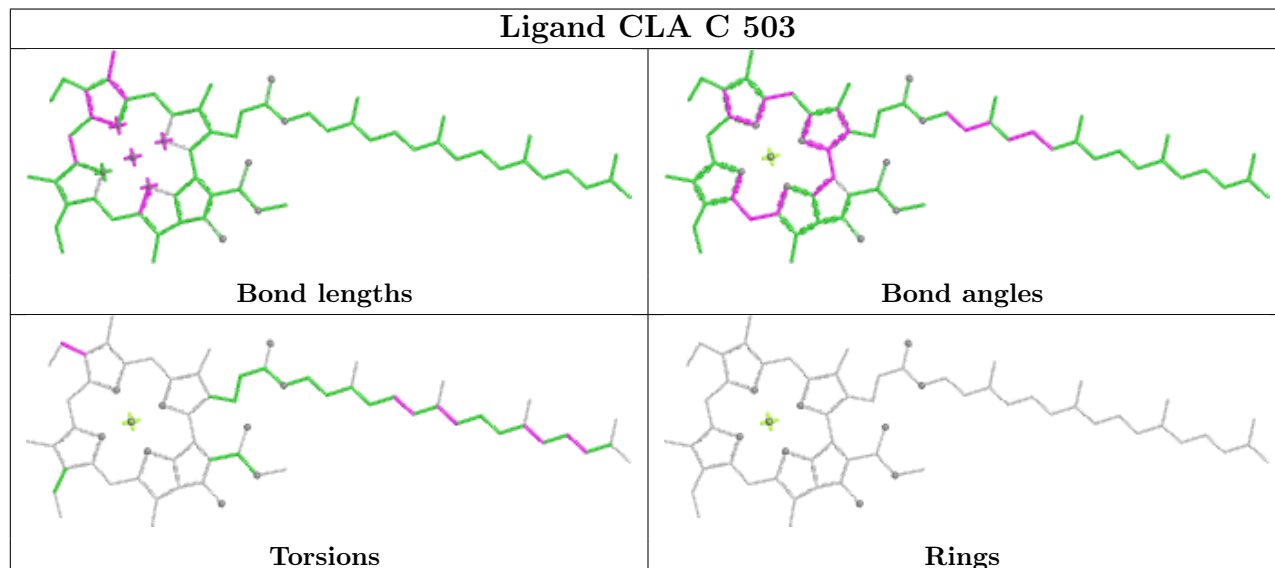
Ligand LMG b 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 A 409	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR D 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG D 407	
 Bond lengths	 Bond angles
 Torsions	 Rings



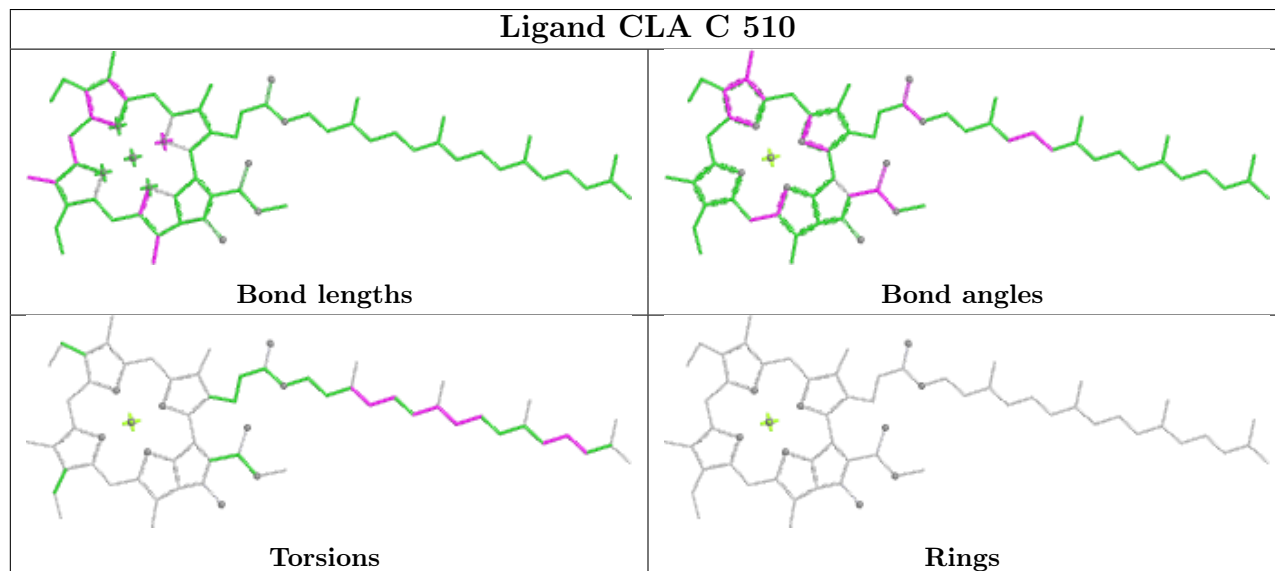
Ligand CLA B 607

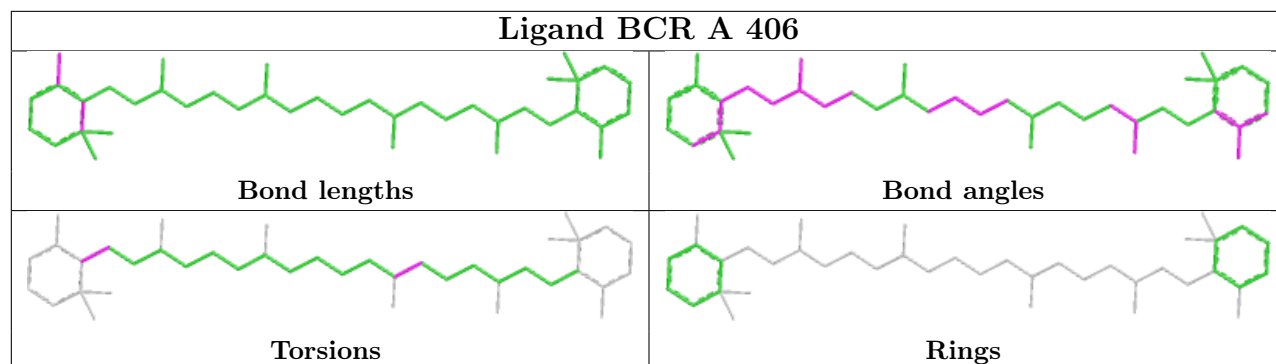
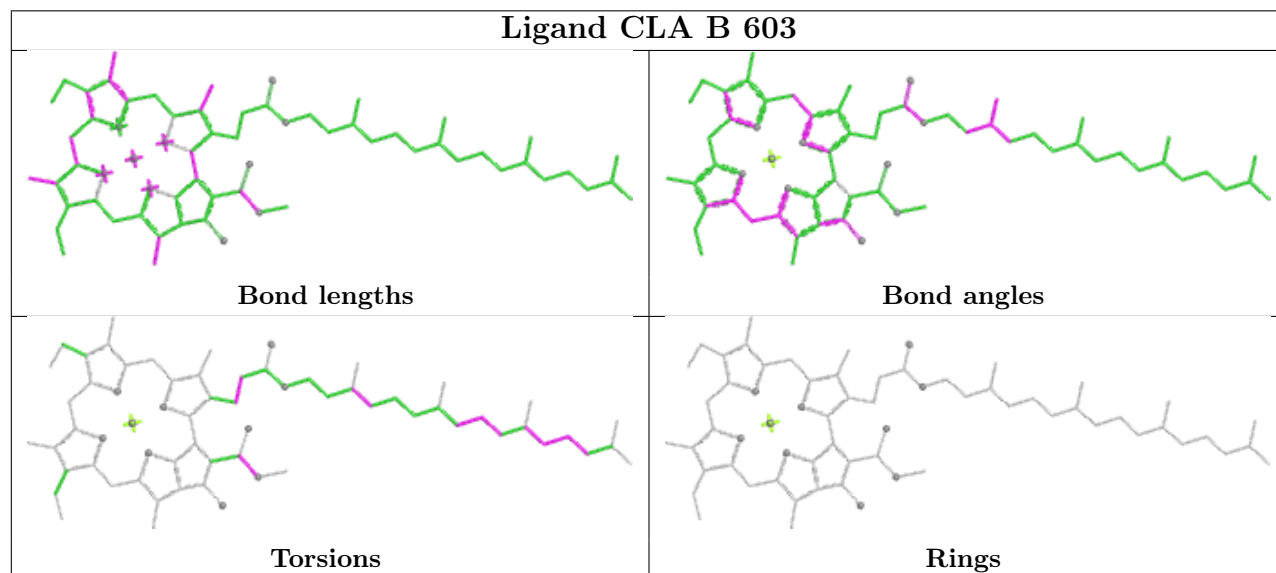
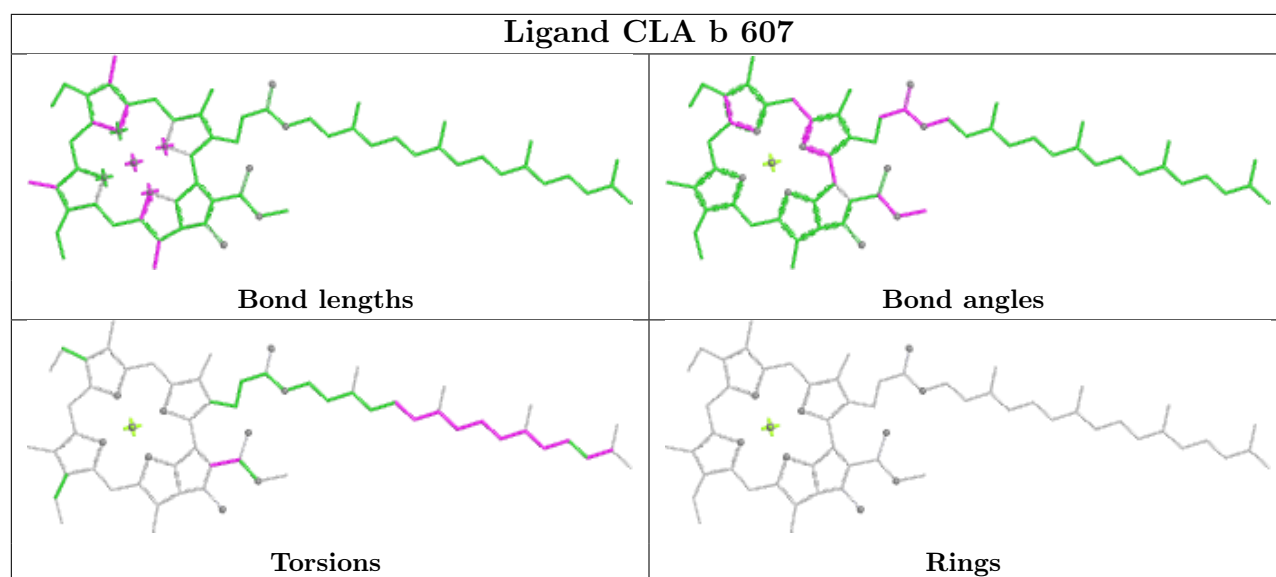


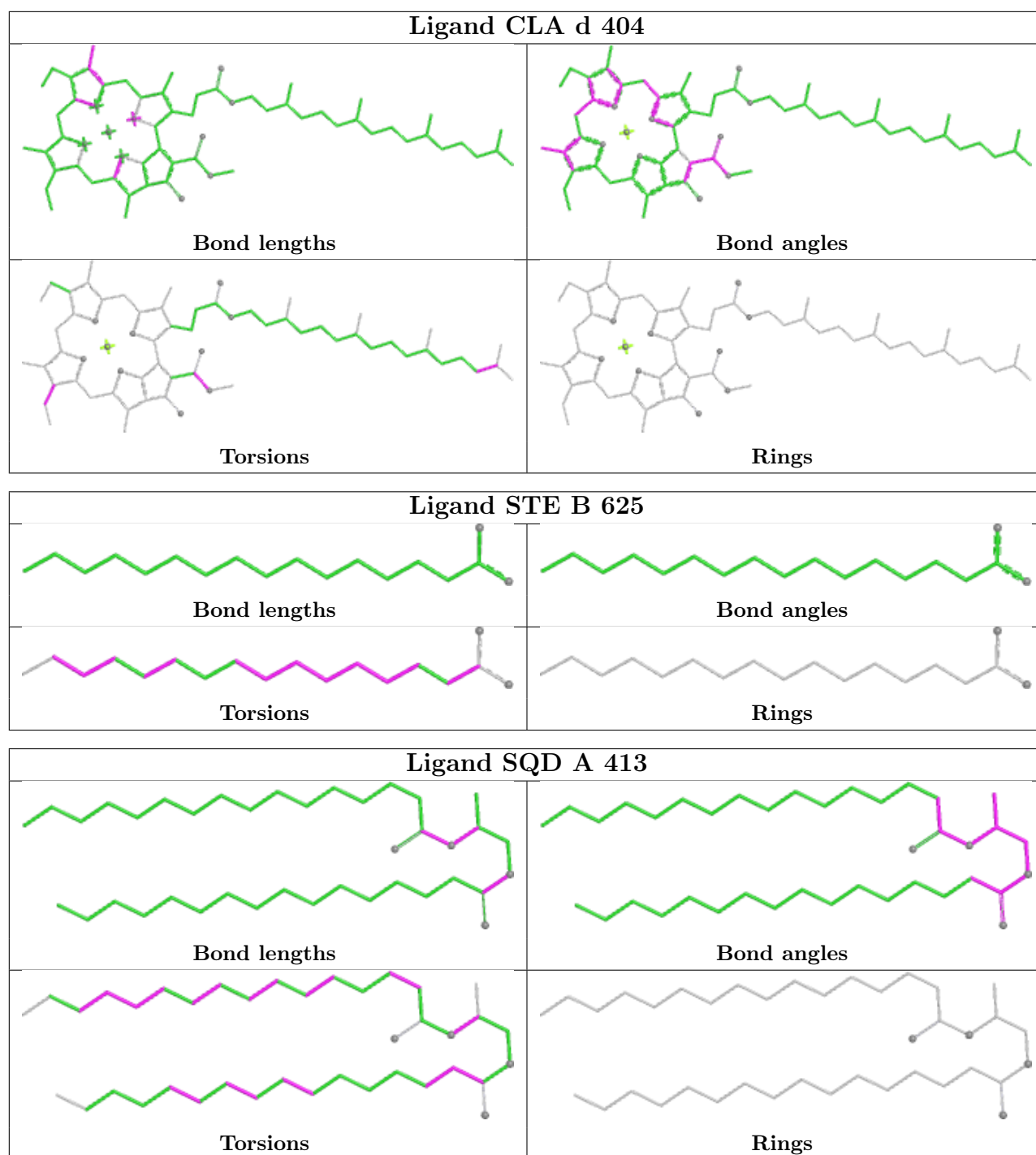
Ligand CLA C 503

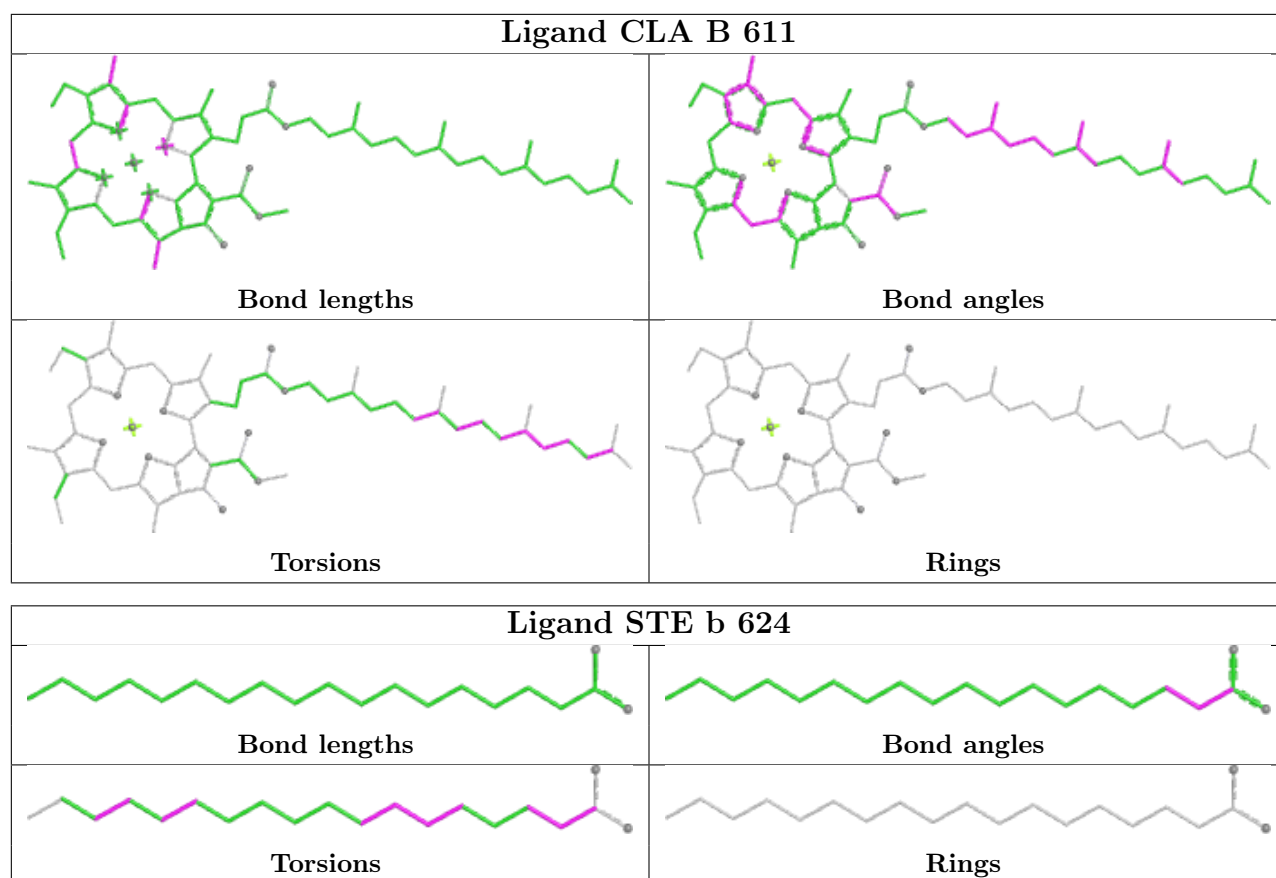


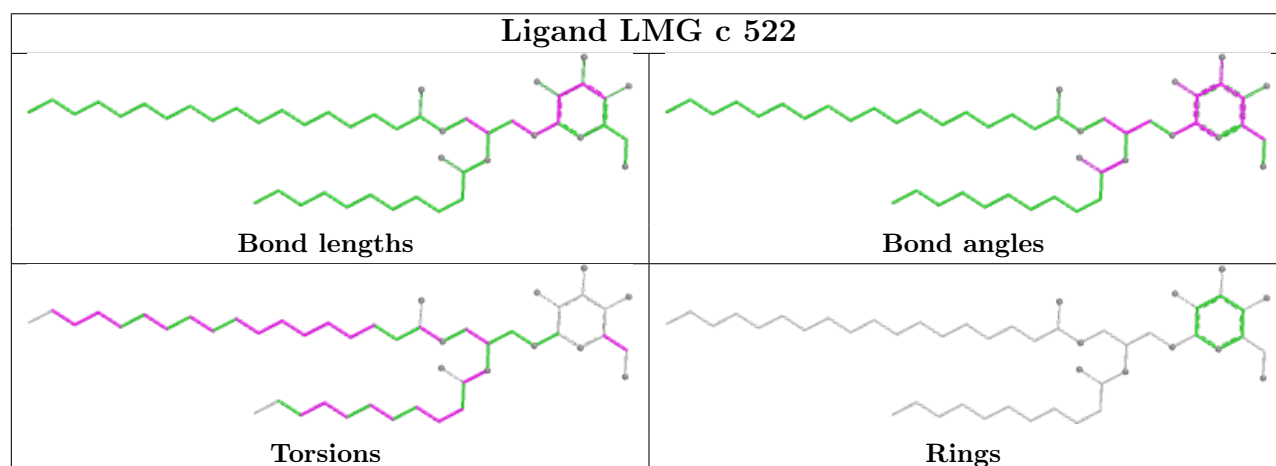
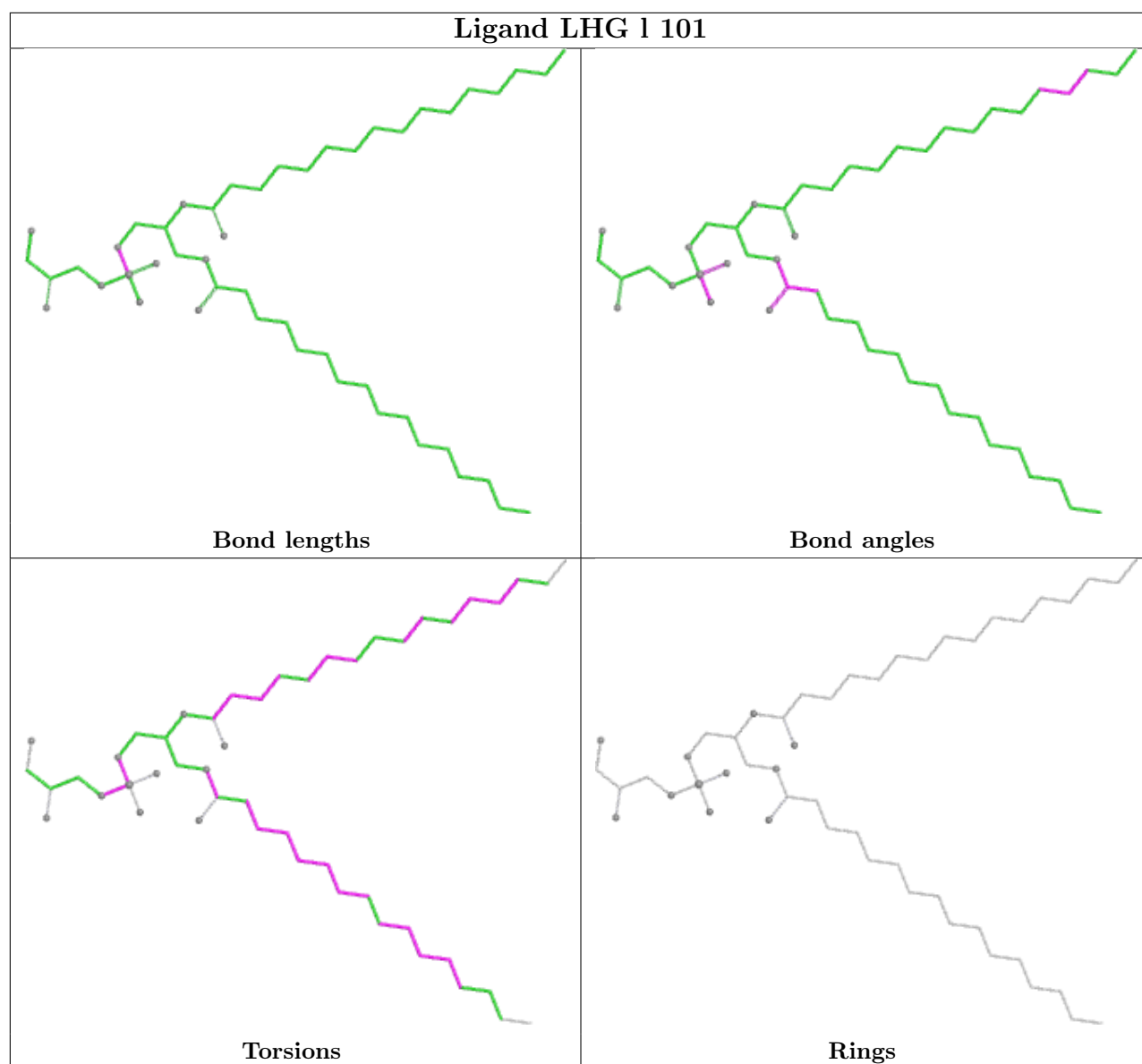
Ligand CLA C 510



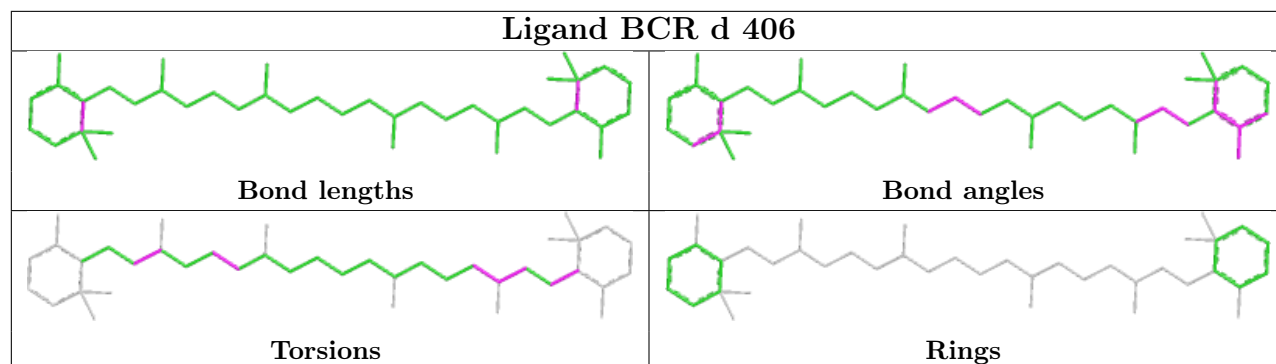




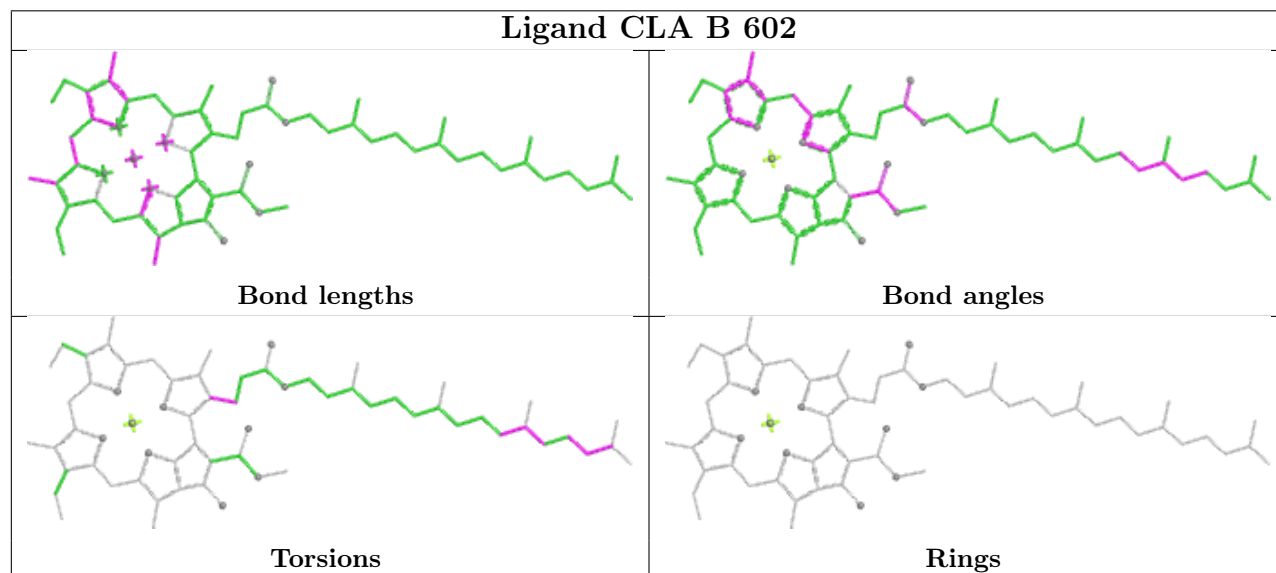




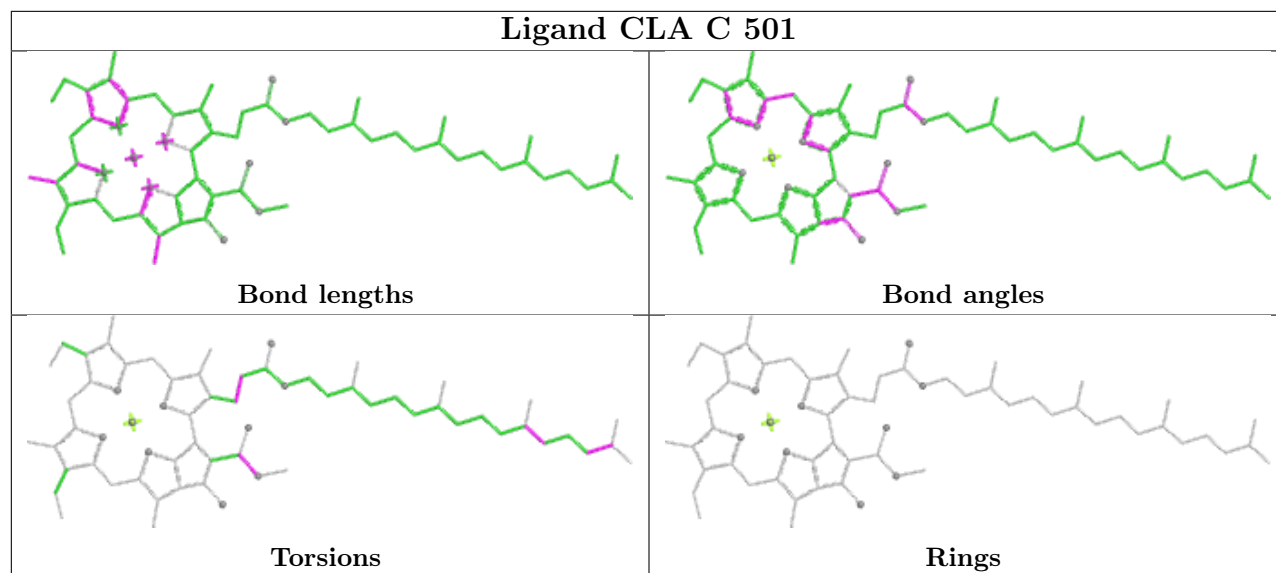
Ligand BCR d 406

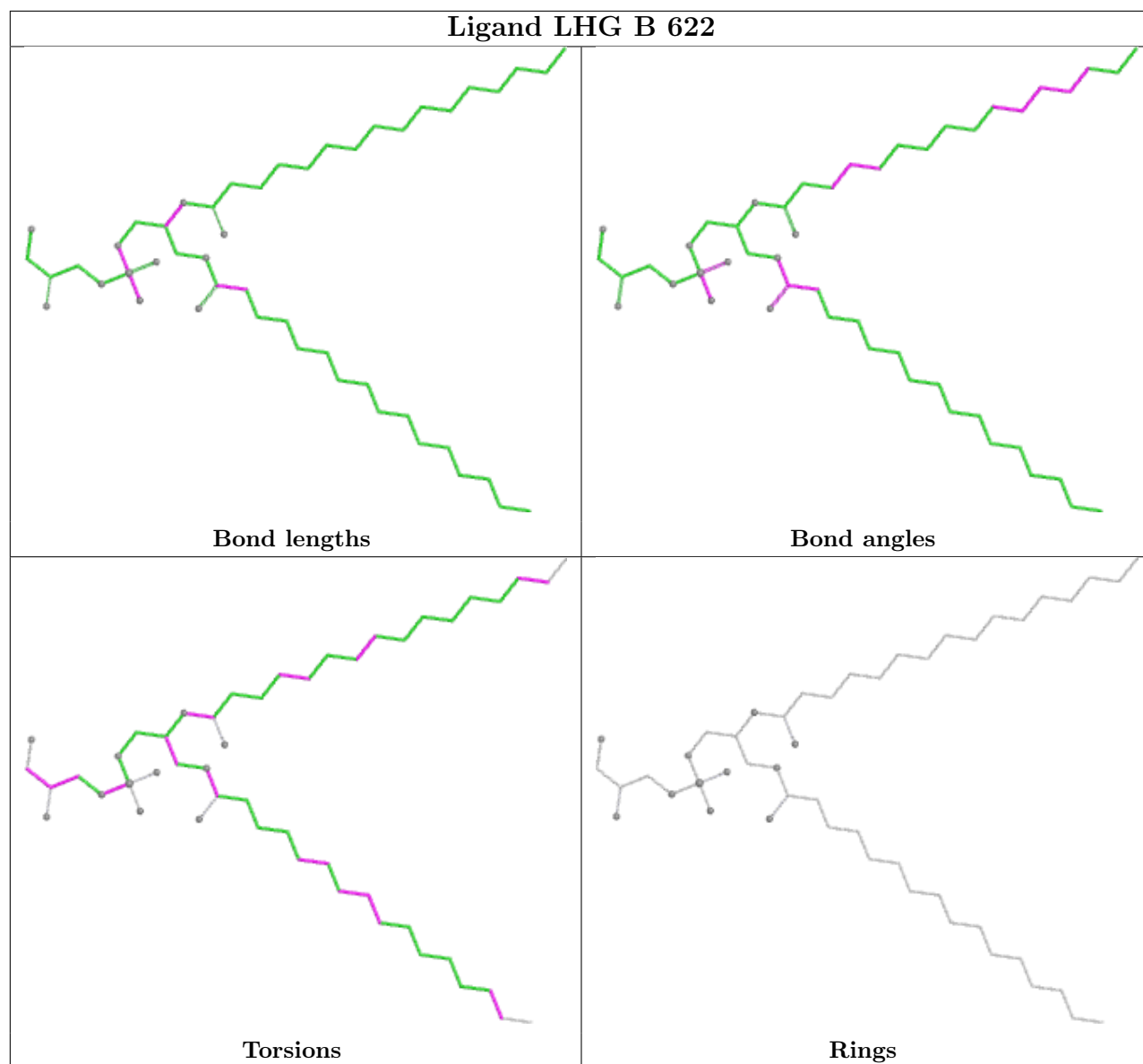
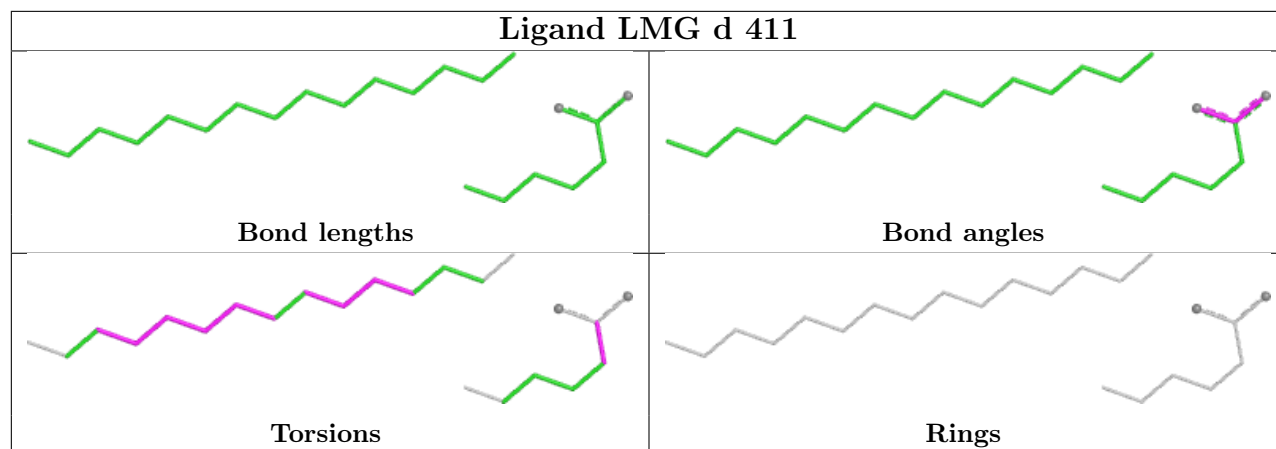


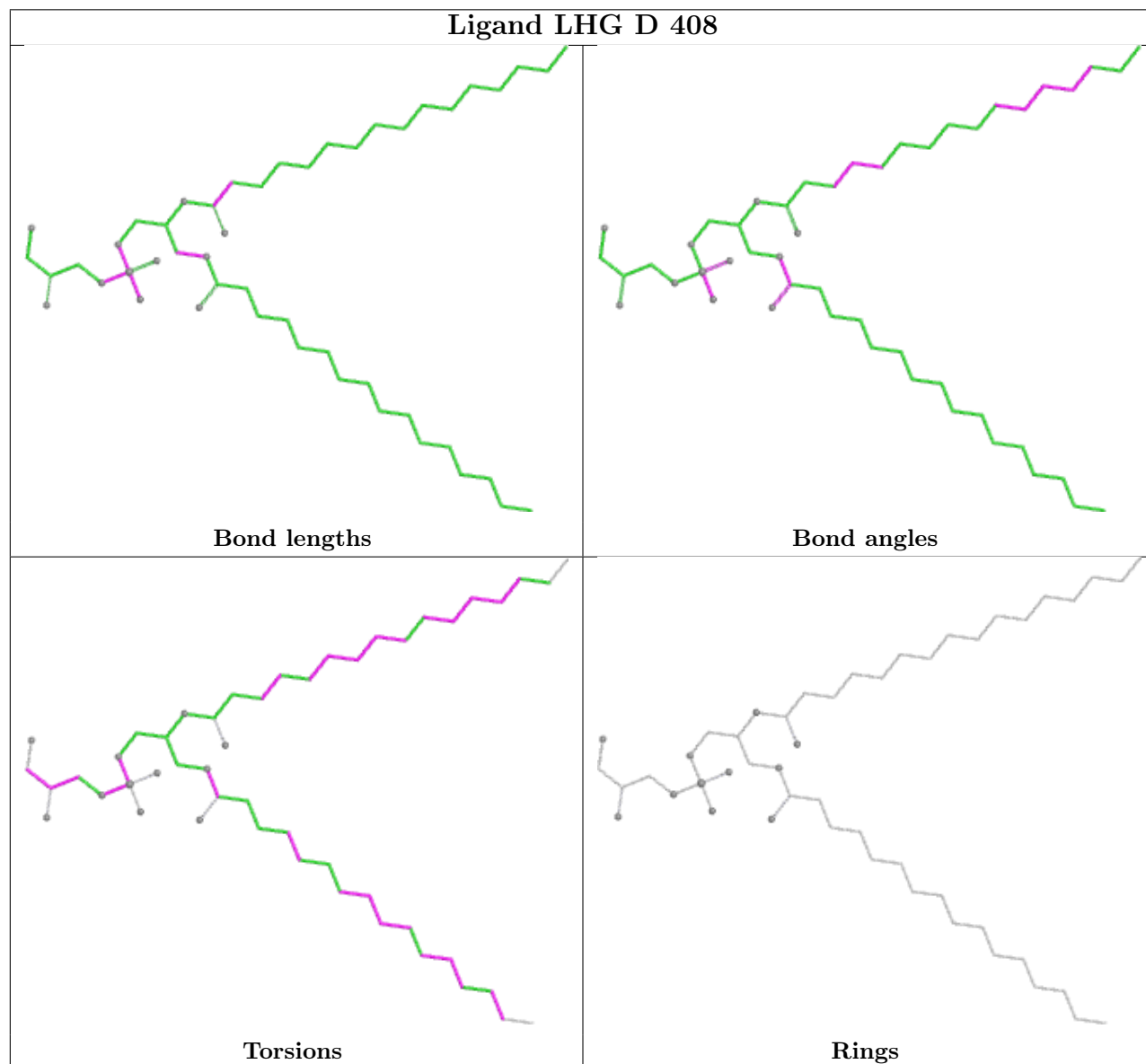
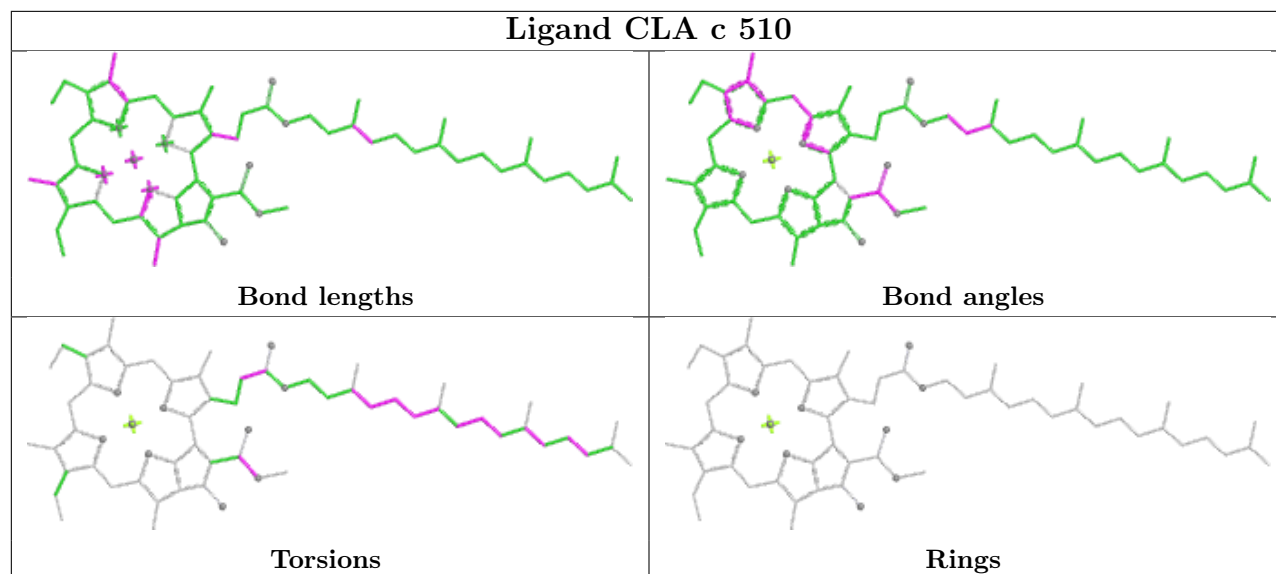
Ligand CLA B 602



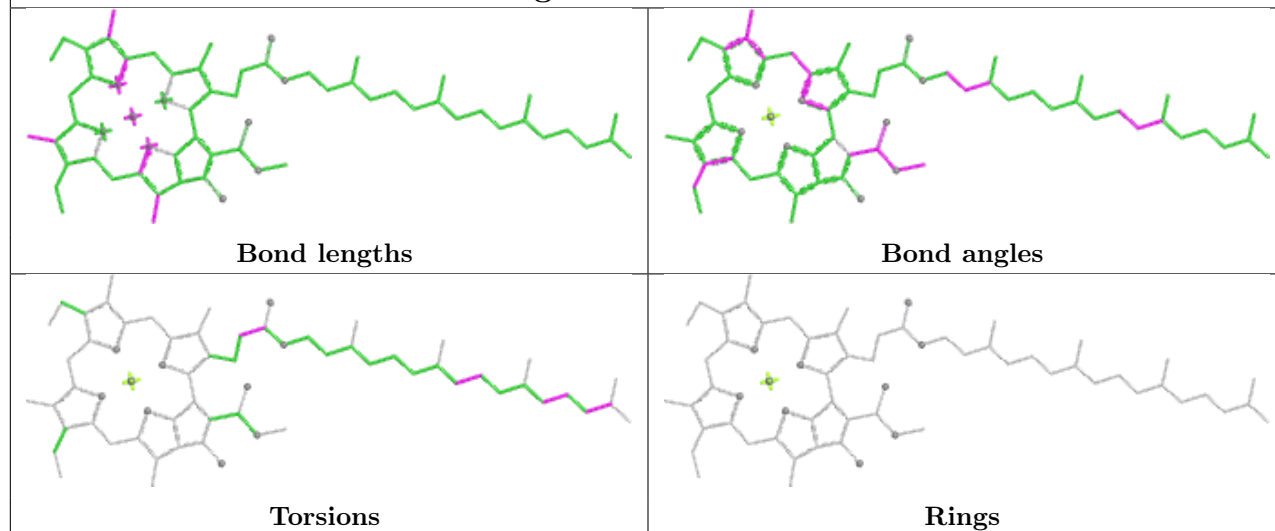
Ligand CLA C 501



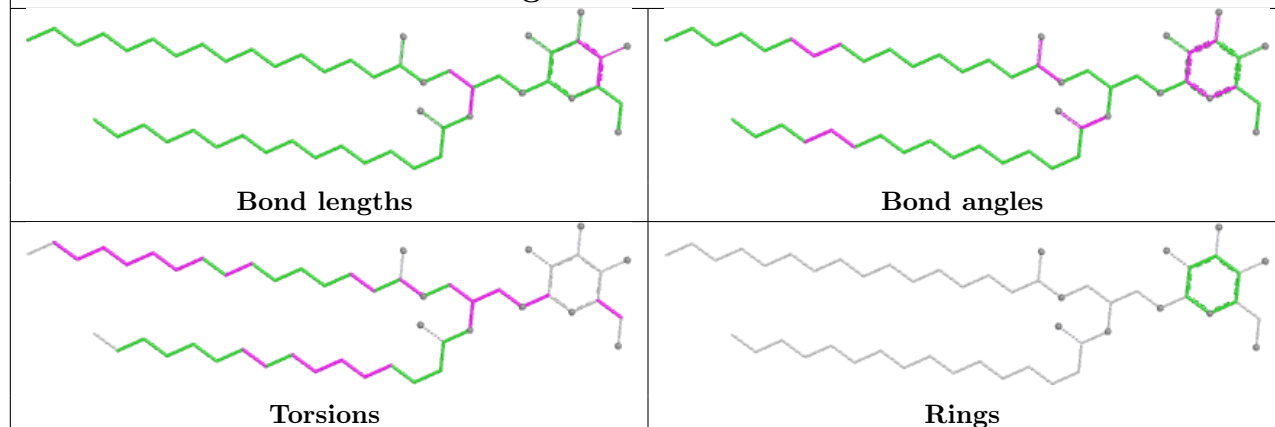




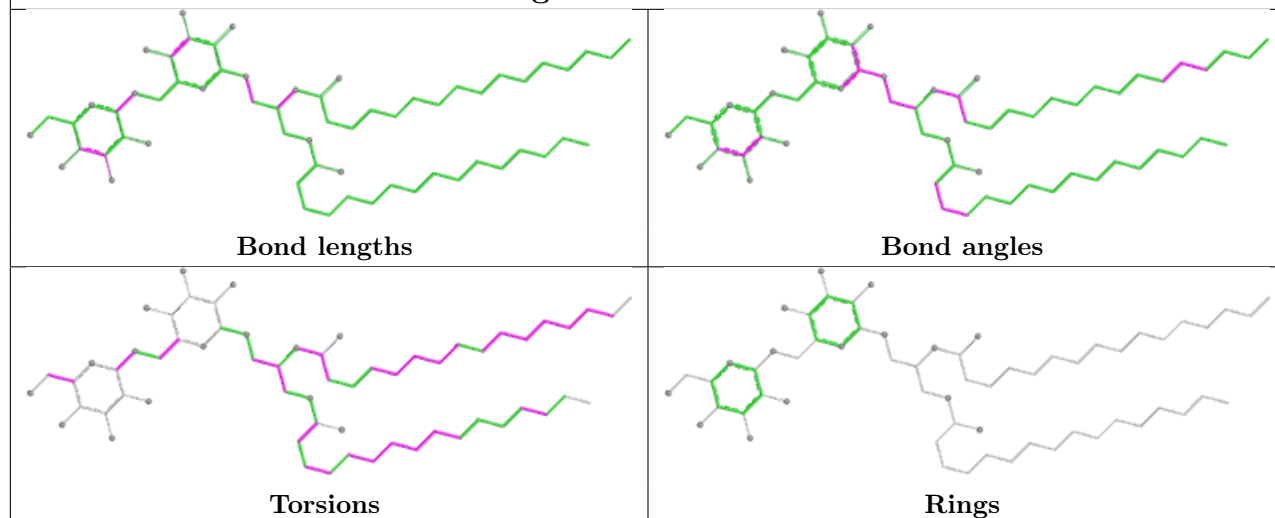
Ligand CLA b 612

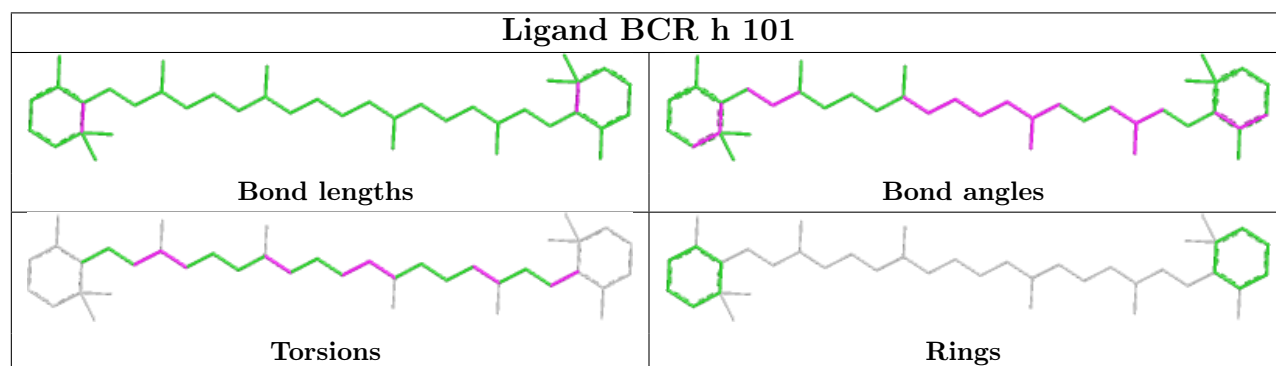
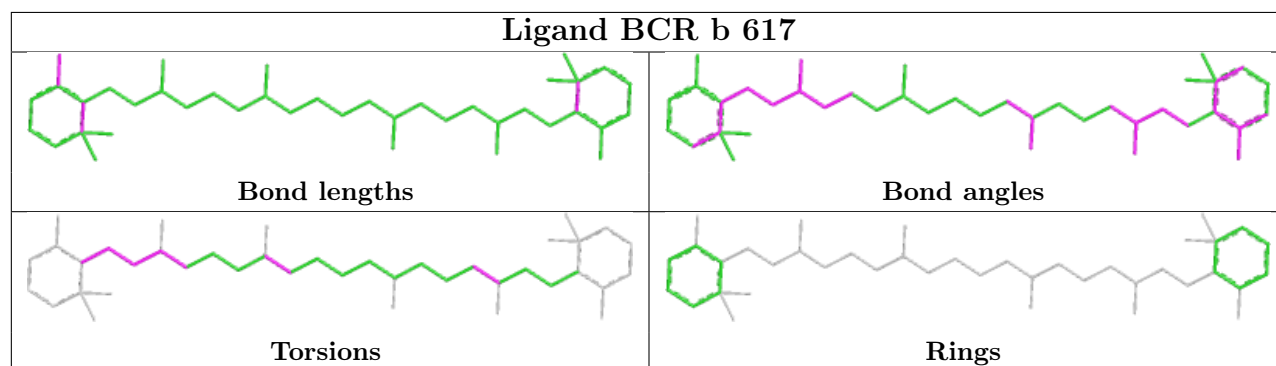
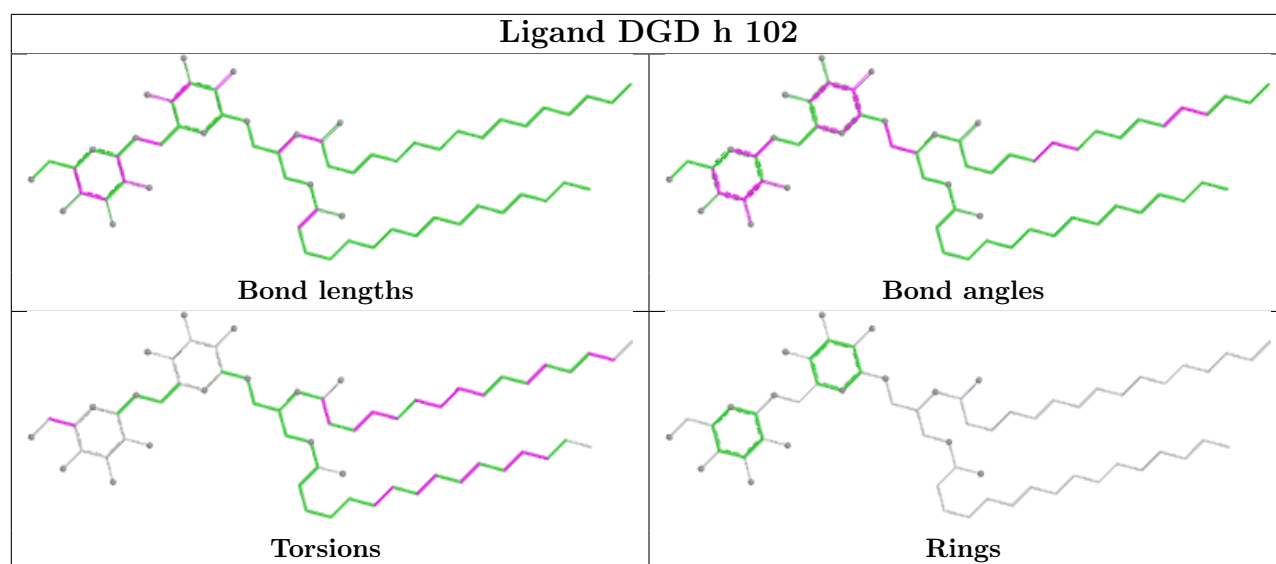


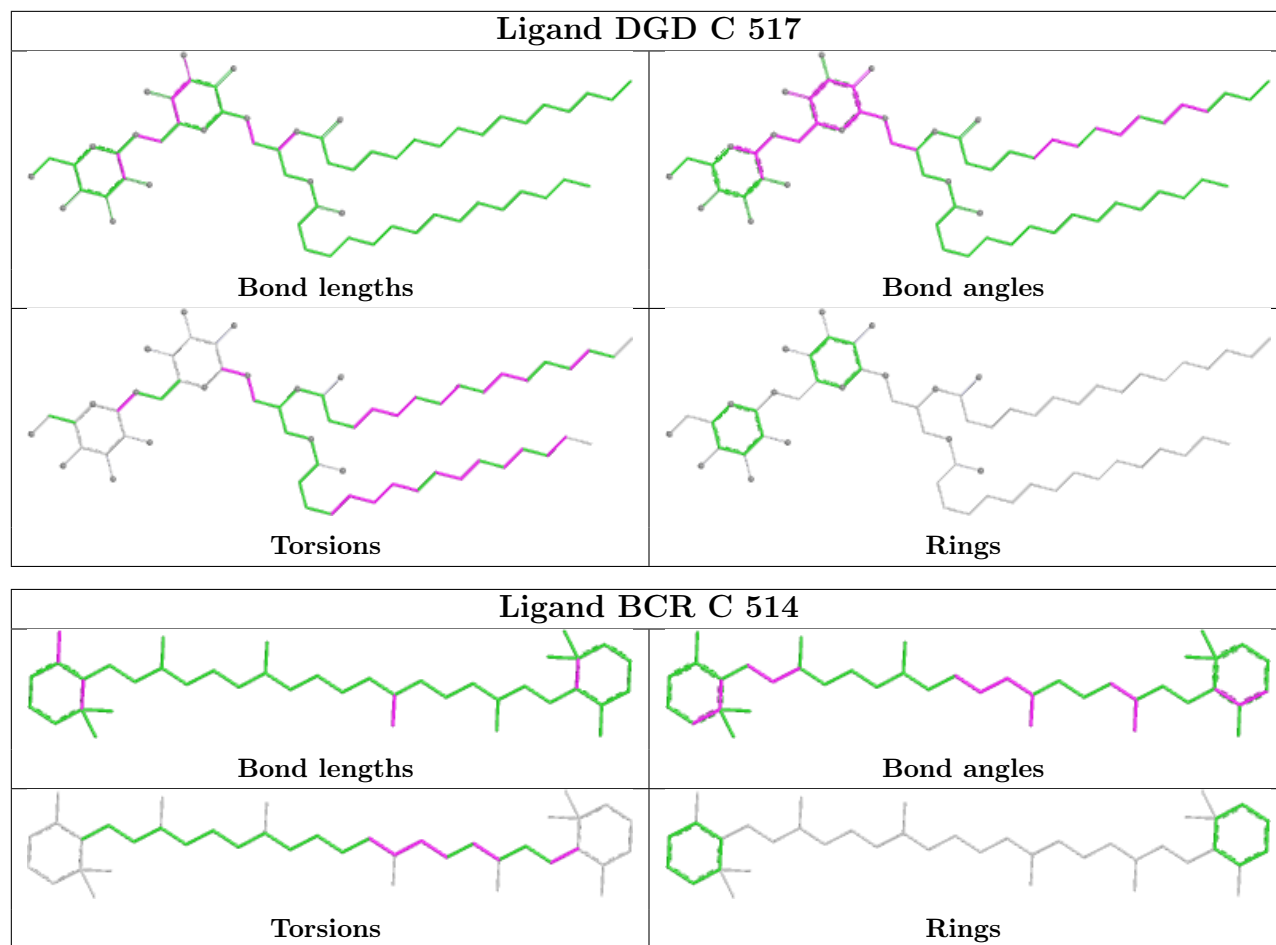
Ligand LMG M 101



Ligand DGD c 517







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.44	0 100 100	15, 35, 57, 92	64 (19%)
1	a	334/344 (97%)	-0.31	4 (1%) 76 78	15, 37, 69, 86	64 (19%)
2	B	505/510 (99%)	-0.39	1 (0%) 91 92	20, 40, 69, 101	4 (0%)
2	b	505/510 (99%)	-0.24	5 (0%) 79 81	31, 43, 80, 129	0
3	C	442/461 (95%)	-0.33	0 100 100	17, 43, 61, 93	11 (2%)
3	c	451/461 (97%)	-0.21	3 (0%) 84 86	17, 47, 70, 107	12 (2%)
4	D	341/352 (96%)	-0.51	0 100 100	17, 37, 56, 88	2 (0%)
4	d	341/352 (96%)	-0.34	1 (0%) 90 91	18, 41, 67, 94	3 (0%)
5	E	82/84 (97%)	0.24	0 100 100	38, 61, 78, 93	1 (1%)
5	e	82/84 (97%)	0.31	1 (1%) 76 78	45, 69, 89, 94	0
6	F	34/45 (75%)	-0.10	0 100 100	46, 53, 77, 98	0
6	f	34/45 (75%)	0.14	0 100 100	48, 57, 88, 102	0
7	H	65/66 (98%)	-0.19	2 (3%) 51 54	40, 49, 65, 83	0
7	h	63/66 (95%)	0.15	1 (1%) 70 73	47, 59, 71, 79	0
8	I	35/38 (92%)	-0.35	0 100 100	38, 45, 79, 89	0
8	i	35/38 (92%)	-0.21	0 100 100	37, 47, 85, 91	0
9	J	36/40 (90%)	-0.10	0 100 100	41, 57, 83, 101	0
9	j	36/40 (90%)	0.24	1 (2%) 55 57	46, 59, 95, 114	0
10	K	37/46 (80%)	0.06	0 100 100	52, 61, 84, 88	0
10	k	37/46 (80%)	0.23	0 100 100	51, 65, 80, 88	0
11	L	37/37 (100%)	-0.54	0 100 100	30, 37, 74, 77	0
11	l	36/37 (97%)	-0.55	0 100 100	28, 37, 79, 97	0
12	M	32/36 (88%)	-0.42	1 (3%) 51 54	31, 40, 68, 79	0
12	m	31/36 (86%)	-0.52	0 100 100	31, 41, 55, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.17	2 (0%) 82 84	31, 49, 89, 147	1 (0%)
13	o	244/272 (89%)	-0.19	1 (0%) 88 90	31, 48, 93, 137	0
14	R	28/41 (68%)	0.84	0 100 100	68, 85, 99, 113	0
14	r	28/41 (68%)	1.33	6 (21%) 2 2	82, 110, 127, 139	0
15	T	29/32 (90%)	-0.56	0 100 100	31, 37, 72, 80	0
15	t	29/32 (90%)	-0.40	1 (3%) 48 50	31, 38, 87, 95	0
16	U	97/134 (72%)	-0.17	0 100 100	36, 51, 77, 100	0
16	u	97/134 (72%)	-0.25	0 100 100	37, 47, 66, 89	0
17	V	137/163 (84%)	-0.32	0 100 100	34, 47, 63, 88	0
17	v	137/163 (84%)	-0.15	0 100 100	38, 54, 78, 93	0
18	X	38/41 (92%)	-0.05	0 100 100	47, 59, 84, 91	0
18	x	39/41 (95%)	0.24	1 (2%) 57 60	58, 69, 100, 115	0
19	Y	27/46 (58%)	0.88	2 (7%) 20 22	61, 83, 99, 111	0
19	y	30/46 (65%)	0.65	0 100 100	70, 85, 101, 108	0
20	Z	62/62 (100%)	0.72	2 (3%) 50 53	62, 79, 123, 138	0
20	z	62/62 (100%)	0.71	4 (6%) 25 26	67, 83, 125, 138	0
All	All	5293/5700 (92%)	-0.22	39 (0%) 84 86	15, 45, 84, 147	162 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	t	30	THR	4.0
13	O	60	ARG	3.8
13	o	58	ASN	3.6
3	c	23	ALA	3.5
18	x	40	SER	3.2
19	Y	22	LEU	3.1
13	O	59	LYS	3.1
5	e	79	PHE	3.1
20	Z	62	VAL	3.1
20	z	33	TRP	3.0
9	j	6	GLY	2.9
7	H	65	LEU	2.8
7	H	41	PHE	2.8
19	Y	25	ILE	2.8
14	r	18	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	2.7
20	z	62	VAL	2.6
7	h	64	ALA	2.6
14	r	3	TRP	2.6
14	r	14	LEU	2.5
2	b	84	THR	2.4
1	a	250	ALA	2.4
3	c	24	THR	2.4
2	b	499	VAL	2.4
2	B	479[A]	PHE	2.3
20	z	40	ILE	2.3
12	M	33	GLN	2.3
2	b	486	LEU	2.3
1	a	248	ILE	2.2
3	c	134	ILE	2.2
14	r	20	VAL	2.2
20	Z	33	TRP	2.2
1	a	249	VAL	2.2
1	a	11	ALA	2.1
14	r	19	ALA	2.1
2	b	496	TYR	2.1
20	z	27	TYR	2.1
14	r	28	VAL	2.1
4	d	239	GLN	2.1

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
15	FME	t	1	10/11	0.94	0.08	33,48,71,72	0
12	FME	M	1	10/11	0.95	0.09	44,54,68,76	0
8	FME	I	1	10/11	0.95	0.08	40,52,64,70	0
15	FME	T	1	10/11	0.96	0.07	29,52,69,69	0
8	FME	i	1	10/11	0.96	0.08	41,51,64,67	0
12	FME	m	1	10/11	0.97	0.08	33,50,72,82	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	STE	H	103	18/20	0.74	0.18	43,78,89,95	0
32	STE	I	101	15/20	0.77	0.18	38,59,77,81	0
32	STE	b	624	20/20	0.78	0.15	51,69,78,93	0
32	STE	a	413	10/20	0.79	0.16	37,66,75,80	0
32	STE	b	625	10/20	0.79	0.14	40,53,63,74	0
32	STE	B	626	16/20	0.80	0.15	39,72,94,94	0
27	LMG	b	622	55/55	0.80	0.16	53,80,98,112	0
33	LHG	E	102	49/49	0.80	0.14	55,87,113,120	0
26	PL9	A	409	55/55	0.81	0.16	44,72,93,105	0
27	LMG	c	522	48/55	0.82	0.14	39,82,115,118	0
27	LMG	d	411	23/55	0.82	0.17	42,72,88,92	0
32	STE	m	101	12/20	0.82	0.16	48,64,76,82	0
32	STE	x	101	20/20	0.82	0.13	49,67,79,79	0
32	STE	b	623	16/20	0.82	0.16	50,68,83,94	0
32	STE	c	524	12/20	0.83	0.11	57,73,82,84	0
29	DGD	a	412	44/66	0.83	0.13	35,58,82,91	0
26	PL9	a	409	55/55	0.83	0.16	42,76,96,107	0
32	STE	E	103	12/20	0.83	0.16	63,80,88,95	0
32	STE	c	521	20/20	0.84	0.12	44,63,94,107	0
32	STE	T	102	16/20	0.84	0.14	41,53,78,79	0
32	STE	j	101	12/20	0.84	0.12	48,62,70,79	0
33	LHG	e	101	42/49	0.84	0.13	56,93,112,132	0
29	DGD	A	414	66/66	0.85	0.11	47,67,82,90	0
28	SQD	A	413	39/54	0.85	0.13	43,66,94,100	0
28	SQD	a	411	36/54	0.85	0.13	32,65,86,91	0
32	STE	J	101	12/20	0.86	0.12	49,62,72,73	0
32	STE	B	627	12/20	0.86	0.14	53,66,83,86	0
32	STE	C	521	16/20	0.86	0.13	38,58,85,88	0
32	STE	a	414	12/20	0.86	0.12	54,67,77,79	0
27	LMG	D	410	33/55	0.86	0.13	41,58,86,90	0
22	CLA	b	601	65/65	0.86	0.11	53,72,92,96	0
27	LMG	A	411	48/55	0.86	0.11	43,65,84,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	B	625	18/20	0.87	0.12	41,59,81,88	0
27	LMG	B	621	28/55	0.87	0.14	37,53,66,72	0
32	STE	B	620	17/20	0.87	0.11	39,59,71,80	0
32	STE	T	103	15/20	0.87	0.14	44,60,81,84	0
32	STE	d	413	17/20	0.88	0.14	48,62,75,82	0
32	STE	M	103	10/20	0.88	0.11	36,54,57,61	0
28	SQD	F	101	36/54	0.88	0.12	43,77,93,98	0
27	LMG	c	520	37/55	0.88	0.12	43,72,92,96	0
28	SQD	f	102	41/54	0.88	0.12	63,89,107,109	0
32	STE	B	624	12/20	0.88	0.10	37,56,70,74	0
32	STE	l	102	18/20	0.89	0.12	37,54,88,89	0
28	SQD	B	623	54/54	0.89	0.10	43,66,97,109	0
27	LMG	b	620	51/55	0.89	0.10	38,57,76,91	0
32	STE	C	520	12/20	0.89	0.12	43,57,68,70	0
27	LMG	C	519	48/55	0.89	0.12	49,74,93,98	0
27	LMG	M	101	51/55	0.90	0.09	33,53,76,92	0
32	STE	b	621	20/20	0.90	0.10	39,58,79,80	0
28	SQD	L	101	49/54	0.90	0.09	40,61,93,97	0
22	CLA	B	601	65/65	0.90	0.10	35,64,90,100	0
32	STE	C	522	12/20	0.90	0.10	34,45,58,64	0
24	BCR	c	514	40/40	0.90	0.10	47,64,79,81	0
24	BCR	d	406	40/40	0.90	0.11	40,57,98,114	0
22	CLA	C	513	65/65	0.91	0.10	45,68,103,112	0
32	STE	D	411	20/20	0.91	0.09	38,55,79,84	0
24	BCR	K	101	40/40	0.91	0.11	51,65,74,78	0
32	STE	t	102	14/20	0.91	0.10	35,55,65,68	0
24	BCR	h	101	40/40	0.91	0.10	43,60,79,91	0
27	LMG	c	523	49/55	0.91	0.10	35,62,83,99	0
24	BCR	k	101	40/40	0.91	0.10	45,67,78,80	0
28	SQD	a	410	54/54	0.92	0.10	44,67,96,99	0
22	CLA	c	512	65/65	0.92	0.10	47,64,99,104	0
24	BCR	Y	101	40/40	0.92	0.09	43,58,76,83	0
24	BCR	b	618	40/40	0.92	0.08	30,44,56,60	0
29	DGD	C	517	62/66	0.92	0.09	41,56,102,121	0
29	DGD	H	102	62/66	0.92	0.09	33,48,61,66	0
24	BCR	B	618	40/40	0.92	0.08	28,41,58,61	0
29	DGD	h	102	62/66	0.92	0.09	33,53,64,71	0
24	BCR	D	405	40/40	0.92	0.10	35,49,85,89	0
24	BCR	H	101	40/40	0.92	0.09	38,53,64,74	0
22	CLA	c	513	65/65	0.93	0.10	49,74,106,110	0
24	BCR	c	515	40/40	0.93	0.08	35,47,58,72	0
32	STE	M	102	15/20	0.93	0.09	37,50,66,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
22	CLA	c	508	64/65	0.93	0.09	37,50,94,112	0
27	LMG	D	407	51/55	0.93	0.10	31,60,86,92	0
28	SQD	A	412	52/54	0.93	0.09	33,66,94,99	0
24	BCR	B	619	40/40	0.93	0.08	33,45,59,61	0
24	BCR	C	514	40/40	0.93	0.09	32,43,56,61	0
29	DGD	c	518	62/66	0.93	0.09	35,58,94,103	0
24	BCR	C	515	40/40	0.93	0.11	45,60,78,81	0
24	BCR	b	619	40/40	0.93	0.08	35,52,70,70	0
34	BCT	a	408	4/4	0.93	0.10	35,40,48,58	0
27	LMG	d	412	44/55	0.94	0.09	37,58,89,92	0
22	CLA	c	509	65/65	0.94	0.09	37,53,70,75	0
22	CLA	c	510	65/65	0.94	0.08	36,53,67,73	0
29	DGD	c	519	62/66	0.94	0.08	31,57,86,101	0
24	BCR	c	516	40/40	0.94	0.11	45,60,71,79	0
22	CLA	C	503	65/65	0.94	0.07	36,47,59,62	0
22	CLA	C	511	65/65	0.94	0.09	36,57,71,76	0
24	BCR	A	406	40/40	0.94	0.07	28,38,49,52	0
24	BCR	T	101	40/40	0.94	0.07	29,44,58,62	0
24	BCR	B	617	40/40	0.94	0.07	30,45,60,65	0
22	CLA	c	506	65/65	0.94	0.09	36,53,94,101	0
33	LHG	d	408	49/49	0.94	0.10	30,55,77,83	0
33	LHG	d	410	39/49	0.94	0.08	34,50,72,74	0
29	DGD	C	516	62/66	0.94	0.09	25,48,84,91	0
22	CLA	C	512	65/65	0.94	0.09	35,61,88,97	0
22	CLA	c	502	65/65	0.95	0.07	34,49,69,75	0
22	CLA	c	503	65/65	0.95	0.08	35,48,61,64	0
24	BCR	a	405	40/40	0.95	0.06	25,36,52,56	0
24	BCR	b	617	40/40	0.95	0.07	29,43,52,56	0
22	CLA	c	504	60/65	0.95	0.07	35,50,87,88	0
22	CLA	c	505	65/65	0.95	0.08	28,45,71,75	0
22	CLA	C	505	65/65	0.95	0.08	22,44,72,75	0
22	CLA	c	507	65/65	0.95	0.08	30,49,61,66	0
22	CLA	C	506	65/65	0.95	0.09	29,49,89,94	0
22	CLA	C	508	65/65	0.95	0.08	32,46,104,115	0
22	CLA	C	509	65/65	0.95	0.09	32,50,65,74	0
22	CLA	c	511	65/65	0.95	0.09	43,60,78,82	0
24	BCR	t	101	40/40	0.95	0.06	27,39,55,58	0
22	CLA	C	510	65/65	0.95	0.07	34,49,66,74	0
29	DGD	C	518	62/66	0.95	0.08	33,54,82,91	0
26	PL9	D	406	55/55	0.95	0.07	24,38,49,50	0
22	CLA	B	609	65/65	0.95	0.08	29,42,56,59	0
26	PL9	d	407	55/55	0.95	0.07	27,38,45,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	d	405	65/65	0.95	0.09	32,53,93,101	0
22	CLA	B	615	65/65	0.95	0.07	29,42,67,77	0
22	CLA	C	502	65/65	0.95	0.07	35,47,60,68	0
22	CLA	a	403	65/65	0.95	0.09	30,45,99,107	0
22	CLA	B	606	65/65	0.95	0.07	28,41,71,77	0
33	LHG	B	622	49/49	0.95	0.09	28,48,68,77	0
33	LHG	D	409	47/49	0.95	0.09	29,53,82,99	0
22	CLA	b	606	65/65	0.95	0.08	29,45,77,78	0
33	LHG	L	102	49/49	0.95	0.07	30,44,59,74	0
22	CLA	b	608	65/65	0.95	0.07	34,48,64,68	0
22	CLA	b	614	65/65	0.95	0.08	25,44,78,85	0
22	CLA	b	615	65/65	0.95	0.07	31,45,61,65	0
33	LHG	l	101	49/49	0.95	0.07	34,48,59,67	0
22	CLA	b	616	60/65	0.95	0.09	34,48,89,91	0
22	CLA	a	402	65/65	0.96	0.06	24,35,48,62	0
22	CLA	B	602	65/65	0.96	0.07	27,40,62,65	0
22	CLA	a	404	65/65	0.96	0.08	21,40,80,85	0
22	CLA	d	403	65/65	0.96	0.07	23,40,60,68	0
22	CLA	d	404	65/65	0.96	0.06	24,35,46,50	0
22	CLA	B	616	60/65	0.96	0.09	28,45,84,100	0
23	PHO	A	404	64/64	0.96	0.05	20,31,40,48	0
23	PHO	D	401	64/64	0.96	0.06	25,37,45,53	0
23	PHO	d	401	64/64	0.96	0.06	23,35,43,48	0
23	PHO	d	402	64/64	0.96	0.06	32,43,54,63	0
22	CLA	b	602	65/65	0.96	0.08	31,46,65,71	0
22	CLA	b	603	65/65	0.96	0.07	24,40,71,79	0
22	CLA	b	604	65/65	0.96	0.07	24,39,80,93	0
22	CLA	b	605	65/65	0.96	0.07	24,39,54,60	0
22	CLA	C	501	65/65	0.96	0.07	26,41,54,58	0
22	CLA	b	607	65/65	0.96	0.07	21,40,65,77	0
22	CLA	B	604	65/65	0.96	0.07	26,38,75,80	0
22	CLA	b	609	65/65	0.96	0.08	32,50,71,77	0
22	CLA	b	610	65/65	0.96	0.08	28,42,53,58	0
22	CLA	b	611	65/65	0.96	0.07	27,39,57,66	0
22	CLA	b	612	65/65	0.96	0.07	26,39,54,63	0
22	CLA	b	613	65/65	0.96	0.07	26,40,76,83	0
22	CLA	B	605	65/65	0.96	0.07	24,35,49,54	0
22	CLA	C	504	59/65	0.96	0.07	32,47,85,92	0
22	CLA	A	403	65/65	0.96	0.09	26,40,103,112	0
22	CLA	c	501	65/65	0.96	0.07	31,44,54,62	0
22	CLA	B	608	65/65	0.96	0.06	22,39,59,65	0
22	CLA	C	507	65/65	0.96	0.07	27,45,60,65	0

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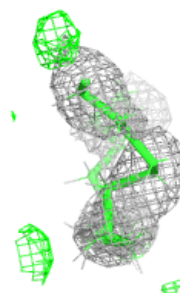
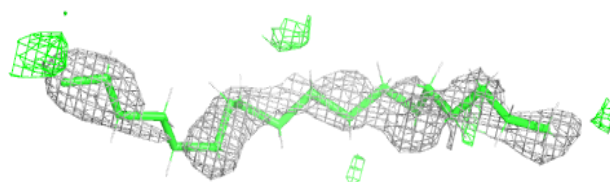
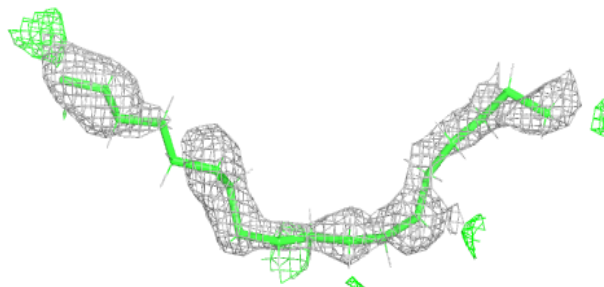
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	D	408	49/49	0.96	0.07	26,44,56,63	0
29	DGD	c	517	62/66	0.96	0.07	25,46,77,83	0
22	CLA	A	402	65/65	0.96	0.06	21,32,46,56	0
22	CLA	B	610	65/65	0.96	0.07	23,35,47,51	0
22	CLA	B	611	65/65	0.96	0.07	23,35,50,56	0
33	LHG	d	409	49/49	0.96	0.07	30,49,61,71	0
22	CLA	B	612	65/65	0.96	0.07	25,36,50,55	0
22	CLA	B	613	65/65	0.96	0.07	21,35,71,75	0
22	CLA	B	614	65/65	0.96	0.08	26,43,77,92	0
34	BCT	D	402	4/4	0.96	0.09	32,33,37,44	0
22	CLA	D	404	65/65	0.96	0.08	27,47,106,117	0
22	CLA	A	410	65/65	0.97	0.06	20,32,52,58	0
22	CLA	B	607	65/65	0.97	0.07	17,37,68,76	0
22	CLA	B	603	65/65	0.97	0.06	24,38,63,64	0
22	CLA	D	403	65/65	0.97	0.06	22,32,59,60	0
35	HEM	E	101	43/43	0.97	0.08	42,57,75,75	0
35	HEM	f	101	43/43	0.97	0.09	46,64,89,90	0
22	CLA	A	405	54/65	0.98	0.06	20,34,68,73	0
25	CL	a	406	1/1	0.98	0.05	30,30,30,30	0
36	HEC	V	201	43/43	0.98	0.07	24,37,49,51	0
36	HEC	v	201	43/43	0.98	0.06	32,41,52,55	0
31	OEX	a	416[A]	10/10	0.99	0.03	32,38,41,41	10
25	CL	a	407	1/1	0.99	0.08	33,33,33,33	0
25	CL	A	407	1/1	0.99	0.04	33,33,33,33	0
25	CL	A	408	1/1	0.99	0.07	32,32,32,32	0
21	FE2	a	401	1/1	0.99	0.02	37,37,37,37	0
31	OEX	A	416[A]	10/10	0.99	0.03	35,37,41,41	10
30	OXY	A	415[B]	11/11	1.00	0.03	21,26,30,34	11
30	OXY	a	415[B]	11/11	1.00	0.02	25,27,31,37	11
21	FE2	A	401	1/1	1.00	0.02	33,33,33,33	0

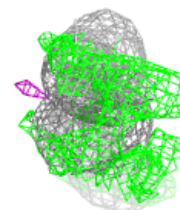
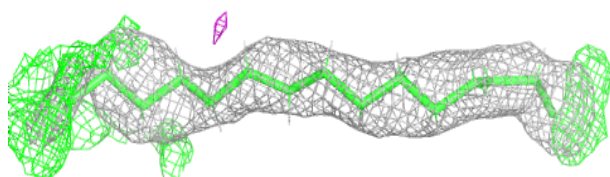
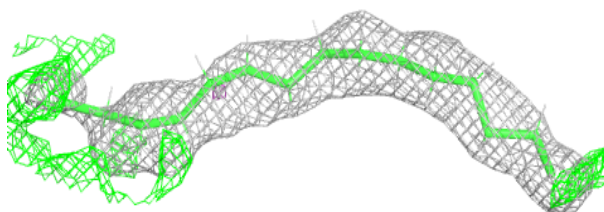
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE H 103:

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

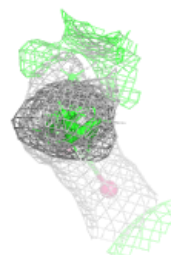
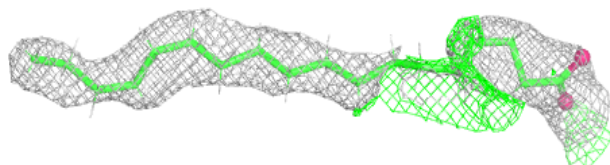
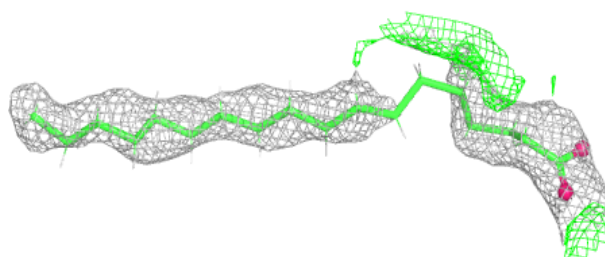
**Electron density around STE I 101:**

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

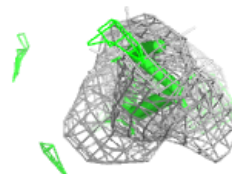
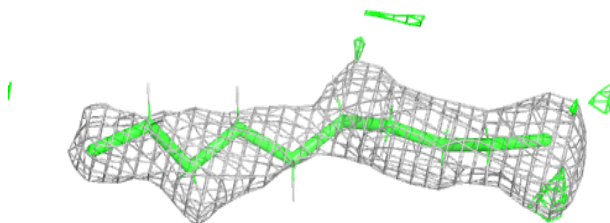
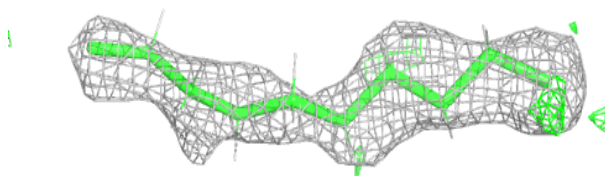


Electron density around STE b 624:

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

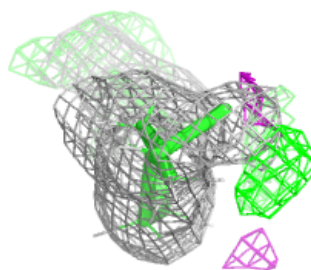
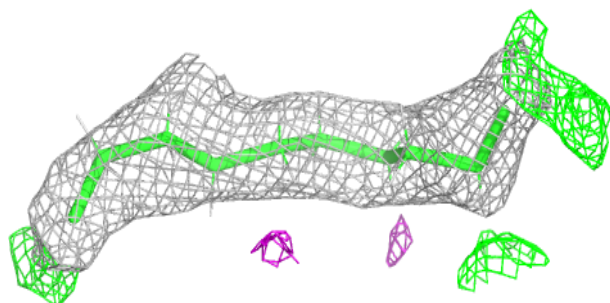
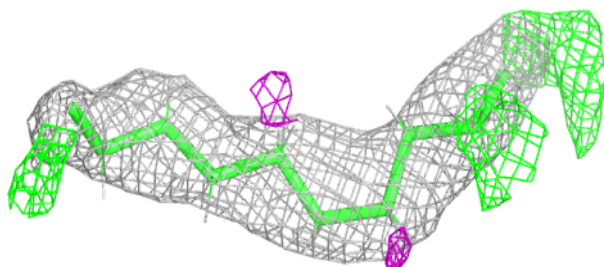
**Electron density around STE a 413:**

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

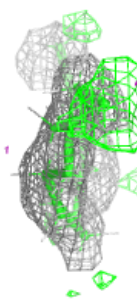
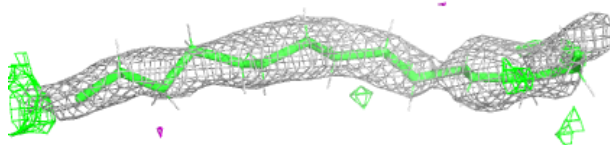


Electron density around STE b 625:

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

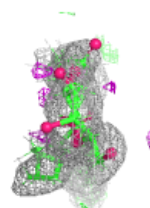
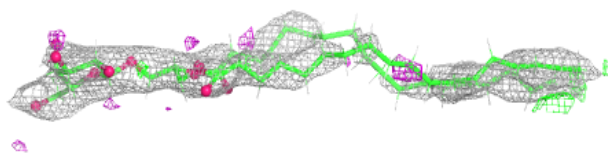
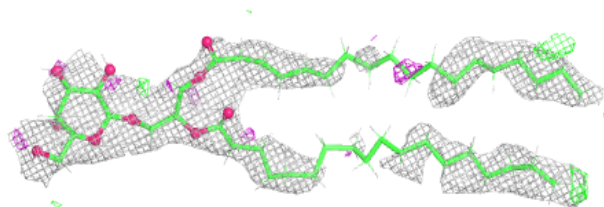
**Electron density around STE B 626:**

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



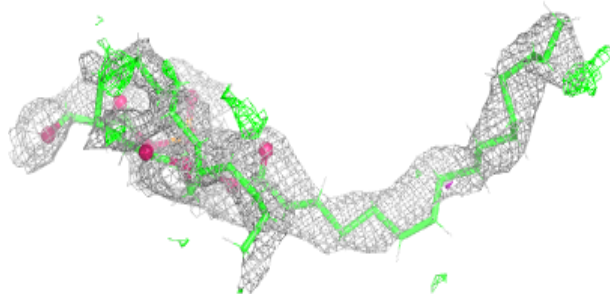
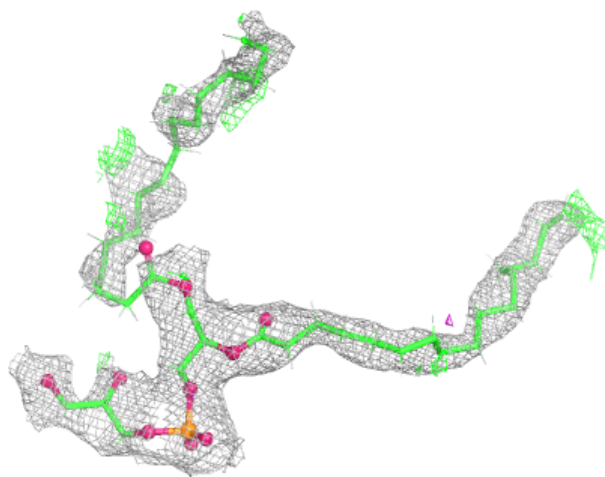
Electron density around LMG b 622:

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



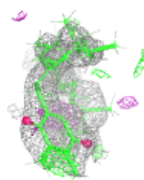
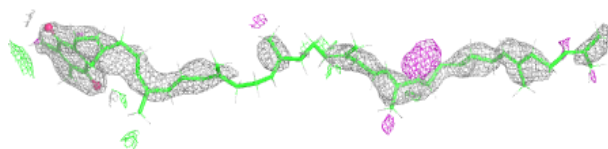
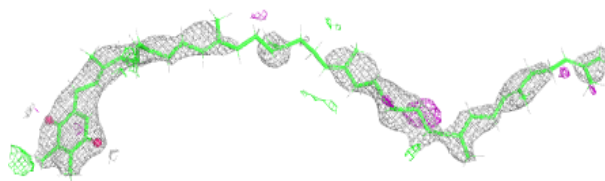
Electron density around LHG E 102:

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

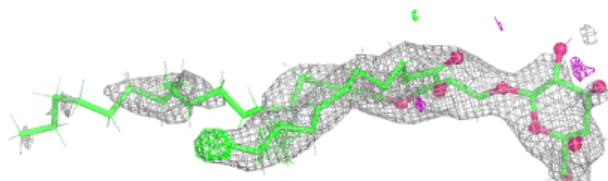


Electron density around PL9 A 409:

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

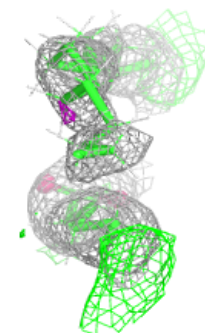
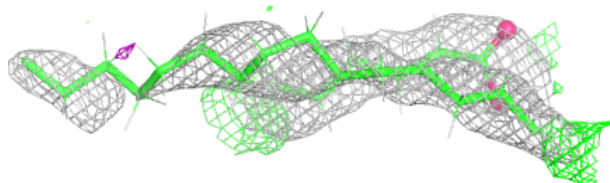
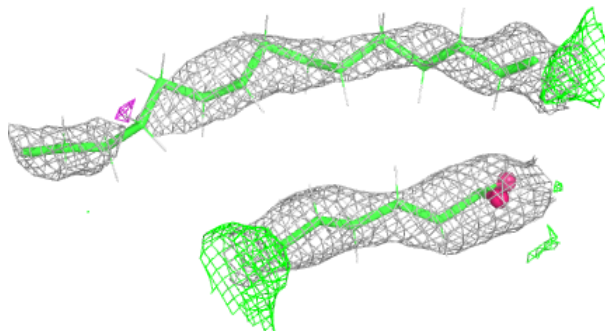
**Electron density around LMG c 522:**

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

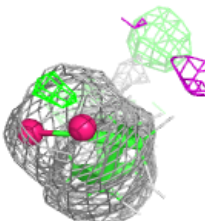
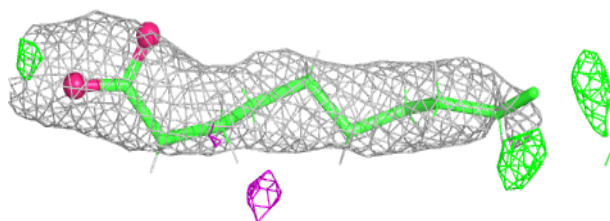
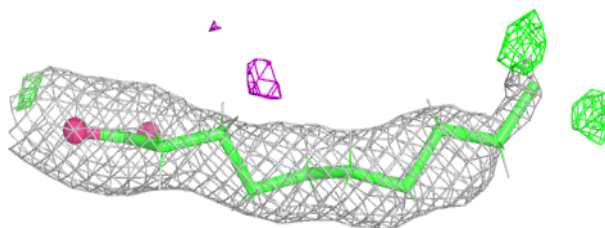


Electron density around LMG d 411:

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

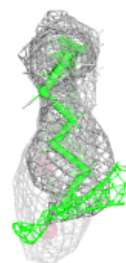
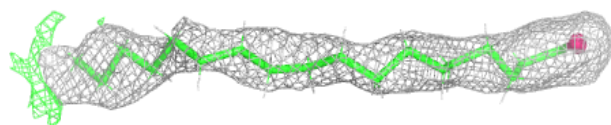
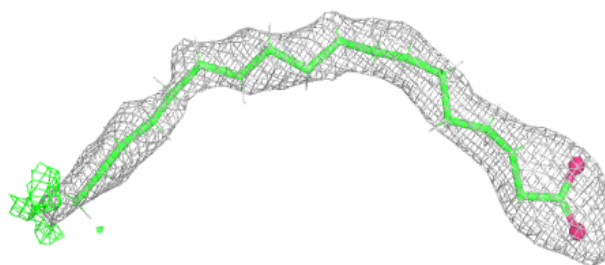
**Electron density around STE m 101:**

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

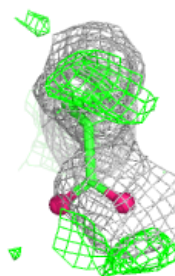
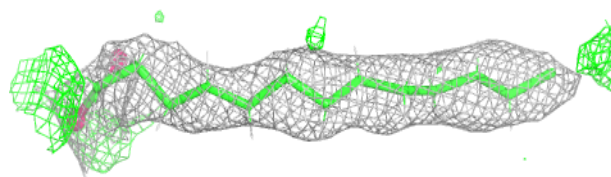
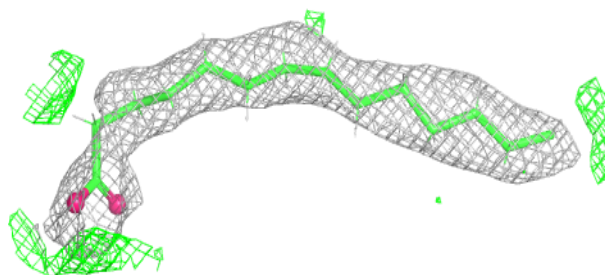


Electron density around STE x 101:

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

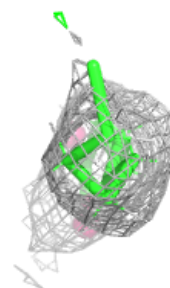
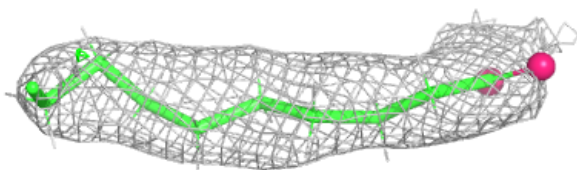
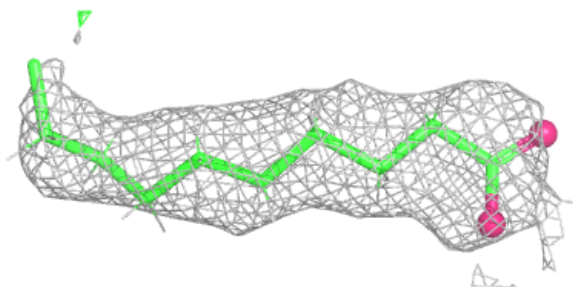
**Electron density around STE b 623:**

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

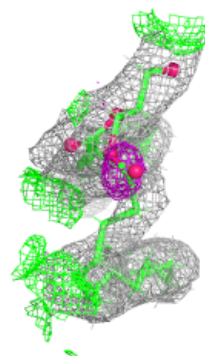
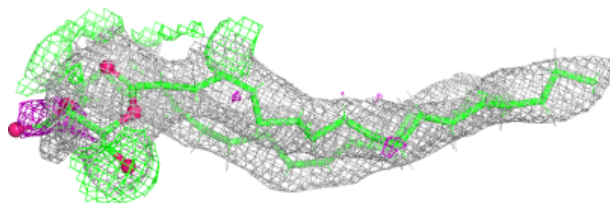
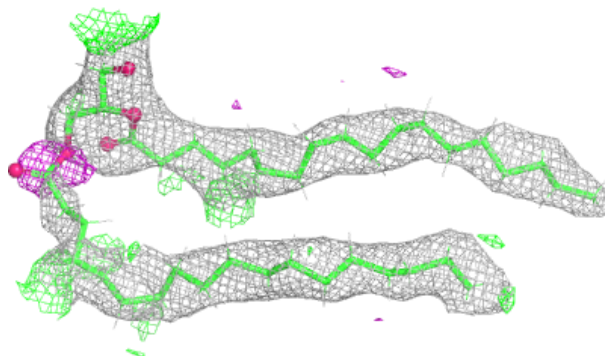


Electron density around STE c 524:

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

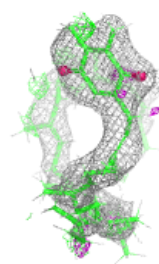
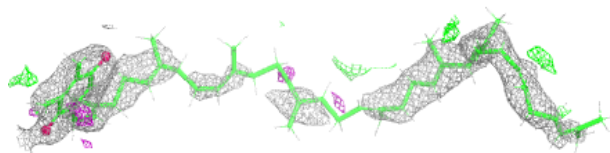
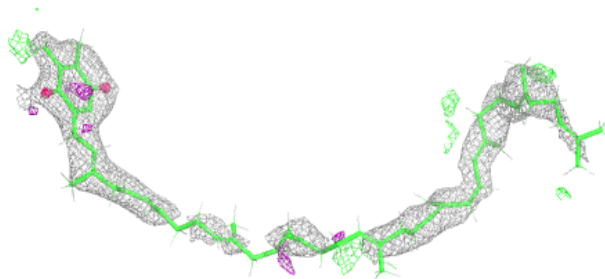
**Electron density around DGD a 412:**

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

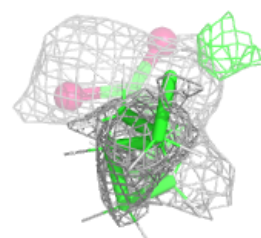
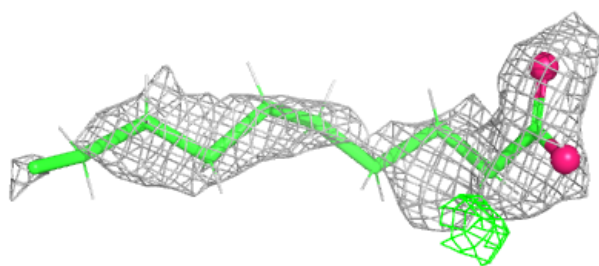
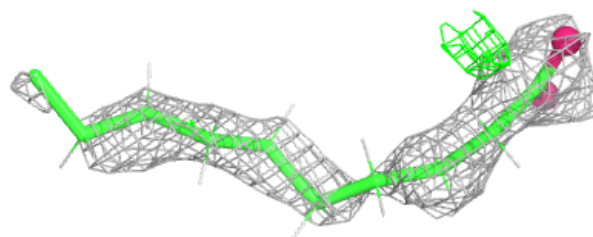


Electron density around PL9 a 409:

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

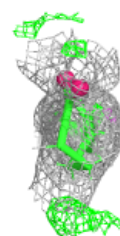
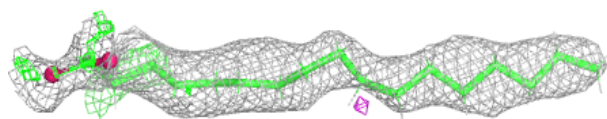
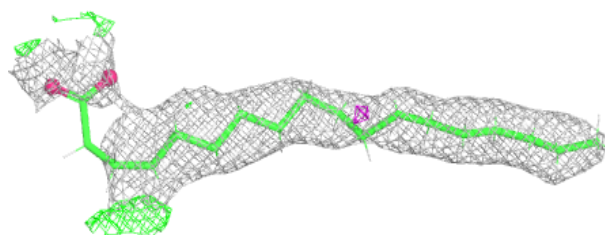
**Electron density around STE E 103:**

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

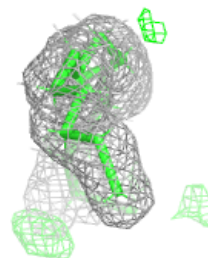
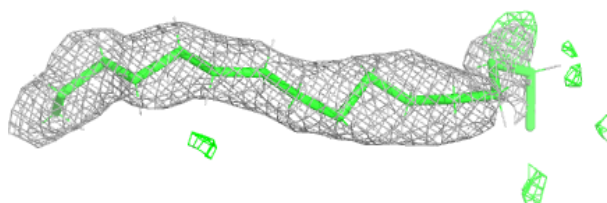
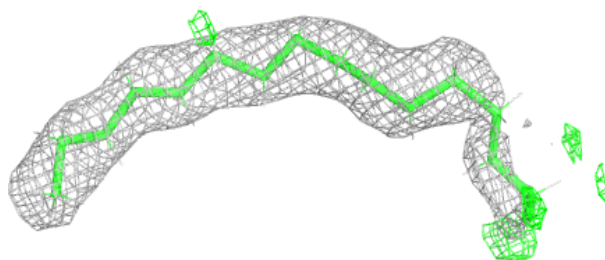


Electron density around STE c 521:

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

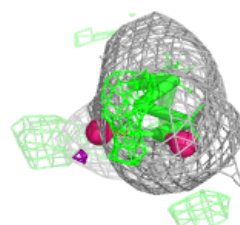
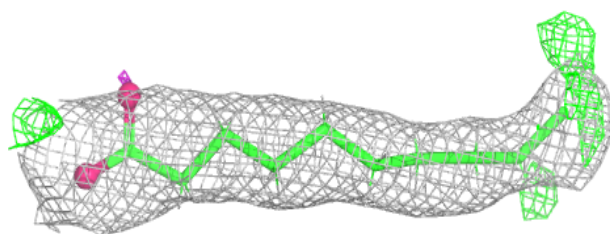
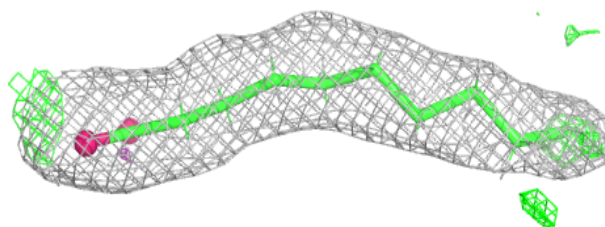
**Electron density around STE T 102:**

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

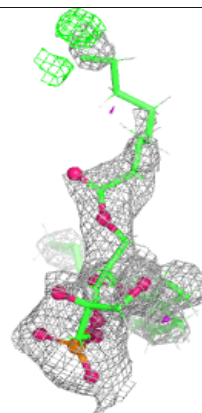
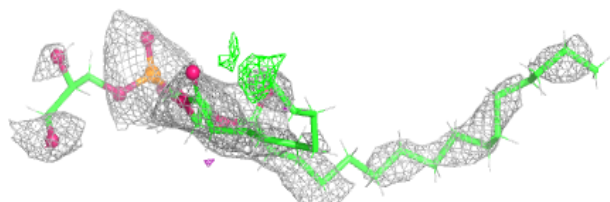
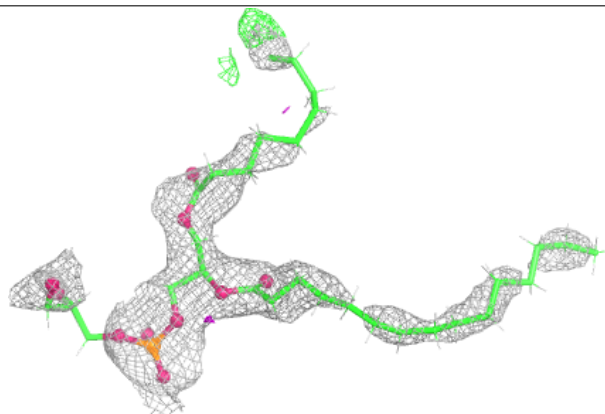


Electron density around STE j 101:

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

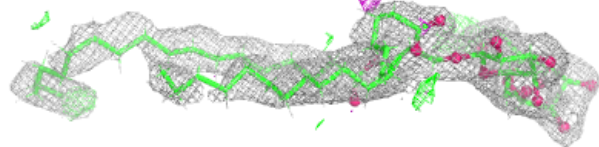
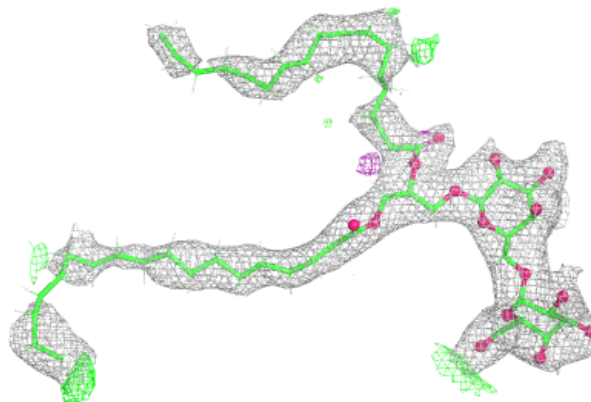
**Electron density around LHG e 101:**

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



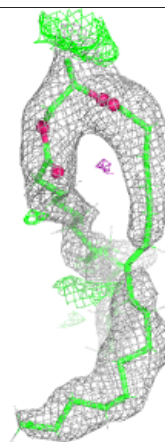
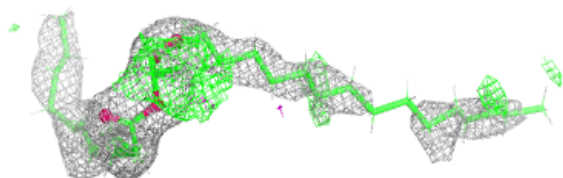
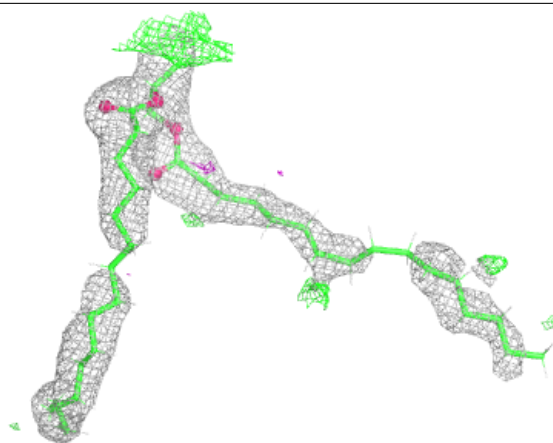
Electron density around DGD A 414:

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



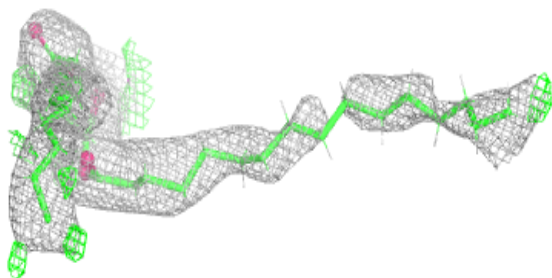
Electron density around SQD A 413:

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



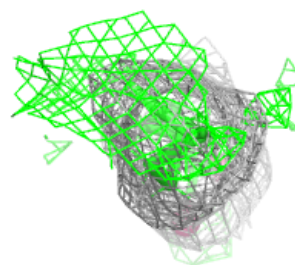
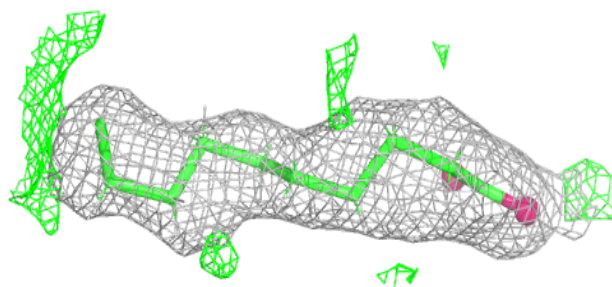
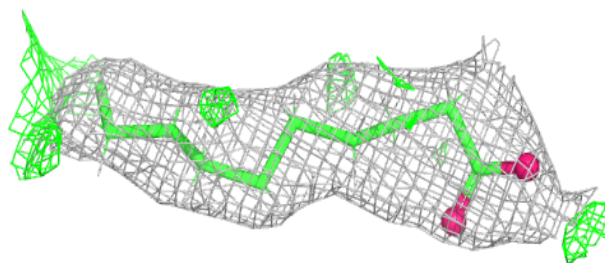
Electron density around SQD a 411:

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

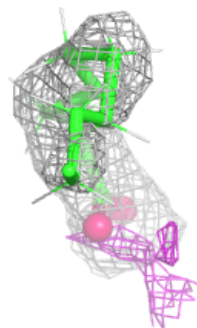
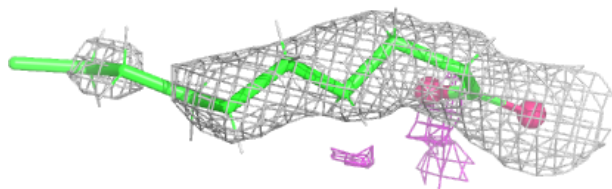
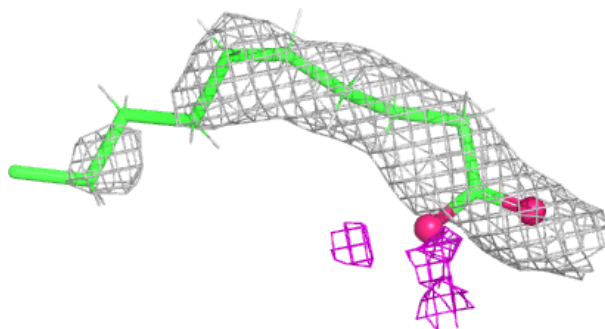


Electron density around STE J 101:

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

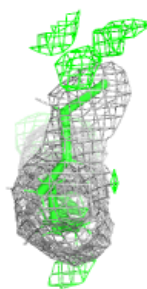
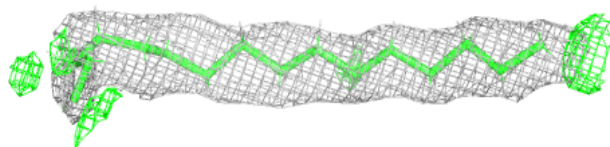
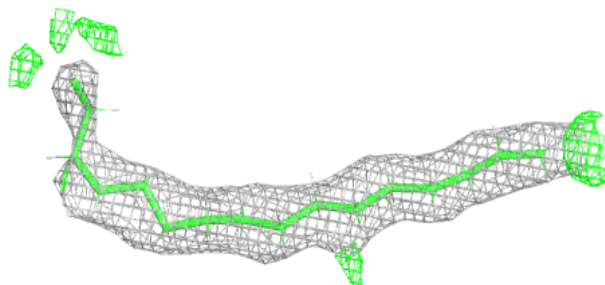
**Electron density around STE B 627:**

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

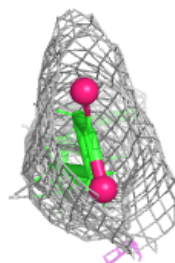
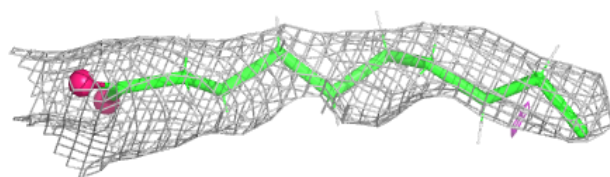
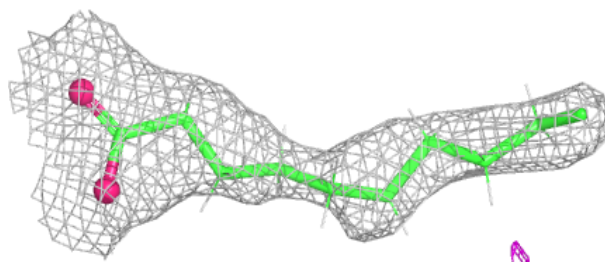


Electron density around STE C 521:

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

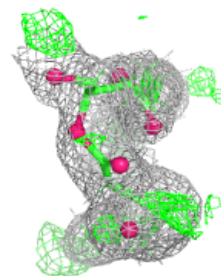
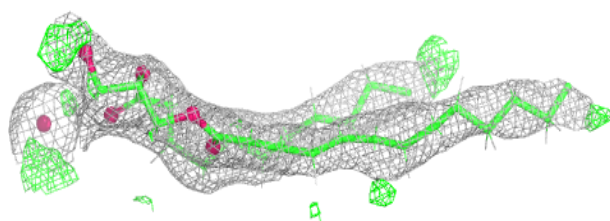
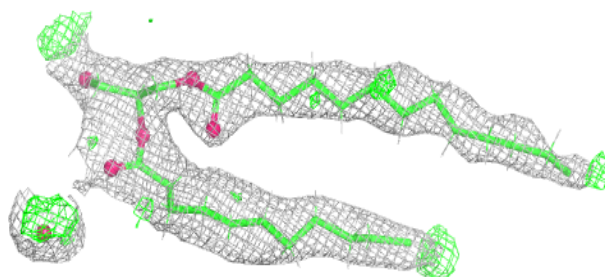
**Electron density around STE a 414:**

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

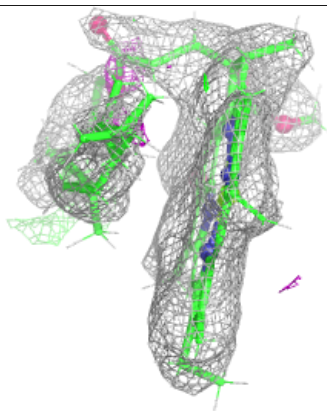
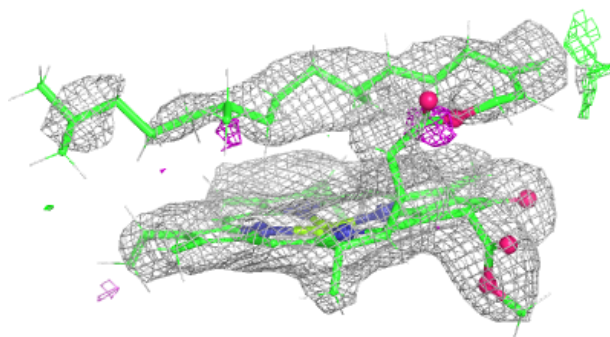
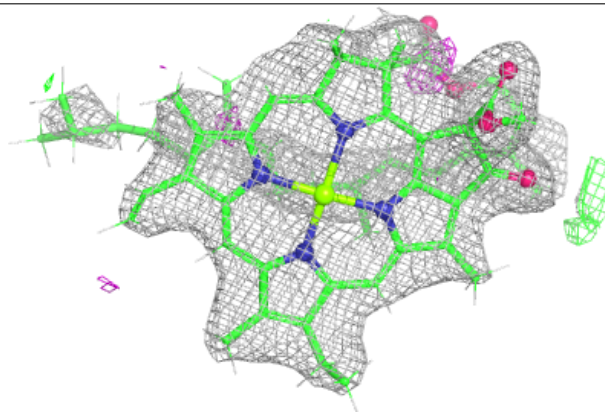


Electron density around LMG D 410:

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

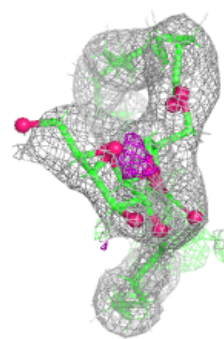
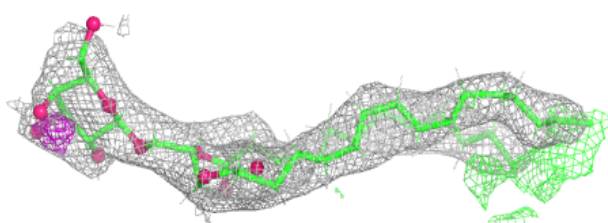
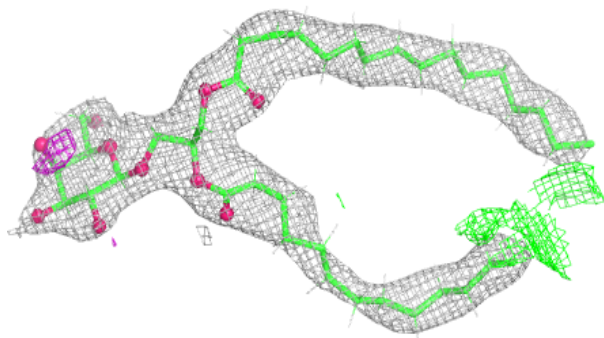
**Electron density around CLA b 601:**

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

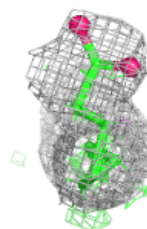
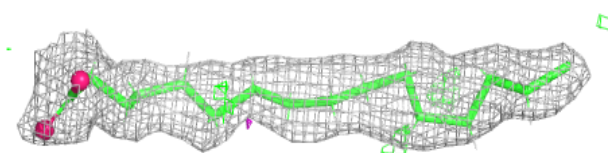
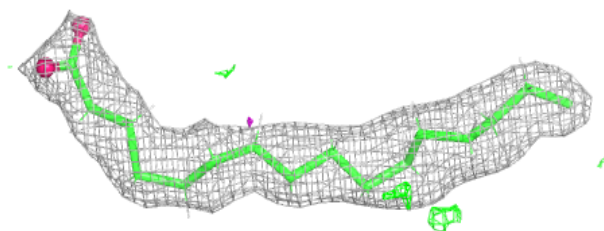


Electron density around LMG A 411:

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

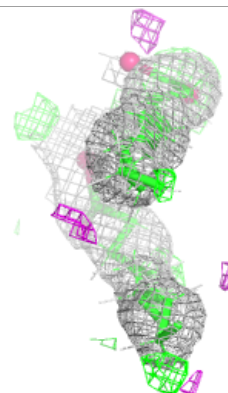
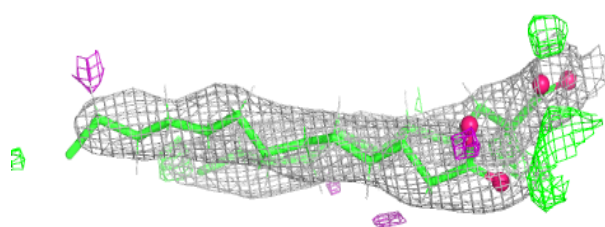
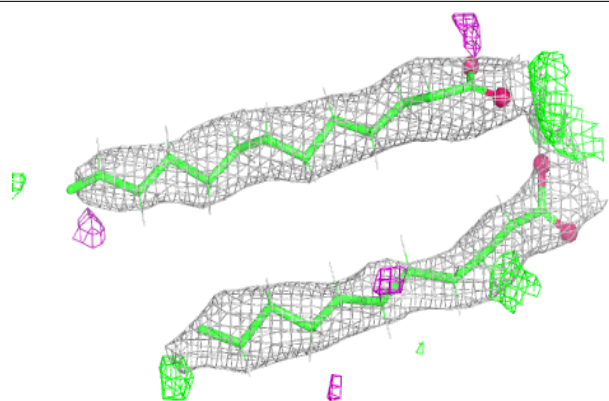
**Electron density around STE B 625:**

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

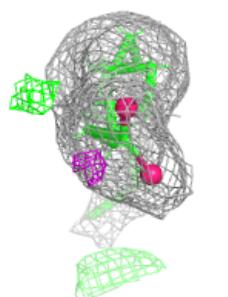
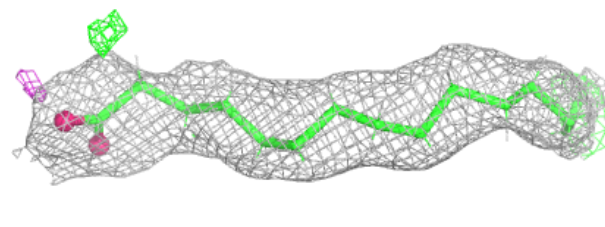
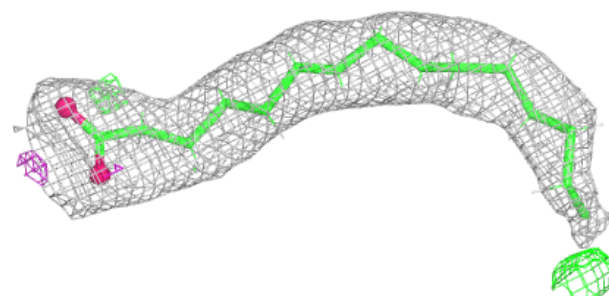


Electron density around LMG B 621:

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

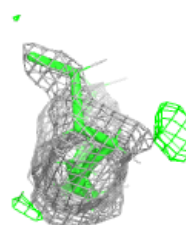
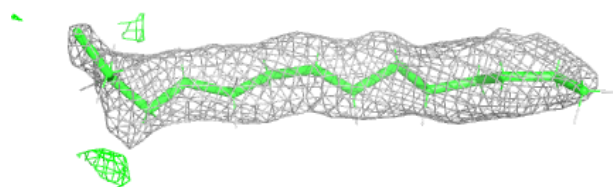
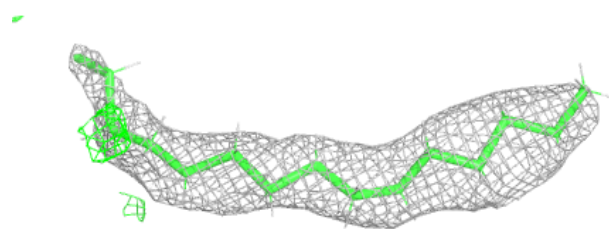
**Electron density around STE B 620:**

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

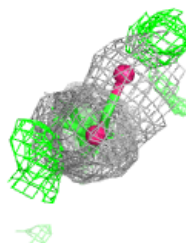
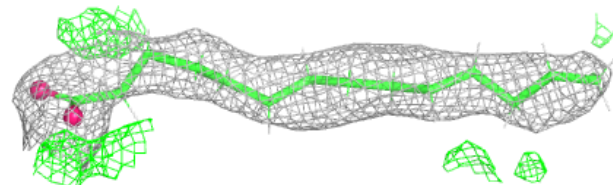
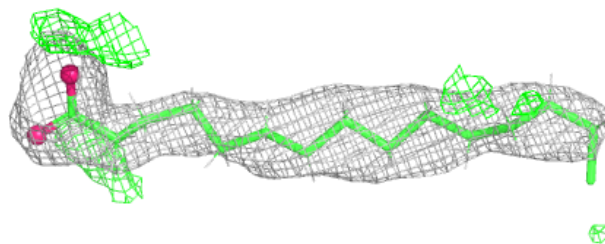


Electron density around STE T 103:

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

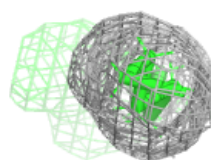
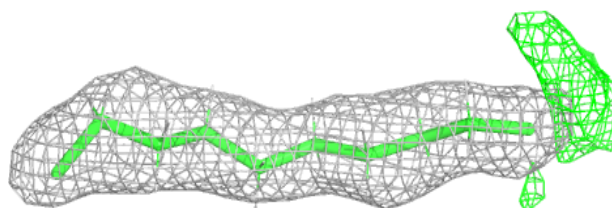
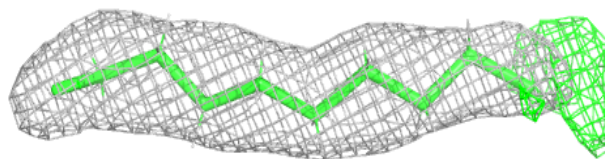
**Electron density around STE d 413:**

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

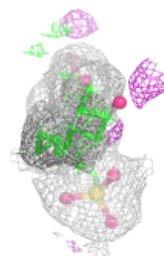
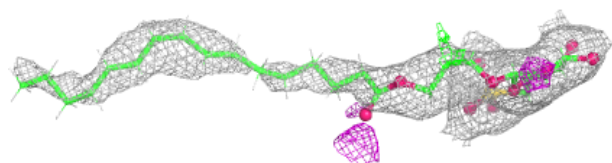
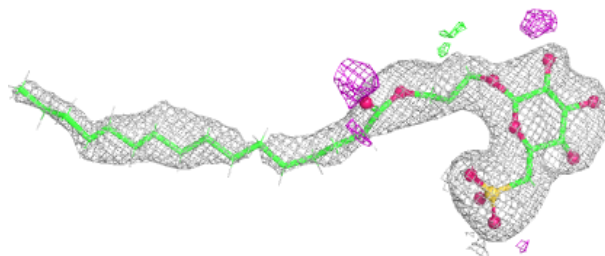


Electron density around STE M 103:

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

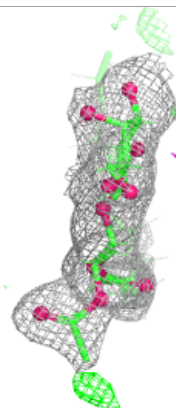
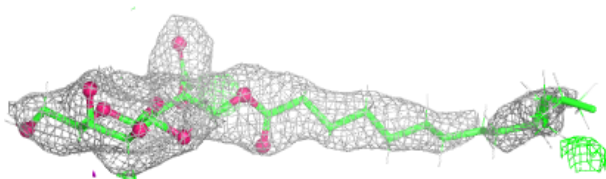
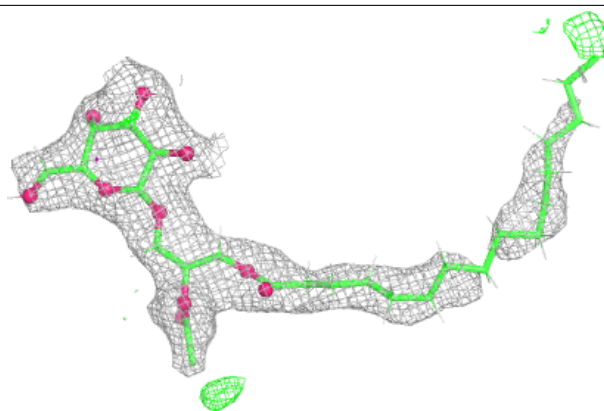
**Electron density around SQD F 101:**

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

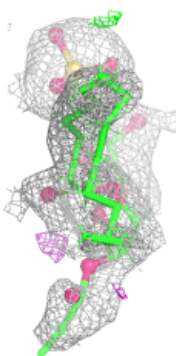
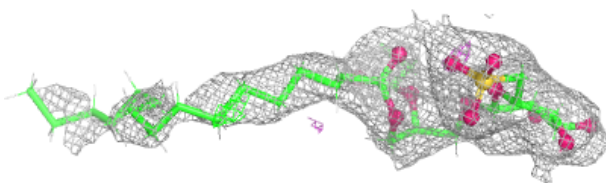
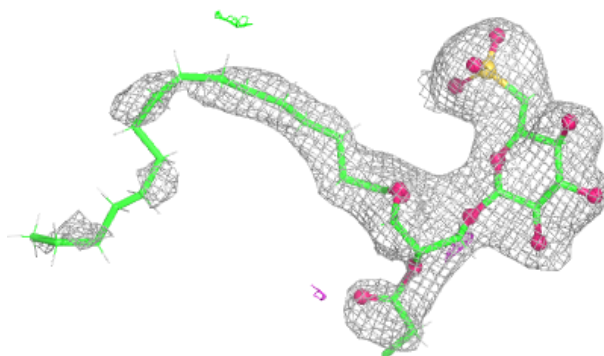


Electron density around LMG c 520:

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

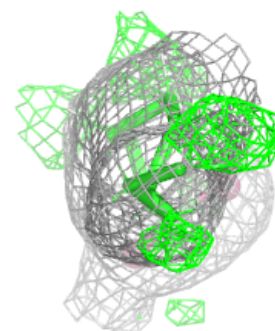
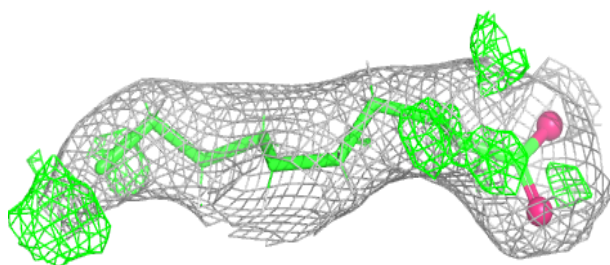
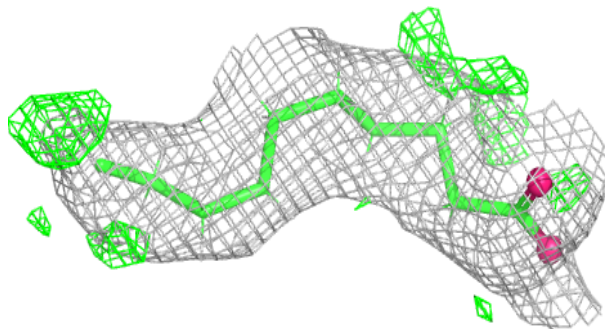
**Electron density around SQD f 102:**

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

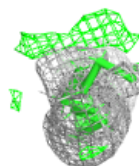
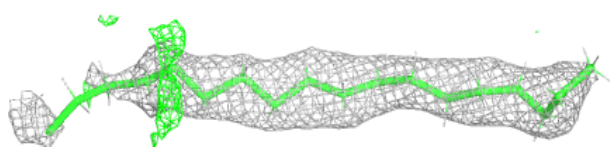
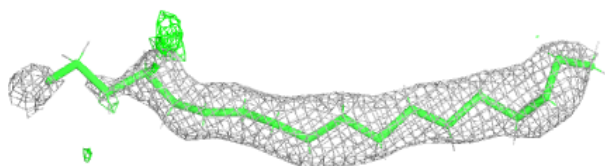


Electron density around STE B 624:

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

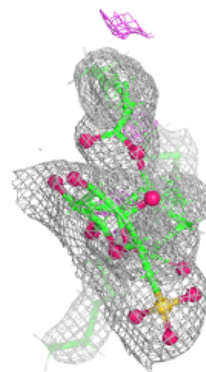
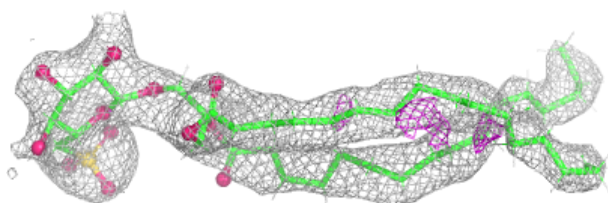
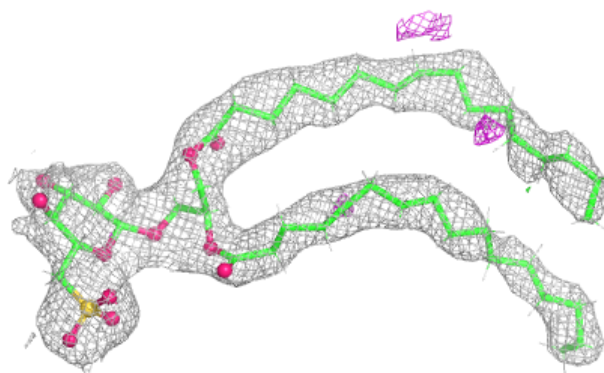
**Electron density around STE I 102:**

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

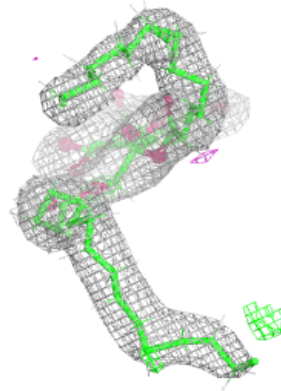
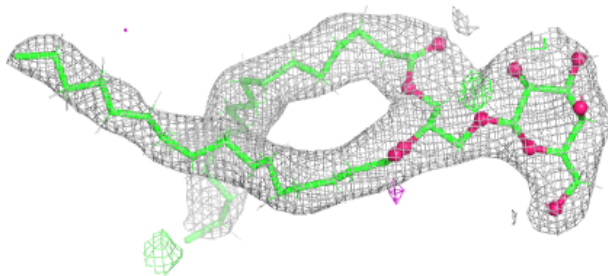
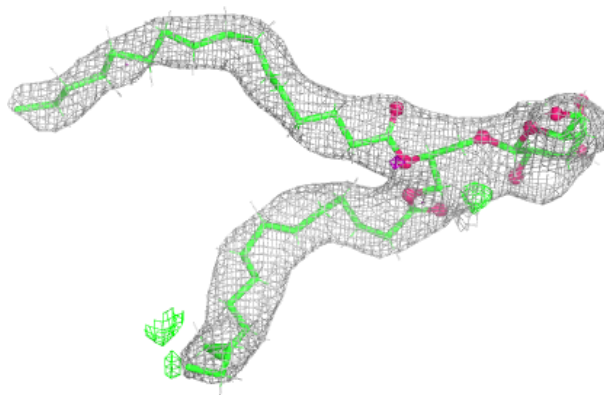


Electron density around SQD B 623:

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

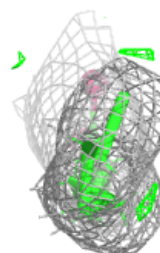
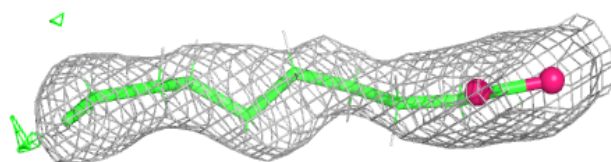
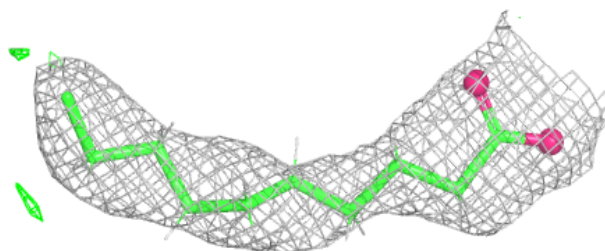
**Electron density around LMG b 620:**

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



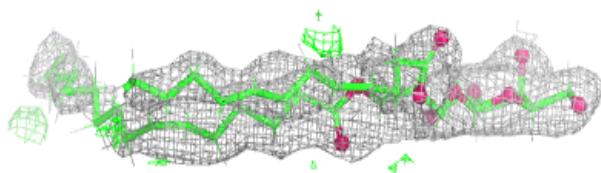
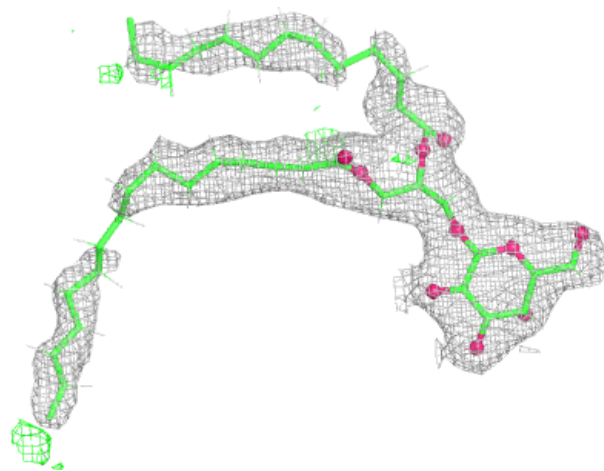
Electron density around STE C 520:

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



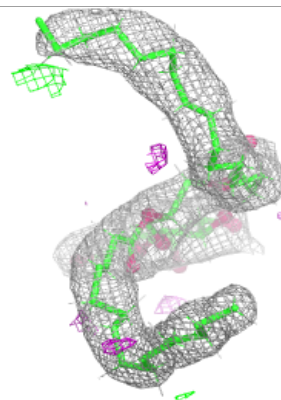
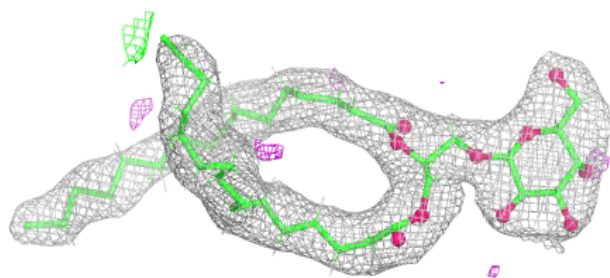
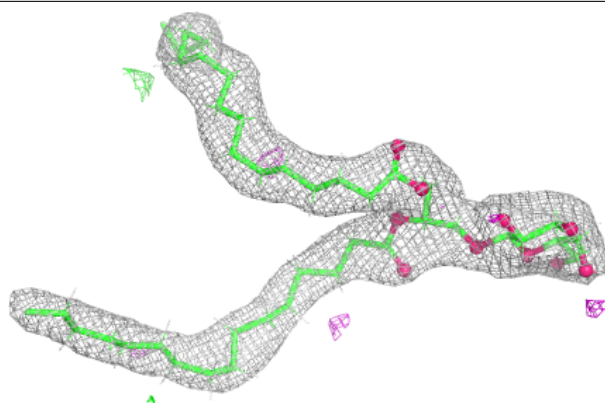
Electron density around LMG C 519:

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

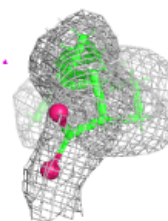
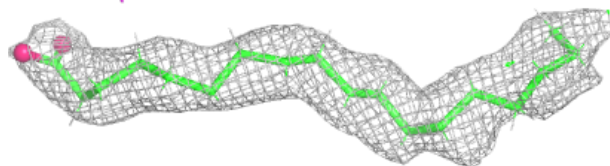
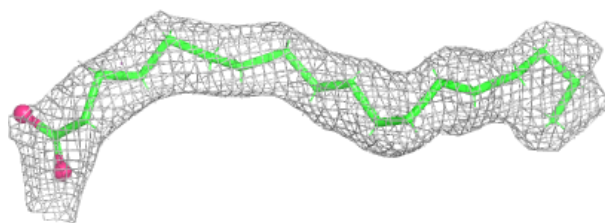


Electron density around LMG M 101:

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

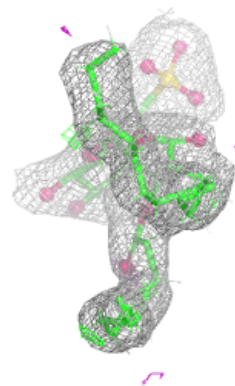
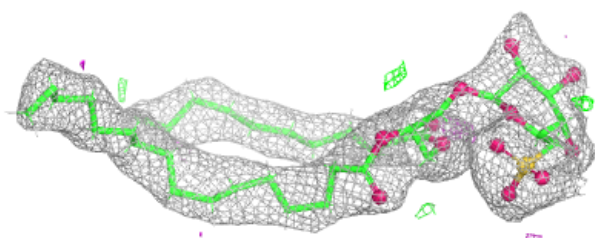
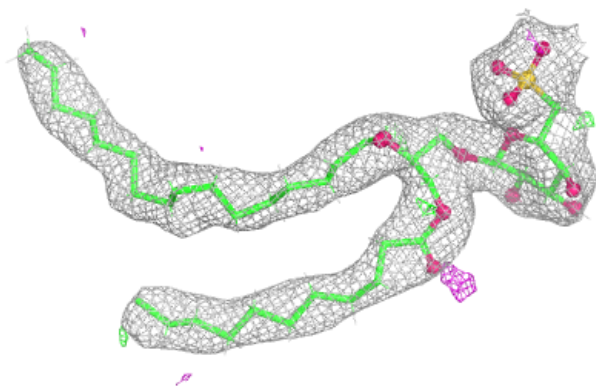
**Electron density around STE b 621:**

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

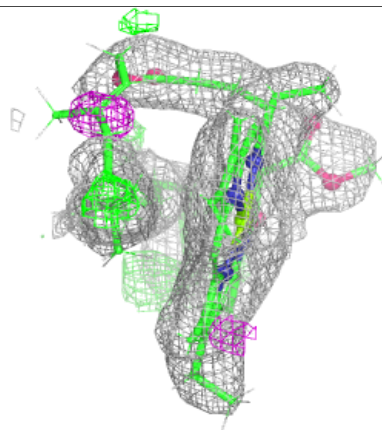
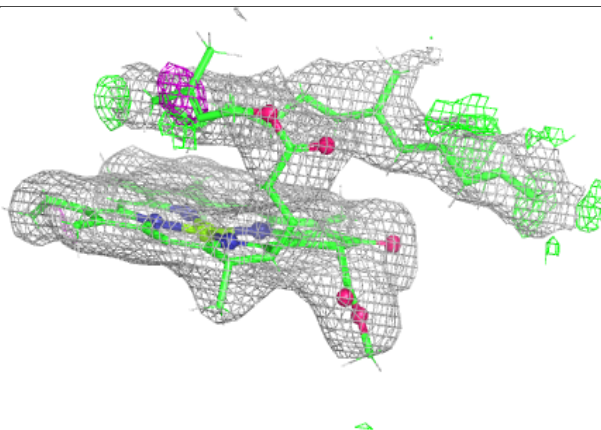
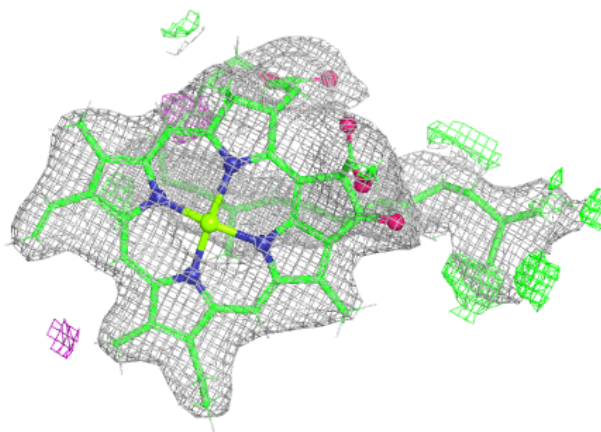


Electron density around SQD L 101:

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

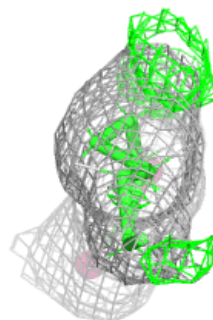
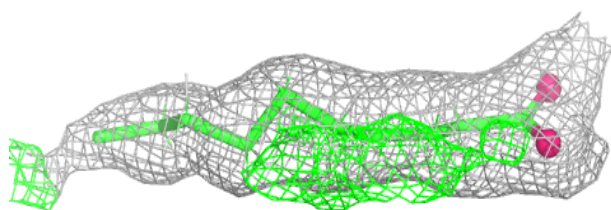
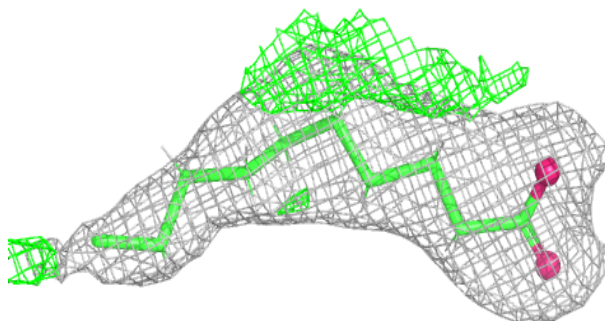
**Electron density around CLA B 601:**

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

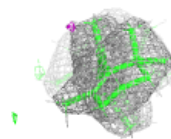
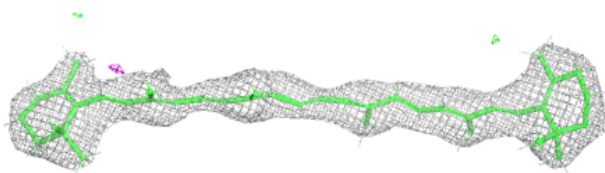
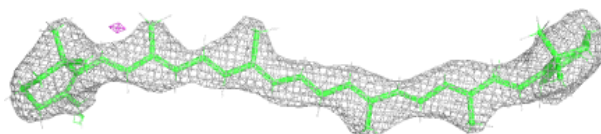


Electron density around STE C 522:

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

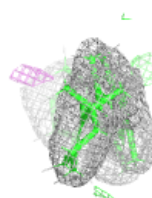
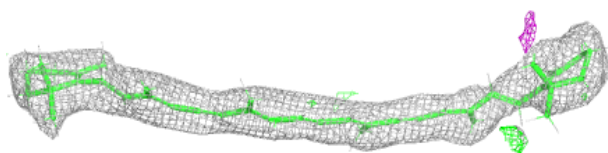
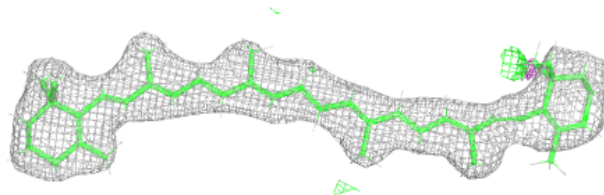
**Electron density around BCR c 514:**

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

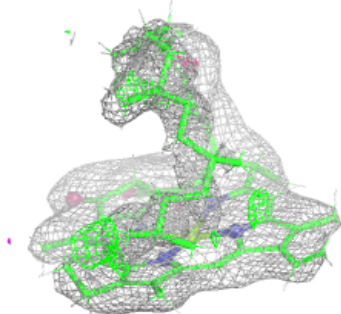
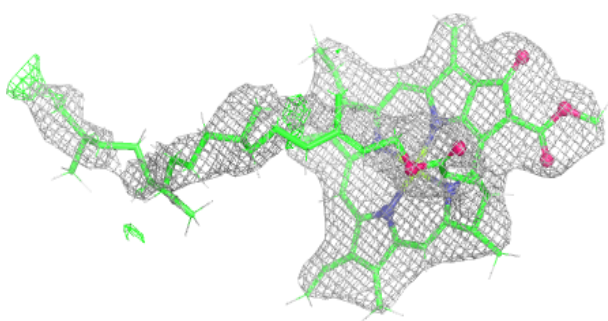
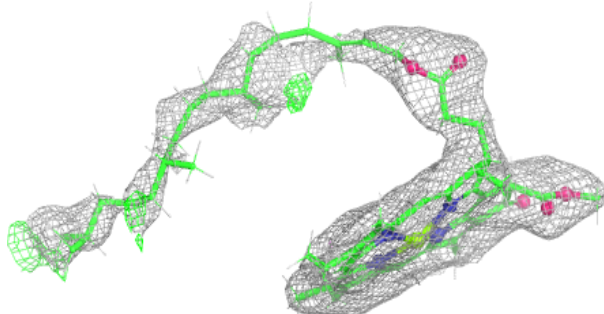


Electron density around BCR d 406:

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

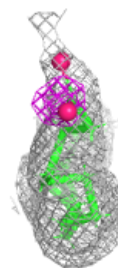
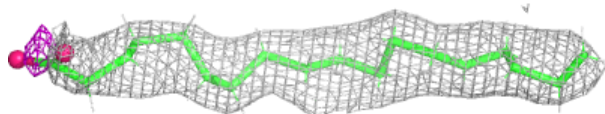
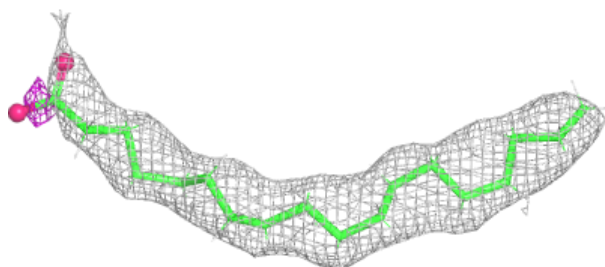
**Electron density around CLA C 513:**

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

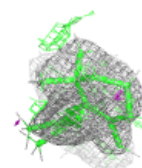
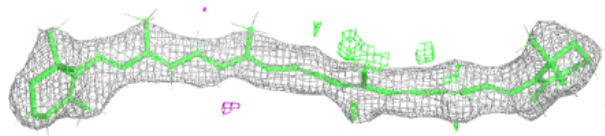
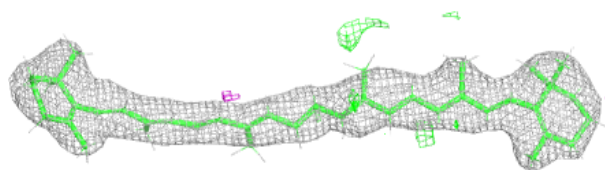


Electron density around STE D 411:

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

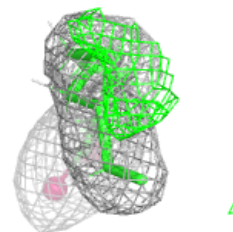
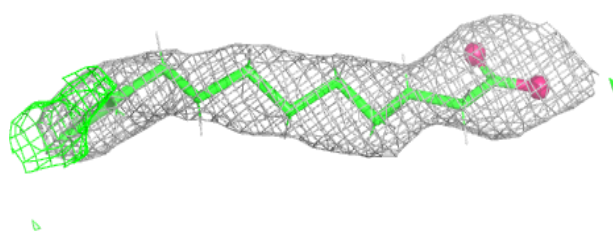
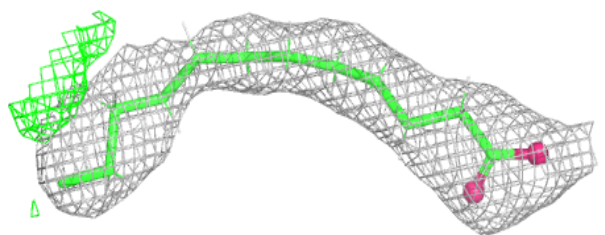
**Electron density around BCR K 101:**

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

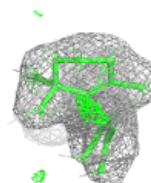
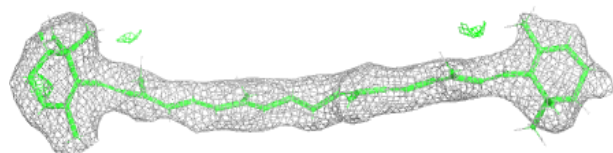
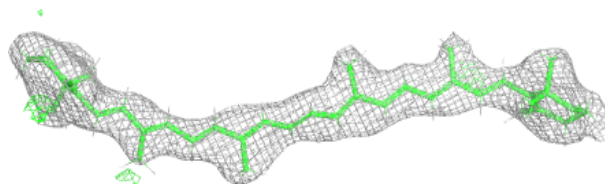


Electron density around STE t 102:

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

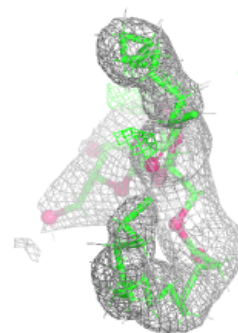
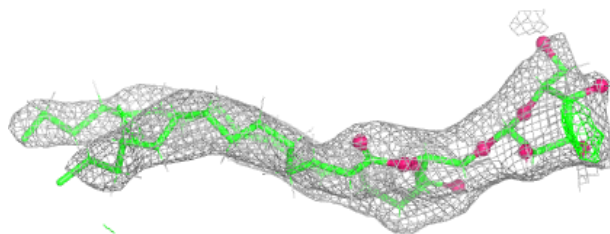
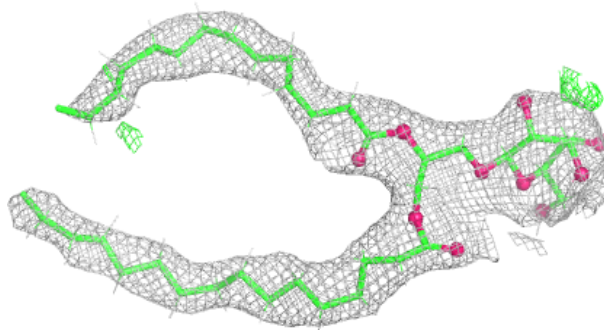
**Electron density around BCR h 101:**

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

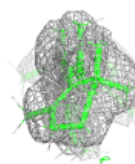
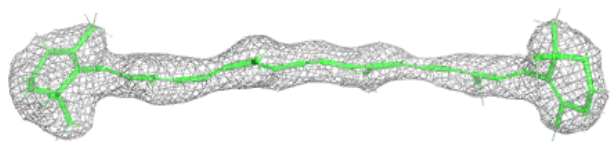


Electron density around LMG c 523:

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

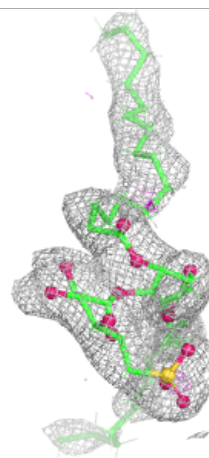
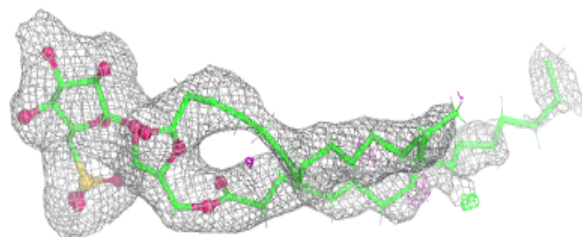
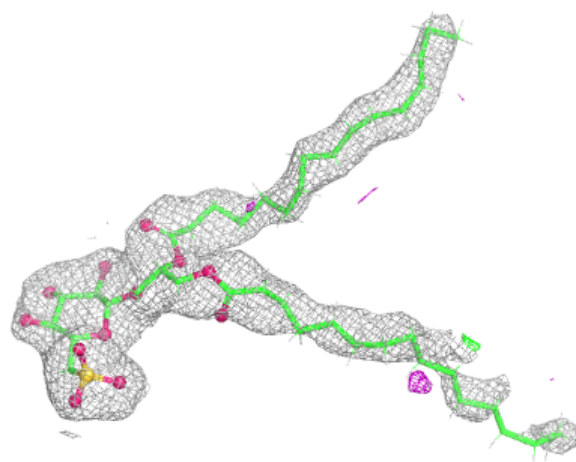
**Electron density around BCR k 101:**

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



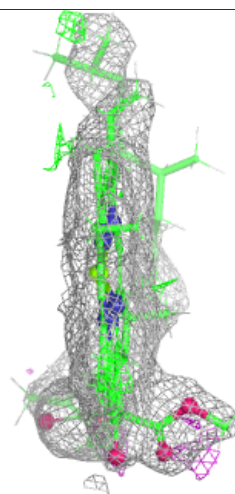
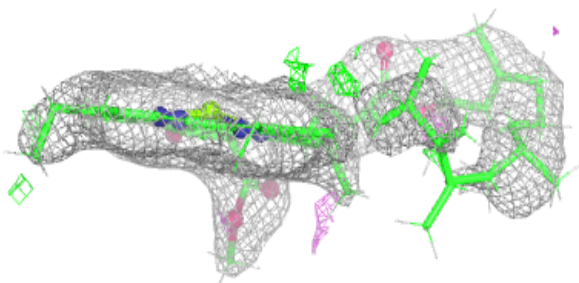
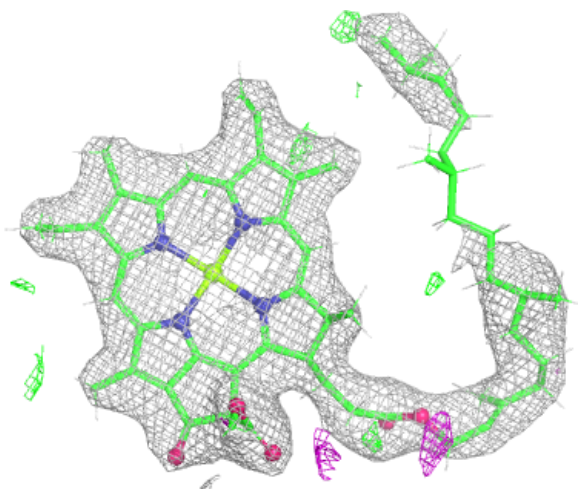
Electron density around SQD a 410:

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



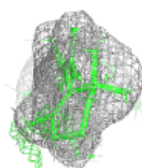
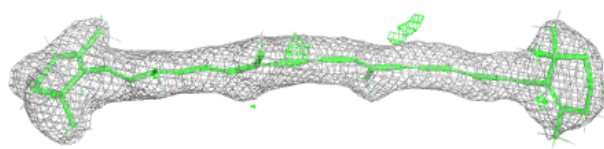
Electron density around CLA c 512:

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

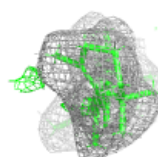
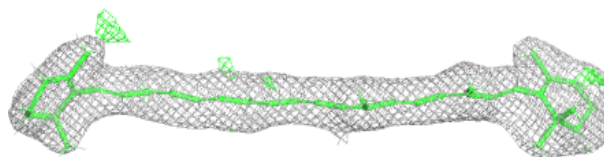
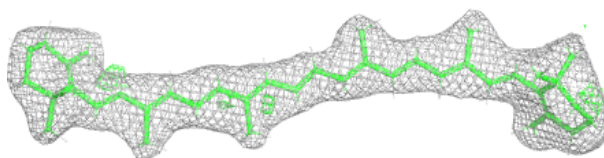


Electron density around BCR Y 101:

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

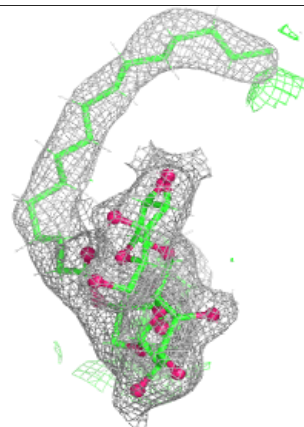
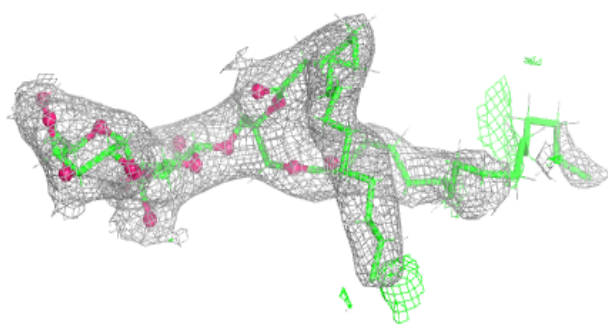
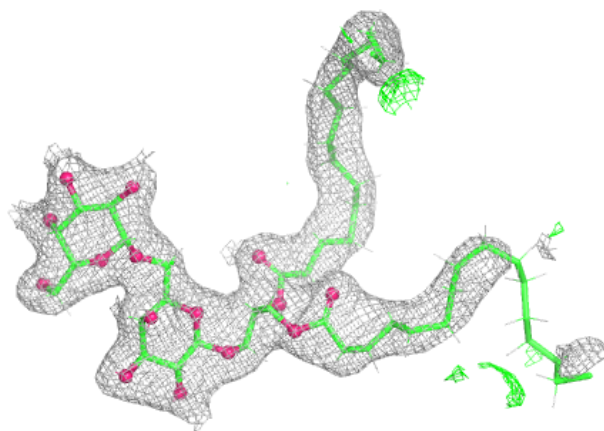
**Electron density around BCR b 618:**

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

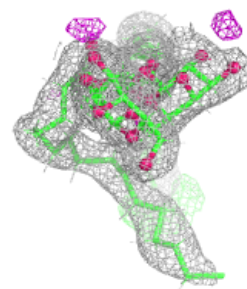
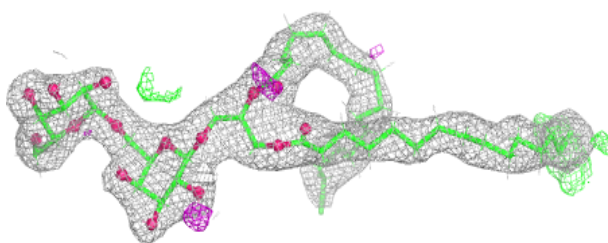
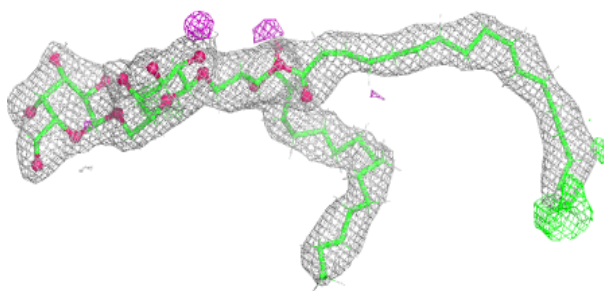


Electron density around DGD C 517:

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

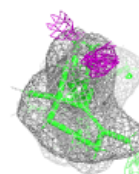
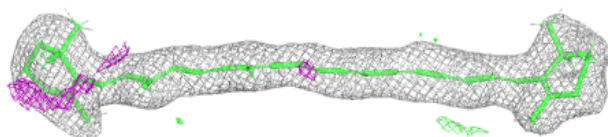
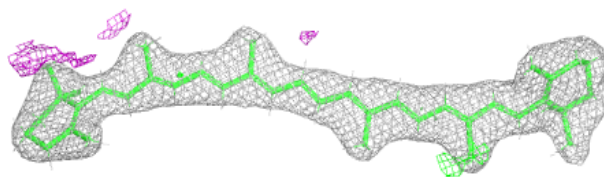
**Electron density around DGD H 102:**

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

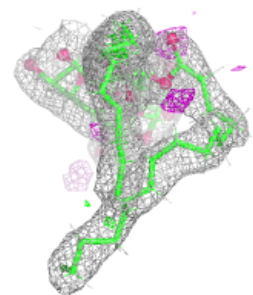
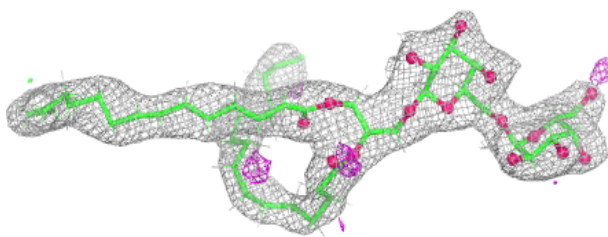
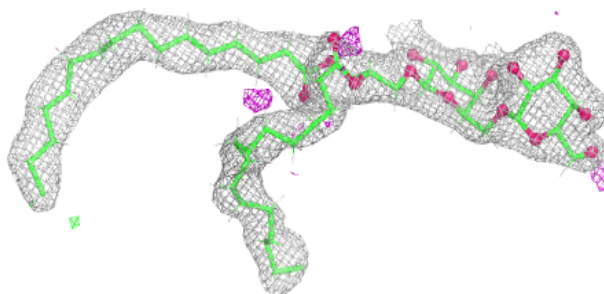


Electron density around BCR B 618:

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

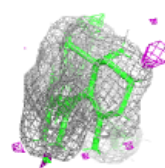
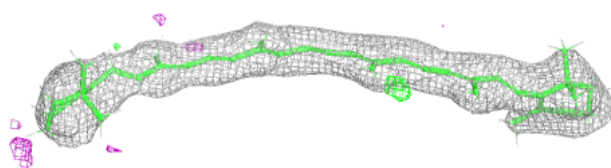
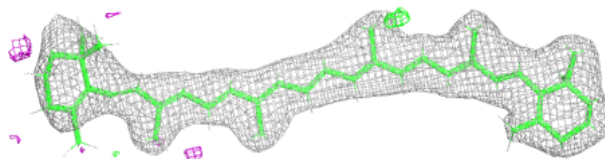
**Electron density around DGD h 102:**

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

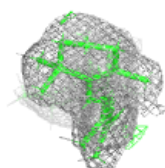
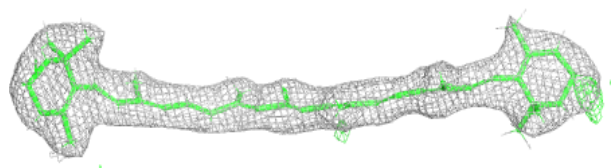
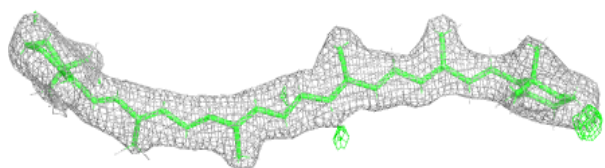


Electron density around BCR D 405:

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

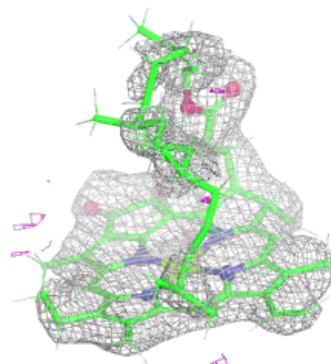
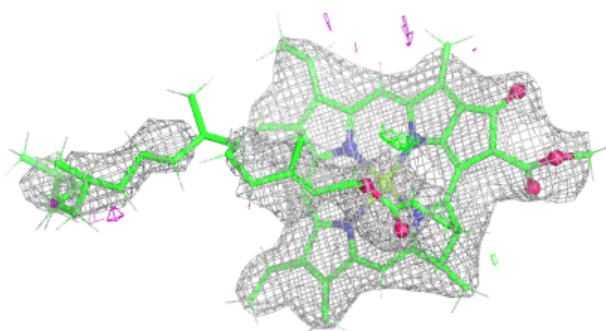
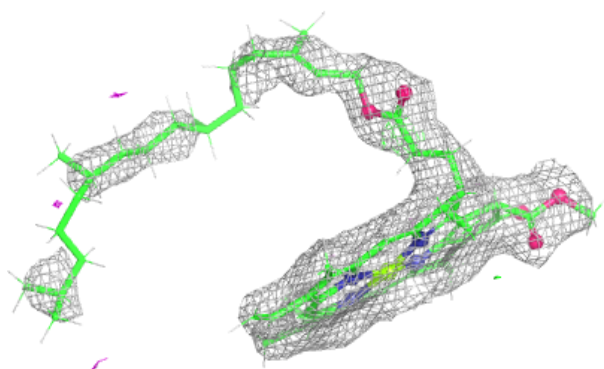
**Electron density around BCR H 101:**

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

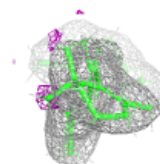
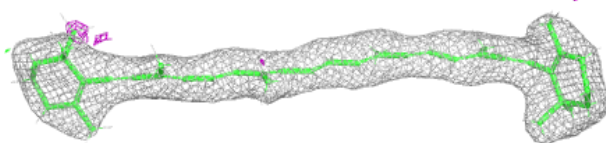
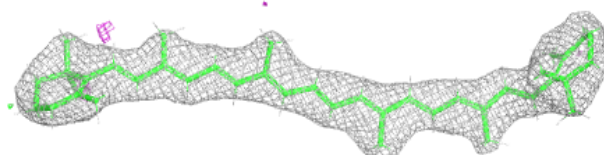


Electron density around CLA c 513:

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

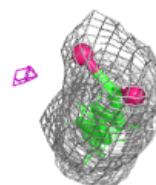
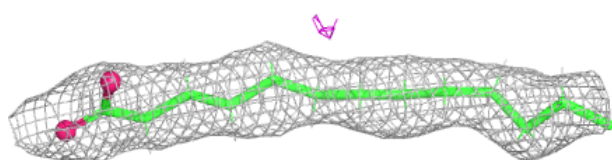
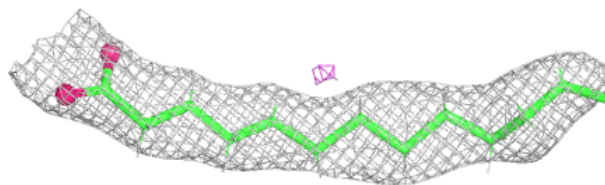
**Electron density around BCR c 515:**

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

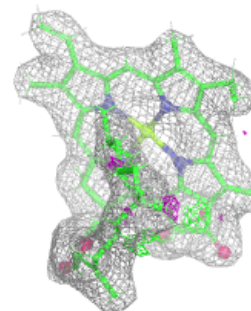
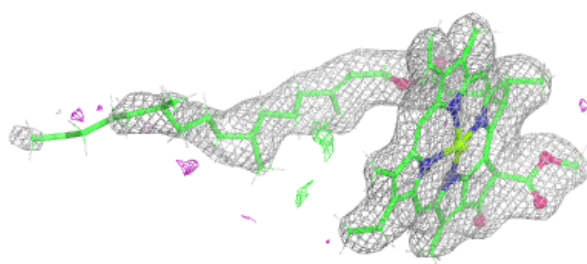
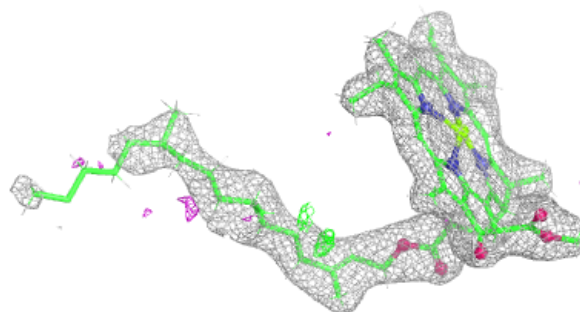


Electron density around STE M 102:

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

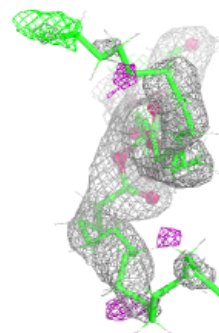
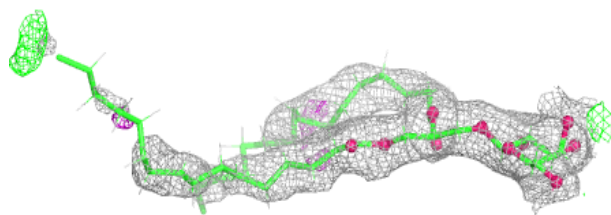
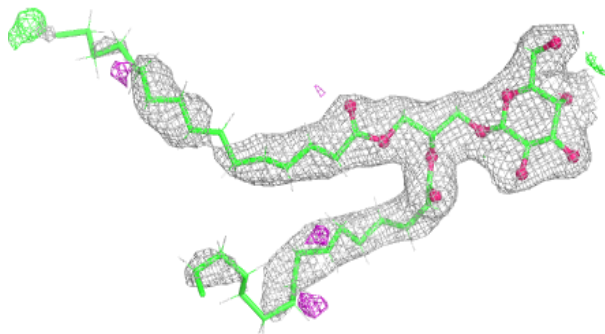
**Electron density around CLA c 508:**

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



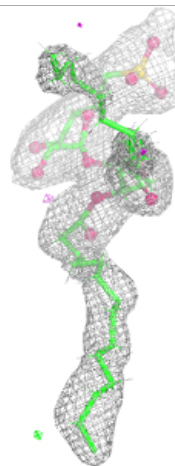
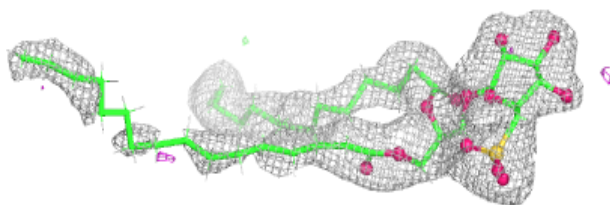
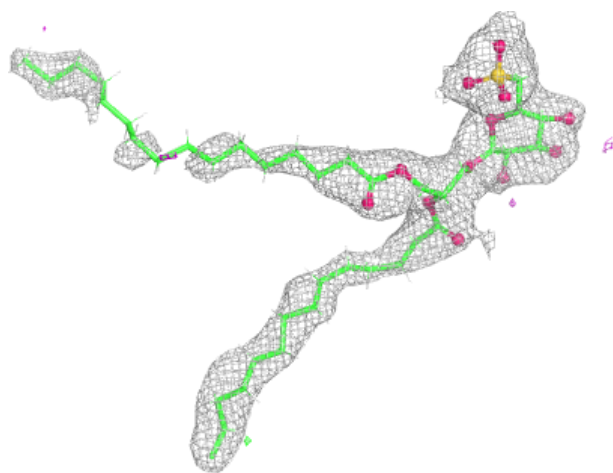
Electron density around LMG D 407:

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



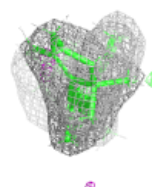
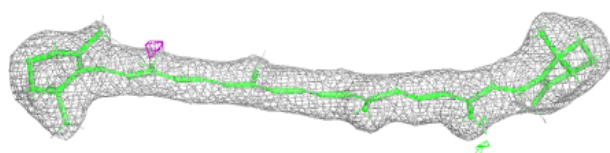
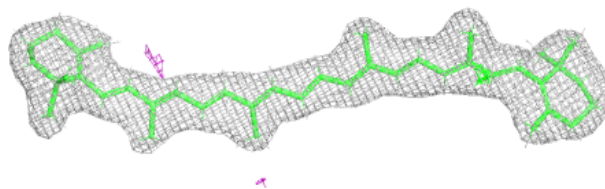
Electron density around SQD A 412:

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

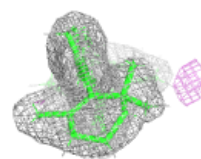
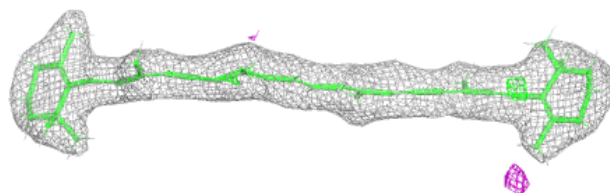
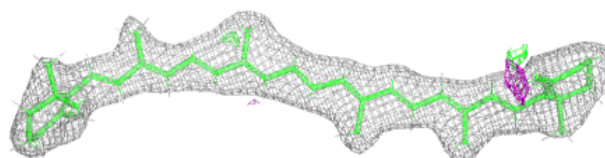


Electron density around BCR B 619:

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

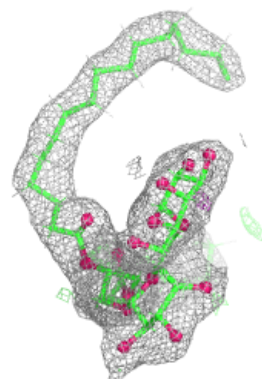
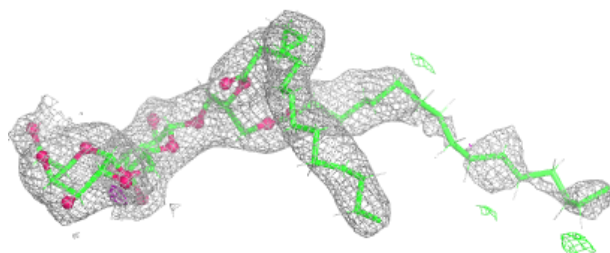
**Electron density around BCR C 514:**

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

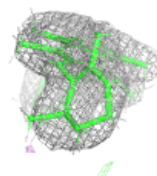
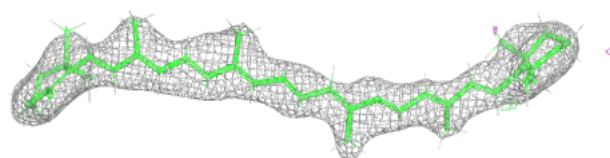
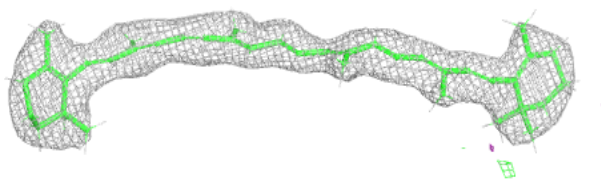


Electron density around DGD c 518:

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

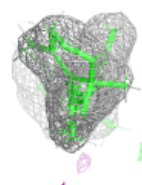
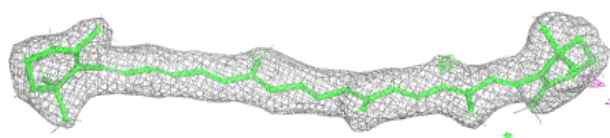
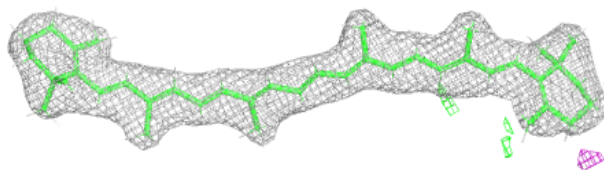
**Electron density around BCR C 515:**

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

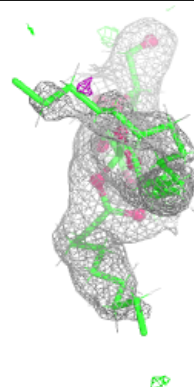
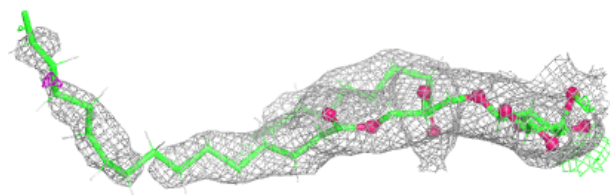
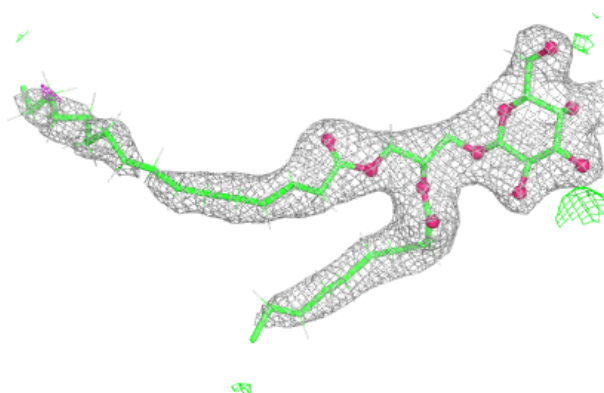


Electron density around BCR b 619:

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

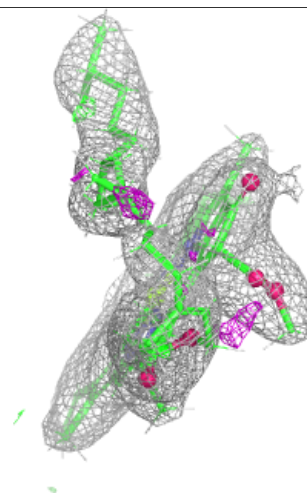
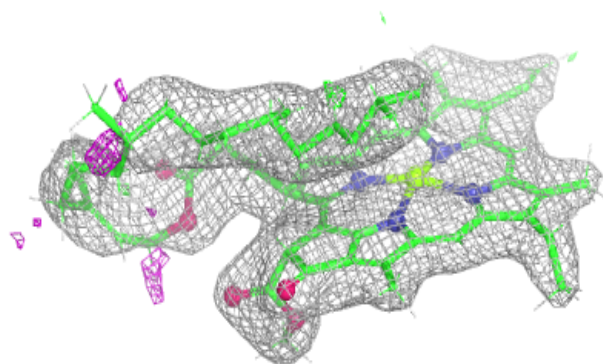
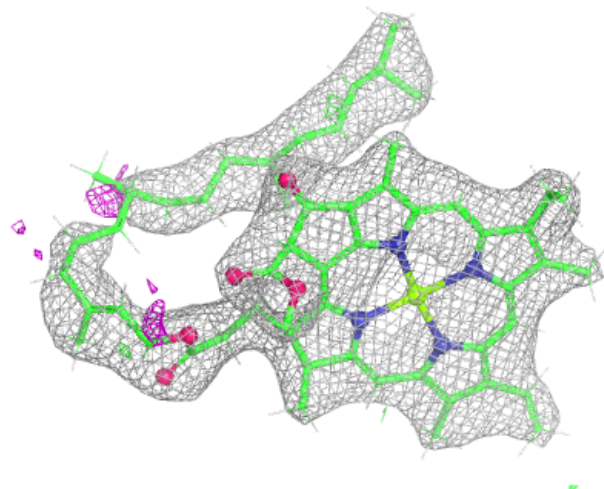
**Electron density around LMG d 412:**

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



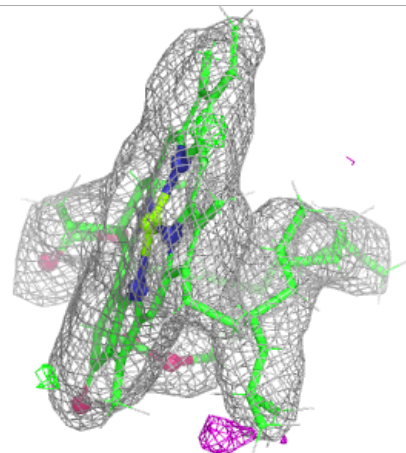
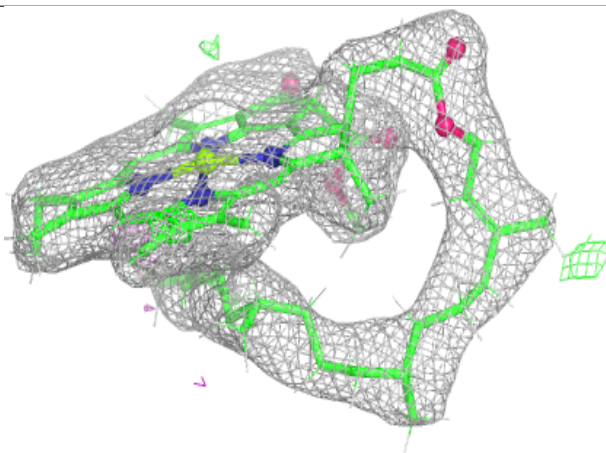
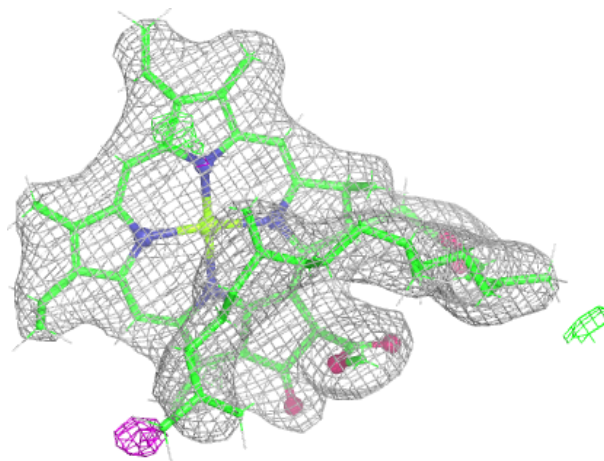
Electron density around CLA c 509:

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



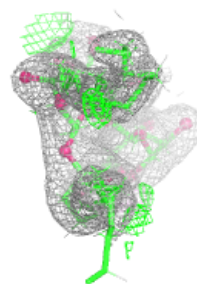
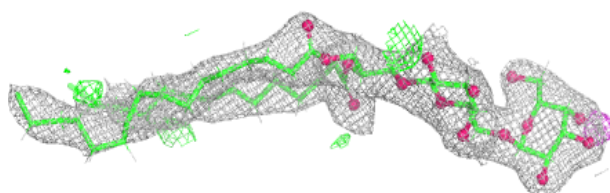
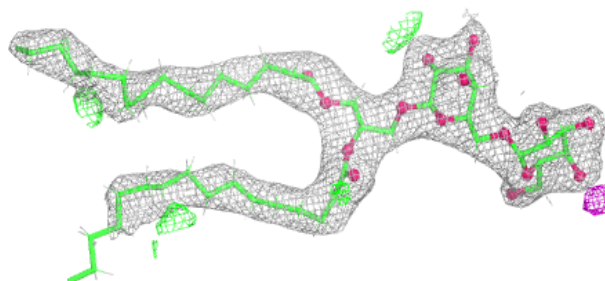
Electron density around CLA c 510:

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

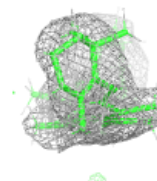
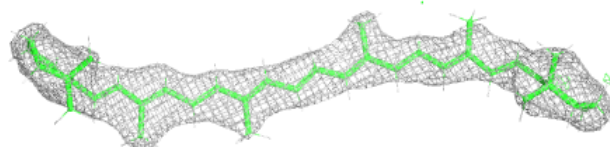
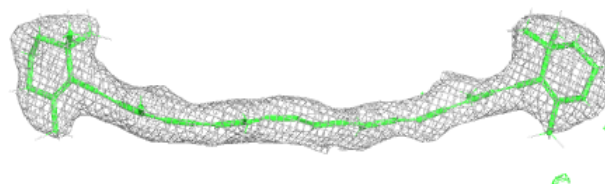


Electron density around DGD c 519:

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

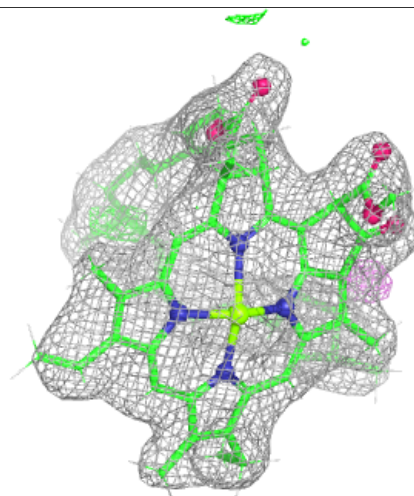
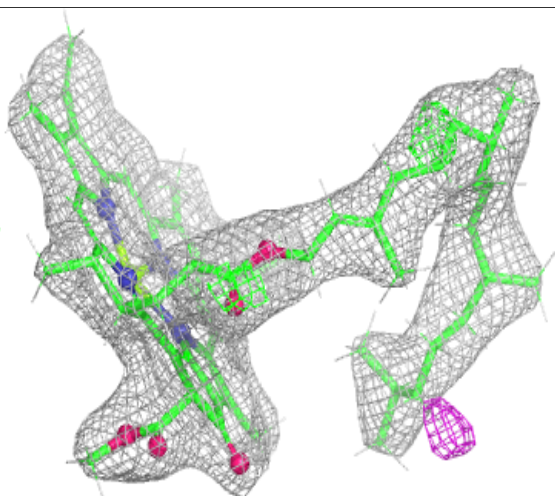
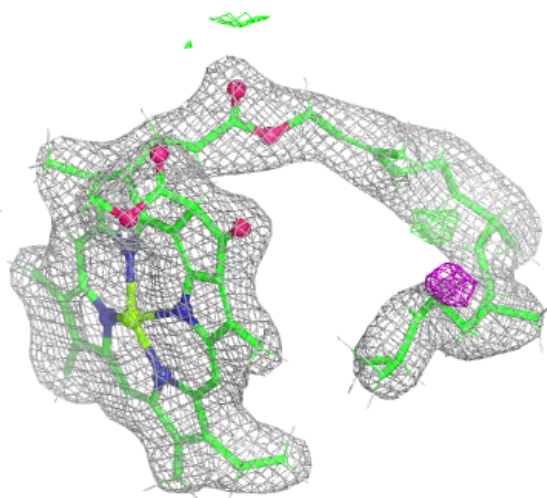
**Electron density around BCR c 516:**

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



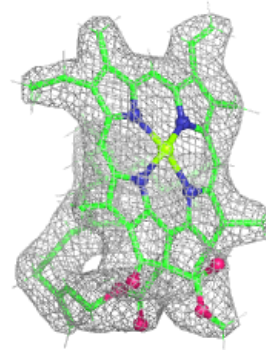
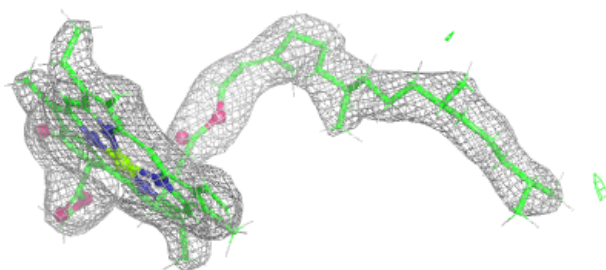
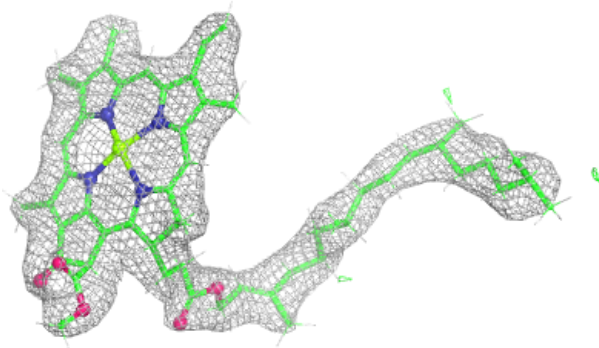
Electron density around CLA C 503:

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

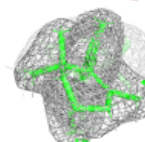
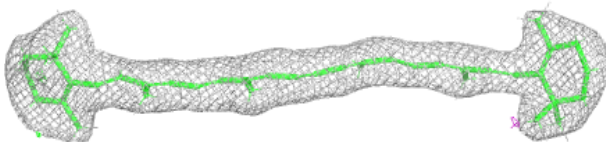
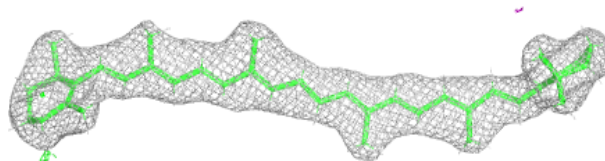


Electron density around CLA C 511:

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

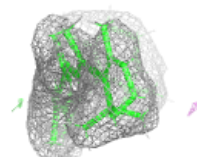
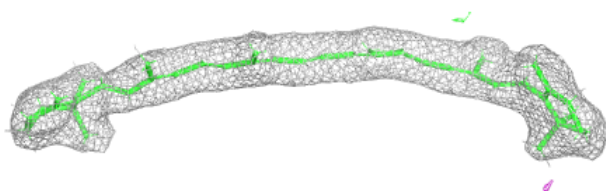
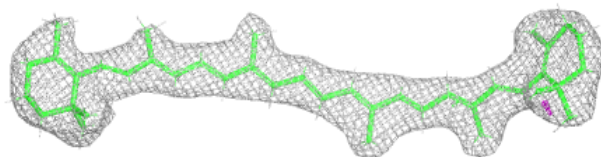
**Electron density around BCR A 406:**

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

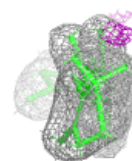
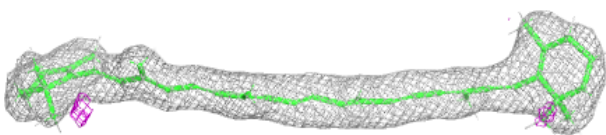
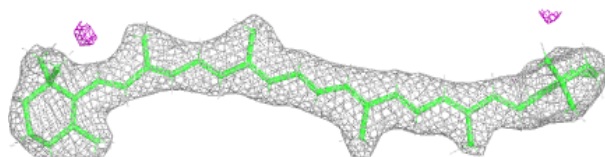


Electron density around BCR T 101:

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

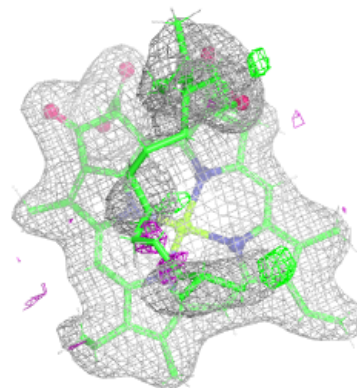
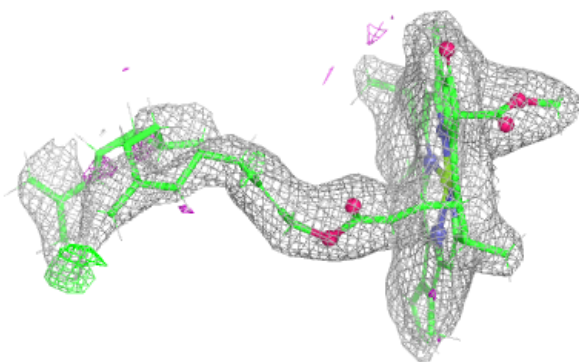
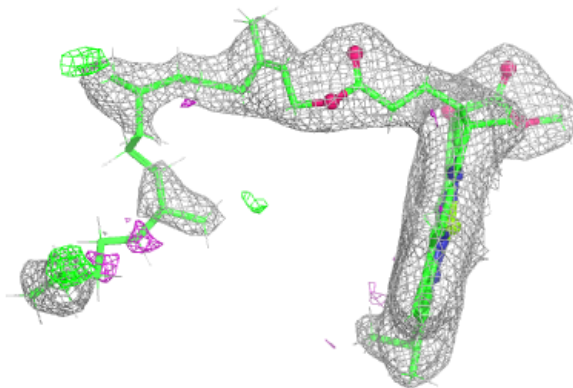
**Electron density around BCR B 617:**

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

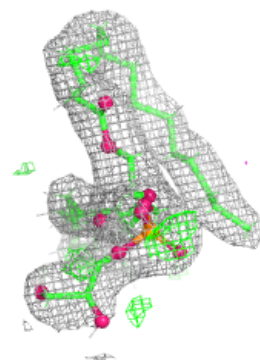
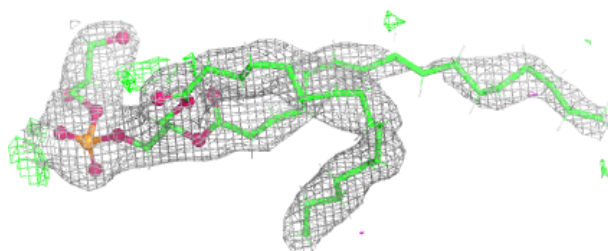
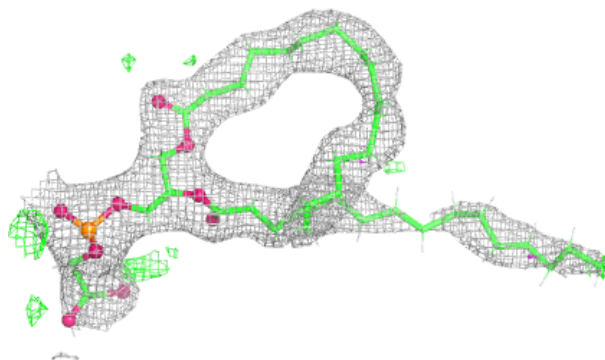


Electron density around CLA c 506:

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

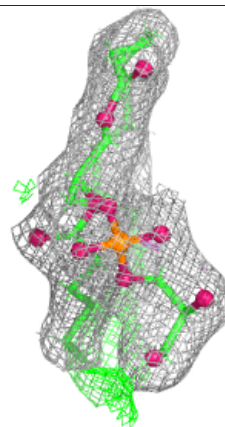
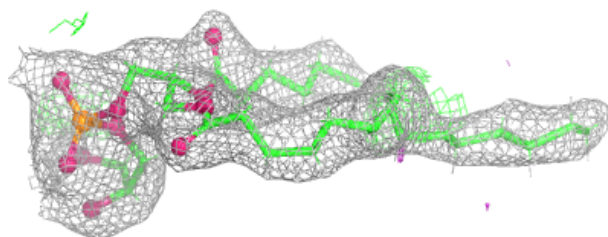
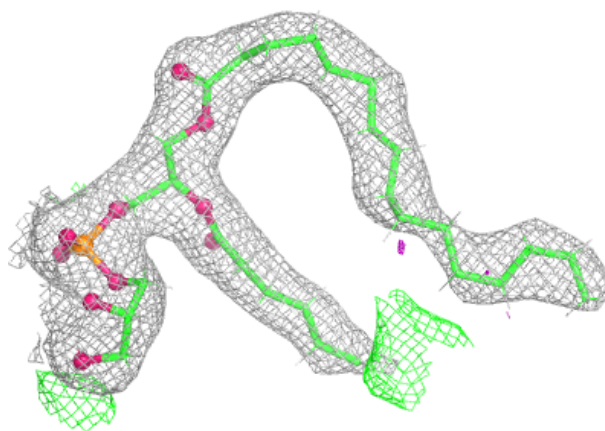
**Electron density around LHG d 408:**

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

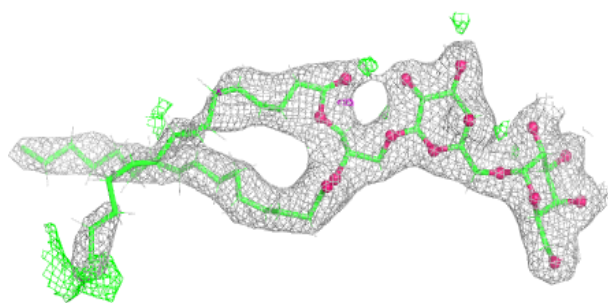
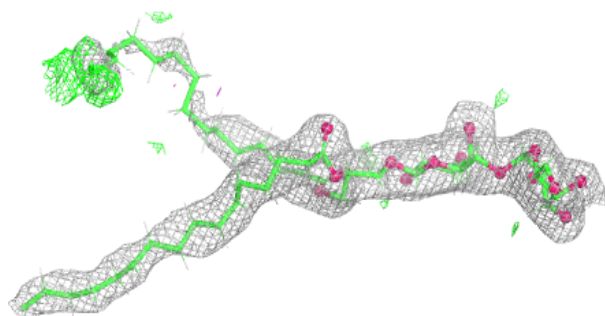


Electron density around LHG d 410:

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

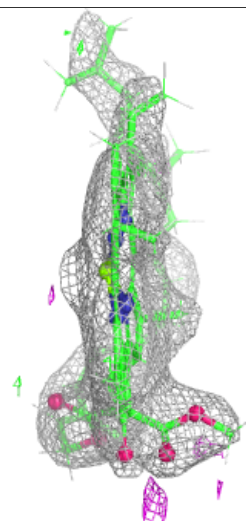
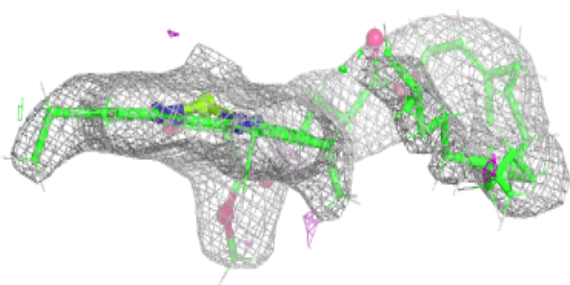
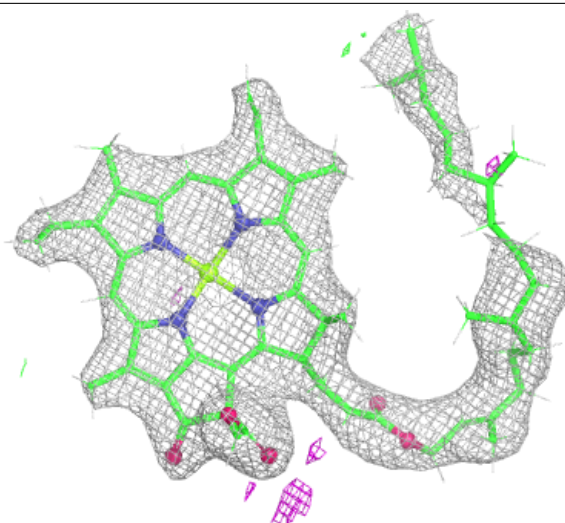
**Electron density around DGD C 516:**

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



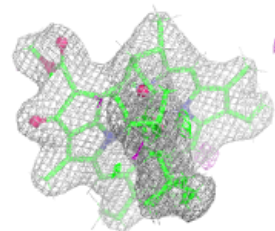
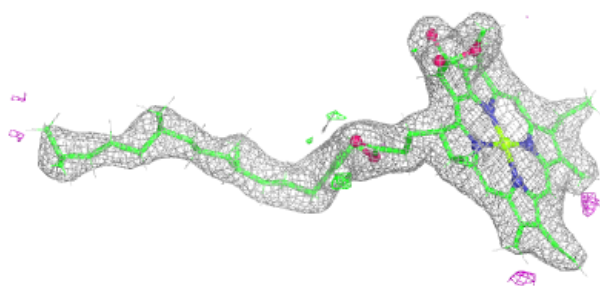
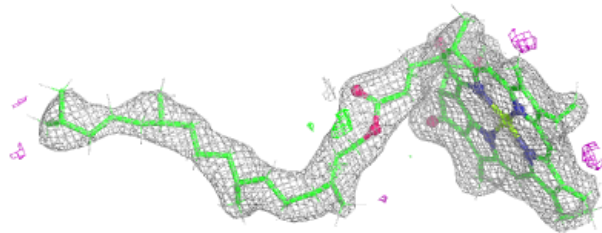
Electron density around CLA C 512:

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



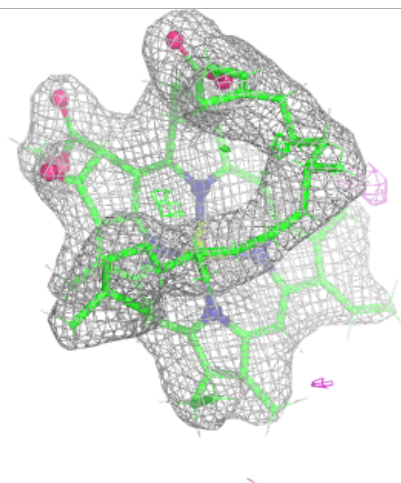
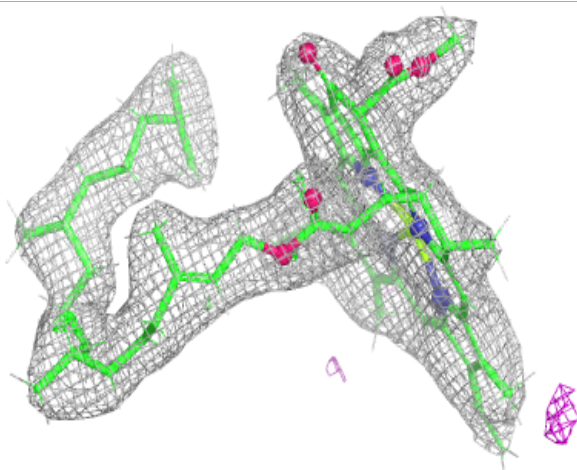
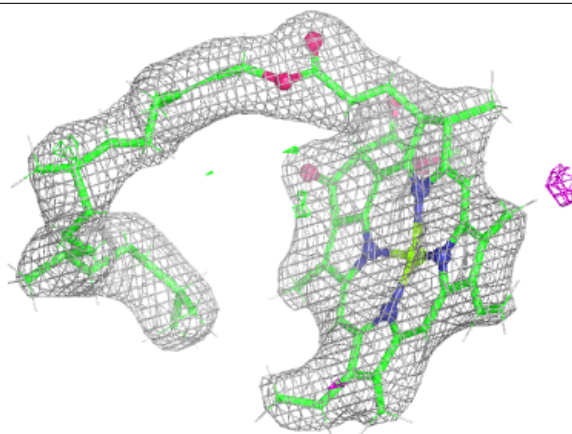
Electron density around CLA c 502:

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



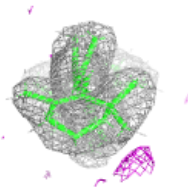
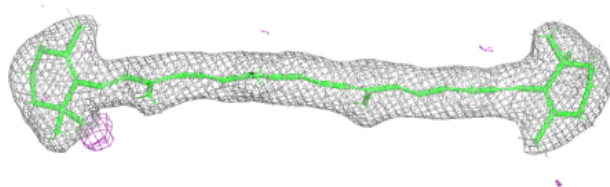
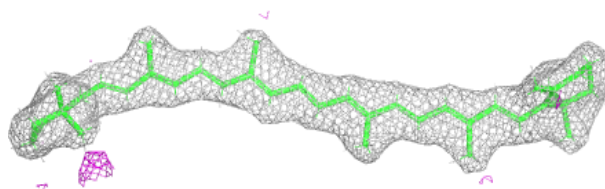
Electron density around CLA c 503:

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

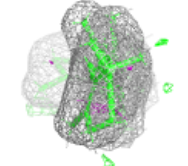
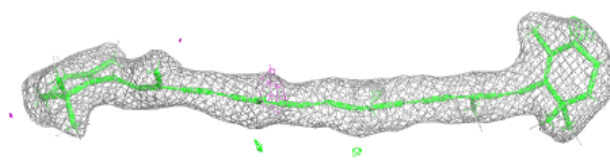
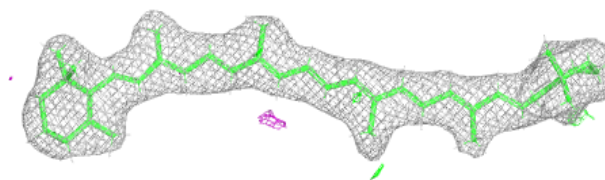


Electron density around BCR a 405:

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

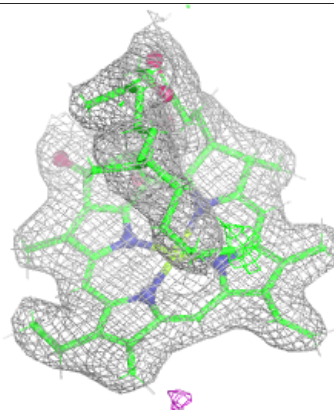
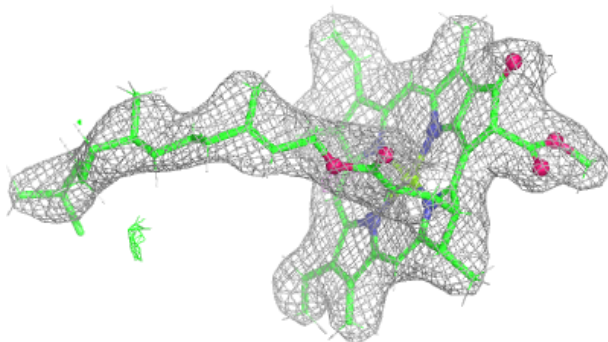
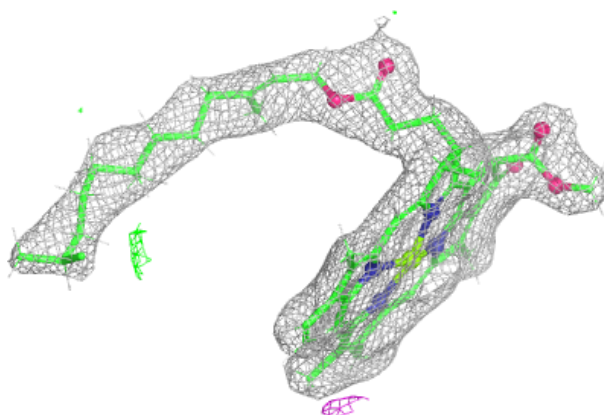
**Electron density around BCR b 617:**

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

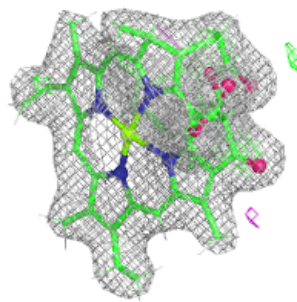
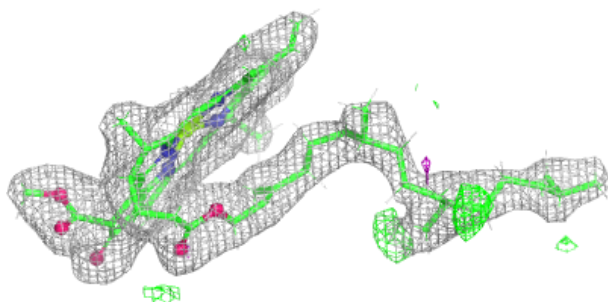
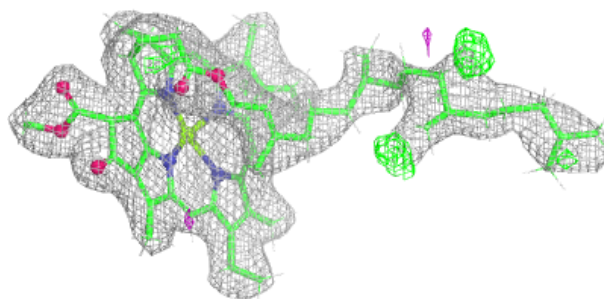


Electron density around CLA c 504:

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

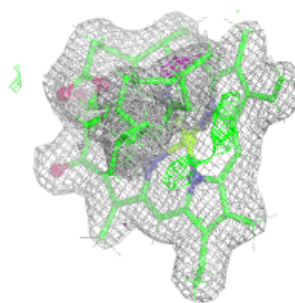
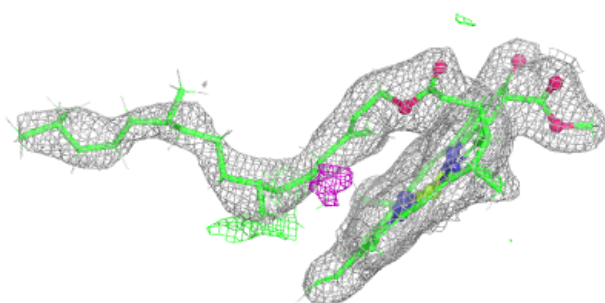
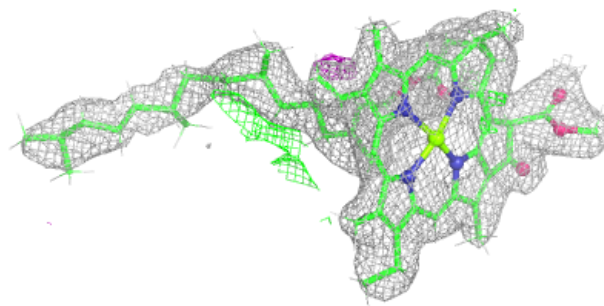
**Electron density around CLA c 505:**

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



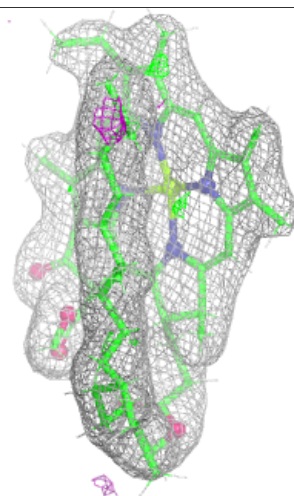
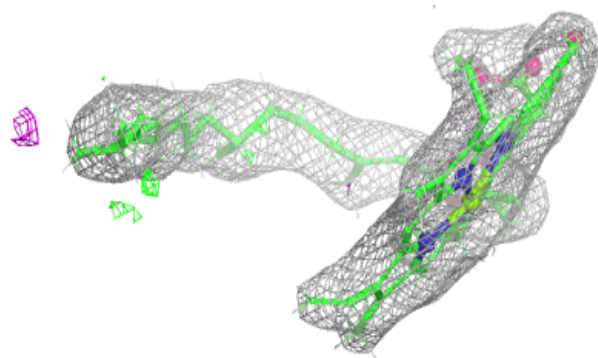
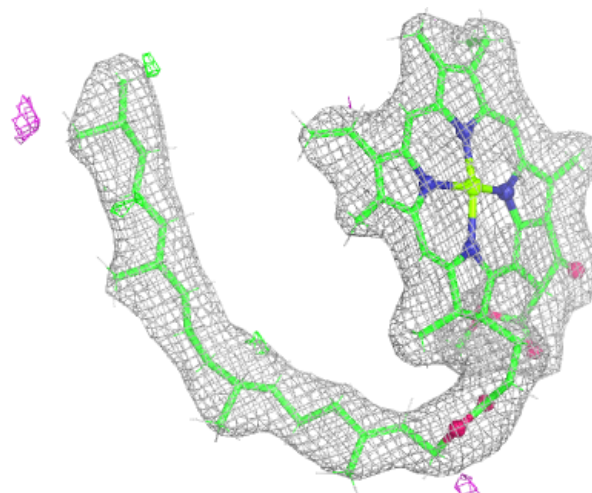
Electron density around CLA C 505:

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



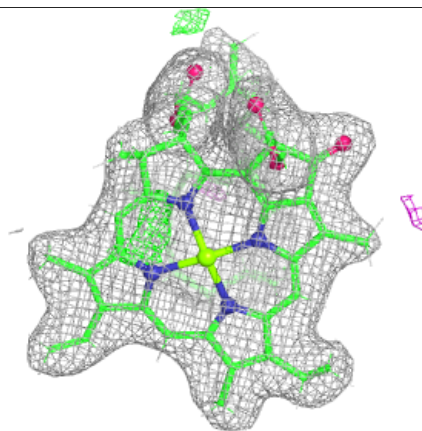
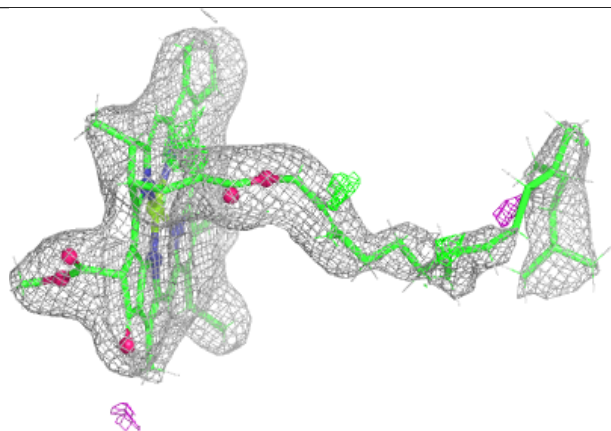
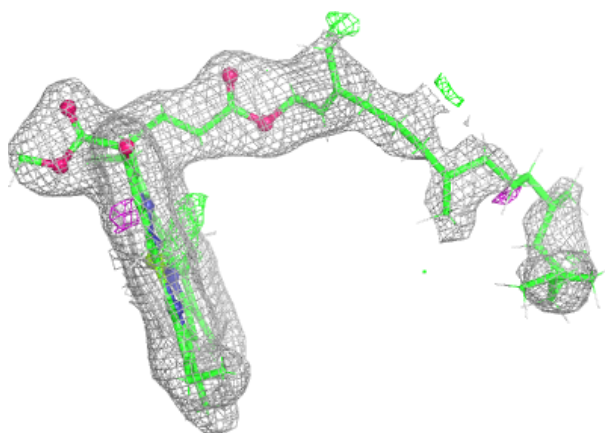
Electron density around CLA c 507:

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

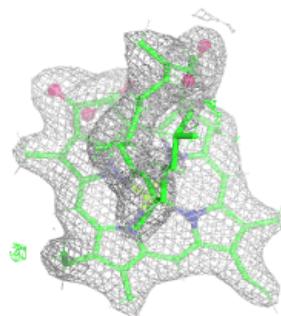
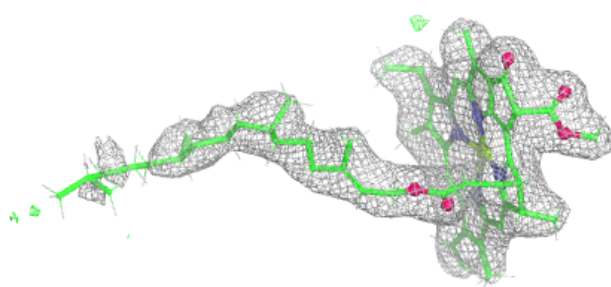
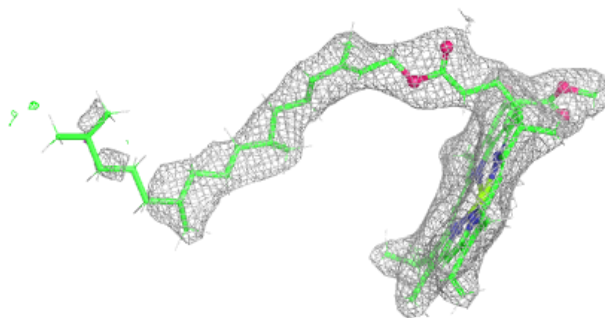


Electron density around CLA C 506:

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

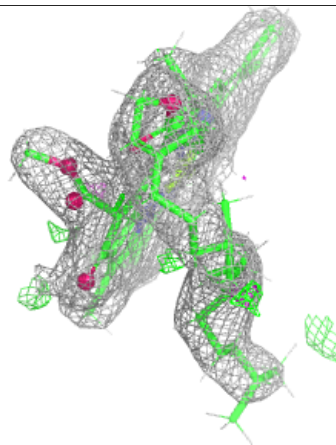
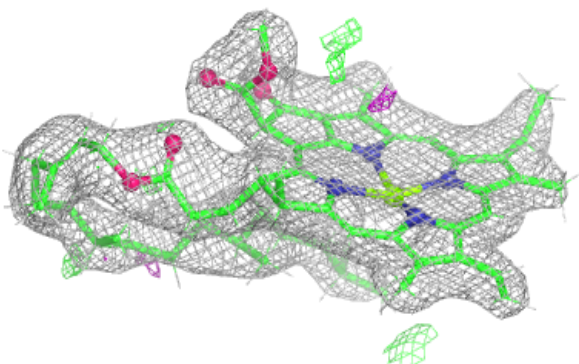
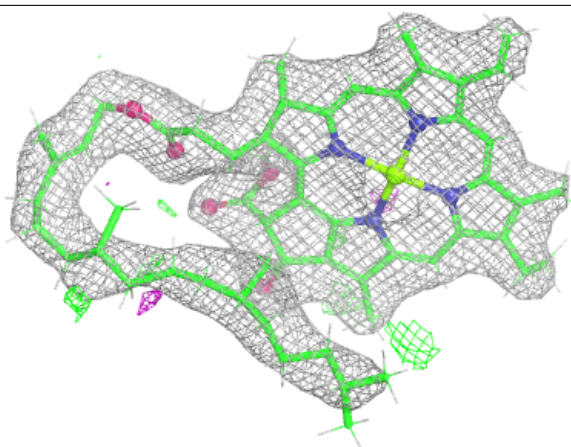
**Electron density around CLA C 508:**

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



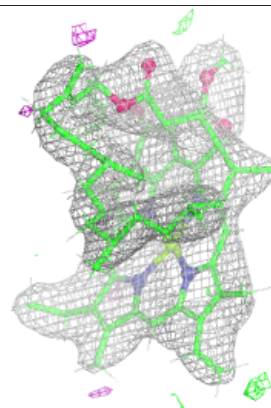
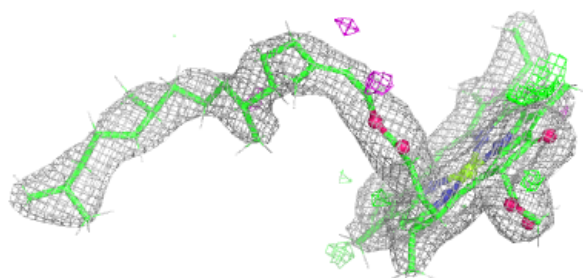
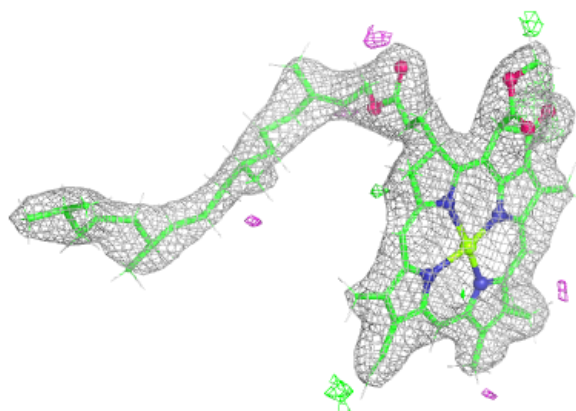
Electron density around CLA C 509:

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

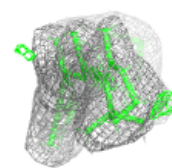
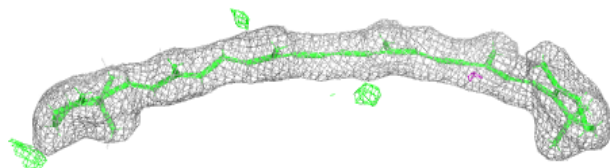
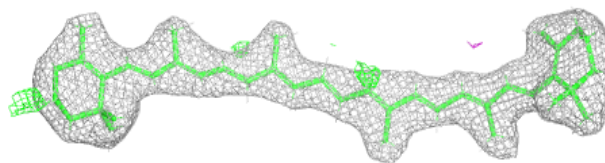


Electron density around CLA c 511:

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

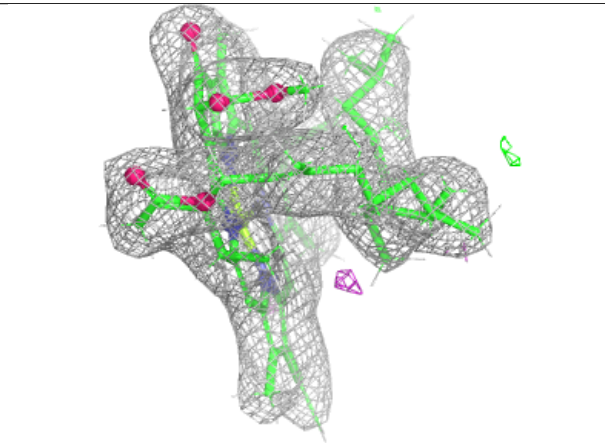
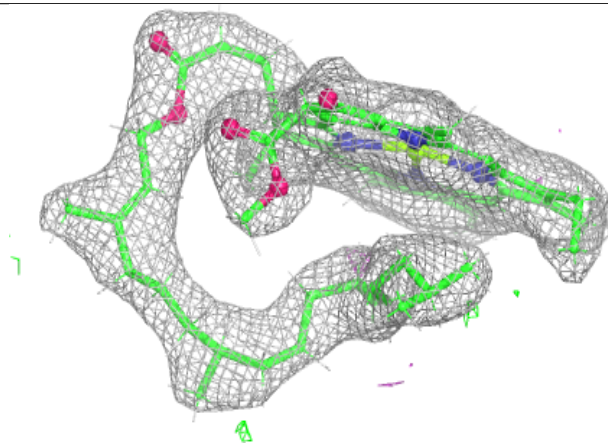
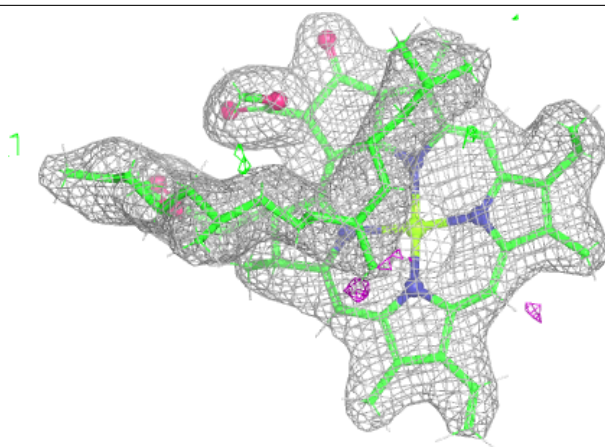
**Electron density around BCR t 101:**

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

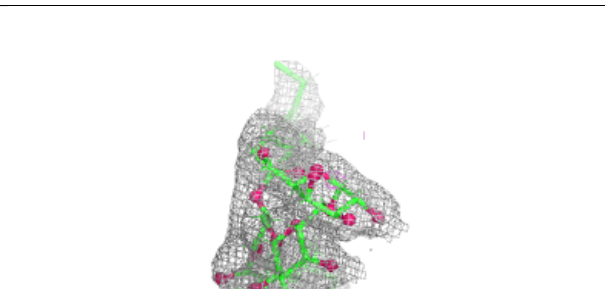
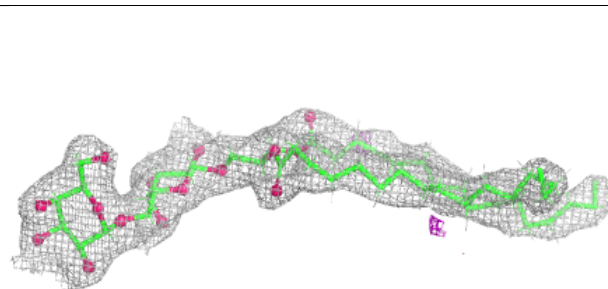
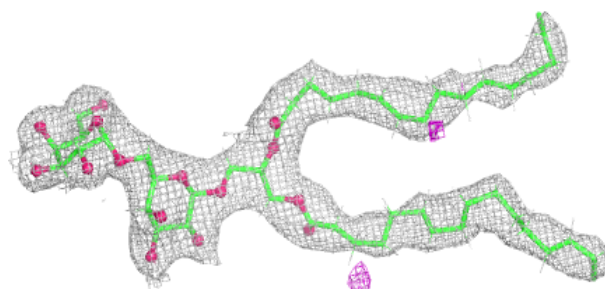


Electron density around CLA C 510:

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

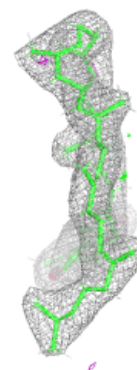
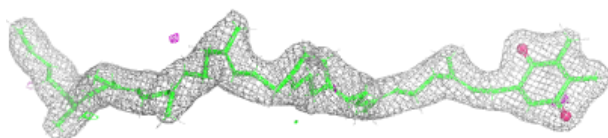
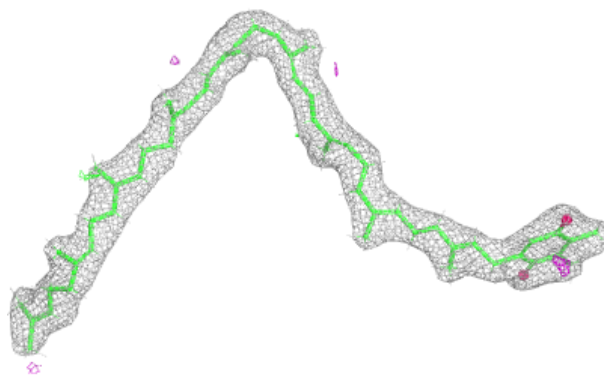
**Electron density around DGD C 518:**

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

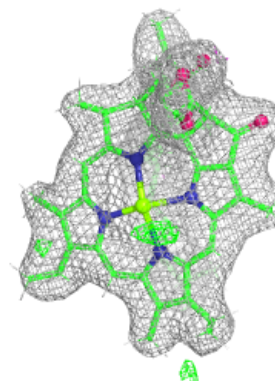
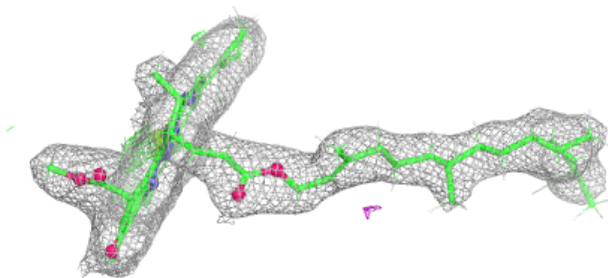
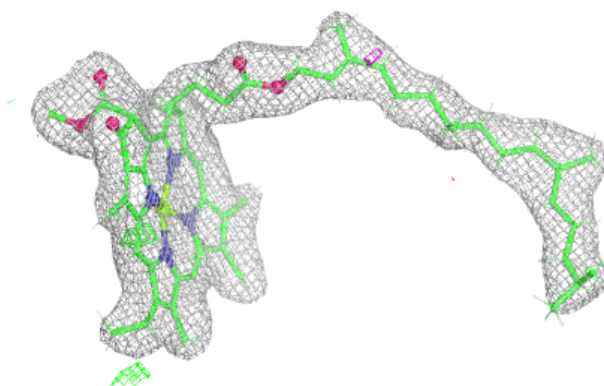


Electron density around PL9 D 406:

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

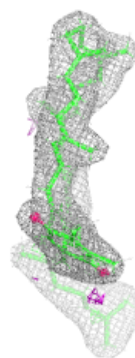
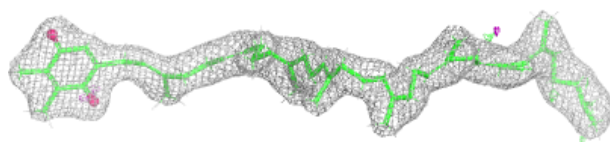
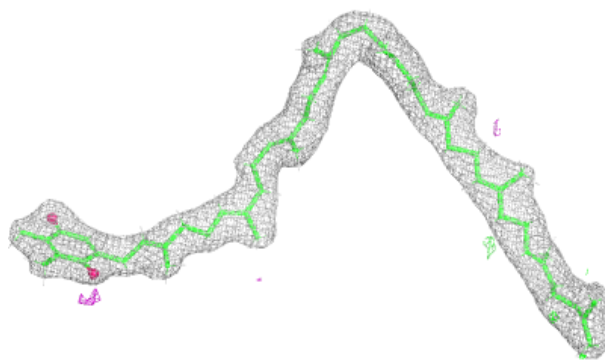
**Electron density around CLA B 609:**

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

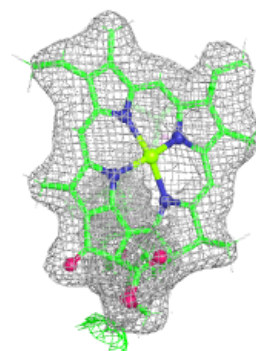
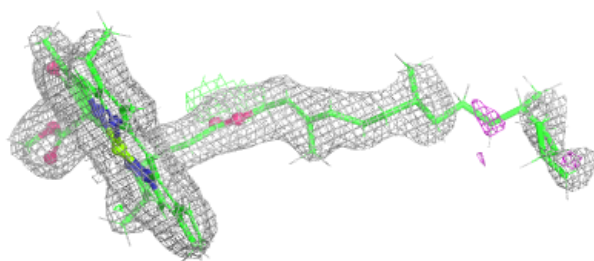
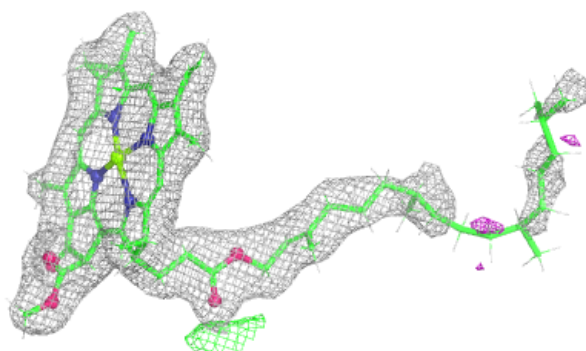


Electron density around PL9 d 407:

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

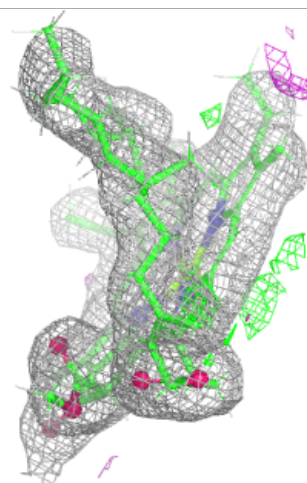
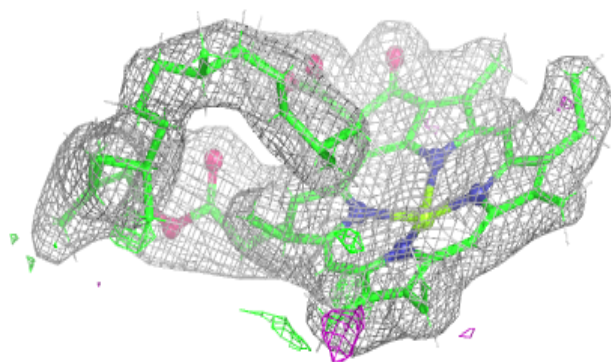
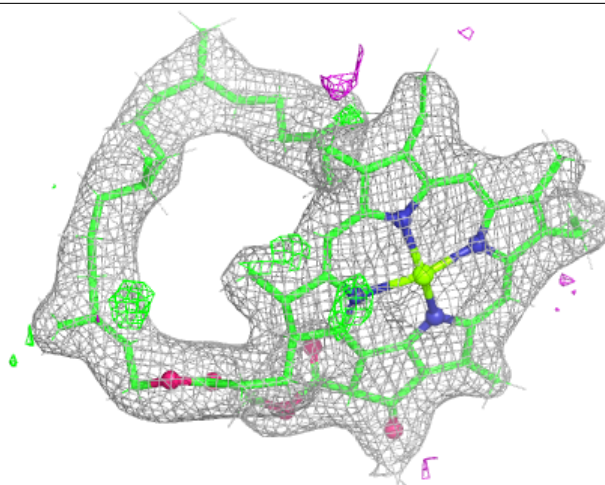
**Electron density around CLA d 405:**

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



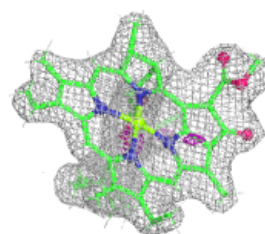
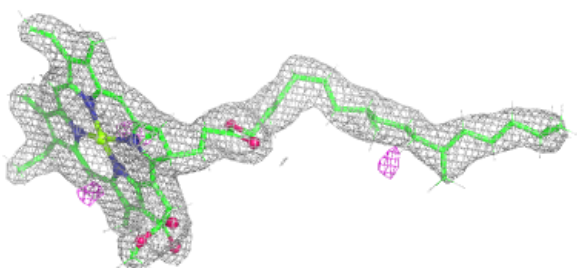
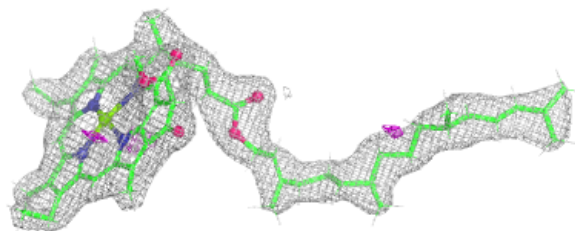
Electron density around CLA B 615:

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

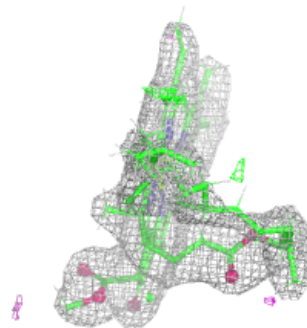
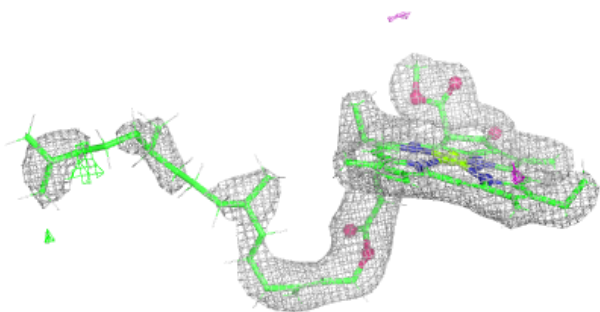
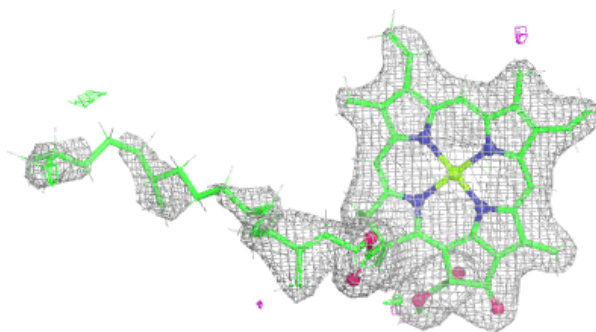


Electron density around CLA C 502:

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

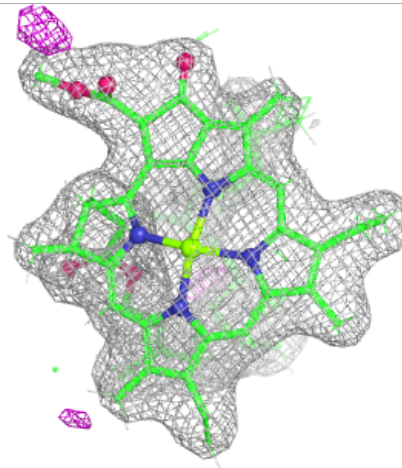
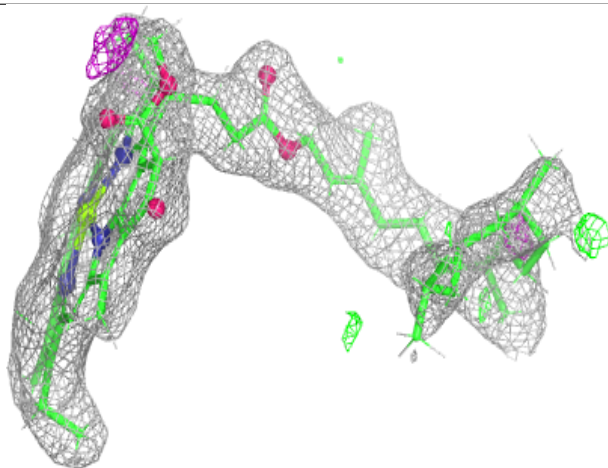
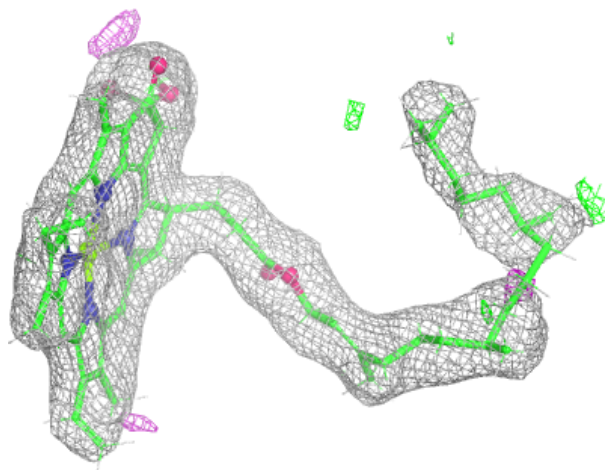
**Electron density around CLA a 403:**

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



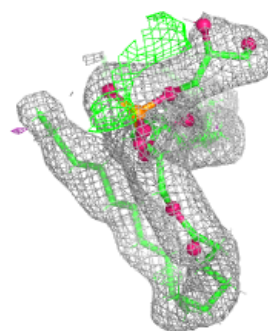
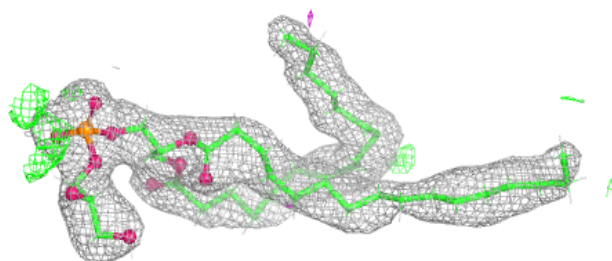
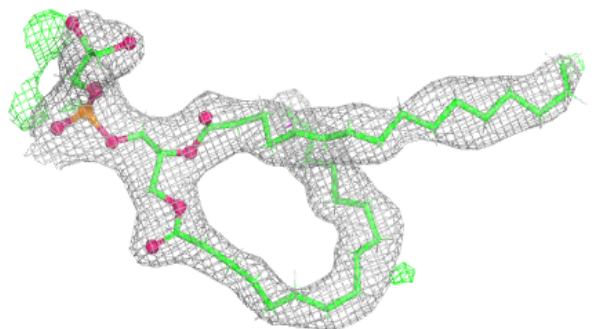
Electron density around CLA B 606:

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

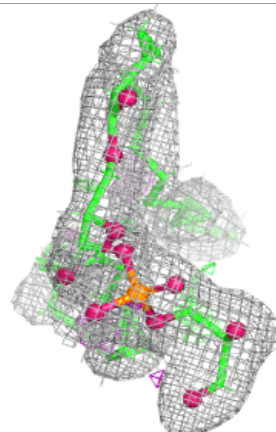
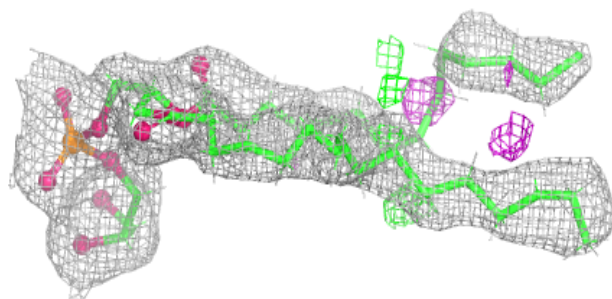
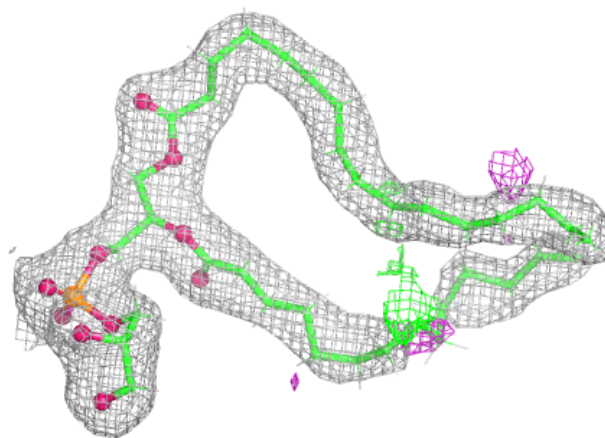


Electron density around LHG B 622:

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

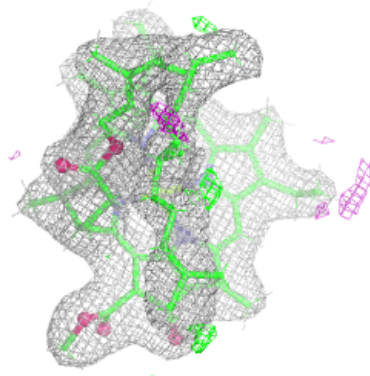
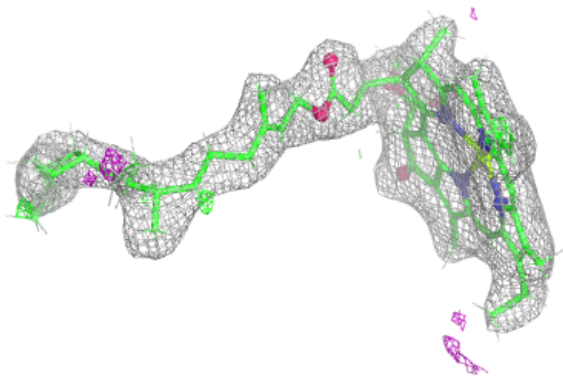
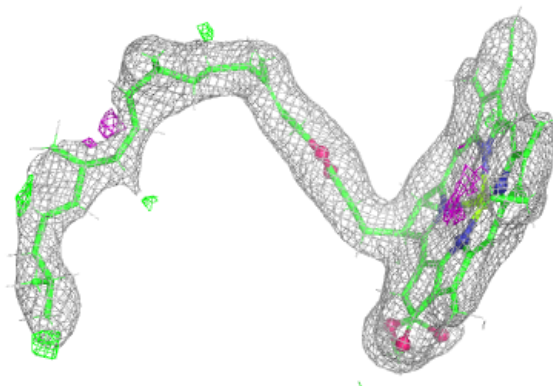
**Electron density around LHG D 409:**

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



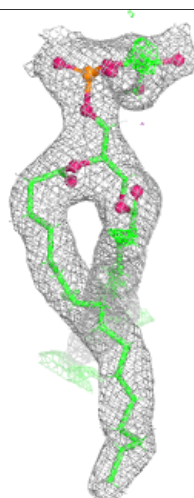
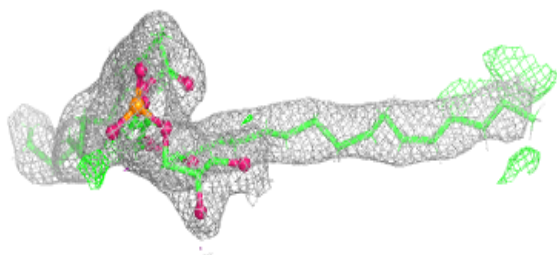
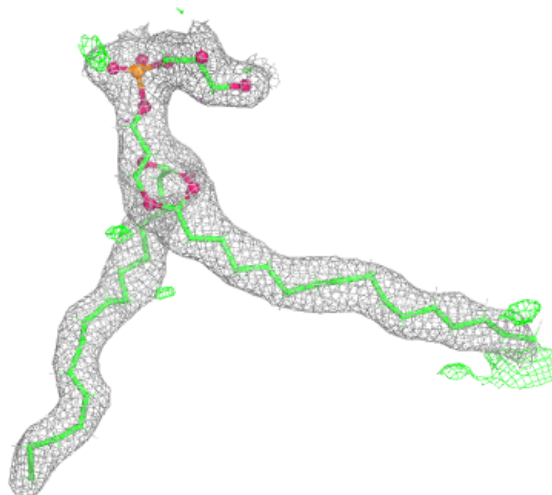
Electron density around CLA b 606:

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



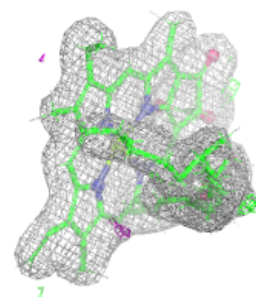
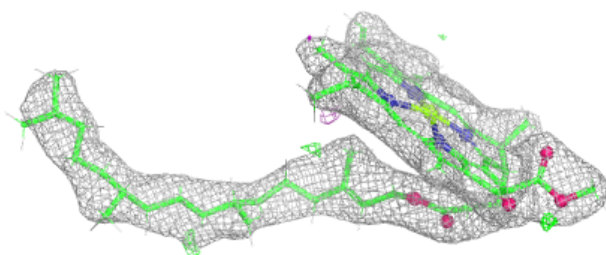
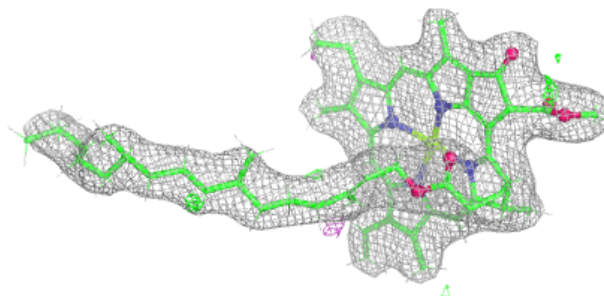
Electron density around LHG L 102:

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

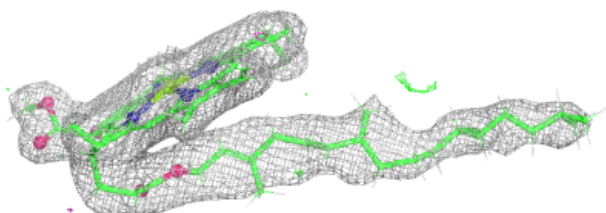
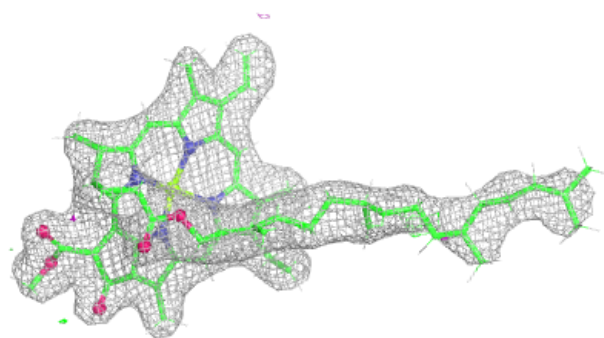


Electron density around CLA b 608:

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

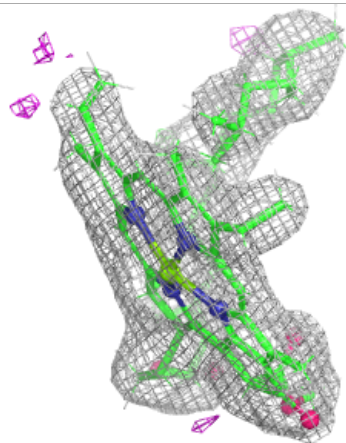
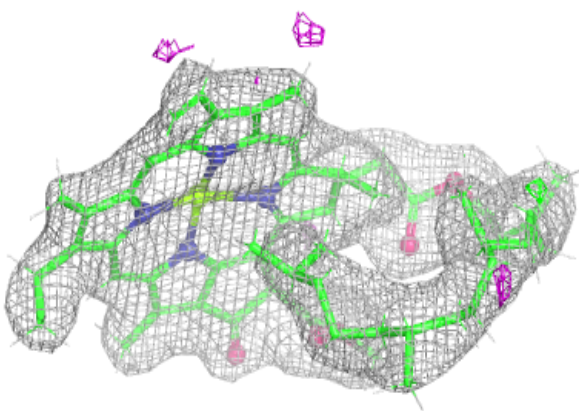
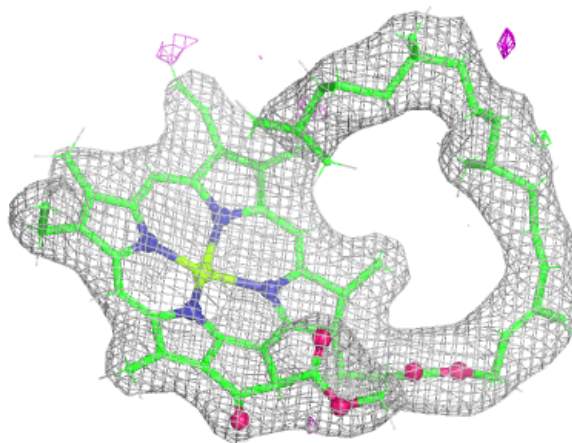
**Electron density around CLA b 614:**

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



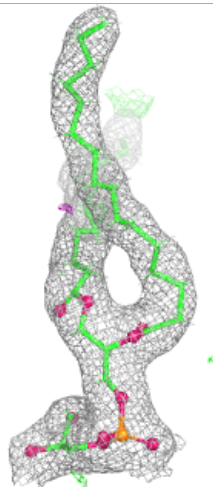
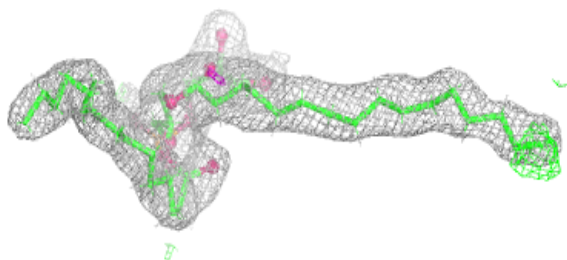
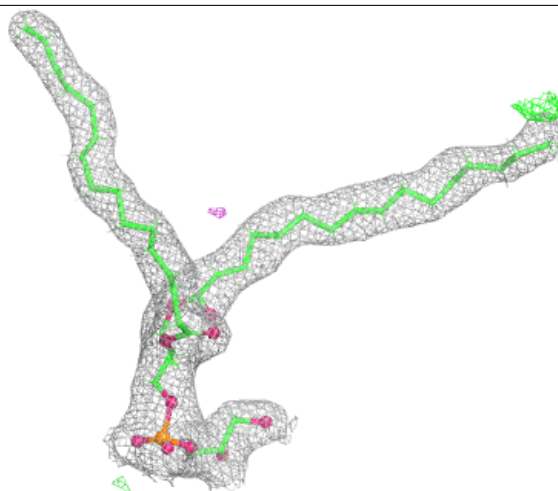
Electron density around CLA b 615:

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



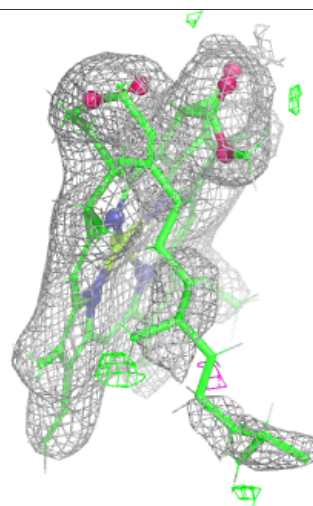
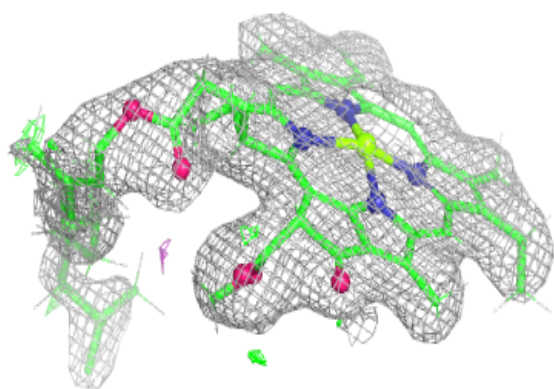
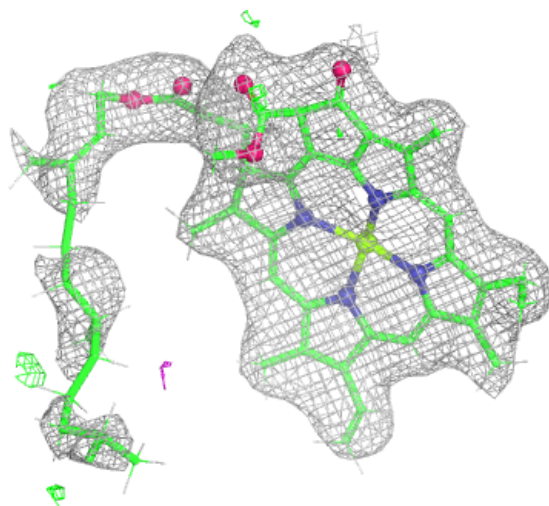
Electron density around LHG 1 101:

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



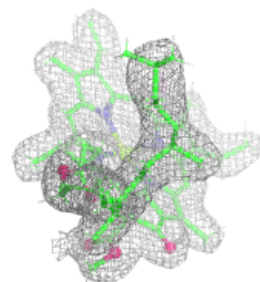
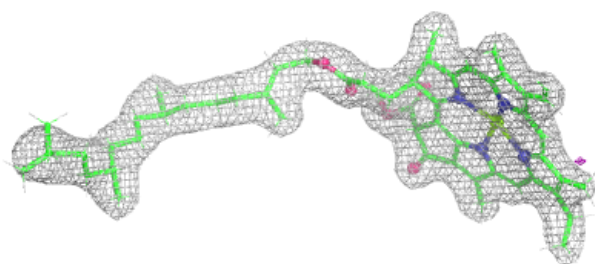
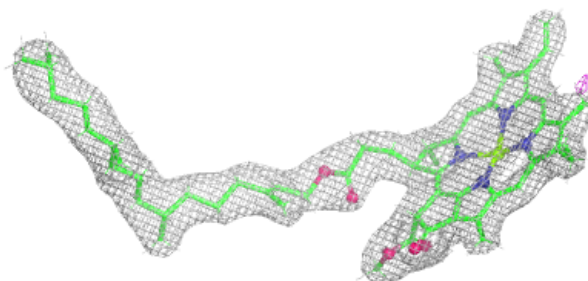
Electron density around CLA b 616:

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

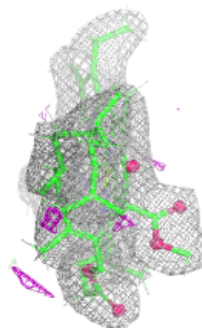
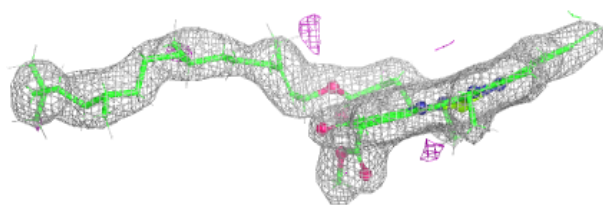
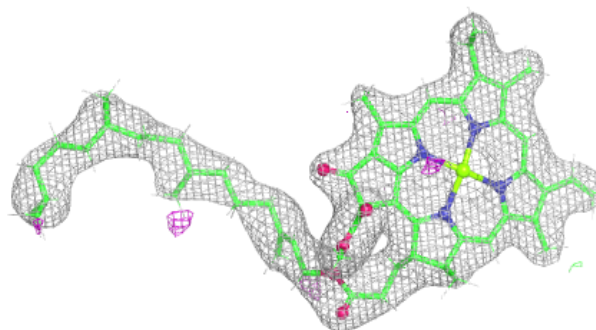


Electron density around CLA a 402:

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

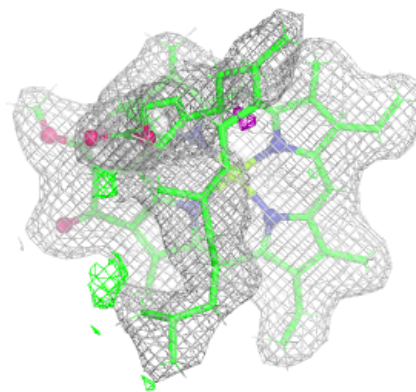
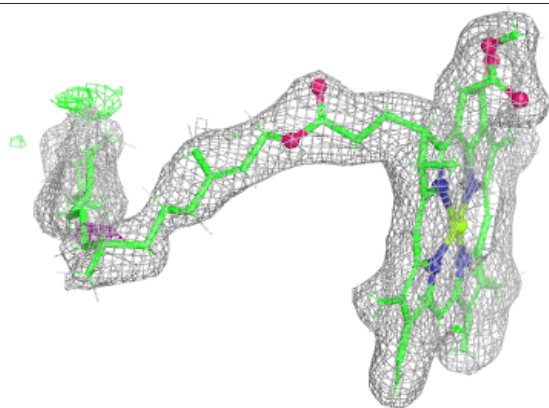
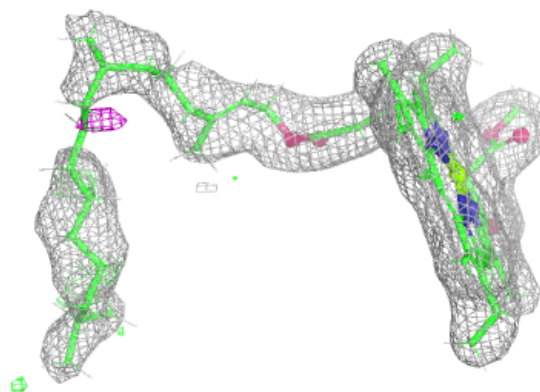
**Electron density around CLA B 602:**

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

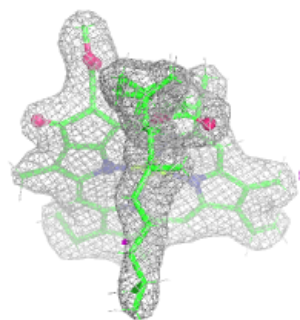
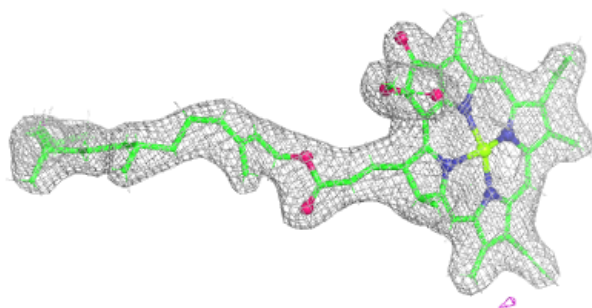
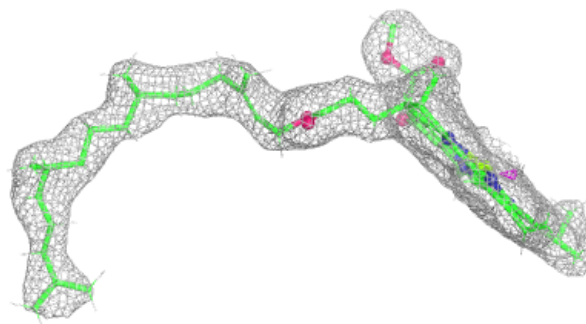


Electron density around CLA a 404:

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

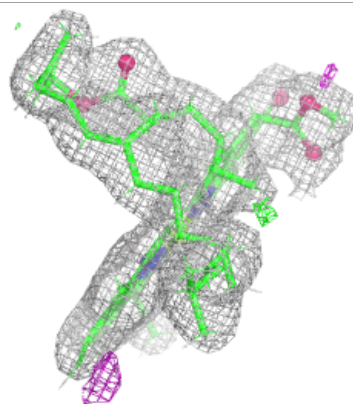
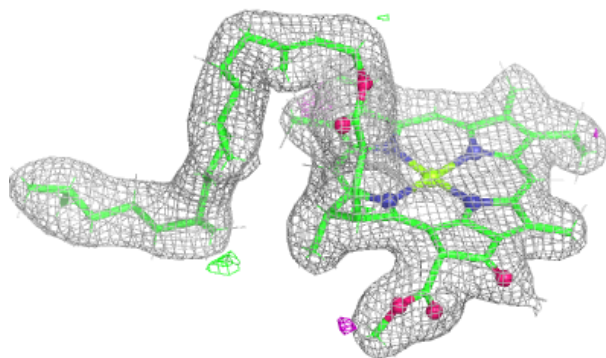
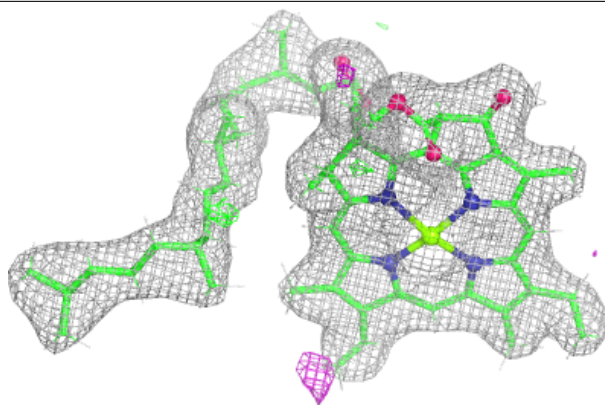
**Electron density around CLA d 403:**

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



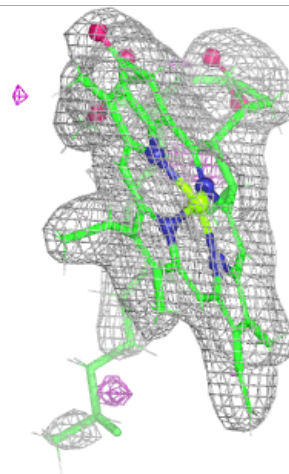
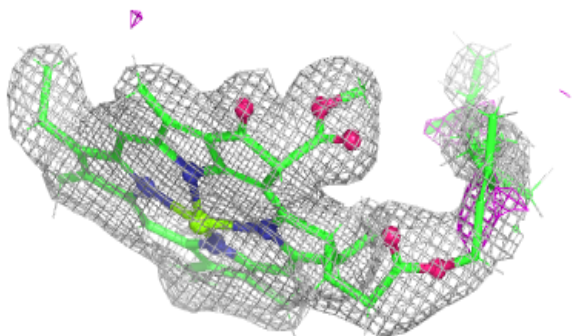
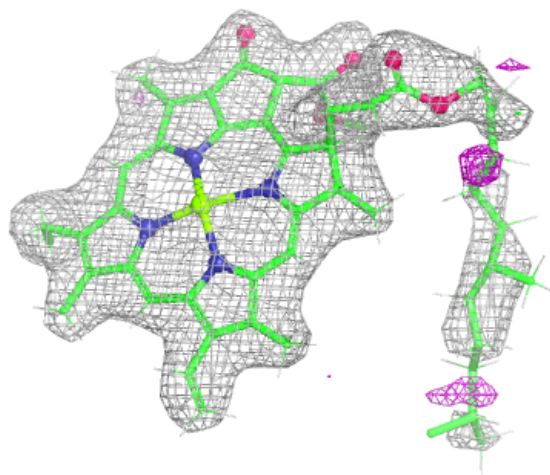
Electron density around CLA d 404:

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



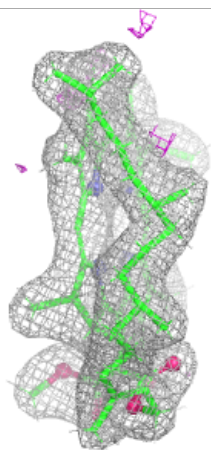
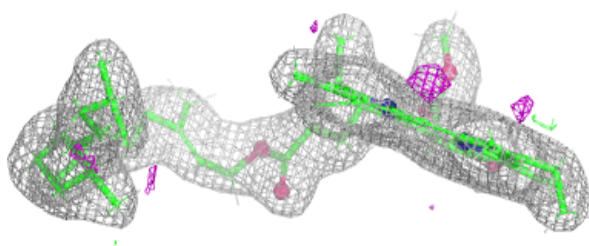
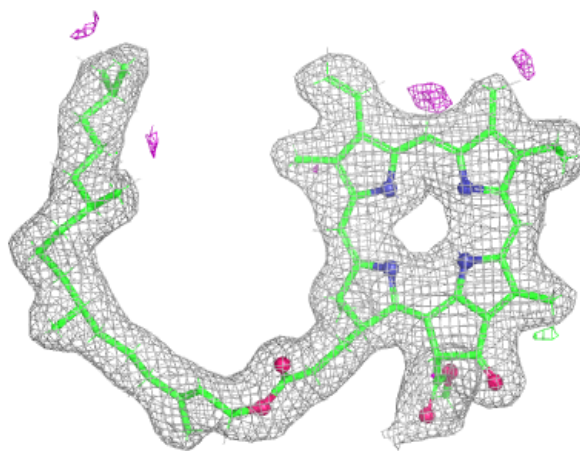
Electron density around CLA B 616:

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



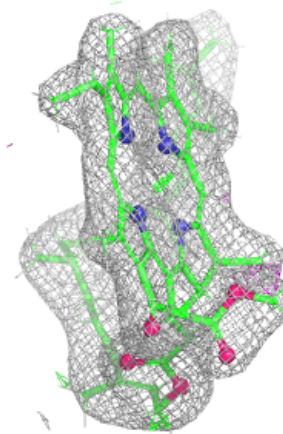
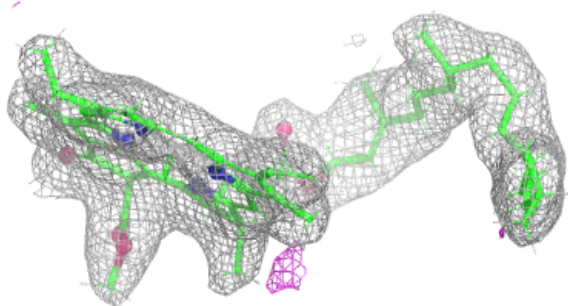
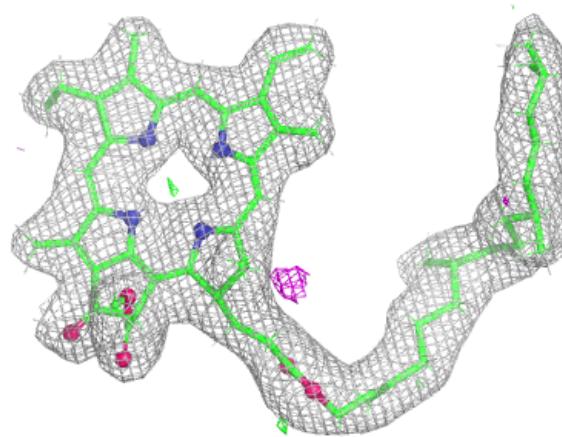
Electron density around PHO A 404:

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



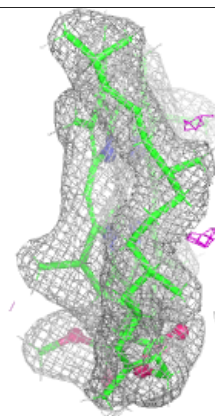
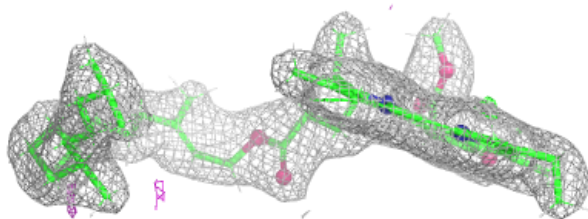
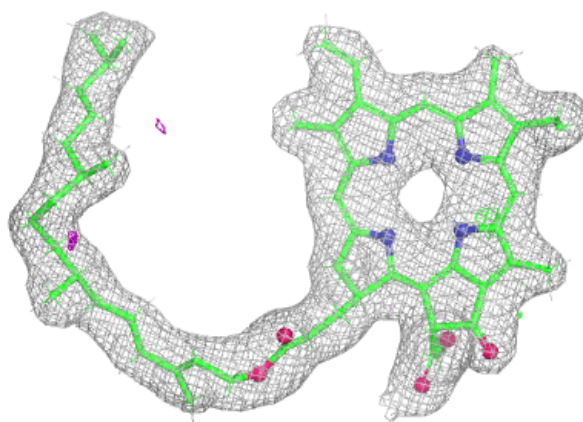
Electron density around PHO D 401:

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



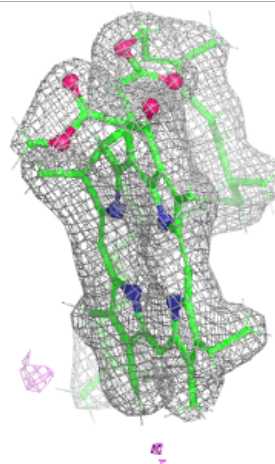
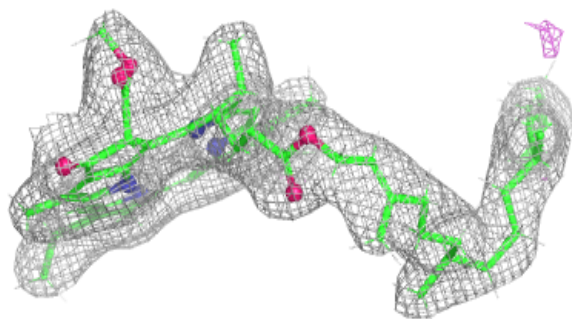
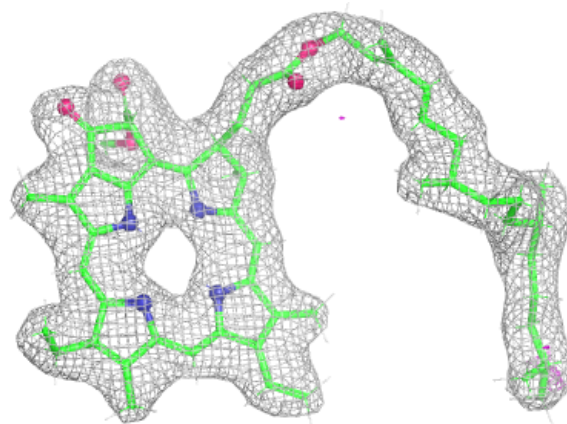
Electron density around PHO d 401:

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



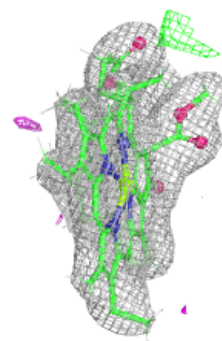
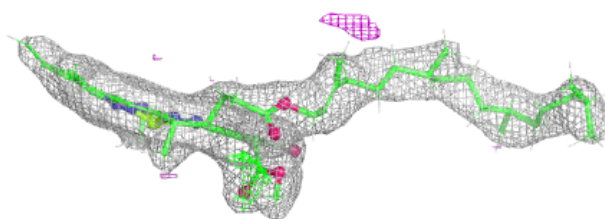
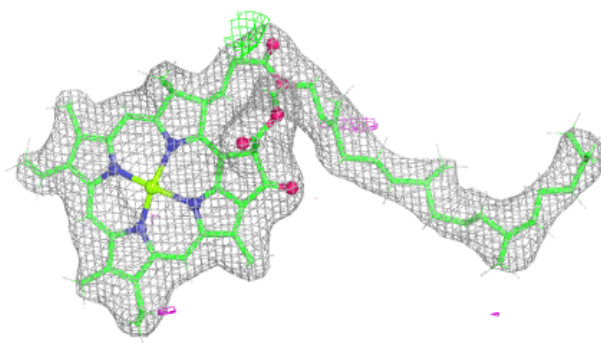
Electron density around PHO d 402:

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

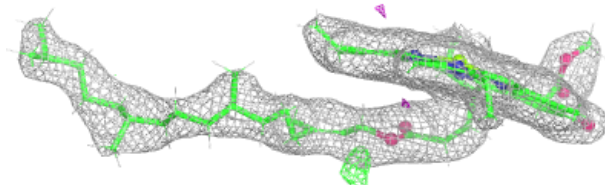
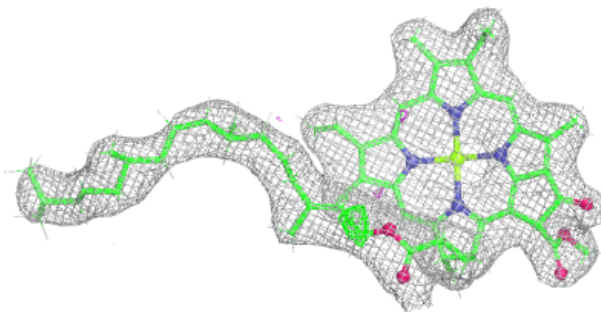


Electron density around CLA b 602:

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

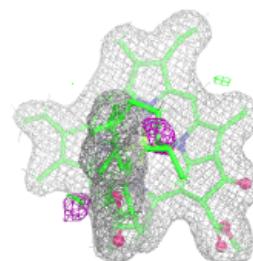
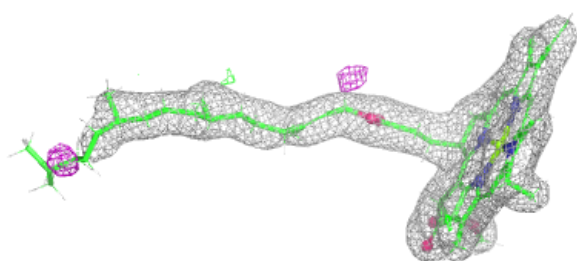
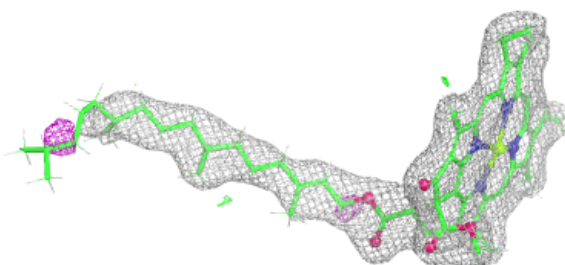
**Electron density around CLA b 603:**

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

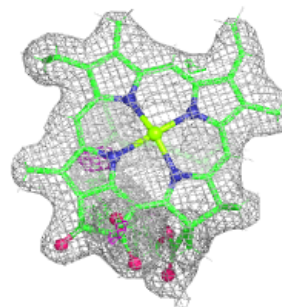
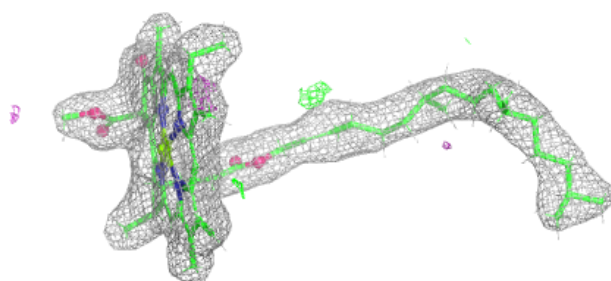
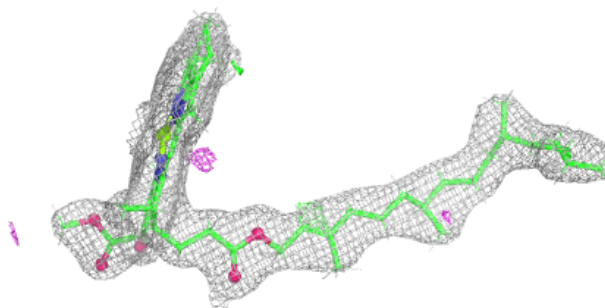


Electron density around CLA b 604:

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

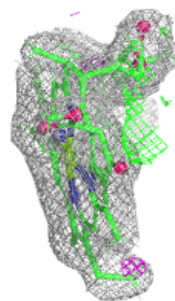
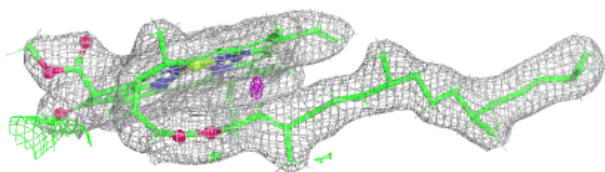
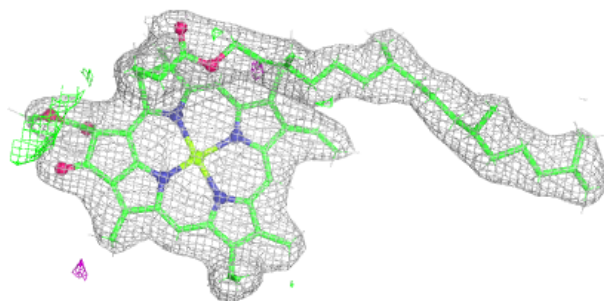
**Electron density around CLA b 605:**

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

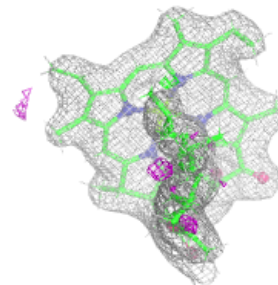
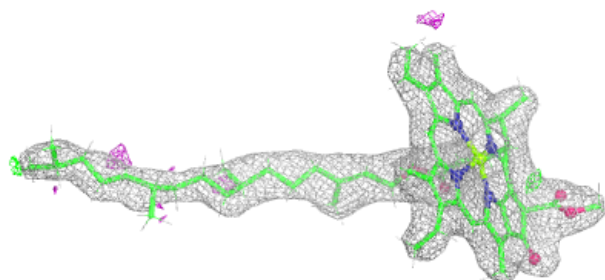
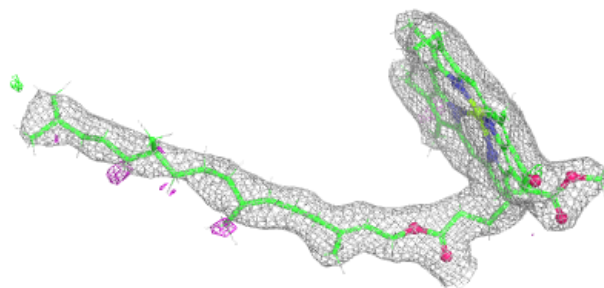


Electron density around CLA C 501:

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

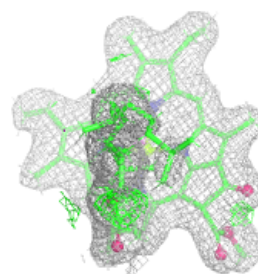
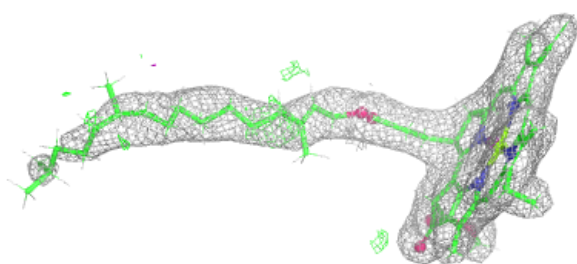
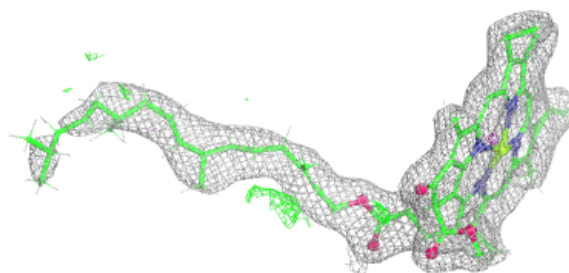
**Electron density around CLA b 607:**

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

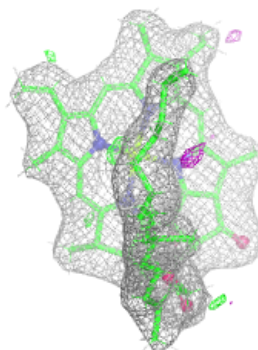
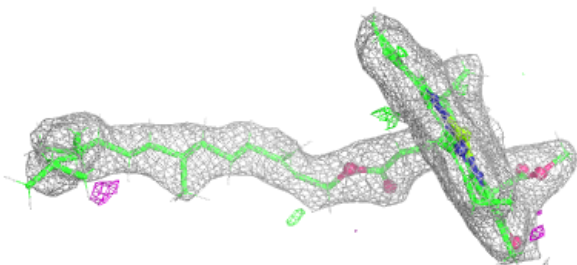
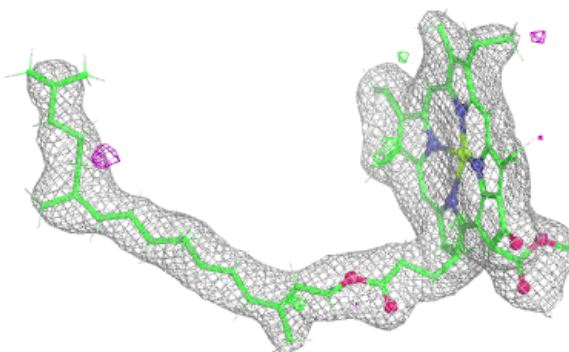


Electron density around CLA B 604:

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

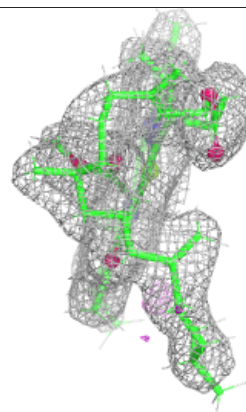
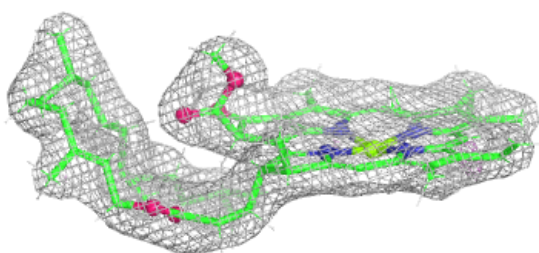
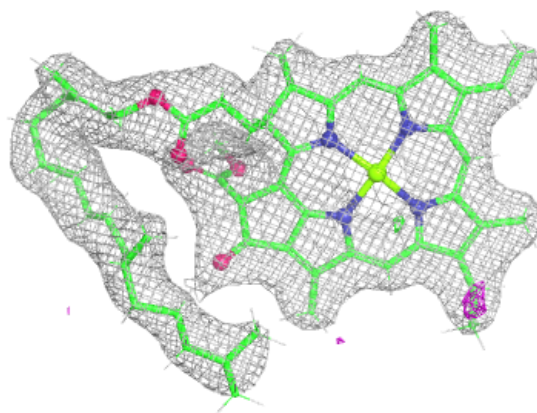
**Electron density around CLA b 609:**

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



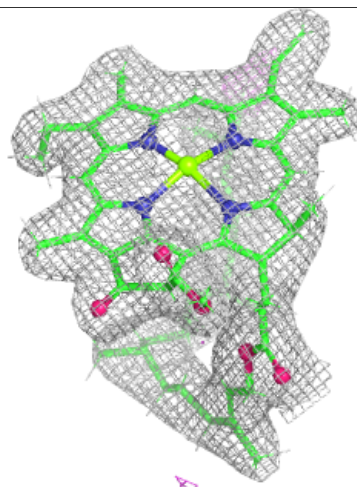
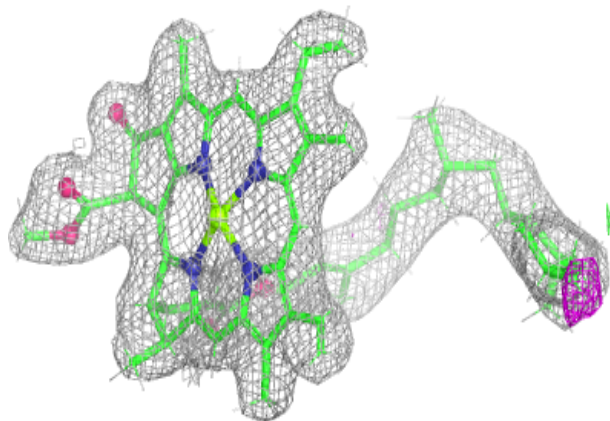
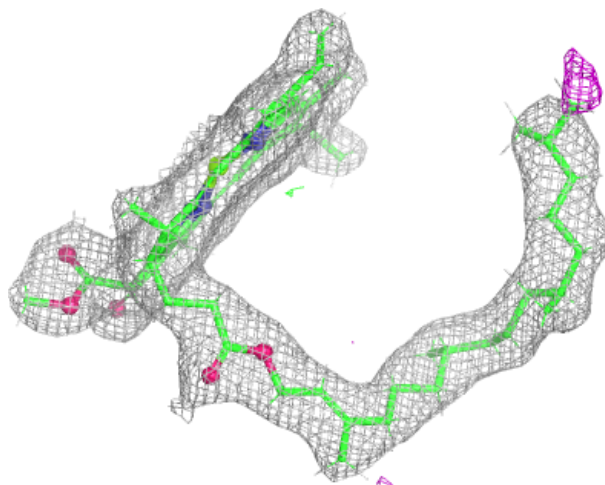
Electron density around CLA b 610:

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



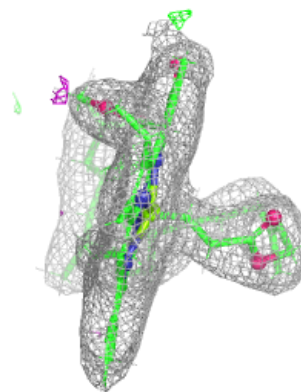
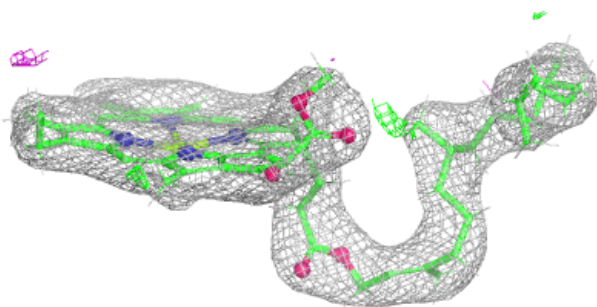
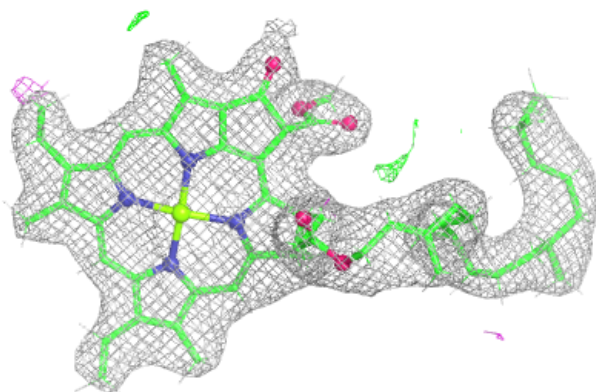
Electron density around CLA b 611:

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



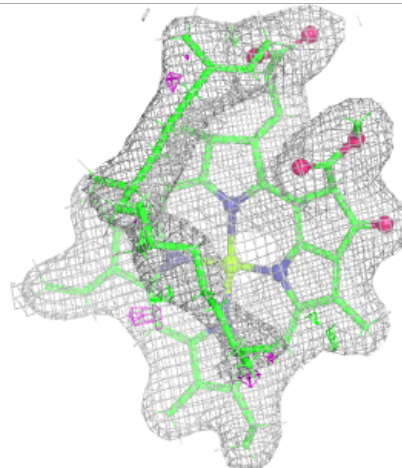
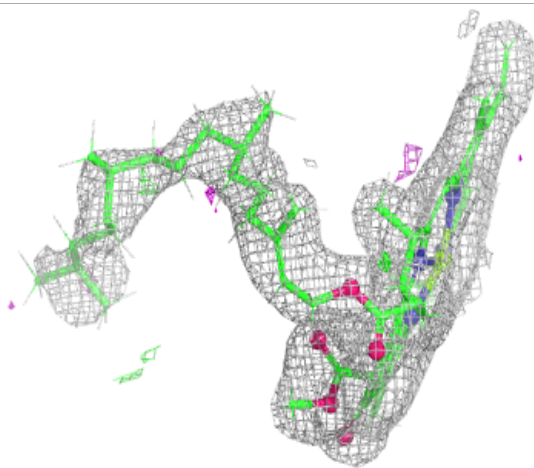
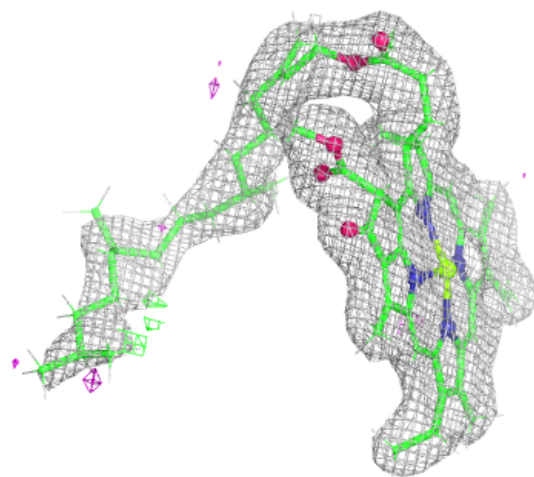
Electron density around CLA b 612:

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



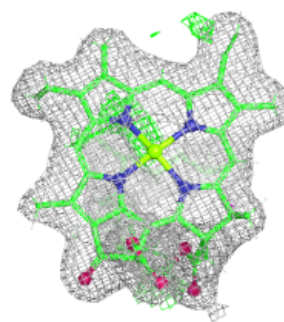
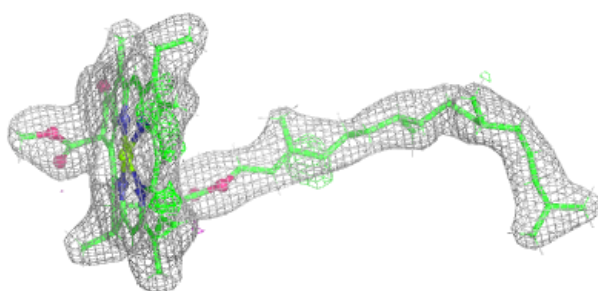
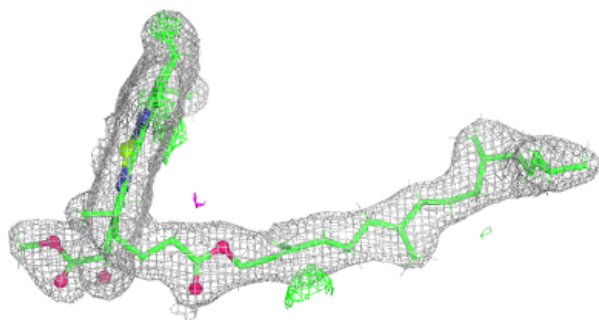
Electron density around CLA b 613:

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

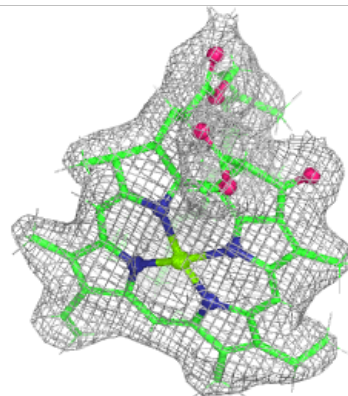
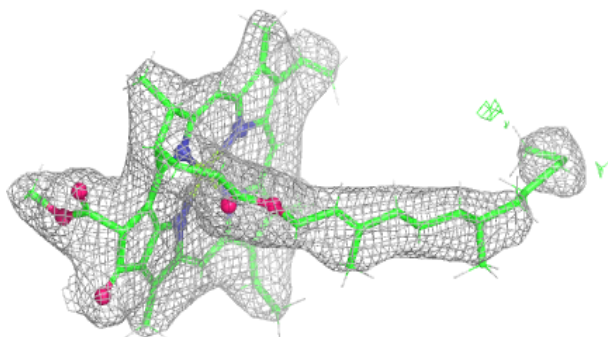
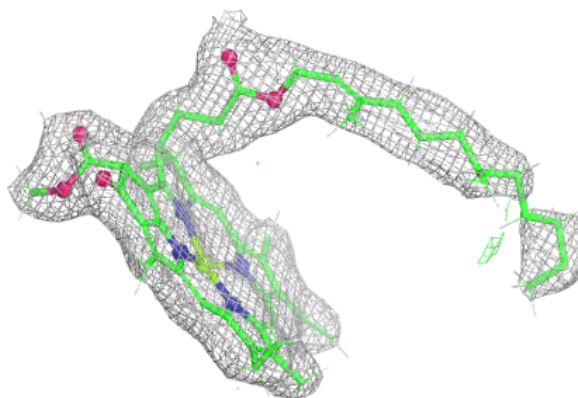


Electron density around CLA B 605:

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

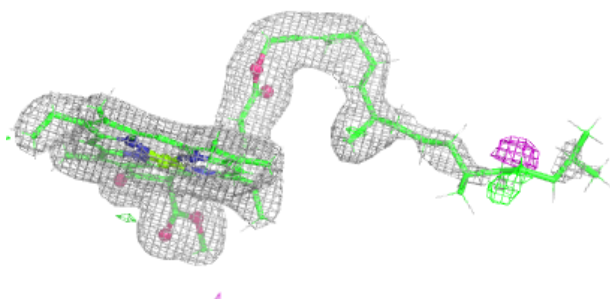
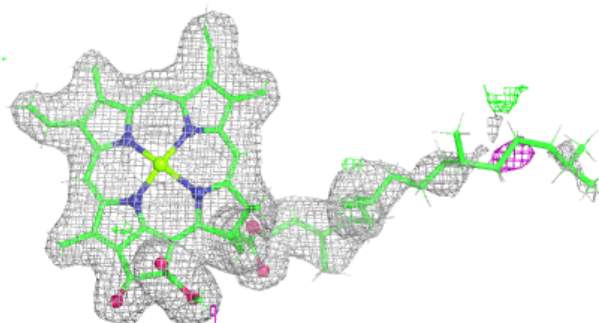
**Electron density around CLA C 504:**

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

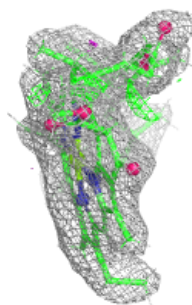
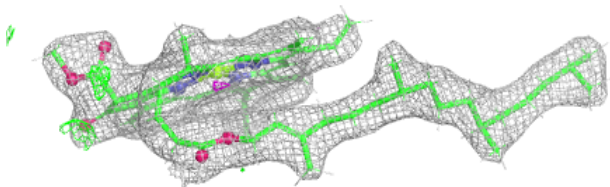
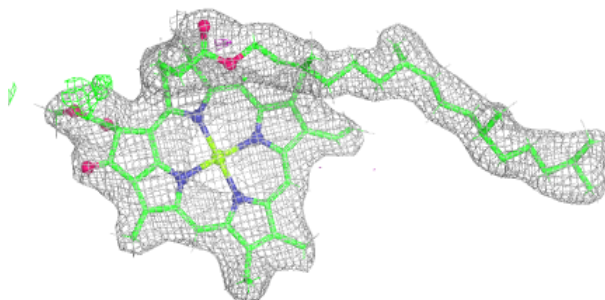


Electron density around CLA A 403:

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

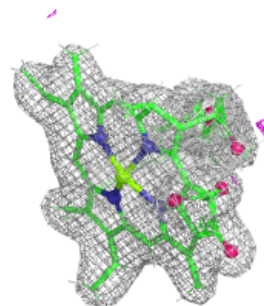
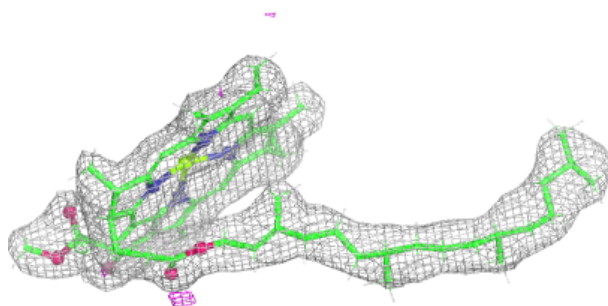
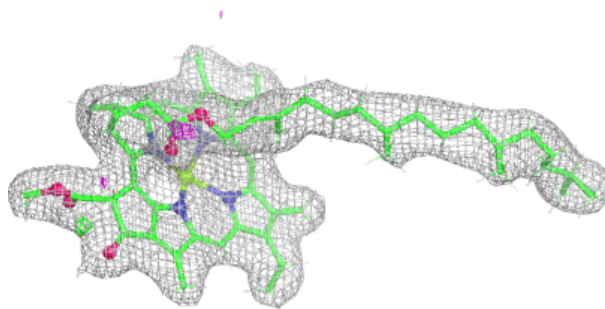
**Electron density around CLA c 501:**

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



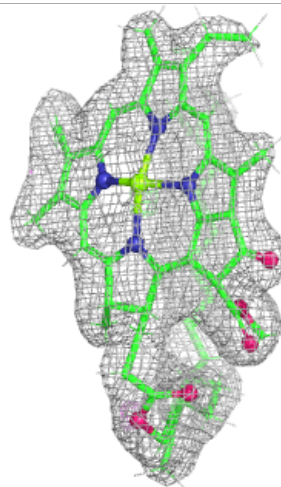
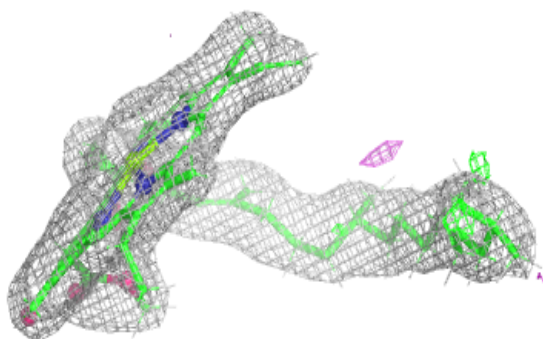
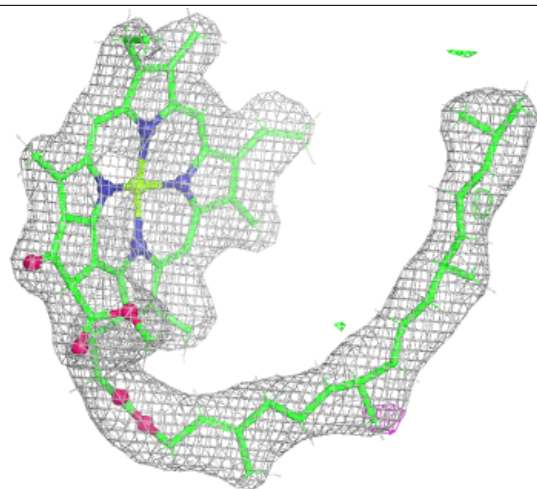
Electron density around CLA B 608:

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



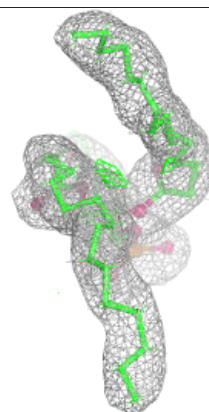
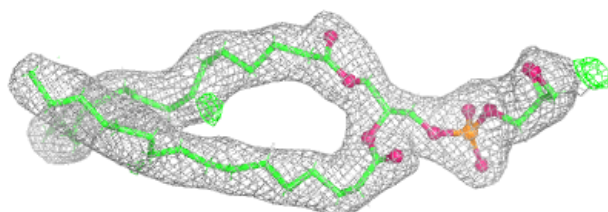
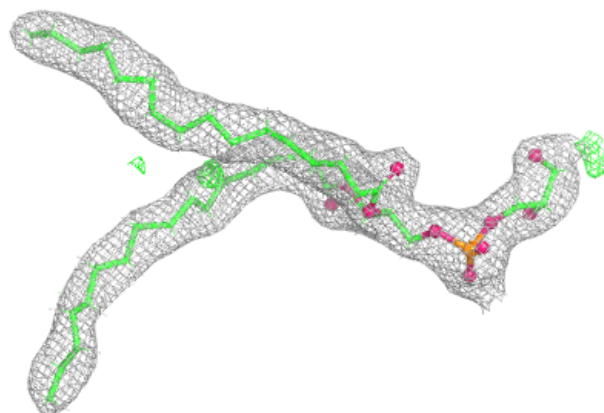
Electron density around CLA C 507:

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

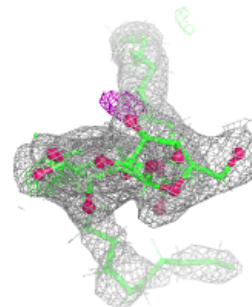
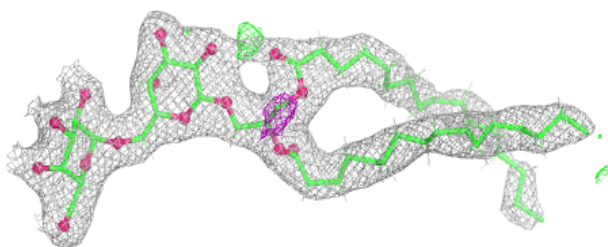
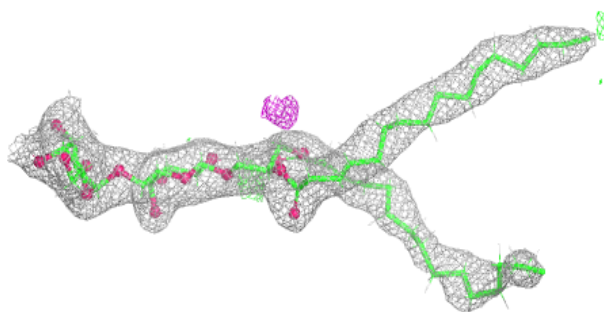


Electron density around LHG D 408:

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

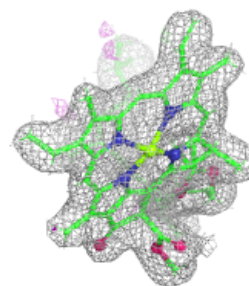
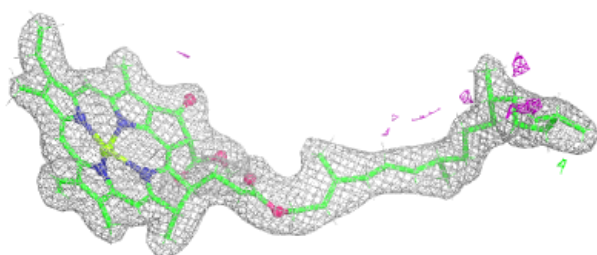
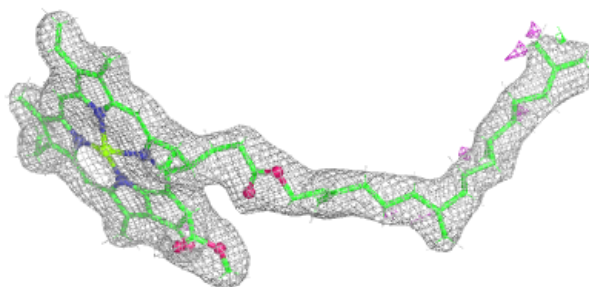
**Electron density around DGD c 517:**

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



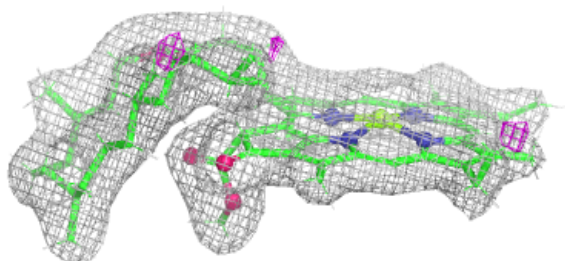
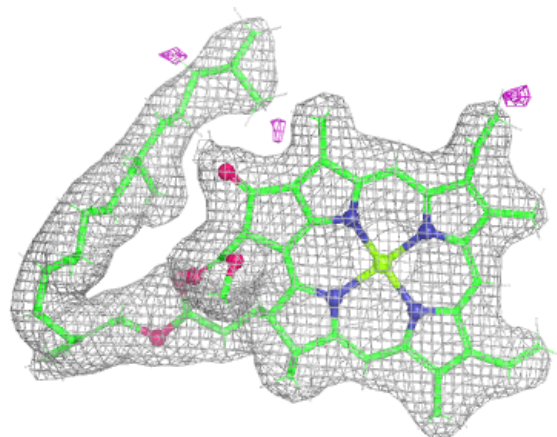
Electron density around CLA A 402:

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



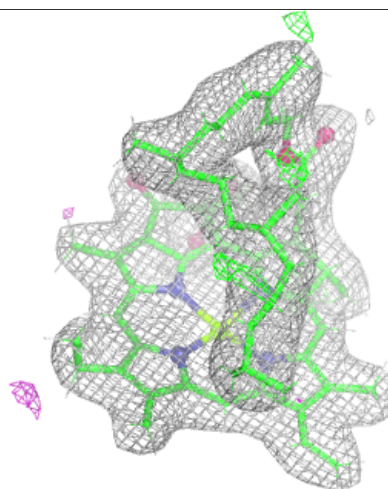
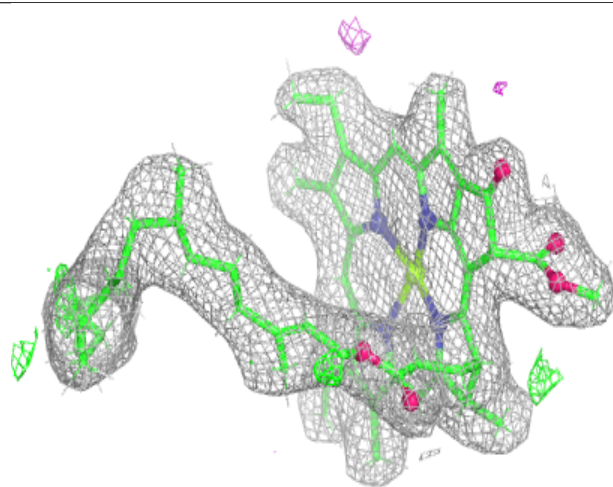
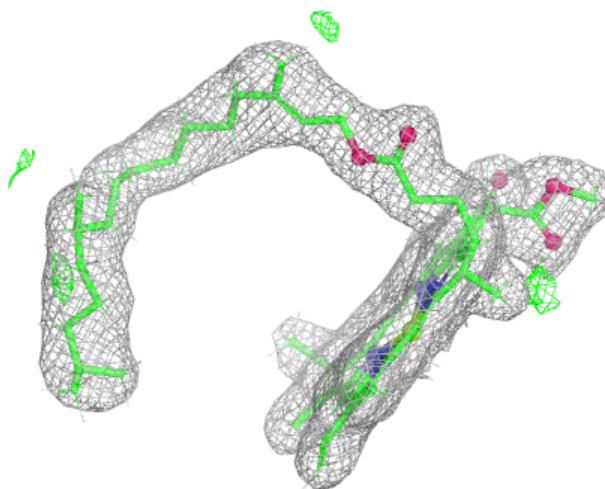
Electron density around CLA B 610:

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



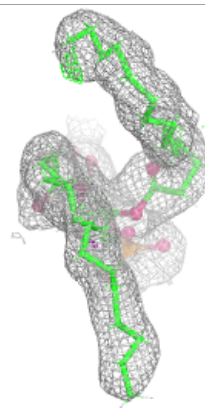
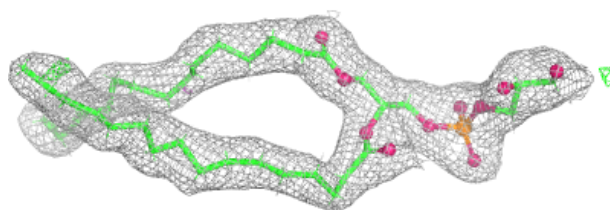
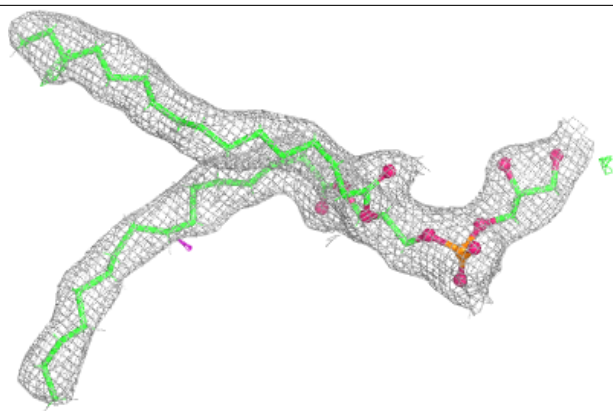
Electron density around CLA B 611:

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

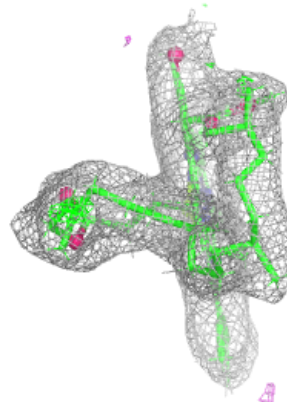
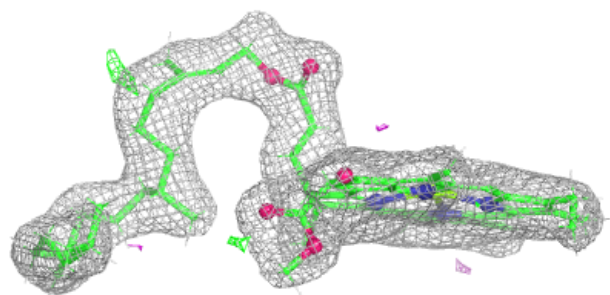
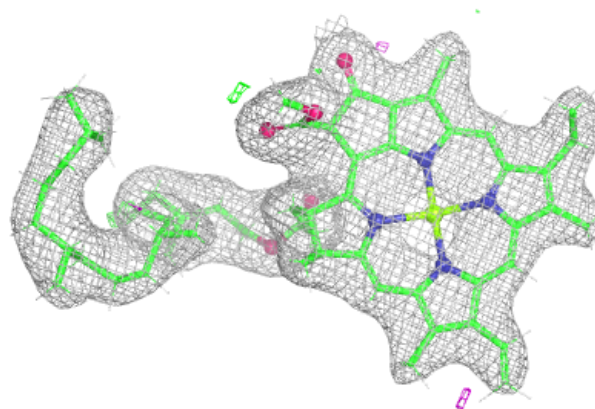


Electron density around LHG d 409:

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

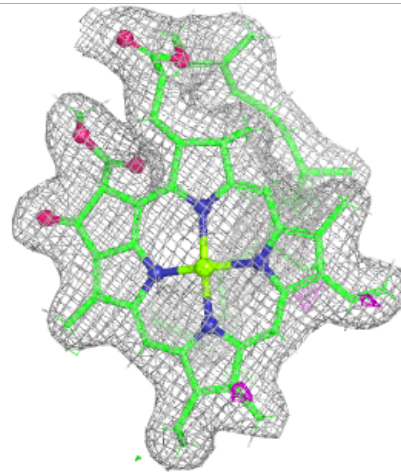
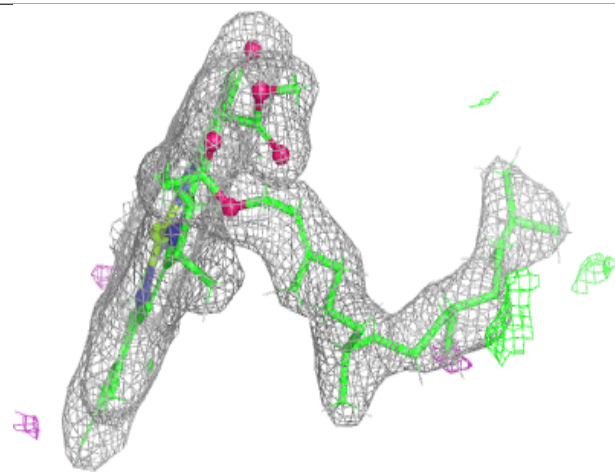
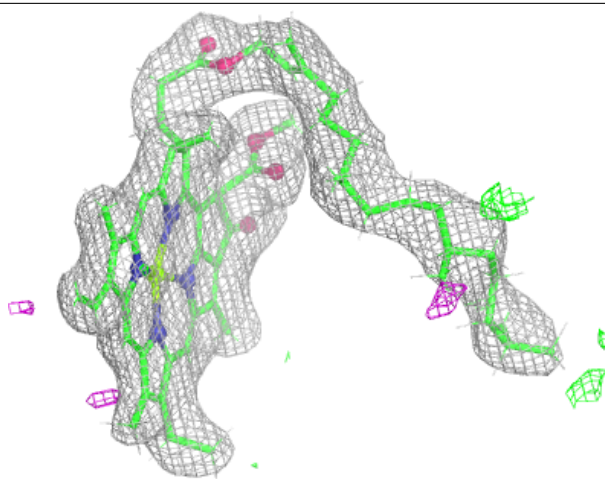
**Electron density around CLA B 612:**

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



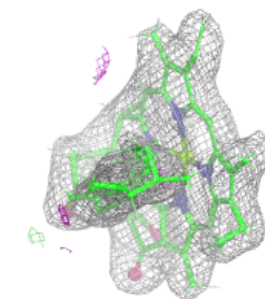
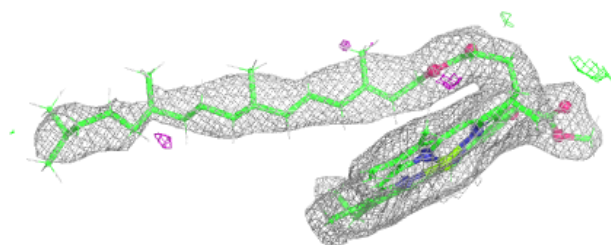
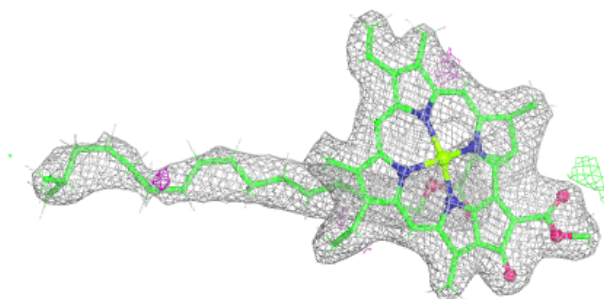
Electron density around CLA B 613:

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

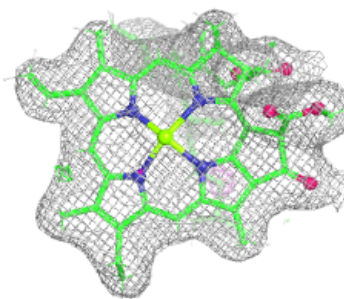
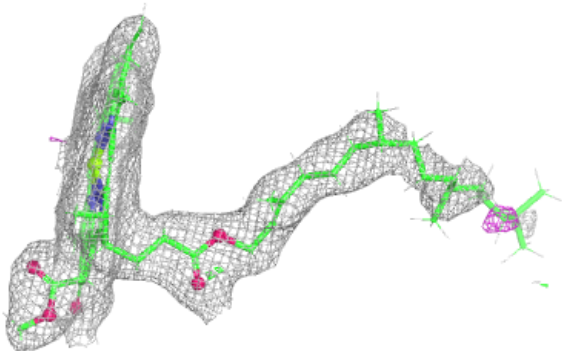
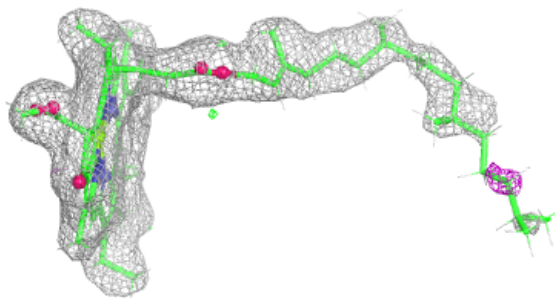


Electron density around CLA B 614:

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

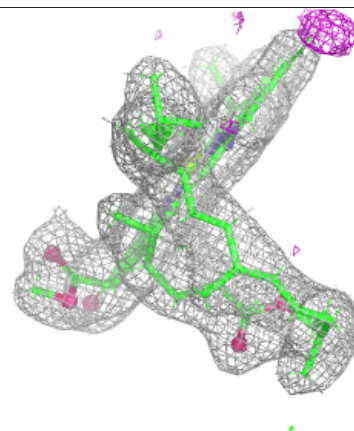
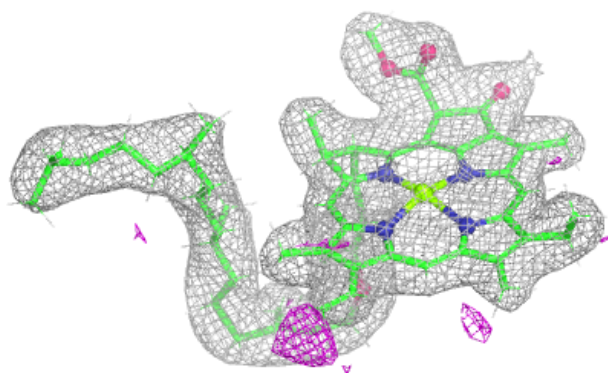
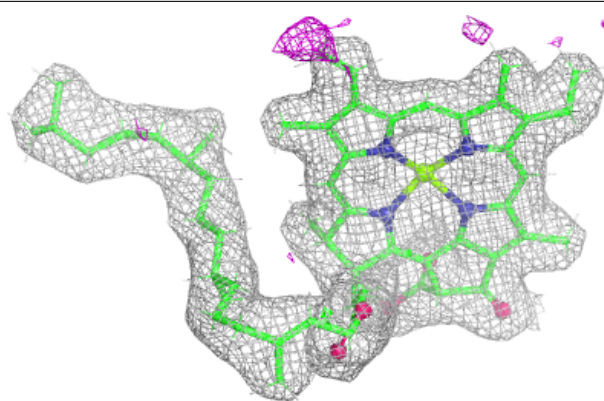
**Electron density around CLA D 404:**

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

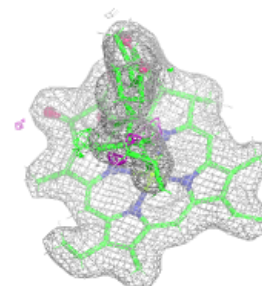
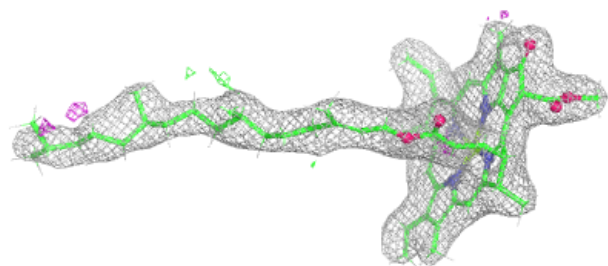
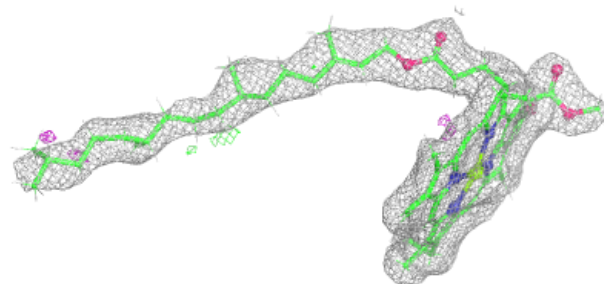


Electron density around CLA A 410:

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

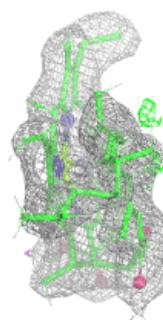
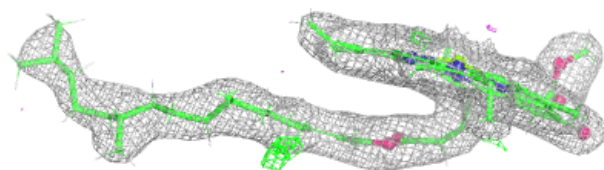
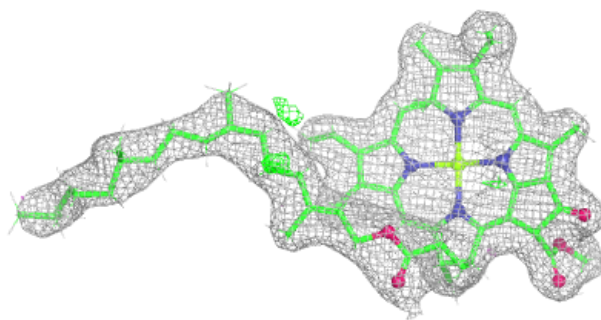
**Electron density around CLA B 607:**

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

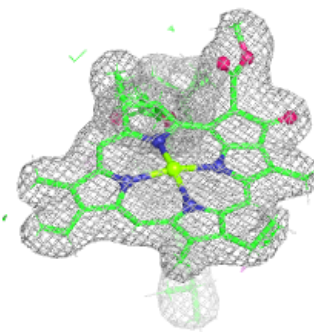
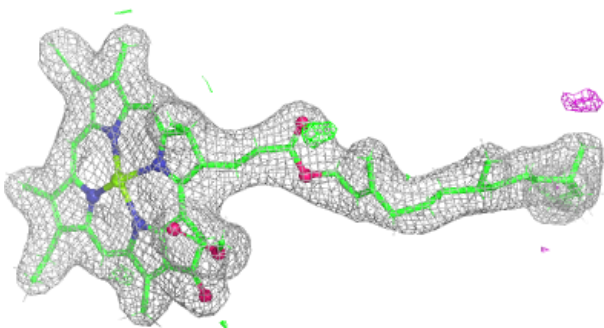
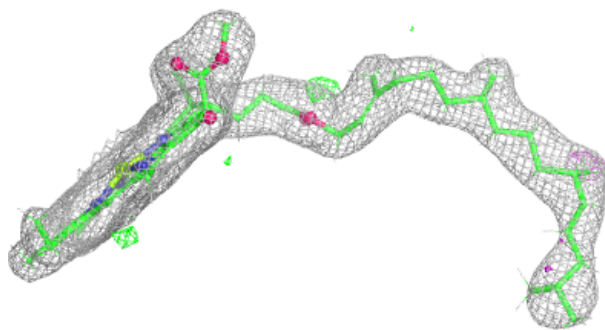


Electron density around CLA B 603:

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

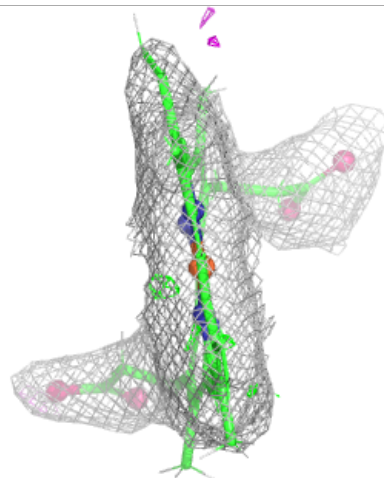
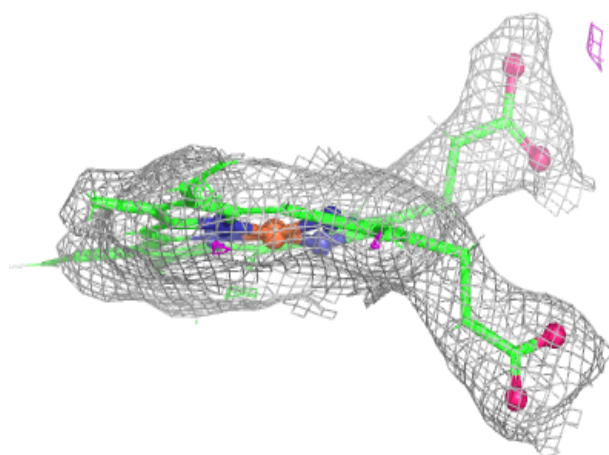
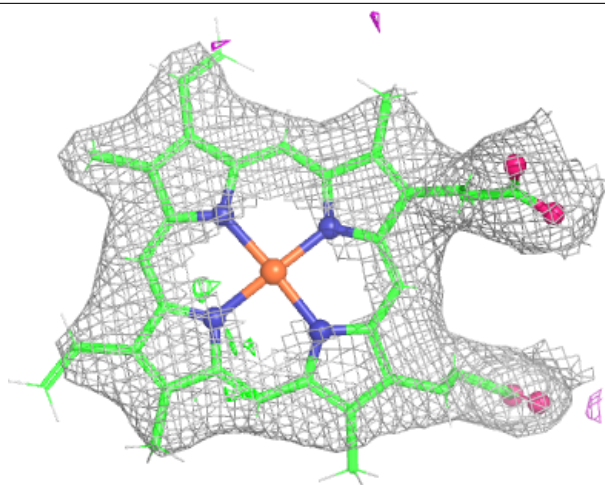
**Electron density around CLA D 403:**

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



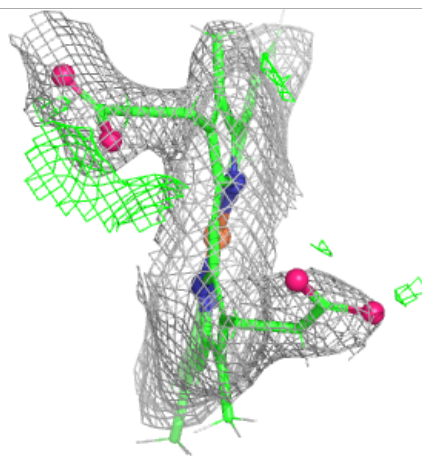
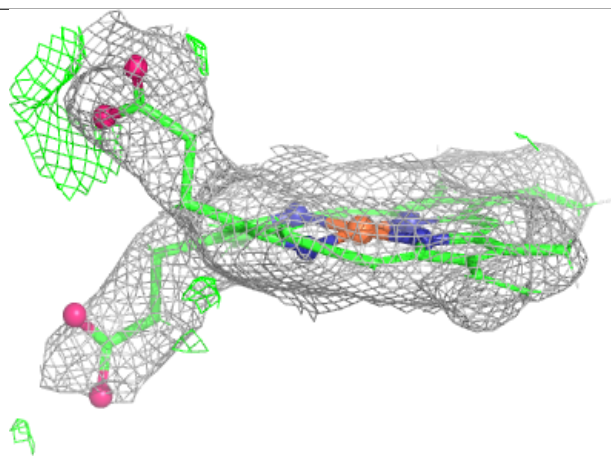
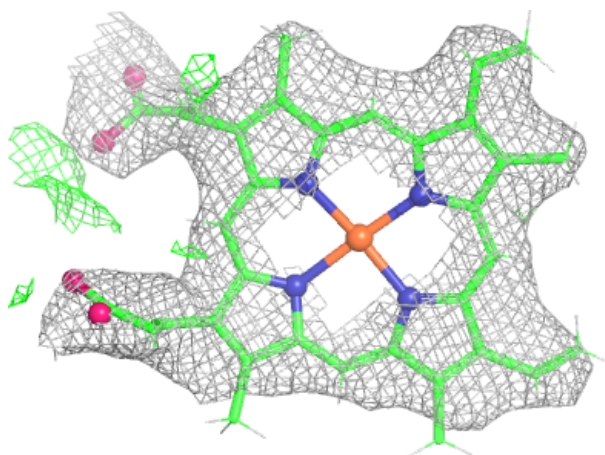
Electron density around HEM E 101:

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



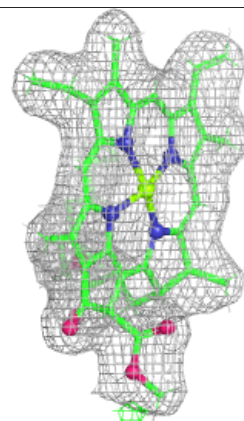
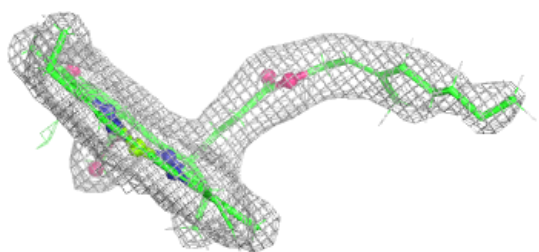
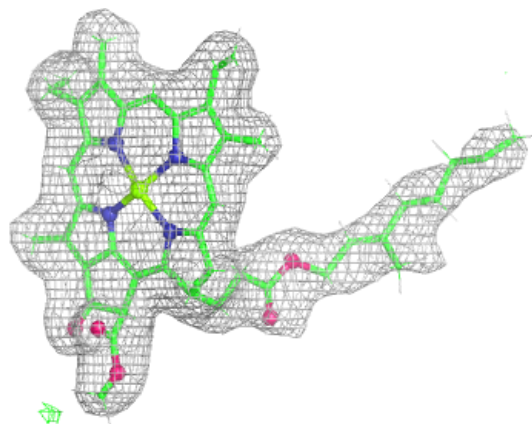
Electron density around HEM f 101:

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



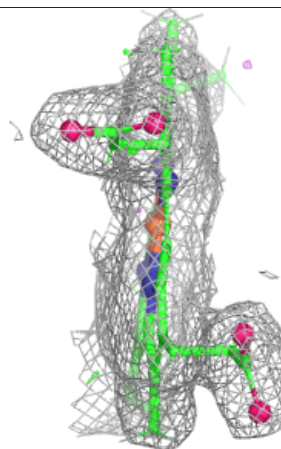
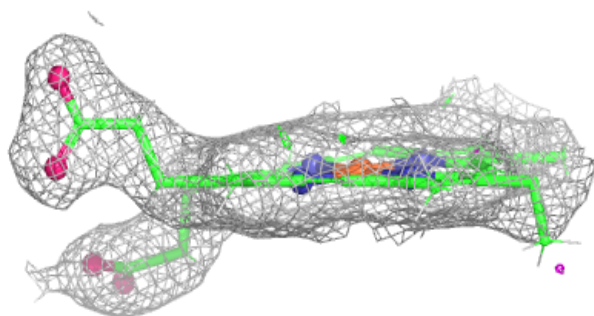
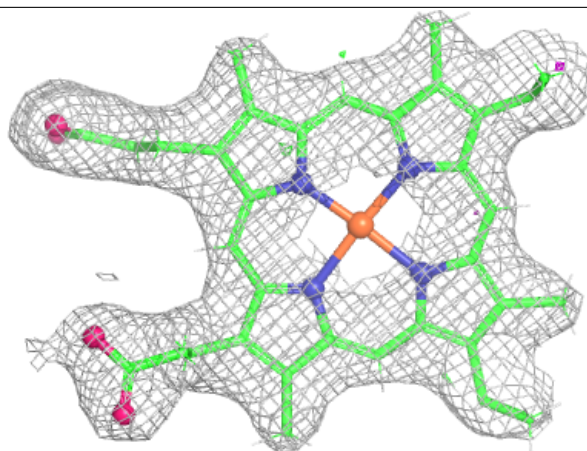
Electron density around CLA A 405:

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



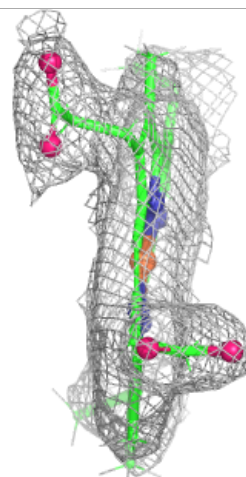
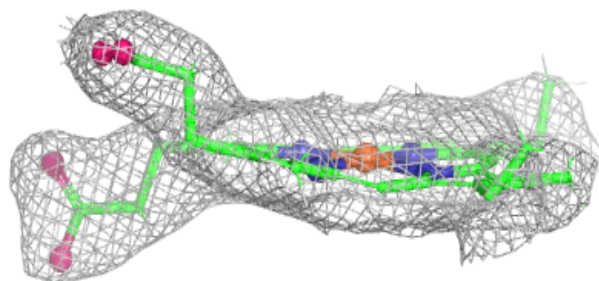
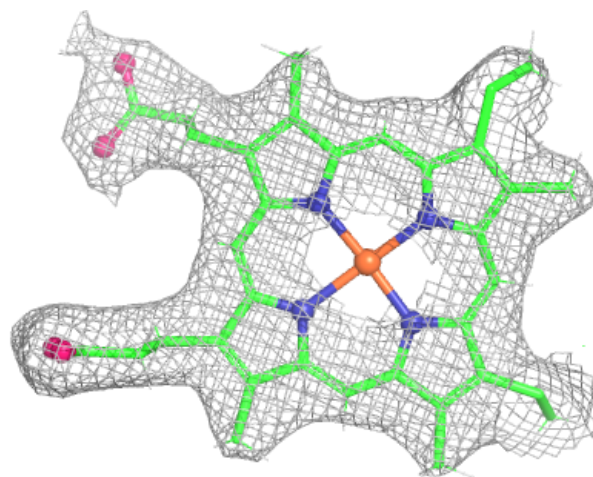
Electron density around HEC V 201:

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



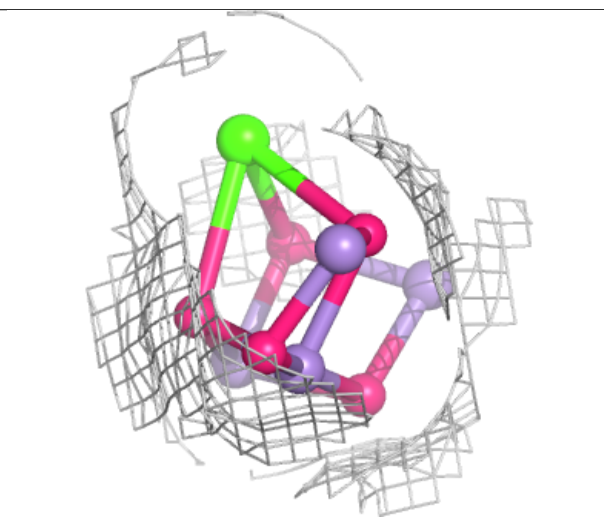
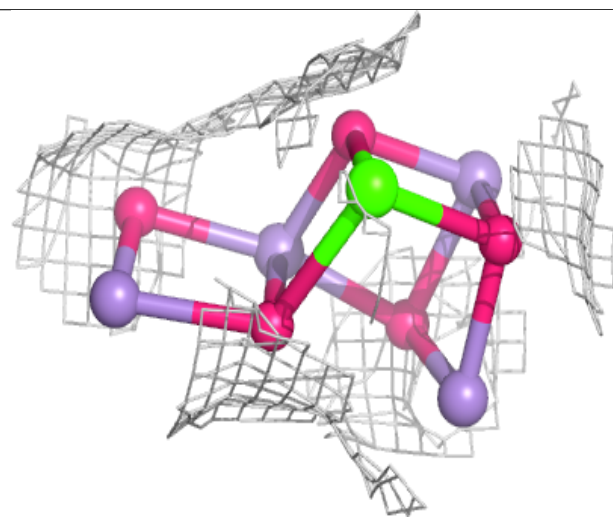
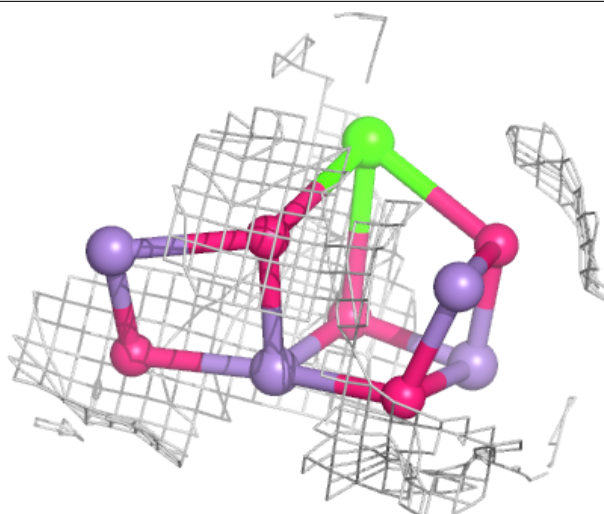
Electron density around HEC v 201:

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



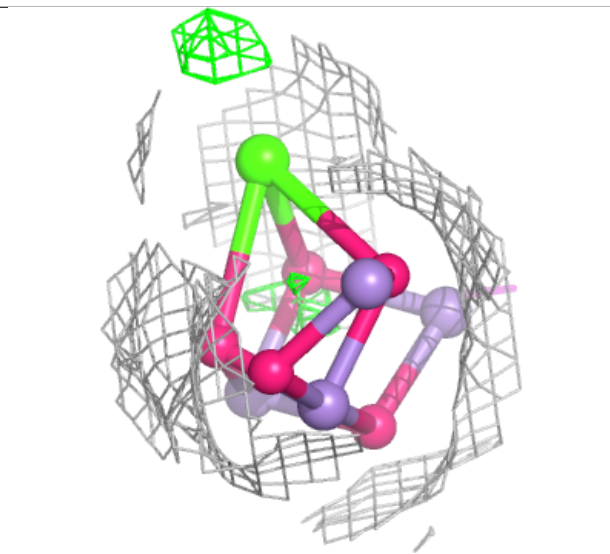
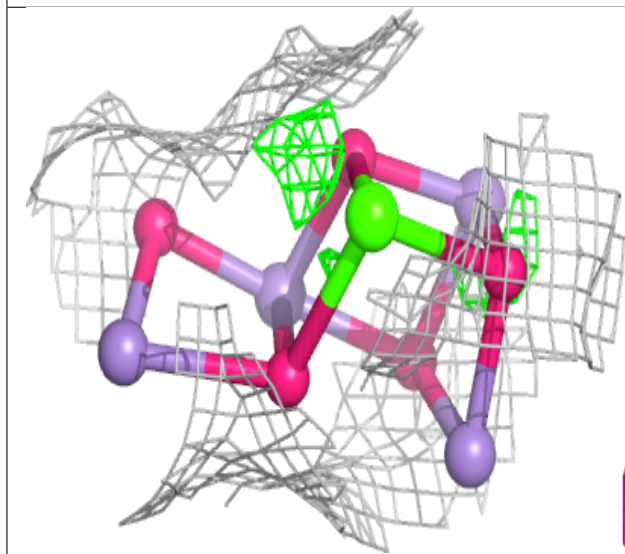
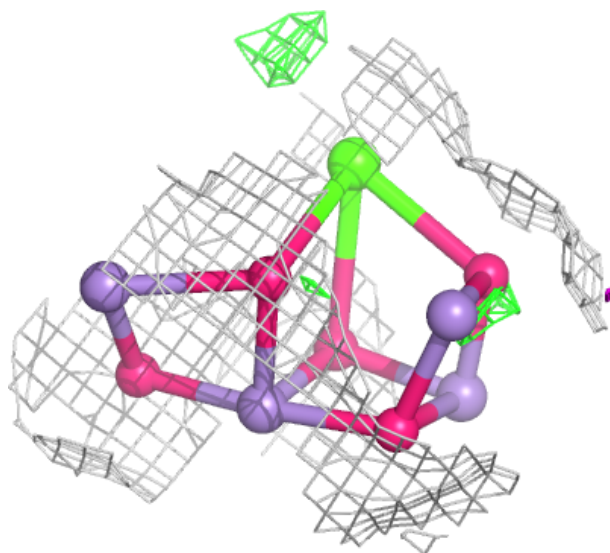
Electron density around OEX a 416 (A):

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



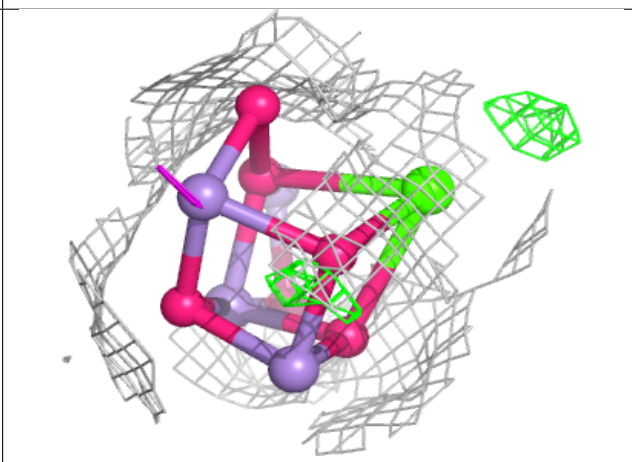
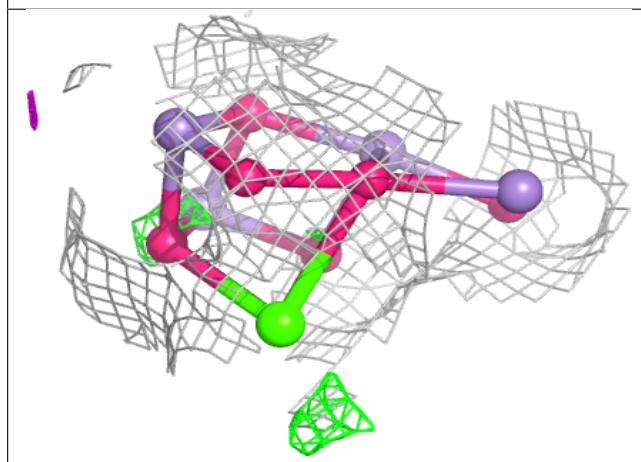
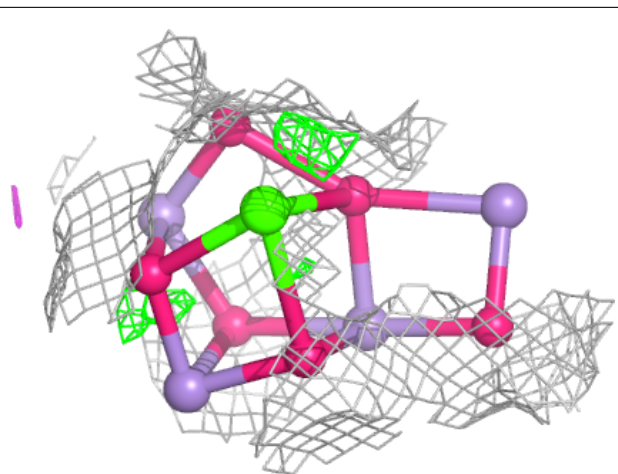
Electron density around OEX A 416 (A):

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



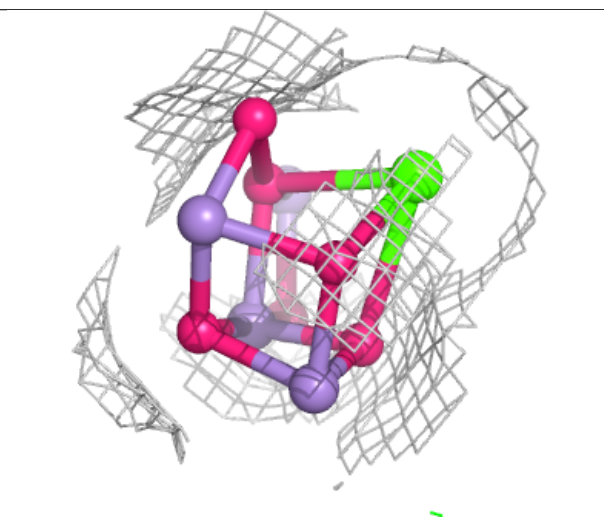
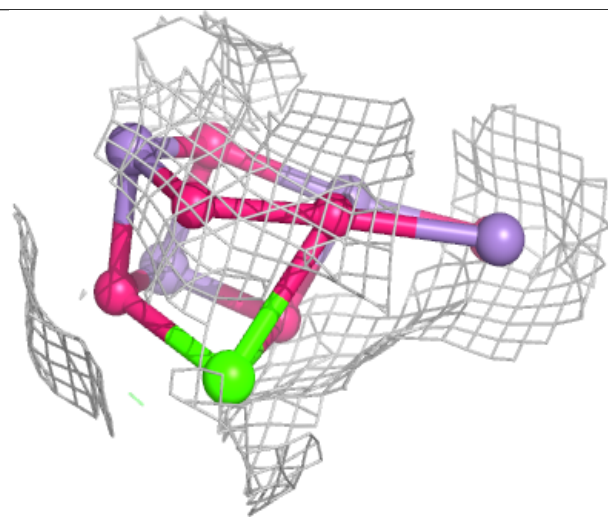
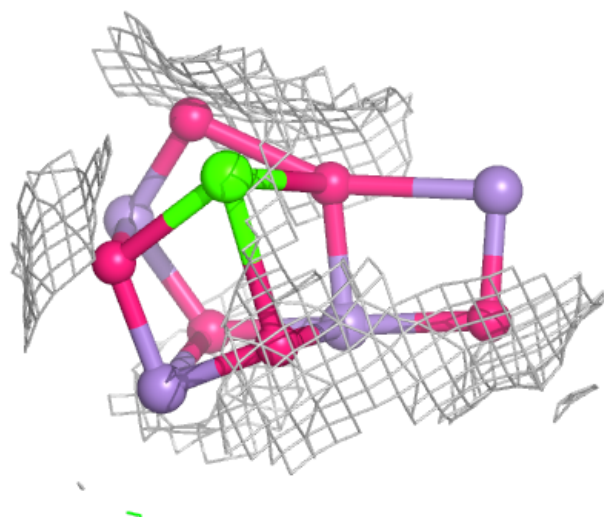
Electron density around OEY A 415 (B):

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



Electron density around OEY a 415 (B):

$2mF_o-DF_c$ (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.