



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:16 AM UTC

PDB ID : 7RF5 / pdb_00007rf5
Title : RT XFEL structure of Photosystem II 150 microseconds after the second illumination at 2.23 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.23 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	: 9.0.010 (Gargrove)

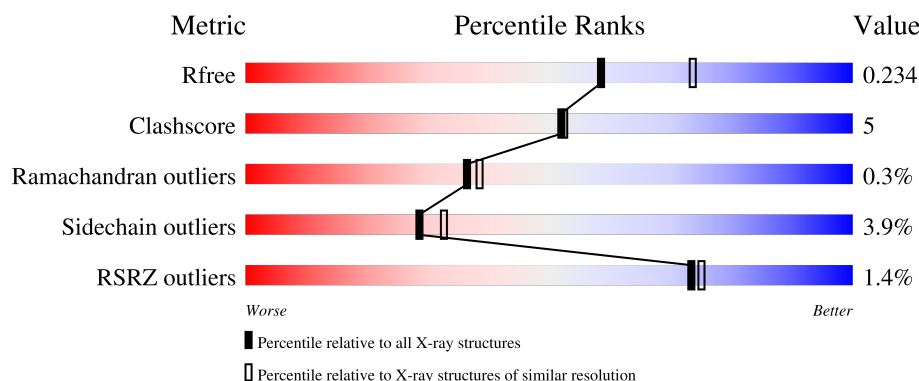
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

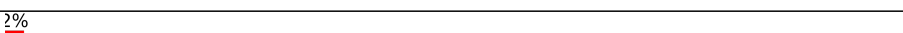
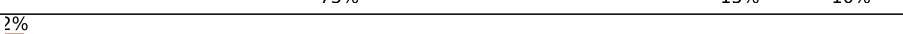
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 84% 12% .
1	a	344	 82% 14% . .

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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) : 2.49

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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
24	CLA	A	604	X	-	-	-
24	CLA	A	605	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	612	X	-	-	-
24	CLA	B	601	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	H	101	X	-	-	-
24	CLA	a	604	X	-	-	-
24	CLA	a	607	X	-	-	-
24	CLA	a	613	X	-	-	-
24	CLA	b	601	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105562 atoms, of which 52760 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	S	0	0
			620	202	316	48	53	1		
11	l	36	Total	C	H	N	O		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	S	0	0
			525	171	269	37	47	1		
12	m	32	Total	C	H	N	O	S	0	0
			518	168	267	36	46	1		

- 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	S	0	1
			3700	1168	1830	313	385	4		0
13	o	244	Total	C	H	N	O	S	0	0
			3720	1170	1846	317	383	4		0

- 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
			519	181	261	36	39	2		
15	t	30	Total	C	H	N	O	S	0	0
			512	180	256	36	38	2		

- 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			

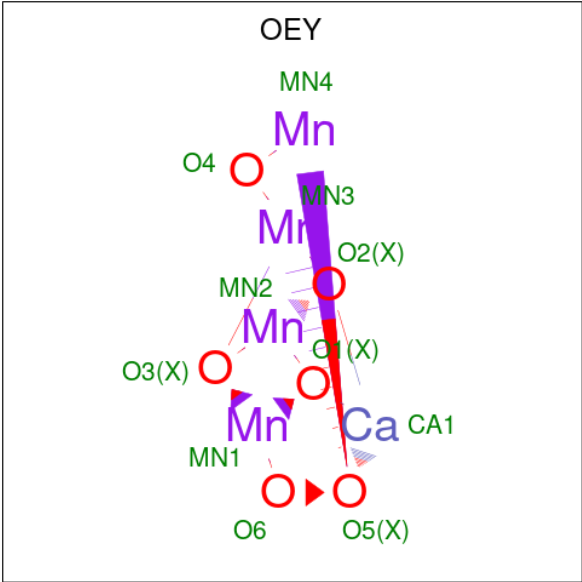
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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.

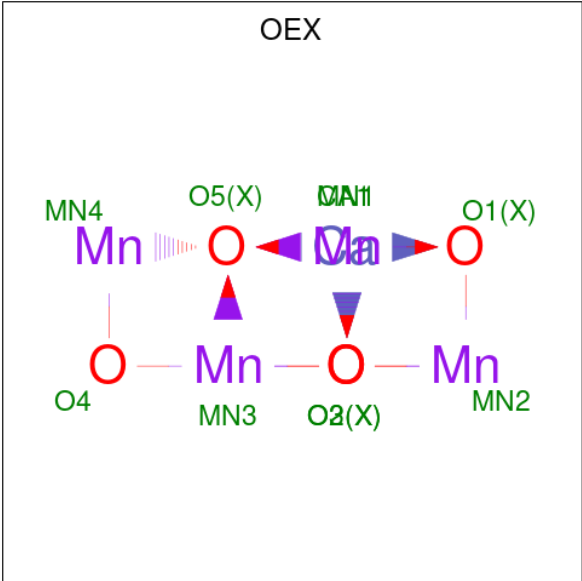
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
20	Z	62	Total 995	C 328	H 516	N 72	O 77	S 2	0	0	0
20	z	62	Total 986	C 326	H 509	N 72	O 77	S 2	0	0	0

- Molecule 21 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
			Total	Ca	Mn	O		
21	A	1	11	1	4	6	0	1
21	a	1	11	1	4	6	0	1

- Molecule 22 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
			Total	Ca	Mn	O		
22	A	1	10	1	4	5	0	1

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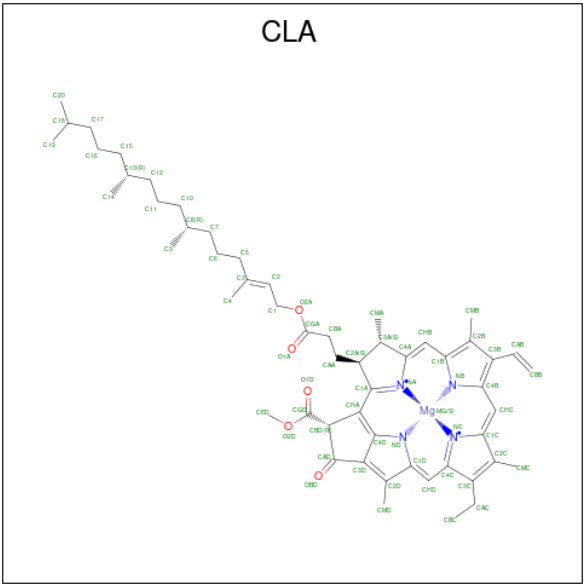
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
24	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	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
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 117	C 49	H 58	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	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
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	D	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	H	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	a	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
24	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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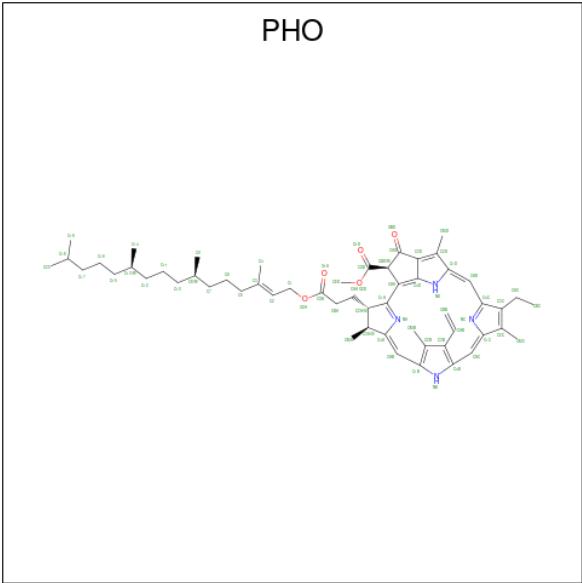
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total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

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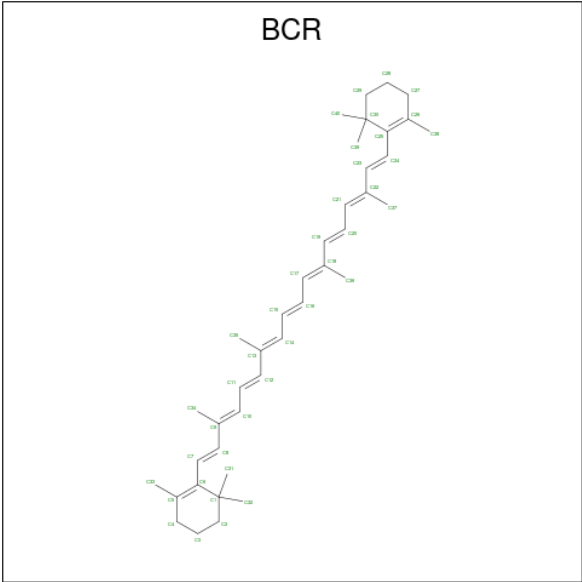
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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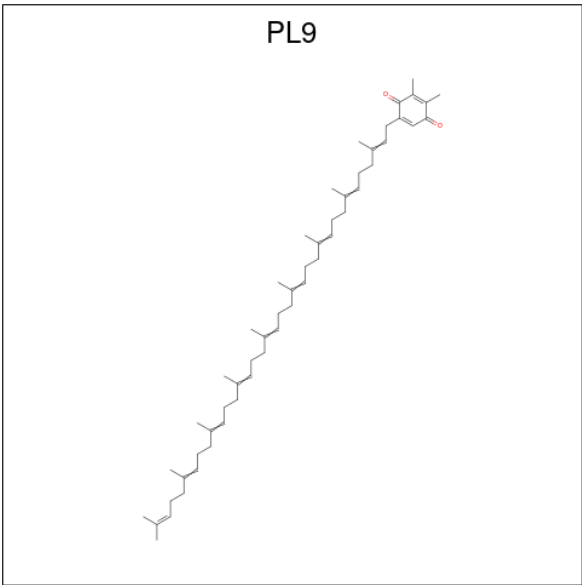
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	h	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40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

- Molecule 27 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

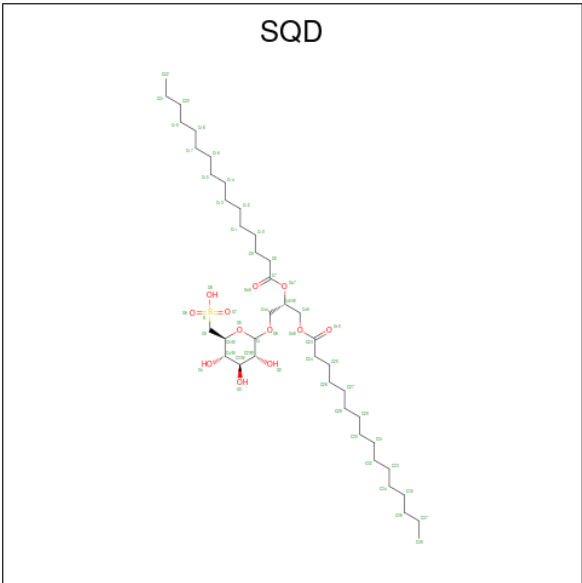
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	2	Total	Cl	0	0
			2	2		
27	a	2	Total	Cl	0	0
			2	2		

- Molecule 28 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).



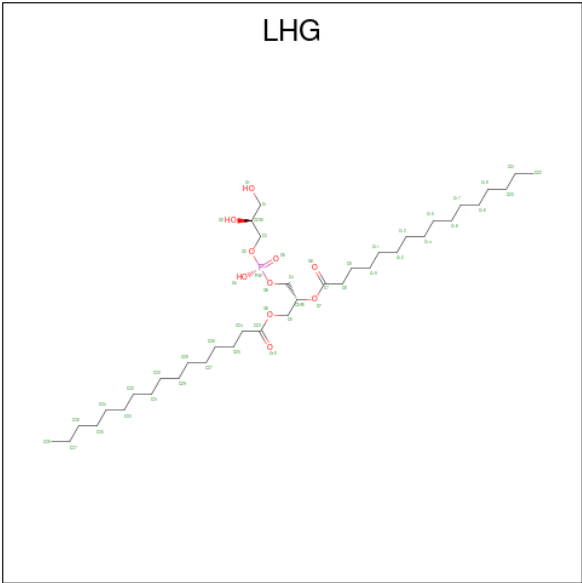
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			135	53	80	2		
28	D	1	Total	C	H	O	0	0
			135	53	80	2		
28	a	1	Total	C	H	O	0	0
			135	53	80	2		
28	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 29 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
29	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
29	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



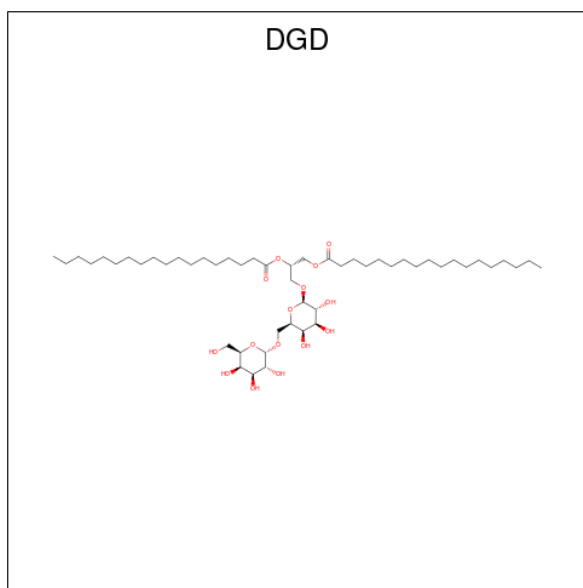
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	a	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			90	28	51	10	1		
30	e	1	Total	C	H	O	P	0	0
			99	31	57	10	1		
30	l	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



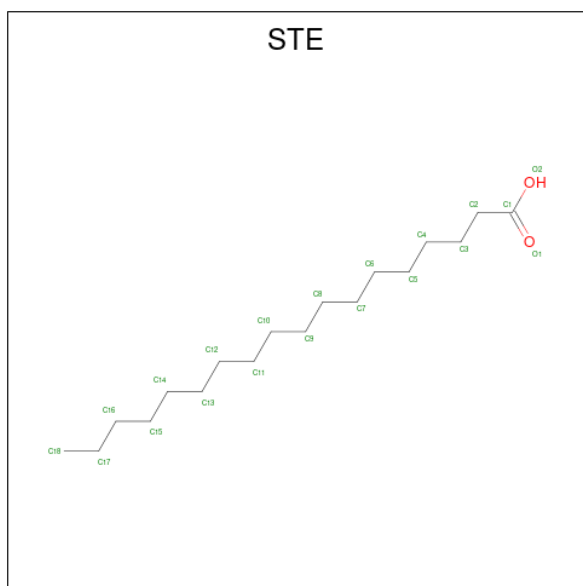
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	H	O	0	0
			162	51	96	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		
31	C	1	Total	C	H	O	0	0
			144	47	82	15		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	H	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	c	1	Total	C	H	O	0	0
			144	47	82	15		
31	h	1	Total	C	H	O	0	0
			144	47	82	15		

- 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
			53	18	35			
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H		0	0
			41	15	26			

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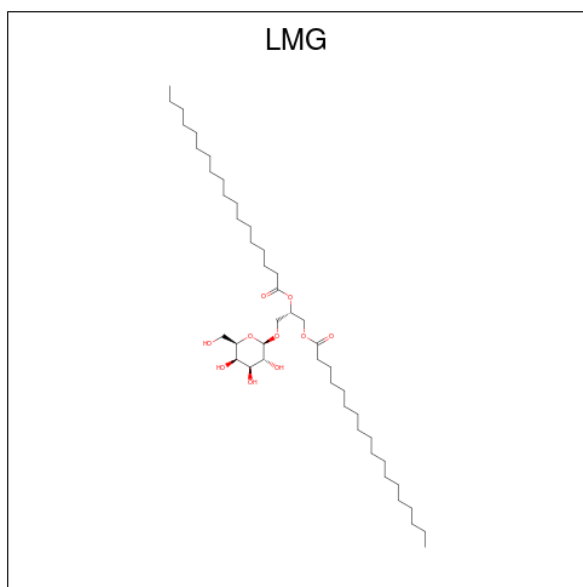
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	L	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	R	1	Total C H O 28 10 16 2	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	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	c	1	Total	C	H	O	0	0
			55	18	35	2		
32	c	1	Total	C	H	O	0	0
			28	10	16	2		
32	d	1	Total	C	H	O	0	0
			43	15	26	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	d	1	Total	C	H	O	0	0
			55	18	35	2		
32	h	1	Total	C	H		0	0
			41	14	27			
32	j	1	Total	C	H	O	0	0
			28	10	16	2		
32	t	1	Total	C	H	O	0	0
			34	12	20	2		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



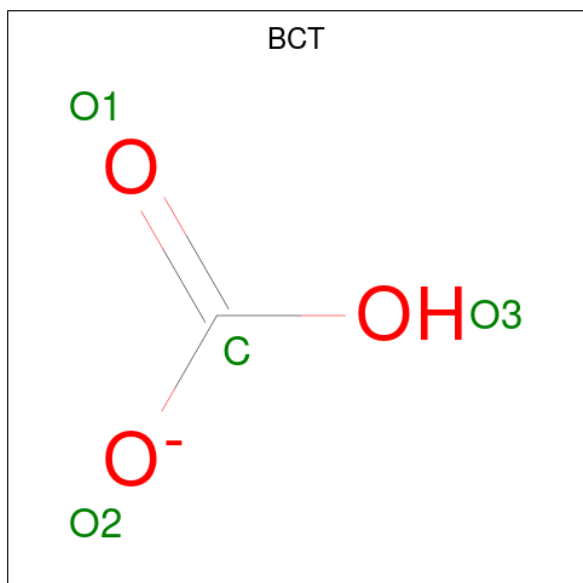
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	C	1	Total	C	H	O	0	0
			114	38	66	10		
33	D	1	Total	C	H	O	0	0
			122	41	71	10		
33	D	1	Total	C	H	O	0	0
			78	27	45	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			68	24	40	4		
33	M	1	Total	C	H	O	0	0
			123	41	72	10		
33	Y	1	Total	C	H	O	0	0
			114	38	66	10		
33	a	1	Total	C	H	O	0	0
			141	45	86	10		
33	b	1	Total	C	H	O	0	0
			141	45	86	10		
33	c	1	Total	C	H	O	0	0
			81	27	44	10		
33	c	1	Total	C	H	O	0	0
			117	38	69	10		
33	c	1	Total	C	H	O	0	0
			117	39	68	10		
33	d	1	Total	C	H	O	0	0
			102	34	58	10		
33	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 34 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



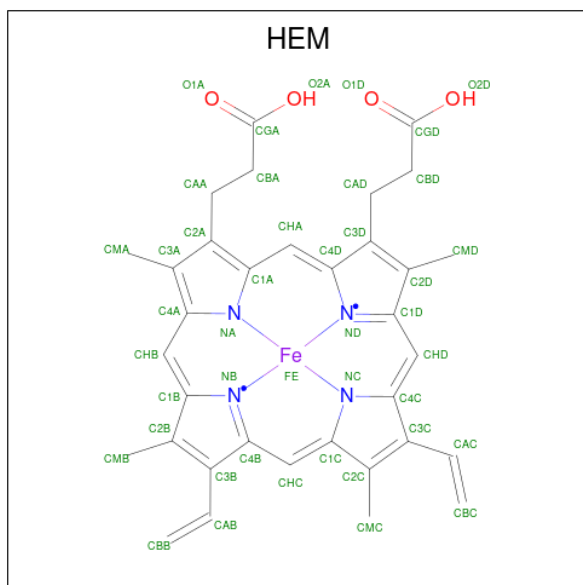
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		

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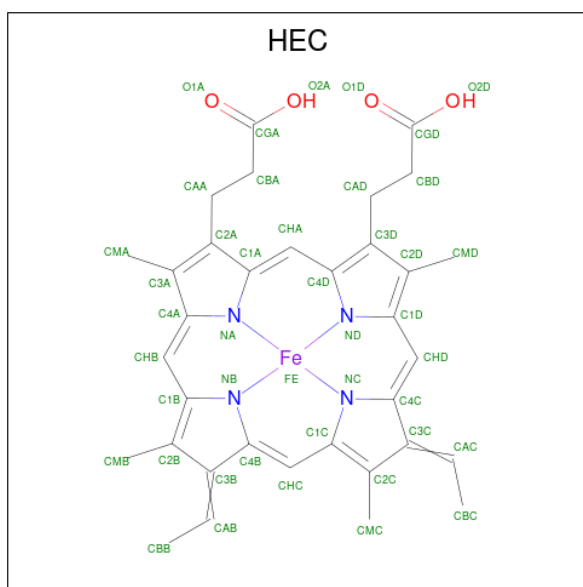
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- 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	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
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: $C_{34}H_{34}FeN_4O_4$).



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	118	Total O 118 118	0	0
37	B	141	Total O 141 141	0	0
37	C	114	Total O 114 114	0	0
37	D	100	Total O 100 100	0	0
37	E	20	Total O 20 20	0	0
37	F	3	Total O 3 3	0	0
37	H	29	Total O 29 29	0	0
37	I	7	Total O 7 7	0	0
37	J	6	Total O 6 6	0	0
37	K	6	Total O 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	10	Total O 10 10	0	0
37	M	5	Total O 5 5	0	0
37	O	71	Total O 71 71	0	0
37	R	1	Total O 1 1	0	0
37	T	5	Total O 5 5	0	0
37	U	33	Total O 33 33	0	0
37	V	49	Total O 49 49	0	0
37	X	7	Total O 7 7	0	0
37	Y	4	Total O 4 4	0	0
37	Z	2	Total O 2 2	0	0
37	a	117	Total O 117 117	0	0
37	b	131	Total O 131 131	0	0
37	c	118	Total O 118 118	0	0
37	d	100	Total O 100 100	0	0
37	e	10	Total O 10 10	0	0
37	f	2	Total O 2 2	0	0
37	h	19	Total O 19 19	0	0
37	i	8	Total O 8 8	0	0
37	j	11	Total O 11 11	0	0
37	k	4	Total O 4 4	0	0
37	l	10	Total O 10 10	0	0

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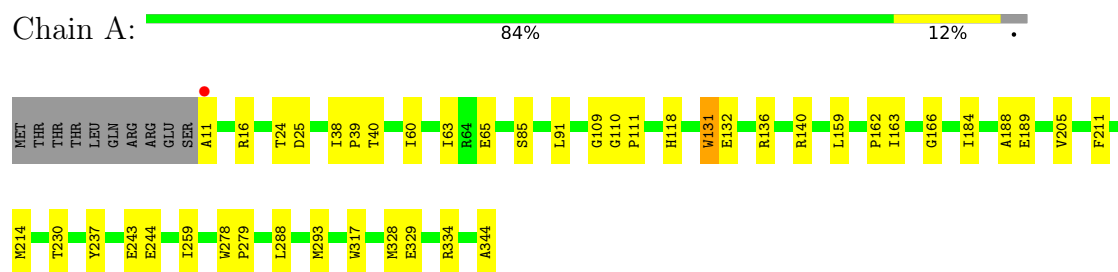
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	m	5	Total 5	O 5	0	0
37	o	65	Total 65	O 65	0	0
37	r	1	Total 1	O 1	0	0
37	t	5	Total 5	O 5	0	0
37	u	41	Total 41	O 41	0	0
37	v	36	Total 36	O 36	0	0
37	x	8	Total 8	O 8	0	0
37	y	1	Total 1	O 1	0	0
37	z	2	Total 2	O 2	0	0

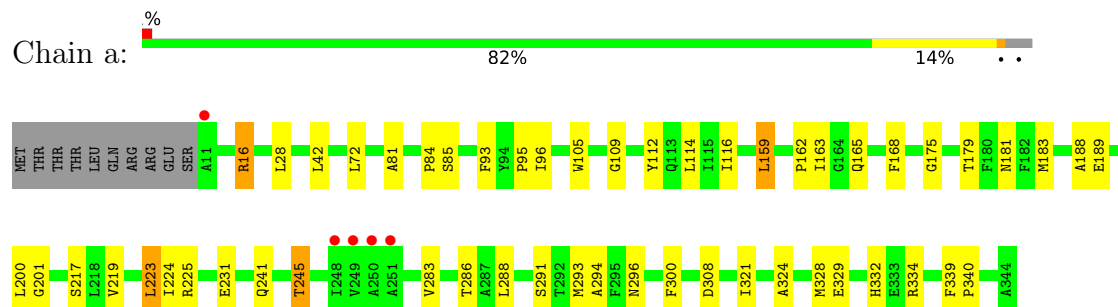
3 Residue-property plots [i](#)

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.

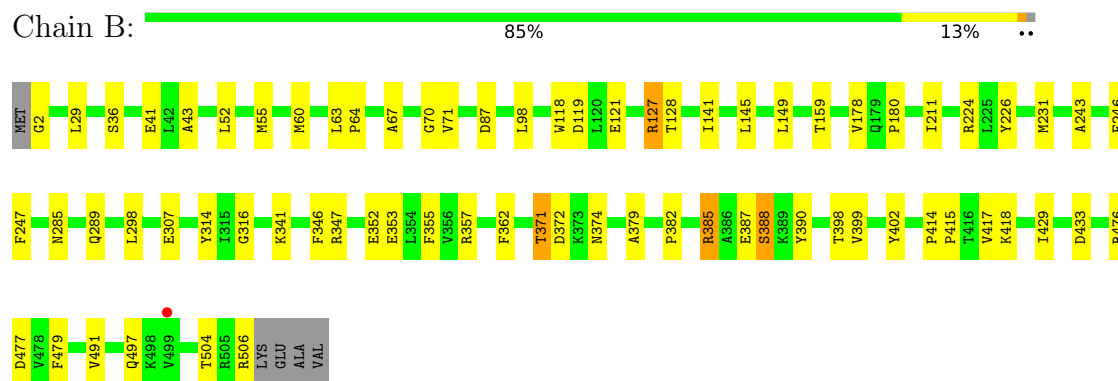
• Molecule 1: Photosystem II protein D1 1



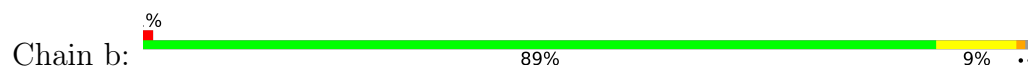
• Molecule 1: Photosystem II protein D1 1

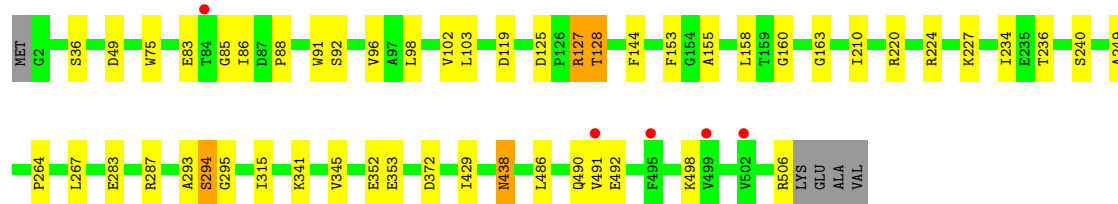


• Molecule 2: Photosystem II CP47 reaction center protein



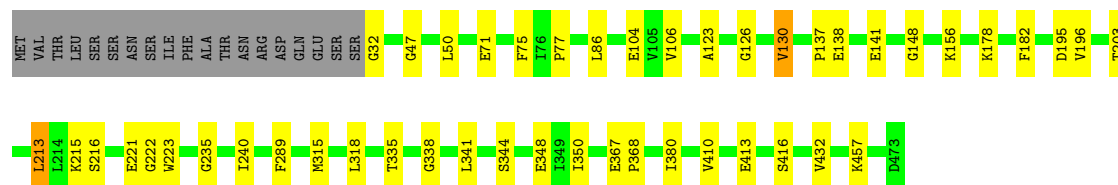
• Molecule 2: Photosystem II CP47 reaction center protein





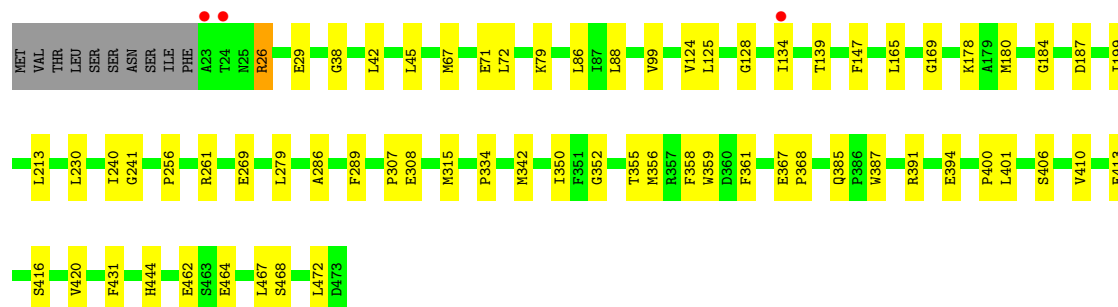
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 86% 10% .



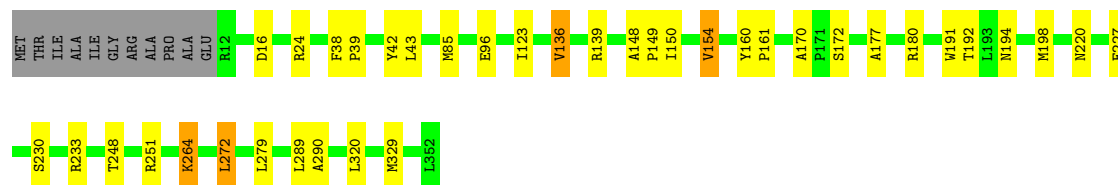
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 83% 14% .



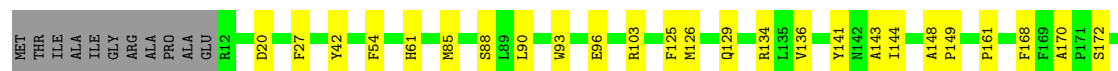
• Molecule 4: Photosystem II D2 protein

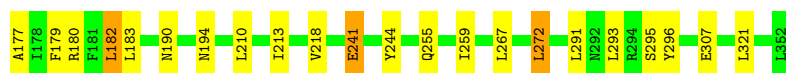
Chain D: 86% 10% . .



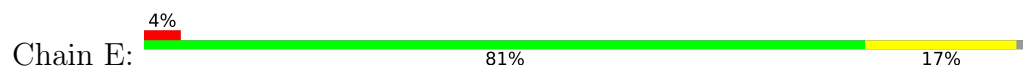
• Molecule 4: Photosystem II D2 protein

Chain d: 84% 13% . .

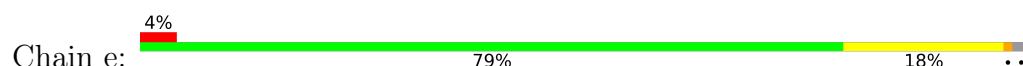




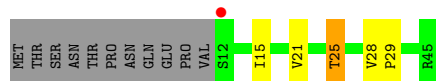
- Molecule 5: Cytochrome b559 subunit alpha



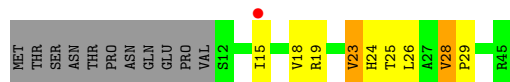
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



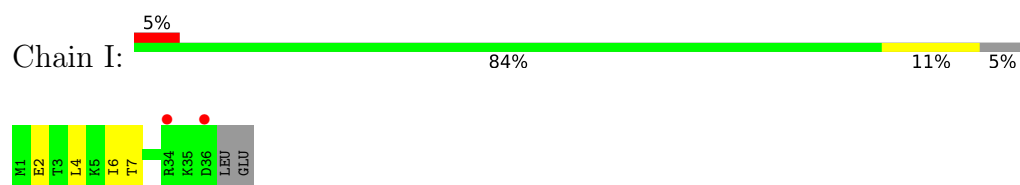
- Molecule 7: Photosystem II reaction center protein H



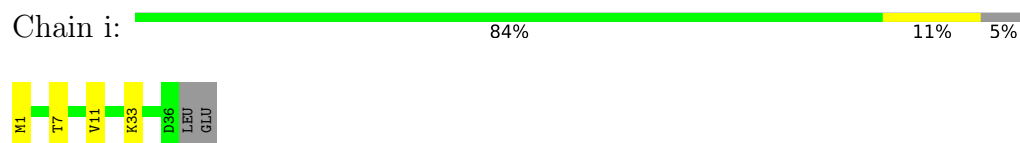
- Molecule 7: Photosystem II reaction center protein H



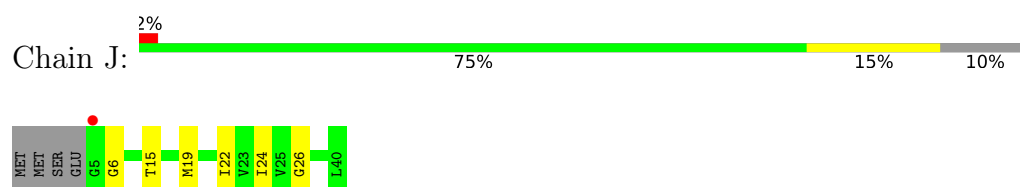
- Molecule 8: Photosystem II reaction center protein I



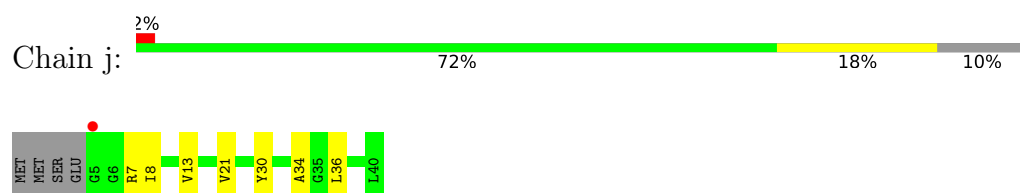
- Molecule 8: Photosystem II reaction center protein I



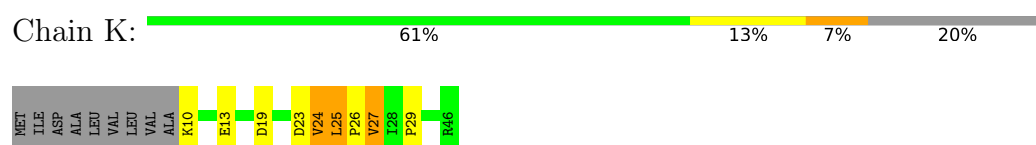
- Molecule 9: Photosystem II reaction center protein J



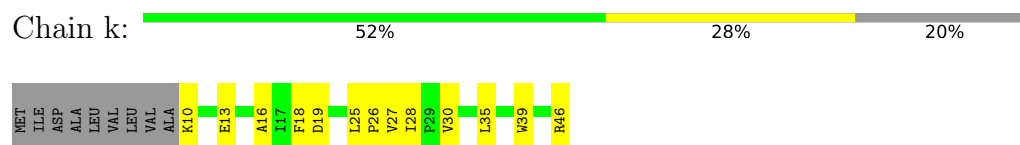
- Molecule 9: Photosystem II reaction center protein J



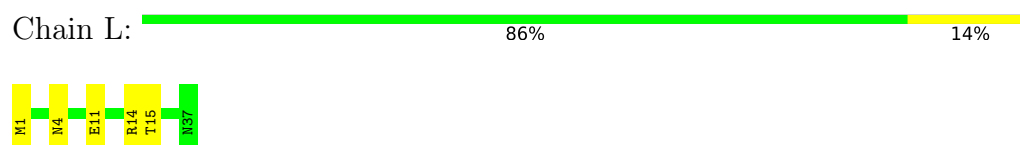
- Molecule 10: Photosystem II reaction center protein K



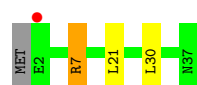
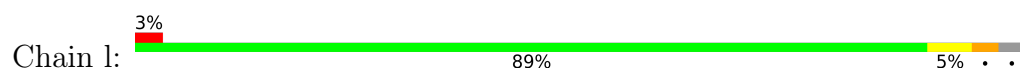
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



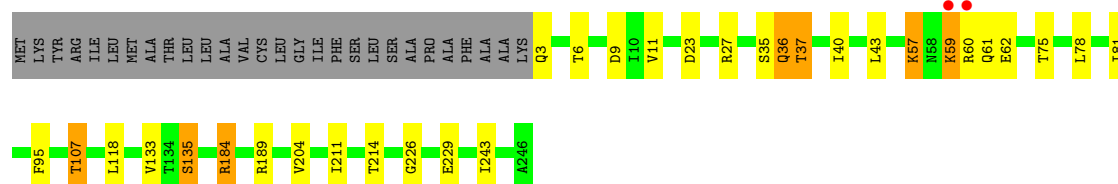
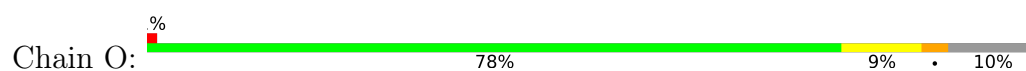
- Molecule 12: Photosystem II reaction center protein M



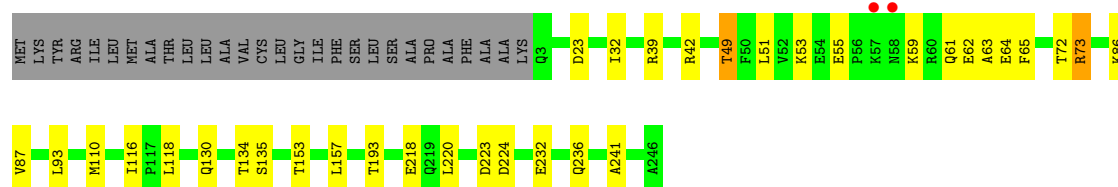
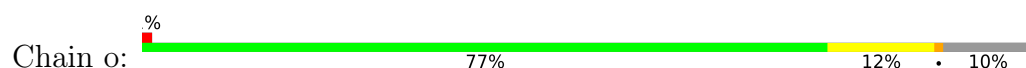
- Molecule 12: Photosystem II reaction center protein M



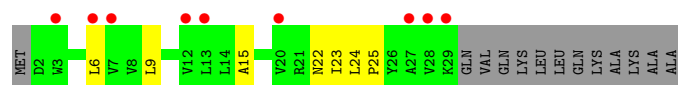
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



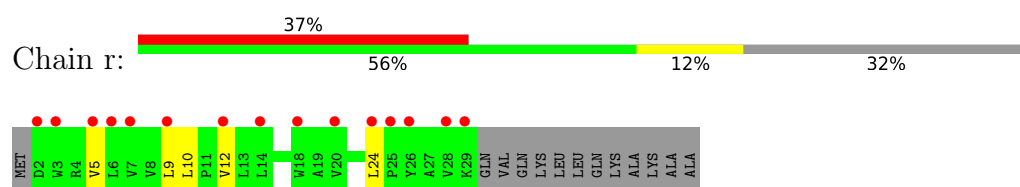
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



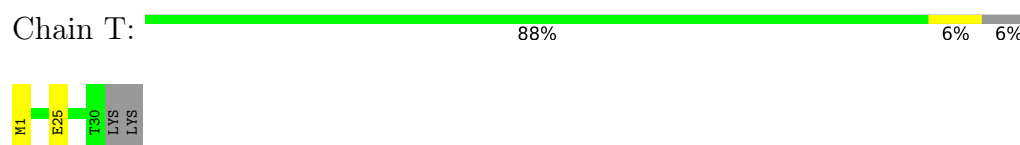
- Molecule 14: Photosystem II protein Y



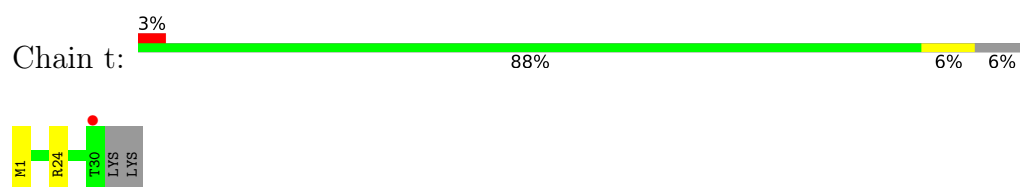
- Molecule 14: Photosystem II protein Y



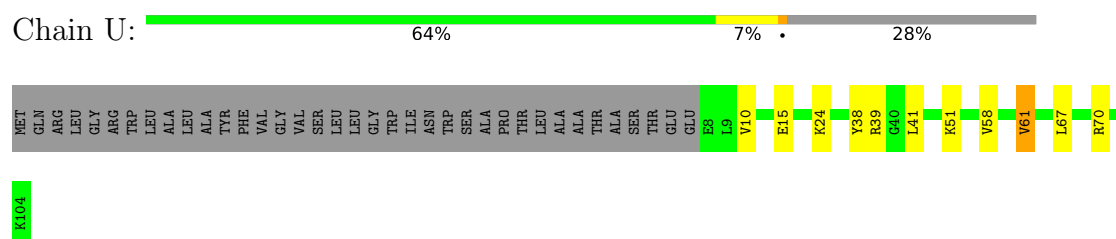
- Molecule 15: Photosystem II reaction center protein T



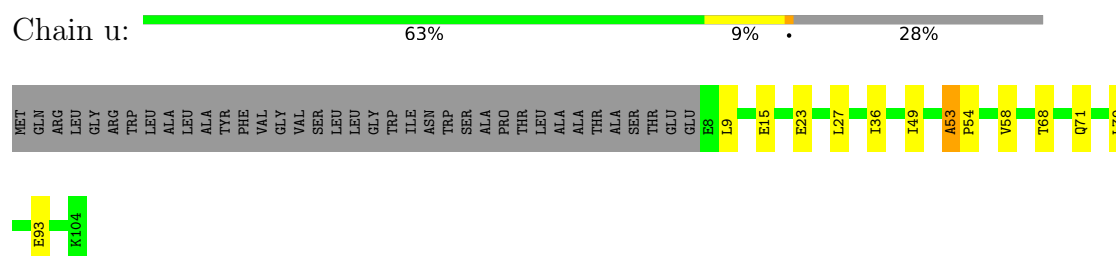
- Molecule 15: Photosystem II reaction center protein T



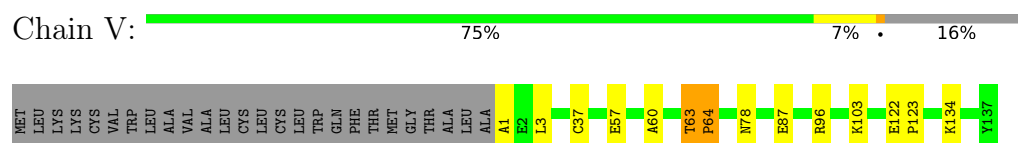
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 17: Cytochrome c-550

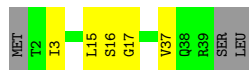
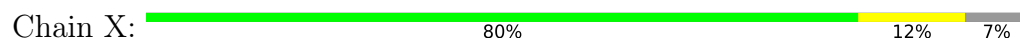


- Molecule 17: Cytochrome c-550

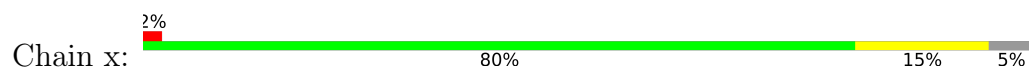




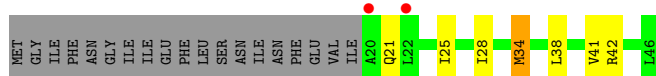
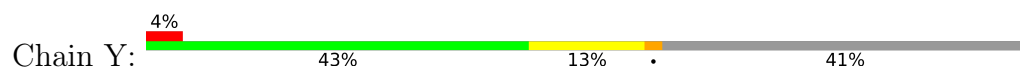
- Molecule 18: Photosystem II reaction center X protein



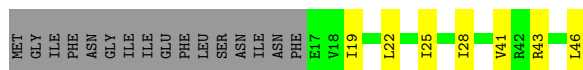
- Molecule 18: Photosystem II reaction center X protein



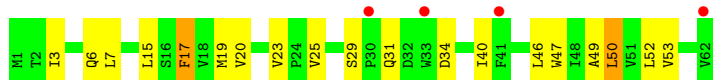
- Molecule 19: Photosystem II reaction center protein Ycf12



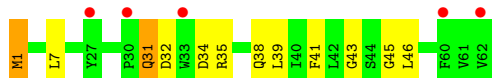
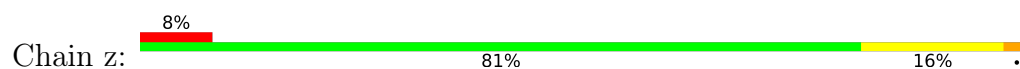
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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	117.02Å 221.78Å 308.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.70 – 2.23 33.70 – 2.23	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.70-2.23) 85.0 (33.70-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.61 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.176 , 0.233 0.177 , 0.234	Depositor DCC
R_{free} test set	3445 reflections (0.55%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	105562	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: BCR, LMG, LHG, STE, OEX, DGD, PHO, FME, FE2, SQD, CLA, CL, OEY, HEC, BCT, PL9, HEM

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	0.50	0/3227	0.60	1/4397 (0.0%)
1	a	0.49	0/3224	0.57	0/4393
2	B	0.57	0/4161	0.64	0/5669
2	b	0.53	0/4118	0.62	0/5611
3	C	0.55	0/3647	0.62	0/4965
3	c	0.51	0/3719	0.60	0/5061
4	D	0.60	0/2825	0.67	0/3847
4	d	0.55	0/2834	0.65	0/3859
5	E	0.46	0/688	0.56	0/940
5	e	0.42	0/683	0.56	0/932
6	F	0.40	0/284	0.56	0/387
6	f	0.47	0/284	0.63	0/387
7	H	0.54	0/523	0.60	0/713
7	h	0.49	0/511	0.58	0/697
8	I	0.53	0/293	0.66	0/396
8	i	0.55	0/293	0.57	0/396
9	J	0.41	0/263	0.55	0/356
9	j	0.43	0/263	0.57	0/356
10	K	0.42	0/303	0.51	0/416
10	k	0.48	0/303	0.53	0/416
11	L	0.63	0/311	0.63	0/422
11	l	0.61	0/303	0.57	0/412
12	M	0.60	0/249	0.67	0/341
12	m	0.62	0/244	0.73	0/334
13	O	0.55	0/1904	0.67	0/2585
13	o	0.56	0/1905	0.63	0/2583
14	R	0.34	0/227	0.44	0/313
14	r	0.32	0/227	0.42	0/313
15	T	0.64	0/257	0.68	0/349
15	t	0.61	0/255	0.64	0/346
16	U	0.48	0/785	0.58	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.56	0/785	0.63	0/1064
17	V	0.54	0/1085	0.65	0/1473
17	v	0.48	0/1085	0.59	0/1473
18	X	0.42	0/284	0.51	0/384
18	x	0.36	0/289	0.46	0/391
19	Y	0.43	0/197	0.47	0/264
19	y	0.36	0/219	0.48	0/294
20	Z	0.36	0/490	0.47	0/669
20	z	0.33	0/488	0.45	0/666
All	All	0.53	0/44035	0.61	1/59934 (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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	TRP	CA-CB-CG	-5.16	103.80	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	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	3110	2976	2954	41	0
2	B	4005	3873	3867	47	0
2	b	3978	3836	3836	33	0
3	C	3509	3432	3409	27	0
3	c	3583	3503	3492	37	0
4	D	2731	2637	2637	28	0
4	d	2737	2643	2643	32	0
5	E	666	651	651	11	0
5	e	664	648	648	12	0
6	F	275	282	282	4	0
6	f	275	282	282	7	0
7	H	510	532	532	4	0
7	h	498	518	518	11	0
8	I	296	311	311	2	0
8	i	296	311	311	1	0
9	J	257	268	268	3	0
9	j	257	268	268	4	0
10	K	293	305	305	6	0
10	k	293	305	305	8	0
11	L	304	316	316	6	0
11	l	296	304	304	1	0
12	M	256	269	269	8	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	19	0
13	o	1874	1846	1846	19	0
14	R	221	238	238	4	0
14	r	221	238	238	0	0
15	T	258	261	261	1	0
15	t	256	256	256	1	0
16	U	774	773	773	5	0
16	u	774	773	773	9	0
17	V	1064	1071	1073	9	0
17	v	1064	1071	1073	18	0
18	X	281	312	312	3	0
18	x	286	316	314	3	0
19	Y	196	217	217	5	0
19	y	218	241	241	3	0
20	Z	479	516	516	8	0
20	z	477	509	509	7	0
21	A	11	0	0	2	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	249	264	264	3	0
24	B	970	1067	1067	12	0
24	C	839	922	922	12	0
24	D	130	144	144	2	0
24	H	65	72	72	3	0
24	a	260	288	288	1	0
24	b	1035	1139	1139	12	0
24	c	839	919	919	17	0
24	d	130	144	144	2	0
25	A	64	74	74	3	0
25	D	64	74	74	0	0
25	a	64	74	74	1	0
25	d	64	74	74	2	0
26	A	40	56	56	0	0
26	B	120	168	168	6	0
26	C	40	56	56	3	0
26	D	40	56	56	2	0
26	K	120	168	168	3	0
26	T	40	56	56	1	0
26	X	40	56	56	1	0
26	a	40	56	56	0	0
26	b	120	168	168	2	0
26	c	80	112	112	3	0
26	d	40	56	56	1	0
26	h	40	56	56	0	0
26	k	80	112	112	1	0
26	t	40	56	56	1	0
27	A	2	0	0	0	0
27	a	2	0	0	0	0
28	A	55	80	80	5	0
28	D	55	80	80	1	0
28	a	55	80	80	1	0
28	d	55	80	80	1	0
29	A	91	135	135	4	0
29	B	54	78	77	3	0
29	D	36	46	45	1	0
29	a	90	134	133	0	0
29	b	49	65	64	0	0
29	f	41	48	48	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	49	74	74	0	0
30	D	145	215	215	4	0
30	L	49	74	74	3	0
30	a	49	74	74	3	0
30	d	88	125	125	0	0
30	e	42	57	57	1	0
30	l	49	74	74	2	0
31	A	66	96	96	3	0
31	C	186	246	245	2	0
31	H	62	82	82	1	0
31	c	186	246	245	2	0
31	h	62	82	81	1	0
32	B	108	178	178	6	0
32	C	40	63	63	1	0
32	I	15	26	26	1	0
32	J	12	16	16	1	0
32	L	12	16	16	0	0
32	M	43	73	73	2	0
32	R	12	16	16	0	0
32	T	31	60	60	2	0
32	X	20	35	35	2	0
32	Z	8	12	12	3	0
32	a	22	32	32	1	0
32	b	66	110	110	2	0
32	c	32	51	51	1	0
32	d	57	96	96	9	0
32	h	14	27	27	1	0
32	j	12	16	16	2	0
32	t	14	20	20	1	0
33	C	48	66	66	2	0
33	D	112	156	156	1	0
33	M	51	72	72	1	0
33	Y	48	66	66	1	0
33	a	55	86	86	1	0
33	b	55	86	86	1	0
33	c	134	181	181	2	0
33	d	44	58	57	0	0
33	m	51	72	72	3	0
34	D	4	1	1	1	0
34	a	4	1	1	0	0
35	F	43	30	30	4	0
35	f	43	30	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	V	43	30	30	0	0
36	v	43	30	30	0	0
37	A	118	0	0	6	0
37	B	141	0	0	4	0
37	C	114	0	0	1	0
37	D	100	0	0	2	0
37	E	20	0	0	4	0
37	F	3	0	0	0	0
37	H	29	0	0	1	0
37	I	7	0	0	0	0
37	J	6	0	0	0	0
37	K	6	0	0	0	0
37	L	10	0	0	0	0
37	M	5	0	0	1	0
37	O	71	0	0	3	0
37	R	1	0	0	0	0
37	T	5	0	0	0	0
37	U	33	0	0	1	0
37	V	49	0	0	2	0
37	X	7	0	0	0	0
37	Y	4	0	0	1	0
37	Z	2	0	0	0	0
37	a	117	0	0	5	0
37	b	131	0	0	7	0
37	c	118	0	0	3	0
37	d	100	0	0	5	0
37	e	10	0	0	1	0
37	f	2	0	0	0	0
37	h	19	0	0	2	0
37	i	8	0	0	0	0
37	j	11	0	0	3	0
37	k	4	0	0	1	0
37	l	10	0	0	3	0
37	m	5	0	0	1	0
37	o	65	0	0	5	0
37	r	1	0	0	0	0
37	t	5	0	0	1	0
37	u	41	0	0	4	0
37	v	36	0	0	6	0
37	x	8	0	0	0	0
37	y	1	0	0	0	0
37	z	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	52802	52760	52670	526	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 (526) 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)
11:l:7:ARG:NH1	37:l:201:HOH:O	1.85	0.96
16:u:23:GLU:O	37:u:201:HOH:O	1.84	0.94
13:o:224:ASP:OD2	37:o:301:HOH:O	1.87	0.93
1:A:25:ASP:OD1	37:A:701:HOH:O	1.89	0.89
10:k:46:ARG:O	37:k:201:HOH:O	1.90	0.89
17:v:34:GLN:NE2	37:v:301:HOH:O	1.86	0.88
4:D:96:GLU:OE1	37:D:501:HOH:O	1.94	0.85
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.58	0.85
5:E:48:GLY:O	37:E:701:HOH:O	1.94	0.85
13:o:223:ASP:OD1	37:o:302:HOH:O	1.95	0.84
1:A:237:TYR:O	37:A:702:HOH:O	1.95	0.84
1:A:244:GLU:OE2	37:A:703:HOH:O	1.95	0.83
17:v:91:VAL:O	37:v:302:HOH:O	1.98	0.81
13:o:218:GLU:OE2	37:o:303:HOH:O	2.00	0.80
1:A:230:THR:OG1	37:A:704:HOH:O	2.00	0.80
4:D:264:LYS:NZ	34:D:402:BCT:O3	2.18	0.76
2:b:492:GLU:OE2	5:e:3:GLY:N	2.19	0.76
17:V:57:GLU:OE1	37:V:301:HOH:O	2.04	0.76
9:j:34:ALA:O	37:j:201:HOH:O	2.02	0.76
2:b:438:ASN:OD1	37:b:701:HOH:O	2.04	0.75
5:e:8:ARG:NH2	37:e:301:HOH:O	2.18	0.75
17:v:75:TYR:OH	37:v:303:HOH:O	1.98	0.75
7:h:64:ALA:O	37:h:201:HOH:O	2.05	0.74
20:z:41:PHE:O	37:z:101:HOH:O	2.04	0.73
17:v:104:MET:HA	17:v:107:LEU:HD22	1.72	0.72
3:c:462:GLU:OE2	37:c:601:HOH:O	2.09	0.71
16:u:36:ILE:O	37:u:202:HOH:O	2.08	0.70
5:E:82:GLN:NE2	37:E:703:HOH:O	2.24	0.70
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.09	0.69
16:u:53:ALA:HB1	16:u:54:PRO:HD2	1.75	0.69
32:d:410:STE:O2	37:d:501:HOH:O	2.11	0.69
28:D:406:PL9:H322	30:L:101:LHG:H223	1.74	0.69
12:m:4:ASN:ND2	33:m:101:LMG:O10	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:86:ILE:HA	37:b:704:HOH:O	1.91	0.68
1:A:11:ALA:O	1:A:16:ARG:NH2	2.28	0.67
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.28	0.67
2:b:119:ASP:OD1	37:b:702:HOH:O	2.11	0.67
28:A:611:PL9:H361	6:F:25:THR:HG21	1.76	0.67
7:h:64:ALA:C	37:h:201:HOH:O	2.37	0.67
16:u:9:LEU:HA	37:u:209:HOH:O	1.95	0.67
13:o:62:GLU:OE2	13:o:63:ALA:N	2.29	0.66
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.78	0.65
13:O:6:THR:HG22	13:O:9:ASP:OD2	1.97	0.64
12:m:30:GLU:OE2	37:m:201:HOH:O	2.15	0.64
32:M:104:STE:H21	37:l:201:HOH:O	1.96	0.64
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.63
20:z:1:MET:SD	20:z:1:MET:N	2.69	0.63
16:U:70:ARG:NH1	37:U:201:HOH:O	1.99	0.62
9:J:15:THR:HG22	9:J:19:MET:HE2	1.82	0.61
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.83	0.61
30:a:614:LHG:O4	4:d:141:TYR:OH	2.06	0.61
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.33	0.61
2:B:127:ARG:HG3	2:B:128:THR:HG23	1.82	0.61
9:j:36:LEU:O	37:j:201:HOH:O	2.16	0.60
2:B:357:ARG:NE	37:B:701:HOH:O	2.19	0.60
6:f:18:VAL:HG22	29:f:102:SQD:H261	1.84	0.60
29:B:620:SQD:H92	29:B:620:SQD:H461	1.84	0.59
17:v:21:LEU:HD11	17:v:117:GLY:HA3	1.84	0.59
32:d:410:STE:C1	37:d:501:HOH:O	2.51	0.59
13:O:184:ARG:NH2	13:O:229[A]:GLU:OE2	2.35	0.59
5:E:68:ASP:OD2	5:E:71:GLU:HB2	2.03	0.58
24:C:506:CLA:H8	26:C:514:BCR:H12C	1.84	0.58
15:t:24:ARG:NH1	37:t:201:HOH:O	2.21	0.58
20:z:45:GLY:N	37:z:101:HOH:O	2.20	0.58
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.69	0.58
32:M:104:STE:C2	37:l:201:HOH:O	2.49	0.58
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.86	0.58
2:B:357:ARG:NH2	37:B:701:HOH:O	2.23	0.58
32:B:623:STE:H152	24:H:101:CLA:H61	1.86	0.57
20:z:34:ASP:O	20:z:38:GLN:NE2	2.35	0.57
13:o:61:GLN:O	37:o:305:HOH:O	2.17	0.57
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.87	0.57
1:a:112:TYR:O	1:a:116:ILE:HG12	2.04	0.57
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:GLY:O	3:C:130:VAL:HG13	2.05	0.56
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.88	0.56
2:B:149[B]:LEU:HD11	24:B:603:CLA:H152	1.87	0.56
3:c:256:PRO:O	3:c:261:ARG:NH1	2.38	0.56
17:v:2:GLU:HB2	37:v:307:HOH:O	2.05	0.56
13:O:59:LYS:O	13:O:61:GLN:N	2.36	0.56
1:A:24:THR:O	4:D:251:ARG:NH2	2.36	0.56
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.88	0.55
5:E:53:ASP:O	17:V:1:ALA:N	2.37	0.55
13:O:57:LYS:HD3	2:b:49:ASP:OD2	2.06	0.55
2:b:352:GLU:OE2	37:b:703:HOH:O	2.18	0.55
5:E:82:GLN:HG3	37:E:703:HOH:O	2.06	0.55
4:D:123:ILE:HD11	31:H:102:DGD:HAH1	1.88	0.55
13:O:35:SER:OG	13:O:36:GLN:N	2.39	0.55
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.36	0.55
25:A:606:PHO:HBC3	4:D:279:LEU:HD22	1.88	0.55
13:O:107:THR:HG22	37:O:311:HOH:O	2.07	0.54
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.88	0.54
13:O:3:GLN:N	37:O:301:HOH:O	2.40	0.54
16:U:58:VAL:O	16:U:61:VAL:HG22	2.08	0.54
25:d:401:PHO:H3A	24:d:402:CLA:H142	1.89	0.54
29:A:613:SQD:H271	30:D:410:LHG:H131	1.90	0.54
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.89	0.54
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.43	0.54
4:d:27:PHE:O	37:d:502:HOH:O	2.18	0.54
17:V:63:THR:HG22	17:V:64:PRO:CD	2.38	0.53
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.43	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.44	0.53
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.89	0.53
29:A:613:SQD:H381	9:J:22:ILE:HD11	1.90	0.53
32:T:103:STE:H71	33:m:101:LMG:HC5	1.91	0.53
24:b:613:CLA:H201	33:m:101:LMG:H352	1.89	0.53
7:h:29:PRO:O	7:h:33:VAL:HG23	2.08	0.53
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.90	0.53
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.53
13:o:110:MET:HE2	13:o:116:ILE:HD11	1.91	0.53
20:Z:29:SER:HB3	20:Z:31:GLN:HG3	1.90	0.52
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.91	0.52
1:a:16:ARG:HH11	1:a:16:ARG:HB3	1.74	0.52
2:b:91:TRP:HE1	32:b:621:STE:H111	1.74	0.52
6:f:24:HIS:O	6:f:28:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:39:ARG:NH2	17:V:60:ALA:O	2.40	0.52
17:v:106:ASN:HA	37:v:324:HOH:O	2.08	0.52
32:d:409:STE:O2	32:d:409:STE:H41	2.09	0.52
2:b:102:VAL:HG11	24:b:606:CLA:H142	1.91	0.52
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.92	0.52
32:d:410:STE:H71	18:x:16:SER:HB3	1.92	0.52
1:a:181[B]:ASN:ND2	37:a:709:HOH:O	2.42	0.51
6:f:19:ARG:O	6:f:23:VAL:HG13	2.11	0.51
2:B:224:ARG:NH2	4:D:16:ASP:OD2	2.39	0.51
26:B:616:BCR:H402	29:B:620:SQD:H82	1.92	0.51
3:C:203:THR:O	3:C:235:GLY:HA3	2.10	0.51
24:b:605:CLA:H8	24:b:612:CLA:H203	1.92	0.51
20:z:32:ASP:HA	20:z:35:ARG:HG3	1.92	0.51
33:a:619:LMG:C28	33:a:619:LMG:H111	2.40	0.51
24:b:615:CLA:H2	24:b:616:CLA:HBB2	1.92	0.51
32:B:625:STE:H41	32:a:617:STE:C1	2.41	0.51
2:b:372:ASP:HB2	37:b:703:HOH:O	2.09	0.51
5:e:30:LEU:HD11	35:f:101:HEM:CBB	2.41	0.51
3:c:45:LEU:HA	3:c:139:THR:HG22	1.92	0.51
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.46	0.50
19:y:22:LEU:HA	19:y:25:ILE:HG22	1.93	0.50
24:C:511:CLA:H143	20:Z:20:VAL:HG13	1.94	0.50
35:F:101:HEM:HBB2	35:F:101:HEM:HMB2	1.92	0.50
3:C:32:GLY:N	37:C:606:HOH:O	2.44	0.50
20:Z:47:TRP:CD2	32:Z:101:STE:H161	2.47	0.50
3:c:464:GLU:HB3	3:c:467:LEU:HD12	1.93	0.50
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.12	0.50
28:a:612:PL9:H261	30:e:101:LHG:H201	1.92	0.50
2:B:371:THR:HG23	2:B:372:ASP:O	2.12	0.50
13:o:39:ARG:NE	37:o:304:HOH:O	2.09	0.50
32:T:102:STE:C3	32:T:103:STE:H72	2.43	0.49
1:A:278:TRP:HB3	1:A:279:PRO:HD3	1.94	0.49
2:b:345:VAL:HG13	2:b:353:GLU:OE2	2.13	0.49
10:k:16:ALA:C	10:k:18:PHE:H	2.20	0.49
2:B:67:ALA:HA	2:B:71:VAL:O	2.11	0.49
16:u:93:GLU:OE1	37:u:203:HOH:O	2.20	0.49
2:B:285:ASN:O	2:B:289:GLN:HG2	2.12	0.49
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.93	0.49
31:C:518:DGD:HAH1	33:D:407:LMG:H201	1.95	0.49
1:a:225:ARG:NH2	37:a:701:HOH:O	2.46	0.49
25:A:606:PHO:HHD	25:A:606:PHO:HBC2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:329[A]:GLU:HG3	37:a:798:HOH:O	2.13	0.49
1:a:334[A]:ARG:NH2	37:a:711:HOH:O	2.44	0.49
30:D:413:LHG:H161	30:L:101:LHG:H292	1.93	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.49
1:a:225:ARG:NE	37:a:701:HOH:O	1.92	0.48
1:A:162[B]:PRO:O	1:A:166[B]:GLY:N	2.44	0.48
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.94	0.48
3:C:338:GLY:HA3	3:C:341:LEU:O	2.13	0.48
3:C:410:VAL:HG22	3:C:413[B]:GLU:HG2	1.94	0.48
1:A:85:SER:HA	1:A:109:GLY:HA3	1.96	0.48
13:O:184:ARG:NE	13:O:226:GLY:O	2.46	0.48
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.29	0.48
32:j:101:STE:O1	37:j:202:HOH:O	2.20	0.48
31:A:616:DGD:HB41	32:I:101:STE:H62	1.94	0.48
2:B:347:ARG:HA	2:B:352:GLU:O	2.14	0.48
4:D:150:ILE:O	4:D:154:VAL:HG13	2.13	0.48
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.95	0.48
3:c:334:PRO:HA	13:o:153:THR:OG1	2.13	0.48
13:o:59:LYS:HB2	13:o:61:GLN:HG2	1.95	0.48
2:B:2:GLY:N	11:L:11:GLU:OE2	2.47	0.48
30:D:409:LHG:HC62	11:L:15:THR:HG23	1.96	0.48
3:c:178:LYS:NZ	3:c:184:GLY:O	2.45	0.48
2:B:385:ARG:O	2:B:388:SER:OG	2.31	0.48
1:a:159[B]:LEU:HD22	1:a:163[B]:ILE:HD11	1.96	0.48
1:a:219:VAL:O	1:a:223:LEU:HD13	2.14	0.48
1:a:324:ALA:O	1:a:328[B]:MET:HG3	2.12	0.48
3:c:128:GLY:HA3	24:c:513:CLA:C3C	2.43	0.48
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.94	0.48
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.49	0.48
18:X:17:GLY:HA2	32:X:102:STE:H152	1.96	0.48
1:a:283:VAL:HA	1:a:286:THR:HG22	1.96	0.48
3:C:348:GLU:O	3:C:350:ILE:HG23	2.15	0.47
2:b:160:GLY:HA2	2:b:163:GLY:O	2.13	0.47
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.28	0.47
24:B:603:CLA:H42	24:B:604:CLA:H42	1.95	0.47
3:c:307:PRO:HA	3:c:358[B]:PHE:CD2	2.50	0.47
2:B:211:ILE:HG23	32:B:626:STE:H51	1.96	0.47
2:B:506:ARG:NH2	37:B:706:HOH:O	2.35	0.47
3:C:123:ALA:HB1	32:Z:101:STE:H162	1.96	0.47
17:V:87:GLU:CD	17:V:96:ARG:HH12	2.21	0.47
24:c:501:CLA:HBB1	26:c:515:BCR:H21C	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:27:ARG:O	13:O:27:ARG:HG2	2.15	0.47
1:a:84:PRO:HA	1:a:112:TYR:CG	2.50	0.47
4:d:134:ARG:HG2	32:d:409:STE:O1	2.14	0.47
2:B:118:TRP:CZ2	11:L:4:ASN:HA	2.49	0.47
30:L:101:LHG:H271	12:M:22:LEU:HD21	1.97	0.47
13:O:133:VAL:C	13:O:135:SER:H	2.22	0.47
1:a:189[B]:GLU:OE1	21:a:601[B]:OEY:O6	2.33	0.47
4:d:180:ARG:HD3	4:d:180:ARG:C	2.40	0.47
17:v:41:HIS:HA	17:v:45:ILE:O	2.15	0.47
1:a:296:ASN:HB3	3:c:401:LEU:HA	1.97	0.47
3:c:286:ALA:HB2	24:c:502:CLA:HMD2	1.97	0.47
9:J:26:GLY:HA2	32:J:101:STE:H81	1.97	0.47
6:f:26:LEU:O	6:f:29:PRO:HD2	2.15	0.47
28:A:611:PL9:H33	4:D:42:TYR:HB2	1.97	0.47
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.97	0.47
3:c:180:MET:HG2	3:c:199:ILE:O	2.15	0.47
24:B:608:CLA:NC	26:X:101:BCR:H332	2.30	0.46
32:B:623:STE:H162	24:H:101:CLA:H92	1.96	0.46
3:C:344:SER:O	13:O:75:THR:HG22	2.14	0.46
2:b:92:SER:O	2:b:96:VAL:HG23	2.16	0.46
20:z:39:LEU:O	20:z:43:GLY:N	2.45	0.46
1:A:288:LEU:HD22	3:C:432:VAL:HG22	1.96	0.46
1:A:329[A]:GLU:OE2	17:V:134:LYS:NZ	2.44	0.46
3:C:137:PRO:HD3	24:C:513:CLA:HED2	1.98	0.46
1:a:291:SER:HB3	3:c:431:PHE:CE2	2.51	0.46
24:b:604:CLA:H42	24:b:605:CLA:H2	1.97	0.46
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	1.98	0.46
31:c:516:DGD:HB42	33:c:522:LMG:H372	1.98	0.46
12:M:29:THR:HA	12:M:32:GLN:OE1	2.15	0.46
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.16	0.46
3:c:213:LEU:HD21	26:c:515:BCR:C20	2.45	0.46
3:c:26:ARG:HA	24:c:511:CLA:OBD	2.16	0.46
19:y:41:VAL:C	19:y:43:ARG:H	2.24	0.46
4:D:160:TYR:HA	4:D:290:ALA:HB2	1.96	0.46
18:x:24:THR:HG22	18:x:28:LEU:HD12	1.97	0.46
10:K:23:ASP:OD2	19:Y:21:GLN:NE2	2.49	0.46
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.51	0.46
3:c:134:ILE:HD12	24:c:511:CLA:H43	1.97	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.97	0.46
16:u:27:LEU:HD22	16:u:49:ILE:HG21	1.98	0.46
2:b:249:ALA:HB2	24:b:604:CLA:HBC3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:623:STE:H32	32:d:411:STE:H62	1.98	0.46
5:e:8:ARG:HG2	5:e:13:ILE:HG13	1.98	0.46
13:O:36:GLN:HG3	13:O:37:THR:N	2.31	0.45
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.52	0.45
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.98	0.45
4:d:148:ALA:HB3	4:d:149:PRO:HD3	1.97	0.45
10:k:35:LEU:HD13	10:k:35:LEU:O	2.16	0.45
10:K:26:PRO:O	10:K:29:PRO:HD2	2.16	0.45
13:O:57:LYS:HE2	13:O:57:LYS:HB3	1.83	0.45
19:Y:42:ARG:NH2	37:Y:201:HOH:O	2.10	0.45
3:c:410:VAL:HG22	3:c:413[A]:GLU:OE1	2.16	0.45
8:i:7:THR:O	8:i:11:VAL:HG23	2.16	0.45
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.98	0.45
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.99	0.45
7:h:6:TRP:NE1	7:h:10:ILE:HD11	2.32	0.45
3:C:318:LEU:C	3:C:318:LEU:HD23	2.42	0.45
3:C:367:GLU:N	3:C:368:PRO:CD	2.79	0.45
2:b:283:GLU:OE2	2:b:287:ARG:NE	2.43	0.45
24:c:508:CLA:HBC3	24:c:510:CLA:H92	1.97	0.45
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.97	0.45
31:A:616:DGD:HD5	2:b:75:TRP:HB3	1.98	0.45
2:B:477:ASP:OD1	2:B:477:ASP:N	2.49	0.45
24:C:503:CLA:HBB1	32:C:520:STE:H171	1.99	0.45
2:B:63:LEU:N	2:B:64:PRO:HD2	2.32	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.98	0.45
5:E:65:LEU:O	5:E:67:THR:HG23	2.16	0.45
10:K:27:VAL:HG21	33:Y:101:LMG:H191	1.98	0.45
2:b:103:LEU:HD22	24:b:606:CLA:H51	1.99	0.45
3:c:38:GLY:HA3	24:c:511:CLA:HMD2	1.98	0.45
24:c:507:CLA:O2A	24:c:507:CLA:HMA2	2.16	0.45
2:B:307:GLU:OE1	13:o:59:LYS:HD3	2.17	0.45
4:D:194:ASN:O	4:D:198:MET:HG3	2.17	0.45
4:d:272:LEU:C	4:d:272:LEU:HD23	2.42	0.45
3:C:71:GLU:HB3	3:C:86:LEU:HD22	1.98	0.45
1:a:296:ASN:HB2	3:c:400:PRO:O	2.17	0.45
4:d:194:ASN:HA	4:d:295:SER:OG	2.17	0.45
17:v:64:PRO:HD2	17:v:66:ARG:NH2	2.32	0.45
6:F:15:ILE:HD13	14:R:23:ILE:HD11	1.99	0.45
1:a:72:LEU:HD21	32:t:102:STE:H41	1.99	0.45
1:a:329[B]:GLU:O	1:a:332[B]:HIS:ND1	2.45	0.45
2:b:224:ARG:HG2	7:h:24:GLY:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:169:GLY:HA2	3:c:241:GLY:HA2	1.99	0.45
2:B:399:VAL:HG12	2:B:417:VAL:HG22	1.99	0.44
32:c:520:STE:C1	32:c:520:STE:H51	2.47	0.44
18:x:27:VAL:O	18:x:31:ILE:HG13	2.16	0.44
2:B:414:PRO:N	2:B:415:PRO:HD2	2.32	0.44
8:I:2:GLU:O	8:I:6:ILE:HG12	2.17	0.44
3:c:67:MET:HB3	3:c:88:LEU:HD12	1.99	0.44
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.44
19:Y:34:MET:O	19:Y:38:LEU:HG	2.18	0.44
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.44
4:D:272:LEU:C	4:D:272:LEU:HD23	2.42	0.44
3:C:213:LEU:HD21	26:C:514:BCR:C20	2.47	0.44
5:E:26:THR:HA	14:R:15:ALA:HB1	1.98	0.44
4:d:210:LEU:HA	4:d:213:ILE:HG22	1.99	0.44
2:b:294:SER:O	37:b:705:HOH:O	2.21	0.44
3:c:26:ARG:HB2	3:c:26:ARG:HH11	1.82	0.44
2:B:36:SER:OG	26:B:617:BCR:H362	2.18	0.44
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.44
12:M:33:GLN:C	37:M:201:HOH:O	2.61	0.44
13:O:204:VAL:HG22	13:O:211:ILE:HG22	1.99	0.44
3:c:394:GLU:OE1	37:c:603:HOH:O	2.21	0.44
4:d:267:LEU:C	4:d:267:LEU:HD23	2.42	0.44
2:B:159:THR:O	2:B:180:PRO:HB3	2.18	0.44
2:B:346:PHE:HA	2:B:398:THR:O	2.18	0.44
1:a:334[A]:ARG:HG3	13:o:157:LEU:HB2	2.00	0.44
26:B:617:BCR:H15C	26:B:617:BCR:H351	1.87	0.44
2:b:155:ALA:HB1	33:b:622:LMG:H122	1.99	0.44
1:A:110:GLY:N	1:A:111:PRO:CD	2.81	0.43
10:K:13:GLU:OE1	10:K:13:GLU:N	2.49	0.43
20:Z:47:TRP:CE3	32:Z:101:STE:H142	2.53	0.43
30:a:614:LHG:H132	30:a:614:LHG:H101	1.73	0.43
3:c:187:ASP:HB2	3:c:230:LEU:HD12	2.00	0.43
2:B:479[A]:PHE:O	4:D:139:ARG:NH2	2.44	0.43
35:F:101:HEM:HHD	35:F:101:HEM:CBC	2.40	0.43
26:b:617:BCR:H23C	26:b:617:BCR:H382	2.01	0.43
3:c:147:PHE:CD2	24:c:513:CLA:H3A	2.54	0.43
17:v:90:GLU:HB2	37:v:327:HOH:O	2.18	0.43
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.53	0.43
24:B:610:CLA:H203	24:B:612:CLA:H8	2.01	0.43
3:C:75:PHE:CZ	3:C:77:PRO:HA	2.53	0.43
11:L:14:ARG:HB3	15:T:25:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:103:LYS:HB2	37:V:339:HOH:O	2.18	0.43
24:b:604:CLA:H91	24:b:615:CLA:H42	2.00	0.43
13:o:72:THR:O	13:o:73:ARG:HB2	2.17	0.43
4:D:38:PHE:N	4:D:39:PRO:CD	2.80	0.43
2:b:293:ALA:C	2:b:295:GLY:H	2.26	0.43
4:d:241:GLU:CD	4:d:241:GLU:H	2.26	0.43
10:k:25:LEU:N	10:k:26:PRO:CD	2.82	0.43
2:B:29:LEU:HD23	29:B:620:SQD:H211	2.00	0.43
4:d:125:PHE:O	4:d:129:GLN:HG3	2.18	0.43
17:v:99:ASP:OD1	17:v:99:ASP:N	2.45	0.43
2:B:247:PHE:HE1	24:B:601:CLA:H102	1.84	0.43
3:C:215:LYS:HE2	3:C:221:GLU:O	2.19	0.43
10:K:24:VAL:HG21	19:Y:25:ILE:HB	1.99	0.43
1:a:339[B]:PHE:HB3	1:a:340[B]:PRO:HD2	1.99	0.43
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.43
16:u:58:VAL:HG12	16:u:79:LEU:HD22	2.00	0.43
2:B:119:ASP:H	11:L:1:MET:CE	2.31	0.43
24:B:605:CLA:H143	24:B:605:CLA:H111	1.84	0.43
3:C:216:SER:HB2	33:C:515:LMG:HC72	2.00	0.43
5:E:51:ARG:NE	37:E:702:HOH:O	2.19	0.43
32:d:410:STE:O1	37:d:501:HOH:O	2.21	0.43
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.01	0.43
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.01	0.43
2:B:414:PRO:O	2:B:418:LYS:HG3	2.18	0.43
7:H:43:LEU:HD22	7:H:47:GLU:OE2	2.19	0.43
24:H:101:CLA:H142	24:H:101:CLA:H112	1.81	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.43
16:U:10:VAL:HG11	16:U:15:GLU:OE2	2.18	0.43
24:b:601:CLA:H91	24:b:601:CLA:H111	1.83	0.43
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.48	0.43
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.84	0.43
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.54	0.43
24:A:612:CLA:HED2	4:D:198:MET:SD	2.58	0.43
2:B:43:ALA:HA	32:B:625:STE:H91	1.99	0.43
3:C:50:LEU:HD21	24:C:513:CLA:C1B	2.48	0.43
24:C:502:CLA:H141	24:C:502:CLA:H161	1.90	0.43
24:b:602:CLA:H43	7:h:45:ILE:HG22	2.00	0.43
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.01	0.43
3:C:457:LYS:HE2	4:D:227:GLU:O	2.19	0.43
24:C:505:CLA:HBC2	26:C:514:BCR:H341	2.01	0.43
6:F:21:VAL:O	6:F:25:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:321:ILE:HD11	4:d:179:PHE:HB2	2.00	0.43
1:a:328[B]:MET:HE1	4:d:183:LEU:HD22	2.00	0.43
3:c:350:ILE:HG21	3:c:359[B]:TRP:HB2	2.01	0.43
1:A:38:ILE:HG12	29:A:615:SQD:H141	2.01	0.42
2:B:353:GLU:HG2	2:B:355:PHE:CZ	2.53	0.42
2:B:506:ARG:NH1	37:B:706:HOH:O	2.42	0.42
10:K:25:LEU:N	10:K:26:PRO:HD2	2.34	0.42
1:a:201:GLY:HA3	1:a:286:THR:HB	2.00	0.42
3:c:342:MET:SD	3:c:356[B]:MET:HE2	2.59	0.42
4:d:85:MET:CE	5:e:69:ARG:HA	2.49	0.42
28:A:611:PL9:H451	28:A:611:PL9:H471	1.86	0.42
2:B:246:PHE:CD1	2:B:246:PHE:C	2.97	0.42
3:C:178:LYS:HA	3:C:182:PHE:HB2	2.00	0.42
4:D:192:THR:HG23	24:D:403:CLA:HBC2	2.01	0.42
5:E:30:LEU:HD11	35:F:101:HEM:HAB	2.00	0.42
2:b:127:ARG:NH2	7:h:18:TYR:O	2.47	0.42
2:b:264:PRO:HG2	2:b:267:LEU:HG	2.00	0.42
9:j:30:TYR:HA	32:j:101:STE:H22	2.01	0.42
24:C:505:CLA:H203	33:C:515:LMG:H132	2.00	0.42
1:a:217:SER:HA	4:d:272:LEU:HD12	2.01	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
1:A:329[A]:GLU:HG3	37:A:803:HOH:O	2.18	0.42
28:A:611:PL9:H422	28:A:611:PL9:H401	1.89	0.42
2:B:433:ASP:OD1	2:B:433:ASP:C	2.61	0.42
24:C:513:CLA:H61	24:C:513:CLA:H41	1.86	0.42
26:T:101:BCR:H321	26:T:101:BCR:HC8	2.02	0.42
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.55	0.42
7:h:49:TYR:CG	31:h:102:DGD:HB22	2.55	0.42
13:o:193:THR:HG21	13:o:220:LEU:HD12	2.02	0.42
2:B:119:ASP:H	11:L:1:MET:HE1	1.84	0.42
1:a:183[A]:MET:HG2	24:a:613:CLA:HBC1	2.01	0.42
2:b:153:PHE:CE2	2:b:158:LEU:HD11	2.55	0.42
13:o:53:LYS:HD2	13:o:232:GLU:OE2	2.19	0.42
16:u:53:ALA:HB1	16:u:54:PRO:CD	2.47	0.42
24:B:606:CLA:H193	24:B:606:CLA:H162	1.92	0.42
13:O:27:ARG:HG3	37:O:312:HOH:O	2.19	0.42
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.55	0.42
26:t:101:BCR:H23C	26:t:101:BCR:H382	2.02	0.42
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.45	0.42
24:A:612:CLA:H201	29:A:615:SQD:H222	2.01	0.42
24:B:610:CLA:H72	24:B:610:CLA:H112	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:9:LEU:HD23	14:R:9:LEU:HA	1.95	0.42
1:a:85:SER:HA	1:a:109:GLY:HA3	2.01	0.42
20:Z:46:LEU:O	20:Z:50:LEU:HB2	2.19	0.42
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.08	0.42
4:d:126:MET:HE3	4:d:143:ALA:O	2.20	0.42
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.55	0.42
1:A:344[B]:ALA:HA	37:A:736:HOH:O	2.20	0.42
24:B:605:CLA:H72	26:B:618:BCR:H311	2.00	0.42
24:B:605:CLA:H93	24:B:605:CLA:H112	1.79	0.42
20:Z:49:ALA:O	20:Z:53:VAL:HG23	2.19	0.42
4:d:161:PRO:HB3	4:d:170:ALA:HB2	2.01	0.42
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.02	0.42
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.02	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.55	0.41
3:C:148:GLY:O	3:C:156:LYS:NZ	2.49	0.41
3:C:222:GLY:O	3:C:223:TRP:C	2.63	0.41
14:R:24:LEU:N	14:R:25:PRO:HD2	2.34	0.41
4:d:93:TRP:HZ3	32:d:410:STE:H62	1.84	0.41
10:k:18:PHE:O	10:k:19:ASP:C	2.63	0.41
10:k:28:ILE:HD11	19:y:28:ILE:HD13	2.02	0.41
12:m:5:GLN:HA	12:m:5:GLN:HE21	1.85	0.41
1:A:40:THR:O	1:A:118:HIS:HB3	2.20	0.41
1:A:132:GLU:O	1:A:136:ARG:HG2	2.20	0.41
1:A:334[A]:ARG:HD3	4:D:320:LEU:HD13	2.02	0.41
1:a:114:LEU:C	1:a:114:LEU:HD23	2.45	0.41
2:b:486:LEU:HD11	2:b:490:GLN:NE2	2.35	0.41
28:d:405:PL9:H322	30:l:101:LHG:H222	2.02	0.41
16:u:68:THR:OG1	16:u:71:GLN:HG3	2.20	0.41
2:B:497:GLN:HB2	2:B:504:THR:HB	2.02	0.41
24:B:601:CLA:H43	7:H:45:ILE:HG22	2.01	0.41
12:M:6:LEU:HD12	33:M:101:LMG:HC92	2.02	0.41
12:M:25:LEU:HD12	12:M:25:LEU:HA	1.91	0.41
1:a:165[B]:GLN:NE2	1:a:294:ALA:O	2.53	0.41
1:a:300:PHE:HZ	31:c:518:DGD:HB61	1.85	0.41
30:a:614:LHG:H162	30:l:101:LHG:H281	2.02	0.41
2:b:86:ILE:HD12	2:b:88:PRO:HD3	2.02	0.41
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.56	0.41
4:d:96:GLU:HB2	37:d:503:HOH:O	2.21	0.41
17:v:93:PRO:HA	17:v:101:PHE:CD2	2.54	0.41
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	2.02	0.41
4:D:230:SER:HB2	37:D:530:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:K:102:BCR:H322	20:Z:17:PHE:CE2	2.56	0.41
12:M:12:ALA:O	12:M:16:LEU:HB2	2.20	0.41
13:O:133:VAL:O	13:O:135:SER:N	2.50	0.41
1:a:308:ASP:OD1	1:a:308:ASP:C	2.64	0.41
2:b:85:GLY:O	37:b:704:HOH:O	2.21	0.41
5:e:68:ASP:OD2	5:e:71:GLU:HB2	2.20	0.41
7:h:59:ASN:O	7:h:61:SER:N	2.52	0.41
1:A:163[A]:ILE:HD11	31:C:516:DGD:HA32	2.01	0.41
24:A:604:CLA:H122	24:A:604:CLA:H161	1.79	0.41
24:B:613:CLA:H41	24:B:613:CLA:H62	1.82	0.41
3:C:47:GLY:HA3	3:C:137:PRO:O	2.20	0.41
24:C:508:CLA:H142	24:C:508:CLA:H112	1.91	0.41
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.02	0.41
26:D:405:BCR:H20C	26:D:405:BCR:H361	1.94	0.41
1:a:81:ALA:HB2	1:a:175[B]:GLY:HA3	2.02	0.41
17:v:120:LEU:HD23	17:v:120:LEU:HA	1.95	0.41
1:A:334[B]:ARG:HD3	4:D:320:LEU:HD13	2.03	0.41
2:B:141:ILE:O	2:B:145:LEU:HG	2.20	0.41
3:C:195:ASP:OD1	3:C:196:VAL:N	2.54	0.41
2:b:36:SER:OG	26:b:618:BCR:H362	2.20	0.41
24:b:609:CLA:HBA1	24:b:610:CLA:CBB	2.50	0.41
24:d:403:CLA:H91	24:d:403:CLA:H111	1.87	0.41
17:v:3:LEU:HD12	17:v:3:LEU:HA	1.93	0.41
31:A:616:DGD:HBN1	8:I:7:THR:HG21	2.02	0.41
26:D:405:BCR:H23C	26:D:405:BCR:H392	2.03	0.41
17:v:76:MET:HE1	17:v:115:ILE:HD12	2.02	0.41
7:H:47:GLU:OE2	37:H:201:HOH:O	2.21	0.41
3:c:269:GLU:OE2	3:c:444:HIS:ND1	2.37	0.41
7:h:25:TRP:O	7:h:26:GLY:C	2.64	0.41
10:k:16:ALA:C	10:k:18:PHE:N	2.79	0.41
17:v:32:LEU:HD13	17:v:111:ASP:HB3	2.02	0.41
1:A:211:PHE:CD1	28:A:611:PL9:H111	2.55	0.41
2:B:52:LEU:HD12	13:o:59:LYS:HE2	2.02	0.41
2:b:220:ARG:HG3	7:h:20:LYS:HG2	2.03	0.41
3:c:367:GLU:N	3:c:368:PRO:CD	2.83	0.41
33:c:521:LMG:H411	33:c:521:LMG:H441	1.83	0.41
26:d:404:BCR:C8	26:d:404:BCR:H331	2.50	0.41
2:B:55:MET:HE2	2:B:55:MET:HB3	1.98	0.41
26:B:617:BCR:H20C	26:B:617:BCR:H361	1.92	0.41
3:C:213:LEU:HG	24:C:506:CLA:H193	2.03	0.41
17:V:122:GLU:N	17:V:123:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:283:VAL:HG21	25:a:606:PHO:HBC3	2.02	0.41
3:c:147:PHE:CE2	24:c:513:CLA:H3A	2.56	0.41
24:c:511:CLA:H11	10:k:39:TRP:CZ2	2.56	0.41
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.55	0.41
2:B:382:PRO:HG2	2:B:385:ARG:HD2	2.03	0.40
12:M:17:VAL:HB	12:M:18:PRO:HD3	2.02	0.40
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.02	0.40
24:b:602:CLA:H193	24:b:602:CLA:H161	1.86	0.40
24:c:501:CLA:CBB	26:c:515:BCR:H21C	2.51	0.40
32:d:411:STE:H82	32:h:103:STE:H62	2.03	0.40
5:e:36:LEU:HD23	5:e:36:LEU:HA	1.95	0.40
1:A:65[B]:GLU:OE2	1:A:334[B]:ARG:NH2	2.54	0.40
24:D:403:CLA:HBC3	24:D:403:CLA:HHD	2.02	0.40
29:D:408:SQD:H341	29:D:408:SQD:H372	1.90	0.40
1:a:16:ARG:HB3	1:a:16:ARG:NH1	2.34	0.40
24:c:508:CLA:H142	24:c:508:CLA:H111	1.91	0.40
24:c:513:CLA:H101	24:c:513:CLA:H62	1.89	0.40
1:A:91:LEU:HD11	1:A:166[B]:GLY:HA2	2.03	0.40
1:A:214:MET:SD	25:A:606:PHO:CAD	3.10	0.40
2:B:41:GLU:HB3	2:B:60:MET:SD	2.61	0.40
26:B:618:BCR:H323	32:B:619:STE:H91	2.03	0.40
24:C:507:CLA:H192	24:C:507:CLA:H162	1.92	0.40
26:k:101:BCR:H321	26:k:101:BCR:HC8	2.03	0.40
20:z:31:GLN:H	20:z:31:GLN:HG3	1.59	0.40
1:A:189[B]:GLU:OE1	21:A:601[B]:OEY:O6	2.39	0.40
26:K:101:BCR:H24C	26:K:101:BCR:H371	1.86	0.40
26:K:102:BCR:H10C	19:Y:28:ILE:HG23	2.03	0.40
18:X:16:SER:HB3	32:X:102:STE:H112	2.03	0.40
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.56	0.40
24:c:509:CLA:H141	24:c:509:CLA:H161	1.81	0.40
35:f:101:HEM:HBC2	35:f:101:HEM:CMC	2.52	0.40
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.03	0.40
17:v:55:ARG:O	17:v:59:LEU:HG	2.22	0.40
1:A:184[B]:ILE:HG23	1:A:328[B]:MET:SD	2.61	0.40
30:D:410:LHG:H141	30:D:410:LHG:H322	2.04	0.40
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	2.03	0.40
2:b:341:LYS:HG3	2:b:429:ILE:HG22	2.04	0.40
3:c:352:GLY:O	3:c:355[A]:THR:HG22	2.21	0.40
25:d:401:PHO:H72	25:d:401:PHO:H112	1.84	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%)	384 (97%)	12 (3%)	1 (0%)	36	38
1	a	397/344 (115%)	390 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	499 (98%)	9 (2%)	0	100	100
2	b	503/510 (99%)	488 (97%)	13 (3%)	2 (0%)	30	30
3	C	454/461 (98%)	441 (97%)	12 (3%)	1 (0%)	43	48
3	c	463/461 (100%)	453 (98%)	9 (2%)	1 (0%)	43	48
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	330 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	77 (96%)	2 (2%)	1 (1%)	9	5
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%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	57 (93%)	3 (5%)	1 (2%)	7	4
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	1 (3%)	1 (3%)	3	1
9	J	34/40 (85%)	31 (91%)	2 (6%)	1 (3%)	3	1
9	j	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	33 (94%)	2 (6%)	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%)	226 (93%)	12 (5%)	5 (2%)	5	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	30	30
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	24 (92%)	2 (8%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	7
17	V	135/163 (83%)	128 (95%)	6 (4%)	1 (1%)	18	16
17	v	135/163 (83%)	130 (96%)	5 (4%)	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
20	Z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
20	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5387/5700 (94%)	5206 (97%)	164 (3%)	17 (0%)	36	38

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	V	64	PRO
3	c	416	SER
3	C	416	SER
13	O	36	GLN
13	O	59	LYS
13	O	60	ARG
16	u	53	ALA
13	O	57	LYS
13	O	62	GLU
13	o	73	ARG
2	b	127	ARG
2	b	294	SER
5	e	83	LEU
8	i	33	LYS
9	J	6	GLY
1	A	259	ILE
7	h	60	VAL

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%)	320 (99%)	4 (1%)	63	72
1	a	323/280 (115%)	312 (97%)	11 (3%)	32	38
2	B	408/407 (100%)	397 (97%)	11 (3%)	39	47
2	b	402/407 (99%)	392 (98%)	10 (2%)	42	50
3	C	356/362 (98%)	346 (97%)	10 (3%)	38	45
3	c	364/362 (101%)	351 (96%)	13 (4%)	31	36
4	D	277/283 (98%)	269 (97%)	8 (3%)	37	44
4	d	278/283 (98%)	267 (96%)	11 (4%)	28	32
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	45
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	29
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	36
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	59
7	h	53/55 (96%)	48 (91%)	5 (9%)	8	5
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	41
8	i	32/34 (94%)	32 (100%)	0	100	100
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	29
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	2
10	K	30/37 (81%)	25 (83%)	5 (17%)	2	0
10	k	30/37 (81%)	26 (87%)	4 (13%)	4	2
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/32 (88%)	26 (93%)	2 (7%)	13	11
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	11
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	23
13	o	207/228 (91%)	197 (95%)	10 (5%)	23	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	R	22/33 (67%)	20 (91%)	2 (9%)	9	5
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	0
15	T	26/28 (93%)	26 (100%)	0	100	100
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	23
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	72
17	V	117/138 (85%)	115 (98%)	2 (2%)	53	63
17	v	117/138 (85%)	114 (97%)	3 (3%)	40	48
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	13
18	x	31/34 (91%)	30 (97%)	1 (3%)	34	40
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	3
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	5
20	Z	52/52 (100%)	42 (81%)	10 (19%)	1	0
20	z	51/52 (98%)	47 (92%)	4 (8%)	11	8
All	All	4451/4654 (96%)	4279 (96%)	172 (4%)	28	33

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	205	VAL
1	A	243	GLU
2	B	87	ASP
2	B	98	LEU
2	B	121	GLU
2	B	127	ARG
2	B	362	PHE
2	B	371	THR
2	B	374	ASN
2	B	385	ARG
2	B	387	GLU
2	B	388	SER
2	B	476	ARG
3	C	104	GLU
3	C	106	VAL
3	C	130	VAL

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Mol	Chain	Res	Type
3	C	138	GLU
3	C	141	GLU
3	C	213	LEU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	380	ILE
4	D	43	LEU
4	D	136	VAL
4	D	154	VAL
4	D	233	ARG
4	D	248	THR
4	D	264	LYS
4	D	272	LEU
4	D	329	MET
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
7	H	56	ASP
8	I	4	LEU
9	J	24	ILE
10	K	10	LYS
10	K	19	ASP
10	K	24	VAL
10	K	25	LEU
10	K	27	VAL
12	M	16	LEU
12	M	25	LEU
13	O	23	ASP
13	O	37	THR
13	O	78	LEU
13	O	107	THR
13	O	118	LEU
13	O	135	SER
13	O	184	ARG
13	O	189	ARG
13	O	214	THR
13	O	243	ILE
14	R	6	LEU
14	R	22	ASN
16	U	24	LYS
16	U	51	LYS

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Mol	Chain	Res	Type
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	37	CYS
18	X	3	ILE
18	X	15	LEU
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	6	GLN
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	19	MET
20	Z	25	VAL
20	Z	34	ASP
20	Z	50	LEU
20	Z	52	LEU
1	a	16	ARG
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	224	ILE
1	a	231	GLU
1	a	245	THR
1	a	288	LEU
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	227	LYS
2	b	234	ILE
2	b	236	THR
2	b	240	SER
2	b	315	ILE
2	b	438	ASN
2	b	506	ARG
3	c	26	ARG
3	c	29	GLU
3	c	72	LEU

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Mol	Chain	Res	Type
3	c	79	LYS
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	289	PHE
3	c	315	MET
3	c	468	SER
4	d	90	LEU
4	d	103	ARG
4	d	144	ILE
4	d	182	LEU
4	d	241	GLU
4	d	259	ILE
4	d	272	LEU
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	8	ARG
5	e	65	LEU
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	12	ARG
7	h	27	THR
7	h	41	PHE
7	h	56	ASP
9	j	7	ARG
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	27	VAL
10	k	30	VAL
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU

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Mol	Chain	Res	Type
12	m	13	LEU
12	m	16	LEU
13	o	23	ASP
13	o	49	THR
13	o	55	GLU
13	o	64	GLU
13	o	86	LYS
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	135	SER
14	r	5	VAL
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	24	LEU
16	u	15	GLU
17	v	14	SER
17	v	52	LEU
17	v	107	LEU
18	x	15	LEU
19	y	19	ILE
19	y	46	LEU
20	z	1	MET
20	z	7	LEU
20	z	31	GLN
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	223	GLN
2	B	289	GLN
2	B	394	GLN
2	B	409	GLN
2	B	490	GLN
3	C	74	HIS
3	C	201	ASN
4	D	336	HIS
11	L	8	GLN
13	O	3	GLN

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Mol	Chain	Res	Type
13	O	88	ASN
13	O	155	ASN
13	O	231	HIS
14	R	22	ASN
16	U	81	HIS
17	V	86	GLN
17	V	106	ASN
18	X	38	GLN
19	Y	21	GLN
19	Y	45	ASN
1	a	19	ASN
1	a	234	ASN
2	b	338	GLN
2	b	409	GLN
2	b	490	GLN
3	c	415	ASN
4	d	255	GLN
12	m	5	GLN
13	o	61	GLN
13	o	155	ASN
18	x	33	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	$\# Z > 2$
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	1.01	0
15	FME	T	1	15	8,9,10	1.11	1 (12%)	8,9,11	1.48	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	FME	M	1	12	8,9,10	0.88	0	8,9,11	0.87	0
15	FME	t	1	15	8,9,10	1.26	1 (12%)	8,9,11	0.79	0
8	FME	i	1	8	8,9,10	1.14	1 (12%)	8,9,11	1.06	1 (12%)
12	FME	m	1	12	8,9,10	0.90	0	8,9,11	1.09	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
8	FME	I	1	8	-	1/7/9/11	-
15	FME	T	1	15	-	1/7/9/11	-
12	FME	M	1	12	-	2/7/9/11	-
15	FME	t	1	15	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-2.96	1.42	1.46
8	i	1	FME	CA-N	-2.42	1.43	1.46
15	T	1	FME	CA-N	-2.03	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	CA-N-CN	3.03	127.49	122.82
15	T	1	FME	CB-CA-N	2.09	114.32	110.52
12	m	1	FME	CA-N-CN	-2.06	119.65	122.82
8	i	1	FME	CB-CA-N	2.01	114.18	110.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
12	m	1	FME	O-C-CA-CB
15	t	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
15	T	1	FME	CB-CG-SD-CE
15	t	1	FME	CB-CG-SD-CE
12	M	1	FME	CA-CB-CG-SD
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 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
26	BCR	c	515	-	41,41,41	1.28	5 (12%)	56,56,56	1.48	10 (17%)
32	STE	t	102	-	13,13,19	0.70	0	13,13,19	1.33	2 (15%)
32	STE	B	622	-	17,17,19	0.71	0	17,17,19	0.97	1 (5%)
24	CLA	C	502	-	69,73,73	1.12	5 (7%)	82,113,113	1.24	7 (8%)
32	STE	M	104	-	17,17,19	0.37	0	16,16,19	0.86	0
33	LMG	C	515	-	48,48,55	1.21	5 (10%)	56,56,63	1.57	12 (21%)
26	BCR	T	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.26	4 (7%)
33	LMG	a	619	-	55,55,55	1.40	8 (14%)	63,63,63	1.49	10 (15%)
26	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.31	9 (16%)
33	LMG	c	519	-	37,37,55	1.23	5 (13%)	45,45,63	1.33	6 (13%)
22	OEX	a	602[A]	3,37,1	0,15,15	-	-	-	-	-
26	BCR	d	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	4 (7%)
25	PHO	D	401	-	58,69,69	1.83	13 (22%)	55,99,99	1.50	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	d	409	-	16,16,19	0.67	0	16,16,19	1.30	2 (12%)
30	LHG	L	101	-	48,48,48	0.76	2 (4%)	51,54,54	1.18	3 (5%)
29	SQD	D	408	-	34,36,54	0.95	2 (5%)	42,45,65	1.75	8 (19%)
32	STE	b	621	-	19,19,19	0.79	1 (5%)	19,19,19	1.05	0
26	BCR	k	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.09	4 (7%)
24	CLA	A	605	37	69,73,73	1.39	8 (11%)	82,113,113	1.31	10 (12%)
34	BCT	a	611	23	3,3,3	1.03	0	2,3,3	3.16	1 (50%)
24	CLA	B	612	-	69,73,73	1.48	8 (11%)	82,113,113	1.51	11 (13%)
21	OEY	a	601[B]	3,37,1	0,16,16	-	-	-	-	-
24	CLA	c	507	37	69,73,73	1.71	7 (10%)	82,113,113	1.42	9 (10%)
21	OEY	A	601[B]	3,37,1	0,16,16	-	-	-	-	-
24	CLA	C	508	-	69,73,73	1.35	6 (8%)	82,113,113	1.29	9 (10%)
24	CLA	b	609	-	69,73,73	1.49	8 (11%)	82,113,113	1.39	7 (8%)
24	CLA	B	613	-	69,73,73	1.52	9 (13%)	82,113,113	1.29	10 (12%)
24	CLA	c	510	-	69,73,73	1.26	7 (10%)	82,113,113	1.50	9 (10%)
26	BCR	B	618	-	41,41,41	1.19	3 (7%)	56,56,56	1.38	10 (17%)
31	DGD	C	517	-	63,63,67	1.12	4 (6%)	77,77,81	1.38	9 (11%)
30	LHG	D	409	-	48,48,48	1.19	5 (10%)	51,54,54	1.24	5 (9%)
32	STE	B	621	-	11,11,19	1.01	1 (9%)	11,11,19	1.11	0
24	CLA	b	615	-	69,73,73	1.45	11 (15%)	82,113,113	1.25	7 (8%)
24	CLA	B	602	-	69,73,73	1.23	11 (15%)	82,113,113	1.32	8 (9%)
36	HEC	v	201	17	46,50,50	1.87	6 (13%)	58,82,82	1.97	12 (20%)
30	LHG	a	614	-	48,48,48	1.09	4 (8%)	51,54,54	1.36	7 (13%)
24	CLA	B	606	37	69,73,73	1.34	9 (13%)	82,113,113	1.46	6 (7%)
33	LMG	Y	101	-	48,48,55	1.27	7 (14%)	56,56,63	1.29	5 (8%)
32	STE	d	410	-	19,19,19	0.62	0	19,19,19	1.02	1 (5%)
29	SQD	b	620	-	47,49,54	0.96	2 (4%)	57,60,65	2.50	15 (26%)
24	CLA	B	607	-	69,73,73	1.39	9 (13%)	82,113,113	1.54	11 (13%)
24	CLA	C	501	-	69,73,73	1.37	10 (14%)	82,113,113	1.31	10 (12%)
32	STE	a	618	-	11,11,19	0.92	0	11,11,19	0.98	0
32	STE	c	520	-	19,19,19	0.78	1 (5%)	19,19,19	1.00	1 (5%)
32	STE	C	521	-	11,11,19	0.84	0	11,11,19	1.02	1 (9%)
24	CLA	b	606	-	69,73,73	1.30	7 (10%)	82,113,113	1.63	12 (14%)
32	STE	C	520	-	15,15,19	0.46	0	14,14,19	0.63	0
24	CLA	C	511	3	69,73,73	1.51	11 (15%)	82,113,113	1.18	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	613	-	69,73,73	1.26	8 (11%)	82,113,113	1.25	7 (8%)
33	LMG	c	522	-	49,49,55	0.99	4 (8%)	57,57,63	1.26	3 (5%)
26	BCR	K	103	-	41,41,41	1.29	4 (9%)	56,56,56	1.29	7 (12%)
32	STE	T	102	-	15,15,19	0.38	0	14,14,19	0.82	0
33	LMG	d	408	-	44,44,55	1.00	3 (6%)	52,52,63	1.25	4 (7%)
33	LMG	D	407	-	51,51,55	1.00	4 (7%)	59,59,63	1.35	6 (10%)
32	STE	C	519	-	11,11,19	1.08	2 (18%)	11,11,19	0.75	0
32	STE	d	411	-	19,19,19	0.58	0	19,19,19	1.10	1 (5%)
34	BCT	D	402	23	3,3,3	1.05	0	2,3,3	2.99	1 (50%)
26	BCR	t	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.45	8 (14%)
24	CLA	C	505	-	69,73,73	1.44	10 (14%)	82,113,113	1.28	9 (10%)
29	SQD	a	615	-	52,54,54	0.96	6 (11%)	62,65,65	2.01	11 (17%)
33	LMG	D	411	-	31,31,55	1.02	3 (9%)	33,33,63	1.20	3 (9%)
32	STE	Z	101	-	7,7,19	0.50	0	6,6,19	0.39	0
26	BCR	a	608	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	9 (16%)
30	LHG	d	406	-	48,48,48	0.84	2 (4%)	51,54,54	1.21	4 (7%)
24	CLA	C	506	-	69,73,73	1.45	8 (11%)	82,113,113	1.36	7 (8%)
30	LHG	e	101	-	41,41,48	1.01	1 (2%)	44,47,54	1.31	6 (13%)
32	STE	R	101	-	11,11,19	0.88	0	11,11,19	1.18	1 (9%)
32	STE	c	523	-	11,11,19	0.80	0	11,11,19	1.08	1 (9%)
24	CLA	A	612	37	69,73,73	1.04	3 (4%)	82,113,113	1.40	10 (12%)
31	DGD	A	616	-	67,67,67	1.26	9 (13%)	81,81,81	1.45	14 (17%)
29	SQD	A	613	-	50,52,54	1.11	6 (12%)	60,63,65	2.02	13 (21%)
24	CLA	b	603	-	69,73,73	1.25	9 (13%)	82,113,113	1.39	6 (7%)
24	CLA	B	615	-	64,68,73	1.44	10 (15%)	76,107,113	1.52	5 (6%)
32	STE	b	624	-	19,19,19	0.64	0	19,19,19	1.05	1 (5%)
26	BCR	B	617	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	8 (14%)
24	CLA	B	603	-	69,73,73	1.51	9 (13%)	82,113,113	1.85	11 (13%)
24	CLA	C	509	-	69,73,73	1.30	9 (13%)	82,113,113	1.41	11 (13%)
24	CLA	B	614	-	69,73,73	1.48	10 (14%)	82,113,113	1.40	6 (7%)
28	PL9	d	405	-	55,55,55	1.50	5 (9%)	68,69,69	1.56	14 (20%)
26	BCR	B	616	-	41,41,41	1.15	3 (7%)	56,56,56	1.46	8 (14%)
32	STE	b	623	-	15,15,19	0.92	1 (6%)	15,15,19	1.02	2 (13%)
24	CLA	a	604	-	69,73,73	1.52	13 (18%)	82,113,113	1.21	6 (7%)
25	PHO	a	606	-	58,69,69	2.10	8 (13%)	55,99,99	1.39	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	T	103	-	14,14,19	0.42	0	13,13,19	0.83	0
26	BCR	D	405	-	41,41,41	1.25	2 (4%)	56,56,56	1.15	5 (8%)
31	DGD	H	102	-	63,63,67	1.32	7 (11%)	77,77,81	1.40	8 (10%)
26	BCR	c	514	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
32	STE	B	625	-	14,14,19	0.45	0	13,13,19	0.82	0
24	CLA	a	607	-	69,73,73	1.34	10 (14%)	82,113,113	1.18	6 (7%)
24	CLA	a	605	37	69,73,73	1.50	9 (13%)	82,113,113	1.23	6 (7%)
30	LHG	D	413	-	48,48,48	1.05	3 (6%)	51,54,54	1.34	7 (13%)
24	CLA	d	403	-	69,73,73	1.33	9 (13%)	82,113,113	1.08	5 (6%)
26	BCR	A	608	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	8 (14%)
24	CLA	c	509	-	69,73,73	1.21	7 (10%)	82,113,113	1.46	7 (8%)
24	CLA	C	503	-	69,73,73	1.40	9 (13%)	82,113,113	1.45	10 (12%)
26	BCR	h	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.32	10 (17%)
32	STE	h	103	-	13,13,19	0.44	0	12,12,19	0.64	0
32	STE	j	101	-	11,11,19	0.90	0	11,11,19	0.96	0
29	SQD	A	615	-	38,38,54	1.06	3 (7%)	40,40,65	1.42	4 (10%)
24	CLA	H	101	37	69,73,73	1.37	8 (11%)	82,113,113	1.32	6 (7%)
26	BCR	b	617	-	41,41,41	1.07	4 (9%)	56,56,56	1.27	6 (10%)
30	LHG	A	614	-	48,48,48	0.84	2 (4%)	51,54,54	1.24	6 (11%)
35	HEM	f	101	5,6	50,50,50	1.40	10 (20%)	67,82,82	1.20	6 (8%)
24	CLA	B	610	-	69,73,73	1.21	7 (10%)	82,113,113	1.25	7 (8%)
24	CLA	b	608	-	69,73,73	1.58	12 (17%)	82,113,113	1.30	12 (14%)
24	CLA	B	609	37	69,73,73	1.54	12 (17%)	82,113,113	1.35	9 (10%)
24	CLA	c	502	-	69,73,73	1.50	9 (13%)	82,113,113	1.40	11 (13%)
24	CLA	C	504	37	63,67,73	1.53	10 (15%)	74,105,113	1.29	12 (16%)
30	LHG	d	407	-	38,38,48	0.97	2 (5%)	41,44,54	1.18	3 (7%)
35	HEM	F	101	5,6	50,50,50	1.67	7 (14%)	67,82,82	1.04	2 (2%)
32	STE	a	617	-	9,9,19	0.54	0	8,8,19	0.57	0
32	STE	B	624	-	15,15,19	0.53	0	14,14,19	0.57	0
32	STE	b	625	-	9,9,19	0.42	0	8,8,19	0.53	0
26	BCR	C	514	-	41,41,41	1.34	3 (7%)	56,56,56	1.19	3 (5%)
24	CLA	b	605	-	69,73,73	1.21	8 (11%)	82,113,113	1.40	8 (9%)
30	LHG	l	101	-	48,48,48	0.79	2 (4%)	51,54,54	1.26	5 (9%)
31	DGD	c	517	-	63,63,67	1.12	4 (6%)	77,77,81	1.31	7 (9%)
32	STE	M	102	-	14,14,19	0.81	0	14,14,19	0.99	0
24	CLA	b	616	-	64,68,73	1.20	9 (14%)	76,107,113	1.44	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	604	-	69,73,73	1.44	11 (15%)	82,113,113	1.16	5 (6%)
31	DGD	c	516	-	63,63,67	1.28	7 (11%)	77,77,81	1.44	14 (18%)
26	BCR	K	102	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	4 (7%)
24	CLA	B	601	-	69,73,73	1.25	9 (13%)	82,113,113	1.33	11 (13%)
30	LHG	D	410	-	46,46,48	1.15	4 (8%)	49,52,54	1.19	2 (4%)
32	STE	J	101	-	11,11,19	0.77	0	11,11,19	1.31	2 (18%)
32	STE	M	103	-	9,9,19	0.50	0	8,8,19	0.57	0
24	CLA	B	608	-	69,73,73	1.27	8 (11%)	82,113,113	1.41	6 (7%)
24	CLA	d	402	-	69,73,73	1.08	6 (8%)	82,113,113	1.18	6 (7%)
24	CLA	b	604	-	69,73,73	1.20	5 (7%)	82,113,113	1.84	13 (15%)
24	CLA	b	607	37	69,73,73	1.52	9 (13%)	82,113,113	1.31	8 (9%)
24	CLA	B	605	-	69,73,73	1.53	9 (13%)	82,113,113	1.25	10 (12%)
33	LMG	D	412	-	26,26,55	0.80	1 (3%)	26,26,63	1.26	1 (3%)
24	CLA	b	601	37	69,73,73	1.35	8 (11%)	82,113,113	1.50	7 (8%)
25	PHO	d	401	-	58,69,69	2.18	11 (18%)	55,99,99	1.62	9 (16%)
31	DGD	c	518	-	63,63,67	1.09	6 (9%)	77,77,81	1.39	12 (15%)
24	CLA	c	505	-	69,73,73	1.18	6 (8%)	82,113,113	1.59	11 (13%)
33	LMG	b	622	-	55,55,55	0.92	3 (5%)	63,63,63	1.51	11 (17%)
32	STE	B	623	-	17,17,19	0.45	0	16,16,19	0.77	0
25	PHO	A	606	-	58,69,69	1.92	9 (15%)	55,99,99	1.71	11 (20%)
26	BCR	b	618	-	41,41,41	1.39	3 (7%)	56,56,56	1.35	9 (16%)
24	CLA	c	512	-	69,73,73	1.14	8 (11%)	82,113,113	1.41	9 (10%)
22	OEX	A	602[A]	3,37,1	0,15,15	-	-	-	-	-
24	CLA	C	507	37	69,73,73	1.64	10 (14%)	82,113,113	1.54	9 (10%)
24	CLA	b	612	-	69,73,73	1.46	8 (11%)	82,113,113	1.38	13 (15%)
24	CLA	c	501	-	69,73,73	1.26	9 (13%)	82,113,113	1.32	6 (7%)
29	SQD	f	102	-	39,41,54	1.09	3 (7%)	49,52,65	1.76	10 (20%)
24	CLA	D	403	-	69,73,73	1.39	9 (13%)	82,113,113	1.33	9 (10%)
28	PL9	a	612	-	55,55,55	0.92	1 (1%)	68,69,69	1.52	11 (16%)
24	CLA	C	513	-	69,73,73	1.40	12 (17%)	82,113,113	1.49	13 (15%)
32	STE	B	619	-	16,16,19	0.76	1 (6%)	16,16,19	1.03	1 (6%)
24	CLA	b	614	-	69,73,73	1.21	8 (11%)	82,113,113	1.28	7 (8%)
32	STE	X	102	-	19,19,19	0.63	0	19,19,19	1.03	0
26	BCR	K	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.22	7 (12%)
26	BCR	k	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.13	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	604	-	69,73,73	1.48	11 (15%)	82,113,113	1.42	11 (13%)
24	CLA	c	506	-	69,73,73	1.32	9 (13%)	82,113,113	1.29	7 (8%)
29	SQD	B	620	-	52,54,54	0.96	2 (3%)	62,65,65	2.16	13 (20%)
24	CLA	c	508	-	68,72,73	1.42	11 (16%)	80,111,113	1.38	9 (11%)
33	LMG	m	101	-	51,51,55	1.23	4 (7%)	59,59,63	1.57	8 (13%)
31	DGD	C	516	-	63,63,67	1.40	11 (17%)	77,77,81	1.33	12 (15%)
24	CLA	B	611	-	69,73,73	1.31	10 (14%)	82,113,113	1.53	10 (12%)
32	STE	L	102	-	11,11,19	0.77	0	11,11,19	1.36	2 (18%)
31	DGD	h	102	-	63,63,67	1.19	8 (12%)	77,77,81	1.35	9 (11%)
24	CLA	c	513	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	11 (13%)
24	CLA	c	511	3	69,73,73	1.50	10 (14%)	82,113,113	1.38	7 (8%)
24	CLA	a	613	37	69,73,73	1.45	9 (13%)	82,113,113	1.26	9 (10%)
24	CLA	b	610	37	69,73,73	1.09	6 (8%)	82,113,113	1.44	10 (12%)
24	CLA	b	611	-	69,73,73	1.29	7 (10%)	82,113,113	1.36	10 (12%)
32	STE	B	626	-	11,11,19	0.74	0	11,11,19	0.99	0
24	CLA	c	504	37	64,68,73	1.24	5 (7%)	76,107,113	1.36	13 (17%)
24	CLA	b	602	-	69,73,73	1.18	9 (13%)	82,113,113	1.39	10 (12%)
24	CLA	A	607	-	58,62,73	1.35	11 (18%)	68,99,113	1.41	9 (13%)
26	BCR	X	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.39	7 (12%)
29	SQD	a	616	-	35,35,54	1.07	2 (5%)	37,37,65	1.18	3 (8%)
36	HEC	V	201	17	46,50,50	1.75	6 (13%)	58,82,82	1.83	6 (10%)
24	CLA	C	510	-	69,73,73	1.30	10 (14%)	82,113,113	1.27	5 (6%)
31	DGD	C	518	-	63,63,67	1.18	8 (12%)	77,77,81	1.39	8 (10%)
24	CLA	D	404	-	69,73,73	1.40	10 (14%)	82,113,113	1.28	10 (12%)
28	PL9	A	611	-	55,55,55	1.22	5 (9%)	68,69,69	1.70	15 (22%)
32	STE	I	101	-	14,14,19	0.53	0	13,13,19	0.61	0
33	LMG	M	101	-	51,51,55	1.03	5 (9%)	59,59,63	1.40	9 (15%)
28	PL9	D	406	-	55,55,55	1.27	5 (9%)	68,69,69	1.83	17 (25%)
24	CLA	c	503	-	69,73,73	1.18	5 (7%)	82,113,113	1.16	4 (4%)
33	LMG	c	521	-	48,48,55	1.20	5 (10%)	56,56,63	1.30	5 (8%)
24	CLA	C	512	-	69,73,73	1.57	9 (13%)	82,113,113	1.36	11 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	c	515	-	-	5/29/63/63	0/2/2/2
32	STE	t	102	-	-	2/11/11/17	-
32	STE	B	622	-	-	8/15/15/17	-
24	CLA	C	502	-	1/1/20/20	5/39/115/115	-
32	STE	M	104	-	-	10/15/15/17	-
33	LMG	C	515	-	-	16/43/63/70	0/1/1/1
26	BCR	T	101	-	-	11/29/63/63	0/2/2/2
33	LMG	a	619	-	-	36/50/70/70	0/1/1/1
26	BCR	b	619	-	-	4/29/63/63	0/2/2/2
33	LMG	c	519	-	-	9/31/51/70	0/1/1/1
26	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	PHO	D	401	-	-	2/37/103/103	0/5/6/6
32	STE	d	409	-	-	12/14/14/17	-
30	LHG	L	101	-	-	19/53/53/53	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
32	STE	b	621	-	-	9/17/17/17	-
26	BCR	k	101	-	-	11/29/63/63	0/2/2/2
24	CLA	A	605	37	1/1/20/20	11/39/115/115	-
24	CLA	B	612	-	1/1/20/20	10/39/115/115	-
24	CLA	c	507	37	1/1/20/20	11/39/115/115	-
24	CLA	B	613	-	1/1/20/20	15/39/115/115	-
24	CLA	C	508	-	-	5/39/115/115	-
24	CLA	b	609	-	-	8/39/115/115	-
24	CLA	c	510	-	1/1/20/20	11/39/115/115	-
26	BCR	B	618	-	-	5/29/63/63	0/2/2/2
31	DGD	C	517	-	-	18/51/91/95	0/2/2/2
30	LHG	D	409	-	-	21/53/53/53	-
32	STE	B	621	-	-	6/9/9/17	-
24	CLA	b	615	-	1/1/20/20	4/39/115/115	-
24	CLA	B	602	-	1/1/20/20	12/39/115/115	-
36	HEC	v	201	17	-	6/14/54/54	-
30	LHG	a	614	-	-	24/53/53/53	-
24	CLA	B	606	37	1/1/20/20	13/39/115/115	-
33	LMG	Y	101	-	-	24/43/63/70	0/1/1/1
32	STE	d	410	-	-	11/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	SQD	b	620	-	-	21/44/64/69	0/1/1/1
24	CLA	B	607	-	1/1/20/20	5/39/115/115	-
24	CLA	C	501	-	1/1/20/20	4/39/115/115	-
32	STE	a	618	-	-	4/9/9/17	-
32	STE	c	520	-	-	7/17/17/17	-
32	STE	C	521	-	-	2/9/9/17	-
24	CLA	b	606	-	1/1/20/20	4/39/115/115	-
32	STE	C	520	-	-	7/13/13/17	-
24	CLA	C	511	3	1/1/20/20	9/39/115/115	-
24	CLA	b	613	-	1/1/20/20	4/39/115/115	-
33	LMG	c	522	-	-	27/44/64/70	0/1/1/1
26	BCR	K	103	-	-	6/29/63/63	0/2/2/2
32	STE	T	102	-	-	9/13/13/17	-
33	LMG	d	408	-	-	12/39/59/70	0/1/1/1
33	LMG	D	407	-	-	14/46/66/70	0/1/1/1
32	STE	C	519	-	-	4/9/9/17	-
32	STE	d	411	-	-	11/17/17/17	-
26	BCR	t	101	-	-	8/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/20/20	11/39/115/115	-
29	SQD	a	615	-	-	25/49/69/69	0/1/1/1
33	LMG	D	411	-	-	14/33/33/70	-
32	STE	Z	101	-	-	2/5/5/17	-
26	BCR	a	608	-	-	5/29/63/63	0/2/2/2
30	LHG	d	406	-	-	26/53/53/53	-
24	CLA	C	506	-	1/1/20/20	13/39/115/115	-
30	LHG	e	101	-	-	21/46/46/53	-
32	STE	R	101	-	-	4/9/9/17	-
32	STE	c	523	-	-	7/9/9/17	-
24	CLA	A	612	37	1/1/20/20	4/39/115/115	-
31	DGD	A	616	-	-	29/55/95/95	0/2/2/2
29	SQD	A	613	-	-	22/47/67/69	0/1/1/1
24	CLA	b	603	-	1/1/20/20	4/39/115/115	-
24	CLA	B	615	-	1/1/19/20	7/33/109/115	-
32	STE	b	624	-	-	11/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
24	CLA	B	603	-	1/1/20/20	11/39/115/115	-
24	CLA	C	509	-	1/1/20/20	13/39/115/115	-
24	CLA	B	614	-	1/1/20/20	8/39/115/115	-
28	PL9	d	405	-	-	13/53/73/73	0/1/1/1
26	BCR	B	616	-	-	7/29/63/63	0/2/2/2
32	STE	b	623	-	-	8/13/13/17	-
24	CLA	a	604	-	1/1/20/20	4/39/115/115	-
25	PHO	a	606	-	-	2/37/103/103	0/5/6/6
32	STE	T	103	-	-	8/12/12/17	-
26	BCR	D	405	-	-	5/29/63/63	0/2/2/2
31	DGD	H	102	-	-	16/51/91/95	0/2/2/2
26	BCR	c	514	-	-	6/29/63/63	0/2/2/2
32	STE	B	625	-	-	8/12/12/17	-
24	CLA	a	607	-	1/1/20/20	10/39/115/115	-
24	CLA	a	605	37	-	7/39/115/115	-
30	LHG	D	413	-	-	15/53/53/53	-
24	CLA	d	403	-	1/1/20/20	9/39/115/115	-
26	BCR	A	608	-	-	6/29/63/63	0/2/2/2
24	CLA	c	509	-	1/1/20/20	13/39/115/115	-
24	CLA	C	503	-	1/1/20/20	6/39/115/115	-
26	BCR	h	101	-	-	5/29/63/63	0/2/2/2
32	STE	h	103	-	-	6/11/11/17	-
32	STE	j	101	-	-	5/9/9/17	-
29	SQD	A	615	-	-	17/39/39/69	-
24	CLA	H	101	37	1/1/20/20	18/39/115/115	-
26	BCR	b	617	-	-	5/29/63/63	0/2/2/2
30	LHG	A	614	-	-	30/53/53/53	-
35	HEM	f	101	5,6	-	4/14/54/54	-
24	CLA	B	610	-	1/1/20/20	6/39/115/115	-
24	CLA	b	608	-	1/1/20/20	6/39/115/115	-
24	CLA	B	609	37	1/1/20/20	6/39/115/115	-
24	CLA	c	502	-	1/1/20/20	9/39/115/115	-
24	CLA	C	504	37	1/1/18/20	8/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	d	407	-	-	16/43/43/53	-
35	HEM	F	101	5,6	-	4/14/54/54	-
32	STE	a	617	-	-	4/7/7/17	-
32	STE	B	624	-	-	11/13/13/17	-
32	STE	b	625	-	-	5/7/7/17	-
26	BCR	C	514	-	-	7/29/63/63	0/2/2/2
24	CLA	b	605	-	1/1/20/20	7/39/115/115	-
30	LHG	l	101	-	-	14/53/53/53	-
31	DGD	c	517	-	-	17/51/91/95	0/2/2/2
32	STE	M	102	-	-	6/12/12/17	-
24	CLA	b	616	-	1/1/19/20	9/33/109/115	-
24	CLA	B	604	-	1/1/20/20	14/39/115/115	-
31	DGD	c	516	-	-	21/51/91/95	0/2/2/2
26	BCR	K	102	-	-	6/29/63/63	0/2/2/2
24	CLA	B	601	-	1/1/20/20	8/39/115/115	-
30	LHG	D	410	-	-	21/51/51/53	-
32	STE	J	101	-	-	2/9/9/17	-
32	STE	M	103	-	-	2/7/7/17	-
24	CLA	B	608	-	-	1/39/115/115	-
24	CLA	d	402	-	-	8/39/115/115	-
24	CLA	b	604	-	1/1/20/20	10/39/115/115	-
24	CLA	b	607	37	1/1/20/20	13/39/115/115	-
24	CLA	B	605	-	1/1/20/20	13/39/115/115	-
33	LMG	D	412	-	-	9/22/22/70	-
24	CLA	b	601	37	1/1/20/20	20/39/115/115	-
25	PHO	d	401	-	-	9/37/103/103	0/5/6/6
31	DGD	c	518	-	-	14/51/91/95	0/2/2/2
24	CLA	c	505	-	1/1/20/20	11/39/115/115	-
33	LMG	b	622	-	-	25/50/70/70	0/1/1/1
32	STE	B	623	-	-	9/15/15/17	-
25	PHO	A	606	-	-	1/37/103/103	0/5/6/6
26	BCR	b	618	-	-	2/29/63/63	0/2/2/2
24	CLA	c	512	-	1/1/20/20	17/39/115/115	-
24	CLA	C	507	37	1/1/20/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	612	-	1/1/20/20	5/39/115/115	-
24	CLA	c	501	-	1/1/20/20	3/39/115/115	-
29	SQD	f	102	-	-	17/36/56/69	0/1/1/1
24	CLA	D	403	-	-	12/39/115/115	-
28	PL9	a	612	-	-	20/53/73/73	0/1/1/1
24	CLA	C	513	-	1/1/20/20	10/39/115/115	-
32	STE	B	619	-	-	9/14/14/17	-
24	CLA	b	614	-	1/1/20/20	12/39/115/115	-
32	STE	X	102	-	-	14/17/17/17	-
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
26	BCR	k	102	-	-	6/29/63/63	0/2/2/2
24	CLA	A	604	-	1/1/20/20	9/39/115/115	-
24	CLA	c	506	-	1/1/20/20	15/39/115/115	-
29	SQD	B	620	-	-	23/49/69/69	0/1/1/1
24	CLA	c	508	-	1/1/19/20	7/38/114/115	-
33	LMG	m	101	-	-	22/46/66/70	0/1/1/1
31	DGD	C	516	-	-	22/51/91/95	0/2/2/2
24	CLA	B	611	-	1/1/20/20	11/39/115/115	-
32	STE	L	102	-	-	3/9/9/17	-
31	DGD	h	102	-	-	18/51/91/95	0/2/2/2
24	CLA	c	513	-	1/1/20/20	7/39/115/115	-
24	CLA	c	511	3	1/1/20/20	6/39/115/115	-
24	CLA	a	613	37	1/1/20/20	2/39/115/115	-
24	CLA	b	610	37	1/1/20/20	10/39/115/115	-
24	CLA	b	611	-	1/1/20/20	4/39/115/115	-
32	STE	B	626	-	-	4/9/9/17	-
24	CLA	c	504	37	1/1/19/20	9/33/109/115	-
24	CLA	b	602	-	-	8/39/115/115	-
24	CLA	A	607	-	1/1/17/20	2/26/102/115	-
26	BCR	X	101	-	-	5/29/63/63	0/2/2/2
29	SQD	a	616	-	-	18/37/37/69	-
36	HEC	V	201	17	-	6/14/54/54	-
24	CLA	C	510	-	1/1/20/20	5/39/115/115	-
31	DGD	C	518	-	-	18/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	404	-	1/1/20/20	11/39/115/115	-
28	PL9	A	611	-	-	22/53/73/73	0/1/1/1
32	STE	I	101	-	-	7/12/12/17	-
33	LMG	M	101	-	-	24/46/66/70	0/1/1/1
28	PL9	D	406	-	-	11/53/73/73	0/1/1/1
24	CLA	c	503	-	1/1/20/20	6/39/115/115	-
33	LMG	c	521	-	-	26/43/63/70	0/1/1/1
24	CLA	C	512	-	1/1/20/20	11/39/115/115	-

All (939) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	606	PHO	C1B-C2B	10.15	1.50	1.39
25	d	401	PHO	C1B-C2B	9.46	1.49	1.39
25	d	401	PHO	C3B-C4B	8.85	1.50	1.41
24	c	507	CLA	MG-NB	-8.83	1.88	2.05
25	A	606	PHO	C1B-C2B	8.50	1.48	1.39
25	a	606	PHO	C3B-C4B	8.15	1.49	1.41
24	B	605	CLA	MG-NA	8.14	2.25	2.06
24	c	502	CLA	MG-NB	-7.78	1.90	2.05
24	C	512	CLA	MG-NA	7.74	2.24	2.06
24	B	603	CLA	MG-NA	7.61	2.24	2.06
24	b	612	CLA	MG-ND	-7.40	1.91	2.05
24	B	613	CLA	MG-ND	-7.29	1.91	2.05
24	C	511	CLA	MG-NA	7.14	2.23	2.06
25	A	606	PHO	C3B-C4B	7.11	1.48	1.41
24	B	609	CLA	MG-ND	-6.94	1.92	2.05
24	C	505	CLA	MG-NA	6.93	2.22	2.06
24	C	507	CLA	MG-NA	6.88	2.22	2.06
24	a	613	CLA	MG-NA	6.87	2.22	2.06
24	b	608	CLA	MG-NA	6.78	2.22	2.06
36	v	201	HEC	CAC-C3C	6.71	1.56	1.35
28	d	405	PL9	C6-C1	-6.69	1.37	1.48
24	C	508	CLA	MG-NA	6.59	2.21	2.06
24	b	609	CLA	MG-NC	6.59	2.21	2.06
24	c	511	CLA	MG-NA	6.56	2.21	2.06
36	V	201	HEC	CAC-C3C	6.52	1.56	1.35
25	D	401	PHO	C1B-C2B	6.52	1.46	1.39
24	B	615	CLA	MG-NA	6.37	2.21	2.06
35	F	101	HEM	FE-NB	6.35	2.14	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	MG-NB	-6.10	1.93	2.05
24	C	507	CLA	MG-NC	-5.99	1.92	2.06
25	D	401	PHO	C3B-C4B	5.99	1.47	1.41
24	B	614	CLA	MG-NA	5.94	2.20	2.06
24	b	615	CLA	MG-NB	5.93	2.17	2.05
36	v	201	HEC	CAB-C3B	5.91	1.54	1.35
24	B	608	CLA	MG-NA	5.88	2.20	2.06
24	B	612	CLA	MG-ND	-5.78	1.94	2.05
24	b	608	CLA	MG-NC	-5.73	1.92	2.06
24	C	503	CLA	MG-NA	5.68	2.19	2.06
24	c	508	CLA	MG-NA	5.61	2.19	2.06
24	C	506	CLA	MG-NA	5.58	2.19	2.06
24	B	607	CLA	MG-NA	5.54	2.19	2.06
24	A	605	CLA	MG-NB	-5.49	1.94	2.05
24	C	513	CLA	MG-NA	5.26	2.18	2.06
24	b	606	CLA	MG-NA	5.22	2.18	2.06
36	V	201	HEC	CAB-C3B	5.21	1.51	1.35
24	c	510	CLA	MG-NA	5.13	2.18	2.06
24	B	612	CLA	MG-NA	5.06	2.18	2.06
24	a	604	CLA	MG-NA	5.03	2.18	2.06
36	v	201	HEC	C3D-C2D	5.03	1.52	1.38
26	b	618	BCR	C30-C25	-4.99	1.47	1.53
24	B	604	CLA	MG-NB	4.93	2.15	2.05
24	C	504	CLA	MG-NB	4.91	2.15	2.05
24	B	606	CLA	MG-NA	4.76	2.17	2.06
24	b	601	CLA	MG-ND	4.72	2.15	2.05
24	C	504	CLA	MG-ND	-4.72	1.96	2.05
24	C	506	CLA	MG-ND	-4.69	1.96	2.05
24	D	404	CLA	MG-NB	-4.68	1.96	2.05
24	a	605	CLA	MG-NA	-4.67	1.95	2.06
26	K	103	BCR	C30-C25	-4.67	1.47	1.53
25	d	401	PHO	C1D-C2D	4.65	1.44	1.39
24	A	604	CLA	MG-NA	4.65	2.17	2.06
24	c	507	CLA	MG-ND	4.63	2.15	2.05
24	d	403	CLA	MG-NA	4.63	2.17	2.06
24	A	604	CLA	MG-NB	4.58	2.14	2.05
24	b	607	CLA	MG-ND	4.56	2.14	2.05
24	D	404	CLA	MG-ND	-4.56	1.96	2.05
33	a	619	LMG	C4-C5	4.56	1.62	1.53
36	V	201	HEC	C3D-C2D	4.55	1.50	1.38
24	c	506	CLA	MG-ND	-4.54	1.96	2.05
26	C	514	BCR	C1-C6	-4.53	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	MG-ND	-4.44	1.97	2.05
26	t	101	BCR	C30-C25	-4.44	1.48	1.53
24	A	607	CLA	MG-NB	-4.41	1.97	2.05
24	a	605	CLA	MG-ND	-4.39	1.97	2.05
26	C	514	BCR	C30-C25	-4.35	1.48	1.53
24	b	613	CLA	MG-NA	4.35	2.16	2.06
33	Y	101	LMG	C4-C5	4.32	1.62	1.53
24	c	509	CLA	MG-ND	4.32	2.14	2.05
24	H	101	CLA	MG-NB	-4.28	1.97	2.05
33	C	515	LMG	C4-C3	4.25	1.63	1.52
31	C	516	DGD	O5D-C6D	-4.22	1.36	1.43
30	a	614	LHG	O7-C5	-4.22	1.36	1.46
24	b	604	CLA	MG-NA	4.21	2.16	2.06
24	b	611	CLA	MG-NA	4.21	2.16	2.06
26	D	405	BCR	C1-C6	-4.19	1.48	1.53
31	A	616	DGD	C4D-C5D	4.18	1.61	1.53
26	K	101	BCR	C1-C6	-4.16	1.48	1.53
26	k	102	BCR	C30-C25	-4.16	1.48	1.53
24	C	501	CLA	MG-NA	4.14	2.16	2.06
24	c	507	CLA	MG-NA	4.13	2.16	2.06
24	B	614	CLA	C1D-ND	4.10	1.43	1.37
24	D	403	CLA	C1D-ND	4.10	1.43	1.37
24	B	604	CLA	MG-ND	-4.08	1.97	2.05
26	X	101	BCR	C30-C25	-4.08	1.48	1.53
24	a	604	CLA	MG-ND	-4.07	1.97	2.05
24	c	505	CLA	MG-NA	4.06	2.15	2.06
24	b	606	CLA	MG-NC	4.06	2.15	2.06
26	B	616	BCR	C1-C6	-4.02	1.48	1.53
26	d	404	BCR	C1-C6	-3.99	1.48	1.53
33	m	101	LMG	C4-C3	3.99	1.62	1.52
24	c	501	CLA	MG-NB	-3.97	1.97	2.05
28	a	612	PL9	C53-C6	-3.97	1.42	1.50
24	B	611	CLA	MG-NC	3.95	2.15	2.06
33	m	101	LMG	O7-C8	-3.95	1.37	1.46
24	D	404	CLA	C1D-ND	3.93	1.43	1.37
26	c	515	BCR	C1-C6	-3.92	1.48	1.53
24	a	607	CLA	MG-NB	-3.91	1.98	2.05
31	H	102	DGD	C4E-C5E	3.90	1.61	1.53
24	A	604	CLA	MG-NC	-3.89	1.97	2.06
26	a	608	BCR	C30-C25	-3.88	1.48	1.53
24	d	403	CLA	MG-NB	-3.88	1.98	2.05
28	A	611	PL9	C7-C3	-3.87	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	CMC-C2C	-3.87	1.44	1.50
24	C	512	CLA	MG-NB	3.86	2.13	2.05
24	B	607	CLA	MG-NB	-3.84	1.98	2.05
26	k	101	BCR	C30-C25	-3.84	1.48	1.53
26	d	404	BCR	C30-C25	-3.83	1.48	1.53
24	a	604	CLA	C1D-ND	3.83	1.42	1.37
24	a	607	CLA	MG-ND	-3.81	1.98	2.05
24	D	403	CLA	MG-NA	3.79	2.15	2.06
26	D	405	BCR	C30-C25	-3.79	1.48	1.53
26	K	102	BCR	C1-C6	-3.79	1.48	1.53
25	D	401	PHO	CAC-C3C	-3.79	1.44	1.51
25	A	606	PHO	C4D-ND	-3.79	1.32	1.38
24	a	605	CLA	MG-NB	3.78	2.13	2.05
24	C	507	CLA	C1D-ND	3.77	1.42	1.37
24	B	613	CLA	MG-NC	3.76	2.15	2.06
24	C	509	CLA	MG-NC	-3.74	1.97	2.06
24	b	615	CLA	MG-NA	3.73	2.15	2.06
24	B	613	CLA	MG-NB	3.72	2.13	2.05
24	B	612	CLA	C4B-NB	3.70	1.42	1.37
30	D	409	LHG	O7-C5	-3.69	1.37	1.46
30	D	409	LHG	O8-C6	-3.69	1.36	1.45
24	C	512	CLA	MG-NC	-3.69	1.97	2.06
24	a	605	CLA	MG-NC	3.68	2.15	2.06
33	m	101	LMG	O1-C7	-3.68	1.37	1.43
24	D	404	CLA	CMD-C2D	-3.66	1.43	1.50
26	K	101	BCR	C30-C25	-3.66	1.49	1.53
24	H	101	CLA	C1D-ND	3.65	1.42	1.37
35	F	101	HEM	FE-ND	-3.64	1.83	1.94
24	b	601	CLA	C1B-C2B	3.64	1.51	1.43
24	c	508	CLA	C1D-ND	3.64	1.42	1.37
31	C	517	DGD	C4D-C3D	3.62	1.61	1.52
30	D	410	LHG	P-O6	3.61	1.73	1.59
31	c	516	DGD	O6E-C1E	-3.61	1.32	1.41
24	C	504	CLA	MG-NA	3.60	2.14	2.06
29	A	615	SQD	O48-C23	3.59	1.43	1.33
24	B	604	CLA	C1B-NB	-3.58	1.33	1.37
24	c	504	CLA	MG-ND	-3.58	1.98	2.05
29	a	616	SQD	O47-C7	3.57	1.44	1.34
31	A	616	DGD	C3E-C2E	3.56	1.61	1.52
29	B	620	SQD	O47-C7	3.56	1.44	1.34
24	b	615	CLA	C1D-ND	3.56	1.42	1.37
24	D	403	CLA	CAA-C2A	-3.56	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	H	101	CLA	MG-NA	3.55	2.14	2.06
33	D	407	LMG	O2-C2	-3.55	1.34	1.43
35	F	101	HEM	FE-NC	3.53	2.06	1.95
24	C	512	CLA	C1D-ND	3.53	1.42	1.37
24	b	609	CLA	MG-NA	3.53	2.14	2.06
24	A	605	CLA	CMD-C2D	-3.52	1.43	1.50
24	C	511	CLA	C1D-ND	3.52	1.42	1.37
24	c	511	CLA	C1D-ND	3.50	1.42	1.37
24	b	614	CLA	C1D-ND	3.50	1.42	1.37
26	A	608	BCR	C1-C6	-3.49	1.49	1.53
26	b	619	BCR	C30-C25	-3.48	1.49	1.53
25	a	606	PHO	C1D-C2D	3.48	1.43	1.39
24	B	613	CLA	C4B-NB	3.48	1.42	1.37
26	B	618	BCR	C1-C6	-3.48	1.49	1.53
24	B	611	CLA	MG-NB	3.47	2.12	2.05
29	b	620	SQD	O48-C23	3.47	1.43	1.33
31	c	517	DGD	O5D-C1E	3.47	1.46	1.40
24	H	101	CLA	C4B-NB	3.47	1.42	1.37
24	A	605	CLA	C4B-NB	3.46	1.42	1.37
24	A	604	CLA	CHC-C1C	3.45	1.45	1.38
30	a	614	LHG	C24-C23	3.43	1.60	1.50
24	c	506	CLA	MG-NB	3.43	2.12	2.05
24	C	503	CLA	C4B-NB	3.42	1.42	1.37
30	D	413	LHG	O7-C5	-3.42	1.38	1.46
29	D	408	SQD	O48-C23	3.40	1.43	1.33
24	B	604	CLA	C1D-ND	3.39	1.42	1.37
24	D	403	CLA	MG-NB	3.38	2.12	2.05
24	C	505	CLA	C1D-ND	3.38	1.42	1.37
24	B	601	CLA	C4B-NB	3.38	1.42	1.37
26	B	618	BCR	C30-C25	-3.37	1.49	1.53
33	D	411	LMG	C7-C8	3.37	1.59	1.51
24	C	513	CLA	C1D-ND	3.37	1.42	1.37
31	H	102	DGD	O5D-C1E	3.37	1.45	1.40
28	d	405	PL9	C11-C9	-3.36	1.44	1.51
24	a	605	CLA	C1B-NB	-3.35	1.33	1.37
31	H	102	DGD	C1E-C2E	3.34	1.62	1.52
29	B	620	SQD	O48-C23	3.34	1.43	1.33
24	B	611	CLA	C1D-ND	3.32	1.42	1.37
30	e	101	LHG	P-O6	3.32	1.72	1.59
24	C	501	CLA	C1D-ND	3.32	1.42	1.37
24	b	611	CLA	C1B-NB	-3.31	1.33	1.37
24	c	501	CLA	C1D-ND	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	C4B-NB	3.31	1.42	1.37
26	B	617	BCR	C30-C25	-3.30	1.49	1.53
26	K	102	BCR	C30-C25	-3.29	1.49	1.53
29	A	615	SQD	O47-C7	3.28	1.43	1.34
29	A	613	SQD	O48-C23	3.28	1.42	1.33
24	b	609	CLA	C4B-NB	3.27	1.42	1.37
24	b	602	CLA	C1D-ND	3.26	1.42	1.37
24	B	610	CLA	C1D-ND	3.26	1.42	1.37
29	a	616	SQD	O48-C23	3.25	1.42	1.33
24	c	509	CLA	C1B-C2B	3.24	1.50	1.43
24	b	616	CLA	MG-NA	3.23	2.13	2.06
33	c	521	LMG	C3-C2	3.23	1.60	1.52
25	d	401	PHO	C4D-CHA	3.22	1.44	1.39
24	C	510	CLA	MG-NB	3.22	2.12	2.05
24	B	609	CLA	C1D-ND	3.21	1.42	1.37
33	c	521	LMG	C7-C8	3.21	1.60	1.50
26	T	101	BCR	C30-C25	-3.20	1.49	1.53
24	B	604	CLA	C1B-C2B	3.20	1.50	1.43
29	f	102	SQD	O48-C23	3.20	1.42	1.33
33	a	619	LMG	C4-C3	3.19	1.60	1.52
33	c	519	LMG	C4-C3	3.19	1.60	1.52
24	a	605	CLA	C1D-ND	3.18	1.42	1.37
26	k	101	BCR	C1-C6	-3.18	1.49	1.53
24	B	610	CLA	MG-NC	3.18	2.13	2.06
30	D	413	LHG	C24-C23	3.18	1.59	1.50
24	C	507	CLA	C1B-C2B	3.17	1.50	1.43
24	b	602	CLA	MG-NA	3.17	2.13	2.06
24	C	505	CLA	MG-ND	-3.17	1.99	2.05
24	b	601	CLA	C4B-NB	3.17	1.42	1.37
24	B	614	CLA	C4B-NB	3.17	1.42	1.37
24	A	605	CLA	C1D-ND	3.16	1.42	1.37
24	b	613	CLA	C4B-NB	3.15	1.42	1.37
24	a	607	CLA	CMD-C2D	-3.15	1.44	1.50
24	b	605	CLA	C1B-C2B	3.15	1.50	1.43
26	c	515	BCR	C30-C25	-3.15	1.49	1.53
24	a	607	CLA	C1D-ND	3.15	1.42	1.37
35	f	101	HEM	FE-NA	3.15	2.05	1.95
24	B	614	CLA	CHC-C1C	3.15	1.44	1.38
24	c	511	CLA	C1B-C2B	3.14	1.50	1.43
24	B	612	CLA	C1B-C2B	3.14	1.50	1.43
24	B	615	CLA	CMC-C2C	-3.14	1.44	1.50
24	B	606	CLA	C1D-ND	3.13	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	MG-NB	-3.13	1.99	2.05
24	C	505	CLA	CHC-C1C	3.12	1.44	1.38
24	b	609	CLA	C1D-ND	3.12	1.42	1.37
35	f	101	HEM	FE-NB	3.12	2.04	1.94
24	c	513	CLA	C4B-NB	3.12	1.42	1.37
31	C	516	DGD	O5D-C1E	3.11	1.45	1.40
24	B	613	CLA	C1D-ND	3.11	1.41	1.37
29	f	102	SQD	O47-C7	3.10	1.43	1.34
24	B	609	CLA	CMB-C2B	-3.10	1.44	1.50
24	C	504	CLA	C4B-NB	3.10	1.41	1.37
24	C	508	CLA	C3B-C4B	3.10	1.51	1.42
24	C	510	CLA	C1D-ND	3.10	1.41	1.37
24	C	506	CLA	C4B-NB	3.09	1.41	1.37
24	B	607	CLA	CMD-C2D	-3.09	1.44	1.50
29	a	615	SQD	O48-C23	3.09	1.42	1.33
24	b	603	CLA	C1D-ND	3.08	1.41	1.37
24	B	603	CLA	MG-NB	3.08	2.11	2.05
24	B	605	CLA	MG-NC	-3.08	1.99	2.06
24	C	511	CLA	C1B-C2B	3.08	1.50	1.43
26	K	103	BCR	C1-C6	-3.07	1.49	1.53
24	C	513	CLA	C1B-C2B	3.07	1.50	1.43
24	C	513	CLA	MG-ND	-3.07	1.99	2.05
31	C	518	DGD	C6D-C5D	3.07	1.60	1.51
25	d	401	PHO	CMD-C2D	-3.06	1.45	1.51
33	a	619	LMG	C7-C8	3.05	1.60	1.50
31	C	516	DGD	C6E-C5E	3.05	1.62	1.51
24	c	508	CLA	C1B-C2B	3.04	1.50	1.43
24	C	501	CLA	MG-NB	-3.04	1.99	2.05
24	C	509	CLA	MG-NA	3.04	2.13	2.06
31	c	516	DGD	O3E-C3E	-3.04	1.35	1.43
24	c	511	CLA	MG-ND	3.04	2.11	2.05
24	b	609	CLA	CMB-C2B	-3.03	1.44	1.50
29	b	620	SQD	O47-C7	3.02	1.42	1.34
24	C	506	CLA	C1D-ND	3.01	1.41	1.37
24	c	507	CLA	C1D-ND	3.01	1.41	1.37
24	c	505	CLA	C4B-NB	3.01	1.41	1.37
24	B	603	CLA	C3B-C4B	3.01	1.51	1.42
24	b	607	CLA	C1D-ND	3.00	1.41	1.37
31	c	516	DGD	O2G-C2G	-2.99	1.39	1.46
24	a	613	CLA	CMB-C2B	-2.99	1.44	1.50
24	C	509	CLA	C1D-ND	2.99	1.41	1.37
31	h	102	DGD	O1G-C1G	-2.99	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	606	PHO	CAC-C3C	-2.99	1.46	1.51
30	D	410	LHG	O3-C3	-2.99	1.33	1.44
24	b	615	CLA	C1B-NB	-2.98	1.33	1.37
24	a	604	CLA	C1B-C2B	2.98	1.50	1.43
24	A	607	CLA	CMB-C2B	-2.98	1.44	1.50
24	b	607	CLA	C4B-NB	2.97	1.41	1.37
26	b	619	BCR	C1-C6	-2.97	1.50	1.53
24	C	510	CLA	C1B-C2B	2.97	1.50	1.43
24	B	615	CLA	C1B-C2B	2.97	1.50	1.43
33	a	619	LMG	C3-C2	2.96	1.60	1.52
24	C	503	CLA	C3B-C4B	2.96	1.51	1.42
24	B	614	CLA	CMB-C2B	-2.96	1.44	1.50
31	C	517	DGD	O3E-C3E	-2.96	1.35	1.43
24	C	504	CLA	C1D-ND	2.95	1.41	1.37
24	b	605	CLA	MG-NA	2.95	2.13	2.06
30	d	407	LHG	P-O6	2.95	1.70	1.59
28	A	611	PL9	C21-C19	2.95	1.57	1.51
24	A	604	CLA	C1D-ND	2.95	1.41	1.37
24	b	609	CLA	C1B-C2B	2.95	1.50	1.43
24	C	511	CLA	MG-NC	-2.94	1.99	2.06
24	d	403	CLA	C1B-C2B	2.94	1.50	1.43
26	c	514	BCR	C1-C6	-2.93	1.50	1.53
24	a	607	CLA	CMC-C2C	-2.93	1.44	1.50
28	D	406	PL9	C52-C5	-2.93	1.44	1.50
33	c	521	LMG	O1-C1	2.93	1.45	1.40
24	c	503	CLA	C1B-C2B	2.93	1.50	1.43
26	h	101	BCR	C30-C25	-2.93	1.50	1.53
31	A	616	DGD	C1E-C2E	2.92	1.61	1.52
24	B	602	CLA	C3B-C4B	2.92	1.51	1.42
24	A	604	CLA	C1B-C2B	2.92	1.50	1.43
35	F	101	HEM	CAB-C3B	2.92	1.55	1.47
31	h	102	DGD	O2G-C1B	2.92	1.42	1.34
28	d	405	PL9	C7-C3	2.91	1.55	1.51
26	b	617	BCR	C1-C6	-2.91	1.50	1.53
24	B	614	CLA	C1B-C2B	2.91	1.50	1.43
24	C	501	CLA	CMD-C2D	-2.91	1.44	1.50
31	C	518	DGD	O5D-C1E	2.90	1.45	1.40
24	c	513	CLA	C1D-ND	2.90	1.41	1.37
24	b	613	CLA	CMB-C2B	-2.89	1.44	1.50
24	a	607	CLA	C1B-C2B	2.88	1.49	1.43
31	C	518	DGD	O1G-C1G	-2.88	1.38	1.45
26	T	101	BCR	C1-C6	-2.88	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Y	101	LMG	C1-C2	2.88	1.60	1.52
26	B	616	BCR	C33-C5	-2.87	1.46	1.50
24	A	607	CLA	MG-ND	-2.86	2.00	2.05
24	B	608	CLA	C1B-C2B	2.86	1.49	1.43
24	B	612	CLA	C1D-ND	2.86	1.41	1.37
24	c	510	CLA	C1D-ND	2.86	1.41	1.37
25	A	606	PHO	CMB-C2B	-2.86	1.45	1.51
25	d	401	PHO	CAC-C3C	-2.86	1.46	1.51
31	C	516	DGD	O1G-C1G	-2.86	1.38	1.45
24	B	609	CLA	MG-NA	2.85	2.13	2.06
24	b	603	CLA	MG-NC	2.85	2.13	2.06
25	d	401	PHO	CMC-C2C	-2.85	1.46	1.50
24	a	605	CLA	CMD-C2D	-2.85	1.44	1.50
33	m	101	LMG	C1-C2	2.85	1.60	1.52
31	c	516	DGD	C4D-C3D	2.85	1.59	1.52
24	C	507	CLA	MG-ND	-2.85	2.00	2.05
24	b	616	CLA	MG-NB	-2.84	2.00	2.05
24	C	507	CLA	CMD-C2D	-2.84	1.45	1.50
31	C	516	DGD	C4E-C3E	2.84	1.59	1.52
24	b	610	CLA	C1D-ND	2.83	1.41	1.37
30	D	409	LHG	P-O6	2.83	1.70	1.59
25	D	401	PHO	C1D-C2D	2.83	1.42	1.39
24	C	508	CLA	C1B-C2B	2.83	1.49	1.43
24	c	504	CLA	C1D-ND	2.83	1.41	1.37
24	c	508	CLA	C3B-C4B	2.83	1.50	1.42
24	c	510	CLA	CMB-C2B	-2.82	1.45	1.50
24	C	502	CLA	MG-NC	-2.82	1.99	2.06
33	a	619	LMG	O7-C10	2.81	1.42	1.34
31	c	518	DGD	C6D-C5D	2.81	1.60	1.51
31	H	102	DGD	C4D-C5D	2.81	1.59	1.53
24	c	504	CLA	C1B-NB	-2.81	1.34	1.37
24	C	513	CLA	MG-NB	2.81	2.11	2.05
26	b	618	BCR	C1-C6	-2.81	1.50	1.53
24	b	605	CLA	CHC-C4B	-2.80	1.33	1.39
33	Y	101	LMG	O7-C8	-2.80	1.40	1.46
24	B	609	CLA	C4B-NB	2.80	1.41	1.37
24	C	504	CLA	C1B-NB	-2.80	1.34	1.37
24	a	613	CLA	C1D-ND	2.80	1.41	1.37
24	c	507	CLA	C1B-C2B	2.79	1.49	1.43
24	B	611	CLA	CHC-C1C	2.78	1.44	1.38
24	c	513	CLA	MG-NB	-2.78	2.00	2.05
24	b	611	CLA	C1D-ND	2.77	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	503	CLA	C1D-ND	2.77	1.41	1.37
24	c	501	CLA	CHC-C4B	-2.77	1.33	1.39
24	B	605	CLA	C1B-C2B	2.77	1.49	1.43
24	c	504	CLA	CMD-C2D	-2.76	1.45	1.50
24	C	511	CLA	C4B-NB	2.76	1.41	1.37
24	a	604	CLA	CMB-C2B	-2.76	1.45	1.50
24	b	608	CLA	C3B-C4B	2.76	1.50	1.42
24	c	506	CLA	MG-NA	2.76	2.12	2.06
26	c	514	BCR	C30-C25	-2.75	1.50	1.53
24	d	403	CLA	CMD-C2D	-2.75	1.45	1.50
24	B	602	CLA	C1D-ND	2.75	1.41	1.37
31	c	516	DGD	O3G-C3G	-2.75	1.39	1.43
24	c	506	CLA	C1B-NB	-2.75	1.34	1.37
24	C	501	CLA	C1B-NB	-2.74	1.34	1.37
24	b	615	CLA	CMB-C2B	-2.74	1.45	1.50
24	B	615	CLA	C1D-ND	2.74	1.41	1.37
24	a	613	CLA	MG-NC	-2.74	1.99	2.06
24	d	402	CLA	C1D-ND	2.74	1.41	1.37
24	c	511	CLA	C4B-NB	2.74	1.41	1.37
24	b	603	CLA	CMD-C2D	-2.74	1.45	1.50
26	k	102	BCR	C1-C6	-2.74	1.50	1.53
33	Y	101	LMG	C4-C3	2.74	1.59	1.52
24	C	506	CLA	CMC-C2C	-2.74	1.45	1.50
24	D	403	CLA	CMB-C2B	-2.74	1.45	1.50
24	C	503	CLA	CMD-C2D	-2.73	1.45	1.50
24	C	509	CLA	C3B-C4B	2.73	1.50	1.42
31	C	518	DGD	O6D-C5D	-2.73	1.37	1.44
24	b	605	CLA	MG-NC	-2.73	1.99	2.06
24	C	501	CLA	C3B-C4B	2.73	1.50	1.42
24	C	503	CLA	C1B-C2B	2.73	1.49	1.43
24	C	501	CLA	CMB-C2B	-2.72	1.45	1.50
24	A	612	CLA	C1D-ND	2.72	1.41	1.37
24	b	604	CLA	C1B-C2B	2.72	1.49	1.43
30	D	410	LHG	C24-C23	-2.71	1.42	1.50
26	a	608	BCR	C1-C6	-2.71	1.50	1.53
33	d	408	LMG	O7-C8	-2.71	1.40	1.46
24	b	614	CLA	MG-NA	2.71	2.12	2.06
24	B	606	CLA	MG-NC	2.71	2.12	2.06
25	D	401	PHO	C3D-C4D	2.70	1.44	1.41
24	b	604	CLA	C1D-ND	2.70	1.41	1.37
24	c	502	CLA	CMD-C2D	-2.70	1.45	1.50
33	c	519	LMG	O1-C1	2.70	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	613	SQD	O2-C2	-2.70	1.36	1.43
24	b	607	CLA	C1B-C2B	2.70	1.49	1.43
33	d	408	LMG	O2-C2	-2.70	1.36	1.43
25	a	606	PHO	C4D-ND	-2.70	1.34	1.38
30	A	614	LHG	P-O6	2.69	1.69	1.59
24	C	506	CLA	C1B-NB	-2.69	1.34	1.37
24	b	607	CLA	CHC-C1C	2.68	1.43	1.38
26	c	515	BCR	C33-C5	-2.68	1.46	1.50
24	a	604	CLA	O2D-CED	-2.68	1.39	1.45
24	b	605	CLA	C3B-C4B	2.68	1.50	1.42
33	c	522	LMG	C4-C5	2.68	1.58	1.53
24	A	604	CLA	C3B-C4B	2.68	1.50	1.42
24	b	602	CLA	C1B-C2B	2.68	1.49	1.43
25	D	401	PHO	CMD-C2D	-2.68	1.46	1.51
24	b	606	CLA	C3B-C4B	2.68	1.50	1.42
25	A	606	PHO	CMD-C2D	-2.67	1.46	1.51
31	C	517	DGD	C6D-C5D	2.67	1.59	1.51
33	b	622	LMG	C4-C3	2.67	1.59	1.52
24	d	402	CLA	C3B-C4B	2.67	1.50	1.42
24	A	605	CLA	MG-NC	2.67	2.12	2.06
25	A	606	PHO	CAC-C3C	-2.67	1.47	1.51
24	c	513	CLA	C1B-C2B	2.67	1.49	1.43
24	C	509	CLA	CMD-C2D	-2.67	1.45	1.50
24	C	511	CLA	C3B-C4B	2.67	1.50	1.42
24	C	501	CLA	C1B-C2B	2.67	1.49	1.43
26	a	608	BCR	C38-C26	-2.66	1.46	1.50
31	H	102	DGD	C4D-C3D	2.66	1.59	1.52
24	c	501	CLA	CMD-C2D	-2.65	1.45	1.50
24	B	609	CLA	C1D-C2D	2.65	1.50	1.45
26	A	608	BCR	C30-C25	-2.65	1.50	1.53
24	C	513	CLA	C3B-C4B	2.64	1.50	1.42
24	C	503	CLA	C1D-ND	2.64	1.41	1.37
31	A	616	DGD	C3G-C2G	2.64	1.59	1.50
24	b	605	CLA	C1D-ND	2.64	1.41	1.37
24	H	101	CLA	C1B-C2B	2.64	1.49	1.43
24	B	602	CLA	CMC-C2C	-2.64	1.45	1.50
33	M	101	LMG	O1-C1	2.63	1.44	1.40
28	d	405	PL9	C3-C4	-2.63	1.45	1.49
24	C	509	CLA	C1B-C2B	2.63	1.49	1.43
33	c	519	LMG	C4-C5	2.63	1.58	1.53
24	B	604	CLA	MG-NC	-2.63	2.00	2.06
25	D	401	PHO	C3B-C2B	-2.63	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	616	DGD	C4E-C5E	2.62	1.58	1.53
24	c	511	CLA	MG-NC	2.62	2.12	2.06
24	b	613	CLA	CMD-C2D	-2.62	1.45	1.50
24	C	513	CLA	MG-NC	-2.62	2.00	2.06
30	a	614	LHG	P-O6	2.62	1.69	1.59
24	C	504	CLA	C3B-C4B	2.62	1.50	1.42
24	C	502	CLA	C1B-C2B	2.61	1.49	1.43
24	c	504	CLA	C4B-NB	2.61	1.41	1.37
31	h	102	DGD	C4E-C5E	2.61	1.58	1.53
24	B	614	CLA	MG-NC	2.60	2.12	2.06
28	D	406	PL9	C3-C4	-2.60	1.45	1.49
26	C	514	BCR	C33-C5	-2.60	1.46	1.50
24	C	510	CLA	MG-NA	2.60	2.12	2.06
26	h	101	BCR	C33-C5	-2.59	1.46	1.50
24	C	501	CLA	C4B-NB	2.59	1.41	1.37
24	c	512	CLA	CHC-C1C	2.59	1.43	1.38
24	b	616	CLA	C1D-ND	2.59	1.41	1.37
24	b	606	CLA	C1D-ND	2.59	1.41	1.37
24	B	610	CLA	CMB-C2B	-2.59	1.45	1.50
26	b	617	BCR	C30-C25	-2.59	1.50	1.53
24	B	601	CLA	C3B-C4B	2.59	1.50	1.42
24	b	608	CLA	C1D-ND	2.59	1.41	1.37
24	B	609	CLA	MG-NC	-2.59	2.00	2.06
24	c	509	CLA	C1B-NB	-2.59	1.34	1.37
24	C	509	CLA	MG-NB	2.58	2.10	2.05
24	b	607	CLA	C3B-C4B	2.58	1.50	1.42
24	b	603	CLA	CMC-C2C	-2.58	1.45	1.50
24	B	615	CLA	CMD-C2D	-2.58	1.45	1.50
31	c	517	DGD	C6D-C5D	2.57	1.59	1.51
24	b	613	CLA	C1C-NC	-2.57	1.33	1.37
35	f	101	HEM	FE-ND	2.57	2.02	1.94
24	c	508	CLA	C4B-NB	2.57	1.41	1.37
31	h	102	DGD	O2D-C2D	-2.57	1.36	1.43
24	b	615	CLA	C3B-C4B	2.56	1.50	1.42
24	b	608	CLA	C1B-C2B	2.56	1.49	1.43
35	F	101	HEM	FE-NA	2.56	2.03	1.95
24	B	609	CLA	C3B-C4B	2.56	1.50	1.42
24	a	607	CLA	C3B-C4B	2.56	1.50	1.42
24	C	510	CLA	CHC-C1C	2.55	1.43	1.38
33	c	519	LMG	C7-C8	2.55	1.58	1.50
24	C	510	CLA	MG-NC	2.55	2.12	2.06
24	B	606	CLA	C1B-C2B	2.55	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C4B-NB	2.55	1.41	1.37
25	D	401	PHO	O2D-CGD	2.55	1.39	1.33
24	B	603	CLA	CMB-C2B	-2.55	1.45	1.50
33	M	101	LMG	C4-C3	2.54	1.58	1.52
24	c	512	CLA	MG-NC	2.54	2.12	2.06
31	A	616	DGD	C4D-C3D	2.54	1.58	1.52
24	b	614	CLA	CMC-C2C	-2.54	1.45	1.50
24	c	511	CLA	C3B-C4B	2.54	1.50	1.42
24	B	609	CLA	CMC-C2C	-2.53	1.45	1.50
31	A	616	DGD	O2G-C2G	-2.53	1.40	1.46
24	D	404	CLA	MG-NC	2.53	2.12	2.06
31	c	518	DGD	O2G-C2G	-2.53	1.40	1.46
25	D	401	PHO	C4D-CHA	2.53	1.43	1.39
24	c	510	CLA	CHC-C1C	2.53	1.43	1.38
24	H	101	CLA	CMB-C2B	-2.52	1.45	1.50
24	c	506	CLA	C1B-C2B	2.52	1.49	1.43
24	a	604	CLA	C3B-C4B	2.52	1.50	1.42
35	f	101	HEM	CAC-C3C	2.52	1.54	1.47
24	A	607	CLA	CMD-C2D	-2.52	1.45	1.50
24	c	513	CLA	C3B-C4B	2.52	1.50	1.42
24	b	601	CLA	CHC-C1C	2.51	1.43	1.38
24	c	509	CLA	CHC-C1C	2.51	1.43	1.38
24	b	607	CLA	MG-NA	2.51	2.12	2.06
24	B	611	CLA	CMC-C2C	-2.50	1.45	1.50
24	c	508	CLA	CMD-C2D	-2.50	1.45	1.50
24	B	611	CLA	CMD-C2D	-2.50	1.45	1.50
24	B	605	CLA	CMB-C2B	-2.49	1.45	1.50
24	C	507	CLA	CMC-C2C	-2.49	1.45	1.50
31	c	516	DGD	C4E-C3E	2.49	1.58	1.52
33	d	408	LMG	C7-C8	2.49	1.58	1.50
24	b	601	CLA	MG-NA	2.49	2.12	2.06
24	a	604	CLA	C4B-NB	2.48	1.41	1.37
31	C	516	DGD	C3D-C2D	2.48	1.58	1.52
24	c	509	CLA	C4B-NB	2.48	1.41	1.37
30	L	101	LHG	P-O6	2.48	1.69	1.59
24	c	505	CLA	CMC-C2C	-2.47	1.45	1.50
24	b	610	CLA	C1B-C2B	2.47	1.48	1.43
31	c	518	DGD	C2A-C1A	-2.47	1.43	1.50
24	A	605	CLA	CAA-C2A	-2.47	1.49	1.54
24	C	507	CLA	C3D-C4D	2.47	1.49	1.44
24	c	512	CLA	C1D-C2D	2.47	1.50	1.45
31	h	102	DGD	C6D-C5D	2.47	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C4B-NB	2.47	1.41	1.37
24	b	612	CLA	C1B-NB	-2.47	1.34	1.37
30	D	410	LHG	O8-C23	2.47	1.40	1.33
24	b	603	CLA	C4B-NB	2.46	1.41	1.37
31	C	517	DGD	C1E-C2E	2.46	1.59	1.52
24	c	505	CLA	C1D-ND	2.46	1.41	1.37
24	c	512	CLA	C1B-C2B	2.46	1.48	1.43
24	C	507	CLA	C3B-C4B	2.46	1.49	1.42
24	B	603	CLA	O2D-CED	-2.46	1.39	1.45
24	d	402	CLA	MG-NB	-2.46	2.00	2.05
33	c	519	LMG	C3-C2	2.45	1.58	1.52
24	c	501	CLA	C1B-C2B	2.45	1.48	1.43
24	b	614	CLA	C1B-C2B	2.44	1.48	1.43
24	C	513	CLA	C4B-NB	2.44	1.41	1.37
24	B	603	CLA	C1B-C2B	2.44	1.48	1.43
25	A	606	PHO	C4D-CHA	2.44	1.43	1.39
24	b	606	CLA	C4B-NB	2.44	1.41	1.37
29	a	615	SQD	O3-C3	-2.44	1.36	1.43
24	B	604	CLA	C3B-C4B	2.44	1.49	1.42
29	A	615	SQD	O47-C45	-2.44	1.42	1.47
24	b	608	CLA	CHC-C1C	2.44	1.43	1.38
24	b	608	CLA	CMD-C2D	-2.44	1.45	1.50
24	C	507	CLA	MG-NB	-2.43	2.01	2.05
24	C	505	CLA	CMC-C2C	-2.43	1.45	1.50
24	B	607	CLA	C1D-ND	2.43	1.41	1.37
24	b	602	CLA	CMD-C2D	-2.43	1.45	1.50
24	H	101	CLA	C3B-C4B	2.43	1.49	1.42
24	b	611	CLA	MG-ND	2.43	2.10	2.05
24	B	609	CLA	C3D-C4D	2.43	1.49	1.44
36	V	201	HEC	C3B-C2B	-2.43	1.33	1.41
25	a	606	PHO	CBD-CGD	-2.42	1.49	1.52
26	K	101	BCR	C33-C5	-2.42	1.47	1.50
24	D	403	CLA	C1B-NB	-2.42	1.34	1.37
24	c	512	CLA	C1D-ND	2.42	1.41	1.37
29	a	615	SQD	O2-C2	-2.42	1.37	1.43
24	c	502	CLA	C1D-ND	2.42	1.41	1.37
24	C	510	CLA	C3B-C4B	2.42	1.49	1.42
24	c	501	CLA	CMB-C2B	-2.42	1.45	1.50
24	B	602	CLA	C1B-C2B	2.42	1.48	1.43
24	c	502	CLA	C1B-C2B	2.42	1.48	1.43
24	c	513	CLA	CMB-C2B	-2.42	1.45	1.50
24	b	613	CLA	C1D-ND	2.42	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	MG-ND	-2.41	2.01	2.05
24	b	608	CLA	CMB-C2B	-2.41	1.45	1.50
24	b	612	CLA	CMC-C2C	-2.41	1.45	1.50
31	A	616	DGD	O5D-C6D	-2.40	1.39	1.43
24	c	502	CLA	C3B-C4B	2.40	1.49	1.42
24	b	606	CLA	C1B-C2B	2.40	1.48	1.43
24	B	610	CLA	CHC-C1C	2.40	1.43	1.38
24	A	607	CLA	CHC-C4B	-2.40	1.34	1.39
24	b	603	CLA	MG-NA	2.40	2.12	2.06
26	B	616	BCR	C30-C25	-2.40	1.50	1.53
24	b	603	CLA	C3B-C4B	2.39	1.49	1.42
31	c	518	DGD	O6D-C5D	-2.39	1.38	1.44
24	a	607	CLA	MG-NA	2.39	2.12	2.06
26	T	101	BCR	C38-C26	-2.39	1.47	1.50
29	A	613	SQD	O3-C3	-2.39	1.37	1.43
29	A	613	SQD	O48-C46	-2.39	1.39	1.45
24	C	506	CLA	C3B-C4B	2.39	1.49	1.42
29	A	613	SQD	O4-C4	-2.38	1.37	1.43
24	B	609	CLA	CMD-C2D	-2.38	1.45	1.50
24	b	610	CLA	CMB-C2B	-2.38	1.45	1.50
24	B	601	CLA	C1B-C2B	2.38	1.48	1.43
24	b	607	CLA	CMD-C2D	-2.38	1.45	1.50
24	B	603	CLA	CMC-C2C	-2.38	1.45	1.50
24	b	612	CLA	CMD-C2D	-2.38	1.45	1.50
29	f	102	SQD	O2-C2	-2.37	1.37	1.43
33	a	619	LMG	C1-C2	2.37	1.59	1.52
24	b	615	CLA	CMC-C2C	-2.37	1.45	1.50
31	c	517	DGD	O3E-C3E	-2.37	1.37	1.43
26	A	608	BCR	C33-C5	-2.37	1.47	1.50
31	C	518	DGD	O2E-C2E	-2.37	1.37	1.43
30	L	101	LHG	O7-C5	-2.37	1.41	1.46
28	d	405	PL9	C53-C6	-2.37	1.45	1.50
35	f	101	HEM	CMC-C2C	2.36	1.55	1.50
24	b	612	CLA	C1D-ND	2.36	1.41	1.37
24	b	615	CLA	C4B-NB	2.36	1.41	1.37
24	B	606	CLA	C4B-NB	2.36	1.41	1.37
24	C	510	CLA	C4B-NB	2.36	1.41	1.37
24	c	513	CLA	CMC-C2C	-2.36	1.45	1.50
24	c	511	CLA	CHC-C1C	2.36	1.43	1.38
24	B	608	CLA	CMD-C2D	-2.36	1.45	1.50
24	c	502	CLA	C4B-NB	2.36	1.41	1.37
33	c	521	LMG	O7-C10	2.36	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	601	CLA	O2D-CGD	2.36	1.39	1.33
35	f	101	HEM	C2A-C3A	-2.35	1.32	1.38
29	A	613	SQD	O47-C7	2.35	1.40	1.34
24	a	604	CLA	MG-NB	2.35	2.10	2.05
24	B	610	CLA	CMC-C2C	-2.35	1.46	1.50
24	b	611	CLA	CMD-C2D	-2.35	1.46	1.50
24	d	403	CLA	CHC-C1C	2.35	1.43	1.38
33	C	515	LMG	O1-C7	-2.35	1.39	1.43
24	c	512	CLA	C4B-NB	2.34	1.40	1.37
33	D	412	LMG	O8-C28	2.34	1.38	1.30
24	B	611	CLA	C1B-C2B	2.34	1.48	1.43
28	D	406	PL9	C36-C34	2.34	1.56	1.51
24	B	601	CLA	CMB-C2B	-2.34	1.46	1.50
24	c	512	CLA	C3B-C4B	2.34	1.49	1.42
24	b	616	CLA	CMD-C2D	-2.33	1.46	1.50
24	b	615	CLA	MG-NC	-2.33	2.00	2.06
30	D	413	LHG	P-O4	-2.33	1.44	1.55
33	C	515	LMG	C6-C5	2.33	1.59	1.51
24	b	601	CLA	C1D-ND	2.33	1.40	1.37
35	f	101	HEM	C3B-C2B	-2.33	1.32	1.37
24	b	614	CLA	C3B-C4B	2.32	1.49	1.42
24	b	614	CLA	C5-C3	-2.32	1.46	1.51
26	K	103	BCR	C33-C5	-2.32	1.47	1.50
24	b	602	CLA	CMC-C2C	-2.32	1.46	1.50
24	B	615	CLA	C1B-NB	-2.31	1.34	1.37
26	B	617	BCR	C1-C6	-2.31	1.50	1.53
24	B	602	CLA	MG-ND	2.31	2.10	2.05
24	b	603	CLA	CMB-C2B	-2.31	1.46	1.50
24	B	602	CLA	CAB-C3B	-2.31	1.41	1.47
24	d	403	CLA	CMC-C2C	-2.31	1.46	1.50
24	C	511	CLA	CMB-C2B	-2.31	1.46	1.50
24	c	506	CLA	O2D-CGD	2.31	1.38	1.33
24	B	601	CLA	C1D-ND	2.31	1.40	1.37
26	K	103	BCR	C27-C26	-2.30	1.46	1.51
25	d	401	PHO	C3B-C2B	-2.30	1.37	1.40
24	C	512	CLA	C1B-C2B	2.30	1.48	1.43
24	C	511	CLA	CMC-C2C	-2.30	1.46	1.50
25	a	606	PHO	CMB-C2B	-2.30	1.47	1.51
24	a	613	CLA	C1B-C2B	2.30	1.48	1.43
24	C	503	CLA	CMC-C2C	-2.30	1.46	1.50
35	F	101	HEM	C3C-C2C	-2.30	1.32	1.37
24	C	501	CLA	CMC-C2C	-2.30	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	613	CLA	C3B-C4B	2.30	1.49	1.42
24	a	605	CLA	CMB-C2B	-2.30	1.46	1.50
24	c	507	CLA	C4B-NB	2.30	1.40	1.37
26	b	617	BCR	C4-C5	-2.30	1.46	1.51
24	b	615	CLA	C1B-C2B	2.30	1.48	1.43
24	c	502	CLA	CHC-C4B	-2.29	1.34	1.39
24	B	605	CLA	MG-NB	-2.29	2.01	2.05
24	c	511	CLA	CMB-C2B	-2.29	1.46	1.50
33	c	522	LMG	C7-C8	2.29	1.58	1.50
24	B	615	CLA	C4B-NB	2.28	1.40	1.37
25	D	401	PHO	C4D-ND	-2.28	1.35	1.38
33	a	619	LMG	C9-C8	2.28	1.57	1.50
30	l	101	LHG	O7-C5	-2.28	1.41	1.46
24	c	508	CLA	CHC-C1C	2.28	1.43	1.38
24	c	509	CLA	CMB-C2B	-2.28	1.46	1.50
24	C	503	CLA	C3D-C4D	2.28	1.49	1.44
24	H	101	CLA	CHC-C1C	2.27	1.43	1.38
24	b	601	CLA	O2A-CGA	2.27	1.40	1.33
24	b	615	CLA	CMD-C2D	-2.27	1.46	1.50
24	b	613	CLA	C1B-NB	-2.27	1.34	1.37
35	F	101	HEM	CAC-C3C	2.27	1.53	1.47
24	C	512	CLA	CMD-C2D	-2.27	1.46	1.50
31	C	518	DGD	C6E-C5E	2.27	1.59	1.51
24	B	611	CLA	C4B-NB	2.27	1.40	1.37
24	b	601	CLA	C3B-C4B	2.27	1.49	1.42
33	Y	101	LMG	C6-C5	2.27	1.59	1.51
29	a	615	SQD	O47-C7	2.27	1.40	1.34
24	d	403	CLA	C3B-C4B	2.27	1.49	1.42
24	c	505	CLA	C1B-C2B	2.26	1.48	1.43
24	b	616	CLA	CMB-C2B	-2.26	1.46	1.50
24	C	511	CLA	C1B-NB	-2.26	1.34	1.37
24	c	501	CLA	MG-ND	-2.26	2.01	2.05
24	c	513	CLA	CHC-C1C	2.26	1.43	1.38
24	B	602	CLA	CMB-C2B	-2.26	1.46	1.50
24	b	610	CLA	MG-ND	-2.26	2.01	2.05
25	A	606	PHO	CBD-CGD	-2.26	1.49	1.52
30	D	409	LHG	P-O3	2.26	1.68	1.59
26	k	101	BCR	C33-C5	-2.25	1.47	1.50
24	C	509	CLA	CMB-C2B	-2.25	1.46	1.50
24	B	602	CLA	CMD-C2D	-2.25	1.46	1.50
36	V	201	HEC	CMB-C2B	2.25	1.55	1.50
24	B	611	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	407	LHG	O7-C5	-2.25	1.41	1.46
24	B	607	CLA	C1B-C2B	2.25	1.48	1.43
26	b	617	BCR	C33-C5	-2.25	1.47	1.50
24	B	610	CLA	C1B-C2B	2.25	1.48	1.43
24	B	606	CLA	O2D-CGD	2.25	1.38	1.33
25	d	401	PHO	CMB-C2B	-2.25	1.47	1.51
24	B	605	CLA	CAB-C3B	-2.25	1.41	1.47
24	B	608	CLA	CMC-C2C	-2.24	1.46	1.50
32	b	623	STE	C2-C1	2.24	1.55	1.50
24	B	613	CLA	CMB-C2B	-2.24	1.46	1.50
26	t	101	BCR	C27-C26	-2.24	1.46	1.51
33	Y	101	LMG	C3-C2	2.24	1.58	1.52
31	C	516	DGD	C4D-C3D	2.23	1.58	1.52
24	b	602	CLA	CAC-C3C	-2.23	1.45	1.51
33	Y	101	LMG	O1-C7	-2.23	1.39	1.43
33	C	515	LMG	C3-C2	2.23	1.58	1.52
33	c	522	LMG	C6-C5	2.23	1.59	1.51
24	b	616	CLA	CAB-C3B	-2.23	1.41	1.47
24	A	604	CLA	C1B-NB	-2.23	1.34	1.37
24	a	607	CLA	C4B-NB	2.23	1.40	1.37
24	C	513	CLA	CMB-C2B	-2.23	1.46	1.50
24	c	506	CLA	C1D-ND	2.23	1.40	1.37
24	c	502	CLA	MG-ND	2.23	2.10	2.05
24	C	512	CLA	MG-ND	-2.23	2.01	2.05
24	C	513	CLA	CMC-C2C	-2.22	1.46	1.50
24	D	404	CLA	C3B-C4B	2.22	1.49	1.42
24	B	605	CLA	C3B-C4B	2.22	1.49	1.42
24	b	605	CLA	O2D-CED	-2.22	1.40	1.45
30	l	101	LHG	O8-C23	2.22	1.39	1.33
24	c	503	CLA	C4-C3	-2.22	1.45	1.50
24	B	610	CLA	CAA-C2A	-2.22	1.50	1.54
24	A	604	CLA	C3C-C2C	2.22	1.41	1.36
24	D	404	CLA	CMB-C2B	-2.22	1.46	1.50
24	A	605	CLA	CHC-C1C	2.22	1.42	1.38
24	C	510	CLA	CMD-C2D	-2.21	1.46	1.50
24	d	402	CLA	CMB-C2B	-2.21	1.46	1.50
24	a	613	CLA	C4B-NB	2.21	1.40	1.37
24	c	501	CLA	CMC-C2C	-2.21	1.46	1.50
24	D	403	CLA	C1B-C2B	2.21	1.48	1.43
24	B	607	CLA	C1D-C2D	2.21	1.49	1.45
24	a	607	CLA	CMB-C2B	-2.21	1.46	1.50
24	C	511	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C1B-NB	-2.20	1.35	1.37
24	B	611	CLA	C1B-NB	-2.20	1.35	1.37
24	C	505	CLA	C3B-C4B	2.20	1.49	1.42
24	c	512	CLA	CMB-C2B	-2.20	1.46	1.50
28	A	611	PL9	C35-C34	-2.20	1.45	1.50
24	c	506	CLA	C4B-NB	2.20	1.40	1.37
24	a	613	CLA	CHC-C1C	2.20	1.42	1.38
24	C	509	CLA	O2D-CGD	2.20	1.38	1.33
33	a	619	LMG	C14-C13	2.20	1.62	1.51
24	c	502	CLA	CMC-C2C	-2.20	1.46	1.50
24	b	616	CLA	C4B-NB	2.20	1.40	1.37
24	b	608	CLA	O2A-CGA	2.20	1.39	1.33
24	B	608	CLA	C3D-C4D	2.19	1.49	1.44
24	C	502	CLA	C3B-C4B	2.19	1.49	1.42
31	h	102	DGD	C4E-C3E	2.19	1.58	1.52
30	D	409	LHG	O6-C4	-2.19	1.36	1.44
24	c	503	CLA	CMC-C2C	-2.19	1.46	1.50
24	A	605	CLA	CMB-C2B	-2.19	1.46	1.50
26	B	617	BCR	C33-C5	-2.18	1.47	1.50
28	D	406	PL9	C12-C13	2.18	1.57	1.50
31	H	102	DGD	O3D-C3D	-2.18	1.37	1.43
24	b	611	CLA	CMC-C2C	-2.18	1.46	1.50
26	c	515	BCR	C38-C26	-2.18	1.47	1.50
24	a	604	CLA	CMD-C2D	-2.18	1.46	1.50
24	B	601	CLA	CHC-C1C	2.18	1.42	1.38
24	b	614	CLA	O2D-CGD	2.18	1.38	1.33
25	D	401	PHO	CBD-CGD	-2.18	1.49	1.52
24	C	502	CLA	MG-NA	2.18	2.11	2.06
24	A	607	CLA	C1D-ND	2.17	1.40	1.37
36	v	201	HEC	CMA-C3A	2.17	1.55	1.50
24	B	614	CLA	CMD-C2D	-2.17	1.46	1.50
24	b	612	CLA	C4B-NB	2.17	1.40	1.37
31	C	516	DGD	O1G-C1A	2.17	1.39	1.33
28	A	611	PL9	C37-C38	2.17	1.57	1.50
24	B	613	CLA	C1B-C2B	2.17	1.48	1.43
36	V	201	HEC	C2A-C3A	-2.17	1.32	1.36
31	H	102	DGD	O2D-C2D	-2.17	1.37	1.43
29	a	615	SQD	O47-C45	-2.17	1.41	1.46
33	M	101	LMG	C9-C8	2.17	1.57	1.50
28	D	406	PL9	C26-C24	-2.16	1.46	1.51
24	a	604	CLA	CAC-C3C	-2.16	1.45	1.51
36	v	201	HEC	C3B-C2B	-2.16	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	522	LMG	C3-C2	2.16	1.57	1.52
24	C	505	CLA	C1B-C2B	2.16	1.48	1.43
24	B	603	CLA	CHC-C1C	2.16	1.42	1.38
25	a	606	PHO	C3B-C2B	-2.16	1.37	1.40
25	A	606	PHO	O2D-CGD	2.16	1.38	1.33
24	C	504	CLA	CHC-C1C	2.16	1.42	1.38
24	C	502	CLA	CMD-C2D	-2.15	1.46	1.50
24	B	606	CLA	MG-ND	-2.15	2.01	2.05
24	B	607	CLA	CMC-C2C	-2.15	1.46	1.50
31	C	516	DGD	C6D-C5D	2.15	1.58	1.51
24	B	615	CLA	CHC-C4B	-2.15	1.34	1.39
24	b	606	CLA	CMB-C2B	-2.15	1.46	1.50
24	B	615	CLA	O2D-CED	-2.15	1.40	1.45
24	D	403	CLA	C1A-CHA	-2.15	1.34	1.43
32	c	520	STE	C2-C1	2.15	1.55	1.50
24	B	602	CLA	O2D-CGD	2.15	1.38	1.33
24	B	604	CLA	CMB-C2B	-2.15	1.46	1.50
35	f	101	HEM	CAB-C3B	2.15	1.53	1.47
24	B	604	CLA	O2D-CED	-2.15	1.40	1.45
24	C	505	CLA	C4B-NB	2.15	1.40	1.37
24	b	609	CLA	CMC-C2C	-2.15	1.46	1.50
24	B	601	CLA	CHC-C4B	-2.14	1.34	1.39
24	C	505	CLA	CMB-C2B	-2.14	1.46	1.50
32	C	519	STE	O1-C1	2.14	1.29	1.22
24	b	613	CLA	CAA-C2A	-2.14	1.50	1.54
25	D	401	PHO	CMA-C3A	-2.14	1.49	1.53
24	B	613	CLA	O2D-CED	-2.14	1.40	1.45
33	c	521	LMG	C4-C5	2.14	1.57	1.53
24	B	605	CLA	CHC-C1C	2.14	1.42	1.38
24	c	507	CLA	C1B-NB	-2.14	1.35	1.37
24	B	612	CLA	O2D-CED	-2.14	1.40	1.45
24	C	504	CLA	CMD-C2D	-2.13	1.46	1.50
36	v	201	HEC	CMD-C2D	2.13	1.55	1.50
30	d	406	LHG	C1-C2	-2.13	1.43	1.51
24	a	604	CLA	CMC-C2C	-2.13	1.46	1.50
24	A	604	CLA	CMB-C2B	-2.13	1.46	1.50
24	d	402	CLA	CMC-C2C	-2.13	1.46	1.50
24	D	404	CLA	C3D-C4D	2.12	1.49	1.44
24	b	604	CLA	CHC-C1C	2.12	1.42	1.38
24	b	610	CLA	CMD-C2D	-2.12	1.46	1.50
24	c	501	CLA	C4B-NB	2.12	1.40	1.37
24	A	607	CLA	C1B-C2B	2.12	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	f	101	HEM	CMB-C2B	2.12	1.55	1.50
25	d	401	PHO	C3D-C4D	2.12	1.44	1.41
24	B	613	CLA	C1A-CHA	-2.12	1.34	1.43
24	d	402	CLA	CMD-C2D	-2.12	1.46	1.50
25	d	401	PHO	C3D-CAD	-2.12	1.43	1.47
33	M	101	LMG	O4-C4	-2.12	1.37	1.43
32	b	621	STE	C2-C1	2.12	1.55	1.50
24	b	609	CLA	C3B-C4B	2.12	1.48	1.42
31	C	516	DGD	O2G-C1B	2.12	1.40	1.34
24	b	612	CLA	C3B-C4B	2.11	1.48	1.42
24	b	602	CLA	C4B-NB	2.11	1.40	1.37
24	b	608	CLA	C4B-NB	2.11	1.40	1.37
24	b	608	CLA	C3C-C2C	2.11	1.41	1.36
31	h	102	DGD	C4D-C3D	2.11	1.57	1.52
26	X	101	BCR	C4-C5	-2.11	1.47	1.51
29	D	408	SQD	O3-C3	-2.11	1.37	1.43
24	B	607	CLA	CMB-C2B	-2.11	1.46	1.50
24	B	612	CLA	CMB-C2B	-2.11	1.46	1.50
24	A	607	CLA	C3B-C4B	2.11	1.48	1.42
30	a	614	LHG	O8-C23	2.10	1.39	1.33
35	f	101	HEM	CMA-C3A	2.10	1.55	1.50
24	D	403	CLA	MG-ND	-2.10	2.01	2.05
24	C	513	CLA	CHC-C4B	-2.10	1.34	1.39
33	D	407	LMG	O1-C7	-2.10	1.40	1.43
24	b	603	CLA	CAC-C3C	-2.10	1.45	1.51
24	B	615	CLA	CMB-C2B	-2.10	1.46	1.50
24	b	602	CLA	CHC-C4B	-2.09	1.34	1.39
24	A	612	CLA	OBD-CAD	2.09	1.26	1.22
24	C	512	CLA	C3B-C4B	2.09	1.48	1.42
24	A	607	CLA	C1B-NB	-2.09	1.35	1.37
24	c	508	CLA	MG-NB	2.09	2.09	2.05
26	b	618	BCR	C33-C5	-2.09	1.47	1.50
24	b	616	CLA	CMC-C2C	-2.09	1.46	1.50
24	C	503	CLA	CMB-C2B	-2.09	1.46	1.50
24	B	608	CLA	O2D-CGD	2.09	1.38	1.33
24	B	606	CLA	CMA-C3A	-2.08	1.48	1.53
31	C	518	DGD	C4D-C5D	2.08	1.57	1.53
33	C	515	LMG	C7-C8	2.08	1.57	1.50
24	B	604	CLA	CHC-C1C	2.08	1.42	1.38
24	B	604	CLA	C4-C3	-2.08	1.45	1.50
24	B	612	CLA	C1B-NB	-2.08	1.35	1.37
24	A	607	CLA	CAC-C3C	-2.08	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	CHC-C4B	-2.08	1.34	1.39
32	B	619	STE	O1-C1	2.08	1.28	1.22
24	c	511	CLA	C1B-NB	-2.08	1.35	1.37
24	c	510	CLA	CMD-C2D	-2.08	1.46	1.50
24	c	509	CLA	O2D-CED	-2.08	1.40	1.45
24	d	403	CLA	O2D-CGD	2.08	1.38	1.33
24	a	605	CLA	CMC-C2C	-2.08	1.46	1.50
24	c	505	CLA	C3B-C4B	2.08	1.48	1.42
24	B	606	CLA	MG-NB	-2.07	2.01	2.05
24	B	602	CLA	CHC-C1C	2.07	1.42	1.38
31	c	518	DGD	O1G-C1G	-2.07	1.40	1.45
31	A	616	DGD	O2G-C1B	2.07	1.40	1.34
24	C	506	CLA	C3D-C4D	2.07	1.48	1.44
24	C	508	CLA	CMD-C2D	-2.07	1.46	1.50
31	C	516	DGD	O1A-C1A	2.06	1.28	1.22
24	C	512	CLA	CHC-C1C	2.06	1.42	1.38
24	b	602	CLA	MG-NB	-2.06	2.01	2.05
24	A	607	CLA	CMC-C2C	-2.06	1.46	1.50
31	h	102	DGD	C1G-C2G	2.06	1.57	1.50
24	B	602	CLA	O2D-CED	-2.06	1.40	1.45
24	B	609	CLA	CMA-C3A	-2.06	1.48	1.53
30	d	406	LHG	O7-C5	-2.06	1.41	1.46
24	b	612	CLA	CAC-C3C	-2.06	1.45	1.51
24	b	616	CLA	CAC-C3C	-2.06	1.45	1.51
24	C	513	CLA	CHC-C1C	2.06	1.42	1.38
24	D	404	CLA	C1B-C2B	2.05	1.47	1.43
24	C	505	CLA	CMD-C2D	-2.05	1.46	1.50
24	C	511	CLA	CHC-C1C	2.05	1.42	1.38
24	b	610	CLA	C1C-C2C	2.05	1.48	1.44
24	c	506	CLA	CMB-C2B	-2.05	1.46	1.50
24	B	603	CLA	CMD-C2D	-2.05	1.46	1.50
31	c	518	DGD	C3E-C2E	2.05	1.57	1.52
24	a	613	CLA	CHD-C4C	2.05	1.43	1.39
24	A	612	CLA	C1B-C2B	2.05	1.47	1.43
33	D	407	LMG	O1-C1	2.04	1.43	1.40
33	D	411	LMG	C9-C8	2.04	1.57	1.50
26	c	515	BCR	C27-C26	-2.04	1.47	1.51
33	b	622	LMG	O6-C1	2.04	1.47	1.41
33	b	622	LMG	C3-C2	2.04	1.57	1.52
24	b	608	CLA	MG-NB	2.04	2.09	2.05
28	A	611	PL9	C41-C39	2.03	1.55	1.51
24	C	510	CLA	C1B-NB	-2.03	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	407	LMG	C4-C5	2.03	1.57	1.53
26	B	618	BCR	C31-C1	-2.03	1.49	1.53
24	c	510	CLA	CMC-C2C	-2.03	1.46	1.50
30	A	614	LHG	O8-C23	2.03	1.39	1.33
24	B	607	CLA	O2A-CGA	2.03	1.39	1.33
26	t	101	BCR	C1-C6	-2.03	1.51	1.53
31	c	517	DGD	C4E-C5E	2.02	1.57	1.53
24	B	614	CLA	CAC-C3C	-2.02	1.45	1.51
24	c	503	CLA	C4B-NB	2.02	1.40	1.37
31	c	516	DGD	C4D-C5D	2.02	1.57	1.53
32	B	621	STE	O1-C1	2.02	1.28	1.22
24	c	508	CLA	CMA-C3A	-2.02	1.48	1.53
31	C	518	DGD	O4E-C4E	-2.02	1.38	1.43
24	b	605	CLA	MG-NB	2.02	2.09	2.05
24	B	608	CLA	C1B-NB	-2.02	1.35	1.37
24	A	604	CLA	C4B-NB	2.02	1.40	1.37
33	D	411	LMG	O8-C28	2.02	1.39	1.33
24	c	510	CLA	MG-ND	-2.02	2.01	2.05
24	c	508	CLA	CMC-C2C	-2.02	1.46	1.50
24	B	605	CLA	C4D-CHA	2.02	1.45	1.38
32	C	519	STE	C2-C1	2.02	1.55	1.50
26	k	102	BCR	C38-C26	-2.02	1.47	1.50
24	b	614	CLA	MG-NB	-2.01	2.01	2.05
24	B	608	CLA	C1D-ND	2.01	1.40	1.37
24	a	604	CLA	O2D-CGD	2.01	1.38	1.33
33	M	101	LMG	O7-C8	-2.01	1.41	1.46
29	a	615	SQD	O4-C4	-2.01	1.38	1.43
24	D	404	CLA	CHC-C4B	-2.01	1.34	1.39
24	C	504	CLA	C1B-C2B	2.01	1.47	1.43

All (1202) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O6-C1-C2	12.20	126.80	108.27
24	B	603	CLA	C4A-NA-C1A	11.81	112.07	106.68
24	b	604	CLA	C4A-NA-C1A	11.14	111.76	106.68
29	B	620	SQD	O6-C1-C2	9.38	122.52	108.27
24	b	606	CLA	C4A-NA-C1A	9.31	110.93	106.68
36	v	201	HEC	CBB-CAB-C3B	-9.29	108.87	127.43
36	V	201	HEC	CBB-CAB-C3B	-9.18	109.08	127.43
24	c	505	CLA	C4A-NA-C1A	9.02	110.79	106.68
29	a	615	SQD	O6-C1-C2	8.79	121.62	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C4A-NA-C1A	8.49	110.55	106.68
24	c	511	CLA	C4A-NA-C1A	8.46	110.54	106.68
24	b	601	CLA	C4A-NA-C1A	8.40	110.51	106.68
24	B	614	CLA	C4A-NA-C1A	8.27	110.45	106.68
24	C	507	CLA	C4A-NA-C1A	8.22	110.43	106.68
24	B	607	CLA	C4A-NA-C1A	8.16	110.40	106.68
24	B	608	CLA	C4A-NA-C1A	7.86	110.27	106.68
24	B	611	CLA	C4A-NA-C1A	7.70	110.19	106.68
24	B	612	CLA	C4A-NA-C1A	7.62	110.16	106.68
24	C	513	CLA	C4A-NA-C1A	7.53	110.12	106.68
24	c	509	CLA	C4A-NA-C1A	7.42	110.06	106.68
24	c	507	CLA	C4A-NA-C1A	7.42	110.06	106.68
24	c	508	CLA	C4A-NA-C1A	6.96	109.85	106.68
29	A	613	SQD	O6-C1-C2	6.90	118.75	108.27
36	v	201	HEC	CBC-CAC-C3C	-6.71	114.02	127.43
24	B	615	CLA	C4A-NA-C1A	6.68	109.73	106.68
24	H	101	CLA	C4A-NA-C1A	6.60	109.69	106.68
24	C	503	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	c	510	CLA	C4A-NA-C1A	6.28	109.54	106.68
24	C	510	CLA	C4A-NA-C1A	6.12	109.47	106.68
24	C	506	CLA	C4A-NA-C1A	6.08	109.45	106.68
28	a	612	PL9	C7-C3-C4	6.01	121.86	116.91
24	b	605	CLA	C4A-NA-C1A	5.98	109.41	106.68
24	A	604	CLA	C4A-NA-C1A	5.83	109.34	106.68
24	b	614	CLA	C4A-NA-C1A	5.79	109.32	106.68
24	C	511	CLA	C4A-NA-C1A	5.74	109.30	106.68
24	c	512	CLA	C4A-NA-C1A	5.73	109.29	106.68
24	b	603	CLA	C4A-NA-C1A	5.55	109.21	106.68
29	A	613	SQD	C1-C2-C3	-5.54	98.36	110.01
36	V	201	HEC	CBC-CAC-C3C	-5.50	116.45	127.43
28	d	405	PL9	C7-C3-C4	5.46	121.41	116.91
24	A	612	CLA	C4A-NA-C1A	5.45	109.17	106.68
24	B	615	CLA	O2D-CGD-O1D	-5.45	113.25	123.85
24	b	602	CLA	C4A-NA-C1A	5.39	109.14	106.68
24	c	501	CLA	O2D-CGD-O1D	-5.39	113.36	123.85
24	c	503	CLA	C4A-NA-C1A	5.36	109.12	106.68
29	f	102	SQD	O6-C1-C2	5.25	116.24	108.27
29	b	620	SQD	O7-S-C6	5.24	114.58	106.76
31	C	518	DGD	O3G-C3G-C2G	-5.18	98.23	110.82
29	b	620	SQD	C1-C2-C3	-5.14	99.20	110.01
25	A	606	PHO	C4D-CHA-CBD	-5.13	105.99	108.45
29	D	408	SQD	O6-C1-C2	5.12	116.05	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	406	PL9	C36-C34-C33	-5.07	109.78	121.17
24	b	609	CLA	C4A-NA-C1A	5.02	108.97	106.68
29	B	620	SQD	C1-C2-C3	-4.98	99.54	110.01
25	A	606	PHO	C2B-C1B-NB	-4.98	105.83	109.43
29	D	408	SQD	O9-S-C6	4.98	114.19	106.76
24	b	607	CLA	C4A-NA-C1A	4.96	108.94	106.68
28	D	406	PL9	C7-C3-C4	4.95	120.98	116.91
24	C	509	CLA	C4A-NA-C1A	4.86	108.90	106.68
24	c	513	CLA	C4A-NA-C1A	4.86	108.90	106.68
24	B	609	CLA	C4A-NA-C1A	4.82	108.88	106.68
29	f	102	SQD	O7-S-C6	4.81	113.94	106.76
29	a	615	SQD	O7-S-C6	4.80	113.93	106.76
24	a	607	CLA	C4A-NA-C1A	4.78	108.86	106.68
24	C	512	CLA	C4A-NA-C1A	4.78	108.86	106.68
24	B	601	CLA	O2D-CGD-CBD	4.76	119.56	111.23
24	B	613	CLA	O2D-CGD-O1D	-4.76	114.58	123.85
24	a	604	CLA	C4A-NA-C1A	4.76	108.85	106.68
28	A	611	PL9	C7-C3-C4	4.74	120.81	116.91
29	A	613	SQD	O7-S-C6	4.73	113.82	106.76
29	a	615	SQD	C1-C2-C3	-4.67	100.18	110.01
24	B	602	CLA	C3B-C4B-NB	-4.66	106.37	110.53
29	b	620	SQD	O2-C2-C1	4.61	121.06	110.08
29	a	615	SQD	C1-O5-C5	-4.59	104.75	113.72
24	c	510	CLA	O2D-CGD-O1D	-4.57	114.95	123.85
24	c	506	CLA	C4A-NA-C1A	4.56	108.76	106.68
31	H	102	DGD	O3G-C3G-C2G	-4.55	99.75	110.82
24	a	613	CLA	C4A-NA-C1A	4.54	108.75	106.68
29	A	613	SQD	O47-C7-C8	4.54	121.29	111.48
25	d	401	PHO	O2D-CGD-O1D	-4.51	115.07	123.85
24	b	611	CLA	O2D-CGD-O1D	-4.51	115.07	123.85
24	b	605	CLA	O1D-CGD-CBD	4.50	133.39	124.52
25	D	401	PHO	C4D-CHA-CBD	-4.49	106.30	108.45
29	A	613	SQD	O47-C7-O49	-4.45	113.30	123.70
30	A	614	LHG	O4-P-O5	4.44	133.11	112.44
24	C	508	CLA	C4A-NA-C1A	4.44	108.71	106.68
30	d	406	LHG	O4-P-O5	4.44	133.09	112.44
30	D	409	LHG	O4-P-O5	4.42	133.01	112.44
24	b	615	CLA	C3B-C4B-NB	-4.40	106.60	110.53
24	b	610	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
25	d	401	PHO	C2B-C1B-NB	-4.36	106.28	109.43
24	C	502	CLA	C4A-NA-C1A	4.35	108.66	106.68
30	e	101	LHG	O4-P-O5	4.31	132.48	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	616	BCR	C2-C1-C6	4.28	116.66	110.44
34	a	611	BCT	O2-C-O1	4.26	130.58	119.68
29	A	615	SQD	C45-O47-C7	4.26	123.92	117.78
29	a	615	SQD	O47-C7-C8	4.21	120.60	111.48
24	C	509	CLA	CMB-C2B-C1B	-4.20	119.02	125.42
29	f	102	SQD	O9-S-O7	-4.19	100.19	113.82
24	C	501	CLA	C4A-NA-C1A	4.16	108.58	106.68
30	L	101	LHG	O4-P-O5	4.16	131.78	112.44
24	c	509	CLA	CHB-C4A-NA	4.14	130.37	124.40
30	d	407	LHG	O4-P-O5	4.13	131.67	112.44
31	C	517	DGD	O3G-C3G-C2G	-4.12	100.79	110.82
24	B	605	CLA	C4A-NA-C1A	4.11	108.55	106.68
30	l	101	LHG	O4-P-O5	4.10	131.54	112.44
24	b	610	CLA	C4A-NA-C1A	4.10	108.55	106.68
24	B	615	CLA	O2D-CGD-CBD	4.09	118.38	111.23
30	D	413	LHG	O4-P-O5	4.08	131.42	112.44
24	b	610	CLA	CHB-C4A-NA	4.08	130.28	124.40
28	A	611	PL9	C40-C39-C41	4.07	122.30	115.23
24	C	501	CLA	O2D-CGD-O1D	-4.07	115.92	123.85
24	b	616	CLA	C4A-NA-C1A	4.07	108.53	106.68
24	d	403	CLA	C4A-NA-C1A	4.06	108.53	106.68
24	c	512	CLA	C1-C2-C3	-4.06	119.55	126.20
24	c	502	CLA	O2D-CGD-O1D	-4.05	115.97	123.85
24	D	404	CLA	C4A-NA-C1A	4.05	108.53	106.68
24	C	502	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
24	b	602	CLA	O2D-CGD-O1D	-4.04	115.99	123.85
28	a	612	PL9	C7-C3-C2	-4.01	118.66	123.39
33	m	101	LMG	O6-C1-O1	-4.01	100.57	110.04
29	B	620	SQD	C1-O5-C5	-4.01	105.89	113.72
24	b	602	CLA	O2D-CGD-CBD	4.00	118.23	111.23
25	D	401	PHO	CMB-C2B-C3B	4.00	132.67	124.68
24	A	604	CLA	CHB-C4A-NA	3.98	130.14	124.40
25	D	401	PHO	C2B-C1B-NB	-3.97	106.56	109.43
29	B	620	SQD	O47-C7-C8	3.97	120.07	111.48
24	a	605	CLA	C4A-NA-C1A	3.96	108.48	106.68
24	C	513	CLA	O2D-CGD-O1D	-3.95	116.16	123.85
24	c	512	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
24	b	614	CLA	C1-C2-C3	-3.93	119.76	126.20
24	B	609	CLA	CHB-C4A-NA	3.92	130.05	124.40
24	b	601	CLA	CHB-C4A-NA	3.91	130.04	124.40
33	a	619	LMG	C1-C2-C3	-3.91	101.79	110.01
24	A	607	CLA	O2D-CGD-O1D	-3.90	116.25	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C3B-C4B-NB	-3.89	107.06	110.53
30	a	614	LHG	O4-P-O5	3.89	130.54	112.44
24	C	512	CLA	C3B-C4B-NB	-3.89	107.06	110.53
25	d	401	PHO	C4D-CHA-CBD	-3.89	106.59	108.45
26	b	617	BCR	C2-C1-C6	3.87	116.06	110.44
34	D	402	BCT	O2-C-O1	3.86	129.54	119.68
24	B	601	CLA	CMB-C2B-C1B	-3.83	119.58	125.42
30	D	410	LHG	O4-P-O5	3.83	130.28	112.44
33	b	622	LMG	C1-O6-C5	-3.83	106.24	113.72
24	B	610	CLA	C4A-NA-C1A	3.83	108.42	106.68
24	c	501	CLA	O2D-CGD-CBD	3.82	117.91	111.23
24	B	607	CLA	O2D-CGD-O1D	-3.81	116.42	123.85
33	m	101	LMG	O7-C10-O9	-3.78	114.86	123.70
24	c	509	CLA	O2A-CGA-O1A	-3.78	114.17	123.63
24	b	616	CLA	C3B-C4B-NB	-3.77	107.17	110.53
24	c	510	CLA	C3B-C4B-NB	-3.77	107.17	110.53
25	d	401	PHO	O1D-CGD-CBD	3.75	130.41	124.72
24	C	507	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
24	b	612	CLA	CMB-C2B-C1B	-3.74	119.72	125.42
24	C	512	CLA	C1-C2-C3	-3.74	120.07	126.20
29	A	615	SQD	O47-C7-C8	3.73	119.55	111.48
26	T	101	BCR	C7-C8-C9	-3.72	120.73	126.23
33	C	515	LMG	O6-C5-C4	-3.72	103.00	109.70
33	b	622	LMG	O1-C1-C2	-3.70	102.65	108.27
29	B	620	SQD	O2-C2-C1	3.70	118.89	110.08
24	A	607	CLA	CMB-C2B-C1B	-3.70	119.79	125.42
24	C	503	CLA	C1-O2A-CGA	3.68	125.57	116.65
24	C	503	CLA	C3B-C4B-NB	-3.67	107.25	110.53
26	B	617	BCR	C15-C16-C17	-3.66	116.02	123.52
24	c	512	CLA	C3B-C4B-NB	-3.66	107.26	110.53
24	b	608	CLA	CMB-C2B-C1B	-3.66	119.85	125.42
24	C	504	CLA	C3B-C4B-NB	-3.66	107.27	110.53
24	b	613	CLA	C1-C2-C3	-3.65	120.22	126.20
33	a	619	LMG	C1-O6-C5	-3.64	106.60	113.72
24	a	605	CLA	CHB-C4A-NA	3.64	129.65	124.40
29	A	613	SQD	C1-O5-C5	-3.64	106.62	113.72
24	B	607	CLA	O2D-CGD-CBD	3.63	117.58	111.23
24	H	101	CLA	C3B-C4B-NB	-3.63	107.29	110.53
24	C	505	CLA	CMB-C2B-C1B	-3.62	119.90	125.42
26	b	618	BCR	C36-C18-C17	-3.62	116.95	122.82
24	c	513	CLA	O2D-CGD-O1D	-3.61	116.81	123.85
28	D	406	PL9	C30-C29-C31	-3.61	108.96	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	612	PL9	C22-C23-C24	-3.61	119.37	127.62
24	D	404	CLA	CMB-C2B-C1B	-3.59	119.95	125.42
24	b	606	CLA	O2D-CGD-CBD	3.59	117.50	111.23
24	B	603	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
31	h	102	DGD	O3G-C3G-C2G	-3.58	102.12	110.82
29	B	620	SQD	C3-C4-C5	3.57	116.71	110.23
28	A	611	PL9	C7-C3-C2	-3.57	119.18	123.39
26	X	101	BCR	C27-C26-C25	3.57	127.52	122.70
24	c	502	CLA	O1D-CGD-CBD	3.57	131.55	124.52
24	c	505	CLA	C3B-C4B-NB	-3.56	107.35	110.53
28	D	406	PL9	C20-C19-C21	3.56	121.41	115.23
24	D	403	CLA	C1-C2-C3	-3.55	120.37	126.20
28	d	405	PL9	C40-C39-C41	3.55	121.39	115.23
24	A	612	CLA	C3B-C4B-NB	-3.55	107.36	110.53
29	A	613	SQD	O8-S-C6	3.55	112.83	105.97
24	B	609	CLA	C3B-C4B-NB	-3.55	107.36	110.53
24	B	611	CLA	C11-C12-C13	-3.55	104.18	115.97
26	t	101	BCR	C15-C16-C17	-3.54	116.27	123.52
24	c	506	CLA	CMB-C2B-C1B	-3.54	120.03	125.42
24	C	509	CLA	CHB-C4A-NA	3.54	129.51	124.40
28	A	611	PL9	O1-C4-C3	-3.53	117.00	120.73
29	B	620	SQD	O8-S-C6	3.53	112.79	105.97
29	b	620	SQD	O9-S-C6	3.51	112.00	106.76
35	f	101	HEM	CBA-CAA-C2A	-3.51	102.82	112.53
24	C	509	CLA	CMB-C2B-C3B	3.51	134.81	126.55
24	c	508	CLA	O2D-CGD-CBD	3.51	117.36	111.23
30	a	614	LHG	O8-C23-C24	3.49	122.48	111.83
26	B	618	BCR	C2-C1-C6	3.49	115.51	110.44
26	d	404	BCR	C38-C26-C25	-3.48	120.69	124.48
29	b	620	SQD	C3-C4-C5	3.47	116.53	110.23
24	b	601	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
33	m	101	LMG	O8-C28-O10	-3.47	114.96	123.63
24	B	612	CLA	CMB-C2B-C1B	-3.46	120.14	125.42
24	c	513	CLA	CHB-C4A-NA	3.46	129.39	124.40
24	A	605	CLA	C3B-C4B-NB	-3.46	107.44	110.53
26	B	616	BCR	C37-C22-C23	3.45	123.36	118.09
24	b	612	CLA	C1-C2-C3	-3.45	120.54	126.20
24	b	611	CLA	C4A-NA-C1A	3.45	108.25	106.68
29	B	620	SQD	O48-C23-C24	3.45	122.34	111.83
31	A	616	DGD	C4E-C3E-C2E	-3.45	104.78	110.83
24	B	605	CLA	C3B-C4B-NB	-3.45	107.45	110.53
24	b	613	CLA	O2D-CGD-O1D	-3.44	117.15	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	606	PHO	C1-C2-C3	-3.43	120.57	126.20
24	C	510	CLA	C3B-C4B-NB	-3.43	107.47	110.53
24	b	615	CLA	C4A-NA-C1A	3.43	108.24	106.68
26	b	617	BCR	C3-C4-C5	-3.42	107.95	114.06
24	B	613	CLA	C4A-NA-C1A	3.42	108.24	106.68
24	a	613	CLA	C3B-C4B-NB	-3.42	107.48	110.53
25	A	606	PHO	C1-C2-C3	-3.41	120.61	126.20
24	c	502	CLA	CMB-C2B-C1B	-3.41	120.23	125.42
24	C	513	CLA	C4-C3-C5	3.40	121.13	115.23
24	b	610	CLA	CAA-CBA-CGA	-3.40	103.55	113.21
24	B	606	CLA	C1-C2-C3	-3.40	120.63	126.20
26	K	103	BCR	C15-C16-C17	-3.40	116.56	123.52
24	C	505	CLA	C3B-C4B-NB	-3.40	107.50	110.53
24	d	402	CLA	C4A-NA-C1A	3.39	108.23	106.68
36	V	201	HEC	C4D-ND-C1D	3.39	111.35	105.82
29	f	102	SQD	O5-C5-C4	3.39	115.80	109.70
28	A	611	PL9	C27-C28-C29	-3.38	119.88	127.62
33	C	515	LMG	O6-C1-O1	-3.38	102.06	110.04
24	a	607	CLA	O2D-CGD-CBD	3.38	117.14	111.23
26	a	608	BCR	C37-C22-C21	-3.38	117.34	122.82
25	a	606	PHO	CMB-C2B-C3B	3.37	131.43	124.68
24	D	404	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
24	B	615	CLA	CHB-C4A-NA	3.36	129.25	124.40
24	b	616	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
26	c	514	BCR	C2-C1-C6	3.35	115.31	110.44
35	f	101	HEM	CBD-CAD-C3D	-3.35	103.28	112.53
24	D	403	CLA	C4-C3-C5	3.34	121.03	115.23
29	b	620	SQD	O48-C23-C24	3.34	122.02	111.83
24	A	612	CLA	CHB-C4A-NA	3.32	129.19	124.40
26	c	515	BCR	C2-C1-C6	3.32	115.26	110.44
25	A	606	PHO	C3B-C4B-NB	-3.31	105.30	107.46
24	b	606	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
30	D	413	LHG	O8-C23-C24	3.30	121.89	111.83
24	d	402	CLA	C3B-C4B-NB	-3.30	107.59	110.53
28	D	406	PL9	C42-C43-C44	-3.29	120.08	127.62
24	b	612	CLA	C11-C12-C13	-3.29	105.02	115.97
31	c	517	DGD	O6D-C1D-O3G	-3.29	102.28	110.04
24	D	403	CLA	O2A-CGA-O1A	-3.28	115.42	123.63
28	a	612	PL9	C20-C19-C21	3.28	120.92	115.23
25	d	401	PHO	C1-C2-C3	-3.27	120.83	126.20
24	b	601	CLA	O2D-CGD-CBD	3.27	116.95	111.23
26	B	617	BCR	C15-C14-C13	-3.27	122.69	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
25	d	401	PHO	O2D-CGD-CBD	3.26	114.53	110.95
29	b	620	SQD	O5-C1-C2	-3.25	103.69	110.37
24	c	504	CLA	C3B-C4B-NB	-3.25	107.63	110.53
24	B	611	CLA	C1D-ND-C4D	3.25	108.59	106.31
24	c	502	CLA	O2A-CGA-O1A	-3.25	115.50	123.63
25	A	606	PHO	CMB-C2B-C3B	3.25	131.17	124.68
24	B	602	CLA	O2A-CGA-O1A	-3.25	115.51	123.63
24	B	609	CLA	O2A-CGA-O1A	-3.25	115.51	123.63
24	C	502	CLA	C3B-C4B-NB	-3.24	107.63	110.53
31	A	616	DGD	C3G-C2G-C1G	-3.24	104.23	111.78
24	b	613	CLA	CMB-C2B-C1B	-3.23	120.50	125.42
24	b	604	CLA	C3B-C4B-NB	-3.23	107.65	110.53
26	d	404	BCR	C27-C26-C25	3.23	127.06	122.70
24	b	615	CLA	CHB-C4A-NA	3.22	129.05	124.40
24	B	611	CLA	CMB-C2B-C1B	-3.22	120.51	125.42
24	c	502	CLA	C1-C2-C3	-3.22	120.92	126.20
24	b	604	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
28	D	406	PL9	C22-C23-C24	-3.22	120.26	127.62
29	B	620	SQD	O9-S-O7	-3.21	103.39	113.82
24	c	504	CLA	C4A-NA-C1A	3.21	108.14	106.68
26	T	101	BCR	C27-C26-C25	3.21	127.04	122.70
24	B	612	CLA	C1-C2-C3	-3.20	120.95	126.20
26	c	515	BCR	C27-C26-C25	3.20	127.03	122.70
24	B	614	CLA	CHB-C4A-NA	3.20	129.02	124.40
24	B	610	CLA	C14-C13-C15	-3.20	99.87	111.27
31	C	518	DGD	O6D-C1D-O3G	-3.20	102.48	110.04
26	A	608	BCR	C40-C30-C25	3.19	115.25	110.24
33	Y	101	LMG	O6-C1-O1	-3.19	102.51	110.04
24	d	403	CLA	C3B-C4B-NB	-3.19	107.69	110.53
26	b	619	BCR	C29-C30-C25	3.19	115.07	110.44
29	B	620	SQD	O7-S-C6	3.18	111.51	106.76
33	m	101	LMG	O1-C1-C2	-3.18	103.44	108.27
33	m	101	LMG	O3-C3-C2	-3.18	102.88	110.38
26	X	101	BCR	C37-C22-C23	3.18	122.95	118.09
29	a	615	SQD	O48-C23-C24	3.17	121.51	111.83
24	b	610	CLA	O2D-CGD-CBD	3.17	116.77	111.23
26	X	101	BCR	C30-C25-C26	-3.17	118.31	122.64
33	c	522	LMG	O6-C1-O1	-3.17	102.56	110.04
24	B	613	CLA	O2D-CGD-CBD	3.17	116.77	111.23
26	B	616	BCR	C37-C22-C21	-3.16	117.69	122.82
24	b	609	CLA	O1D-CGD-CBD	3.16	130.75	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	608	BCR	C27-C26-C25	3.16	126.97	122.70
24	A	605	CLA	CMB-C2B-C1B	-3.15	120.62	125.42
36	v	201	HEC	CMC-C2C-C1C	-3.15	120.62	125.42
24	c	504	CLA	C4-C3-C5	3.14	120.68	115.23
29	D	408	SQD	O8-S-C6	3.14	112.04	105.97
24	C	505	CLA	CHB-C1B-NB	3.14	128.76	124.05
24	A	607	CLA	C4-C3-C5	3.14	120.68	115.23
29	a	616	SQD	O48-C23-O10	-3.13	115.79	123.63
26	b	619	BCR	C2-C1-C6	3.13	114.99	110.44
31	c	518	DGD	O3G-C3G-C2G	-3.12	103.22	110.82
29	a	616	SQD	O48-C23-C24	3.12	121.33	111.83
26	c	514	BCR	C38-C26-C25	-3.11	121.09	124.48
24	C	505	CLA	O2A-CGA-O1A	-3.10	115.87	123.63
24	B	613	CLA	C3B-C4B-NB	-3.10	107.77	110.53
24	C	505	CLA	CMB-C2B-C3B	3.09	133.82	126.55
24	D	403	CLA	C3B-C4B-NB	-3.09	107.78	110.53
29	B	620	SQD	O48-C23-O10	-3.09	115.91	123.63
24	C	512	CLA	CHB-C4A-NA	3.08	128.85	124.40
24	b	614	CLA	O2A-CGA-O1A	-3.08	115.94	123.63
24	c	504	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
31	A	616	DGD	O3G-C3G-C2G	-3.07	103.35	110.82
24	A	605	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
31	C	517	DGD	O6D-C1D-O3G	-3.07	102.80	110.04
24	B	601	CLA	CMB-C2B-C3B	3.07	133.76	126.55
24	c	512	CLA	CHB-C4A-NA	3.06	128.82	124.40
24	b	616	CLA	CHC-C4B-NB	3.06	128.65	124.05
24	H	101	CLA	O2D-CGD-CBD	3.06	116.57	111.23
24	d	402	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
26	D	405	BCR	C27-C26-C25	3.05	126.83	122.70
24	B	611	CLA	C2D-C1D-ND	-3.05	107.11	110.13
28	D	406	PL9	C7-C3-C2	-3.05	119.80	123.39
24	C	512	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
24	B	601	CLA	CHB-C4A-NA	3.04	128.79	124.40
24	D	404	CLA	C4-C3-C5	3.04	120.50	115.23
32	L	102	STE	O2-C1-C2	3.04	123.60	114.00
33	a	619	LMG	O7-C10-O9	-3.03	116.62	123.70
24	B	603	CLA	CHB-C4A-NA	3.03	128.77	124.40
28	A	611	PL9	C12-C13-C14	-3.03	120.69	127.62
24	c	510	CLA	O1D-CGD-CBD	3.02	130.48	124.52
33	C	515	LMG	C1-O6-C5	-3.01	107.83	113.72
24	B	603	CLA	C3B-C4B-NB	-3.01	107.84	110.53
26	t	101	BCR	C36-C18-C19	3.00	122.67	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	620	SQD	O8-S-O7	-3.00	103.90	111.40
29	a	616	SQD	O47-C7-C8	2.99	117.95	111.48
24	C	501	CLA	CHB-C1B-NB	2.99	128.53	124.05
31	c	516	DGD	O3G-C3G-C2G	-2.98	103.56	110.82
24	b	608	CLA	CMB-C2B-C3B	2.98	133.57	126.55
29	b	620	SQD	O47-C7-C8	2.98	117.93	111.48
28	d	405	PL9	C7-C3-C2	-2.98	119.87	123.39
26	K	102	BCR	C27-C26-C25	2.98	126.73	122.70
24	C	508	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
24	b	610	CLA	O2A-CGA-O1A	-2.97	116.19	123.63
26	B	617	BCR	C37-C22-C21	-2.97	118.00	122.82
26	B	618	BCR	C15-C16-C17	-2.97	117.44	123.52
24	C	507	CLA	CHD-C1D-ND	-2.97	120.62	124.80
31	C	516	DGD	O3G-C3G-C2G	-2.97	103.60	110.82
26	A	608	BCR	C37-C22-C21	-2.96	118.01	122.82
26	c	515	BCR	C15-C16-C17	-2.96	117.46	123.52
24	A	607	CLA	O2D-CGD-CBD	2.96	116.40	111.23
24	A	604	CLA	CAA-CBA-CGA	-2.96	104.81	113.21
29	A	615	SQD	O48-C23-C24	2.95	120.83	111.83
26	B	618	BCR	C36-C18-C17	-2.95	118.04	122.82
24	B	605	CLA	O2A-CGA-O1A	-2.95	116.26	123.63
24	b	611	CLA	O2D-CGD-CBD	2.94	116.37	111.23
24	C	501	CLA	O2D-CGD-CBD	2.94	116.37	111.23
28	d	405	PL9	C7-C8-C9	-2.94	121.77	126.83
24	b	615	CLA	C11-C10-C8	-2.93	106.22	115.97
36	v	201	HEC	C4D-ND-C1D	2.93	110.60	105.82
31	c	518	DGD	O5D-C1E-C2E	2.93	112.72	108.27
28	D	406	PL9	C35-C34-C36	2.93	120.31	115.23
24	b	608	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	a	607	CLA	CHB-C4A-NA	2.93	128.63	124.40
28	D	406	PL9	C7-C8-C9	-2.93	121.78	126.83
30	A	614	LHG	O8-C23-C24	2.92	120.74	111.83
28	d	405	PL9	C22-C23-C24	-2.92	120.94	127.62
24	C	504	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
26	h	101	BCR	C27-C26-C25	2.91	126.64	122.70
28	A	611	PL9	C40-C39-C38	-2.91	116.16	123.63
29	a	615	SQD	O9-S-O7	-2.91	104.37	113.82
33	b	622	LMG	C1-C2-C3	-2.91	103.89	110.01
24	A	605	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
25	d	401	PHO	C3B-C4B-NB	-2.91	105.57	107.46
24	c	508	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
24	c	502	CLA	CMB-C2B-C3B	2.89	133.36	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	CHB-C1B-NB	2.89	128.39	124.05
25	A	606	PHO	O1D-CGD-CBD	2.89	129.11	124.72
24	c	508	CLA	C3B-C4B-NB	-2.89	107.95	110.53
24	b	608	CLA	O2D-CGD-CBD	2.89	116.28	111.23
24	A	604	CLA	C3B-C4B-NB	-2.88	107.95	110.53
35	F	101	HEM	CBD-CAD-C3D	-2.88	104.56	112.53
24	D	404	CLA	CMB-C2B-C3B	2.88	133.32	126.55
24	c	506	CLA	CMB-C2B-C3B	2.88	133.32	126.55
26	K	101	BCR	C15-C16-C17	-2.87	117.64	123.52
25	a	606	PHO	C2B-C1B-NB	-2.87	107.36	109.43
25	a	606	PHO	O2D-CGD-O1D	-2.87	118.26	123.85
24	B	613	CLA	CHB-C4A-NA	2.87	128.54	124.40
24	A	604	CLA	C7-C6-C5	-2.87	105.62	113.26
24	C	508	CLA	CMB-C2B-C1B	-2.87	121.06	125.42
24	B	604	CLA	CHD-C1D-ND	-2.86	120.77	124.80
26	A	608	BCR	C27-C26-C25	2.86	126.57	122.70
31	c	518	DGD	C6D-O5D-C1E	2.86	119.93	113.80
24	a	605	CLA	CMB-C2B-C1B	-2.86	121.06	125.42
26	B	616	BCR	C27-C26-C25	2.86	126.57	122.70
26	C	514	BCR	C15-C16-C17	-2.85	117.68	123.52
29	D	408	SQD	C1-C2-C3	-2.85	104.02	110.01
24	D	403	CLA	C4A-NA-C1A	2.85	107.98	106.68
31	c	516	DGD	O6D-C1D-O3G	-2.85	103.32	110.04
24	C	508	CLA	CHB-C1B-NB	2.84	128.31	124.05
24	b	604	CLA	CAA-CBA-CGA	-2.84	105.14	113.21
24	b	612	CLA	CMB-C2B-C3B	2.84	133.23	126.55
31	C	516	DGD	O3E-C3E-C2E	-2.84	103.69	110.38
24	D	403	CLA	CMB-C2B-C1B	-2.83	121.10	125.42
24	B	610	CLA	C1-C2-C3	-2.83	121.55	126.20
24	c	506	CLA	C4-C3-C5	2.83	120.14	115.23
26	B	617	BCR	C29-C30-C25	2.83	114.55	110.44
31	h	102	DGD	O3E-C3E-C2E	-2.83	103.70	110.38
33	Y	101	LMG	O8-C28-O10	-2.83	116.55	123.63
26	b	618	BCR	C27-C26-C25	2.83	126.53	122.70
24	b	609	CLA	CHA-C1A-NA	-2.83	119.99	126.39
29	A	613	SQD	O8-S-O7	-2.82	104.34	111.40
24	A	612	CLA	C1C-C2C-C3C	-2.82	104.01	106.98
24	A	605	CLA	CMB-C2B-C3B	2.82	133.18	126.55
24	b	612	CLA	C3B-C4B-NB	-2.82	108.01	110.53
31	H	102	DGD	O2D-C2D-C1D	-2.82	103.37	110.08
24	B	606	CLA	C3B-C4B-NB	-2.81	108.02	110.53
24	A	607	CLA	CMB-C2B-C3B	2.81	133.16	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	CMD-C2D-C1D	2.81	129.70	125.42
31	c	517	DGD	O3G-C3G-C2G	-2.81	103.99	110.82
28	A	611	PL9	C22-C23-C24	-2.80	121.20	127.62
30	D	413	LHG	C11-C10-C9	-2.80	100.19	114.37
32	d	409	STE	O2-C1-C2	2.80	122.85	114.00
24	B	605	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
30	D	413	LHG	O8-C23-O10	-2.80	116.63	123.63
26	a	608	BCR	C2-C1-C6	2.79	114.50	110.44
26	b	618	BCR	C15-C16-C17	-2.79	117.81	123.52
24	B	603	CLA	C1D-ND-C4D	2.79	108.27	106.31
30	e	101	LHG	O8-C23-C24	2.79	120.33	111.83
28	A	611	PL9	C36-C34-C33	-2.79	114.91	121.17
31	c	516	DGD	C3G-C2G-C1G	-2.79	105.29	111.78
26	K	102	BCR	C37-C22-C21	-2.78	118.30	122.82
24	b	616	CLA	CHB-C4A-NA	2.78	128.42	124.40
24	b	601	CLA	C3B-C4B-NB	-2.78	108.05	110.53
33	C	515	LMG	C9-C8-C7	-2.78	105.30	111.78
31	c	518	DGD	O6E-C1E-O5D	-2.78	103.48	110.04
28	d	405	PL9	C12-C13-C14	-2.78	121.27	127.62
28	D	406	PL9	C27-C28-C29	-2.78	121.27	127.62
24	B	613	CLA	C1-C2-C3	-2.77	121.66	126.20
24	b	603	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
24	b	608	CLA	CHB-C1B-NB	2.77	128.20	124.05
28	a	612	PL9	C32-C33-C34	-2.76	121.30	127.62
24	B	606	CLA	C2A-C1A-CHA	2.76	128.66	123.87
24	b	603	CLA	C3B-C4B-NB	-2.76	108.06	110.53
26	t	101	BCR	C1-C6-C5	-2.76	118.87	122.64
31	h	102	DGD	C3E-C4E-C5E	-2.76	105.23	110.23
24	A	604	CLA	C1-C2-C3	-2.76	121.68	126.20
31	C	517	DGD	O5D-C6D-C5D	-2.75	103.21	109.42
31	c	516	DGD	C3E-C4E-C5E	-2.75	105.24	110.23
26	b	619	BCR	C15-C16-C17	-2.75	117.89	123.52
24	b	616	CLA	O2A-CGA-O1A	-2.75	116.75	123.63
31	A	616	DGD	O6D-C1D-O3G	-2.75	103.55	110.04
36	v	201	HEC	CBA-CAA-C2A	-2.75	104.93	112.53
33	M	101	LMG	O7-C10-O9	-2.75	117.29	123.70
28	D	406	PL9	C12-C13-C14	-2.74	121.34	127.62
26	k	102	BCR	C27-C26-C25	2.74	126.41	122.70
26	B	617	BCR	C2-C1-C6	2.74	114.43	110.44
24	b	603	CLA	C2D-C1D-ND	-2.74	107.41	110.13
24	b	608	CLA	C2D-C1D-ND	-2.74	107.41	110.13
26	B	616	BCR	C3-C4-C5	-2.74	109.17	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	O1D-CGD-CBD	2.74	129.93	124.52
29	f	102	SQD	O9-S-C6	2.74	110.85	106.76
24	b	604	CLA	CHB-C4A-NA	2.74	128.35	124.40
30	D	409	LHG	C18-C17-C16	-2.74	100.54	114.37
24	a	605	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
29	D	408	SQD	O9-S-O7	-2.73	104.94	113.82
24	c	513	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	C	506	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
24	B	601	CLA	C16-C15-C13	-2.73	106.90	115.97
24	C	506	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	D	403	CLA	C6-C5-C3	2.73	120.11	113.47
24	C	511	CLA	CMB-C2B-C1B	-2.72	121.27	125.42
24	b	611	CLA	C1-C2-C3	-2.72	121.73	126.20
24	b	612	CLA	CHB-C4A-NA	2.72	128.33	124.40
24	b	606	CLA	O2A-CGA-O1A	-2.72	116.81	123.63
33	d	408	LMG	O6-C1-O1	-2.72	103.61	110.04
26	K	103	BCR	C37-C22-C21	-2.72	118.41	122.82
24	c	504	CLA	CHB-C1B-NB	2.72	128.13	124.05
31	C	516	DGD	O5D-C6D-C5D	-2.72	103.29	109.42
26	C	514	BCR	C36-C18-C17	-2.72	118.41	122.82
26	c	515	BCR	C8-C9-C10	2.72	123.28	119.01
24	B	610	CLA	C3B-C4B-NB	-2.72	108.11	110.53
24	c	504	CLA	C6-C7-C8	-2.71	106.95	115.97
24	b	607	CLA	C1-O2A-CGA	2.71	123.21	116.65
24	B	602	CLA	C1-C2-C3	-2.71	121.76	126.20
24	d	402	CLA	O2A-CGA-O1A	-2.71	116.86	123.63
32	d	409	STE	O2-C1-O1	-2.71	116.37	123.33
24	B	610	CLA	C7-C6-C5	-2.70	106.05	113.26
29	A	613	SQD	O5-C1-O6	2.70	116.43	110.04
32	t	102	STE	O2-C1-C2	2.70	122.54	114.00
31	h	102	DGD	O6D-C1D-O3G	-2.70	103.66	110.04
25	a	606	PHO	C4D-CHA-CBD	-2.70	107.16	108.45
24	b	601	CLA	CHD-C1D-ND	-2.69	121.01	124.80
24	b	605	CLA	CHB-C4A-NA	2.69	128.29	124.40
30	a	614	LHG	C20-C19-C18	-2.69	100.76	114.37
31	h	102	DGD	C1D-C2D-C3D	-2.69	104.35	110.01
24	A	612	CLA	CMB-C2B-C3B	2.69	132.87	126.55
31	C	516	DGD	O6D-C1D-O3G	-2.69	103.70	110.04
24	a	605	CLA	CMB-C2B-C3B	2.68	132.86	126.55
26	K	103	BCR	C27-C26-C25	2.68	126.33	122.70
33	a	619	LMG	C9-C8-C7	-2.68	105.54	111.78
24	C	509	CLA	C3B-C4B-NB	-2.68	108.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	d	407	LHG	O8-C23-C24	2.68	120.00	111.83
24	C	504	CLA	C4A-NA-C1A	2.68	107.90	106.68
28	A	611	PL9	C35-C34-C36	2.68	119.87	115.23
24	B	603	CLA	C6-C5-C3	-2.67	106.96	113.47
28	D	406	PL9	C31-C29-C28	2.67	127.16	121.17
26	B	617	BCR	C36-C18-C17	-2.66	118.50	122.82
24	B	607	CLA	C11-C10-C8	-2.66	107.11	115.97
24	C	508	CLA	CHD-C1D-ND	-2.66	121.06	124.80
24	c	503	CLA	C3B-C4B-NB	-2.66	108.16	110.53
29	D	408	SQD	C44-O6-C1	2.66	118.22	113.68
33	a	619	LMG	O8-C28-O10	-2.66	116.98	123.63
24	c	510	CLA	CMB-C2B-C1B	-2.66	121.37	125.42
24	c	502	CLA	C4A-NA-C1A	2.66	107.89	106.68
24	C	501	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
24	b	602	CLA	CHB-C4A-NA	2.65	128.23	124.40
24	a	613	CLA	CHD-C1D-ND	-2.64	121.08	124.80
33	c	521	LMG	O3-C3-C2	-2.64	104.14	110.38
29	b	620	SQD	O9-S-O7	-2.64	105.23	113.82
24	C	513	CLA	CHB-C4A-NA	2.64	128.21	124.40
31	A	616	DGD	O5D-C6D-C5D	-2.64	103.47	109.42
29	A	615	SQD	O47-C45-C46	2.64	112.28	106.21
29	A	613	SQD	O9-S-O7	-2.64	105.25	113.82
28	A	611	PL9	O2-C1-C2	-2.64	115.83	121.83
24	c	504	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
24	c	505	CLA	C4D-CHA-C1A	2.63	124.38	121.24
24	c	513	CLA	C4-C3-C5	2.63	119.79	115.23
24	d	402	CLA	C1-C2-C3	-2.63	121.89	126.20
32	R	101	STE	O2-C1-C2	2.63	122.30	114.00
26	a	608	BCR	C37-C22-C23	2.63	122.10	118.09
24	b	615	CLA	CAA-CBA-CGA	-2.63	105.75	113.21
24	C	501	CLA	CHD-C1D-ND	-2.62	121.11	124.80
28	D	406	PL9	C40-C39-C41	2.62	119.78	115.23
24	b	612	CLA	CAA-CBA-CGA	-2.62	105.76	113.21
32	b	624	STE	C3-C2-C1	-2.62	107.67	114.51
24	b	610	CLA	C1D-ND-C4D	-2.62	104.47	106.31
29	B	620	SQD	O9-S-C6	2.62	110.67	106.76
33	M	101	LMG	C40-C39-C38	-2.62	101.14	114.37
30	a	614	LHG	O8-C23-O10	-2.62	117.09	123.63
24	c	508	CLA	C1-C2-C3	-2.61	121.92	126.20
35	F	101	HEM	CBA-CAA-C2A	-2.61	105.33	112.53
24	c	507	CLA	C2C-C1C-NC	2.60	112.72	109.98
33	M	101	LMG	O3-C3-C2	-2.60	104.24	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	605	CLA	CHC-C4B-NB	2.60	127.95	124.05
29	D	408	SQD	C3-C4-C5	2.60	114.95	110.23
31	c	518	DGD	O6D-C1D-O3G	-2.60	103.90	110.04
24	C	513	CLA	CMB-C2B-C1B	-2.60	121.46	125.42
25	a	606	PHO	OBD-CAD-CBD	-2.60	122.01	125.82
26	B	616	BCR	C29-C30-C25	2.60	114.21	110.44
24	b	608	CLA	CHD-C1D-C2D	2.59	130.88	125.49
24	c	502	CLA	CHD-C1D-ND	-2.59	121.16	124.80
24	B	607	CLA	CHC-C4B-NB	2.59	127.93	124.05
31	C	516	DGD	O1G-C1A-C2A	-2.59	103.94	111.83
33	M	101	LMG	C1-O6-C5	-2.59	108.66	113.72
24	b	614	CLA	C3B-C4B-NB	-2.59	108.22	110.53
26	B	618	BCR	C36-C18-C19	2.59	122.04	118.09
33	C	515	LMG	C3-C4-C5	-2.59	105.55	110.23
31	c	516	DGD	O3E-C3E-C2E	-2.58	104.28	110.38
24	b	608	CLA	C3B-C4B-NB	-2.58	108.22	110.53
24	B	601	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
25	A	606	PHO	C4B-NB-C1B	2.58	112.58	108.82
33	D	407	LMG	O1-C7-C8	-2.58	104.54	110.82
24	B	609	CLA	CHD-C1D-ND	-2.58	121.17	124.80
33	b	622	LMG	C4-C3-C2	-2.58	106.30	110.83
33	M	101	LMG	O6-C1-O1	-2.58	103.95	110.04
33	c	519	LMG	C9-C8-C7	-2.58	105.78	111.78
29	b	620	SQD	O5-C5-C4	2.58	114.34	109.70
28	D	406	PL9	C37-C38-C39	-2.57	121.73	127.62
24	b	607	CLA	CHD-C4C-NC	2.57	128.22	124.23
28	D	406	PL9	C8-C7-C3	2.57	118.68	112.03
26	k	102	BCR	C2-C1-C6	2.57	114.17	110.44
24	b	604	CLA	C11-C10-C8	-2.57	107.43	115.97
26	K	101	BCR	C2-C1-C6	2.57	114.17	110.44
24	c	502	CLA	CHB-C1B-NB	2.56	127.90	124.05
24	b	607	CLA	C3B-C4B-NB	-2.56	108.24	110.53
32	d	411	STE	O2-C1-C2	2.56	122.10	114.00
24	C	507	CLA	CHB-C4A-NA	2.56	128.09	124.40
24	b	612	CLA	C4A-NA-C1A	2.56	107.85	106.68
33	m	101	LMG	O1-C7-C8	-2.56	104.60	110.82
24	c	510	CLA	CHB-C1B-NB	2.56	127.89	124.05
24	b	611	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
30	l	101	LHG	C5-O7-C7	-2.56	111.68	117.80
31	C	516	DGD	CDB-CCB-CBB	-2.55	101.45	114.37
24	C	502	CLA	O1D-CGD-CBD	2.55	129.55	124.52
24	a	613	CLA	CHB-C4A-NA	2.55	128.08	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	613	CLA	CHB-C1B-NB	2.55	127.87	124.05
31	C	516	DGD	CBB-CAB-C9B	-2.55	101.49	114.37
35	f	101	HEM	CHD-C4C-NC	2.55	127.23	124.45
33	b	622	LMG	C3-C4-C5	-2.54	105.62	110.23
24	B	605	CLA	O2D-CGD-CBD	2.54	115.67	111.23
31	A	616	DGD	O1G-C1A-O1A	-2.54	117.27	123.63
26	b	618	BCR	C30-C25-C26	-2.54	119.17	122.64
24	c	510	CLA	CHB-C4A-NA	2.54	128.06	124.40
24	B	613	CLA	CHC-C4B-NB	2.54	127.85	124.05
31	A	616	DGD	O5D-C1E-C2E	2.54	112.12	108.27
24	B	612	CLA	CAC-C3C-C4C	2.53	128.09	124.79
24	B	611	CLA	CHB-C4A-NA	2.53	128.05	124.40
24	b	604	CLA	O2D-CGD-CBD	2.53	115.65	111.23
33	m	101	LMG	O6-C1-C2	2.53	115.56	110.37
24	B	611	CLA	CMB-C2B-C3B	2.53	132.49	126.55
24	A	612	CLA	CHD-C1D-ND	-2.52	121.25	124.80
24	B	603	CLA	C11-C10-C8	-2.52	107.58	115.97
26	h	101	BCR	C36-C18-C17	-2.52	118.73	122.82
24	C	512	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
25	D	401	PHO	C3B-C4B-NB	-2.51	105.83	107.46
24	b	616	CLA	CMB-C2B-C3B	2.51	132.46	126.55
24	a	604	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
26	X	101	BCR	C37-C22-C21	-2.51	118.75	122.82
26	C	514	BCR	C2-C1-C6	2.51	114.08	110.44
32	t	102	STE	C3-C2-C1	-2.51	107.97	114.51
24	b	610	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	b	616	CLA	CHD-C1D-ND	-2.51	121.28	124.80
24	b	606	CLA	CHB-C1B-NB	2.51	127.81	124.05
26	t	101	BCR	C7-C8-C9	-2.50	122.53	126.23
24	B	607	CLA	CHB-C4A-NA	2.50	128.01	124.40
24	B	607	CLA	C3B-C4B-NB	-2.50	108.30	110.53
31	A	616	DGD	C1D-C2D-C3D	-2.50	104.75	110.01
24	B	605	CLA	CHA-C1A-NA	-2.50	120.73	126.39
31	c	517	DGD	O2E-C2E-C1E	-2.50	104.11	110.08
24	c	505	CLA	C11-C10-C8	-2.50	107.66	115.97
24	B	611	CLA	C3B-C4B-NB	-2.50	108.30	110.53
24	b	613	CLA	CHB-C4A-NA	2.50	128.00	124.40
25	A	606	PHO	O2D-CGD-O1D	-2.50	118.99	123.85
31	H	102	DGD	C3D-C4D-C5D	-2.50	105.70	110.23
31	c	518	DGD	C3G-C2G-C1G	-2.50	105.96	111.78
24	D	404	CLA	CAC-C3C-C4C	2.49	128.03	124.79
24	C	504	CLA	CHB-C1B-NB	2.49	127.79	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	101	BCR	C38-C26-C25	-2.49	121.76	124.48
24	b	614	CLA	CHB-C4A-NA	2.49	127.99	124.40
24	c	513	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
33	D	407	LMG	O1-C1-C2	-2.49	104.49	108.27
24	B	603	CLA	O2D-CGD-CBD	2.49	115.58	111.23
24	b	603	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	D	404	CLA	C2C-C1C-NC	2.48	112.59	109.98
24	a	607	CLA	CAA-CBA-CGA	-2.48	106.16	113.21
24	c	513	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
24	c	509	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	B	614	CLA	C11-C10-C8	-2.48	107.73	115.97
24	b	609	CLA	CHC-C4B-NB	2.47	127.76	124.05
28	d	405	PL9	C37-C38-C39	-2.47	121.97	127.62
24	c	507	CLA	CHC-C4B-NB	2.47	127.76	124.05
36	v	201	HEC	CHA-C4D-ND	2.47	128.34	123.86
24	A	605	CLA	C1-C2-C3	-2.47	122.15	126.20
24	c	507	CLA	CHD-C1D-ND	-2.47	121.33	124.80
24	b	602	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
30	D	410	LHG	O8-C23-C24	2.47	119.35	111.83
26	b	618	BCR	C15-C14-C13	-2.46	123.82	127.28
28	A	611	PL9	C11-C9-C8	-2.46	115.64	121.17
24	b	604	CLA	OBD-CAD-C3D	2.46	134.17	128.42
24	C	506	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
28	A	611	PL9	C20-C19-C21	2.46	119.50	115.23
26	k	101	BCR	C38-C26-C25	-2.46	121.80	124.48
24	C	504	CLA	C4-C3-C5	2.46	119.49	115.23
31	A	616	DGD	CDB-CCB-CBB	-2.46	101.96	114.37
24	C	508	CLA	CMB-C2B-C3B	2.45	132.32	126.55
25	A	606	PHO	C3D-C4D-ND	2.45	110.85	107.71
33	c	519	LMG	C40-C39-C38	-2.45	101.97	114.37
24	B	612	CLA	C2A-C1A-CHA	2.45	128.12	123.87
26	h	101	BCR	C37-C22-C21	-2.45	118.85	122.82
32	J	101	STE	C3-C2-C1	-2.45	108.12	114.51
24	b	613	CLA	C4A-NA-C1A	2.45	107.80	106.68
32	b	623	STE	O2-C1-C2	2.45	121.73	114.00
24	B	601	CLA	CHA-C1A-NA	-2.45	120.85	126.39
30	l	101	LHG	C20-C19-C18	-2.45	102.00	114.37
26	B	618	BCR	C29-C30-C25	2.44	113.99	110.44
24	b	604	CLA	CHD-C4C-NC	2.44	128.02	124.23
33	D	411	LMG	O8-C28-O10	-2.44	117.52	123.63
26	c	515	BCR	C37-C22-C23	2.44	121.82	118.09
24	A	607	CLA	CAA-CBA-CGA	-2.44	106.28	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	514	BCR	C3-C4-C5	-2.44	109.71	114.06
32	d	410	STE	O2-C1-C2	2.44	121.70	114.00
33	C	515	LMG	O7-C10-C11	2.43	116.75	111.48
24	c	507	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
24	b	611	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	h	102	DGD	CDB-CCB-CBB	-2.43	102.08	114.37
33	c	519	LMG	O6-C1-O1	-2.43	104.30	110.04
33	m	101	LMG	C38-C37-C36	-2.43	102.08	114.37
26	K	101	BCR	C27-C26-C25	2.43	125.99	122.70
25	A	606	PHO	C5-C3-C2	2.43	126.62	121.17
26	k	101	BCR	C27-C26-C25	2.43	125.98	122.70
26	a	608	BCR	C38-C26-C25	-2.43	121.83	124.48
30	l	101	LHG	O8-C23-C24	2.43	119.23	111.83
26	b	618	BCR	C36-C18-C19	2.42	121.79	118.09
31	A	616	DGD	CBB-CAB-C9B	-2.42	102.11	114.37
24	C	504	CLA	O2D-CGD-CBD	2.42	115.47	111.23
26	T	101	BCR	C1-C6-C5	-2.42	119.33	122.64
32	b	623	STE	O2-C1-O1	-2.42	117.11	123.33
31	C	517	DGD	C6D-O5D-C1E	2.42	118.98	113.80
24	B	604	CLA	C7-C6-C5	-2.42	106.81	113.26
32	J	101	STE	O2-C1-C2	2.41	121.62	114.00
26	b	617	BCR	C29-C30-C25	2.41	113.94	110.44
24	c	502	CLA	CHB-C1B-C2B	-2.41	120.43	127.43
33	a	619	LMG	O6-C1-C2	-2.41	105.42	110.37
24	a	604	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
33	b	622	LMG	O7-C10-O9	-2.41	118.08	123.70
26	t	101	BCR	C1-C6-C7	2.40	122.17	115.65
24	C	506	CLA	CMB-C2B-C3B	2.40	132.21	126.55
28	d	405	PL9	C8-C7-C3	2.40	118.24	112.03
24	b	609	CLA	C1-O2A-CGA	2.40	122.46	116.65
24	B	602	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
24	A	605	CLA	CHB-C4A-NA	2.40	127.86	124.40
31	c	518	DGD	CBB-CAB-C9B	-2.40	102.25	114.37
33	c	521	LMG	O2-C2-C1	-2.40	104.36	110.08
24	C	505	CLA	CHA-C1A-NA	-2.40	120.97	126.39
24	b	616	CLA	C2A-C3A-C4A	2.39	105.74	101.87
26	h	101	BCR	C2-C1-C6	2.39	113.92	110.44
24	B	612	CLA	CHA-C1A-NA	-2.39	120.97	126.39
24	C	501	CLA	C3B-C4B-NB	-2.39	108.40	110.53
33	b	622	LMG	O6-C5-C6	2.39	112.36	106.44
30	D	409	LHG	C20-C19-C18	-2.39	102.29	114.37
24	B	606	CLA	CHB-C4A-NA	2.39	127.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	405	BCR	C16-C15-C14	-2.39	118.63	123.52
26	b	619	BCR	C37-C22-C21	-2.39	118.95	122.82
29	b	620	SQD	O47-C45-C46	2.39	116.91	108.34
24	d	403	CLA	CHA-C1A-NA	-2.39	120.99	126.39
24	c	508	CLA	CHB-C4A-NA	2.38	127.84	124.40
24	A	607	CLA	C2C-C1C-NC	2.38	112.48	109.98
24	C	509	CLA	CHD-C1D-ND	-2.38	121.45	124.80
24	b	609	CLA	C5-C3-C2	2.38	126.51	121.17
26	t	101	BCR	C4-C5-C6	2.38	125.92	122.70
24	b	616	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
26	c	515	BCR	C1-C6-C5	-2.38	119.39	122.64
30	d	407	LHG	O8-C23-O10	-2.38	117.69	123.63
24	a	607	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
24	C	513	CLA	O2D-CGD-CBD	2.37	115.38	111.23
24	B	607	CLA	CMB-C2B-C1B	-2.37	121.81	125.42
24	B	612	CLA	CMB-C2B-C3B	2.37	132.12	126.55
24	B	612	CLA	C4-C3-C5	2.37	119.33	115.23
33	D	412	LMG	O7-C10-O9	-2.37	117.25	123.33
24	c	511	CLA	CHB-C4A-NA	2.37	127.81	124.40
26	d	404	BCR	C16-C15-C14	-2.36	118.68	123.52
33	D	407	LMG	O2-C2-C3	-2.36	104.81	110.38
24	B	602	CLA	CHD-C1D-ND	-2.36	121.48	124.80
24	C	503	CLA	C4-C3-C5	2.36	119.33	115.23
31	H	102	DGD	C4D-C3D-C2D	-2.36	106.69	110.83
24	C	511	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
31	c	516	DGD	O1G-C1A-C2A	-2.36	104.65	111.83
33	c	521	LMG	C9-C8-C7	-2.36	106.29	111.78
26	b	617	BCR	C36-C18-C19	2.36	121.69	118.09
24	A	612	CLA	CMB-C2B-C1B	-2.35	121.83	125.42
24	C	510	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
25	D	401	PHO	CED-O2D-CGD	2.35	121.24	115.92
24	c	504	CLA	CMB-C2B-C3B	2.35	132.07	126.55
24	C	509	CLA	C1-C2-C3	-2.35	122.35	126.20
31	c	516	DGD	O3G-C1D-C2D	-2.35	104.71	108.27
24	c	504	CLA	CHD-C4C-NC	2.35	127.87	124.23
24	b	611	CLA	CHB-C4A-NA	2.35	127.79	124.40
24	B	611	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
24	B	614	CLA	C3B-C4B-NB	-2.35	108.44	110.53
24	c	506	CLA	C4-C3-C2	-2.34	117.61	123.63
24	B	604	CLA	C4A-NA-C1A	2.34	107.75	106.68
32	L	102	STE	O2-C1-O1	-2.34	117.31	123.33
24	B	613	CLA	O2A-CGA-O1A	-2.34	117.77	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	CHC-C1C-NC	2.34	127.83	124.31
26	a	608	BCR	C20-C21-C22	-2.34	124.00	127.28
24	B	607	CLA	C11-C12-C13	-2.34	108.19	115.97
31	C	518	DGD	CDB-CCB-CBB	-2.34	102.55	114.37
24	B	602	CLA	O2D-CGD-CBD	2.34	115.31	111.23
26	a	608	BCR	C29-C30-C25	2.33	113.83	110.44
29	a	615	SQD	O8-S-C6	2.33	110.47	105.97
26	B	616	BCR	C15-C16-C17	-2.33	118.75	123.52
30	a	614	LHG	C11-C10-C9	-2.33	102.59	114.37
24	B	612	CLA	CHB-C1B-NB	2.33	127.54	124.05
25	a	606	PHO	O2D-CGD-CBD	2.33	113.51	110.95
33	c	522	LMG	O8-C28-O10	-2.33	117.80	123.63
24	b	604	CLA	CGD-CBD-CAD	-2.32	103.32	110.85
24	b	614	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
24	a	613	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
24	B	603	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
29	A	613	SQD	O3-C3-C4	2.32	115.85	110.38
33	d	408	LMG	O2-C2-C1	-2.32	104.54	110.08
28	a	612	PL9	C26-C24-C23	-2.32	115.96	121.17
24	b	602	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	C	517	DGD	O6E-C1E-O5D	-2.32	104.56	110.04
25	D	401	PHO	CBC-CAC-C3C	-2.32	109.55	112.87
30	a	614	LHG	C18-C17-C16	-2.32	102.65	114.37
24	B	613	CLA	CAC-C3C-C4C	2.32	127.80	124.79
24	C	508	CLA	CHB-C1B-C2B	-2.31	120.71	127.43
24	b	614	CLA	CHD-C1D-ND	-2.31	121.55	124.80
25	a	606	PHO	C3D-C4D-ND	2.31	110.67	107.71
25	a	606	PHO	O2A-CGA-O1A	-2.31	117.84	123.63
25	a	606	PHO	O1D-CGD-CBD	2.31	128.23	124.72
29	f	102	SQD	O47-C7-C8	2.31	119.41	110.93
26	h	101	BCR	C37-C22-C23	2.31	121.61	118.09
24	C	501	CLA	CHD-C1D-C2D	2.31	130.28	125.49
28	a	612	PL9	C27-C28-C29	-2.31	122.35	127.62
24	B	601	CLA	C3B-C4B-NB	-2.31	108.47	110.53
33	c	519	LMG	C38-C37-C36	-2.31	102.72	114.37
24	B	606	CLA	CHA-C1A-NA	-2.30	121.17	126.39
24	B	605	CLA	CHB-C1B-NB	2.30	127.51	124.05
31	c	517	DGD	CDB-CCB-CBB	-2.30	102.72	114.37
33	C	515	LMG	O3-C3-C2	-2.30	104.95	110.38
24	c	510	CLA	CMB-C2B-C3B	2.30	131.96	126.55
31	h	102	DGD	O5E-C6E-C5E	-2.30	103.51	111.33
31	c	516	DGD	O4D-C4D-C5D	-2.30	103.66	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	403	CLA	CMB-C2B-C3B	2.30	131.95	126.55
33	b	622	LMG	C9-C8-C7	-2.30	106.43	111.78
29	B	620	SQD	C46-C45-C44	-2.29	106.43	111.78
29	f	102	SQD	O48-C23-C24	2.29	118.83	111.83
33	a	619	LMG	O7-C10-C11	2.29	116.44	111.48
24	A	605	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
33	D	411	LMG	C38-C37-C36	-2.29	102.78	114.37
26	c	515	BCR	C35-C13-C14	-2.29	119.10	122.82
31	c	516	DGD	O2D-C2D-C1D	-2.29	104.62	110.08
29	f	102	SQD	C3-C4-C5	2.29	114.38	110.23
24	c	505	CLA	C3A-C2A-C1A	2.29	104.77	101.34
24	c	512	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
24	b	604	CLA	CHD-C1D-ND	-2.29	121.58	124.80
28	A	611	PL9	O2-C1-C6	2.29	124.12	120.48
24	A	612	CLA	CHD-C1D-C2D	2.29	130.24	125.49
24	C	510	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
26	b	618	BCR	C35-C13-C14	-2.29	119.11	122.82
24	c	511	CLA	C1D-ND-C4D	2.28	107.91	106.31
26	c	514	BCR	C27-C26-C25	2.28	125.79	122.70
24	b	613	CLA	O1D-CGD-CBD	2.28	129.02	124.52
33	Y	101	LMG	O2-C2-C1	-2.28	104.64	110.08
33	a	619	LMG	O1-C1-C2	2.28	111.74	108.27
24	a	613	CLA	CHD-C4C-NC	2.28	127.77	124.23
24	b	608	CLA	CHD-C1D-ND	-2.28	121.60	124.80
26	b	618	BCR	C1-C6-C5	-2.28	119.52	122.64
26	K	102	BCR	C30-C25-C26	-2.28	119.53	122.64
24	B	602	CLA	CHD-C1D-C2D	2.28	130.22	125.49
24	B	607	CLA	CMB-C2B-C3B	2.28	131.90	126.55
31	C	516	DGD	C9B-C8B-C7B	-2.27	102.88	114.37
24	B	601	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
24	b	616	CLA	C1-C2-C3	-2.27	122.47	126.20
24	C	507	CLA	O1D-CGD-CBD	2.27	129.00	124.52
26	c	515	BCR	C37-C22-C21	-2.27	119.14	122.82
24	b	607	CLA	CMB-C2B-C1B	-2.27	121.96	125.42
26	b	619	BCR	C36-C18-C19	2.27	121.56	118.09
31	c	518	DGD	CDB-CCB-CBB	-2.27	102.91	114.37
31	C	516	DGD	C6D-O5D-C1E	2.27	118.66	113.80
26	c	515	BCR	C7-C8-C9	-2.27	122.88	126.23
24	C	503	CLA	CHD-C1D-ND	-2.26	121.61	124.80
30	D	413	LHG	C18-C17-C16	-2.26	102.92	114.37
30	e	101	LHG	C20-C19-C18	-2.26	102.93	114.37
24	B	604	CLA	O2A-CGA-O1A	-2.26	117.97	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	O1D-CGD-CBD	2.26	128.97	124.52
24	b	612	CLA	OBD-CAD-C3D	2.26	133.70	128.42
26	d	404	BCR	C11-C10-C9	-2.26	124.11	127.28
24	C	504	CLA	CHD-C1D-ND	-2.26	121.63	124.80
24	b	602	CLA	C16-C15-C13	-2.26	108.47	115.97
31	A	616	DGD	O5E-C6E-C5E	-2.26	103.65	111.33
36	V	201	HEC	O1D-CGD-CBD	-2.26	115.94	123.09
33	Y	101	LMG	O1-C7-C8	-2.25	105.33	110.82
24	b	615	CLA	CHC-C1C-NC	2.25	127.70	124.31
24	b	606	CLA	CHB-C4A-NA	2.25	127.65	124.40
36	v	201	HEC	C1D-C2D-C3D	-2.25	104.24	106.82
24	C	513	CLA	CHC-C1C-NC	2.25	127.70	124.31
31	c	516	DGD	CCB-CBB-CAB	-2.25	102.99	114.37
24	c	504	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	C	503	CLA	C7-C6-C5	-2.25	107.27	113.26
26	B	618	BCR	C38-C26-C25	-2.25	122.03	124.48
31	h	102	DGD	CBB-CAB-C9B	-2.25	103.01	114.37
36	v	201	HEC	CHB-C1B-NB	2.25	127.93	123.86
24	c	512	CLA	CHD-C1D-ND	-2.25	121.64	124.80
26	h	101	BCR	C36-C18-C19	2.25	121.52	118.09
24	C	501	CLA	CAA-CBA-CGA	-2.24	106.83	113.21
33	D	407	LMG	O6-C1-O1	-2.24	104.74	110.04
26	h	101	BCR	C38-C26-C25	-2.24	122.04	124.48
28	d	405	PL9	C41-C39-C38	-2.24	116.14	121.17
25	d	401	PHO	CMB-C2B-C3B	2.24	129.15	124.68
24	C	504	CLA	CHC-C1C-NC	2.24	127.68	124.31
24	A	607	CLA	C1C-C2C-C3C	-2.24	104.63	106.98
24	C	507	CLA	C2A-C1A-CHA	2.24	127.75	123.87
30	A	614	LHG	C11-C10-C9	-2.23	103.08	114.37
33	b	622	LMG	C40-C39-C38	-2.23	103.09	114.37
24	C	512	CLA	CHA-C4D-ND	2.23	137.15	132.55
24	a	604	CLA	CMB-C2B-C3B	2.23	131.79	126.55
33	D	411	LMG	O1-C7-C8	-2.23	106.04	111.77
26	A	608	BCR	C16-C15-C14	-2.23	118.96	123.52
26	A	608	BCR	C37-C22-C23	2.23	121.49	118.09
33	M	101	LMG	C38-C37-C36	-2.23	103.11	114.37
26	A	608	BCR	C8-C7-C6	-2.23	121.05	127.00
24	C	513	CLA	CMB-C2B-C3B	2.22	131.78	126.55
24	c	510	CLA	C11-C12-C13	-2.22	108.58	115.97
24	B	610	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	b	611	CLA	CHB-C1B-NB	2.22	127.38	124.05
24	c	505	CLA	C6-C7-C8	-2.22	108.59	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	CLA	C1-C2-C3	-2.22	122.56	126.20
24	a	607	CLA	C3B-C4B-NB	-2.22	108.55	110.53
24	b	602	CLA	CMB-C2B-C3B	2.22	131.77	126.55
24	C	504	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	B	602	CLA	CHD-C4C-NC	2.22	127.67	124.23
24	C	510	CLA	CMB-C2B-C3B	2.21	131.76	126.55
25	D	401	PHO	C1-C2-C3	-2.21	122.57	126.20
24	c	503	CLA	CHC-C4B-NB	2.21	127.36	124.05
26	X	101	BCR	C1-C6-C5	-2.21	119.62	122.64
24	b	606	CLA	C1C-C2C-C3C	-2.21	104.66	106.98
30	l	101	LHG	C11-C10-C9	-2.21	103.21	114.37
29	D	408	SQD	O5-C5-C4	2.21	113.68	109.70
28	A	611	PL9	C25-C24-C26	2.21	119.06	115.23
24	C	508	CLA	CHD-C1D-C2D	2.21	130.08	125.49
24	b	604	CLA	C1-C2-C3	-2.20	122.58	126.20
24	C	505	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
29	A	613	SQD	O5-C1-C2	-2.20	105.84	110.37
24	c	501	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	C	507	CLA	C11-C12-C13	-2.20	108.65	115.97
26	K	103	BCR	C2-C1-C6	2.20	113.64	110.44
26	A	608	BCR	C15-C16-C17	-2.20	119.02	123.52
24	B	609	CLA	C1-C2-C3	-2.20	122.59	126.20
31	H	102	DGD	C3G-C2G-C1G	-2.20	106.66	111.78
24	a	613	CLA	CHA-C1A-NA	-2.20	121.42	126.39
24	b	606	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
33	M	101	LMG	C37-C36-C35	-2.20	103.26	114.37
24	d	403	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
24	b	604	CLA	CHD-C1D-C2D	2.20	130.05	125.49
24	A	612	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
30	a	614	LHG	C15-C14-C13	-2.19	103.28	114.37
26	k	102	BCR	C8-C7-C6	-2.19	121.14	127.00
29	A	613	SQD	O48-C23-C24	2.19	118.52	111.83
24	C	512	CLA	O2D-CGD-CBD	2.19	115.06	111.23
24	B	603	CLA	CHB-C1B-NB	2.19	127.34	124.05
24	b	605	CLA	C1-C2-C3	-2.19	122.61	126.20
30	d	406	LHG	C20-C19-C18	-2.19	103.29	114.37
36	v	201	HEC	CAD-CBD-CGD	-2.19	107.86	113.67
32	C	521	STE	O2-C1-C2	2.19	120.91	114.00
28	a	612	PL9	O2-C1-C2	-2.19	116.86	121.83
31	H	102	DGD	C6D-C5D-C4D	2.18	116.64	112.07
29	a	615	SQD	O10-C23-C24	-2.18	115.25	123.78
24	D	404	CLA	O2D-CGD-CBD	2.18	115.04	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	DGD	C3E-C4E-C5E	-2.18	106.28	110.23
30	D	413	LHG	C20-C19-C18	-2.18	103.36	114.37
25	D	401	PHO	CMD-C2D-C3D	2.18	129.03	124.68
24	c	509	CLA	CHD-C1D-ND	-2.18	121.74	124.80
24	B	611	CLA	C1-C2-C3	-2.17	122.63	126.20
24	c	507	CLA	O1A-CGA-CBA	2.17	132.29	123.78
29	b	620	SQD	O8-S-C6	2.17	110.17	105.97
24	c	505	CLA	O2D-CGD-CBD	2.17	115.03	111.23
24	c	501	CLA	C2C-C1C-NC	2.17	112.26	109.98
24	c	505	CLA	CHC-C4B-NB	2.17	127.31	124.05
24	c	501	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
33	M	101	LMG	O2-C2-C3	-2.17	105.26	110.38
26	b	619	BCR	C38-C26-C25	-2.17	122.11	124.48
24	B	614	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
30	D	413	LHG	C15-C14-C13	-2.17	103.40	114.37
24	C	502	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
33	M	101	LMG	O2-C2-C1	-2.17	104.91	110.08
33	d	408	LMG	C3-C4-C5	-2.17	106.30	110.23
35	f	101	HEM	C3B-C4B-NB	-2.17	107.91	109.47
26	K	103	BCR	C7-C8-C9	-2.17	123.03	126.23
31	C	517	DGD	O2D-C2D-C1D	-2.16	104.92	110.08
24	B	609	CLA	C1D-ND-C4D	-2.16	104.79	106.31
31	C	516	DGD	C7A-C6A-C5A	-2.16	103.43	114.37
24	c	508	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
24	B	608	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
24	c	507	CLA	CHD-C4C-NC	2.16	127.58	124.23
24	a	604	CLA	CHB-C4A-NA	2.16	127.52	124.40
24	b	605	CLA	C3B-C4B-NB	-2.16	108.60	110.53
24	B	601	CLA	CHB-C1B-NB	2.16	127.29	124.05
26	T	101	BCR	C31-C1-C6	2.16	113.63	110.24
24	C	513	CLA	CHD-C1D-ND	-2.16	121.77	124.80
24	C	513	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
30	d	406	LHG	C27-C26-C25	-2.16	103.47	114.37
33	c	519	LMG	C8-O7-C10	2.16	121.65	117.85
29	b	620	SQD	O10-C23-C24	-2.16	115.35	123.78
24	c	513	CLA	CAA-CBA-CGA	-2.15	107.09	113.21
35	f	101	HEM	CAB-C3B-C2B	-2.15	121.44	128.43
26	D	405	BCR	C38-C26-C25	-2.15	122.14	124.48
28	d	405	PL9	C40-C39-C38	-2.15	118.12	123.63
26	A	608	BCR	C15-C14-C13	-2.15	124.27	127.28
28	a	612	PL9	C12-C13-C14	-2.15	122.71	127.62
31	c	518	DGD	C5B-C4B-C3B	-2.14	103.53	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	h	102	DGD	C3G-C2G-C1G	-2.14	106.79	111.78
26	h	101	BCR	C7-C8-C9	-2.14	123.06	126.23
24	b	603	CLA	CHD-C1D-C2D	2.14	129.94	125.49
24	C	503	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
24	A	604	CLA	CMB-C2B-C3B	2.14	131.59	126.55
24	B	608	CLA	CMB-C2B-C3B	2.14	131.59	126.55
26	t	101	BCR	C12-C13-C14	-2.14	115.64	119.01
26	B	618	BCR	C33-C5-C6	-2.14	122.15	124.48
24	c	511	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
31	H	102	DGD	C3E-C4E-C5E	-2.14	106.35	110.23
30	e	101	LHG	C5-O7-C7	-2.14	112.68	117.80
24	b	609	CLA	O2D-CGD-CBD	-2.14	107.49	111.23
24	b	613	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	C	502	CLA	CHD-C1D-ND	-2.14	121.80	124.80
30	A	614	LHG	C27-C26-C25	-2.14	103.57	114.37
26	a	608	BCR	C30-C25-C26	-2.13	119.72	122.64
24	c	504	CLA	O2D-CGD-CBD	2.13	114.96	111.23
24	b	605	CLA	CHD-C4C-NC	2.13	127.54	124.23
24	b	610	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
31	c	516	DGD	CAB-C9B-C8B	-2.13	103.60	114.37
24	B	609	CLA	O1A-CGA-CBA	2.13	132.11	123.78
31	c	516	DGD	O2G-C1B-C2B	-2.13	106.88	111.48
29	f	102	SQD	O5-C1-C2	-2.13	106.00	110.37
26	D	405	BCR	C15-C16-C17	-2.13	119.16	123.52
33	Y	101	LMG	O6-C5-C6	2.13	111.71	106.44
30	D	409	LHG	O8-C23-C24	2.13	118.32	111.83
28	a	612	PL9	O2-C1-C6	2.13	123.86	120.48
24	B	608	CLA	CMC-C2C-C1C	2.13	128.36	125.03
24	C	503	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
30	L	101	LHG	C27-C26-C25	-2.13	103.63	114.37
24	c	511	CLA	O2D-CGD-O1D	-2.12	119.71	123.85
24	H	101	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
24	b	612	CLA	CMD-C2D-C3D	2.12	132.56	127.69
24	A	604	CLA	C11-C12-C13	-2.12	108.92	115.97
24	D	403	CLA	CHB-C1B-NB	2.12	127.23	124.05
24	b	606	CLA	C3B-C4B-NB	-2.12	108.64	110.53
33	C	515	LMG	O8-C28-O10	-2.11	118.34	123.63
28	d	405	PL9	C20-C19-C21	2.11	118.90	115.23
24	C	504	CLA	CHD-C4C-NC	2.11	127.51	124.23
24	c	509	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
26	K	101	BCR	C11-C10-C9	-2.11	124.32	127.28
24	C	511	CLA	O2D-CGD-O1D	-2.11	119.74	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	614	LHG	O8-C23-O10	-2.11	118.35	123.63
31	A	616	DGD	C8B-C7B-C6B	-2.11	103.70	114.37
24	b	610	CLA	C2C-C1C-NC	2.11	112.20	109.98
36	V	201	HEC	CHC-C4B-C3B	2.11	128.76	125.21
24	B	608	CLA	CMD-C2D-C1D	-2.11	121.02	124.73
30	e	101	LHG	O8-C23-O10	-2.11	118.36	123.63
33	c	521	LMG	O7-C10-O9	-2.11	118.78	123.70
24	c	505	CLA	C1D-ND-C4D	2.11	107.79	106.31
24	b	612	CLA	C3D-C4D-ND	2.10	113.41	109.99
24	B	609	CLA	CAA-C2A-C3A	-2.10	107.31	113.00
33	c	521	LMG	C6-C5-C4	-2.10	107.85	113.02
26	a	608	BCR	C39-C30-C25	-2.10	106.94	110.24
24	C	505	CLA	C16-C15-C13	-2.10	108.97	115.97
24	C	512	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
31	c	518	DGD	CAB-C9B-C8B	-2.10	103.74	114.37
30	D	409	LHG	C27-C26-C25	-2.10	103.76	114.37
29	a	615	SQD	O5-C1-O6	2.10	115.00	110.04
24	A	605	CLA	C7-C6-C5	-2.10	107.67	113.26
25	D	401	PHO	CMA-C3A-C4A	-2.10	110.09	114.61
24	B	613	CLA	O1D-CGD-CBD	2.10	128.65	124.52
24	c	511	CLA	CHA-C4D-ND	2.10	136.87	132.55
32	B	622	STE	O2-C1-C2	2.10	120.62	114.00
30	e	101	LHG	C11-C10-C9	-2.10	103.78	114.37
24	c	509	CLA	C2A-C3A-C4A	2.09	105.25	101.87
26	D	405	BCR	C24-C23-C22	-2.09	123.14	126.23
26	k	101	BCR	C7-C8-C9	-2.09	123.14	126.23
24	b	612	CLA	CAC-C3C-C4C	2.09	127.52	124.79
24	c	507	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	c	513	CLA	CHD-C1D-ND	-2.09	121.86	124.80
32	c	523	STE	O2-C1-C2	2.09	120.61	114.00
26	B	617	BCR	C8-C7-C6	-2.09	121.41	127.00
31	C	518	DGD	O5D-C6D-C5D	-2.09	104.70	109.42
24	a	613	CLA	C2A-C1A-CHA	2.09	127.50	123.87
24	c	505	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
31	c	518	DGD	O3G-C1D-C2D	-2.09	105.10	108.27
24	C	505	CLA	C2D-C1D-ND	-2.09	108.06	110.13
24	c	508	CLA	CHD-C4C-NC	2.09	127.47	124.23
33	c	522	LMG	O7-C10-O9	-2.09	118.83	123.70
24	B	615	CLA	C2A-C3A-C4A	2.08	105.23	101.87
36	V	201	HEC	C4D-C3D-C2D	-2.08	103.64	106.87
31	c	518	DGD	C3D-C4D-C5D	-2.08	106.46	110.23
24	C	507	CLA	C1D-ND-C4D	-2.08	104.85	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	517	DGD	O2D-C2D-C1D	-2.08	105.11	110.08
24	b	606	CLA	C1-C2-C3	-2.08	122.79	126.20
26	k	102	BCR	C38-C26-C25	-2.08	122.21	124.48
24	B	612	CLA	CHB-C4A-NA	2.08	127.40	124.40
24	C	512	CLA	CMB-C2B-C3B	2.08	131.44	126.55
24	b	602	CLA	CGD-CBD-CAD	-2.08	104.11	110.85
31	C	517	DGD	O3G-C1D-C2D	-2.08	105.12	108.27
29	f	102	SQD	O47-C7-O49	-2.08	118.85	123.70
31	c	516	DGD	CDB-CCB-CBB	-2.08	103.86	114.37
31	C	518	DGD	O3G-C1D-C2D	-2.08	105.12	108.27
24	c	501	CLA	O1D-CGD-CBD	2.08	128.61	124.52
24	C	513	CLA	CAC-C3C-C4C	2.08	127.49	124.79
24	b	615	CLA	CHB-C1B-NB	2.08	127.16	124.05
24	D	404	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
26	B	618	BCR	C1-C6-C5	-2.07	119.80	122.64
24	C	504	CLA	CHA-C4D-ND	2.07	136.82	132.55
33	c	519	LMG	O8-C28-O10	-2.07	118.44	123.63
24	A	604	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
36	v	201	HEC	CBD-CAD-C3D	-2.07	106.81	112.53
24	c	504	CLA	CHD-C1D-ND	-2.07	121.89	124.80
26	b	617	BCR	C27-C26-C25	2.07	125.50	122.70
33	C	515	LMG	O2-C2-C1	-2.07	105.14	110.08
24	B	605	CLA	C2A-C1A-CHA	2.07	127.46	123.87
28	d	405	PL9	C27-C28-C29	-2.07	122.89	127.62
26	b	617	BCR	C24-C23-C22	-2.07	123.17	126.23
24	b	607	CLA	CHD-C1D-ND	-2.07	121.89	124.80
24	a	605	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
26	k	101	BCR	C8-C7-C6	-2.07	121.47	127.00
31	A	616	DGD	C5B-C4B-C3B	-2.07	103.92	114.37
24	B	603	CLA	CGD-CBD-CAD	-2.07	104.15	110.85
25	A	606	PHO	CBC-CAC-C3C	2.07	115.83	112.87
24	C	508	CLA	CHA-C4D-ND	2.07	136.81	132.55
26	B	616	BCR	C36-C18-C19	2.07	121.25	118.09
31	C	516	DGD	C7B-C6B-C5B	-2.07	103.92	114.37
24	d	402	CLA	C6-C5-C3	2.07	118.50	113.47
26	h	101	BCR	C40-C30-C25	2.07	113.48	110.24
26	K	101	BCR	C24-C23-C22	-2.07	123.18	126.23
26	X	101	BCR	C16-C15-C14	-2.06	119.30	123.52
24	b	607	CLA	CMB-C2B-C3B	2.06	131.40	126.55
26	b	619	BCR	C20-C21-C22	-2.06	124.39	127.28
24	c	512	CLA	O2D-CGD-CBD	2.06	114.84	111.23
31	c	517	DGD	CBB-CAB-C9B	-2.06	103.94	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	407	LMG	O3-C3-C2	-2.06	105.52	110.38
26	K	103	BCR	C20-C21-C22	-2.06	124.39	127.28
24	D	404	CLA	C1-C2-C3	-2.06	122.82	126.20
31	C	518	DGD	O3D-C3D-C4D	-2.06	105.52	110.38
24	b	601	CLA	CBA-CAA-C2A	2.06	119.93	113.79
24	b	612	CLA	CHA-C1A-NA	-2.06	121.72	126.39
30	A	614	LHG	C20-C19-C18	-2.06	103.97	114.37
24	B	604	CLA	CHD-C1D-C2D	2.06	129.76	125.49
26	c	514	BCR	C15-C16-C17	-2.06	119.31	123.52
24	C	509	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
24	c	513	CLA	O2D-CGD-CBD	2.06	114.83	111.23
30	L	101	LHG	C20-C19-C18	-2.06	103.98	114.37
24	C	509	CLA	CHC-C1C-NC	2.05	127.41	124.31
26	c	515	BCR	C38-C26-C25	-2.05	122.24	124.48
26	B	617	BCR	C27-C26-C25	2.05	125.48	122.70
33	C	515	LMG	C38-C37-C36	-2.05	103.99	114.37
31	c	517	DGD	O1G-C1A-O1A	-2.05	118.49	123.63
24	b	608	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
32	B	619	STE	C3-C2-C1	-2.05	109.16	114.51
35	f	101	HEM	O1D-CGD-CBD	-2.05	116.59	123.09
31	C	517	DGD	C1D-C2D-C3D	-2.05	105.70	110.01
24	c	506	CLA	CHB-C4A-NA	2.05	127.36	124.40
24	b	602	CLA	C1-C2-C3	-2.05	122.84	126.20
24	C	507	CLA	C3A-C2A-C1A	2.05	104.41	101.34
26	X	101	BCR	C38-C26-C25	-2.05	122.25	124.48
24	A	612	CLA	C16-C15-C13	-2.05	109.16	115.97
28	D	406	PL9	O2-C1-C2	-2.05	117.17	121.83
24	b	605	CLA	CHD-C1D-ND	-2.05	121.92	124.80
24	c	505	CLA	C16-C15-C13	-2.05	109.16	115.97
24	B	605	CLA	CHD-C1D-ND	-2.04	121.92	124.80
24	a	604	CLA	C3B-C4B-NB	-2.04	108.71	110.53
24	C	501	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
33	C	515	LMG	C35-C34-C33	-2.04	104.05	114.37
33	a	619	LMG	O7-C8-C7	2.04	115.67	108.34
24	c	507	CLA	CHD-C4C-C3C	-2.04	121.80	124.77
24	C	502	CLA	C16-C17-C18	-2.04	106.83	115.94
24	A	604	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
28	D	406	PL9	C32-C33-C34	-2.04	122.95	127.62
24	B	614	CLA	CHC-C4B-NB	2.04	127.11	124.05
33	b	622	LMG	O2-C2-C1	-2.04	105.22	110.08
29	a	615	SQD	O47-C7-O49	-2.04	118.94	123.70
26	B	618	BCR	C8-C7-C6	-2.04	121.56	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	K	103	BCR	C36-C18-C17	-2.04	119.52	122.82
24	B	610	CLA	C20-C18-C19	-2.03	101.45	110.53
33	b	622	LMG	O8-C28-O10	-2.03	118.54	123.63
24	C	504	CLA	O1A-CGA-CBA	2.03	131.74	123.78
24	A	607	CLA	CMA-C3A-C2A	-2.03	106.13	113.98
24	B	607	CLA	C6-C7-C8	-2.03	109.22	115.97
26	b	619	BCR	C36-C18-C17	-2.03	119.53	122.82
24	C	509	CLA	CHD-C1D-C2D	2.03	129.71	125.49
28	d	405	PL9	C15-C14-C13	-2.03	118.42	123.63
24	b	607	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
24	c	503	CLA	CMA-C3A-C4A	2.03	117.22	111.77
24	b	611	CLA	C2C-C1C-NC	2.03	112.11	109.98
28	a	612	PL9	C35-C34-C36	2.03	118.75	115.23
26	K	102	BCR	C8-C7-C6	-2.03	121.58	127.00
26	B	618	BCR	C40-C30-C29	-2.03	101.17	108.95
24	d	403	CLA	CHA-C4D-ND	2.02	136.72	132.55
24	B	605	CLA	CHD-C4C-NC	2.02	127.37	124.23
24	c	506	CLA	C4D-CHA-C1A	2.02	123.66	121.24
26	t	101	BCR	C36-C18-C17	-2.02	119.54	122.82
31	A	616	DGD	O2D-C2D-C1D	-2.02	105.26	110.08
24	B	608	CLA	CMD-C2D-C3D	2.02	132.32	127.69
31	C	518	DGD	C3G-C2G-C1G	-2.02	107.08	111.78
25	d	401	PHO	C4B-NB-C1B	2.02	111.76	108.82
24	c	502	CLA	CHD-C1D-C2D	2.02	129.69	125.49
24	c	511	CLA	C3B-C4B-NB	-2.02	108.73	110.53
24	b	611	CLA	O1D-CGD-CBD	2.02	128.50	124.52
24	C	509	CLA	C1-O2A-CGA	2.02	121.53	116.65
24	c	504	CLA	CHB-C1B-C2B	-2.02	121.58	127.43
32	c	520	STE	O2-C1-C2	2.01	120.36	114.00
24	c	513	CLA	CMB-C2B-C3B	2.01	131.28	126.55
33	C	515	LMG	C12-C11-C10	-2.01	106.32	113.69
25	a	606	PHO	OBD-CAD-C3D	2.01	131.03	127.89
24	B	601	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
26	b	619	BCR	C28-C27-C26	-2.01	110.47	114.06
26	K	101	BCR	C15-C14-C13	-2.01	124.46	127.28
26	h	101	BCR	C16-C17-C18	-2.01	124.46	127.28
24	b	608	CLA	C11-C10-C8	-2.01	109.28	115.97
24	c	508	CLA	C7-C6-C5	-2.01	107.91	113.26
36	v	201	HEC	CHD-C1D-ND	2.01	127.50	123.86
33	D	407	LMG	O8-C28-O10	-2.01	118.61	123.63
33	d	408	LMG	O2-C2-C3	-2.01	105.64	110.38
28	d	405	PL9	C32-C33-C34	-2.01	123.03	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	618	BCR	C38-C26-C25	-2.01	122.29	124.48
31	C	518	DGD	C6B-C5B-C4B	-2.01	104.22	114.37
24	b	606	CLA	CGD-CBD-CAD	-2.01	104.35	110.85
24	B	612	CLA	C2C-C1C-NC	2.01	112.09	109.98
31	C	516	DGD	O2E-C2E-C1E	-2.01	105.30	110.08
24	H	101	CLA	CHB-C4A-NA	2.01	127.29	124.40
24	C	506	CLA	CHA-C1A-NA	-2.01	121.85	126.39
31	H	102	DGD	CAB-C9B-C8B	-2.01	104.23	114.37
31	c	516	DGD	CEB-CDB-CCB	-2.00	104.23	114.37
24	C	511	CLA	CHB-C4A-NA	2.00	127.29	124.40
30	d	406	LHG	O8-C23-C24	2.00	117.94	111.83
24	C	512	CLA	C6-C5-C3	-2.00	108.59	113.47
33	a	619	LMG	C33-C32-C31	-2.00	104.25	114.37
24	C	513	CLA	C1-C2-C3	-2.00	122.92	126.20
24	A	604	CLA	C11-C10-C8	-2.00	109.31	115.97
24	b	606	CLA	CHC-C4B-NB	2.00	127.05	124.05
24	C	513	CLA	O1D-CGD-CBD	2.00	128.46	124.52

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	604	CLA	ND
24	A	605	CLA	ND
24	A	607	CLA	ND
24	A	612	CLA	ND
24	B	601	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	609	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	C	501	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND

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Mol	Chain	Res	Type	Atom
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	404	CLA	ND
24	H	101	CLA	ND
24	a	604	CLA	ND
24	a	607	CLA	ND
24	a	613	CLA	ND
24	b	601	CLA	ND
24	b	603	CLA	ND
24	b	604	CLA	ND
24	b	605	CLA	ND
24	b	606	CLA	ND
24	b	607	CLA	ND
24	b	608	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	c	501	CLA	ND
24	c	502	CLA	ND
24	c	503	CLA	ND
24	c	504	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	d	403	CLA	ND

All (1874) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	613	CLA	CAD-CBD-CGD-O1D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C11-C10-C8-C9
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	512	CLA	C2B-C3B-CAB-CBB
24	C	512	CLA	C4B-C3B-CAB-CBB
24	H	101	CLA	C1A-C2A-CAA-CBA
24	H	101	CLA	C3A-C2A-CAA-CBA
24	H	101	CLA	CAD-CBD-CGD-O1D
24	H	101	CLA	CAD-CBD-CGD-O2D
24	b	601	CLA	C1A-C2A-CAA-CBA
24	b	601	CLA	CAD-CBD-CGD-O1D
24	b	601	CLA	CAD-CBD-CGD-O2D
24	b	610	CLA	C2B-C3B-CAB-CBB
24	b	610	CLA	C4B-C3B-CAB-CBB
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	C11-C12-C13-C15
24	b	616	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	C11-C10-C8-C9
24	c	504	CLA	C2-C3-C5-C6
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
24	c	509	CLA	CBD-CGD-O2D-CED
24	c	509	CLA	C6-C7-C8-C9
24	c	512	CLA	C2B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C11-C10-C8-C9
25	d	401	PHO	CBD-CGD-O2D-CED
26	B	617	BCR	C16-C17-C18-C36
26	C	514	BCR	C37-C22-C23-C24
26	D	405	BCR	C23-C24-C25-C26
26	D	405	BCR	C23-C24-C25-C30
26	K	101	BCR	C16-C17-C18-C36
26	K	102	BCR	C5-C6-C7-C8
26	K	102	BCR	C20-C21-C22-C37
26	K	102	BCR	C37-C22-C23-C24
26	K	103	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	T	101	BCR	C7-C8-C9-C10
26	b	618	BCR	C35-C13-C14-C15
26	c	514	BCR	C11-C12-C13-C14
26	c	514	BCR	C11-C12-C13-C35
26	c	515	BCR	C35-C13-C14-C15
26	c	515	BCR	C20-C21-C22-C37
26	k	101	BCR	C5-C6-C7-C8
26	k	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C10-C9-C34
26	t	101	BCR	C11-C12-C13-C35
28	A	611	PL9	C12-C13-C14-C16
28	A	611	PL9	C18-C19-C21-C22
28	A	611	PL9	C37-C38-C39-C40
28	A	611	PL9	C37-C38-C39-C41
28	D	406	PL9	C32-C33-C34-C35
28	a	612	PL9	C12-C13-C14-C16
28	a	612	PL9	C22-C23-C24-C26
28	d	405	PL9	C32-C33-C34-C35
28	d	405	PL9	C32-C33-C34-C36
28	d	405	PL9	C37-C38-C39-C41
29	A	615	SQD	C44-C45-C46-O48
29	A	615	SQD	C46-C45-O47-C7
29	B	620	SQD	O5-C1-O6-C44
29	B	620	SQD	O6-C44-C45-O47
29	B	620	SQD	O49-C7-O47-C45
29	B	620	SQD	C8-C7-O47-C45
29	B	620	SQD	O10-C23-O48-C46
29	B	620	SQD	C24-C23-O48-C46
29	D	408	SQD	C45-C44-O6-C1
29	a	616	SQD	O49-C7-O47-C45
29	a	616	SQD	C8-C7-O47-C45
29	b	620	SQD	C8-C7-O47-C45
29	b	620	SQD	O10-C23-O48-C46
29	f	102	SQD	C2-C1-O6-C44
30	A	614	LHG	O1-C1-C2-C3
30	A	614	LHG	C4-O6-P-O3
30	A	614	LHG	C4-O6-P-O4
30	D	409	LHG	O2-C2-C3-O3
30	D	409	LHG	C3-O3-P-O5
30	D	409	LHG	C3-O3-P-O6
30	D	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
30	D	409	LHG	C4-O6-P-O4
30	D	410	LHG	C3-O3-P-O6
30	D	413	LHG	C1-C2-C3-O3
30	D	413	LHG	C3-O3-P-O4
30	D	413	LHG	C3-O3-P-O5
30	D	413	LHG	C3-O3-P-O6
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O4
30	a	614	LHG	O1-C1-C2-C3
30	a	614	LHG	C3-O3-P-O6
30	d	406	LHG	O1-C1-C2-C3
30	d	406	LHG	C3-O3-P-O6
30	d	406	LHG	C4-O6-P-O3
30	d	406	LHG	C4-O6-P-O5
30	e	101	LHG	C1-C2-C3-O3
30	e	101	LHG	C3-O3-P-O5
31	A	616	DGD	C2B-C1B-O2G-C2G
31	A	616	DGD	O1B-C1B-O2G-C2G
33	C	515	LMG	O9-C10-O7-C8
33	D	411	LMG	O1-C7-C8-C9
33	D	411	LMG	O1-C7-C8-O7
33	D	411	LMG	C11-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
33	c	522	LMG	O6-C1-O1-C7
36	V	201	HEC	C2B-C3B-CAB-CBB
36	V	201	HEC	C2C-C3C-CAC-CBC
36	V	201	HEC	C4C-C3C-CAC-CBC
36	v	201	HEC	C2B-C3B-CAB-CBB
36	v	201	HEC	C2C-C3C-CAC-CBC
36	v	201	HEC	C4C-C3C-CAC-CBC
24	B	615	CLA	O1D-CGD-O2D-CED
24	b	601	CLA	O1D-CGD-O2D-CED
24	B	602	CLA	CBD-CGD-O2D-CED
24	B	615	CLA	CBD-CGD-O2D-CED
24	C	501	CLA	CBD-CGD-O2D-CED
24	b	601	CLA	CBD-CGD-O2D-CED
33	c	521	LMG	O10-C28-O8-C9
33	c	522	LMG	O10-C28-O8-C9
28	a	612	PL9	C47-C48-C49-C51
29	b	620	SQD	C24-C23-O48-C46
33	c	521	LMG	C29-C28-O8-C9
33	c	522	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
33	c	519	LMG	C11-C10-O7-C8
29	a	616	SQD	O10-C23-O48-C46
30	A	614	LHG	O10-C23-O8-C6
33	M	101	LMG	O10-C28-O8-C9
24	c	509	CLA	O1D-CGD-O2D-CED
29	f	102	SQD	O10-C23-O48-C46
33	D	411	LMG	O9-C10-O7-C8
33	b	622	LMG	O9-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
24	B	604	CLA	C3-C5-C6-C7
24	B	615	CLA	C3-C5-C6-C7
24	C	512	CLA	C3-C5-C6-C7
24	b	602	CLA	C3-C5-C6-C7
24	b	603	CLA	C3-C5-C6-C7
24	b	604	CLA	C3-C5-C6-C7
24	b	614	CLA	C3-C5-C6-C7
29	f	102	SQD	C24-C23-O48-C46
33	M	101	LMG	C29-C28-O8-C9
24	c	512	CLA	CBD-CGD-O2D-CED
33	C	515	LMG	C11-C10-O7-C8
33	Y	101	LMG	C11-C10-O7-C8
25	d	401	PHO	O1D-CGD-O2D-CED
24	D	404	CLA	C4-C3-C5-C6
24	c	504	CLA	C4-C3-C5-C6
28	A	611	PL9	C25-C24-C26-C27
28	D	406	PL9	C35-C34-C36-C37
28	a	612	PL9	C20-C19-C21-C22
24	B	604	CLA	C2-C3-C5-C6
28	A	611	PL9	C43-C44-C46-C47
28	d	405	PL9	C38-C39-C41-C42
24	b	609	CLA	CBD-CGD-O2D-CED
33	c	519	LMG	O9-C10-O7-C8
24	C	506	CLA	C3-C5-C6-C7
24	b	601	CLA	C3-C5-C6-C7
30	A	614	LHG	C24-C23-O8-C6
33	a	619	LMG	C29-C28-O8-C9
28	a	612	PL9	C22-C23-C24-C25
28	D	406	PL9	C32-C33-C34-C36
29	D	408	SQD	O10-C23-O48-C46
30	e	101	LHG	O10-C23-O8-C6
29	f	102	SQD	O49-C7-O47-C45
24	C	501	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	B	613	CLA	CBD-CGD-O2D-CED
24	C	511	CLA	CBD-CGD-O2D-CED
30	D	413	LHG	O2-C2-C3-O3
30	e	101	LHG	O2-C2-C3-O3
29	a	616	SQD	C24-C23-O48-C46
31	C	516	DGD	O6E-C5E-C6E-O5E
33	c	521	LMG	O6-C5-C6-O5
29	f	102	SQD	C8-C7-O47-C45
33	c	522	LMG	O6-C5-C6-O5
28	a	612	PL9	C47-C48-C49-C50
24	C	509	CLA	C3-C5-C6-C7
24	A	607	CLA	C4-C3-C5-C6
24	B	604	CLA	C4-C3-C5-C6
24	C	513	CLA	C4-C3-C5-C6
24	C	513	CLA	C2-C3-C5-C6
24	D	404	CLA	C2-C3-C5-C6
28	A	611	PL9	C38-C39-C41-C42
28	D	406	PL9	C33-C34-C36-C37
28	a	612	PL9	C18-C19-C21-C22
31	c	518	DGD	O1A-C1A-O1G-C1G
28	A	611	PL9	C19-C21-C22-C23
28	A	611	PL9	C39-C41-C42-C43
28	D	406	PL9	C29-C31-C32-C33
28	a	612	PL9	C34-C36-C37-C38
28	a	612	PL9	C39-C41-C42-C43
28	a	612	PL9	C44-C46-C47-C48
29	f	102	SQD	O5-C1-O6-C44
33	Y	101	LMG	O6-C1-O1-C7
33	b	622	LMG	O6-C1-O1-C7
24	C	510	CLA	CBD-CGD-O2D-CED
24	H	101	CLA	CBD-CGD-O2D-CED
28	A	611	PL9	C12-C13-C14-C15
24	a	605	CLA	C3-C5-C6-C7
24	A	604	CLA	C2C-C3C-CAC-CBC
29	b	620	SQD	O49-C7-O47-C45
30	A	614	LHG	C1-C2-C3-O3
24	c	506	CLA	CBA-CGA-O2A-C1
29	D	408	SQD	C24-C23-O48-C46
30	e	101	LHG	C24-C23-O8-C6
33	Y	101	LMG	C29-C28-O8-C9
24	b	607	CLA	CBD-CGD-O2D-CED
32	b	624	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	B	602	CLA	O1D-CGD-O2D-CED
33	c	522	LMG	C4-C5-C6-O5
28	A	611	PL9	C40-C39-C41-C42
24	A	607	CLA	C2-C3-C5-C6
28	A	611	PL9	C23-C24-C26-C27
28	A	611	PL9	C33-C34-C36-C37
28	D	406	PL9	C38-C39-C41-C42
24	A	605	CLA	C14-C13-C15-C16
24	B	604	CLA	C6-C7-C8-C9
24	B	605	CLA	C11-C12-C13-C14
24	B	606	CLA	C14-C13-C15-C16
24	B	610	CLA	C11-C12-C13-C14
24	C	507	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	D	403	CLA	C14-C13-C15-C16
24	H	101	CLA	C14-C13-C15-C16
24	b	601	CLA	C11-C10-C8-C9
24	b	604	CLA	C6-C7-C8-C9
24	b	607	CLA	C11-C10-C8-C9
24	b	610	CLA	C14-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C9
24	c	510	CLA	C14-C13-C15-C16
24	c	512	CLA	C6-C7-C8-C9
24	c	512	CLA	O1D-CGD-O2D-CED
29	A	615	SQD	C44-C45-O47-C7
29	B	620	SQD	C2-C1-O6-C44
33	Y	101	LMG	C2-C1-O1-C7
33	b	622	LMG	C2-C1-O1-C7
30	A	614	LHG	O2-C2-C3-O3
26	B	617	BCR	C37-C22-C23-C24
26	C	514	BCR	C36-C18-C19-C20
26	K	101	BCR	C7-C8-C9-C34
26	K	102	BCR	C7-C8-C9-C34
26	K	102	BCR	C11-C12-C13-C35
26	K	103	BCR	C11-C12-C13-C35
26	b	619	BCR	C37-C22-C23-C24
26	c	515	BCR	C11-C12-C13-C35
26	d	404	BCR	C37-C22-C23-C24
26	h	101	BCR	C7-C8-C9-C34
26	k	101	BCR	C37-C22-C23-C24
26	k	102	BCR	C11-C12-C13-C35
26	k	102	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C2A-CAA-CBA-CGA
24	c	506	CLA	O1A-CGA-O2A-C1
33	a	619	LMG	O10-C28-O8-C9
24	B	605	CLA	C15-C16-C17-C18
24	b	603	CLA	C10-C11-C12-C13
24	C	509	CLA	C2-C1-O2A-CGA
28	D	406	PL9	C22-C23-C24-C25
28	D	406	PL9	C37-C38-C39-C40
24	b	611	CLA	C13-C15-C16-C17
33	m	101	LMG	O6-C5-C6-O5
24	D	403	CLA	C3-C5-C6-C7
30	D	409	LHG	C30-C31-C32-C33
24	C	508	CLA	C12-C13-C15-C16
24	b	602	CLA	C11-C12-C13-C15
24	b	609	CLA	C11-C12-C13-C15
24	c	506	CLA	C11-C12-C13-C15
30	d	407	LHG	C30-C31-C32-C33
32	B	625	STE	C5-C6-C7-C8
32	c	520	STE	C2-C3-C4-C5
24	C	504	CLA	C4-C3-C5-C6
26	K	101	BCR	C13-C14-C15-C16
28	A	611	PL9	C34-C36-C37-C38
28	A	611	PL9	C44-C46-C47-C48
28	a	612	PL9	C24-C26-C27-C28
24	B	615	CLA	C5-C6-C7-C8
24	C	505	CLA	C10-C11-C12-C13
30	A	614	LHG	C27-C28-C29-C30
33	a	619	LMG	O6-C5-C6-O5
33	c	521	LMG	C4-C5-C6-O5
29	A	613	SQD	C7-C8-C9-C10
29	A	615	SQD	C23-C24-C25-C26
30	a	614	LHG	C7-C8-C9-C10
30	a	614	LHG	C23-C24-C25-C26
33	D	407	LMG	C10-C11-C12-C13
33	M	101	LMG	C10-C11-C12-C13
33	c	522	LMG	C10-C11-C12-C13
33	d	408	LMG	C28-C29-C30-C31
24	B	606	CLA	C10-C11-C12-C13
24	b	601	CLA	C8-C10-C11-C12
24	b	605	CLA	C10-C11-C12-C13
24	b	611	CLA	C8-C10-C11-C12
24	b	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	c	509	CLA	C13-C15-C16-C17
24	b	606	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C8-C10-C11-C12
24	B	611	CLA	C10-C11-C12-C13
24	C	503	CLA	C5-C6-C7-C8
24	C	509	CLA	C8-C10-C11-C12
24	a	605	CLA	C10-C11-C12-C13
24	b	602	CLA	C15-C16-C17-C18
24	b	614	CLA	C13-C15-C16-C17
29	A	613	SQD	C23-C24-C25-C26
29	a	616	SQD	C7-C8-C9-C10
31	C	518	DGD	C1A-C2A-C3A-C4A
32	B	619	STE	C1-C2-C3-C4
33	D	412	LMG	C28-C29-C30-C31
24	b	609	CLA	O1D-CGD-O2D-CED
31	A	616	DGD	O6D-C1D-O3G-C3G
31	C	517	DGD	O6E-C1E-O5D-C6D
24	B	607	CLA	C13-C15-C16-C17
24	C	502	CLA	C13-C15-C16-C17
24	C	504	CLA	C8-C10-C11-C12
24	C	509	CLA	C5-C6-C7-C8
24	b	608	CLA	C5-C6-C7-C8
24	b	611	CLA	C15-C16-C17-C18
24	b	613	CLA	C15-C16-C17-C18
24	c	508	CLA	C10-C11-C12-C13
24	d	403	CLA	C10-C11-C12-C13
32	R	101	STE	C1-C2-C3-C4
24	b	607	CLA	C10-C11-C12-C13
24	C	512	CLA	C8-C10-C11-C12
31	c	517	DGD	C1B-C2B-C3B-C4B
33	b	622	LMG	C10-C11-C12-C13
24	C	510	CLA	O1D-CGD-O2D-CED
24	H	101	CLA	C10-C11-C12-C13
24	c	512	CLA	CBA-CGA-O2A-C1
33	b	622	LMG	C11-C10-O7-C8
24	B	613	CLA	O1D-CGD-O2D-CED
24	B	603	CLA	C13-C15-C16-C17
32	M	104	STE	C2-C3-C4-C5
31	c	517	DGD	C1A-C2A-C3A-C4A
24	C	511	CLA	CBA-CGA-O2A-C1
31	c	518	DGD	C2A-C1A-O1G-C1G
32	B	626	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	c	521	LMG	C41-C42-C43-C44
24	A	605	CLA	C10-C11-C12-C13
24	A	612	CLA	C15-C16-C17-C18
24	B	606	CLA	C5-C6-C7-C8
24	B	606	CLA	C8-C10-C11-C12
24	B	606	CLA	C15-C16-C17-C18
24	B	613	CLA	C5-C6-C7-C8
24	b	607	CLA	C8-C10-C11-C12
24	b	614	CLA	C5-C6-C7-C8
24	c	505	CLA	C15-C16-C17-C18
24	c	509	CLA	C10-C11-C12-C13
24	B	603	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	C15-C16-C17-C18
24	c	512	CLA	C13-C15-C16-C17
24	d	403	CLA	C13-C15-C16-C17
24	B	605	CLA	C8-C10-C11-C12
24	B	610	CLA	C8-C10-C11-C12
24	B	613	CLA	C15-C16-C17-C18
24	a	605	CLA	C13-C15-C16-C17
32	b	624	STE	C1-C2-C3-C4
28	A	611	PL9	C45-C44-C46-C47
28	a	612	PL9	C33-C34-C36-C37
24	C	506	CLA	C8-C10-C11-C12
24	c	503	CLA	C15-C16-C17-C18
24	C	511	CLA	O1D-CGD-O2D-CED
29	a	615	SQD	C2-C1-O6-C44
31	C	517	DGD	C2E-C1E-O5D-C6D
31	c	517	DGD	C2E-C1E-O5D-C6D
33	M	101	LMG	C2-C1-O1-C7
24	b	607	CLA	C5-C6-C7-C8
24	c	512	CLA	C8-C10-C11-C12
26	A	608	BCR	C35-C13-C14-C15
26	A	608	BCR	C20-C21-C22-C37
26	B	616	BCR	C11-C10-C9-C34
26	B	616	BCR	C16-C17-C18-C36
26	B	617	BCR	C11-C10-C9-C34
26	B	618	BCR	C35-C13-C14-C15
26	C	514	BCR	C16-C17-C18-C36
26	K	101	BCR	C35-C13-C14-C15
26	K	103	BCR	C20-C21-C22-C37
26	T	101	BCR	C20-C21-C22-C37
26	a	608	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
26	b	617	BCR	C20-C21-C22-C37
26	b	619	BCR	C35-C13-C14-C15
26	c	515	BCR	C16-C17-C18-C36
26	k	102	BCR	C11-C10-C9-C34
24	B	604	CLA	C13-C15-C16-C17
26	D	405	BCR	C37-C22-C23-C24
26	b	619	BCR	C7-C8-C9-C34
24	A	604	CLA	C4C-C3C-CAC-CBC
31	h	102	DGD	O6E-C5E-C6E-O5E
26	A	608	BCR	C11-C12-C13-C14
30	a	614	LHG	C10-C11-C12-C13
24	b	601	CLA	C2A-CAA-CBA-CGA
30	D	409	LHG	O1-C1-C2-C3
30	D	410	LHG	O1-C1-C2-C3
30	d	407	LHG	O1-C1-C2-C3
29	b	620	SQD	C46-C45-O47-C7
33	b	622	LMG	C9-C8-O7-C10
24	A	612	CLA	C16-C17-C18-C20
24	a	604	CLA	C16-C17-C18-C20
24	b	604	CLA	C16-C17-C18-C20
32	d	411	STE	C9-C10-C11-C12
26	A	608	BCR	C12-C13-C14-C15
26	B	616	BCR	C20-C21-C22-C23
26	B	618	BCR	C11-C10-C9-C8
26	B	618	BCR	C12-C13-C14-C15
26	C	514	BCR	C20-C21-C22-C23
26	K	101	BCR	C11-C10-C9-C8
26	K	101	BCR	C16-C17-C18-C19
26	T	101	BCR	C12-C13-C14-C15
26	X	101	BCR	C11-C10-C9-C8
26	b	618	BCR	C12-C13-C14-C15
26	h	101	BCR	C11-C10-C9-C8
26	k	102	BCR	C20-C21-C22-C23
31	c	517	DGD	O6E-C1E-O5D-C6D
33	M	101	LMG	O6-C1-O1-C7
33	a	619	LMG	C11-C10-O7-C8
31	C	516	DGD	C4E-C5E-C6E-O5E
24	a	607	CLA	CBA-CGA-O2A-C1
31	c	516	DGD	O6D-C5D-C6D-O5D
24	B	607	CLA	C16-C17-C18-C20
24	a	604	CLA	C16-C17-C18-C19
24	b	616	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	c	512	CLA	O1A-CGA-O2A-C1
29	f	102	SQD	C28-C29-C30-C31
32	B	622	STE	C3-C4-C5-C6
32	B	623	STE	C3-C4-C5-C6
32	c	523	STE	C4-C5-C6-C7
32	d	409	STE	C2-C3-C4-C5
29	A	615	SQD	C10-C11-C12-C13
29	B	620	SQD	C13-C14-C15-C16
30	A	614	LHG	C11-C10-C9-C8
30	d	406	LHG	C28-C29-C30-C31
31	C	518	DGD	C6A-C7A-C8A-C9A
31	C	518	DGD	CCA-CDA-CEA-CFA
31	c	518	DGD	CCB-CDB-CEB-CFB
32	J	101	STE	C5-C6-C7-C8
32	J	101	STE	C6-C7-C8-C9
32	b	621	STE	C13-C14-C15-C16
33	C	515	LMG	C14-C15-C16-C17
33	C	515	LMG	C33-C34-C35-C36
33	D	407	LMG	C35-C36-C37-C38
33	c	522	LMG	C32-C33-C34-C35
30	A	614	LHG	C23-C24-C25-C26
29	B	620	SQD	C25-C26-C27-C28
29	a	615	SQD	C12-C13-C14-C15
31	A	616	DGD	CAA-CBA-CCA-CDA
31	A	616	DGD	C2B-C3B-C4B-C5B
31	h	102	DGD	C9A-CAA-CBA-CCA
32	B	619	STE	C11-C12-C13-C14
33	M	101	LMG	C31-C32-C33-C34
33	c	521	LMG	C29-C30-C31-C32
33	c	521	LMG	C32-C33-C34-C35
29	A	613	SQD	C10-C11-C12-C13
29	A	615	SQD	C9-C10-C11-C12
29	a	615	SQD	C28-C29-C30-C31
30	A	614	LHG	C12-C13-C14-C15
30	A	614	LHG	C13-C14-C15-C16
30	A	614	LHG	C33-C34-C35-C36
30	D	409	LHG	C32-C33-C34-C35
30	D	410	LHG	C11-C12-C13-C14
30	D	410	LHG	C26-C27-C28-C29
30	a	614	LHG	C11-C10-C9-C8
32	B	622	STE	C10-C11-C12-C13
32	B	624	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	X	102	STE	C5-C6-C7-C8
32	b	625	STE	C2-C3-C4-C5
32	c	523	STE	C3-C4-C5-C6
32	d	410	STE	C13-C14-C15-C16
33	C	515	LMG	C35-C36-C37-C38
33	D	411	LMG	C34-C35-C36-C37
33	a	619	LMG	C12-C13-C14-C15
33	b	622	LMG	C16-C17-C18-C19
33	c	522	LMG	C18-C19-C20-C21
30	A	614	LHG	O1-C1-C2-O2
30	D	410	LHG	O1-C1-C2-O2
33	C	515	LMG	C38-C39-C40-C41
33	a	619	LMG	C13-C14-C15-C16
33	b	622	LMG	C40-C41-C42-C43
33	m	101	LMG	C16-C17-C18-C19
31	c	516	DGD	C4D-C5D-C6D-O5D
24	b	605	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
32	B	626	STE	C1-C2-C3-C4
30	D	410	LHG	C24-C25-C26-C27
31	C	517	DGD	C5A-C6A-C7A-C8A
31	h	102	DGD	C2B-C3B-C4B-C5B
31	h	102	DGD	C5B-C6B-C7B-C8B
32	B	621	STE	C2-C3-C4-C5
32	B	622	STE	C11-C10-C9-C8
32	d	411	STE	C6-C7-C8-C9
33	C	515	LMG	C13-C14-C15-C16
33	a	619	LMG	C33-C34-C35-C36
33	c	522	LMG	C31-C32-C33-C34
24	B	601	CLA	C16-C17-C18-C19
24	B	601	CLA	C16-C17-C18-C20
24	b	604	CLA	C16-C17-C18-C19
24	C	511	CLA	O1A-CGA-O2A-C1
30	l	101	LHG	C14-C15-C16-C17
31	C	518	DGD	C9A-CAA-CBA-CCA
33	Y	101	LMG	C17-C18-C19-C20
24	C	509	CLA	C13-C15-C16-C17
24	D	404	CLA	C5-C6-C7-C8
24	b	615	CLA	C15-C16-C17-C18
24	c	502	CLA	C15-C16-C17-C18
33	c	522	LMG	C11-C10-O7-C8
30	D	413	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
30	a	614	LHG	C14-C15-C16-C17
31	C	518	DGD	C4A-C5A-C6A-C7A
32	C	519	STE	C3-C4-C5-C6
32	B	624	STE	C14-C15-C16-C17
32	d	409	STE	C5-C6-C7-C8
32	d	410	STE	C1-C2-C3-C4
24	a	607	CLA	C5-C6-C7-C8
24	c	507	CLA	C10-C11-C12-C13
29	A	613	SQD	C34-C35-C36-C37
30	d	407	LHG	C27-C28-C29-C30
31	C	518	DGD	C5A-C6A-C7A-C8A
32	B	625	STE	C11-C10-C9-C8
32	T	103	STE	C11-C10-C9-C8
32	b	621	STE	C14-C15-C16-C17
33	D	407	LMG	C30-C31-C32-C33
24	b	601	CLA	C3A-C2A-CAA-CBA
25	d	401	PHO	C3A-C2A-CAA-CBA
29	A	615	SQD	C12-C13-C14-C15
29	a	615	SQD	C30-C31-C32-C33
30	L	101	LHG	C29-C30-C31-C32
31	c	518	DGD	C9B-CAB-CBB-CCB
32	B	623	STE	C5-C6-C7-C8
24	b	608	CLA	C13-C15-C16-C17
24	d	403	CLA	C8-C10-C11-C12
31	C	516	DGD	C8A-C9A-CAA-CBA
24	B	609	CLA	C16-C17-C18-C20
24	b	602	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C20
32	B	621	STE	C5-C6-C7-C8
30	D	410	LHG	C14-C15-C16-C17
30	D	410	LHG	C27-C28-C29-C30
30	d	406	LHG	C11-C10-C9-C8
32	b	625	STE	C3-C4-C5-C6
33	D	407	LMG	O6-C5-C6-O5
24	C	506	CLA	CBA-CGA-O2A-C1
24	H	101	CLA	CBA-CGA-O2A-C1
30	e	101	LHG	C4-C5-C6-O8
29	f	102	SQD	C29-C30-C31-C32
31	c	518	DGD	C3A-C4A-C5A-C6A
32	d	410	STE	C11-C12-C13-C14
29	a	616	SQD	C11-C10-C9-C8
29	b	620	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
31	A	616	DGD	C4B-C5B-C6B-C7B
31	C	516	DGD	C9A-CAA-CBA-CCA
32	T	103	STE	C9-C10-C11-C12
32	X	102	STE	C6-C7-C8-C9
32	h	103	STE	C11-C12-C13-C14
33	D	407	LMG	C15-C16-C17-C18
33	D	412	LMG	C29-C30-C31-C32
33	M	101	LMG	C33-C34-C35-C36
33	a	619	LMG	C40-C41-C42-C43
33	c	522	LMG	C14-C15-C16-C17
32	B	626	STE	C2-C3-C4-C5
32	b	623	STE	C3-C4-C5-C6
33	b	622	LMG	C31-C32-C33-C34
33	c	521	LMG	C15-C16-C17-C18
31	h	102	DGD	C7A-C8A-C9A-CAA
31	h	102	DGD	CBB-CCB-CDB-CEB
32	c	520	STE	C7-C8-C9-C10
24	A	605	CLA	C16-C17-C18-C20
24	C	502	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	B	616	BCR	C1-C6-C7-C8
26	C	514	BCR	C23-C24-C25-C30
26	K	102	BCR	C1-C6-C7-C8
26	K	103	BCR	C1-C6-C7-C8
26	T	101	BCR	C1-C6-C7-C8
26	T	101	BCR	C5-C6-C7-C8
26	b	617	BCR	C1-C6-C7-C8
26	k	101	BCR	C1-C6-C7-C8
29	D	408	SQD	C32-C33-C34-C35
30	L	101	LHG	C12-C13-C14-C15
31	H	102	DGD	C6B-C7B-C8B-C9B
32	a	617	STE	C5-C6-C7-C8
35	F	101	HEM	C3D-CAD-CBD-CGD
31	H	102	DGD	CCA-CDA-CEA-CFA
32	B	619	STE	C6-C7-C8-C9
33	Y	101	LMG	C18-C19-C20-C21
30	D	410	LHG	C9-C10-C11-C12
31	C	517	DGD	C6A-C7A-C8A-C9A
24	C	506	CLA	O1A-CGA-O2A-C1
24	a	607	CLA	O1A-CGA-O2A-C1
28	D	406	PL9	C4-C3-C7-C8
28	a	612	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
31	c	516	DGD	C4A-C5A-C6A-C7A
31	c	518	DGD	CAA-CBA-CCA-CDA
32	Z	101	STE	C11-C12-C13-C14
32	t	102	STE	C6-C7-C8-C9
33	Y	101	LMG	O9-C10-O7-C8
24	C	506	CLA	C4-C3-C5-C6
30	A	614	LHG	C14-C15-C16-C17
31	c	516	DGD	CBA-CCA-CDA-CEA
32	B	624	STE	C9-C10-C11-C12
32	c	523	STE	C6-C7-C8-C9
26	B	617	BCR	C18-C19-C20-C21
26	B	618	BCR	C10-C11-C12-C13
26	t	101	BCR	C18-C19-C20-C21
24	B	613	CLA	C8-C10-C11-C12
24	c	506	CLA	C13-C15-C16-C17
24	C	504	CLA	C2-C3-C5-C6
30	D	409	LHG	C18-C19-C20-C21
30	D	413	LHG	C14-C15-C16-C17
30	L	101	LHG	C18-C19-C20-C21
30	a	614	LHG	C32-C33-C34-C35
30	d	407	LHG	C25-C26-C27-C28
31	H	102	DGD	C7B-C8B-C9B-CAB
31	H	102	DGD	CCB-CDB-CEB-CFB
32	b	624	STE	C14-C15-C16-C17
31	A	616	DGD	C1B-C2B-C3B-C4B
31	C	516	DGD	C1B-C2B-C3B-C4B
29	a	615	SQD	C24-C25-C26-C27
29	f	102	SQD	C26-C27-C28-C29
30	e	101	LHG	C11-C10-C9-C8
30	l	101	LHG	C27-C28-C29-C30
31	H	102	DGD	C5A-C6A-C7A-C8A
32	I	101	STE	C11-C10-C9-C8
32	b	621	STE	C3-C4-C5-C6
32	d	411	STE	C14-C15-C16-C17
30	l	101	LHG	C16-C17-C18-C19
31	c	516	DGD	C4B-C5B-C6B-C7B
31	c	518	DGD	CCA-CDA-CEA-CFA
32	B	623	STE	C13-C14-C15-C16
33	M	101	LMG	C32-C33-C34-C35
33	m	101	LMG	C34-C35-C36-C37
26	B	617	BCR	C22-C23-C24-C25
26	d	404	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
31	c	516	DGD	O6E-C1E-O5D-C6D
29	A	613	SQD	C12-C13-C14-C15
32	B	619	STE	C2-C3-C4-C5
32	X	102	STE	C4-C5-C6-C7
33	Y	101	LMG	C35-C36-C37-C38
33	c	522	LMG	C2-C1-O1-C7
24	B	609	CLA	C8-C10-C11-C12
24	a	607	CLA	C10-C11-C12-C13
24	c	513	CLA	C10-C11-C12-C13
32	B	621	STE	C4-C5-C6-C7
32	B	624	STE	C5-C6-C7-C8
32	B	624	STE	C7-C8-C9-C10
32	M	102	STE	C9-C10-C11-C12
32	Z	101	STE	C13-C14-C15-C16
32	L	102	STE	C1-C2-C3-C4
29	A	615	SQD	C11-C10-C9-C8
29	b	620	SQD	C27-C28-C29-C30
31	h	102	DGD	C7B-C8B-C9B-CAB
32	T	103	STE	C11-C12-C13-C14
33	Y	101	LMG	C11-C12-C13-C14
29	B	620	SQD	C11-C12-C13-C14
30	D	413	LHG	C29-C30-C31-C32
30	e	101	LHG	C27-C28-C29-C30
31	C	517	DGD	CBA-CCA-CDA-CEA
32	C	519	STE	C2-C3-C4-C5
32	T	103	STE	C14-C15-C16-C17
33	D	412	LMG	C32-C33-C34-C35
33	m	101	LMG	C31-C32-C33-C34
24	b	603	CLA	C13-C15-C16-C17
26	k	102	BCR	C9-C10-C11-C12
33	c	519	LMG	O6-C5-C6-O5
24	B	611	CLA	C16-C17-C18-C20
24	b	616	CLA	C11-C12-C13-C15
24	c	510	CLA	C16-C17-C18-C19
33	m	101	LMG	C11-C10-O7-C8
30	e	101	LHG	C7-C8-C9-C10
24	C	506	CLA	C15-C16-C17-C18
24	C	513	CLA	C10-C11-C12-C13
33	Y	101	LMG	C33-C34-C35-C36
33	m	101	LMG	C18-C19-C20-C21
29	B	620	SQD	C33-C34-C35-C36
32	d	411	STE	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
26	A	608	BCR	C11-C12-C13-C35
26	B	616	BCR	C37-C22-C23-C24
33	D	407	LMG	C21-C22-C23-C24
32	B	621	STE	C1-C2-C3-C4
29	B	620	SQD	C35-C36-C37-C38
26	k	101	BCR	C7-C8-C9-C10
24	c	501	CLA	CBA-CGA-O2A-C1
33	a	619	LMG	C8-C7-O1-C1
29	A	613	SQD	C11-C10-C9-C8
30	D	410	LHG	C33-C34-C35-C36
30	d	407	LHG	C26-C27-C28-C29
24	c	512	CLA	C2A-CAA-CBA-CGA
24	A	605	CLA	C16-C17-C18-C19
24	B	605	CLA	C16-C17-C18-C19
24	B	605	CLA	C16-C17-C18-C20
30	A	614	LHG	C18-C19-C20-C21
31	c	517	DGD	CCA-CDA-CEA-CFA
32	I	101	STE	C10-C11-C12-C13
24	c	506	CLA	C4-C3-C5-C6
24	C	504	CLA	C11-C12-C13-C14
29	B	620	SQD	C9-C10-C11-C12
29	a	616	SQD	C12-C13-C14-C15
30	d	406	LHG	C29-C30-C31-C32
32	X	102	STE	C11-C12-C13-C14
33	M	101	LMG	C13-C14-C15-C16
24	B	609	CLA	C15-C16-C17-C18
29	b	620	SQD	C10-C11-C12-C13
31	C	517	DGD	CCB-CDB-CEB-CFB
32	B	625	STE	C10-C11-C12-C13
33	a	619	LMG	C41-C42-C43-C44
24	H	101	CLA	O1A-CGA-O2A-C1
33	d	408	LMG	O6-C5-C6-O5
24	B	605	CLA	C10-C11-C12-C13
32	c	520	STE	C9-C10-C11-C12
32	M	104	STE	C7-C8-C9-C10
24	b	612	CLA	C10-C11-C12-C13
24	c	510	CLA	C16-C17-C18-C20
29	a	615	SQD	C25-C26-C27-C28
32	a	617	STE	C4-C5-C6-C7
32	d	409	STE	C9-C10-C11-C12
30	L	101	LHG	C33-C34-C35-C36
31	c	518	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
32	d	410	STE	C6-C7-C8-C9
33	c	522	LMG	C33-C34-C35-C36
32	c	520	STE	C1-C2-C3-C4
33	a	619	LMG	C10-C11-C12-C13
24	C	511	CLA	C8-C10-C11-C12
30	D	410	LHG	C29-C30-C31-C32
32	X	102	STE	C13-C14-C15-C16
32	d	411	STE	C7-C8-C9-C10
33	D	407	LMG	C12-C13-C14-C15
24	d	402	CLA	C3-C5-C6-C7
29	A	613	SQD	O6-C44-C45-O47
29	a	615	SQD	O6-C44-C45-O47
31	A	616	DGD	O2G-C2G-C3G-O3G
33	c	521	LMG	O1-C7-C8-O7
32	T	102	STE	C7-C8-C9-C10
30	a	614	LHG	C15-C16-C17-C18
31	C	518	DGD	CBA-CCA-CDA-CEA
32	T	103	STE	C10-C11-C12-C13
32	b	621	STE	C11-C10-C9-C8
33	D	412	LMG	C33-C34-C35-C36
33	c	521	LMG	C34-C35-C36-C37
33	c	522	LMG	C17-C18-C19-C20
33	b	622	LMG	O6-C5-C6-O5
30	D	409	LHG	C15-C16-C17-C18
29	D	408	SQD	C31-C32-C33-C34
33	D	407	LMG	C36-C37-C38-C39
33	c	519	LMG	C30-C31-C32-C33
29	A	615	SQD	C16-C17-C18-C19
29	b	620	SQD	C9-C10-C11-C12
30	L	101	LHG	C13-C14-C15-C16
30	d	406	LHG	C15-C16-C17-C18
32	b	624	STE	C10-C11-C12-C13
30	D	413	LHG	C25-C26-C27-C28
24	b	614	CLA	C4-C3-C5-C6
33	c	522	LMG	O9-C10-O7-C8
30	D	409	LHG	C1-C2-C3-O3
24	b	602	CLA	C8-C10-C11-C12
29	D	408	SQD	C30-C31-C32-C33
31	A	616	DGD	C5B-C6B-C7B-C8B
32	C	520	STE	C7-C8-C9-C10
32	d	410	STE	C3-C4-C5-C6
33	a	619	LMG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	H	101	CLA	O1D-CGD-O2D-CED
31	C	516	DGD	CBA-CCA-CDA-CEA
32	b	621	STE	C11-C12-C13-C14
32	d	409	STE	C10-C11-C12-C13
31	A	616	DGD	C5A-C6A-C7A-C8A
32	B	619	STE	C9-C10-C11-C12
32	B	625	STE	C4-C5-C6-C7
24	b	601	CLA	C10-C11-C12-C13
31	c	518	DGD	C4B-C5B-C6B-C7B
29	B	620	SQD	C11-C10-C9-C8
30	d	406	LHG	C33-C34-C35-C36
32	b	624	STE	C12-C13-C14-C15
24	B	609	CLA	C16-C17-C18-C19
30	a	614	LHG	O1-C1-C2-O2
24	B	603	CLA	C1A-C2A-CAA-CBA
24	C	503	CLA	C1A-C2A-CAA-CBA
24	a	605	CLA	C1A-C2A-CAA-CBA
24	a	613	CLA	C1A-C2A-CAA-CBA
24	c	508	CLA	C1A-C2A-CAA-CBA
24	c	513	CLA	C1A-C2A-CAA-CBA
30	L	101	LHG	C26-C27-C28-C29
28	A	611	PL9	C47-C48-C49-C50
31	c	517	DGD	CAB-CBB-CCB-CDB
32	d	410	STE	C9-C10-C11-C12
25	d	401	PHO	C8-C10-C11-C12
33	M	101	LMG	C39-C40-C41-C42
24	A	604	CLA	C12-C13-C15-C16
24	B	602	CLA	C6-C7-C8-C10
24	B	612	CLA	C6-C7-C8-C10
24	C	506	CLA	C11-C12-C13-C15
24	a	607	CLA	C12-C13-C15-C16
24	b	601	CLA	C11-C12-C13-C15
24	b	608	CLA	C11-C12-C13-C15
24	b	609	CLA	C12-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C10
24	b	615	CLA	C11-C12-C13-C15
24	c	506	CLA	C6-C7-C8-C10
24	c	510	CLA	C6-C7-C8-C10
29	a	615	SQD	C14-C15-C16-C17
30	d	406	LHG	C13-C14-C15-C16
24	b	610	CLA	C2C-C3C-CAC-CBC
32	B	622	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	a	619	LMG	C30-C31-C32-C33
31	H	102	DGD	CAB-CBB-CCB-CDB
33	a	619	LMG	C39-C40-C41-C42
24	C	505	CLA	C4-C3-C5-C6
24	C	505	CLA	C2-C3-C5-C6
33	D	412	LMG	C31-C32-C33-C34
31	c	516	DGD	O6E-C5E-C6E-O5E
24	c	504	CLA	C8-C10-C11-C12
24	c	507	CLA	C5-C6-C7-C8
24	c	501	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	C14-C13-C15-C16
24	B	602	CLA	C6-C7-C8-C9
24	B	611	CLA	C11-C10-C8-C9
24	B	612	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16
24	a	607	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	b	608	CLA	C11-C12-C13-C14
24	c	506	CLA	C6-C7-C8-C9
24	c	507	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
33	C	515	LMG	C16-C17-C18-C19
33	M	101	LMG	C19-C20-C21-C22
29	A	615	SQD	C7-C8-C9-C10
24	c	507	CLA	C16-C17-C18-C20
29	a	615	SQD	C17-C18-C19-C20
33	m	101	LMG	C29-C28-O8-C9
28	d	405	PL9	C22-C23-C24-C25
32	b	624	STE	C2-C3-C4-C5
30	e	101	LHG	C16-C17-C18-C19
32	j	101	STE	C4-C5-C6-C7
31	A	616	DGD	C1G-C2G-C3G-O3G
33	Y	101	LMG	O1-C7-C8-C9
33	c	521	LMG	O1-C7-C8-C9
33	c	522	LMG	O1-C7-C8-C9
31	C	516	DGD	C4B-C5B-C6B-C7B
33	a	619	LMG	C38-C39-C40-C41
33	b	622	LMG	C32-C33-C34-C35
29	f	102	SQD	C27-C28-C29-C30
32	B	623	STE	C14-C15-C16-C17
33	D	407	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	R	101	STE	C7-C8-C9-C10
30	l	101	LHG	C7-C8-C9-C10
24	B	614	CLA	C16-C17-C18-C20
24	c	503	CLA	C16-C17-C18-C20
24	c	513	CLA	C16-C17-C18-C19
30	D	410	LHG	C25-C26-C27-C28
31	C	516	DGD	CAB-CBB-CCB-CDB
32	C	520	STE	C12-C13-C14-C15
33	C	515	LMG	C11-C12-C13-C14
33	d	408	LMG	C37-C38-C39-C40
29	D	408	SQD	C25-C26-C27-C28
29	b	620	SQD	C29-C30-C31-C32
29	a	616	SQD	C19-C20-C21-C22
30	l	101	LHG	C32-C33-C34-C35
25	d	401	PHO	CHA-CBD-CGD-O1D
25	d	401	PHO	CHA-CBD-CGD-O2D
26	T	101	BCR	C11-C10-C9-C34
26	b	617	BCR	C35-C13-C14-C15
26	b	619	BCR	C20-C21-C22-C37
26	h	101	BCR	C35-C13-C14-C15
26	k	101	BCR	C20-C21-C22-C37
31	C	517	DGD	C9A-CAA-CBA-CCA
31	H	102	DGD	C4B-C5B-C6B-C7B
29	a	615	SQD	C23-C24-C25-C26
32	c	523	STE	C1-C2-C3-C4
31	C	518	DGD	O1A-C1A-O1G-C1G
31	A	616	DGD	C4A-C5A-C6A-C7A
33	c	522	LMG	C12-C13-C14-C15
24	C	506	CLA	C2-C3-C5-C6
28	a	612	PL9	C38-C39-C41-C42
24	H	101	CLA	C8-C10-C11-C12
30	A	614	LHG	C34-C35-C36-C37
32	d	409	STE	C11-C10-C9-C8
24	c	501	CLA	O1A-CGA-O2A-C1
29	a	615	SQD	C15-C16-C17-C18
33	D	407	LMG	C33-C34-C35-C36
31	c	518	DGD	C5B-C6B-C7B-C8B
33	m	101	LMG	C4-C5-C6-O5
32	d	411	STE	C12-C13-C14-C15
24	b	608	CLA	O2A-C1-C2-C3
29	B	620	SQD	C46-C45-O47-C7
33	D	411	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
30	e	101	LHG	C12-C13-C14-C15
33	M	101	LMG	C14-C15-C16-C17
26	d	404	BCR	C10-C11-C12-C13
29	a	615	SQD	C32-C33-C34-C35
29	f	102	SQD	C24-C25-C26-C27
30	d	407	LHG	C31-C32-C33-C34
31	c	517	DGD	C4B-C5B-C6B-C7B
32	I	101	STE	C2-C3-C4-C5
32	T	102	STE	C12-C13-C14-C15
32	a	617	STE	C2-C3-C4-C5
33	c	522	LMG	C37-C38-C39-C40
32	B	619	STE	C11-C10-C9-C8
30	D	413	LHG	O10-C23-O8-C6
26	b	617	BCR	C12-C13-C14-C15
26	k	101	BCR	C11-C10-C9-C8
29	A	615	SQD	C15-C16-C17-C18
33	c	522	LMG	C29-C30-C31-C32
32	C	521	STE	C6-C7-C8-C9
33	d	408	LMG	C10-C11-C12-C13
30	L	101	LHG	C19-C20-C21-C22
29	A	613	SQD	C14-C15-C16-C17
29	a	616	SQD	C17-C18-C19-C20
30	A	614	LHG	C17-C18-C19-C20
32	M	104	STE	C13-C14-C15-C16
32	d	411	STE	C4-C5-C6-C7
24	B	613	CLA	C4-C3-C5-C6
30	l	101	LHG	C29-C30-C31-C32
33	a	619	LMG	C15-C16-C17-C18
33	a	619	LMG	C32-C33-C34-C35
24	C	513	CLA	CBD-CGD-O2D-CED
30	D	410	LHG	C32-C33-C34-C35
32	d	410	STE	C2-C3-C4-C5
33	M	101	LMG	C36-C37-C38-C39
29	A	613	SQD	C17-C18-C19-C20
30	D	410	LHG	C17-C18-C19-C20
30	d	406	LHG	C35-C36-C37-C38
24	c	503	CLA	C5-C6-C7-C8
30	D	409	LHG	C12-C13-C14-C15
30	D	409	LHG	C25-C26-C27-C28
31	C	517	DGD	C3A-C4A-C5A-C6A
32	B	623	STE	C6-C7-C8-C9
32	b	624	STE	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	a	619	LMG	C35-C36-C37-C38
33	M	101	LMG	O1-C7-C8-O7
33	c	521	LMG	O7-C8-C9-O8
32	M	103	STE	C3-C4-C5-C6
30	L	101	LHG	C10-C11-C12-C13
32	T	102	STE	C9-C10-C11-C12
32	T	102	STE	C13-C14-C15-C16
33	m	101	LMG	C32-C33-C34-C35
24	C	507	CLA	C13-C15-C16-C17
24	C	512	CLA	C13-C15-C16-C17
24	B	604	CLA	C16-C17-C18-C20
32	C	519	STE	C7-C8-C9-C10
32	a	618	STE	C4-C5-C6-C7
30	L	101	LHG	O10-C23-O8-C6
30	D	410	LHG	C35-C36-C37-C38
32	L	102	STE	C7-C8-C9-C10
29	D	408	SQD	C28-C29-C30-C31
31	c	517	DGD	C9A-CAA-CBA-CCA
29	a	616	SQD	C18-C19-C20-C21
31	c	518	DGD	CDA-CEA-CFA-CGA
30	D	410	LHG	C12-C13-C14-C15
24	C	505	CLA	C5-C6-C7-C8
26	c	514	BCR	C14-C15-C16-C17
33	D	407	LMG	C38-C39-C40-C41
24	b	607	CLA	O1D-CGD-O2D-CED
33	c	521	LMG	C42-C43-C44-C45
24	B	603	CLA	C10-C11-C12-C13
28	D	406	PL9	C28-C29-C31-C32
29	f	102	SQD	C25-C26-C27-C28
30	D	409	LHG	C11-C10-C9-C8
24	c	507	CLA	CBA-CGA-O2A-C1
30	d	407	LHG	C35-C36-C37-C38
32	h	103	STE	C5-C6-C7-C8
33	a	619	LMG	C42-C43-C44-C45
33	b	622	LMG	C18-C19-C20-C21
32	T	103	STE	C12-C13-C14-C15
32	d	411	STE	C5-C6-C7-C8
29	A	615	SQD	O49-C7-O47-C45
31	c	516	DGD	O1B-C1B-O2G-C2G
30	d	407	LHG	O1-C1-C2-O2
24	C	508	CLA	C11-C10-C8-C9
24	C	509	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	511	CLA	C6-C7-C8-C9
24	b	601	CLA	C11-C12-C13-C14
24	b	605	CLA	C11-C10-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	b	609	CLA	C14-C13-C15-C16
24	d	402	CLA	C6-C7-C8-C9
30	L	101	LHG	C11-C12-C13-C14
32	b	621	STE	C2-C3-C4-C5
24	B	602	CLA	C5-C6-C7-C8
24	b	604	CLA	C15-C16-C17-C18
32	B	623	STE	C1-C2-C3-C4
24	B	605	CLA	C4B-C3B-CAB-CBB
24	b	601	CLA	C4B-C3B-CAB-CBB
24	c	505	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
29	A	613	SQD	C25-C26-C27-C28
31	A	616	DGD	CBB-CCB-CDB-CEB
32	C	520	STE	C11-C10-C9-C8
32	h	103	STE	C10-C11-C12-C13
31	C	516	DGD	O1G-C1A-C2A-C3A
29	b	620	SQD	C28-C29-C30-C31
33	c	521	LMG	C30-C31-C32-C33
24	A	612	CLA	C13-C15-C16-C17
24	B	606	CLA	C13-C15-C16-C17
30	l	101	LHG	C19-C20-C21-C22
33	Y	101	LMG	C40-C41-C42-C43
31	C	518	DGD	C3B-C4B-C5B-C6B
33	a	619	LMG	C36-C37-C38-C39
33	b	622	LMG	C19-C20-C21-C22
30	D	413	LHG	C19-C20-C21-C22
31	C	517	DGD	CDA-CEA-CFA-CGA
24	A	605	CLA	C12-C13-C15-C16
24	B	601	CLA	C12-C13-C15-C16
24	B	611	CLA	C11-C10-C8-C7
24	C	503	CLA	C11-C10-C8-C7
24	C	506	CLA	C12-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C7
24	C	509	CLA	C12-C13-C15-C16
24	C	511	CLA	C6-C7-C8-C10
24	a	605	CLA	C6-C7-C8-C10
24	b	607	CLA	C6-C7-C8-C10
24	b	607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	b	616	CLA	C11-C10-C8-C7
24	c	507	CLA	C6-C7-C8-C10
24	c	509	CLA	C6-C7-C8-C10
24	c	512	CLA	C6-C7-C8-C10
24	d	402	CLA	C6-C7-C8-C10
29	a	616	SQD	C31-C32-C33-C34
32	B	625	STE	C13-C14-C15-C16
32	I	101	STE	C1-C2-C3-C4
32	M	103	STE	C1-C2-C3-C4
31	A	616	DGD	CDB-CEB-CFB-CGB
24	a	604	CLA	C15-C16-C17-C18
32	M	104	STE	C10-C11-C12-C13
32	M	104	STE	C15-C16-C17-C18
24	a	605	CLA	C3A-C2A-CAA-CBA
28	d	405	PL9	C30-C29-C31-C32
24	b	614	CLA	C2-C3-C5-C6
28	d	405	PL9	C43-C44-C46-C47
32	B	622	STE	C13-C14-C15-C16
29	D	408	SQD	C29-C30-C31-C32
33	Y	101	LMG	C12-C13-C14-C15
31	C	517	DGD	O6D-C1D-O3G-C3G
33	D	412	LMG	C17-C18-C19-C20
33	c	521	LMG	C11-C12-C13-C14
29	a	615	SQD	C34-C35-C36-C37
31	c	516	DGD	C9B-CAB-CBB-CCB
24	C	511	CLA	C3-C5-C6-C7
24	A	612	CLA	C16-C17-C18-C19
24	B	604	CLA	C8-C10-C11-C12
26	T	101	BCR	C11-C12-C13-C35
31	h	102	DGD	C6B-C7B-C8B-C9B
32	b	621	STE	C6-C7-C8-C9
33	a	619	LMG	C37-C38-C39-C40
33	Y	101	LMG	O10-C28-O8-C9
30	a	614	LHG	C18-C19-C20-C21
32	L	102	STE	C2-C3-C4-C5
32	d	411	STE	C15-C16-C17-C18
31	C	516	DGD	C5B-C6B-C7B-C8B
31	H	102	DGD	C9A-CAA-CBA-CCA
29	A	615	SQD	C32-C33-C34-C35
29	a	615	SQD	C11-C12-C13-C14
30	d	406	LHG	C16-C17-C18-C19
31	A	616	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
29	A	613	SQD	O6-C44-C45-C46
29	B	620	SQD	O6-C44-C45-C46
29	a	615	SQD	O6-C44-C45-C46
29	a	616	SQD	C44-C45-C46-O48
30	A	614	LHG	C4-C5-C6-O8
31	C	516	DGD	O1G-C1G-C2G-C3G
33	M	101	LMG	O1-C7-C8-C9
33	M	101	LMG	C7-C8-C9-O8
33	b	622	LMG	O1-C7-C8-C9
32	B	619	STE	C12-C13-C14-C15
32	B	624	STE	C3-C4-C5-C6
24	c	503	CLA	C16-C17-C18-C19
29	b	620	SQD	C13-C14-C15-C16
31	A	616	DGD	CBA-CCA-CDA-CEA
31	A	616	DGD	C7B-C8B-C9B-CAB
32	b	623	STE	C9-C10-C11-C12
33	b	622	LMG	C38-C39-C40-C41
33	c	522	LMG	C19-C20-C21-C22
25	d	401	PHO	C1A-C2A-CAA-CBA
32	X	102	STE	C7-C8-C9-C10
33	D	411	LMG	C14-C15-C16-C17
33	m	101	LMG	C17-C18-C19-C20
28	D	406	PL9	C30-C29-C31-C32
33	C	515	LMG	C31-C32-C33-C34
33	m	101	LMG	C22-C23-C24-C25
24	D	404	CLA	C10-C11-C12-C13
32	a	618	STE	C2-C3-C4-C5
33	c	519	LMG	C39-C40-C41-C42
29	A	615	SQD	O47-C45-C46-O48
31	A	616	DGD	CCB-CDB-CEB-CFB
24	B	607	CLA	C16-C17-C18-C19
24	c	507	CLA	C16-C17-C18-C19
30	e	101	LHG	O6-C4-C5-O7
33	m	101	LMG	C33-C34-C35-C36
29	a	615	SQD	C19-C20-C21-C22
26	c	514	BCR	C1-C6-C7-C8
26	k	101	BCR	C23-C24-C25-C30
30	L	101	LHG	C23-C24-C25-C26
30	d	406	LHG	C31-C32-C33-C34
31	c	517	DGD	C6B-C7B-C8B-C9B
32	h	103	STE	C6-C7-C8-C9
33	a	619	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	f	102	SQD	C33-C34-C35-C36
31	c	518	DGD	C6B-C7B-C8B-C9B
24	c	513	CLA	C5-C6-C7-C8
32	R	101	STE	C3-C4-C5-C6
24	B	606	CLA	C16-C17-C18-C20
24	b	602	CLA	C16-C17-C18-C19
29	a	616	SQD	O47-C45-C46-O48
30	A	614	LHG	C35-C36-C37-C38
28	A	611	PL9	C4-C3-C7-C8
33	c	521	LMG	C12-C13-C14-C15
33	c	521	LMG	C33-C34-C35-C36
33	M	101	LMG	C15-C16-C17-C18
33	c	521	LMG	C31-C32-C33-C34
26	K	101	BCR	C18-C19-C20-C21
28	d	405	PL9	C28-C29-C31-C32
29	A	615	SQD	C28-C29-C30-C31
30	d	406	LHG	C17-C18-C19-C20
32	B	622	STE	C2-C3-C4-C5
24	B	604	CLA	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C19
30	l	101	LHG	C34-C35-C36-C37
32	c	523	STE	C2-C3-C4-C5
33	b	622	LMG	C41-C42-C43-C44
24	b	604	CLA	C10-C11-C12-C13
33	Y	101	LMG	C10-C11-C12-C13
32	M	104	STE	C6-C7-C8-C9
33	D	412	LMG	C35-C36-C37-C38
24	B	602	CLA	C14-C13-C15-C16
24	C	508	CLA	C14-C13-C15-C16
24	C	510	CLA	C11-C10-C8-C9
24	H	101	CLA	C6-C7-C8-C9
24	a	605	CLA	C6-C7-C8-C9
32	B	625	STE	C3-C4-C5-C6
29	b	620	SQD	C30-C31-C32-C33
33	M	101	LMG	C28-C29-C30-C31
30	a	614	LHG	C25-C26-C27-C28
31	C	516	DGD	C6A-C7A-C8A-C9A
33	C	515	LMG	C39-C40-C41-C42
31	c	517	DGD	CDA-CEA-CFA-CGA
24	B	606	CLA	C16-C17-C18-C19
24	B	614	CLA	C16-C17-C18-C19
30	D	413	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
31	c	516	DGD	C2E-C1E-O5D-C6D
29	B	620	SQD	C24-C25-C26-C27
32	M	102	STE	C3-C4-C5-C6
24	b	610	CLA	C4C-C3C-CAC-CBC
32	B	625	STE	C6-C7-C8-C9
32	B	621	STE	C7-C8-C9-C10
32	B	625	STE	C2-C3-C4-C5
32	b	625	STE	C1-C2-C3-C4
30	D	409	LHG	O1-C1-C2-O2
30	d	406	LHG	O1-C1-C2-O2
24	B	611	CLA	CBA-CGA-O2A-C1
31	A	616	DGD	C2A-C1A-O1G-C1G
24	H	101	CLA	C4-C3-C5-C6
28	d	405	PL9	C45-C44-C46-C47
26	A	608	BCR	C9-C10-C11-C12
30	e	101	LHG	C8-C7-O7-C5
29	b	620	SQD	C7-C8-C9-C10
29	a	615	SQD	C26-C27-C28-C29
33	c	522	LMG	C11-C12-C13-C14
33	D	412	LMG	C37-C38-C39-C40
24	B	614	CLA	C10-C11-C12-C13
24	D	403	CLA	C10-C11-C12-C13
32	a	618	STE	C3-C4-C5-C6
32	d	410	STE	C12-C13-C14-C15
26	a	608	BCR	C35-C13-C14-C15
33	a	619	LMG	C16-C17-C18-C19
30	A	614	LHG	O6-C4-C5-C6
30	d	406	LHG	O6-C4-C5-C6
24	B	610	CLA	C16-C17-C18-C20
24	c	504	CLA	C11-C12-C13-C15
32	b	625	STE	C7-C8-C9-C10
31	h	102	DGD	C8B-C9B-CAB-CBB
24	B	610	CLA	C13-C15-C16-C17
24	b	610	CLA	C8-C10-C11-C12
32	C	520	STE	C3-C4-C5-C6
30	a	614	LHG	C29-C30-C31-C32
32	b	623	STE	C11-C10-C9-C8
24	A	605	CLA	C11-C12-C13-C15
24	B	602	CLA	C12-C13-C15-C16
24	B	604	CLA	C11-C10-C8-C7
24	B	606	CLA	C12-C13-C15-C16
24	B	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C11-C10-C8-C7
24	C	509	CLA	C11-C10-C8-C7
24	C	510	CLA	C11-C10-C8-C7
24	D	403	CLA	C6-C7-C8-C10
24	D	404	CLA	C12-C13-C15-C16
24	b	612	CLA	C12-C13-C15-C16
24	c	503	CLA	C6-C7-C8-C10
24	c	505	CLA	C6-C7-C8-C10
24	c	508	CLA	C6-C7-C8-C10
29	f	102	SQD	C32-C33-C34-C35
30	d	407	LHG	C29-C30-C31-C32
32	M	102	STE	C4-C5-C6-C7
32	b	624	STE	C6-C7-C8-C9
24	b	616	CLA	C5-C6-C7-C8
26	K	103	BCR	C17-C18-C19-C20
26	T	101	BCR	C21-C22-C23-C24
26	k	101	BCR	C21-C22-C23-C24
31	c	516	DGD	O1A-C1A-O1G-C1G
31	C	517	DGD	C2G-C3G-O3G-C1D
31	c	517	DGD	C5D-C6D-O5D-C1E
33	b	622	LMG	C39-C40-C41-C42
33	d	408	LMG	C32-C33-C34-C35
31	h	102	DGD	C9B-CAB-CBB-CCB
33	Y	101	LMG	C37-C38-C39-C40
24	B	611	CLA	O1A-CGA-O2A-C1
24	c	507	CLA	O1A-CGA-O2A-C1
24	H	101	CLA	C2-C3-C5-C6
33	c	519	LMG	C35-C36-C37-C38
31	C	517	DGD	C8B-C9B-CAB-CBB
24	c	511	CLA	CBA-CGA-O2A-C1
33	a	619	LMG	C9-C8-O7-C10
33	c	522	LMG	C9-C8-O7-C10
26	T	101	BCR	C13-C14-C15-C16
32	B	624	STE	C10-C11-C12-C13
30	a	614	LHG	C9-C10-C11-C12
31	C	518	DGD	C4B-C5B-C6B-C7B
29	a	615	SQD	O10-C23-O48-C46
31	A	616	DGD	CEA-CFA-CGA-CHA
33	d	408	LMG	C14-C15-C16-C17
26	h	101	BCR	C20-C21-C22-C23
30	A	614	LHG	O6-C4-C5-O7
33	a	619	LMG	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
24	C	513	CLA	O1D-CGD-O2D-CED
30	d	407	LHG	C4-C5-C6-O8
24	C	507	CLA	C10-C11-C12-C13
25	d	401	PHO	C5-C6-C7-C8
35	F	101	HEM	C4C-C3C-CAC-CBC
31	H	102	DGD	C8B-C9B-CAB-CBB
28	d	405	PL9	C35-C34-C36-C37
24	B	613	CLA	C2-C3-C5-C6
32	B	619	STE	C4-C5-C6-C7
33	m	101	LMG	C35-C36-C37-C38
33	m	101	LMG	C15-C16-C17-C18
29	a	616	SQD	C15-C16-C17-C18
29	b	620	SQD	C16-C17-C18-C19
33	c	521	LMG	C16-C17-C18-C19
30	L	101	LHG	C27-C28-C29-C30
31	c	517	DGD	CCB-CDB-CEB-CFB
32	b	623	STE	C5-C6-C7-C8
30	A	614	LHG	O7-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-O2G
33	M	101	LMG	O7-C8-C9-O8
33	a	619	LMG	O7-C8-C9-O8
24	A	605	CLA	C11-C12-C13-C14
24	C	504	CLA	C11-C10-C8-C9
24	b	602	CLA	C11-C12-C13-C14
24	b	607	CLA	C6-C7-C8-C9
24	c	502	CLA	C14-C13-C15-C16
25	D	401	PHO	C14-C13-C15-C16
31	c	517	DGD	C7A-C8A-C9A-CAA
30	e	101	LHG	C28-C29-C30-C31
32	T	103	STE	C13-C14-C15-C16
33	D	407	LMG	C34-C35-C36-C37
33	c	522	LMG	C39-C40-C41-C42
29	A	615	SQD	C31-C32-C33-C34
32	M	104	STE	C12-C13-C14-C15
32	X	102	STE	C10-C11-C12-C13
32	b	624	STE	C13-C14-C15-C16
33	M	101	LMG	C34-C35-C36-C37
33	c	521	LMG	C36-C37-C38-C39
32	d	411	STE	C2-C3-C4-C5
24	b	616	CLA	C2-C1-O2A-CGA
24	c	506	CLA	C2-C1-O2A-CGA
24	A	604	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	a	607	CLA	C16-C17-C18-C20
32	b	623	STE	C10-C11-C12-C13
32	c	520	STE	C6-C7-C8-C9
32	B	626	STE	C5-C6-C7-C8
33	M	101	LMG	C12-C13-C14-C15
24	c	510	CLA	C4-C3-C5-C6
24	c	513	CLA	C8-C10-C11-C12
24	d	403	CLA	C15-C16-C17-C18
30	a	614	LHG	C31-C32-C33-C34
32	b	621	STE	C5-C6-C7-C8
31	c	516	DGD	CDA-CEA-CFA-CGA
29	A	613	SQD	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
24	b	616	CLA	C10-C11-C12-C13
31	H	102	DGD	O1A-C1A-O1G-C1G
32	B	624	STE	C4-C5-C6-C7
24	B	611	CLA	C8-C10-C11-C12
25	A	606	PHO	C2C-C3C-CAC-CBC
24	c	511	CLA	C16-C17-C18-C20
32	T	102	STE	C6-C7-C8-C9
24	D	403	CLA	C4B-C3B-CAB-CBB
24	H	101	CLA	C4B-C3B-CAB-CBB
26	C	514	BCR	C22-C23-C24-C25
30	a	614	LHG	C27-C28-C29-C30
30	D	409	LHG	C13-C14-C15-C16
31	h	102	DGD	CAB-CBB-CCB-CDB
32	j	101	STE	C7-C8-C9-C10
33	c	519	LMG	C37-C38-C39-C40
30	e	101	LHG	O6-C4-C5-C6
31	c	518	DGD	C2A-C3A-C4A-C5A
32	T	102	STE	C10-C11-C12-C13
32	M	102	STE	C2-C3-C4-C5
24	B	603	CLA	C12-C13-C15-C16
24	B	606	CLA	C11-C10-C8-C7
24	B	610	CLA	C11-C12-C13-C15
24	B	614	CLA	C12-C13-C15-C16
24	C	505	CLA	C6-C7-C8-C10
24	C	505	CLA	C11-C12-C13-C15
24	C	505	CLA	C12-C13-C15-C16
24	C	507	CLA	C12-C13-C15-C16
24	D	404	CLA	C6-C7-C8-C10
24	b	601	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C11-C10-C8-C7
29	a	615	SQD	C9-C10-C11-C12
30	A	614	LHG	C29-C30-C31-C32
24	b	608	CLA	C16-C17-C18-C19
33	C	515	LMG	C40-C41-C42-C43
32	C	521	STE	C2-C3-C4-C5
31	c	516	DGD	C6B-C7B-C8B-C9B
32	j	101	STE	C5-C6-C7-C8
24	D	404	CLA	C15-C16-C17-C18
32	B	622	STE	C4-C5-C6-C7
30	d	407	LHG	C24-C25-C26-C27
33	a	619	LMG	C21-C22-C23-C24
30	D	413	LHG	C23-C24-C25-C26
29	A	613	SQD	C9-C10-C11-C12
32	T	102	STE	C4-C5-C6-C7
33	a	619	LMG	C34-C35-C36-C37
24	c	505	CLA	C4-C3-C5-C6
36	V	201	HEC	C4B-C3B-CAB-CBB
36	v	201	HEC	C4B-C3B-CAB-CBB
33	m	101	LMG	C38-C39-C40-C41
31	C	516	DGD	CDA-CEA-CFA-CGA
30	e	101	LHG	O9-C7-O7-C5
30	d	406	LHG	O6-C4-C5-O7
33	a	619	LMG	C11-C12-C13-C14
29	b	620	SQD	C12-C13-C14-C15
24	B	612	CLA	C14-C13-C15-C16
24	D	403	CLA	C6-C7-C8-C9
24	D	404	CLA	C14-C13-C15-C16
24	b	607	CLA	C14-C13-C15-C16
24	b	612	CLA	C14-C13-C15-C16
29	A	613	SQD	C32-C33-C34-C35
30	d	406	LHG	C9-C10-C11-C12
32	c	523	STE	C5-C6-C7-C8
24	B	613	CLA	C16-C17-C18-C20
24	d	402	CLA	C16-C17-C18-C19
24	d	402	CLA	C16-C17-C18-C20
31	H	102	DGD	C9B-CAB-CBB-CCB
30	a	614	LHG	C26-C27-C28-C29
31	H	102	DGD	CBB-CCB-CDB-CEB
29	f	102	SQD	C30-C31-C32-C33
24	c	511	CLA	O1A-CGA-O2A-C1
30	d	407	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	b	620	SQD	O6-C44-C45-O47
29	f	102	SQD	O47-C45-C46-O48
30	e	101	LHG	O7-C5-C6-O8
31	C	516	DGD	O1G-C1G-C2G-O2G
33	Y	101	LMG	O1-C7-C8-O7
33	b	622	LMG	O1-C7-C8-O7
33	c	522	LMG	O1-C7-C8-O7
30	L	101	LHG	C16-C17-C18-C19
29	b	620	SQD	C19-C20-C21-C22
31	h	102	DGD	C2A-C3A-C4A-C5A
32	B	619	STE	C7-C8-C9-C10
30	l	101	LHG	C4-C5-C6-O8
31	c	516	DGD	O1G-C1G-C2G-C3G
31	c	516	DGD	C1G-C2G-C3G-O3G
33	c	521	LMG	C7-C8-C9-O8
28	a	612	PL9	C15-C14-C16-C17
32	X	102	STE	C9-C10-C11-C12
24	D	403	CLA	C2C-C3C-CAC-CBC
24	B	606	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
32	B	621	STE	C6-C7-C8-C9
24	B	604	CLA	CBA-CGA-O2A-C1
30	d	406	LHG	C26-C27-C28-C29
31	c	516	DGD	CCB-CDB-CEB-CFB
31	H	102	DGD	CDA-CEA-CFA-CGA
33	d	408	LMG	C33-C34-C35-C36
24	A	604	CLA	C15-C16-C17-C18
24	C	509	CLA	C10-C11-C12-C13
31	C	516	DGD	O1A-C1A-O1G-C1G
29	a	615	SQD	C18-C19-C20-C21
24	A	605	CLA	C2C-C3C-CAC-CBC
30	A	614	LHG	C24-C25-C26-C27
33	c	522	LMG	C13-C14-C15-C16
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	CHA-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O1D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
26	X	101	BCR	C9-C10-C11-C12
30	A	614	LHG	C4-O6-P-O5
30	D	409	LHG	C4-O6-P-O5
30	D	410	LHG	C3-O3-P-O5
30	L	101	LHG	C4-O6-P-O3
30	a	614	LHG	C3-O3-P-O5
30	d	406	LHG	C3-O3-P-O5
33	m	101	LMG	C28-C29-C30-C31
31	C	517	DGD	C4A-C5A-C6A-C7A
24	b	601	CLA	C2B-C3B-CAB-CBB
24	b	605	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
29	A	613	SQD	C31-C32-C33-C34
32	B	623	STE	C2-C3-C4-C5
32	b	623	STE	C4-C5-C6-C7
24	c	506	CLA	C2-C3-C5-C6
26	B	618	BCR	C37-C22-C23-C24
32	T	102	STE	C5-C6-C7-C8
24	c	509	CLA	C16-C17-C18-C19
30	e	101	LHG	C26-C27-C28-C29
24	c	509	CLA	CAA-CBA-CGA-O2A
26	d	404	BCR	C21-C22-C23-C24
30	d	406	LHG	C25-C26-C27-C28
32	b	625	STE	C5-C6-C7-C8
30	d	407	LHG	C32-C33-C34-C35
32	X	102	STE	C3-C4-C5-C6
32	d	409	STE	C11-C12-C13-C14
33	c	521	LMG	C39-C40-C41-C42
30	d	406	LHG	C14-C15-C16-C17
24	B	612	CLA	C8-C10-C11-C12
24	b	612	CLA	C13-C15-C16-C17
32	X	102	STE	C15-C16-C17-C18
32	C	520	STE	C11-C12-C13-C14
33	m	101	LMG	C11-C12-C13-C14
24	D	404	CLA	C13-C15-C16-C17
24	c	510	CLA	C2-C3-C5-C6
28	a	612	PL9	C43-C44-C46-C47
32	B	623	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	M	102	STE	C11-C10-C9-C8
31	C	516	DGD	CDB-CEB-CFB-CGB
33	m	101	LMG	C13-C14-C15-C16
31	h	102	DGD	CDA-CEA-CFA-CGA
31	C	517	DGD	C3B-C4B-C5B-C6B
33	Y	101	LMG	C32-C33-C34-C35
24	B	606	CLA	C11-C10-C8-C9
24	B	612	CLA	C11-C12-C13-C14
24	C	513	CLA	C6-C7-C8-C9
24	c	505	CLA	C6-C7-C8-C9
24	c	511	CLA	C6-C7-C8-C9
30	d	406	LHG	C30-C31-C32-C33
24	c	511	CLA	C6-C7-C8-C10
26	T	101	BCR	C16-C17-C18-C19
29	B	620	SQD	C23-C24-C25-C26
30	d	407	LHG	C23-C24-C25-C26
29	A	613	SQD	C11-C12-C13-C14
32	c	520	STE	C3-C4-C5-C6
29	b	620	SQD	O5-C1-O6-C44
24	B	610	CLA	C16-C17-C18-C19
33	a	619	LMG	O8-C28-C29-C30
33	a	619	LMG	C24-C25-C26-C27
32	C	520	STE	C10-C11-C12-C13
24	a	607	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C19
31	A	616	DGD	O1G-C1G-C2G-O2G
30	D	410	LHG	O2-C2-C3-O3
29	A	615	SQD	C27-C28-C29-C30
29	f	102	SQD	C23-C24-C25-C26
31	C	516	DGD	C1A-C2A-C3A-C4A
33	m	101	LMG	C10-C11-C12-C13
26	t	101	BCR	C13-C14-C15-C16
31	c	517	DGD	C3A-C4A-C5A-C6A
31	C	517	DGD	CDB-CEB-CFB-CGB
32	d	409	STE	C4-C5-C6-C7
31	A	616	DGD	O6D-C5D-C6D-O5D
32	X	102	STE	C2-C3-C4-C5
24	A	604	CLA	C16-C17-C18-C19
31	A	616	DGD	O1G-C1G-C2G-C3G
32	d	411	STE	C1-C2-C3-C4
30	A	614	LHG	C10-C11-C12-C13
31	C	516	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
33	a	619	LMG	C4-C5-C6-O5
24	c	505	CLA	C16-C17-C18-C20
32	T	102	STE	C15-C16-C17-C18
31	C	518	DGD	C7B-C8B-C9B-CAB
29	B	620	SQD	C45-C44-O6-C1
31	C	517	DGD	C5D-C6D-O5D-C1E
33	C	515	LMG	C8-C7-O1-C1
24	b	606	CLA	C15-C16-C17-C18
24	b	610	CLA	C2A-CAA-CBA-CGA
24	A	604	CLA	O1D-CGD-O2D-CED
26	k	101	BCR	C19-C20-C21-C22
24	c	504	CLA	C11-C12-C13-C14
24	c	512	CLA	C4-C3-C5-C6
24	B	612	CLA	C5-C6-C7-C8
24	B	612	CLA	C15-C16-C17-C18
24	c	505	CLA	C2-C3-C5-C6
29	B	620	SQD	C29-C30-C31-C32
29	a	616	SQD	C29-C30-C31-C32
32	I	101	STE	C5-C6-C7-C8
32	d	409	STE	C7-C8-C9-C10
24	c	509	CLA	C5-C6-C7-C8
31	C	517	DGD	O1B-C1B-O2G-C2G
31	C	518	DGD	C8A-C9A-CAA-CBA
24	B	603	CLA	C14-C13-C15-C16
24	C	505	CLA	C6-C7-C8-C9
24	b	601	CLA	C14-C13-C15-C16
33	Y	101	LMG	C36-C37-C38-C39
24	B	613	CLA	CBA-CGA-O2A-C1
32	d	409	STE	C12-C13-C14-C15
24	B	613	CLA	O1A-CGA-O2A-C1
24	B	614	CLA	C4B-C3B-CAB-CBB
31	C	518	DGD	O6D-C5D-C6D-O5D
33	D	412	LMG	C30-C31-C32-C33
33	c	521	LMG	C38-C39-C40-C41
24	B	603	CLA	C16-C17-C18-C20
30	a	614	LHG	C13-C14-C15-C16
31	C	518	DGD	C5B-C6B-C7B-C8B
32	t	102	STE	C11-C10-C9-C8
24	B	604	CLA	O1A-CGA-O2A-C1
29	A	613	SQD	C30-C31-C32-C33
24	b	604	CLA	C6-C7-C8-C10
24	c	502	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	b	604	CLA	C13-C15-C16-C17
31	H	102	DGD	O2G-C1B-C2B-C3B
32	b	621	STE	C12-C13-C14-C15
24	B	603	CLA	C16-C17-C18-C19
30	D	410	LHG	C10-C11-C12-C13
24	B	603	CLA	O1D-CGD-O2D-CED
29	b	620	SQD	O47-C45-C46-O48
30	L	101	LHG	C15-C16-C17-C18
32	B	624	STE	C6-C7-C8-C9
33	M	101	LMG	C17-C18-C19-C20
33	c	521	LMG	C14-C15-C16-C17
31	C	518	DGD	CAB-CBB-CCB-CDB
24	b	603	CLA	C8-C10-C11-C12
33	D	411	LMG	C36-C37-C38-C39
26	D	405	BCR	C16-C17-C18-C36
26	X	101	BCR	C16-C17-C18-C36
31	A	616	DGD	CCA-CDA-CEA-CFA
24	d	402	CLA	C2-C1-O2A-CGA
26	c	515	BCR	C13-C14-C15-C16
32	d	409	STE	C6-C7-C8-C9
24	b	604	CLA	C8-C10-C11-C12
26	a	608	BCR	C37-C22-C23-C24
32	T	103	STE	C4-C5-C6-C7
31	A	616	DGD	C4E-C5E-C6E-O5E
24	C	507	CLA	C15-C16-C17-C18
24	C	512	CLA	C10-C11-C12-C13
24	B	602	CLA	C4-C3-C5-C6
30	D	410	LHG	C4-C5-C6-O8
30	e	101	LHG	C14-C15-C16-C17
29	D	408	SQD	O10-C23-C24-C25
30	a	614	LHG	C19-C20-C21-C22
32	a	617	STE	C1-C2-C3-C4
30	L	101	LHG	C9-C10-C11-C12
33	d	408	LMG	C39-C40-C41-C42
32	b	624	STE	O1-C1-C2-C3
24	C	512	CLA	C11-C12-C13-C14
24	D	403	CLA	C11-C10-C8-C9
24	b	605	CLA	C11-C12-C13-C14
24	c	505	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C10-C8-C9
24	c	506	CLA	C11-C12-C13-C14
29	a	616	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	a	615	SQD	C35-C36-C37-C38
33	c	522	LMG	C20-C21-C22-C23
33	a	619	LMG	C29-C30-C31-C32
29	A	613	SQD	C35-C36-C37-C38
30	D	409	LHG	C28-C29-C30-C31
28	A	611	PL9	C13-C14-C16-C17
32	B	622	STE	C6-C7-C8-C9
36	v	201	HEC	CAD-CBD-CGD-O1D
30	l	101	LHG	C26-C27-C28-C29
24	c	512	CLA	C1A-C2A-CAA-CBA
26	B	616	BCR	C12-C13-C14-C15
33	b	622	LMG	C36-C37-C38-C39
24	C	508	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C19
32	b	623	STE	O1-C1-C2-C3
31	H	102	DGD	C7A-C8A-C9A-CAA
24	B	612	CLA	C13-C15-C16-C17
24	B	602	CLA	C2B-C3B-CAB-CBB
24	B	614	CLA	C2B-C3B-CAB-CBB
24	H	101	CLA	C2B-C3B-CAB-CBB
24	c	505	CLA	C2B-C3B-CAB-CBB
26	B	616	BCR	C5-C6-C7-C8
26	B	617	BCR	C23-C24-C25-C30
26	C	514	BCR	C23-C24-C25-C26
26	K	103	BCR	C5-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	c	514	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C30
26	k	101	BCR	C23-C24-C25-C26
26	t	101	BCR	C1-C6-C7-C8
30	l	101	LHG	C8-C7-O7-C5
33	Y	101	LMG	C15-C16-C17-C18
30	d	407	LHG	C2-C3-O3-P
32	b	624	STE	O2-C1-C2-C3
32	d	409	STE	O2-C1-C2-C3
29	B	620	SQD	C34-C35-C36-C37
24	c	512	CLA	C2-C3-C5-C6
31	H	102	DGD	CDB-CEB-CFB-CGB
30	D	413	LHG	C7-C8-C9-C10
30	a	614	LHG	C12-C13-C14-C15
33	d	408	LMG	C30-C31-C32-C33
24	B	605	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	C	512	CLA	C11-C12-C13-C15
24	b	607	CLA	C11-C10-C8-C7
33	b	622	LMG	C34-C35-C36-C37
24	b	602	CLA	C2A-CAA-CBA-CGA
30	l	101	LHG	O7-C5-C6-O8
33	a	619	LMG	O1-C7-C8-O7
32	d	409	STE	O1-C1-C2-C3
35	f	101	HEM	CAD-CBD-CGD-O1D
33	b	622	LMG	C11-C12-C13-C14
29	A	613	SQD	C15-C16-C17-C18
32	B	623	STE	C10-C11-C12-C13
36	v	201	HEC	CAD-CBD-CGD-O2D
31	c	517	DGD	CBB-CCB-CDB-CEB
26	T	101	BCR	C7-C8-C9-C34
24	c	508	CLA	C4-C3-C5-C6
28	d	405	PL9	C33-C34-C36-C37
30	a	614	LHG	C33-C34-C35-C36
24	B	615	CLA	O1A-CGA-O2A-C1
24	a	607	CLA	C15-C16-C17-C18
24	b	605	CLA	C5-C6-C7-C8
24	H	101	CLA	C16-C17-C18-C19
24	B	611	CLA	C13-C15-C16-C17
24	B	601	CLA	C11-C12-C13-C14
24	b	611	CLA	C10-C11-C12-C13
33	Y	101	LMG	C38-C39-C40-C41
24	c	513	CLA	C4-C3-C5-C6
28	a	612	PL9	C45-C44-C46-C47
24	c	502	CLA	C13-C15-C16-C17
32	b	623	STE	O2-C1-C2-C3
30	A	614	LHG	C2-C3-O3-P
30	D	410	LHG	C2-C3-O3-P
32	X	102	STE	O2-C1-C2-C3
35	f	101	HEM	CAD-CBD-CGD-O2D
31	h	102	DGD	CAA-CBA-CCA-CDA
24	c	506	CLA	C8-C10-C11-C12
31	h	102	DGD	C4A-C5A-C6A-C7A
33	a	619	LMG	O1-C7-C8-C9
33	a	619	LMG	C7-C8-C9-O8
32	M	104	STE	C1-C2-C3-C4
32	B	624	STE	C11-C12-C13-C14
31	A	616	DGD	CFB-CGB-CHB-CIB
31	C	516	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C4-C3-C5-C6
31	C	516	DGD	O6D-C5D-C6D-O5D
24	B	602	CLA	C2-C3-C5-C6
24	A	605	CLA	C15-C16-C17-C18
24	c	509	CLA	C8-C10-C11-C12
30	e	101	LHG	C9-C10-C11-C12
33	D	407	LMG	C39-C40-C41-C42
24	B	602	CLA	C4B-C3B-CAB-CBB
24	b	601	CLA	O1A-CGA-O2A-C1
33	Y	101	LMG	O6-C5-C6-O5
31	h	102	DGD	C5A-C6A-C7A-C8A
24	b	609	CLA	C15-C16-C17-C18
31	c	517	DGD	CAA-CBA-CCA-CDA
24	C	511	CLA	C16-C17-C18-C19
32	M	102	STE	C1-C2-C3-C4
30	e	101	LHG	C15-C16-C17-C18
26	a	608	BCR	C16-C17-C18-C36
24	B	604	CLA	C10-C11-C12-C13
24	D	403	CLA	C16-C17-C18-C19
29	a	615	SQD	O47-C45-C46-O48
29	D	408	SQD	O48-C23-C24-C25
30	D	409	LHG	C33-C34-C35-C36
33	D	407	LMG	C17-C18-C19-C20
24	B	601	CLA	C11-C12-C13-C15
24	B	605	CLA	C11-C12-C13-C15
24	D	403	CLA	C11-C12-C13-C15
24	b	612	CLA	C11-C10-C8-C7
24	c	510	CLA	C12-C13-C15-C16
32	C	520	STE	C4-C5-C6-C7
32	M	104	STE	C11-C10-C9-C8
24	B	603	CLA	C11-C10-C8-C9
24	B	604	CLA	C11-C10-C8-C9
24	B	605	CLA	C11-C10-C8-C9
24	b	614	CLA	C11-C12-C13-C14
24	c	504	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C10-C8-C9
32	a	618	STE	C6-C7-C8-C9
31	h	102	DGD	CCA-CDA-CEA-CFA
33	d	408	LMG	C15-C16-C17-C18
31	C	516	DGD	C5D-C6D-O5D-C1E
31	c	516	DGD	C5D-C6D-O5D-C1E
31	c	517	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
33	M	101	LMG	C8-C7-O1-C1
33	C	515	LMG	C30-C31-C32-C33
24	D	403	CLA	C2-C1-O2A-CGA
32	d	410	STE	C10-C11-C12-C13
24	c	504	CLA	C10-C11-C12-C13
24	b	601	CLA	CBA-CGA-O2A-C1
24	D	404	CLA	C3A-C2A-CAA-CBA
24	d	403	CLA	C3A-C2A-CAA-CBA
31	h	102	DGD	O2G-C1B-C2B-C3B
29	a	616	SQD	C27-C28-C29-C30
31	C	517	DGD	C2D-C1D-O3G-C3G
25	a	606	PHO	O2A-C1-C2-C3
30	d	406	LHG	C34-C35-C36-C37
33	C	515	LMG	C36-C37-C38-C39
30	D	413	LHG	C11-C12-C13-C14
33	Y	101	LMG	C30-C31-C32-C33
33	d	408	LMG	C35-C36-C37-C38
32	X	102	STE	O1-C1-C2-C3
26	d	404	BCR	C16-C17-C18-C19
26	k	102	BCR	C22-C23-C24-C25
24	B	608	CLA	C3-C5-C6-C7
28	a	612	PL9	C12-C13-C14-C15
32	X	102	STE	C14-C15-C16-C17
28	A	611	PL9	C12-C11-C9-C10
26	K	101	BCR	C9-C10-C11-C12
32	h	103	STE	C11-C10-C9-C8
36	V	201	HEC	CAD-CBD-CGD-O1D
24	B	609	CLA	C14-C13-C15-C16
24	C	505	CLA	C11-C12-C13-C14
24	C	512	CLA	C11-C10-C8-C9
24	D	404	CLA	C6-C7-C8-C9
24	c	502	CLA	C6-C7-C8-C9
24	c	508	CLA	C6-C7-C8-C9
24	c	510	CLA	C11-C12-C13-C14
29	D	408	SQD	C44-C45-C46-O48
29	a	615	SQD	O47-C7-C8-C9
32	c	523	STE	C7-C8-C9-C10
31	C	518	DGD	CDB-CEB-CFB-CGB
30	l	101	LHG	O6-C4-C5-C6
24	B	613	CLA	C2A-CAA-CBA-CGA
24	A	605	CLA	C11-C10-C8-C7
24	B	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	H	101	CLA	C12-C13-C15-C16
24	b	605	CLA	C11-C12-C13-C15
24	b	610	CLA	C11-C12-C13-C15
24	b	610	CLA	C12-C13-C15-C16
24	c	505	CLA	C11-C10-C8-C7
24	c	506	CLA	C11-C10-C8-C7
24	c	508	CLA	C12-C13-C15-C16
36	V	201	HEC	CAD-CBD-CGD-O2D
24	B	605	CLA	C2B-C3B-CAB-CBB
24	C	509	CLA	C2B-C3B-CAB-CBB
24	D	403	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C23-C24-C25-C26
26	a	608	BCR	C23-C24-C25-C30
26	c	514	BCR	C23-C24-C25-C30
26	d	404	BCR	C23-C24-C25-C26
26	h	101	BCR	C23-C24-C25-C26
26	t	101	BCR	C5-C6-C7-C8
33	D	411	LMG	C32-C33-C34-C35
32	I	101	STE	C3-C4-C5-C6
31	c	516	DGD	O1G-C1A-C2A-C3A
33	m	101	LMG	O8-C28-C29-C30
29	a	615	SQD	O5-C1-O6-C44
24	b	601	CLA	C16-C17-C18-C20
33	b	622	LMG	O7-C10-C11-C12
33	D	411	LMG	C13-C14-C15-C16
32	d	410	STE	C5-C6-C7-C8
24	c	506	CLA	C10-C11-C12-C13
31	C	516	DGD	O2G-C1B-C2B-C3B
24	c	512	CLA	C3-C5-C6-C7
32	d	410	STE	C11-C10-C9-C8
28	d	405	PL9	C4-C3-C7-C8
25	d	401	PHO	C2C-C3C-CAC-CBC
24	B	605	CLA	C5-C6-C7-C8
24	b	613	CLA	CAA-CBA-CGA-O2A
29	A	613	SQD	O47-C7-C8-C9
32	I	101	STE	C12-C13-C14-C15
29	A	613	SQD	C29-C30-C31-C32
26	X	101	BCR	C11-C10-C9-C34
24	C	513	CLA	C5-C6-C7-C8
31	c	518	DGD	O6E-C5E-C6E-O5E
24	b	613	CLA	C13-C15-C16-C17
32	M	104	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	a	613	CLA	C4C-C3C-CAC-CBC
24	B	614	CLA	C14-C13-C15-C16
24	C	501	CLA	C14-C13-C15-C16
24	b	604	CLA	C11-C12-C13-C14
29	B	620	SQD	O47-C7-C8-C9
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	609	CLA	C4B-C3B-CAB-CBB
24	C	503	CLA	C4B-C3B-CAB-CBB
32	h	103	STE	C7-C8-C9-C10
33	b	622	LMG	C42-C43-C44-C45
24	C	510	CLA	C2-C3-C5-C6
28	a	612	PL9	C28-C29-C31-C32
26	D	405	BCR	C21-C22-C23-C24
26	X	101	BCR	C15-C16-C17-C18
24	A	604	CLA	CBD-CGD-O2D-CED
28	a	612	PL9	C42-C43-C44-C46
24	c	503	CLA	C8-C10-C11-C12
35	F	101	HEM	CAD-CBD-CGD-O1D
24	C	501	CLA	C2A-CAA-CBA-CGA
31	A	616	DGD	C9A-CAA-CBA-CCA
30	a	614	LHG	C17-C18-C19-C20
24	B	612	CLA	CAA-CBA-CGA-O2A
32	B	624	STE	C15-C16-C17-C18
30	A	614	LHG	C31-C32-C33-C34
24	c	502	CLA	C4C-C3C-CAC-CBC
24	A	604	CLA	C2-C1-O2A-CGA
24	B	603	CLA	C11-C10-C8-C7
24	B	607	CLA	C11-C12-C13-C15
24	a	607	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15
24	b	609	CLA	C8-C10-C11-C12
24	c	505	CLA	O1A-CGA-O2A-C1
30	D	409	LHG	C31-C32-C33-C34
33	C	515	LMG	C28-C29-C30-C31
24	C	512	CLA	O2A-C1-C2-C3
25	D	401	PHO	O2A-C1-C2-C3
24	a	604	CLA	C13-C15-C16-C17
31	c	516	DGD	C2A-C3A-C4A-C5A
24	B	611	CLA	CAA-CBA-CGA-O2A
33	D	411	LMG	C12-C13-C14-C15
24	c	510	CLA	C13-C15-C16-C17
30	A	614	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
33	c	519	LMG	C33-C34-C35-C36
24	c	509	CLA	C2A-CAA-CBA-CGA
29	b	620	SQD	C11-C10-C9-C8
33	m	101	LMG	C20-C21-C22-C23
24	b	610	CLA	CBD-CGD-O2D-CED
24	B	601	CLA	C3A-C2A-CAA-CBA
24	C	512	CLA	C4-C3-C5-C6
24	c	512	CLA	C3A-C2A-CAA-CBA
28	A	611	PL9	C15-C14-C16-C17
31	A	616	DGD	C4D-C5D-C6D-O5D
30	l	101	LHG	C17-C18-C19-C20
33	c	519	LMG	C29-C28-O8-C9
30	a	614	LHG	O6-C4-C5-O7
33	M	101	LMG	C22-C23-C24-C25
29	A	613	SQD	C13-C14-C15-C16
33	D	411	LMG	C15-C16-C17-C18
28	d	405	PL9	C21-C22-C23-C24
24	A	605	CLA	C4C-C3C-CAC-CBC
24	C	505	CLA	C8-C10-C11-C12
24	C	505	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C10-C8-C9
24	b	609	CLA	C11-C12-C13-C14
29	a	615	SQD	O49-C7-C8-C9
29	a	616	SQD	C30-C31-C32-C33
32	c	520	STE	C4-C5-C6-C7
33	d	408	LMG	C11-C12-C13-C14
31	C	518	DGD	C7A-C8A-C9A-CAA
31	c	516	DGD	CAB-CBB-CCB-CDB
33	D	411	LMG	C29-C28-O8-C9
24	C	506	CLA	C13-C15-C16-C17
24	B	613	CLA	C16-C17-C18-C19
32	j	101	STE	O2-C1-C2-C3
24	b	613	CLA	CAA-CBA-CGA-O1A
33	Y	101	LMG	C31-C32-C33-C34
33	c	522	LMG	C8-C7-O1-C1
33	m	101	LMG	C8-C7-O1-C1
30	d	406	LHG	O9-C7-O7-C5
30	d	407	LHG	O7-C5-C6-O8
29	B	620	SQD	O49-C7-C8-C9
33	D	411	LMG	C35-C36-C37-C38
28	A	611	PL9	C9-C11-C12-C13
33	b	622	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
24	B	614	CLA	C5-C6-C7-C8
24	c	510	CLA	CAA-CBA-CGA-O2A
24	c	508	CLA	C2-C3-C5-C6
32	C	519	STE	O2-C1-C2-C3
26	t	101	BCR	C9-C10-C11-C12
33	b	622	LMG	C13-C14-C15-C16
24	C	503	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	d	403	CLA	CAD-CBD-CGD-O2D
25	a	606	PHO	CAD-CBD-CGD-O2D
24	B	613	CLA	C13-C15-C16-C17
30	D	409	LHG	C23-C24-C25-C26
24	B	607	CLA	C11-C10-C8-C7
30	L	101	LHG	O7-C7-C8-C9
32	j	101	STE	O1-C1-C2-C3
35	f	101	HEM	CAA-CBA-CGA-O1A
24	b	607	CLA	C16-C17-C18-C19
31	C	518	DGD	O1G-C1A-C2A-C3A
31	A	616	DGD	C6B-C7B-C8B-C9B
24	c	502	CLA	O1A-CGA-O2A-C1
35	F	101	HEM	CAD-CBD-CGD-O2D
35	f	101	HEM	CAA-CBA-CGA-O2A
24	B	611	CLA	CAA-CBA-CGA-O1A
30	d	406	LHG	C11-C12-C13-C14
32	R	101	STE	C6-C7-C8-C9

There are no ring outliers.

121 monomers are involved in 163 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	c	515	BCR	3	0
32	t	102	STE	1	0
24	C	502	CLA	1	0
32	M	104	STE	2	0
33	C	515	LMG	2	0
26	T	101	BCR	1	0
33	a	619	LMG	1	0
26	d	404	BCR	1	0
32	d	409	STE	2	0
30	L	101	LHG	3	0
29	D	408	SQD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	b	621	STE	1	0
26	k	101	BCR	1	0
24	B	612	CLA	1	0
21	a	601[B]	OEY	1	0
24	c	507	CLA	1	0
21	A	601[B]	OEY	2	0
24	C	508	CLA	1	0
24	b	609	CLA	1	0
24	B	613	CLA	1	0
24	c	510	CLA	1	0
26	B	618	BCR	2	0
30	D	409	LHG	1	0
24	b	615	CLA	2	0
30	a	614	LHG	3	0
24	B	606	CLA	1	0
33	Y	101	LMG	1	0
32	d	410	STE	5	0
32	c	520	STE	1	0
24	b	606	CLA	2	0
32	C	520	STE	1	0
24	C	511	CLA	1	0
24	b	613	CLA	1	0
33	c	522	LMG	1	0
32	T	102	STE	1	0
33	D	407	LMG	1	0
32	d	411	STE	2	0
34	D	402	BCT	1	0
26	t	101	BCR	1	0
24	C	505	CLA	2	0
32	Z	101	STE	3	0
24	C	506	CLA	2	0
30	e	101	LHG	1	0
24	A	612	CLA	2	0
31	A	616	DGD	3	0
29	A	613	SQD	2	0
26	B	617	BCR	3	0
24	B	603	CLA	2	0
28	d	405	PL9	1	0
26	B	616	BCR	1	0
32	b	623	STE	1	0
25	a	606	PHO	1	0
32	T	103	STE	2	0

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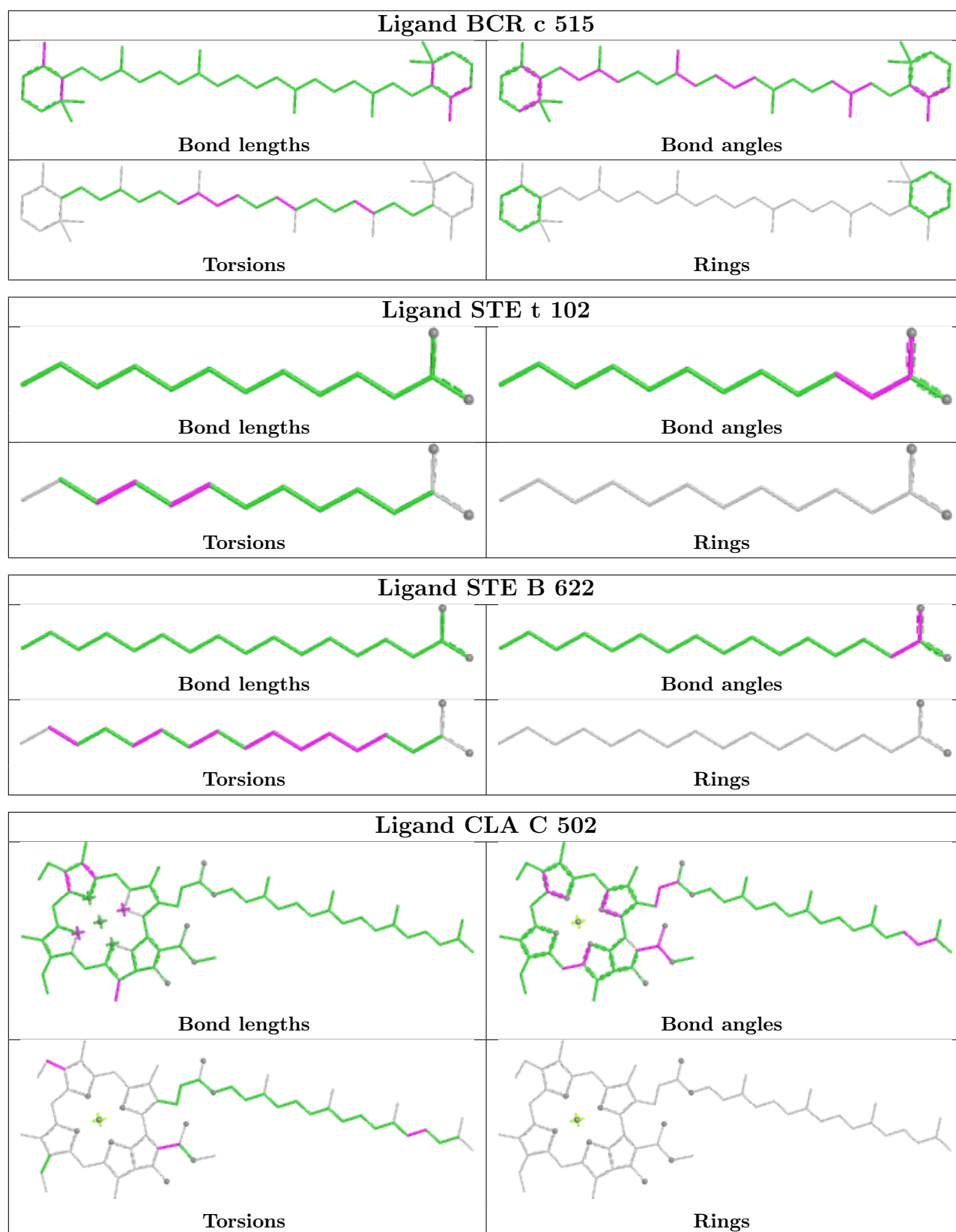
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	D	405	BCR	2	0
31	H	102	DGD	1	0
32	B	625	STE	2	0
30	D	413	LHG	1	0
24	d	403	CLA	1	0
24	c	509	CLA	1	0
24	C	503	CLA	1	0
32	h	103	STE	1	0
32	j	101	STE	2	0
29	A	615	SQD	2	0
24	H	101	CLA	3	0
26	b	617	BCR	1	0
35	f	101	HEM	3	0
24	B	610	CLA	2	0
24	c	502	CLA	1	0
35	F	101	HEM	4	0
32	a	617	STE	1	0
26	C	514	BCR	3	0
24	b	605	CLA	2	0
30	l	101	LHG	2	0
24	b	616	CLA	1	0
24	B	604	CLA	1	0
31	c	516	DGD	1	0
26	K	102	BCR	2	0
24	B	601	CLA	2	0
30	D	410	LHG	2	0
32	J	101	STE	1	0
24	B	608	CLA	1	0
24	d	402	CLA	1	0
24	b	604	CLA	3	0
24	B	605	CLA	3	0
24	b	601	CLA	1	0
25	d	401	PHO	2	0
31	c	518	DGD	1	0
33	b	622	LMG	1	0
32	B	623	STE	2	0
25	A	606	PHO	3	0
26	b	618	BCR	1	0
24	C	507	CLA	1	0
24	b	612	CLA	1	0
24	c	501	CLA	3	0
29	f	102	SQD	1	0

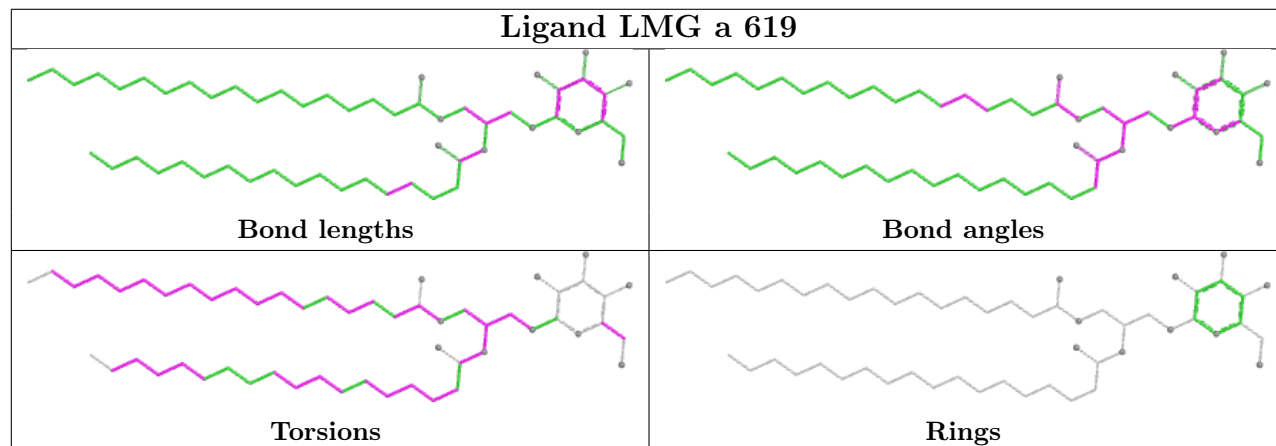
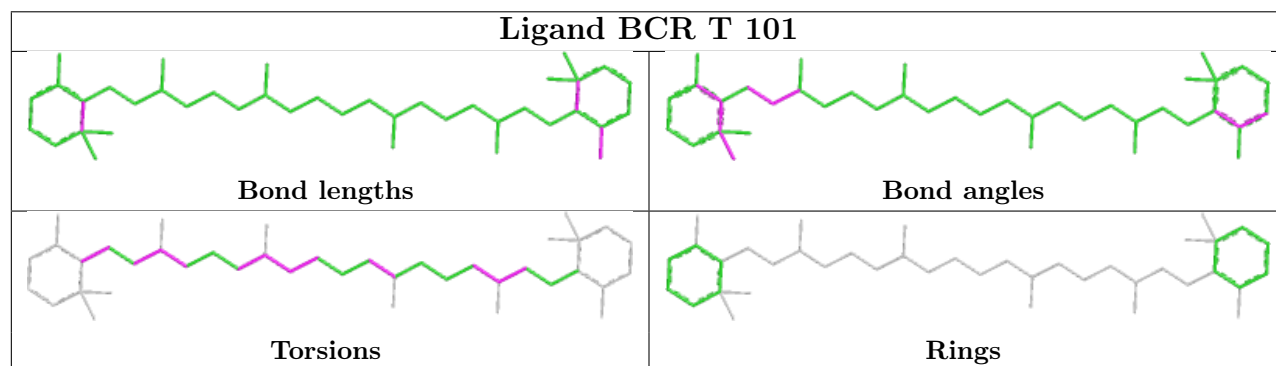
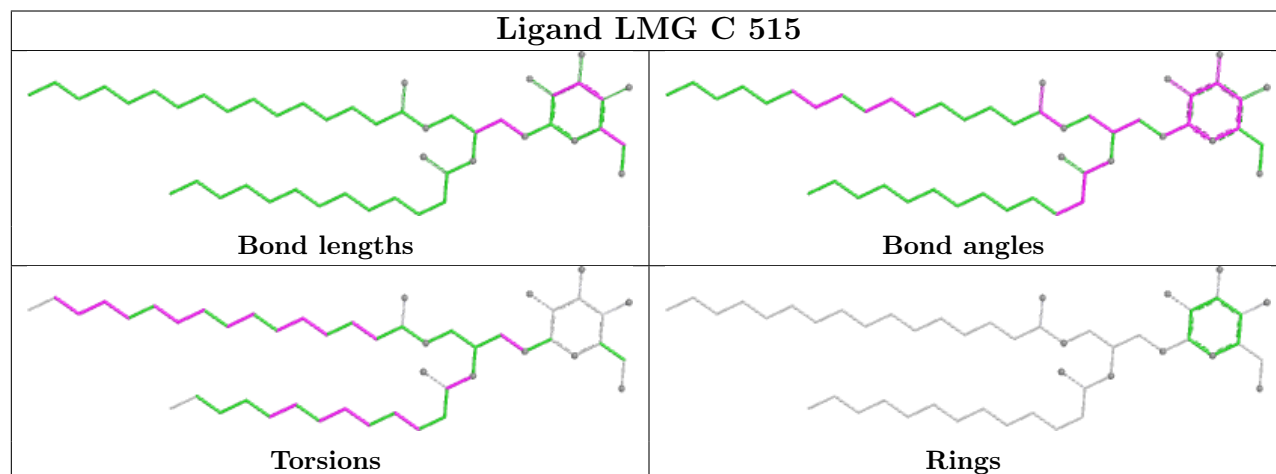
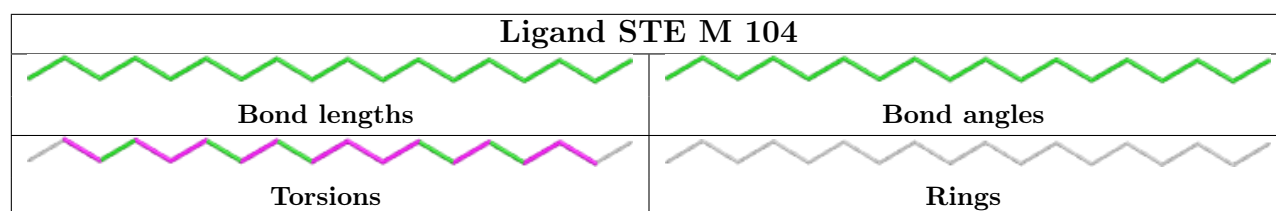
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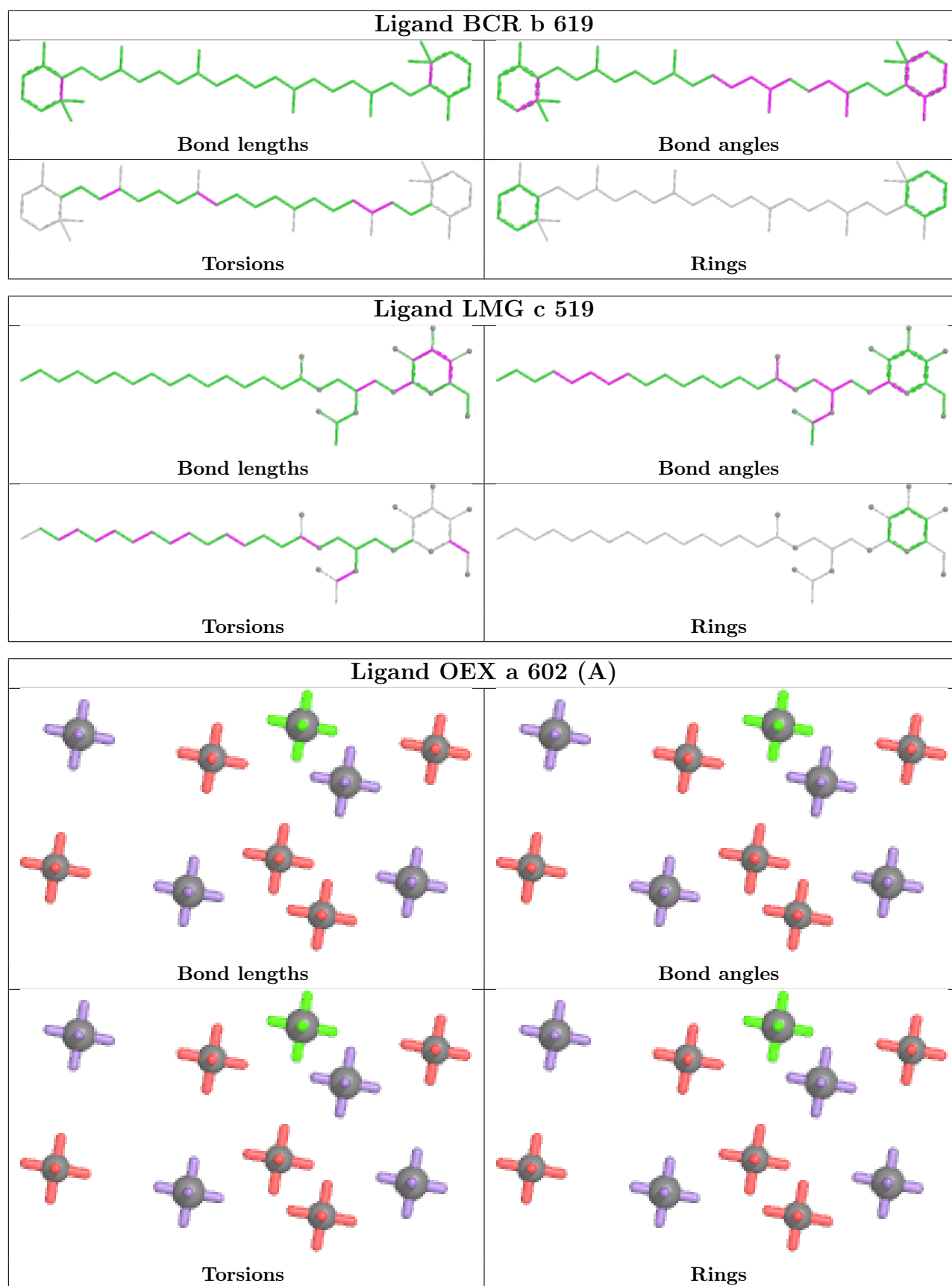
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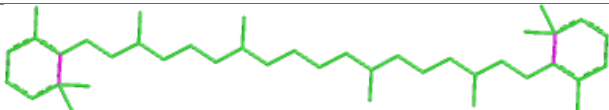
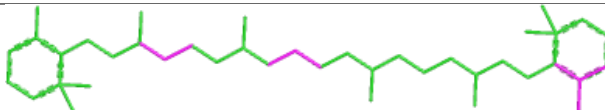
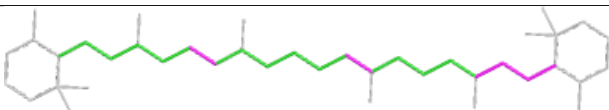
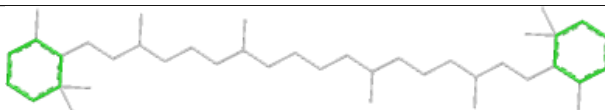
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	403	CLA	2	0
28	a	612	PL9	1	0
24	C	513	CLA	3	0
32	B	619	STE	1	0
32	X	102	STE	2	0
26	K	101	BCR	1	0
24	A	604	CLA	1	0
29	B	620	SQD	3	0
24	c	508	CLA	2	0
33	m	101	LMG	3	0
31	C	516	DGD	1	0
31	h	102	DGD	1	0
24	c	513	CLA	4	0
24	c	511	CLA	5	0
24	a	613	CLA	1	0
24	b	610	CLA	1	0
32	B	626	STE	1	0
24	b	602	CLA	2	0
26	X	101	BCR	1	0
31	C	518	DGD	1	0
28	A	611	PL9	5	0
32	I	101	STE	1	0
33	M	101	LMG	1	0
28	D	406	PL9	1	0
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33	c	521	LMG	1	0

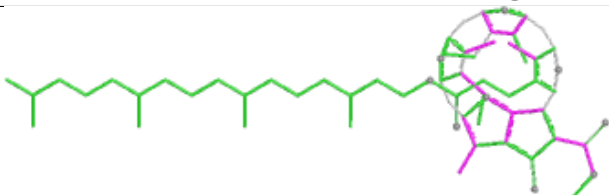
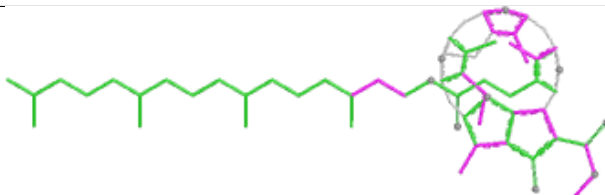
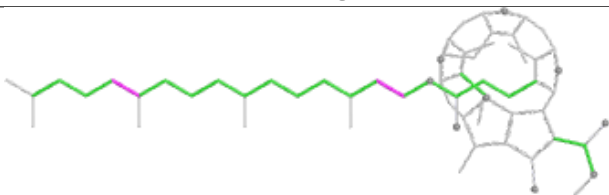
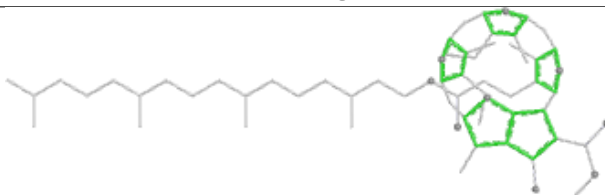
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

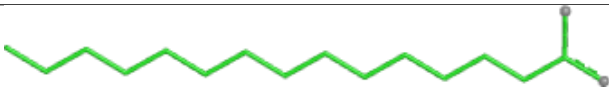
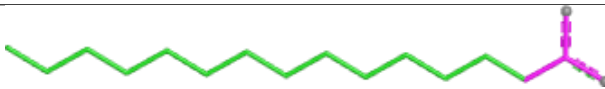
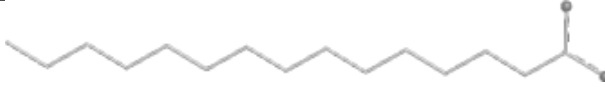


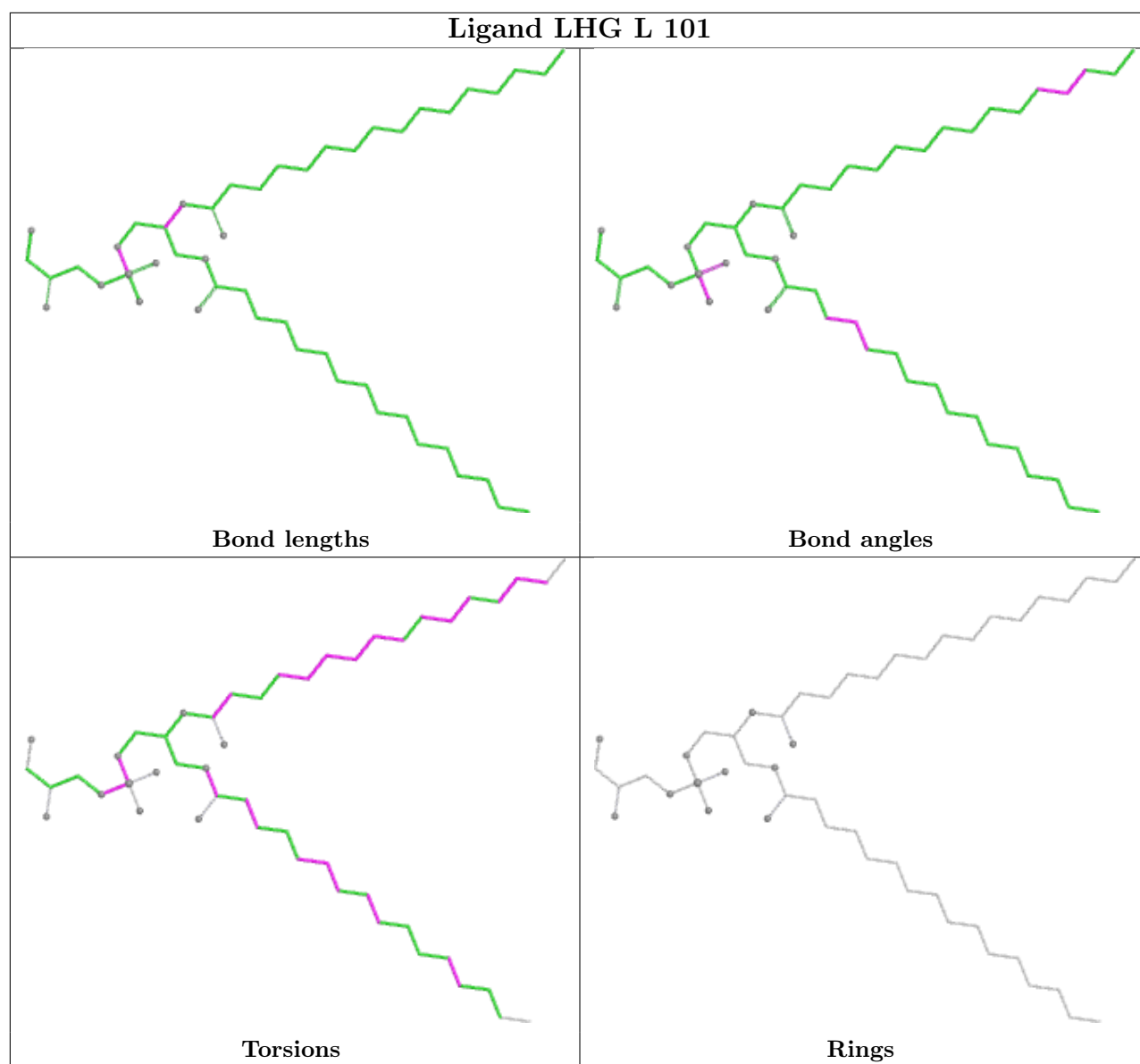


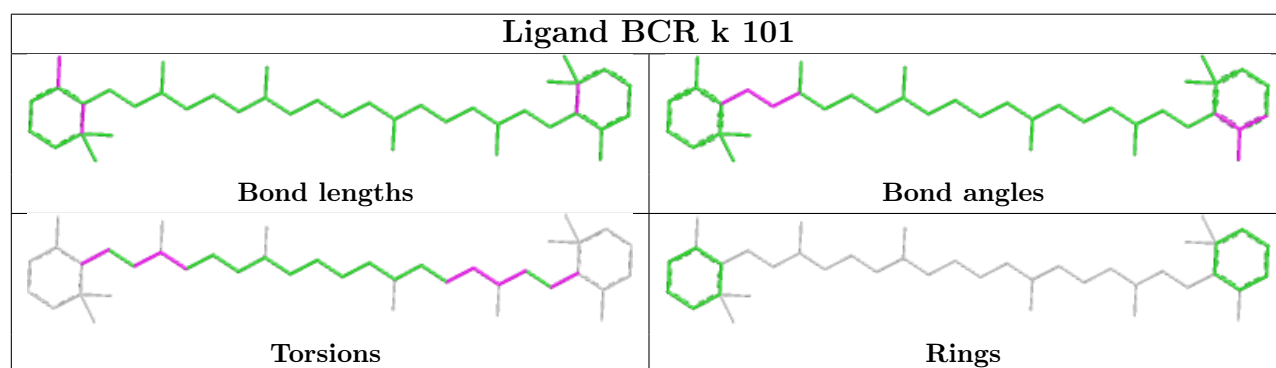
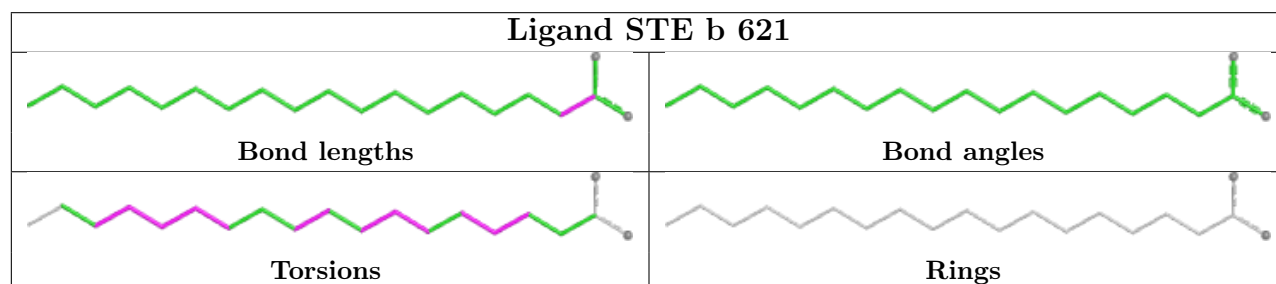
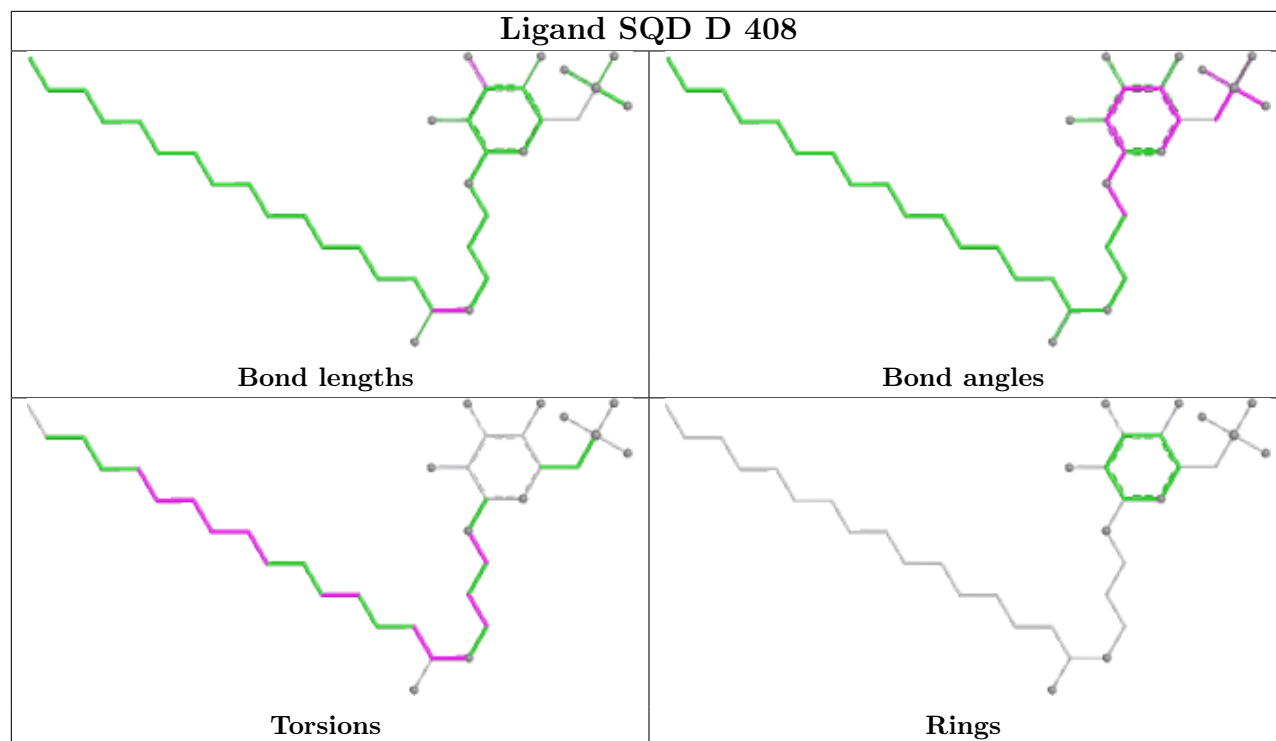


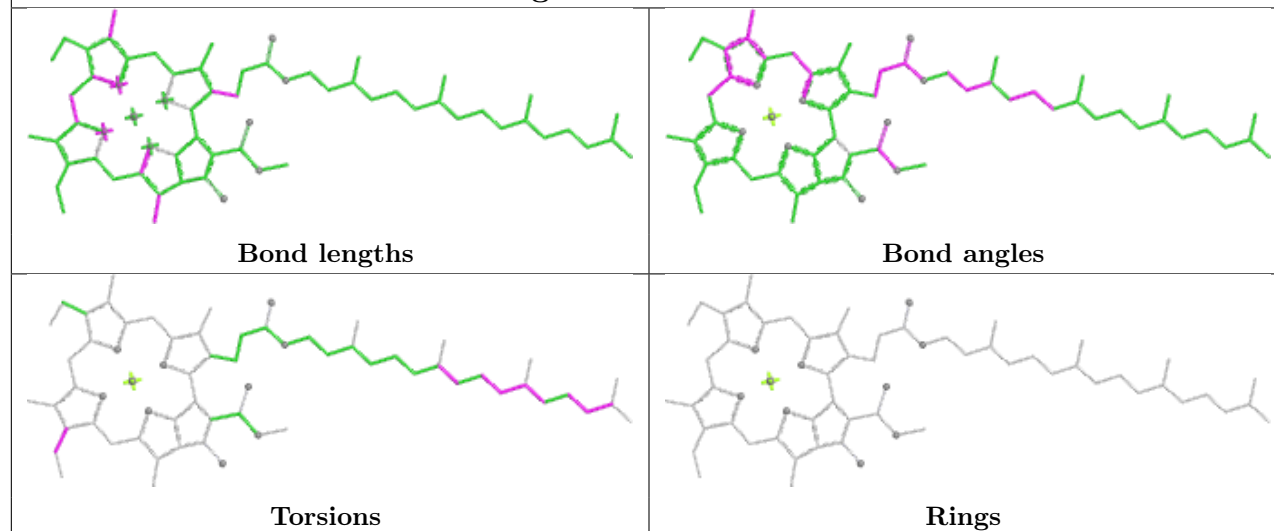
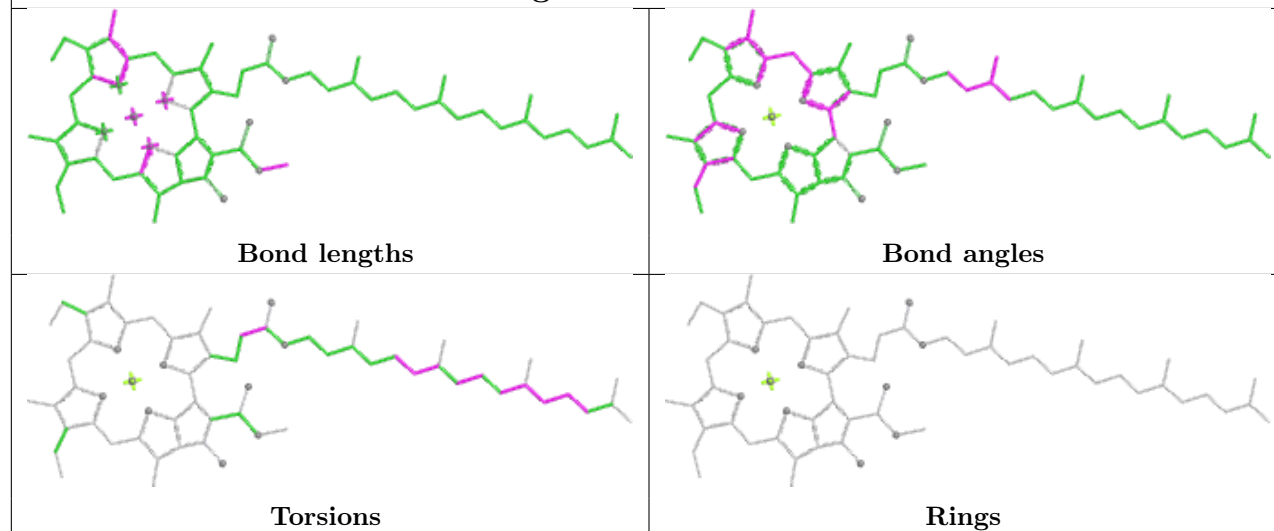
Ligand BCR d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO D 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

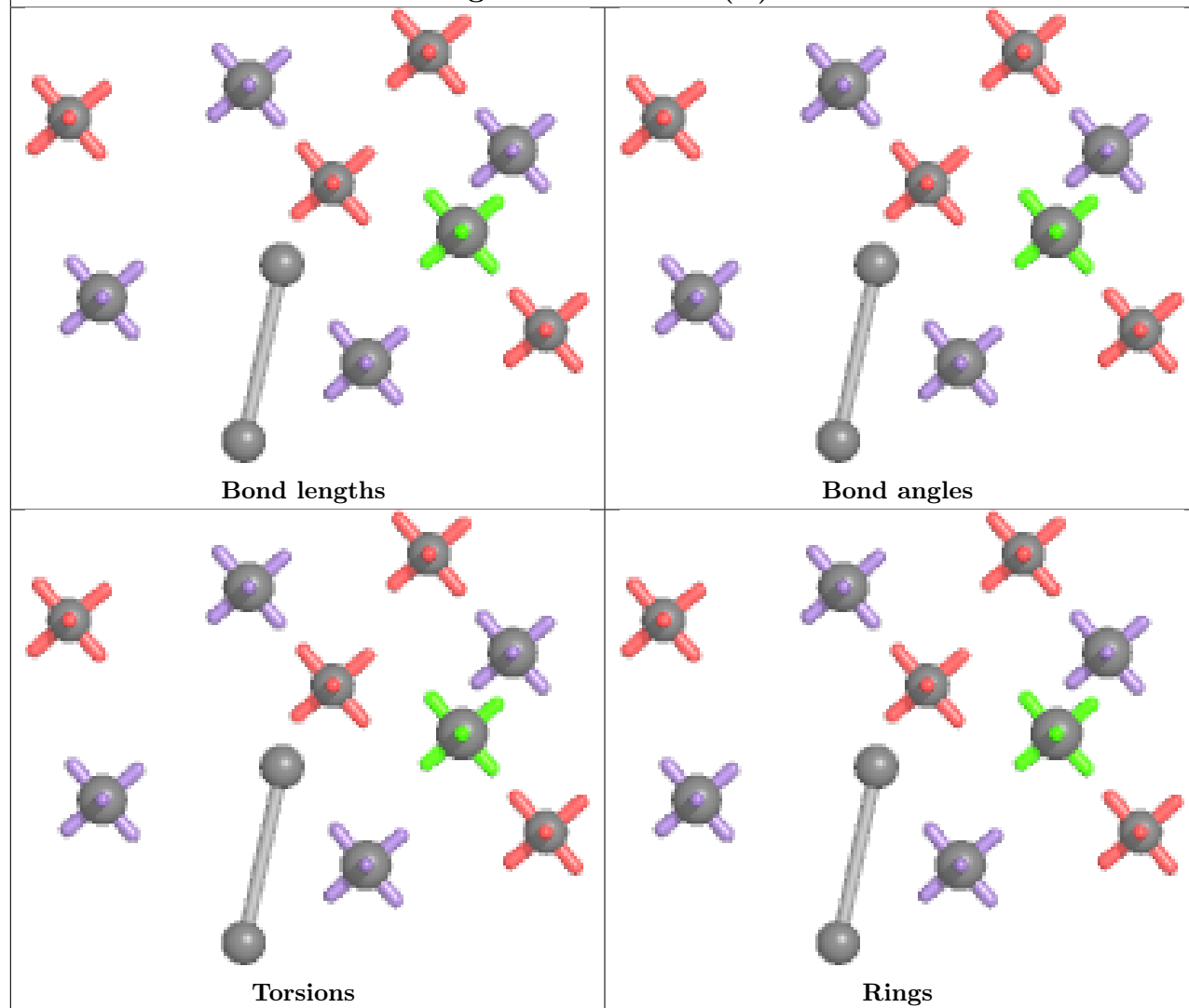
Ligand STE d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings



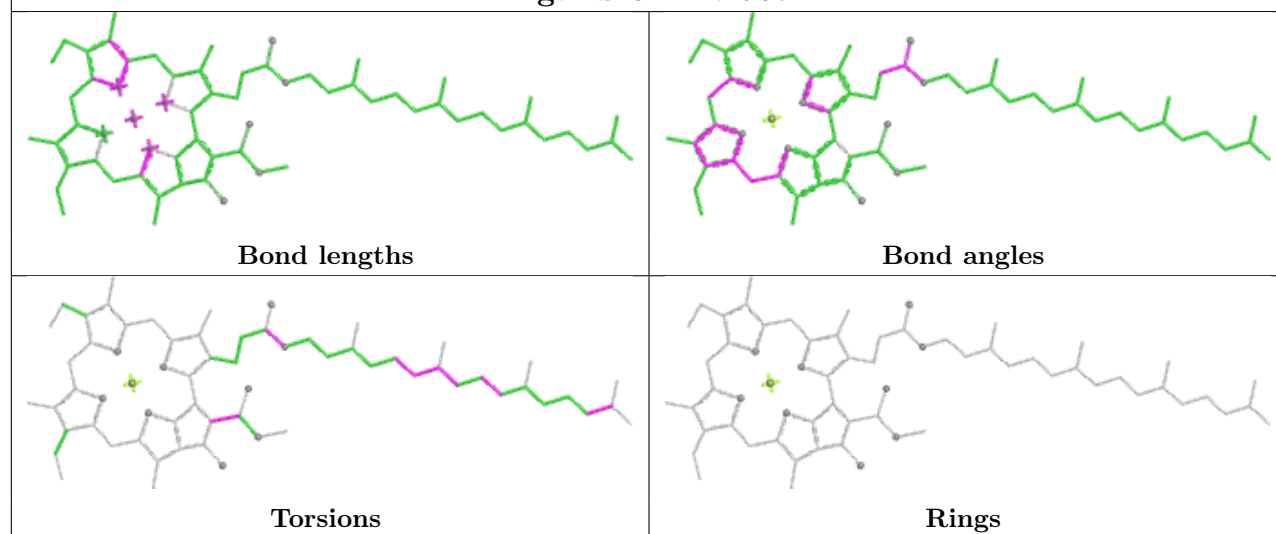


Ligand CLA A 605**Ligand CLA B 612**

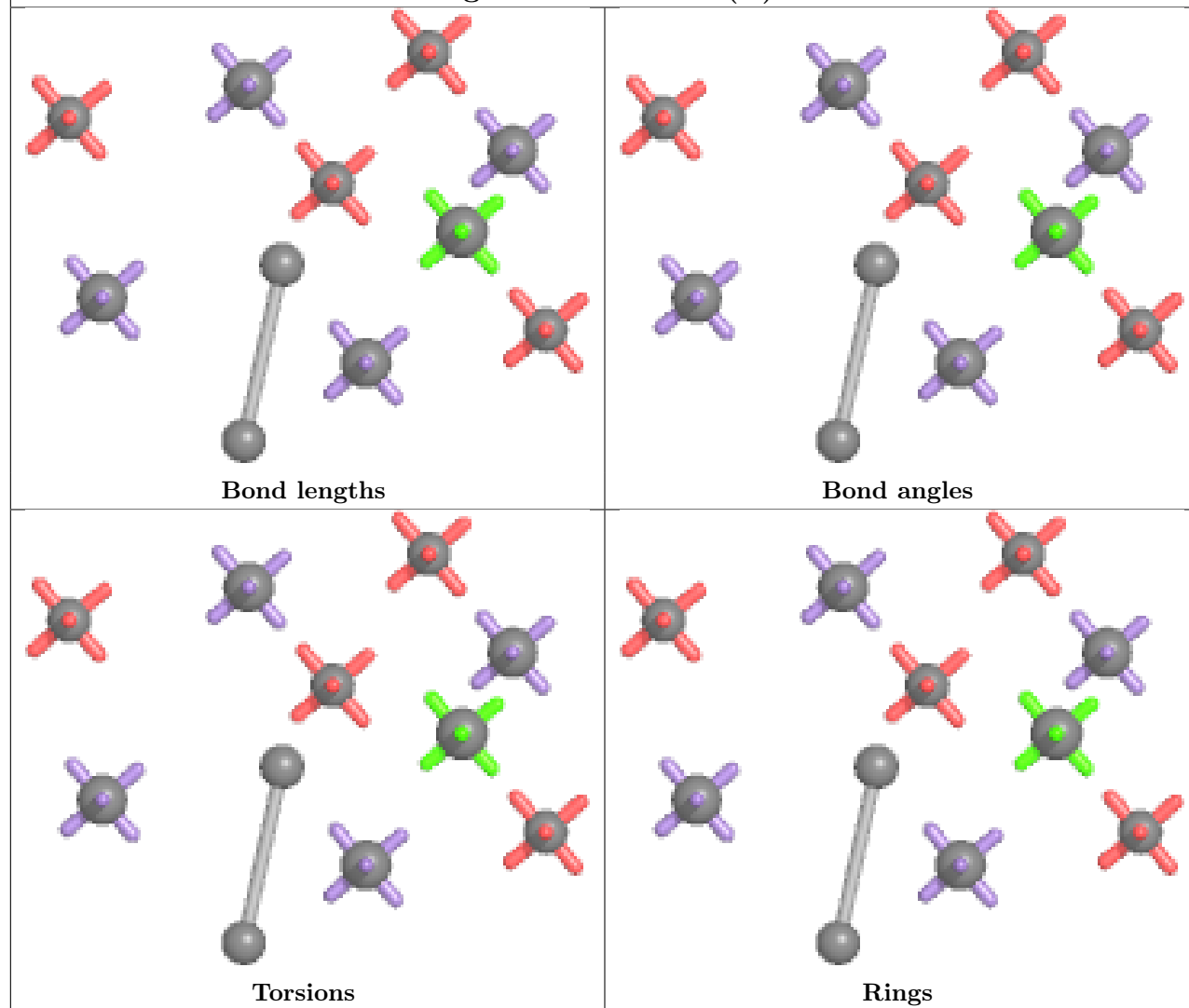
Ligand OEY a 601 (B)



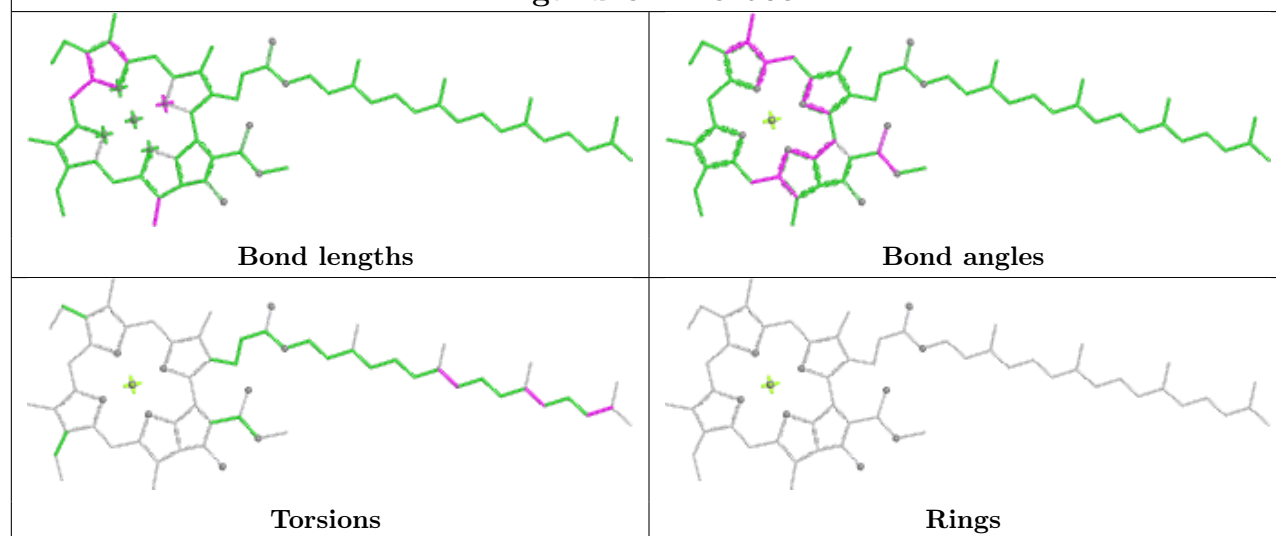
Ligand CLA c 507



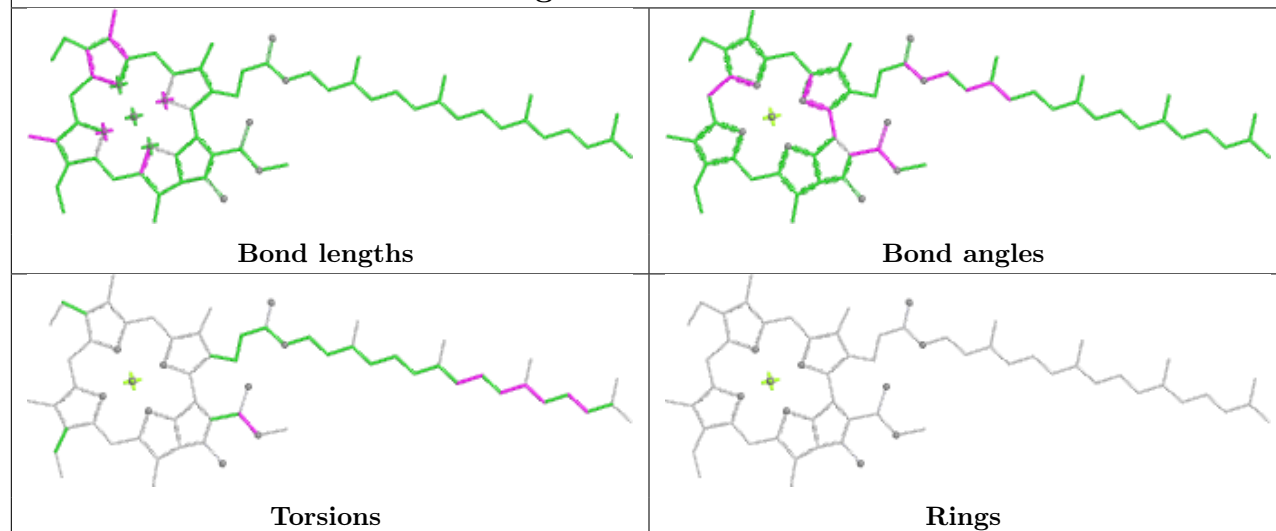
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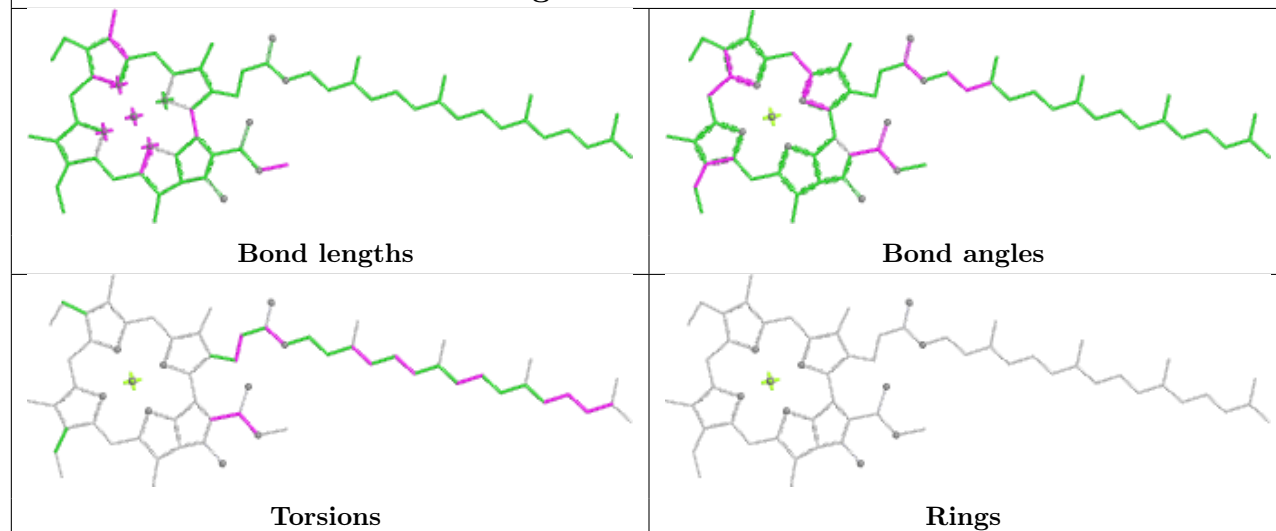
Ligand CLA C 508



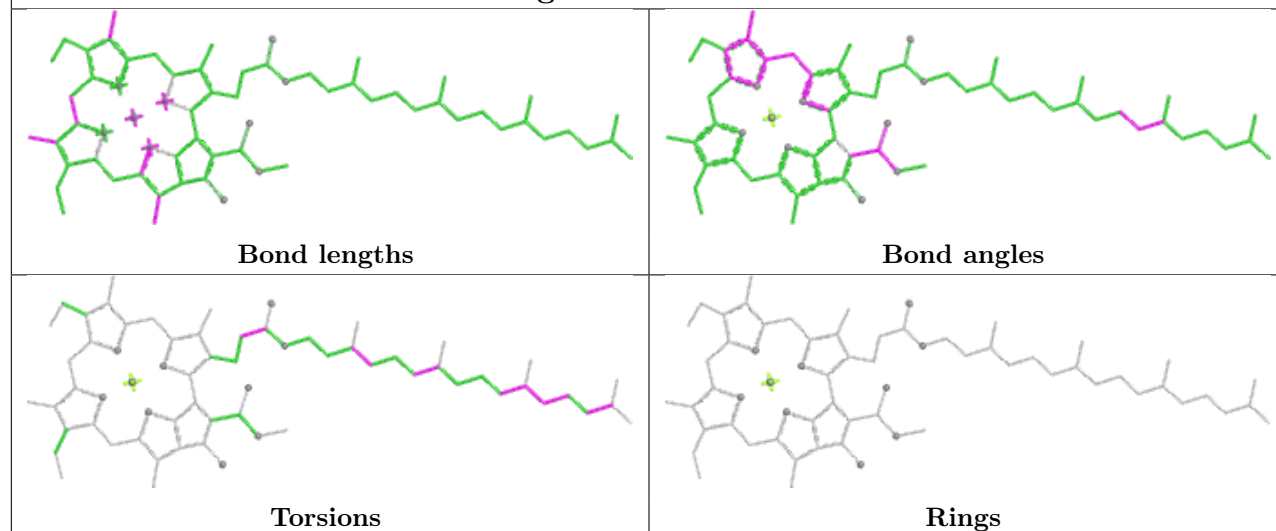
Ligand CLA b 609

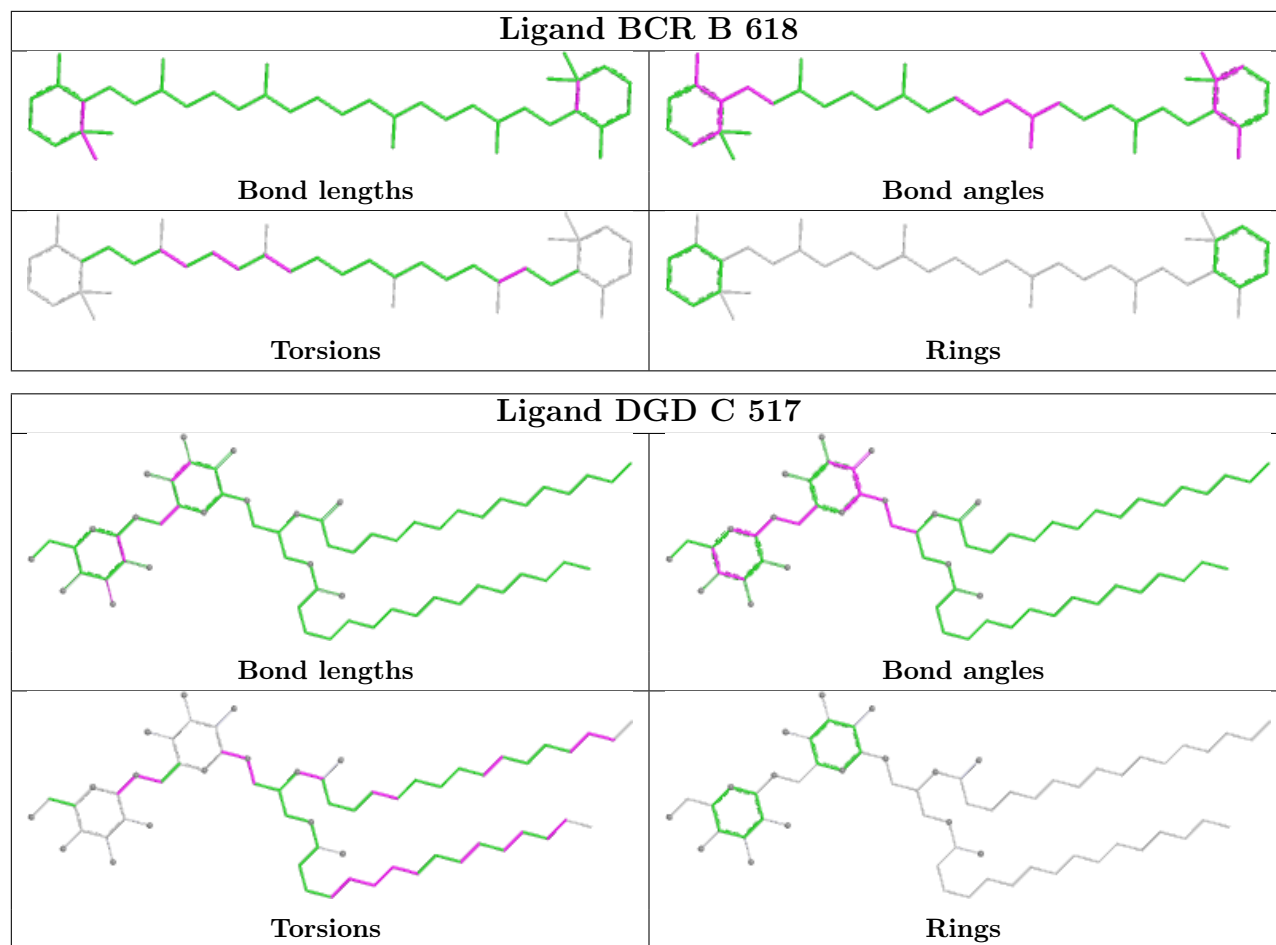


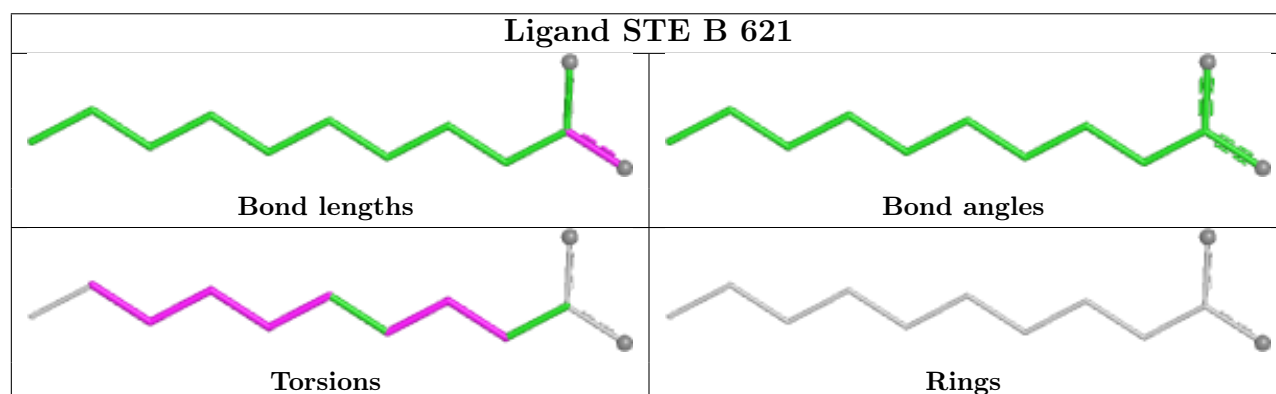
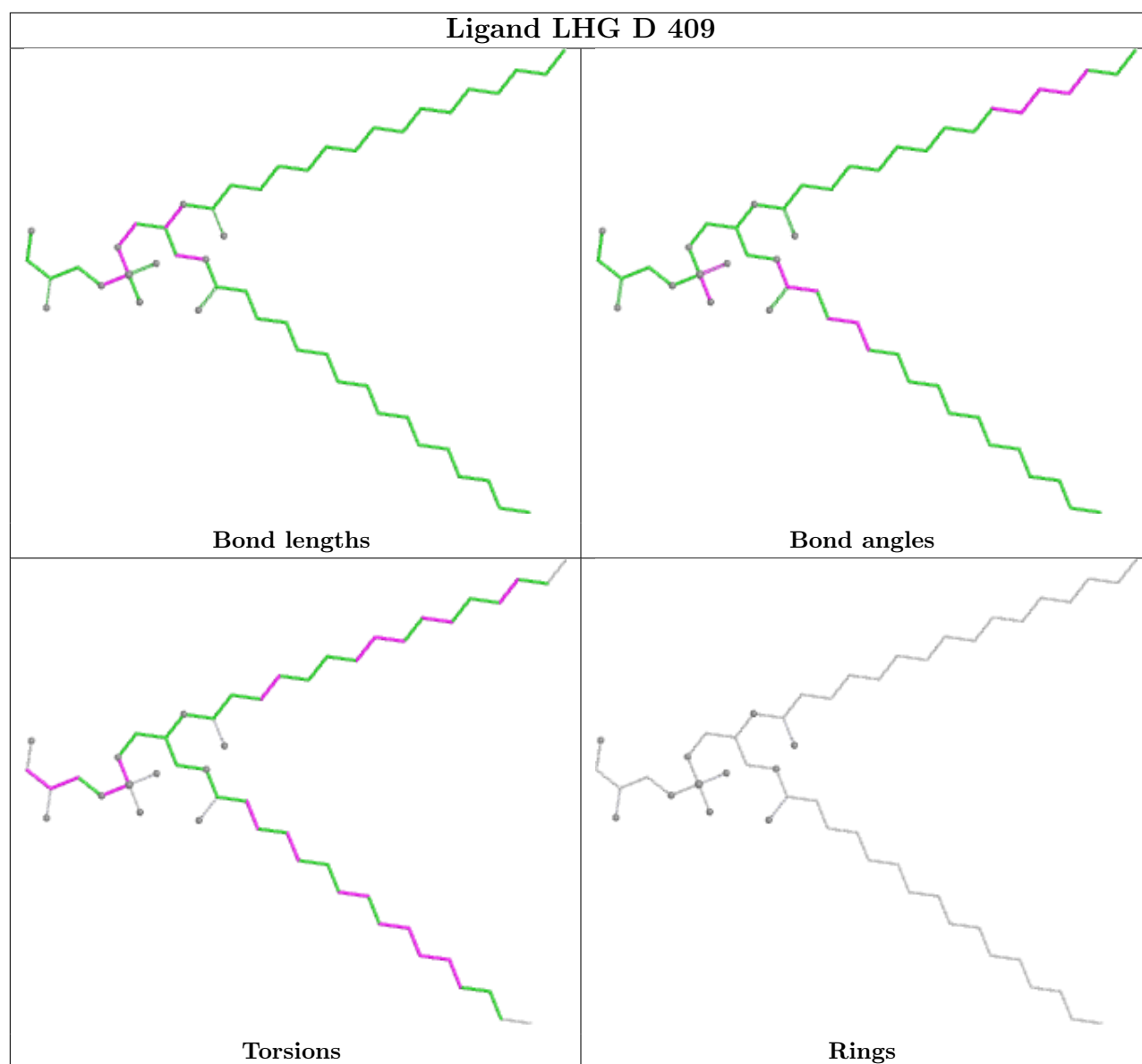
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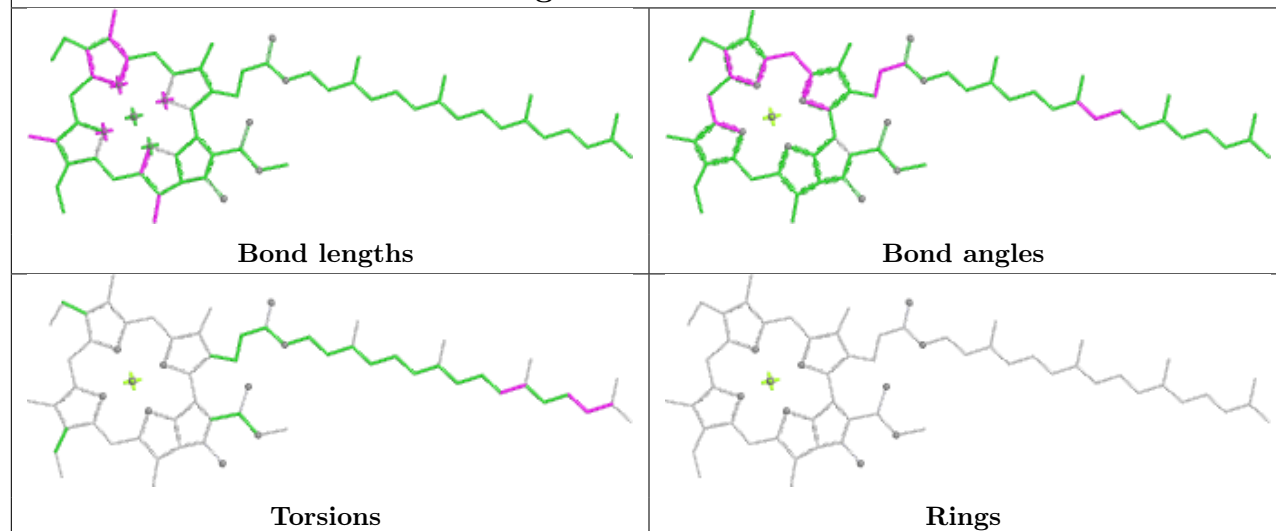
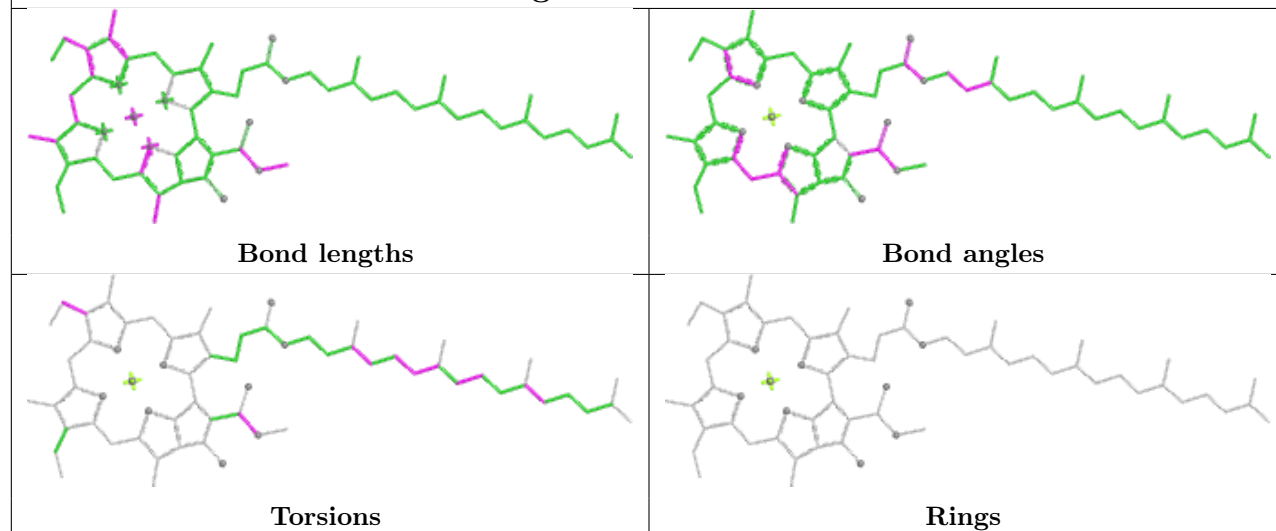


Ligand CLA c 510

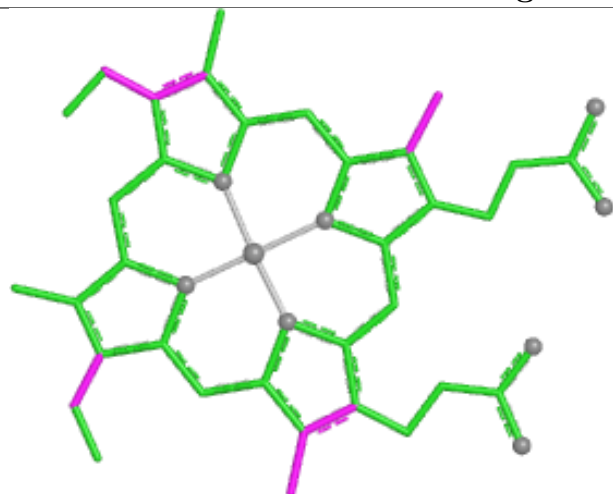




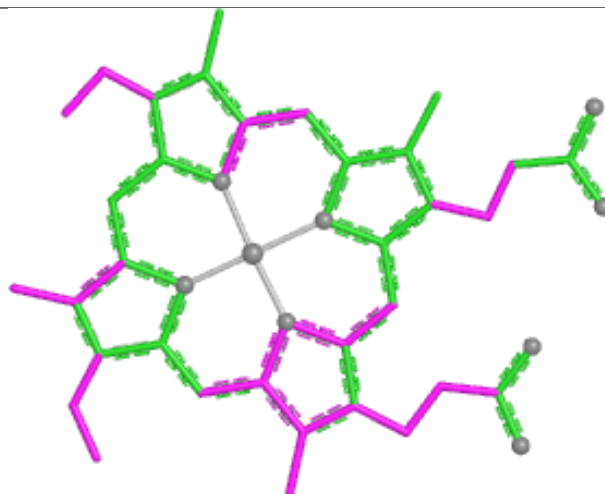


Ligand CLA b 615**Ligand CLA B 602**

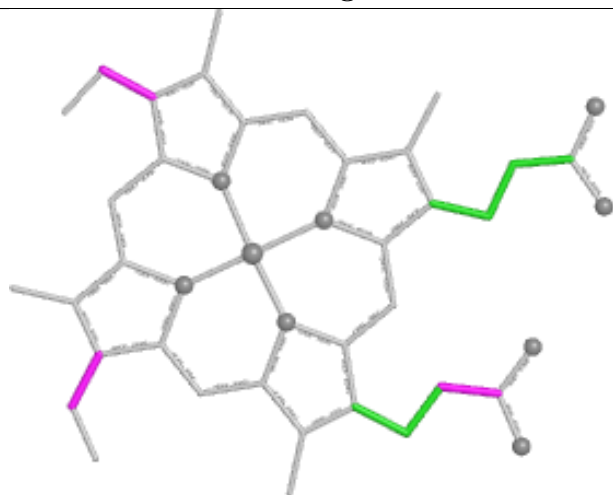
Ligand HEC v 201



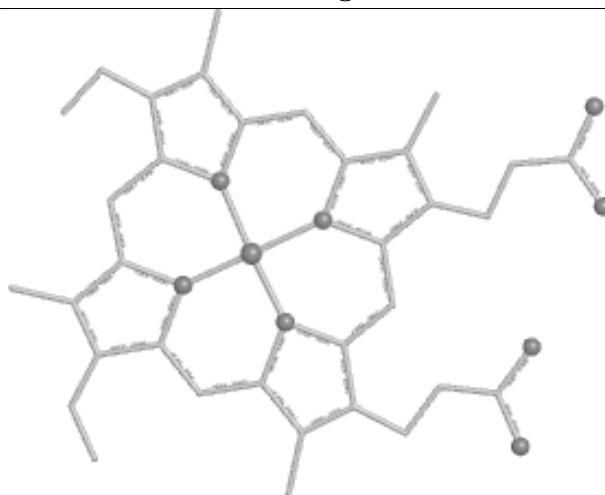
Bond lengths



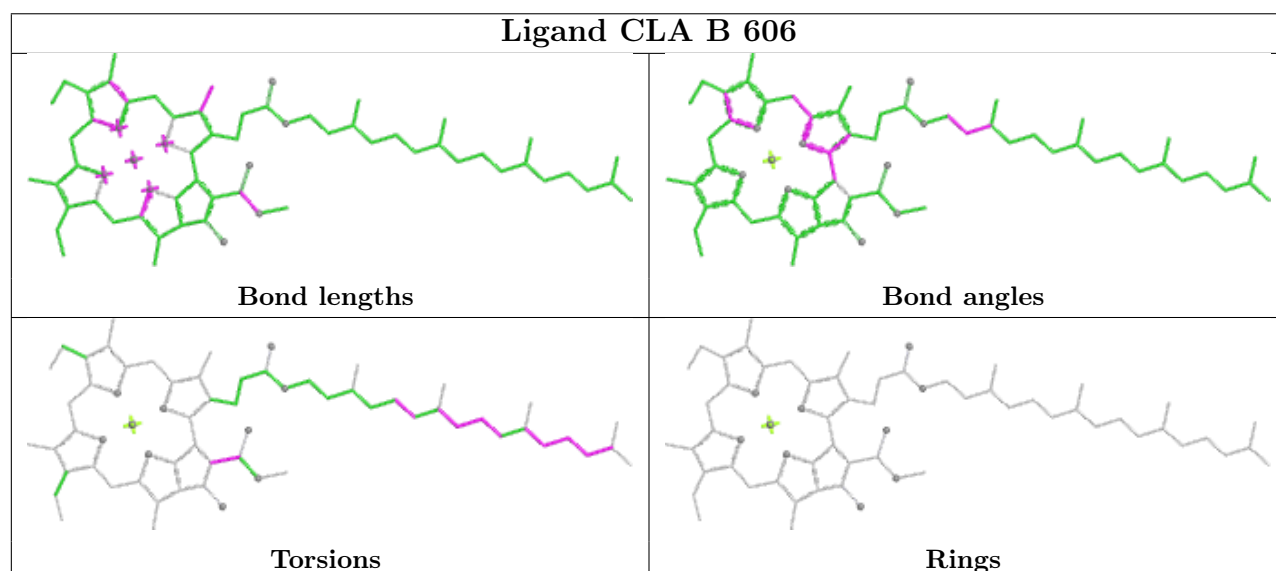
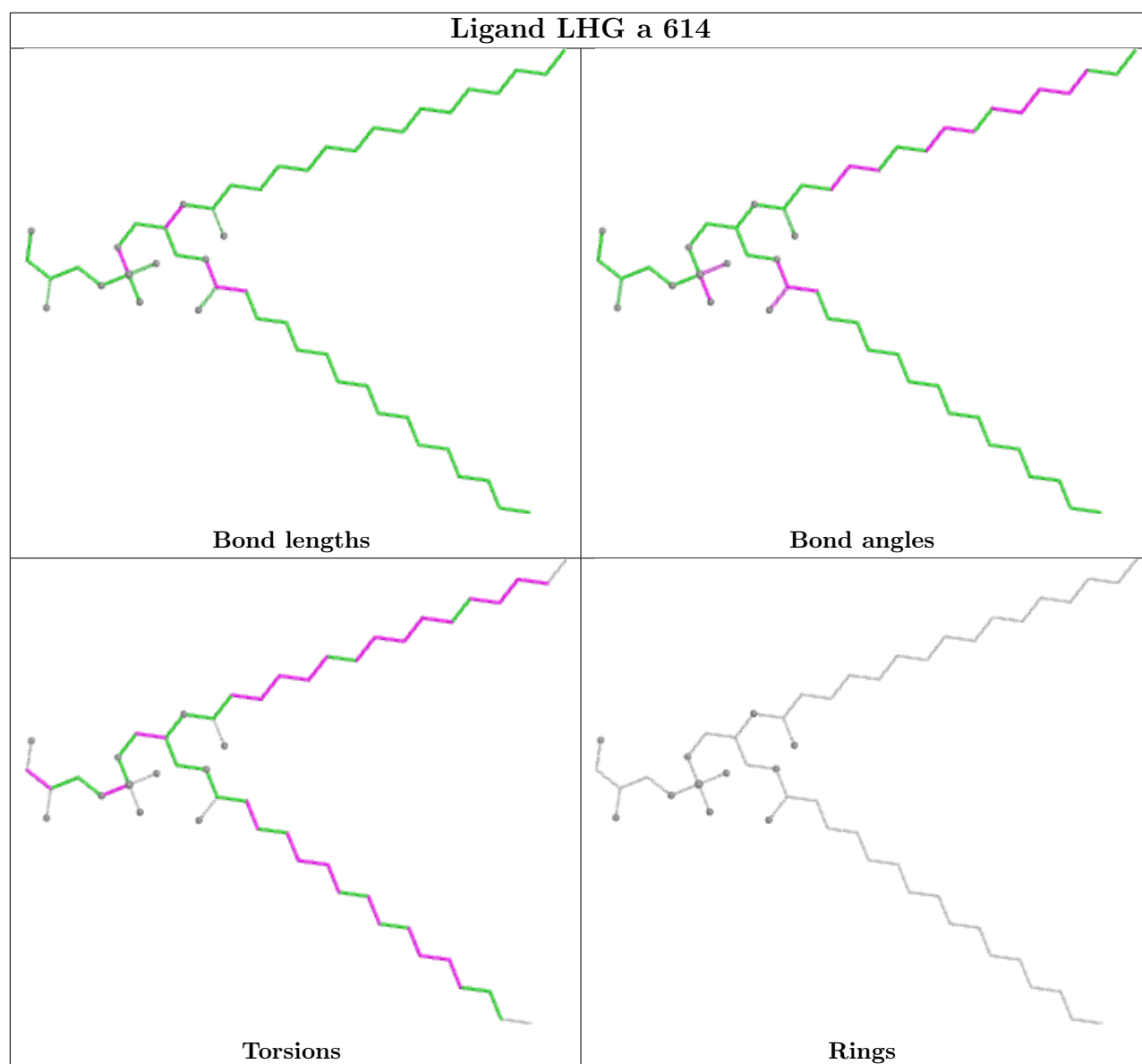
Bond angles

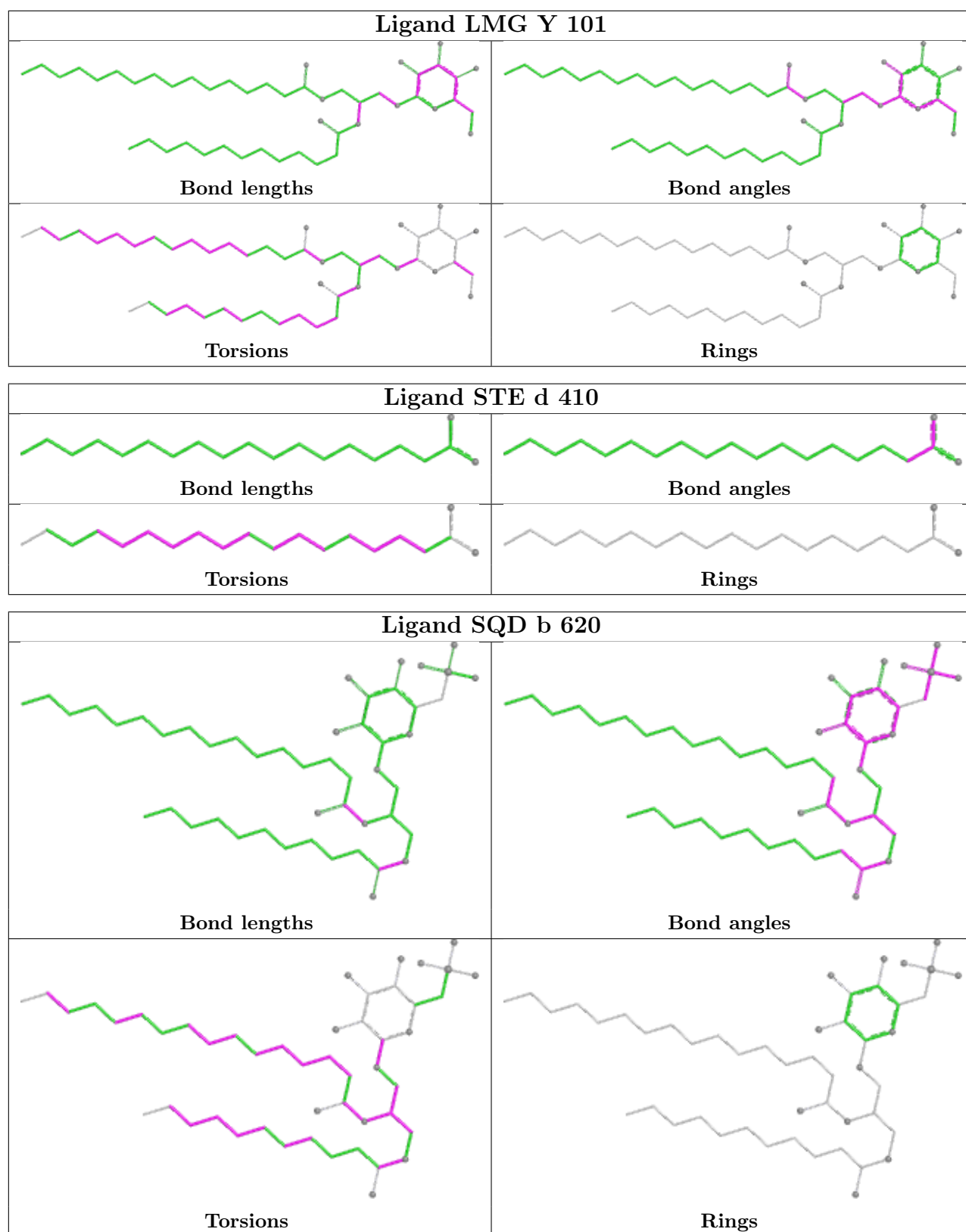


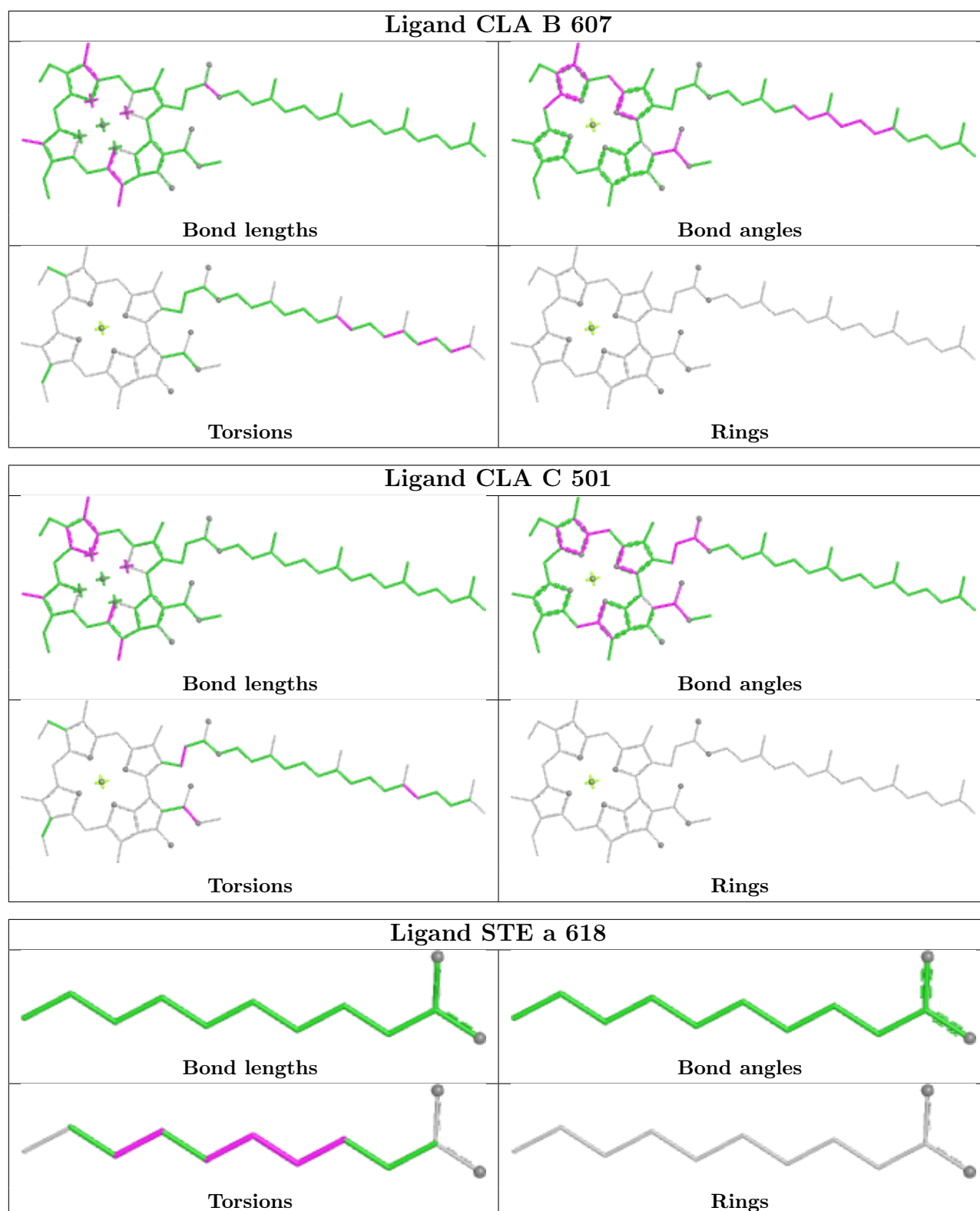
Torsions

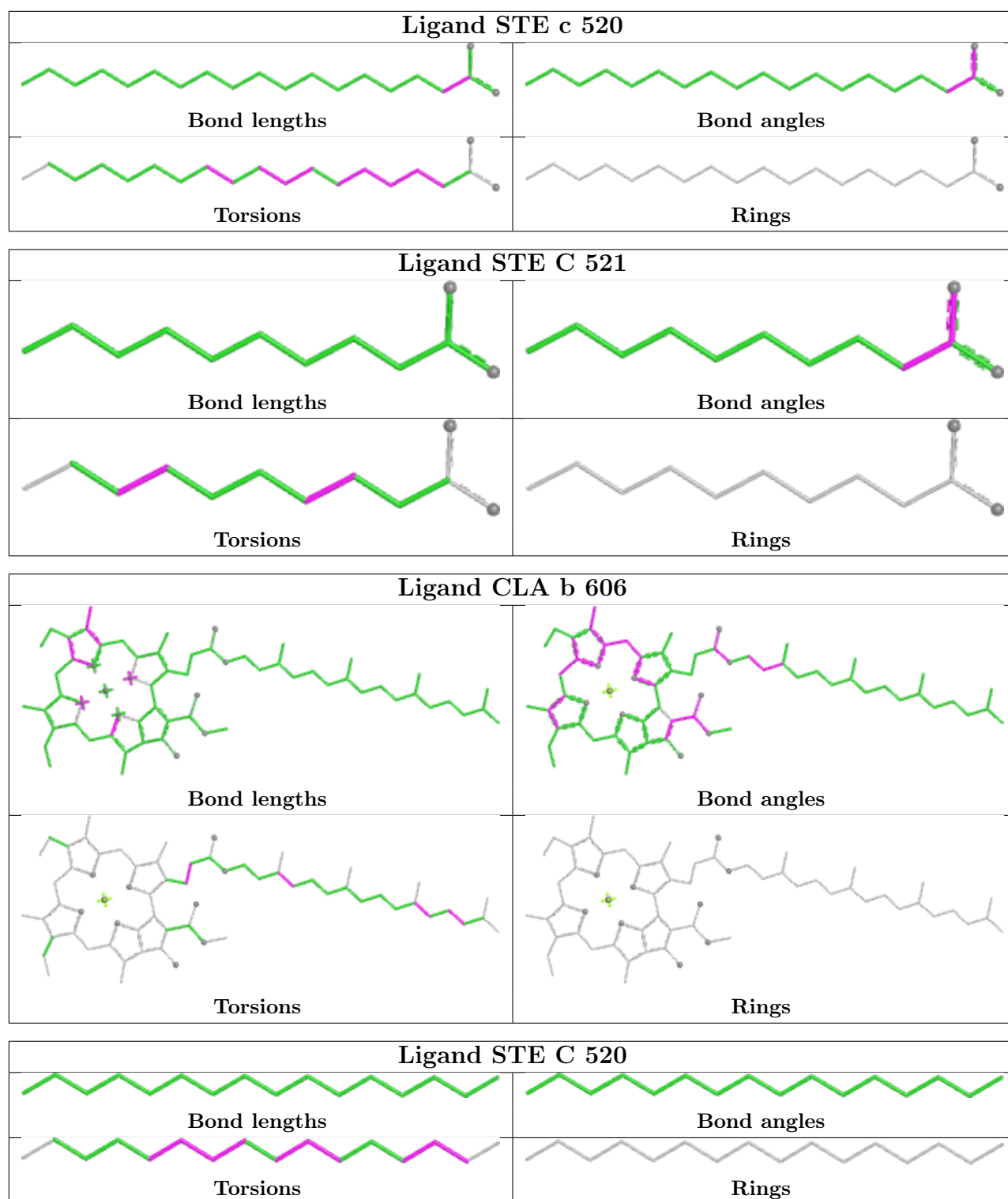


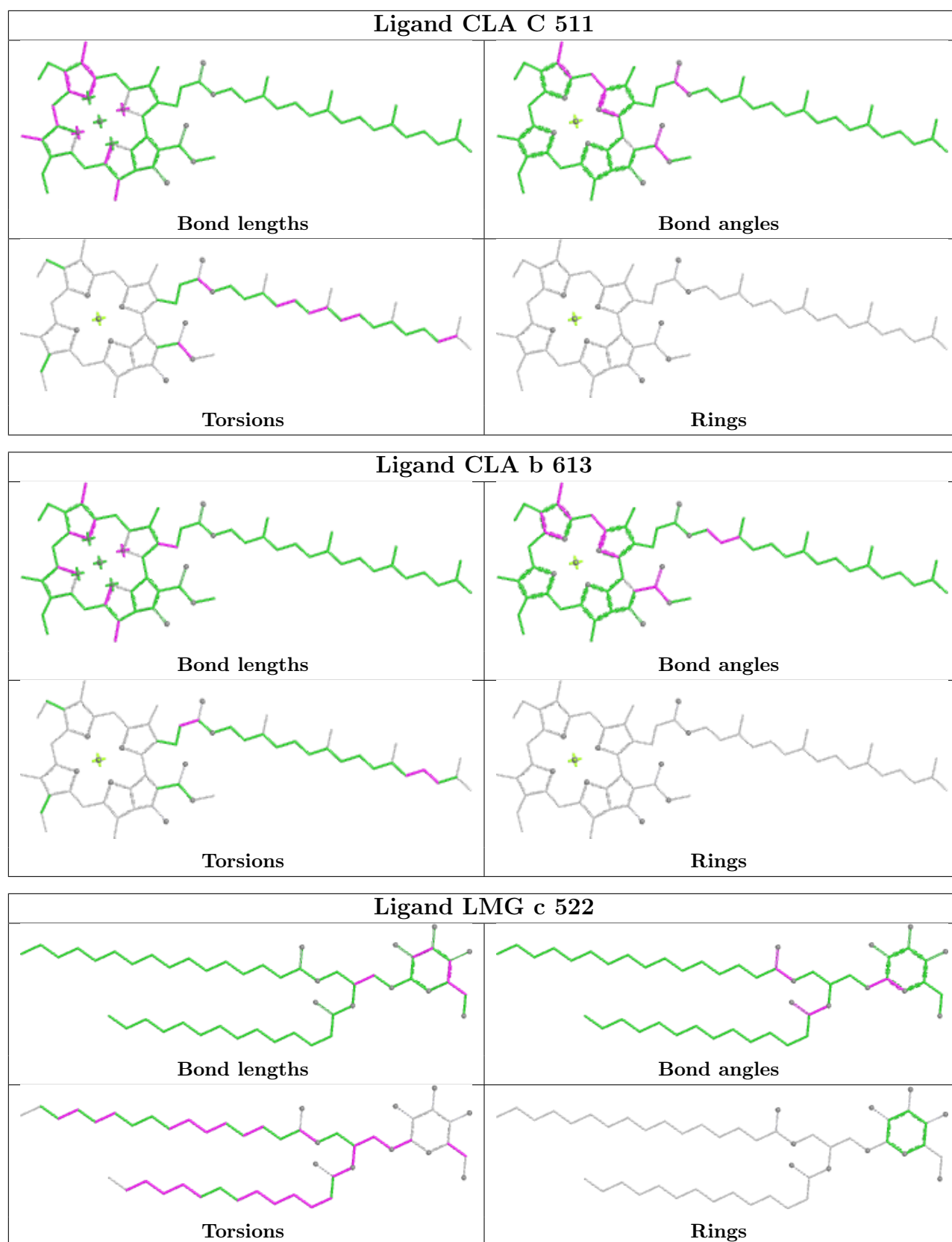
Rings

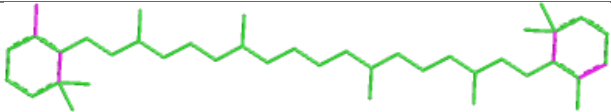
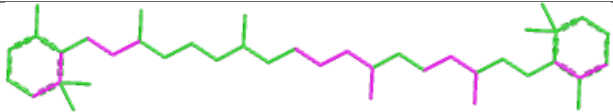
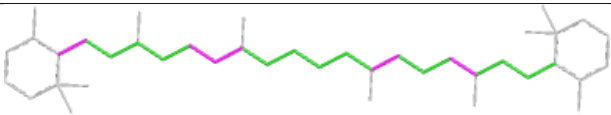
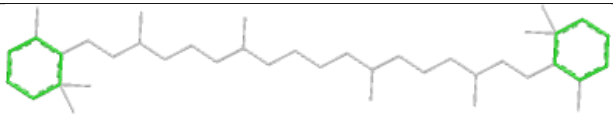




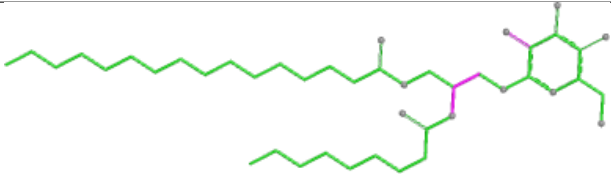
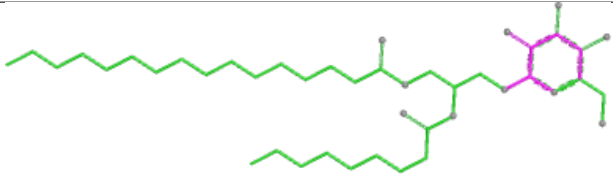
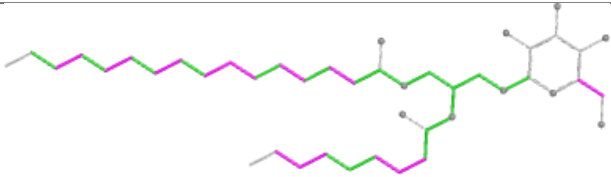
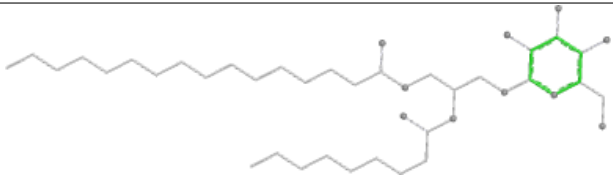


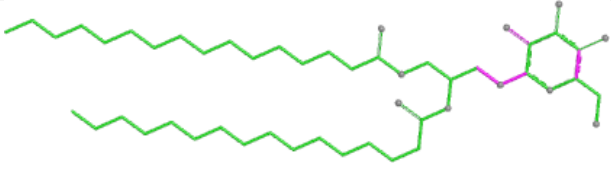
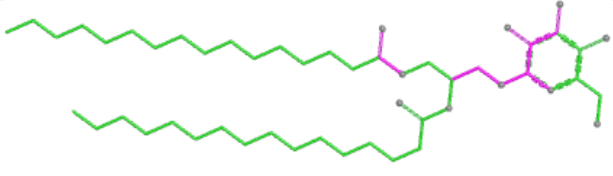
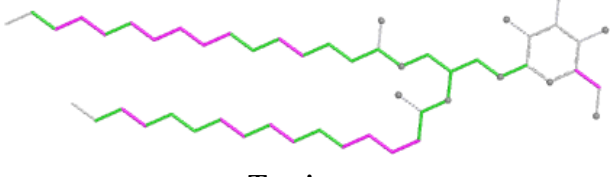
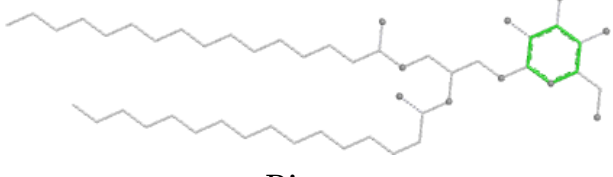


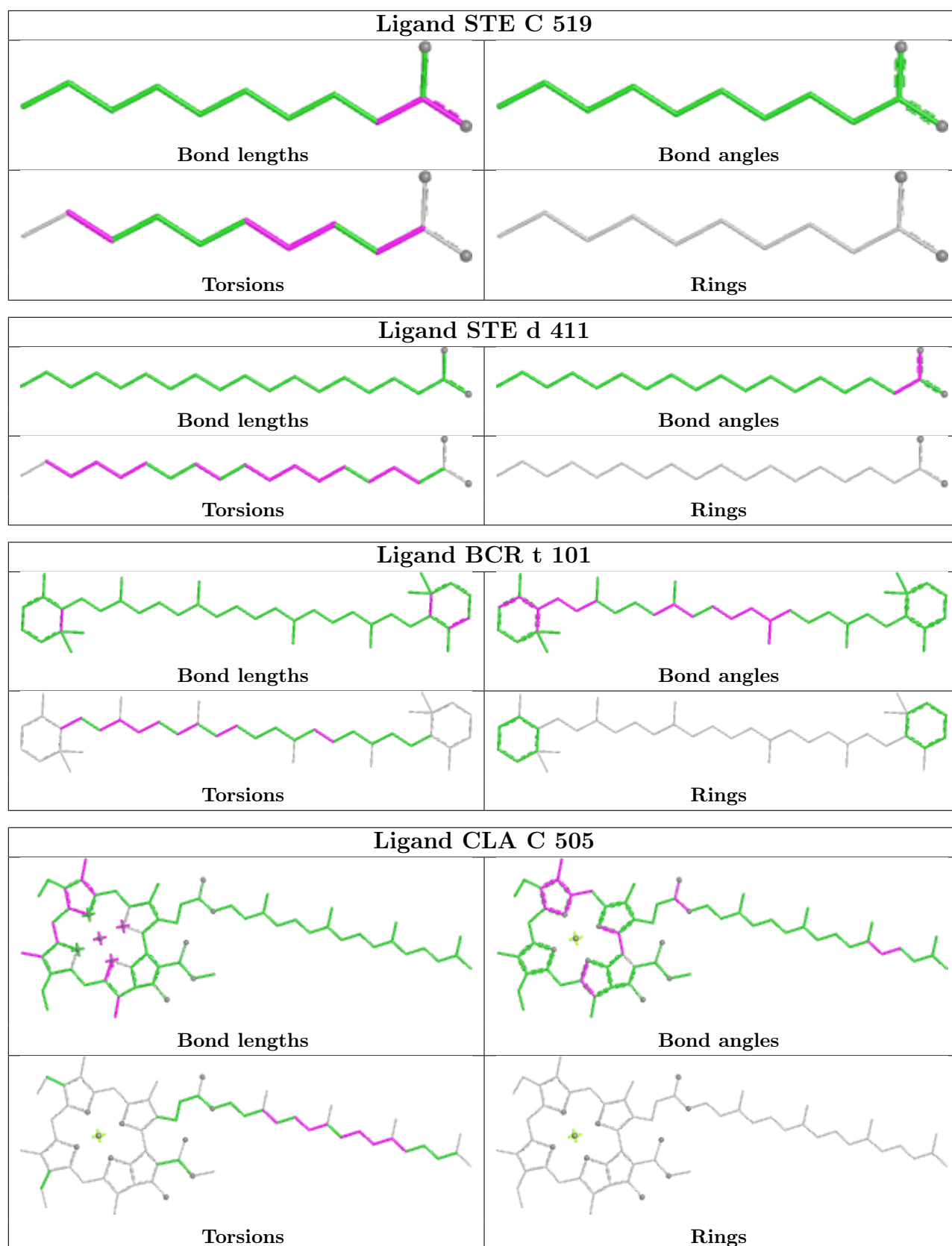


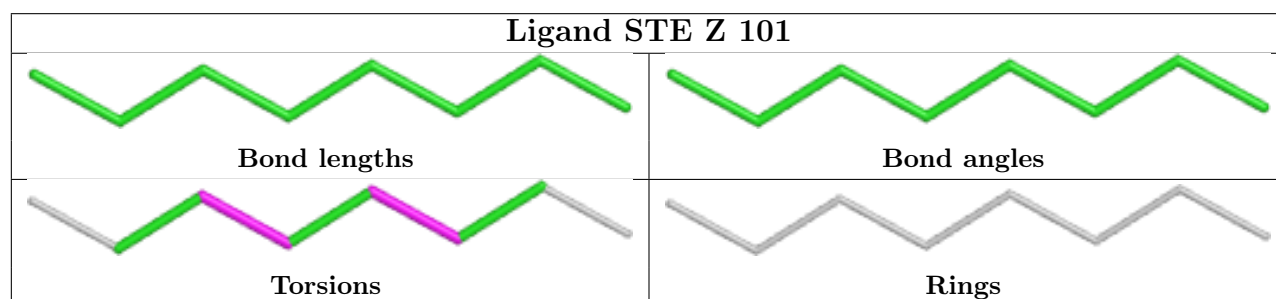
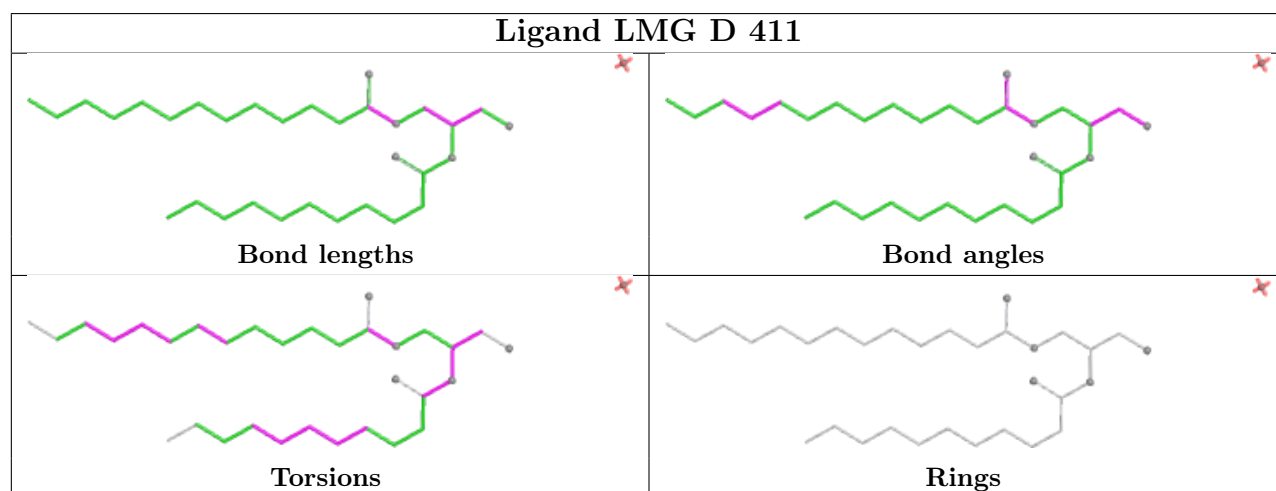
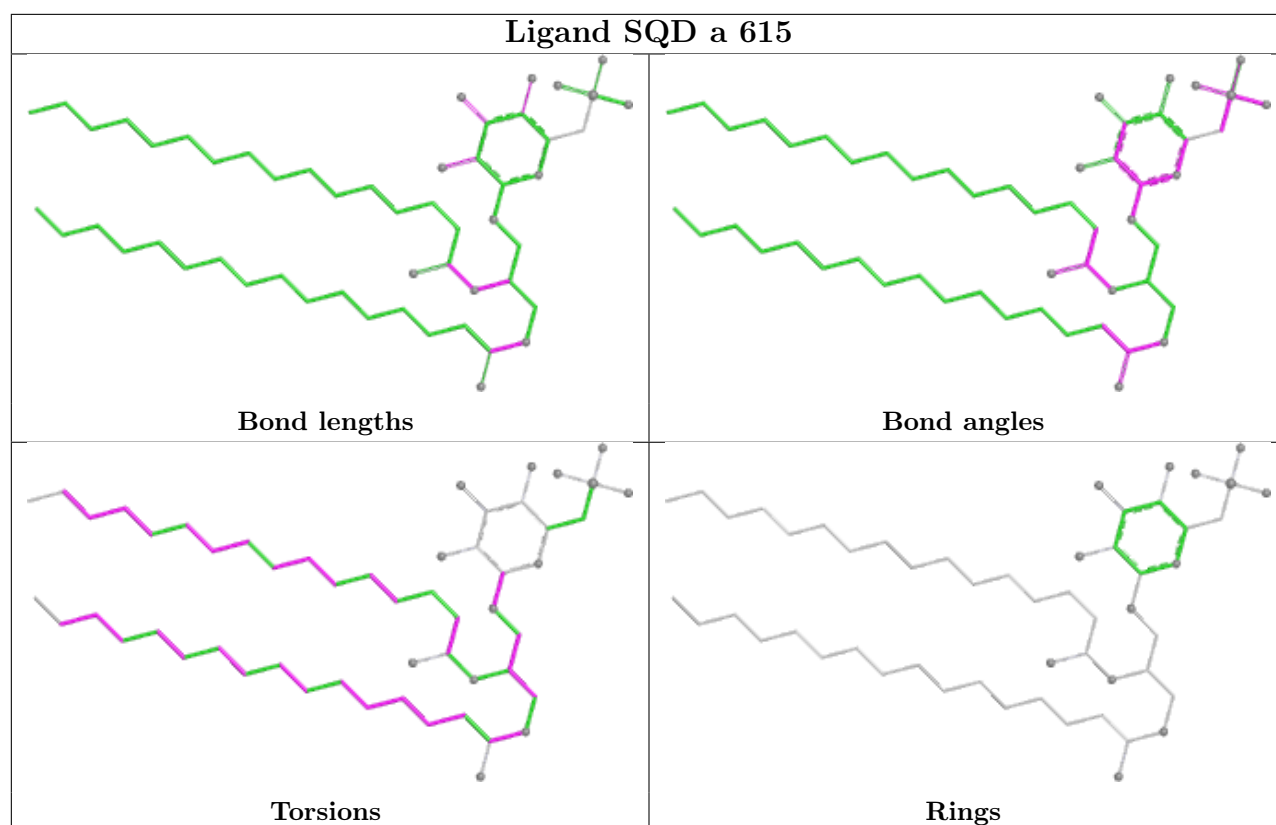
Ligand BCR K 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

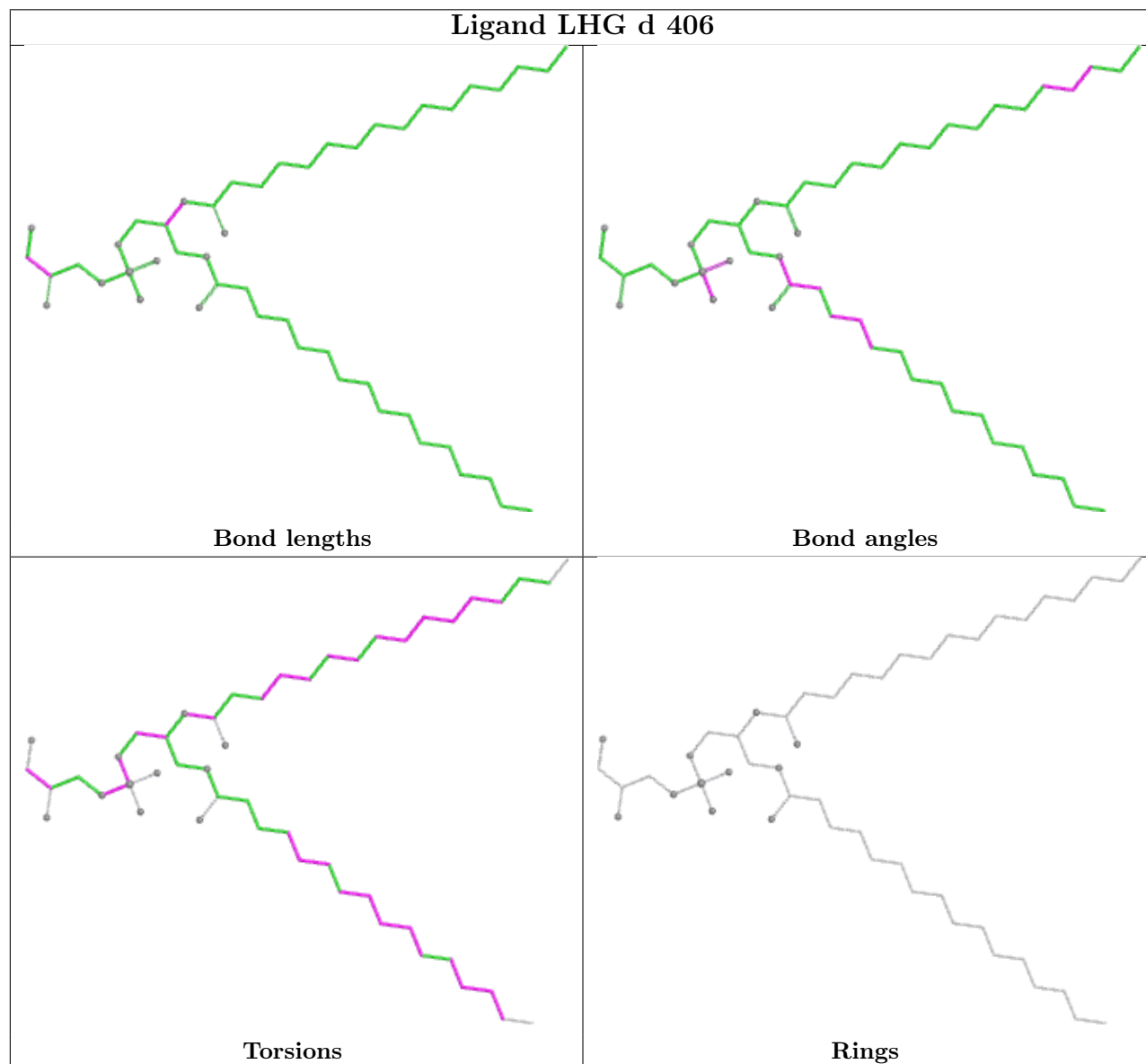
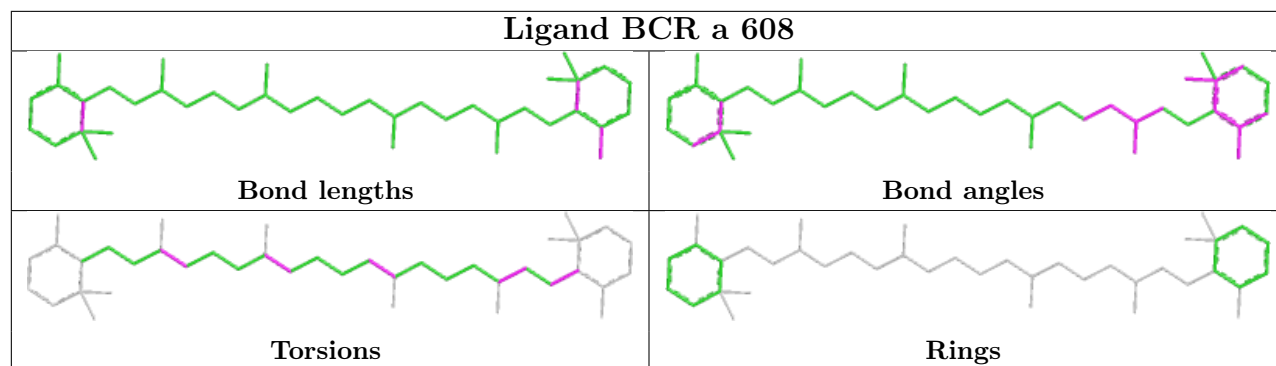
Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

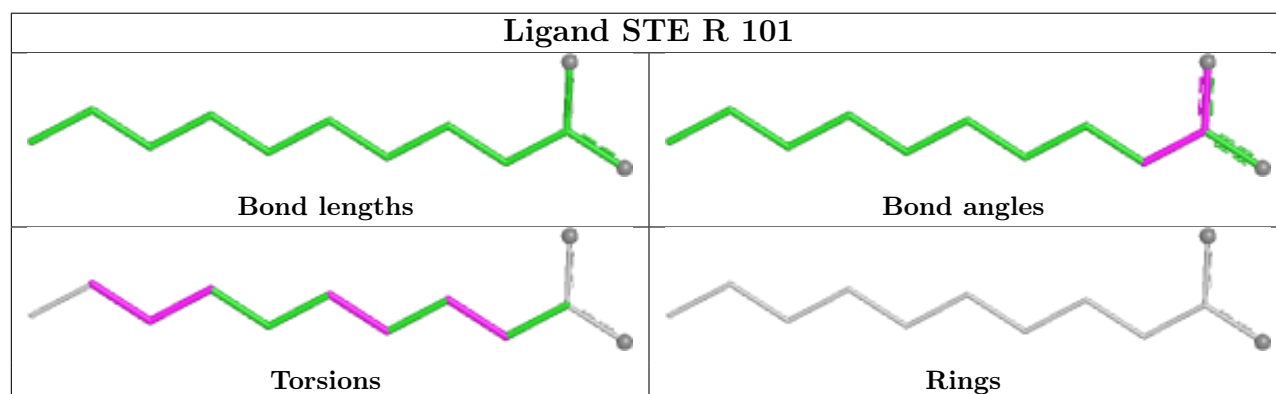
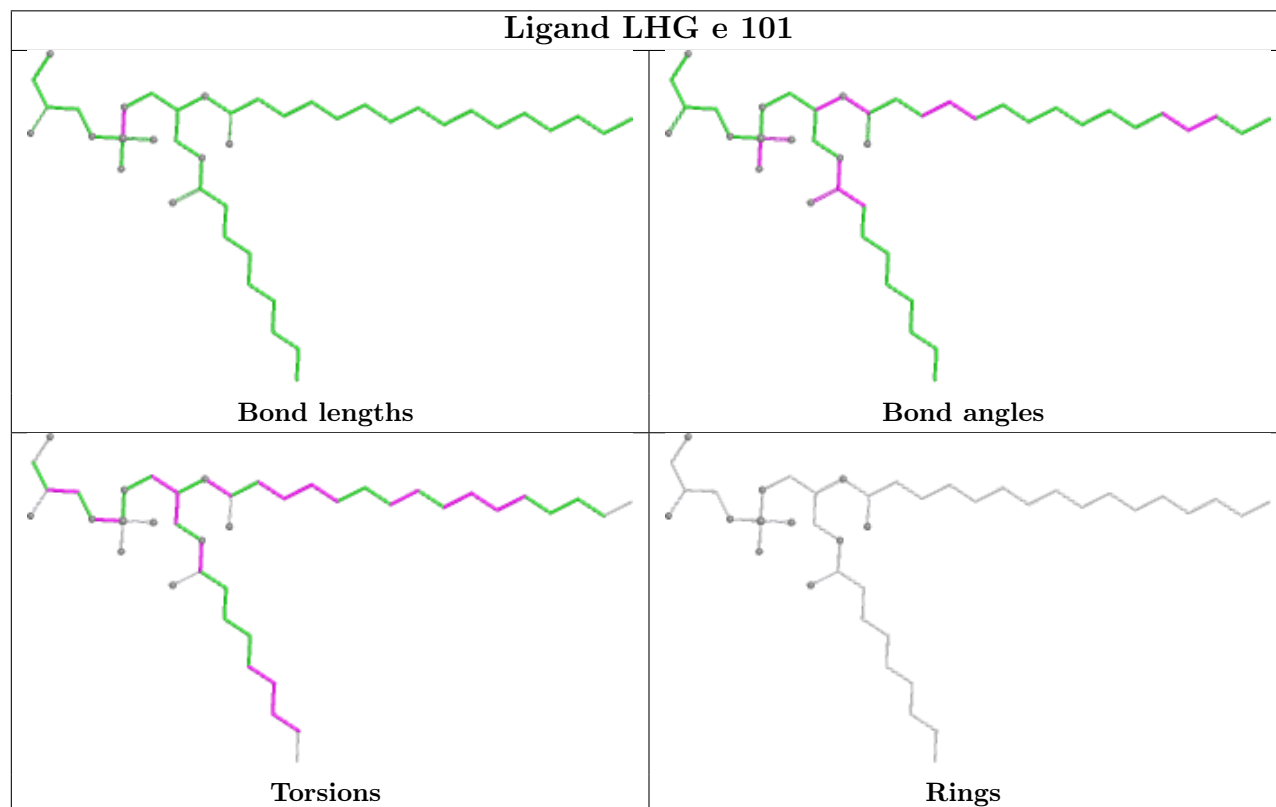
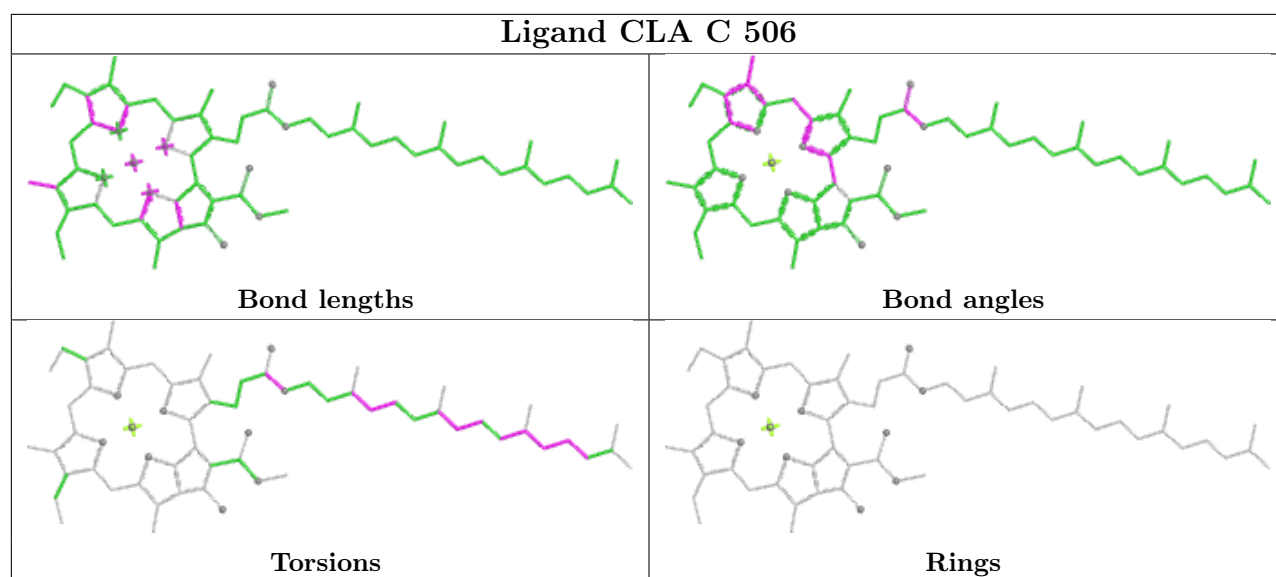
Ligand LMG d 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

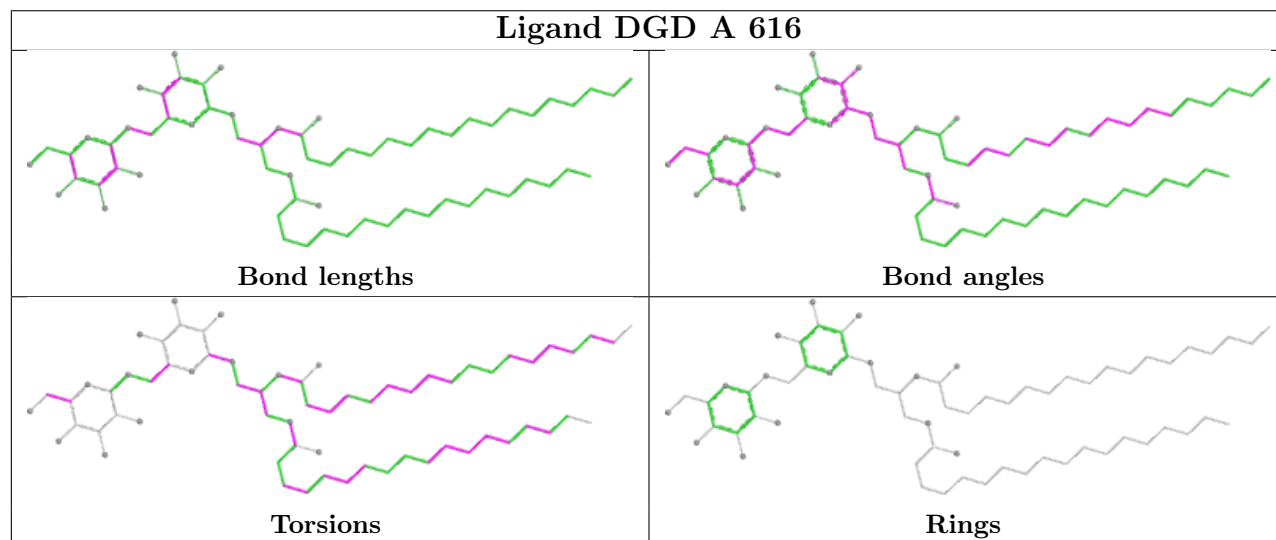
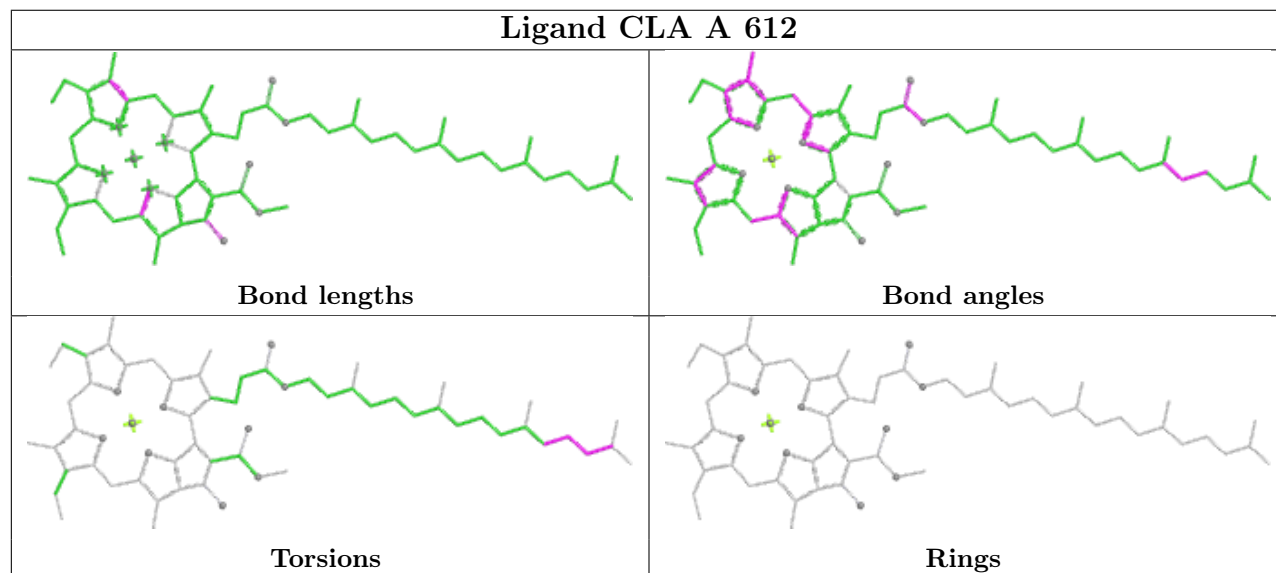
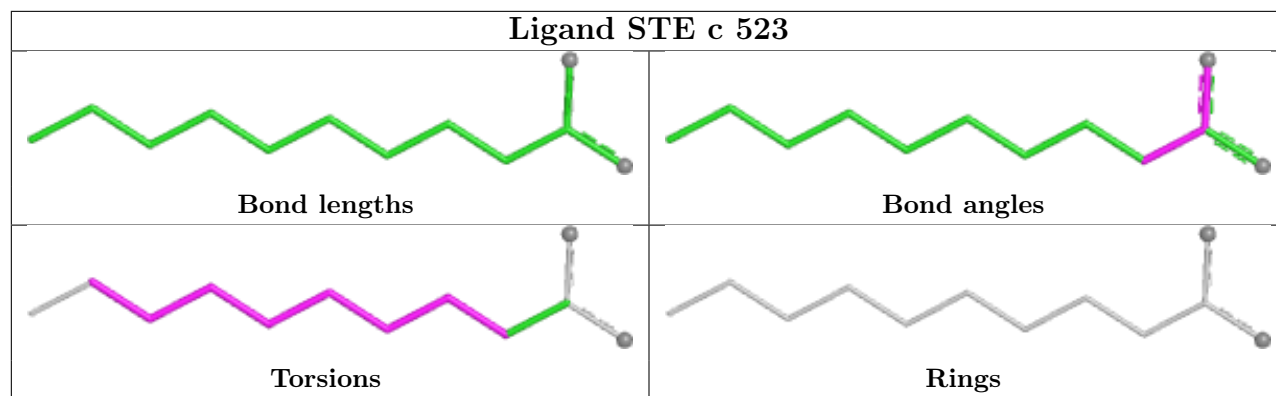
Ligand LMG D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

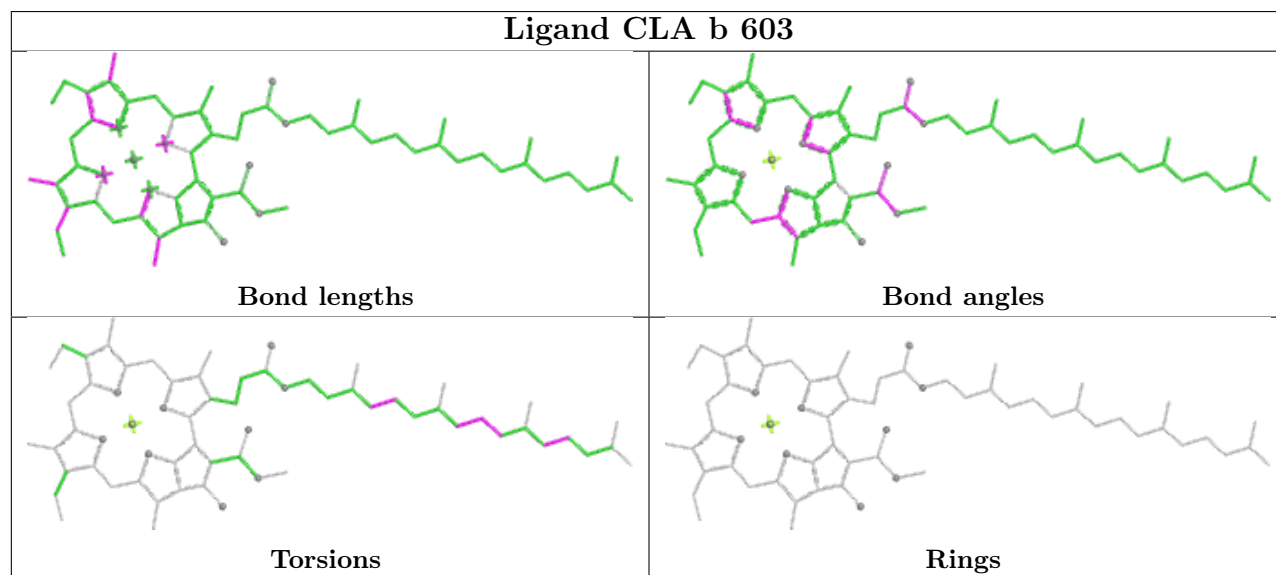
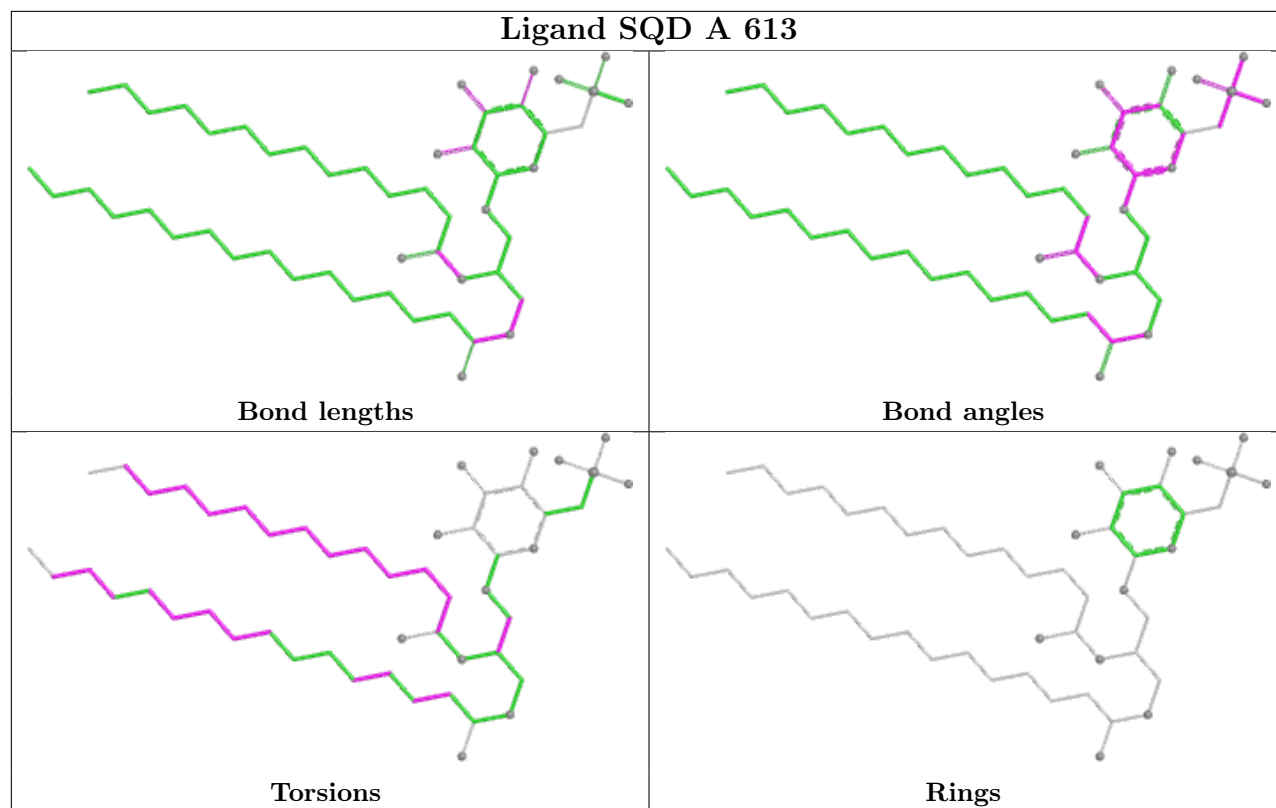


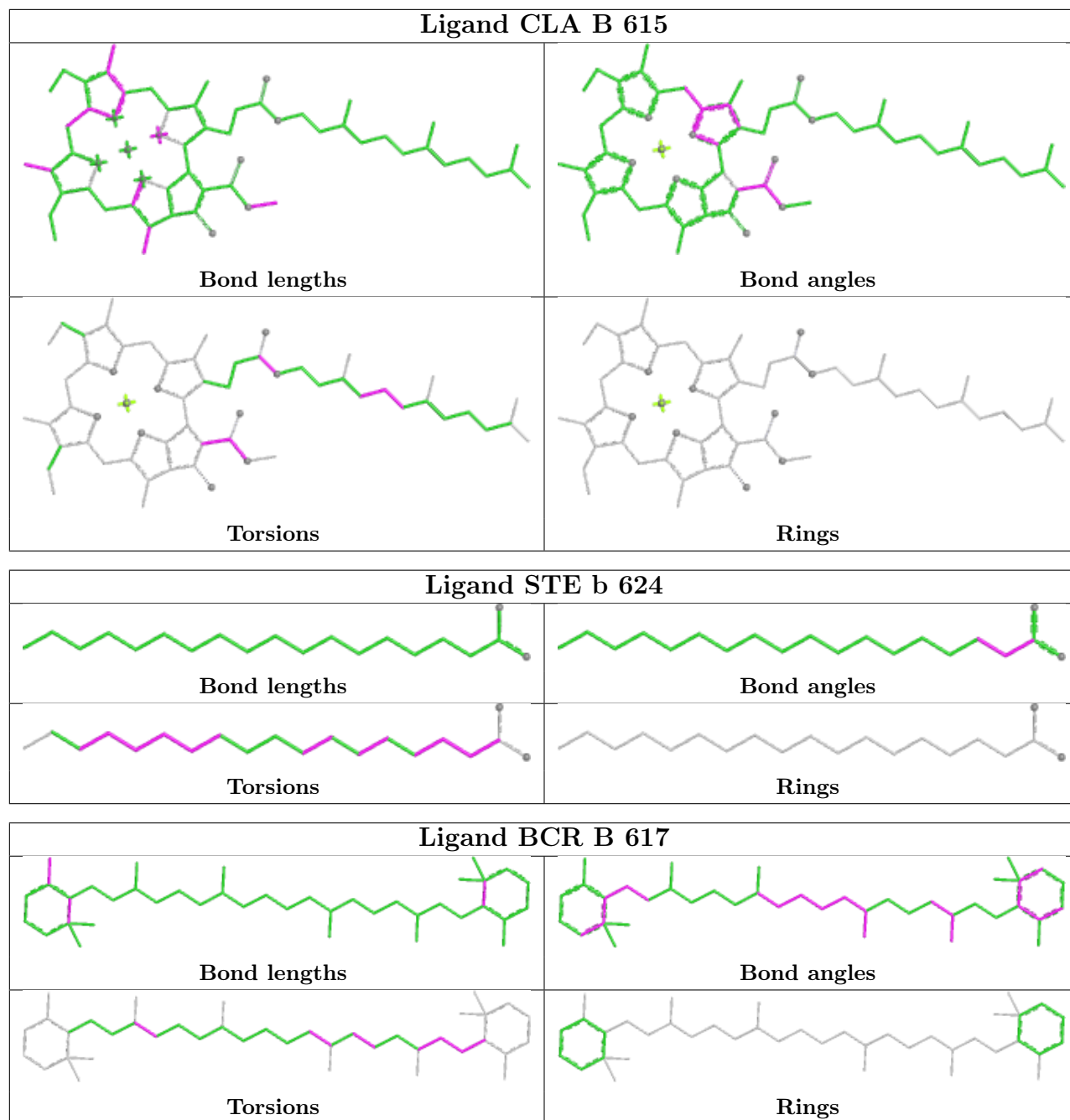




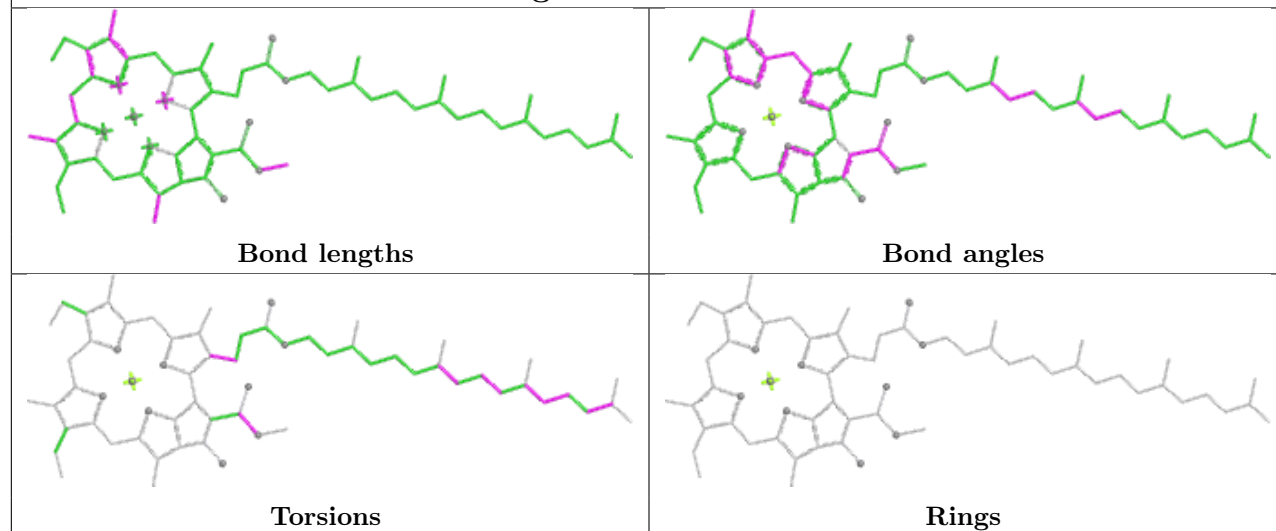




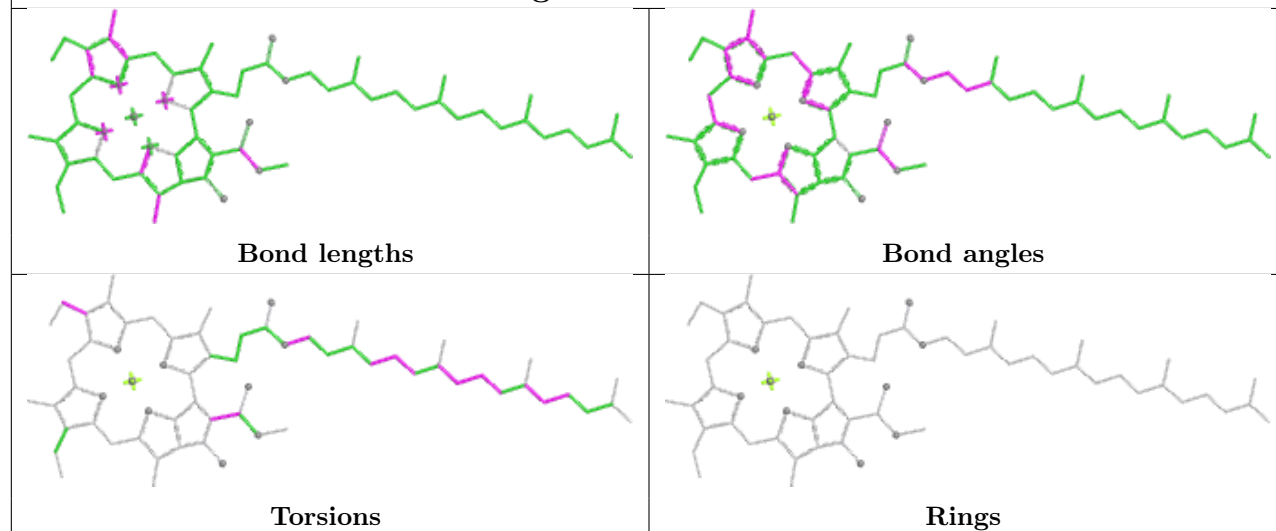




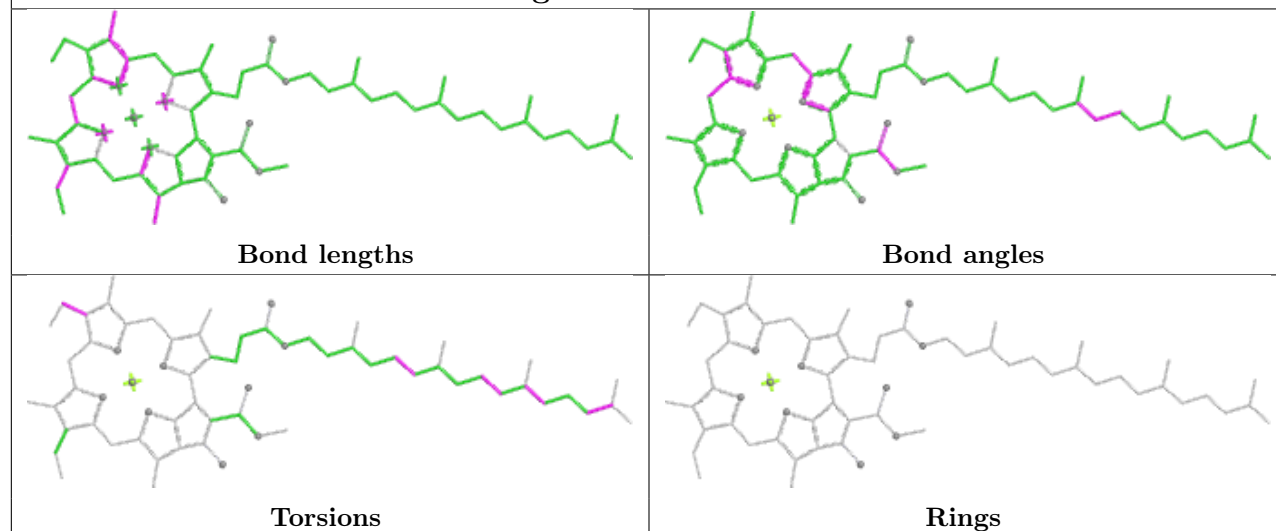
Ligand CLA B 603

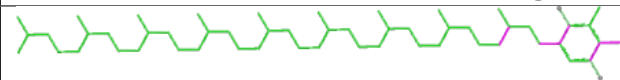
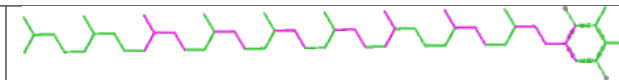
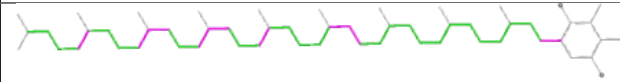
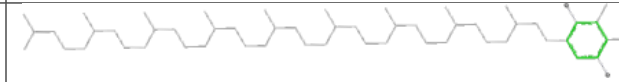
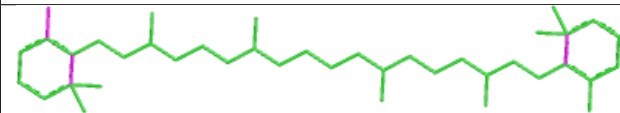
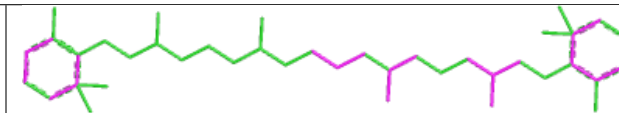
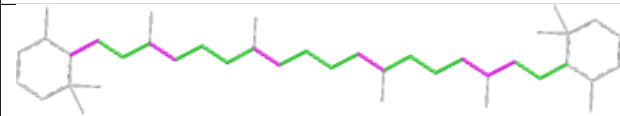
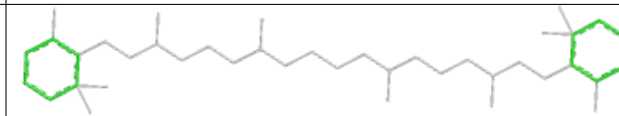
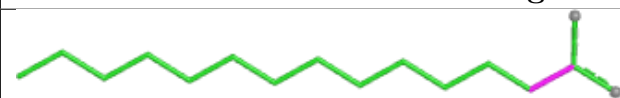
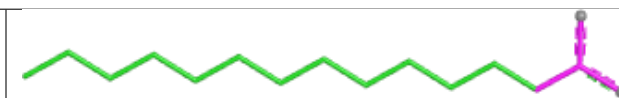
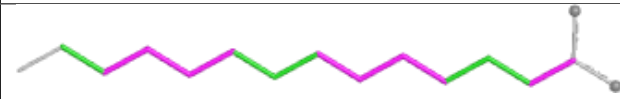
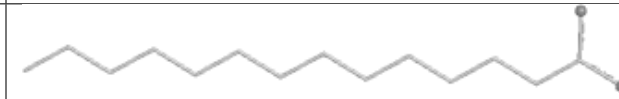
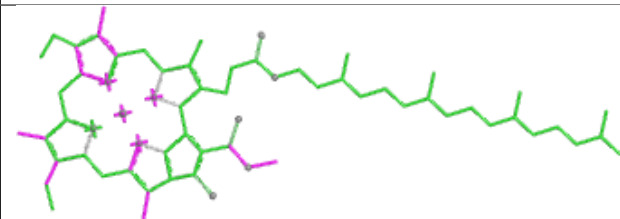
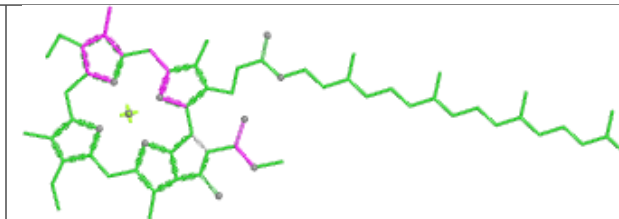
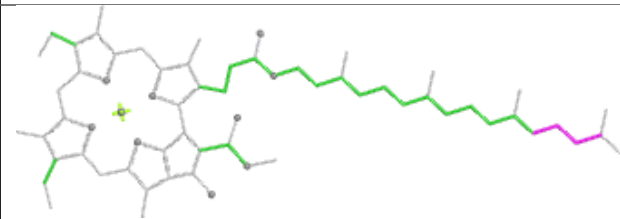
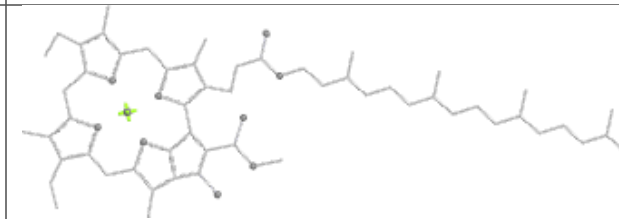


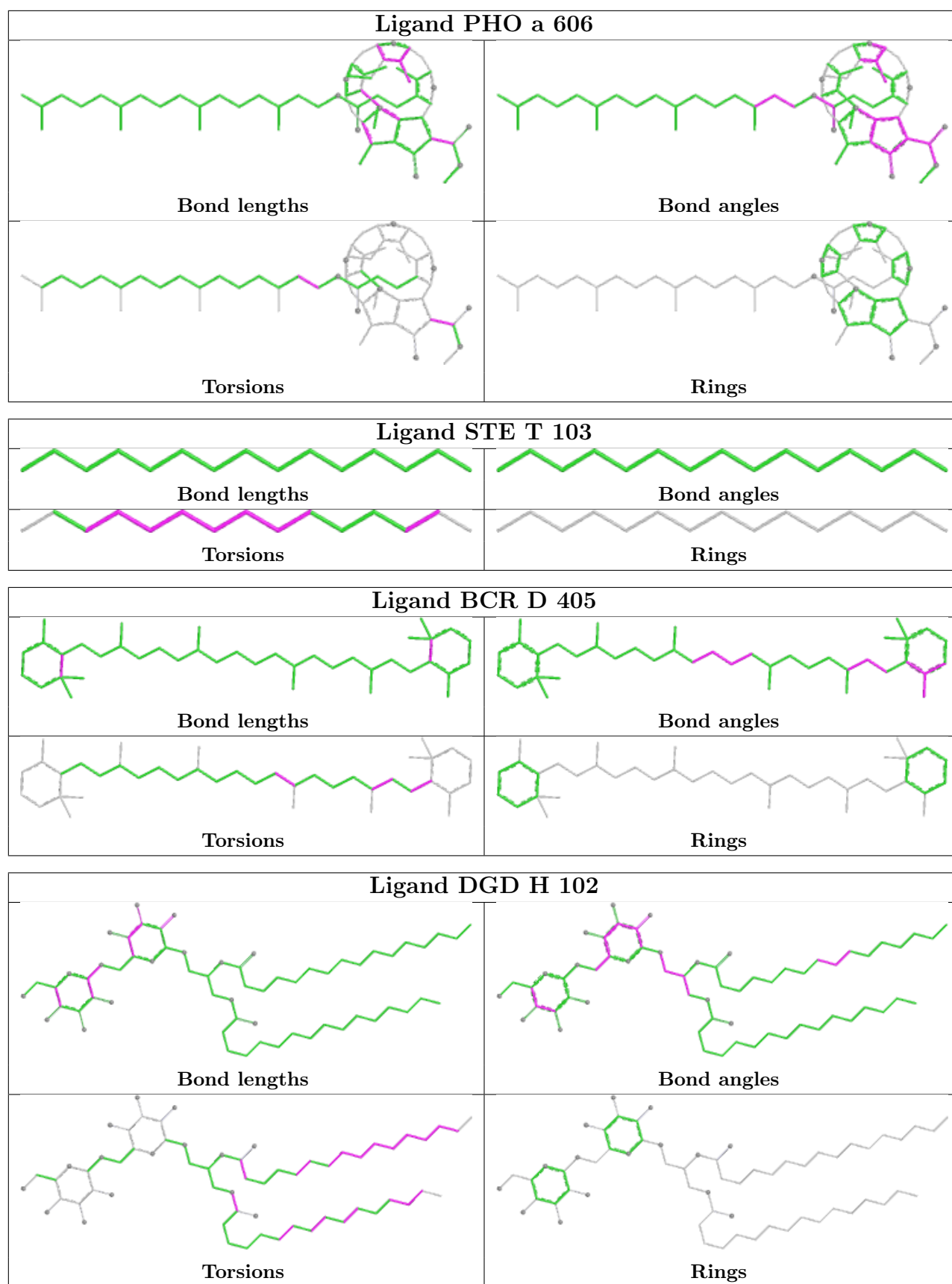
Ligand CLA C 509

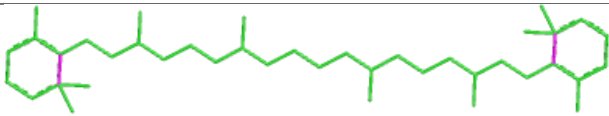
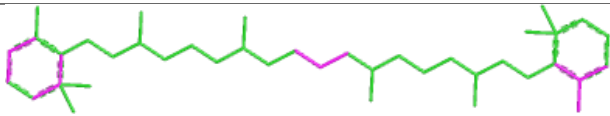
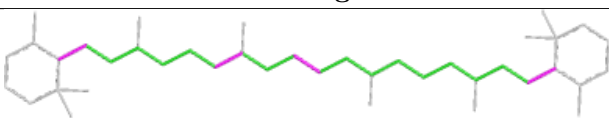
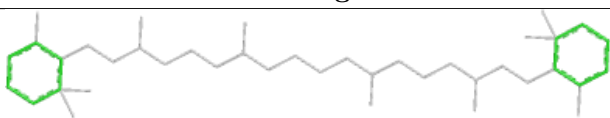


Ligand CLA B 614

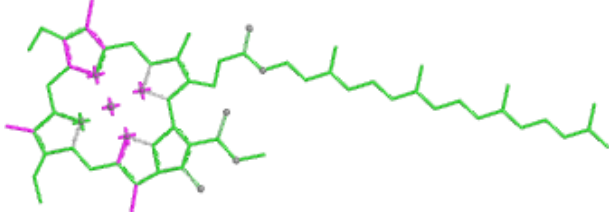
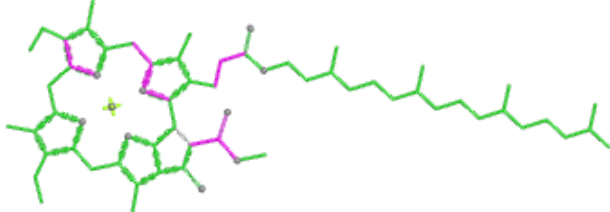
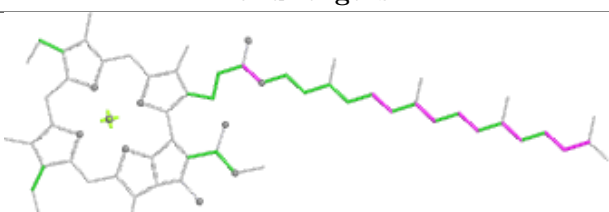
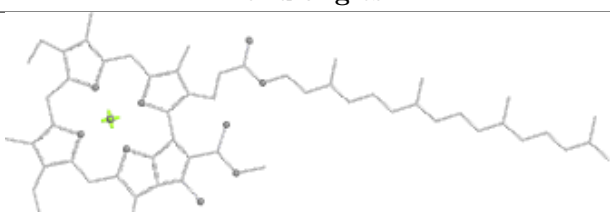


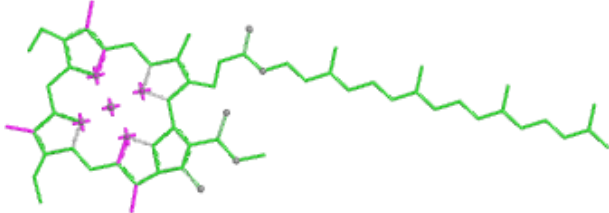
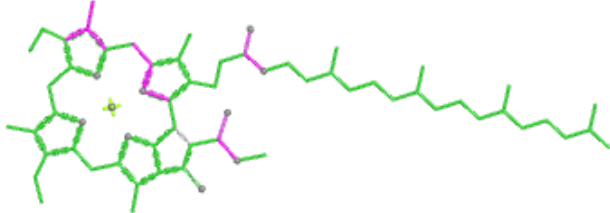
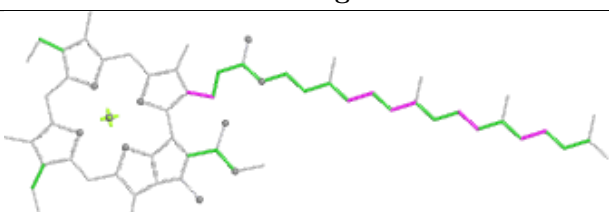
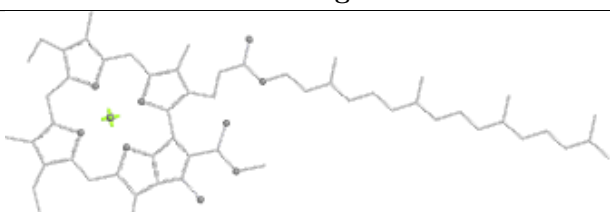
Ligand PL9 d 405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE b 623	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

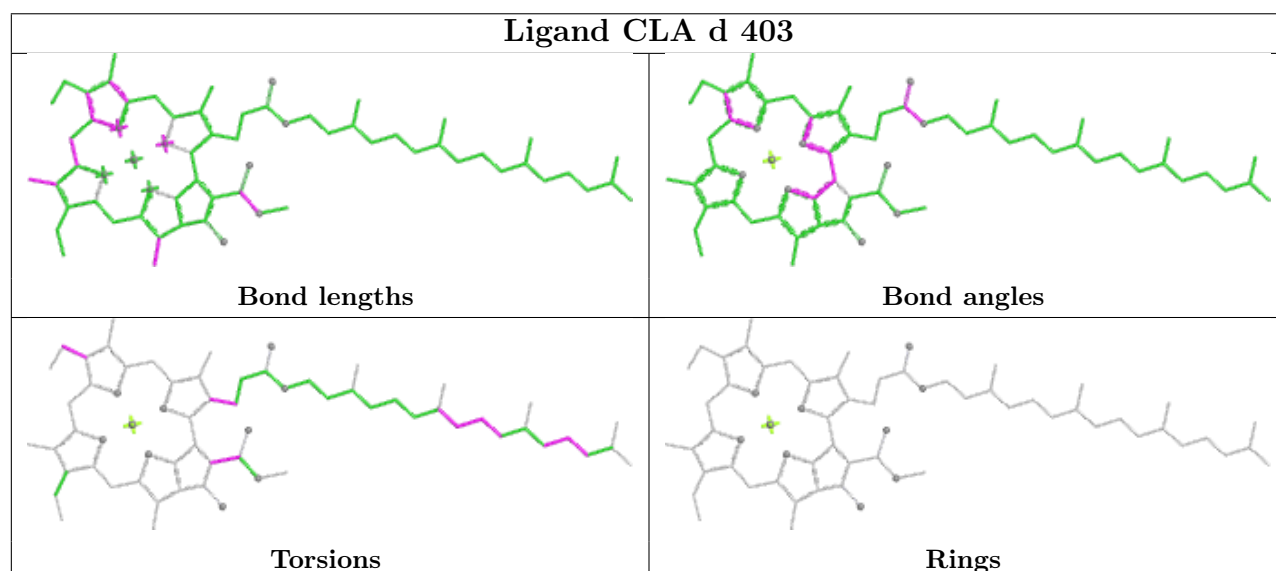
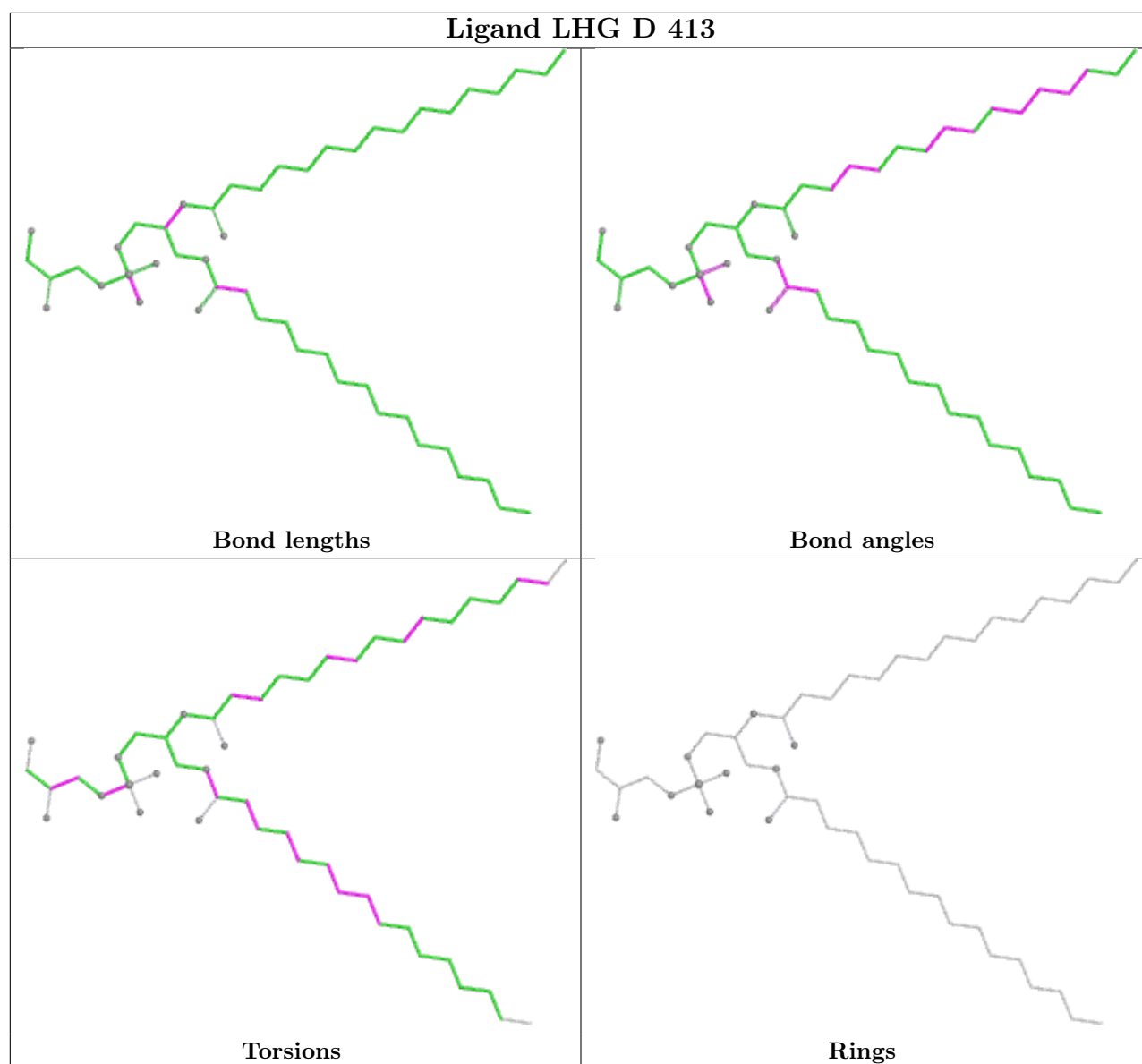


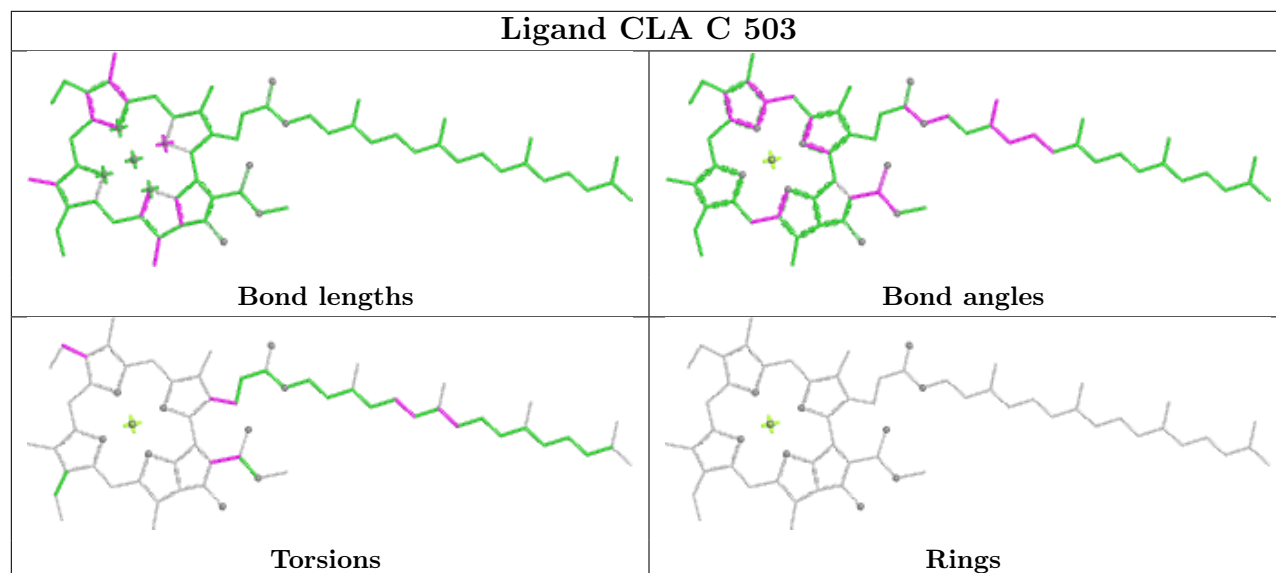
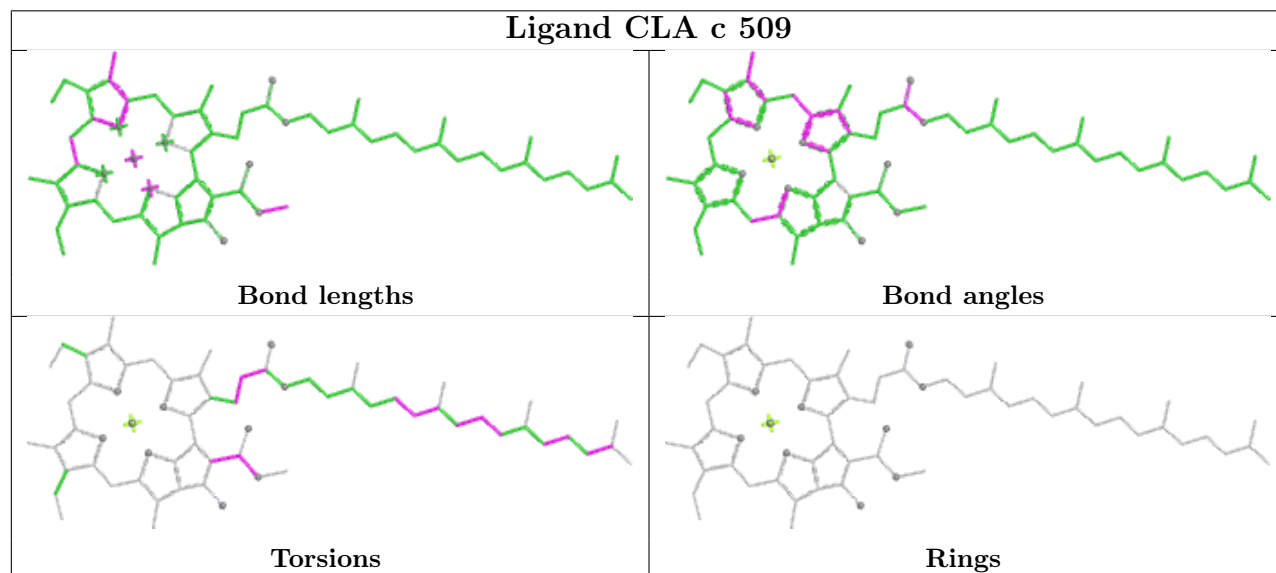
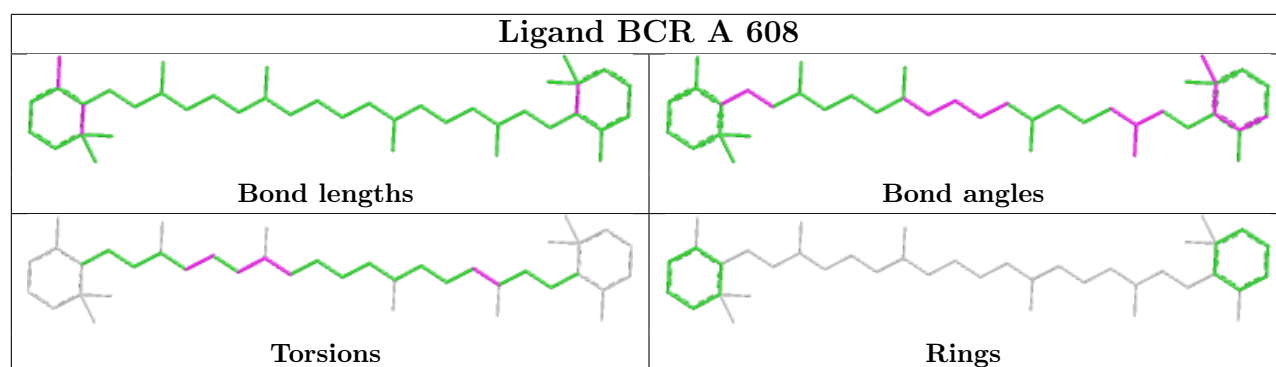
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

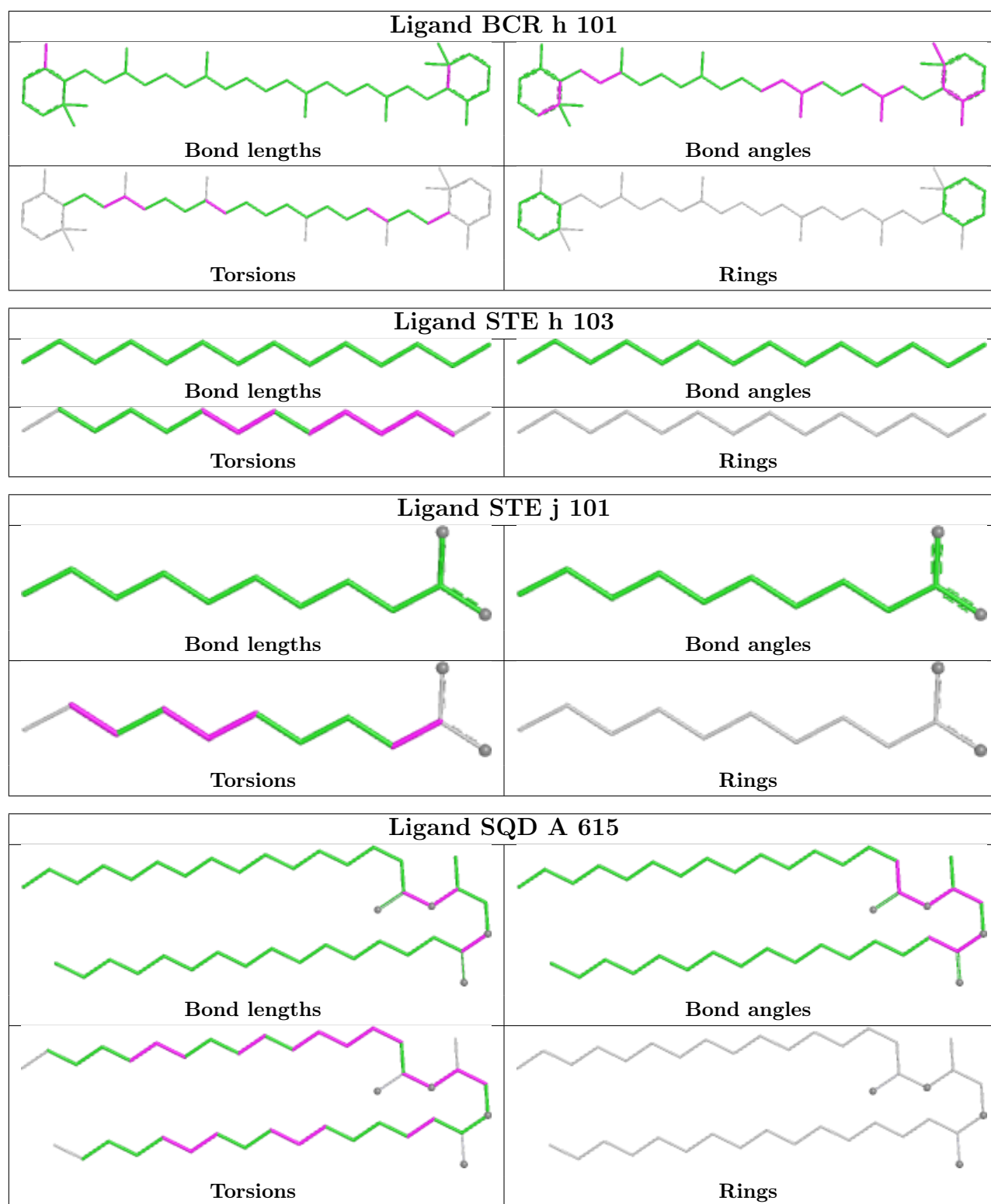
Ligand STE B 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

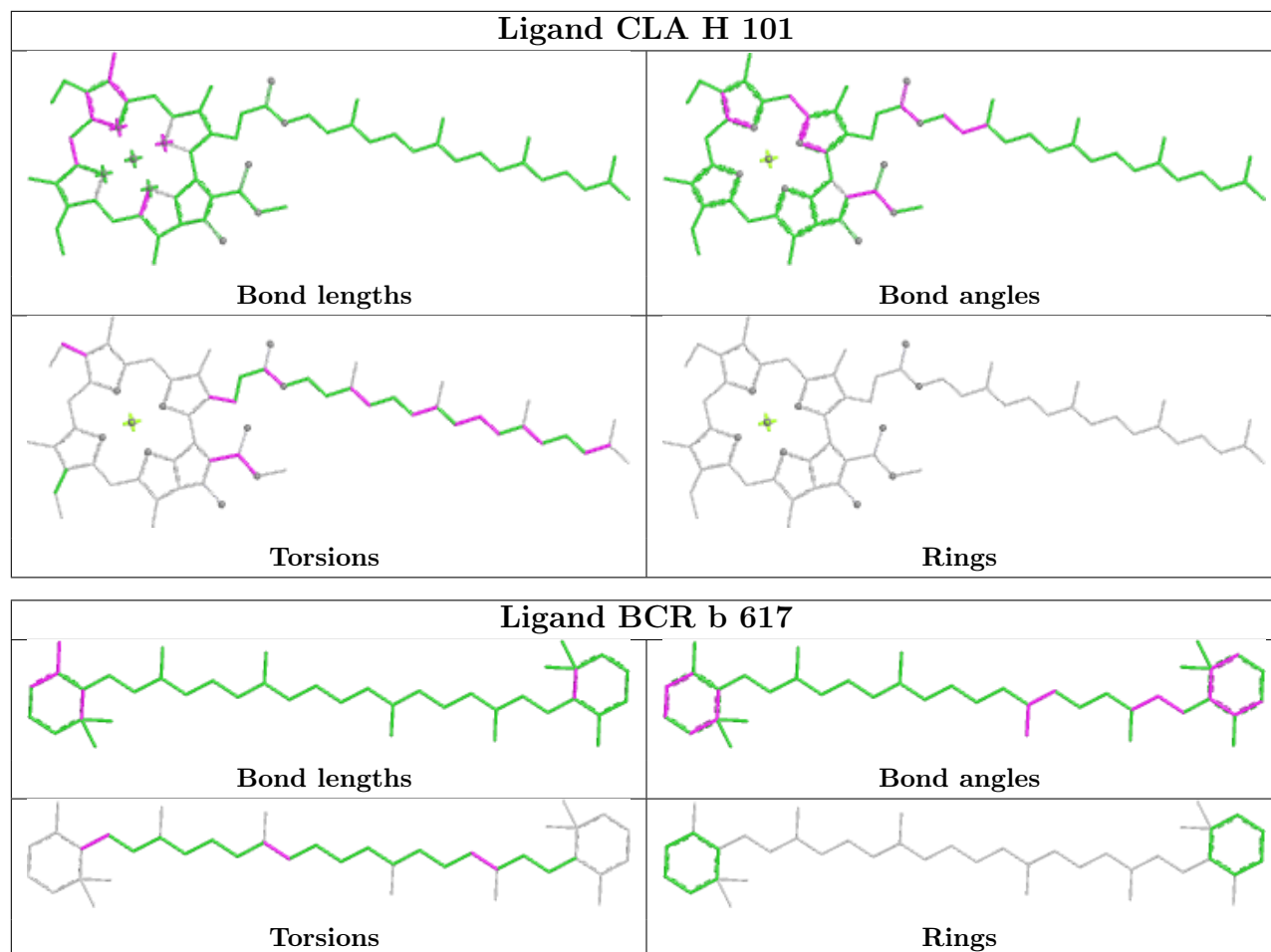
Ligand CLA a 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

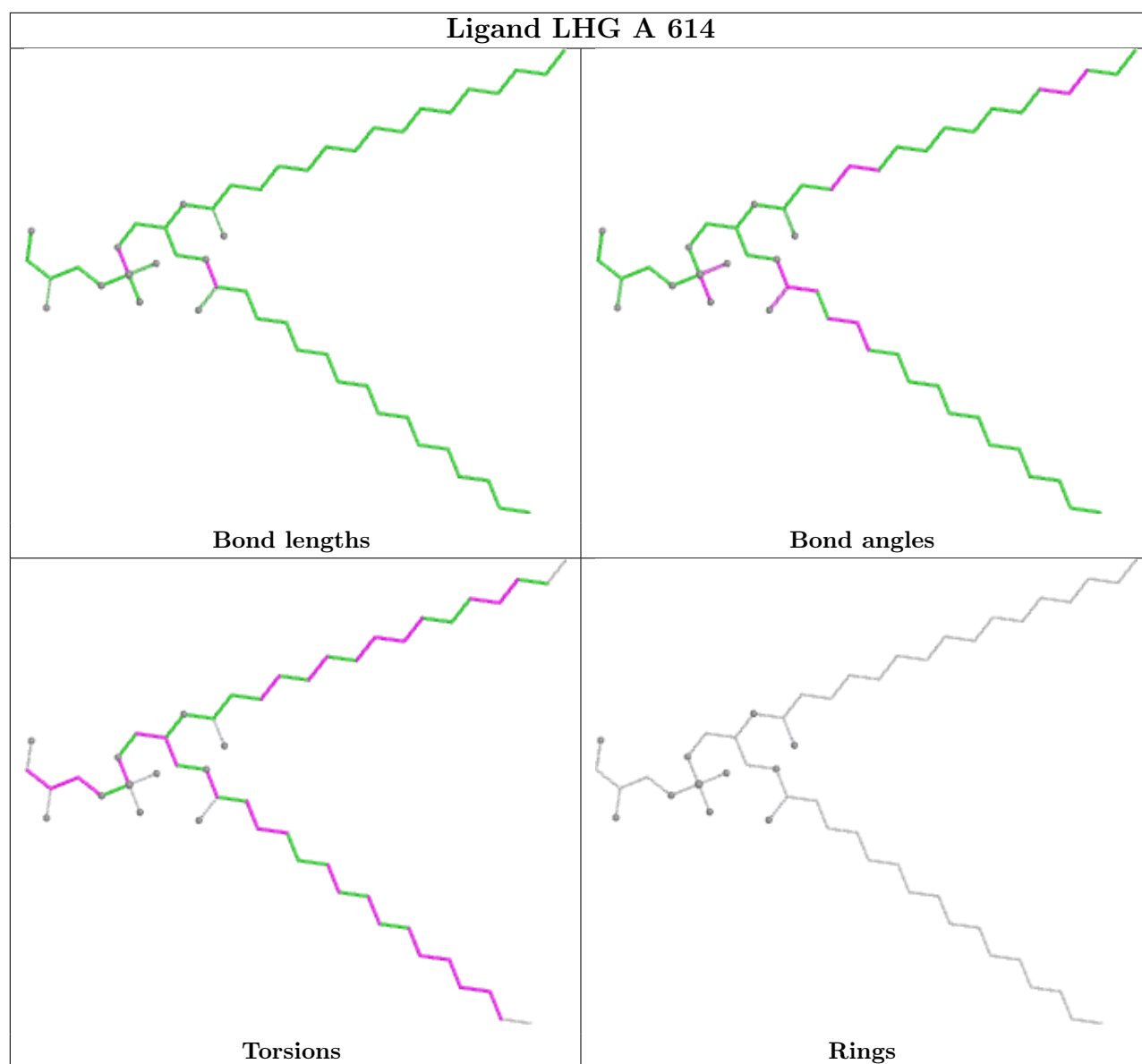
Ligand CLA a 605	
	
Bond lengths	Bond angles
	
Torsions	Rings



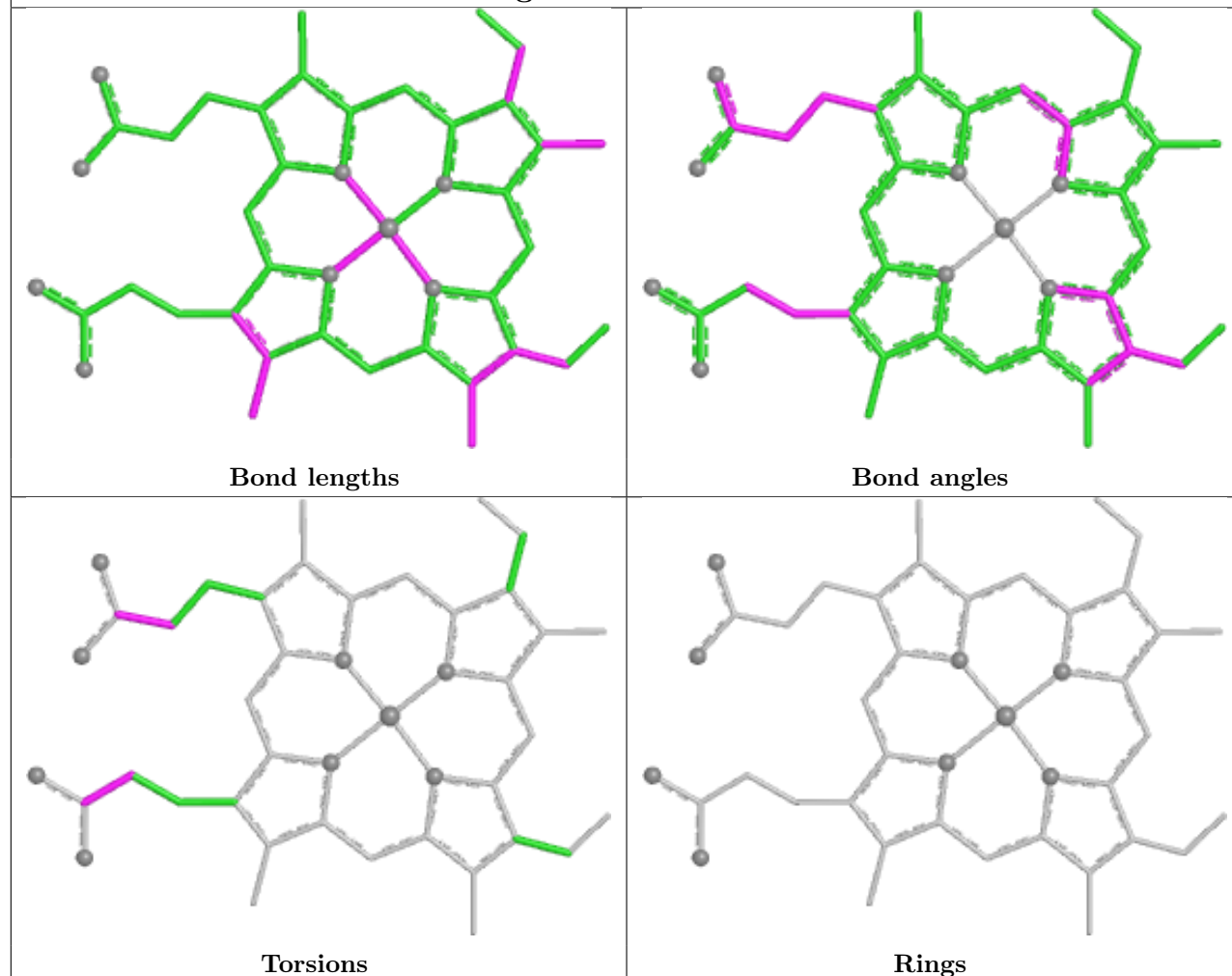




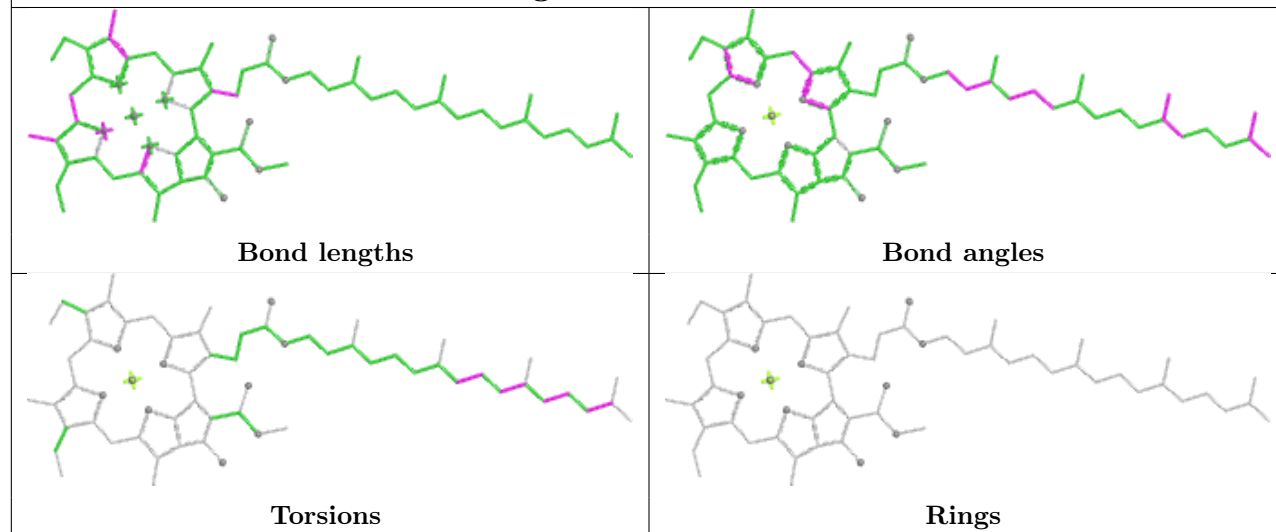




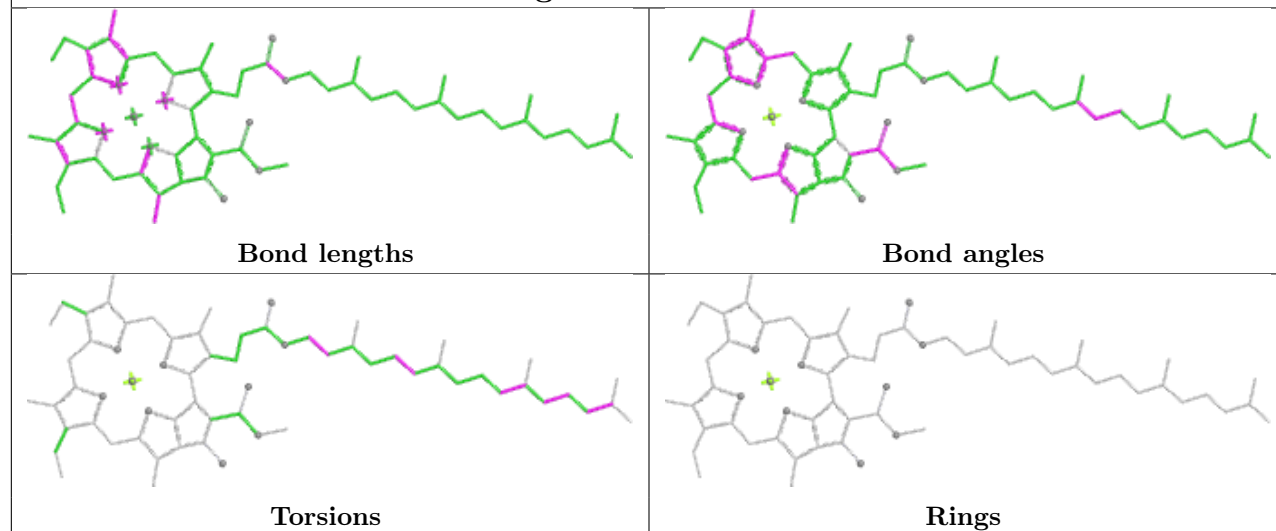
Ligand HEM f 101



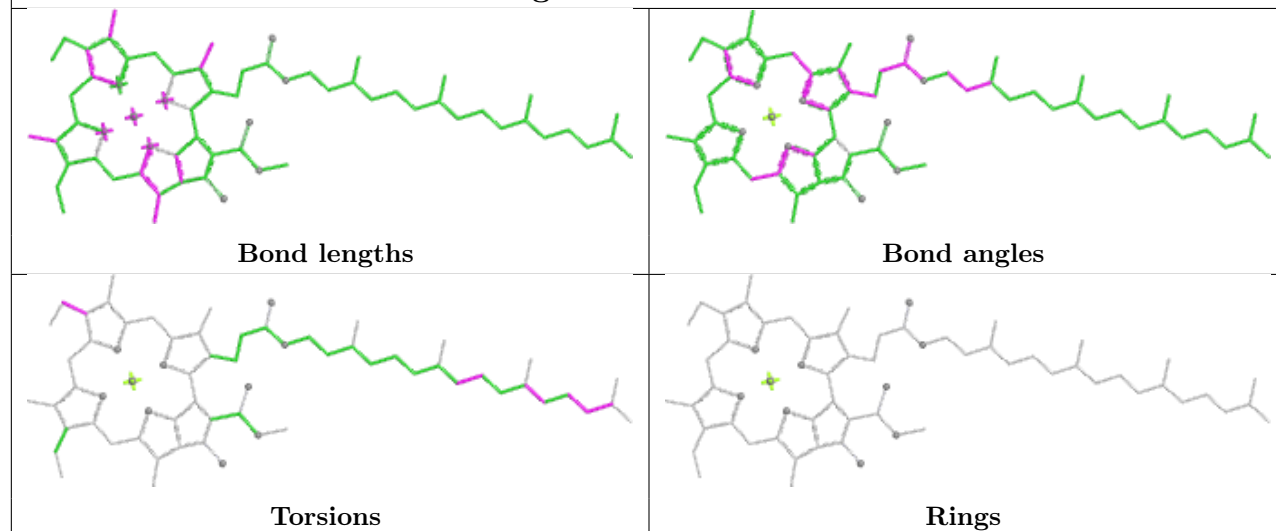
Ligand CLA B 610



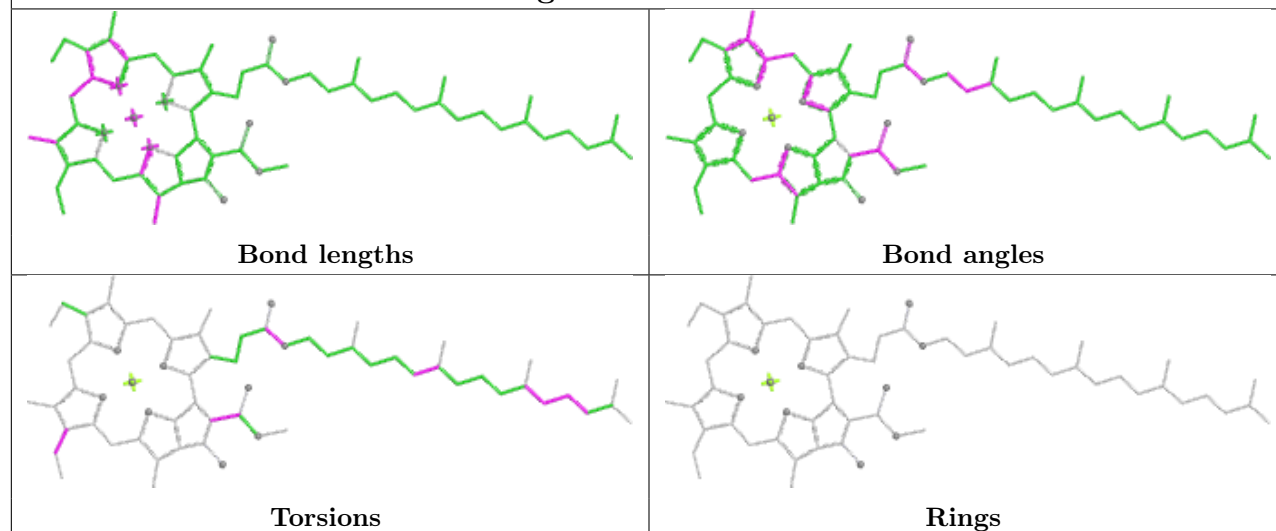
Ligand CLA b 608



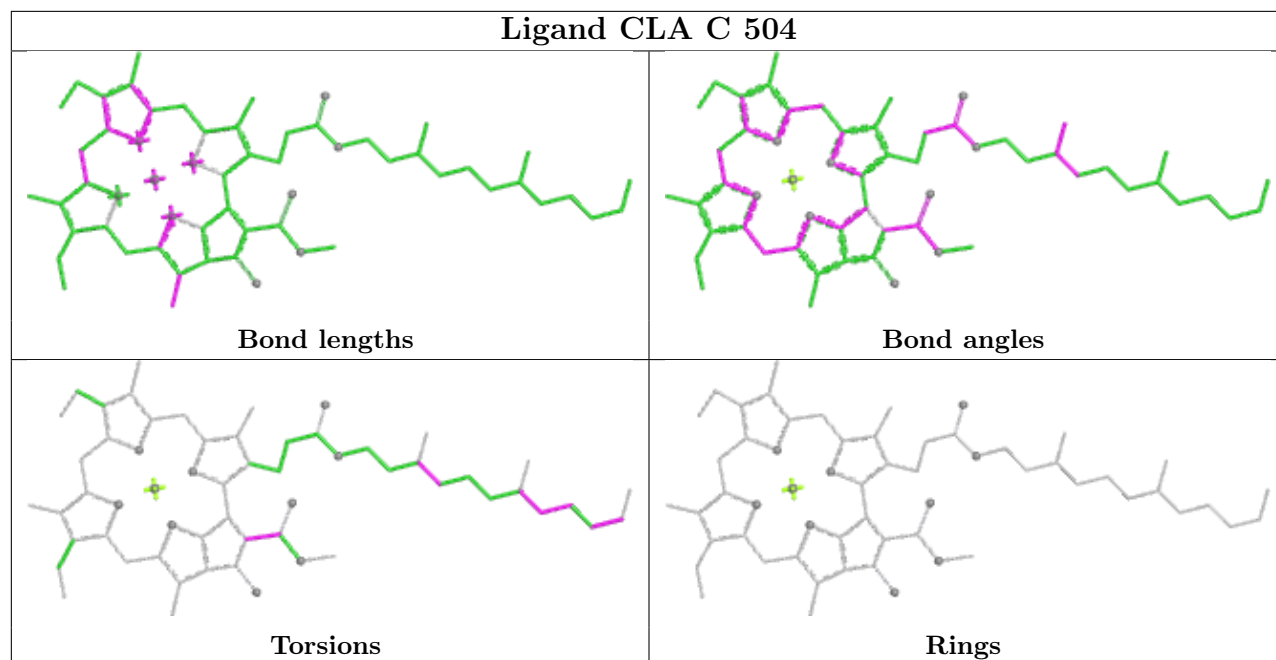
Ligand CLA B 609



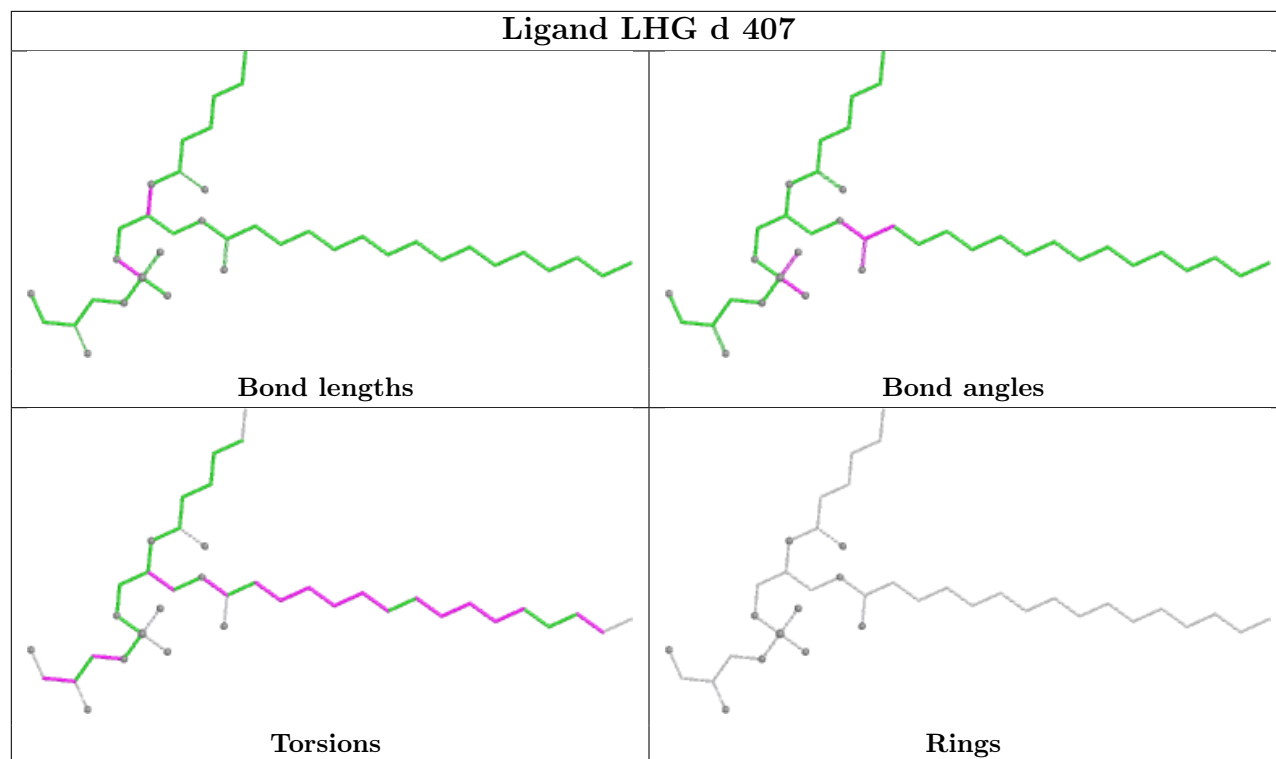
Ligand CLA c 502

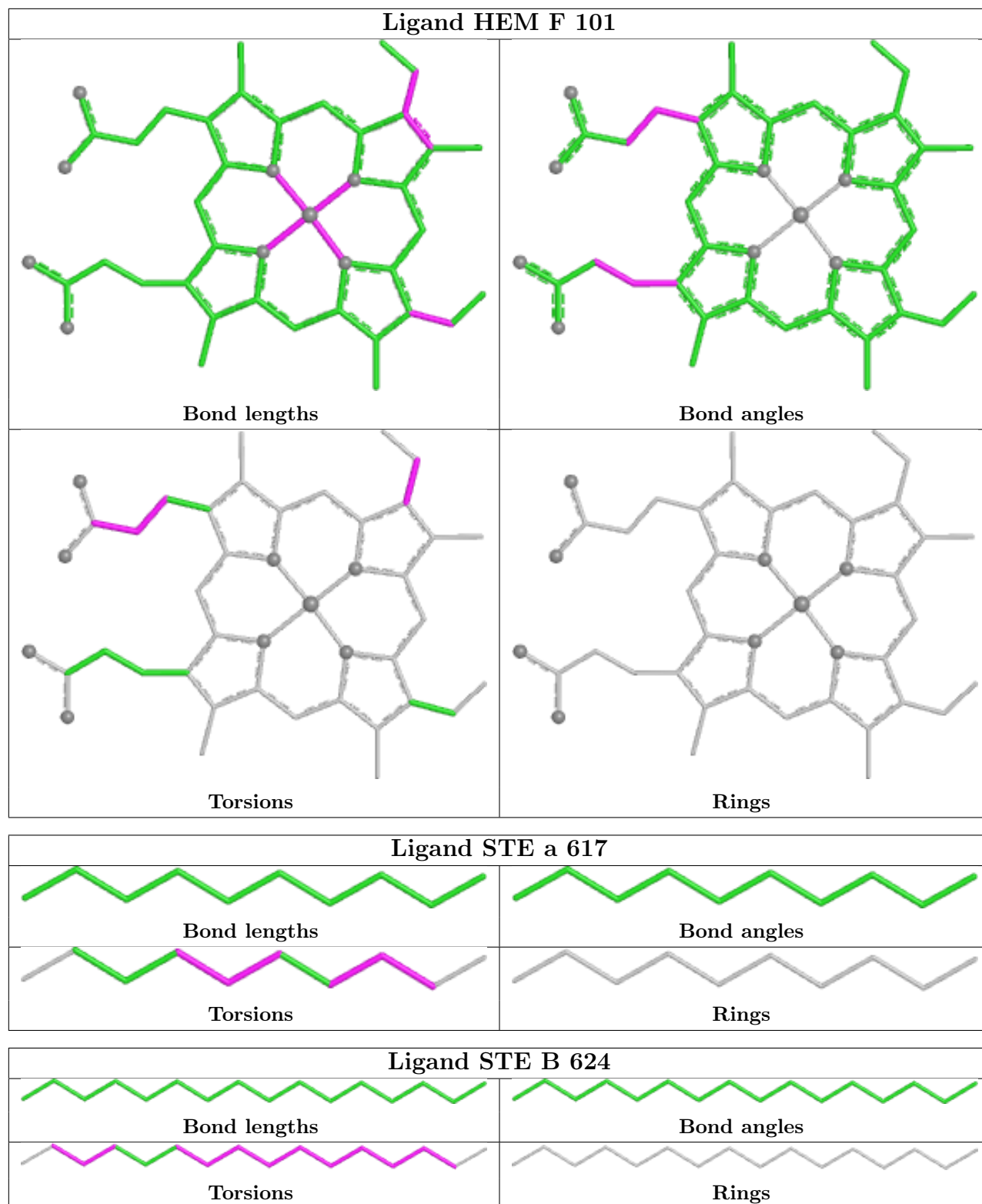


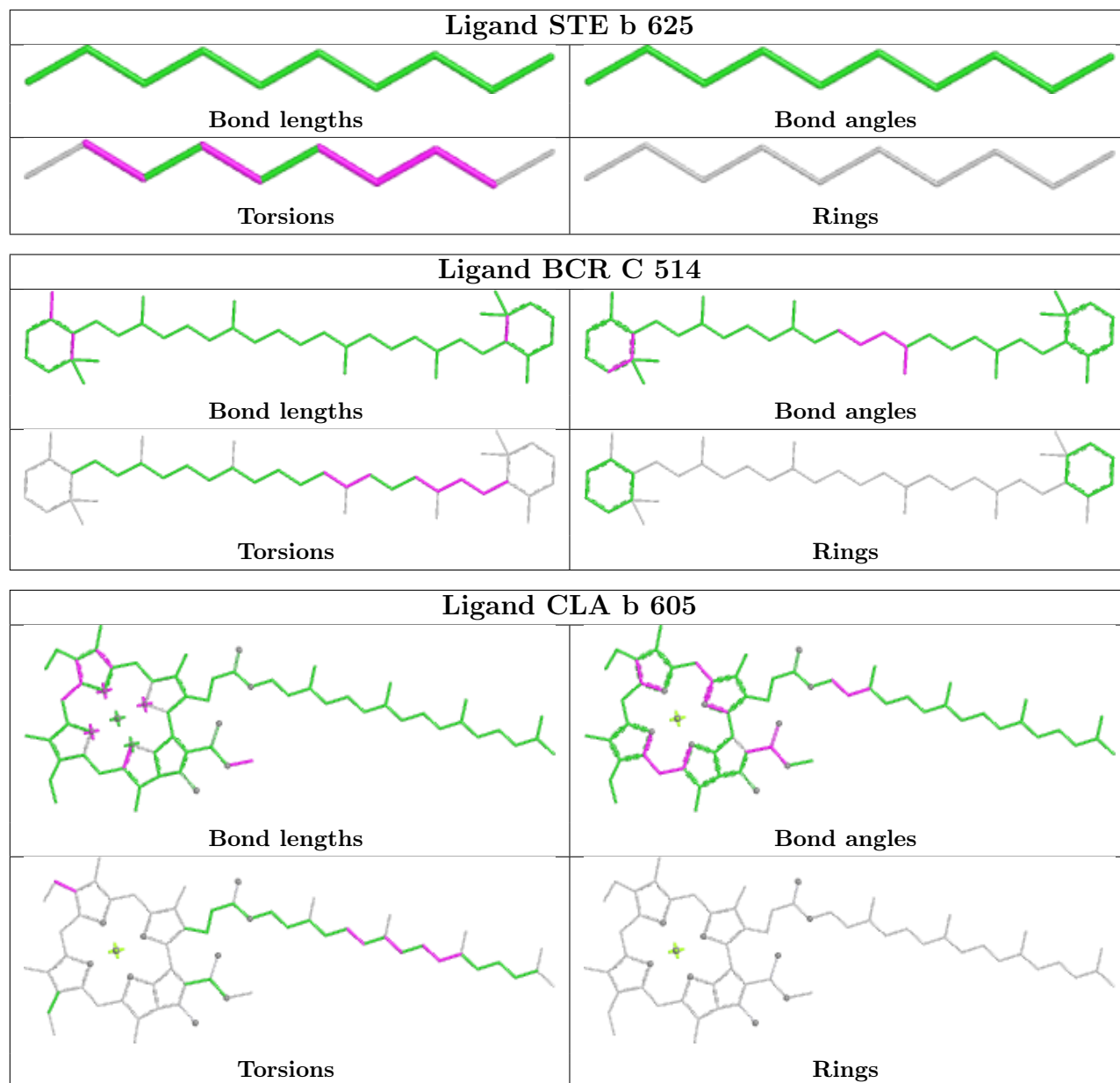
Ligand CLA C 504

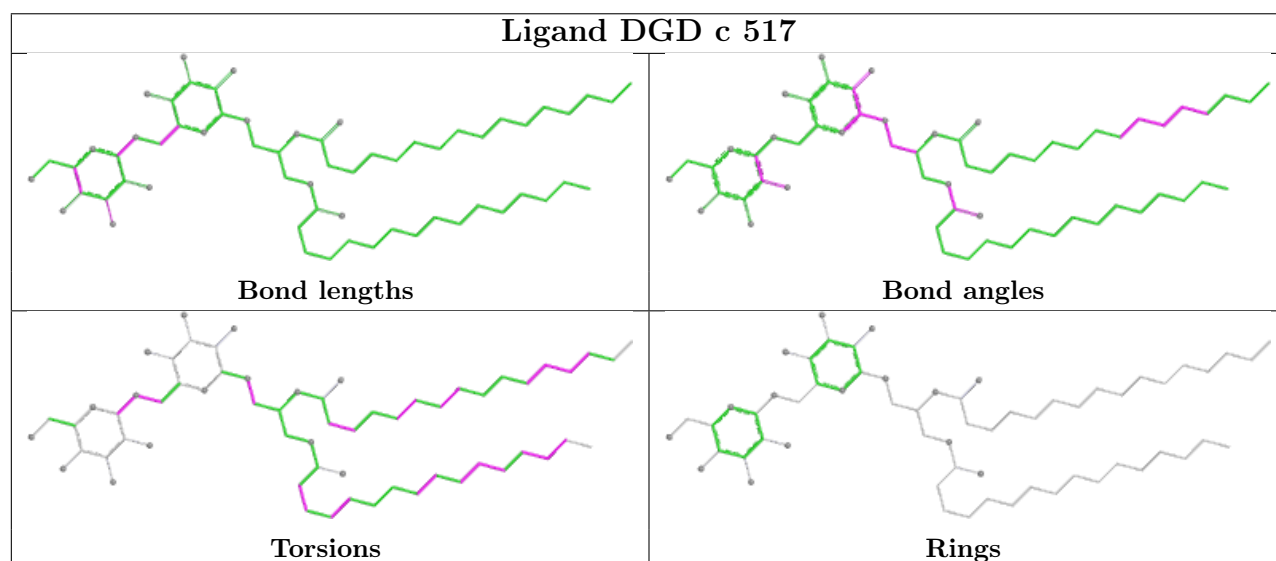
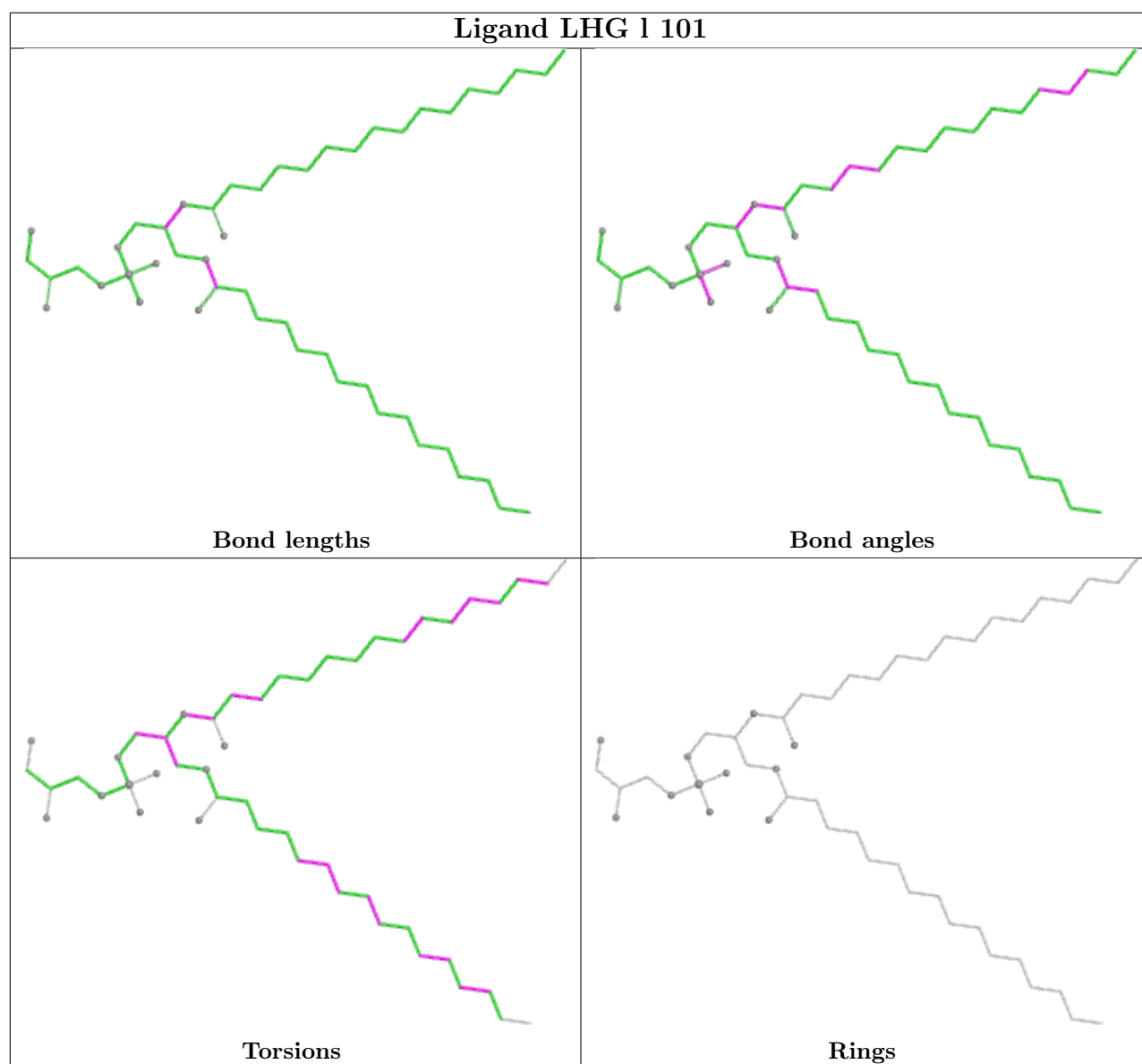


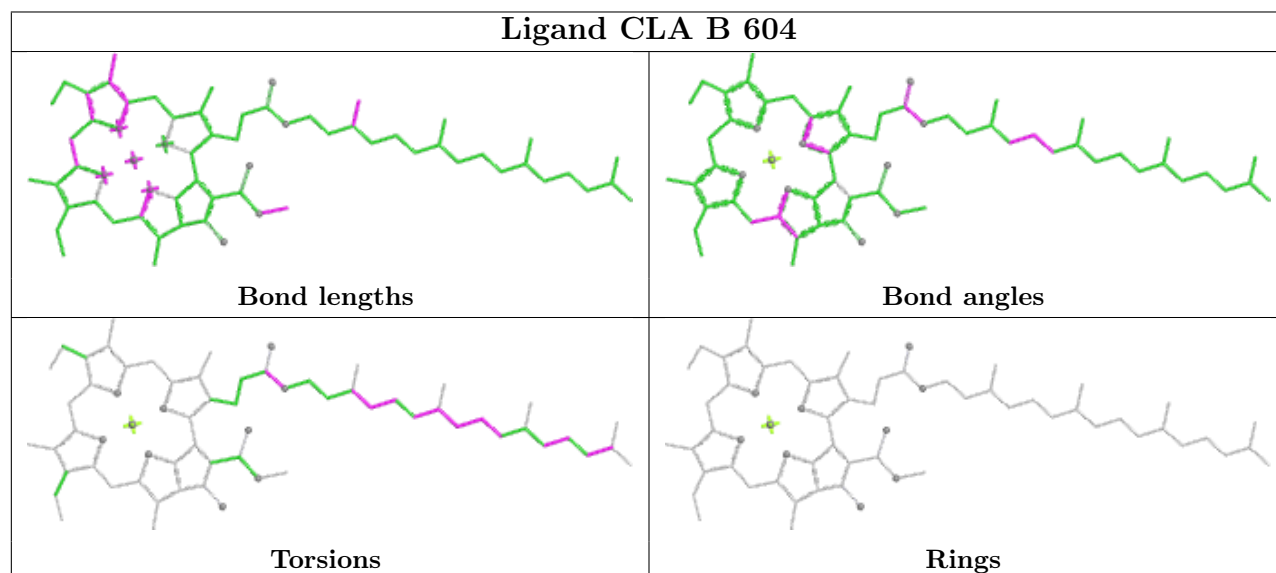
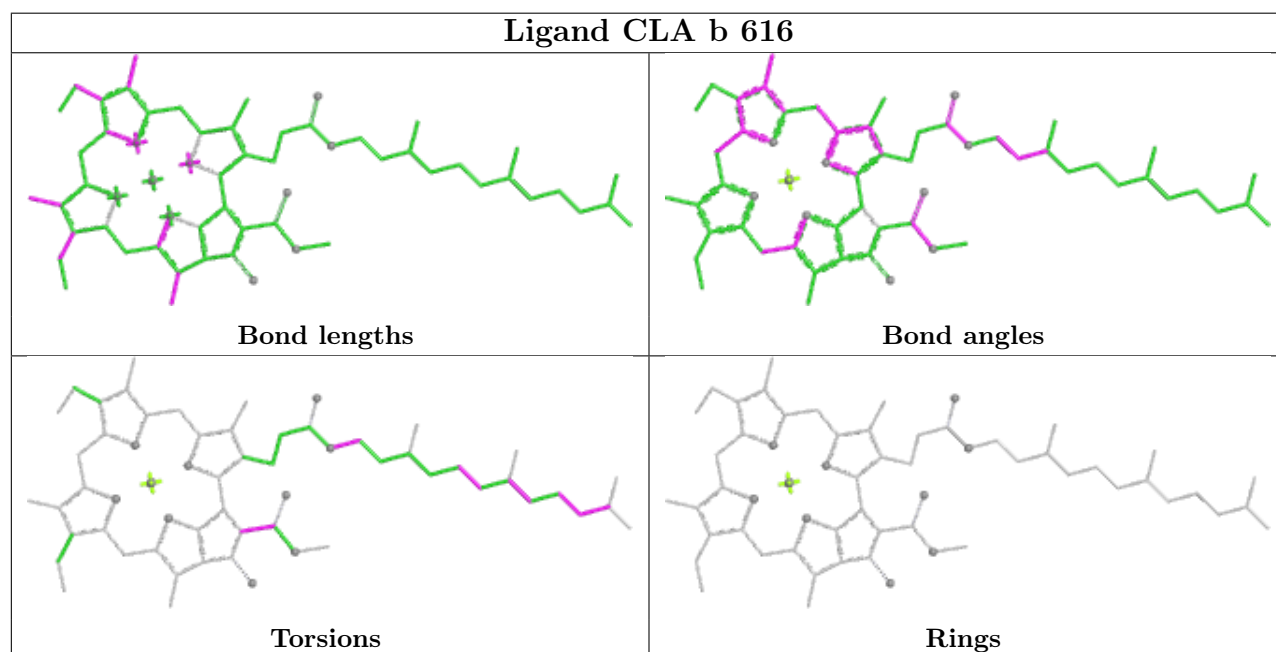
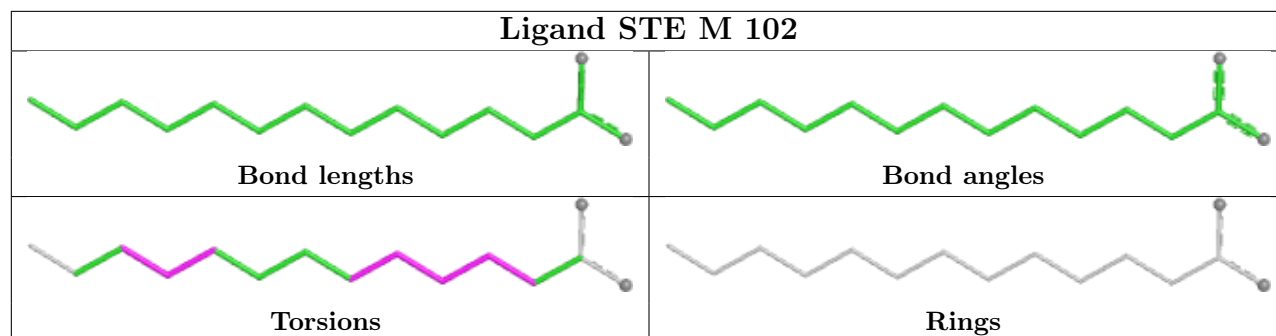
Ligand LHG d 407

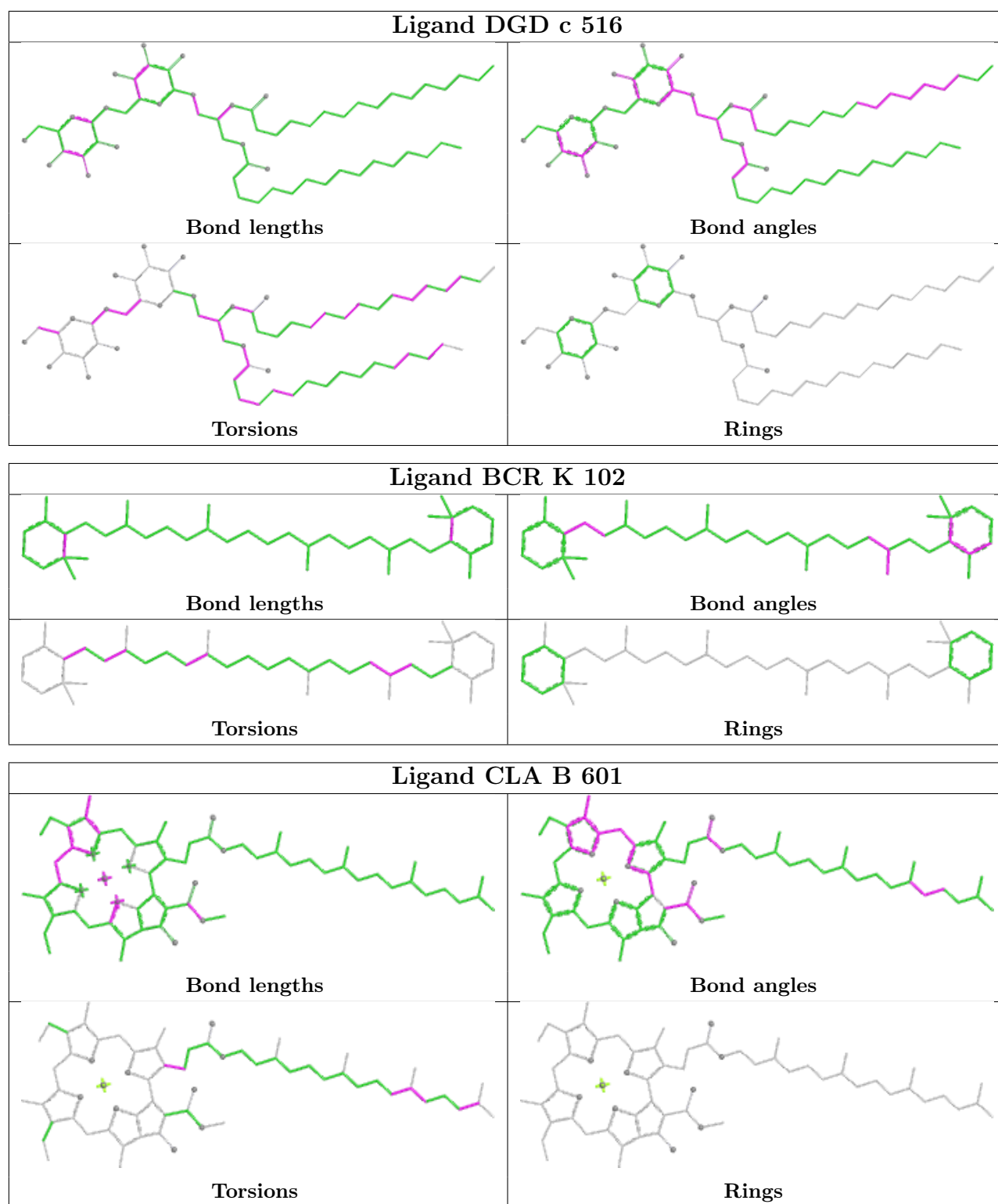


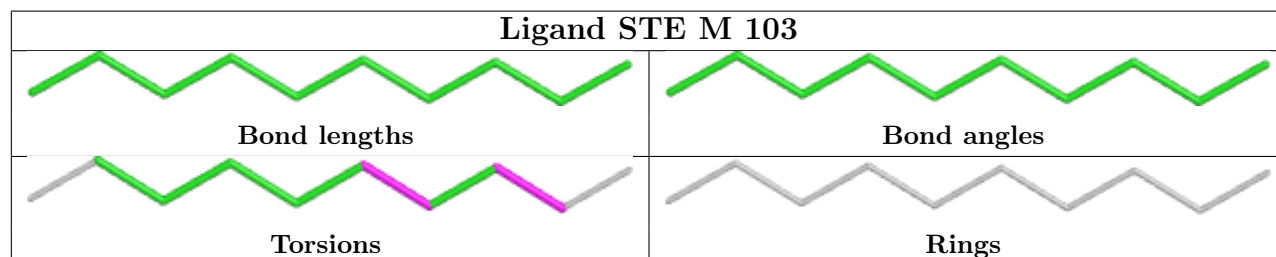
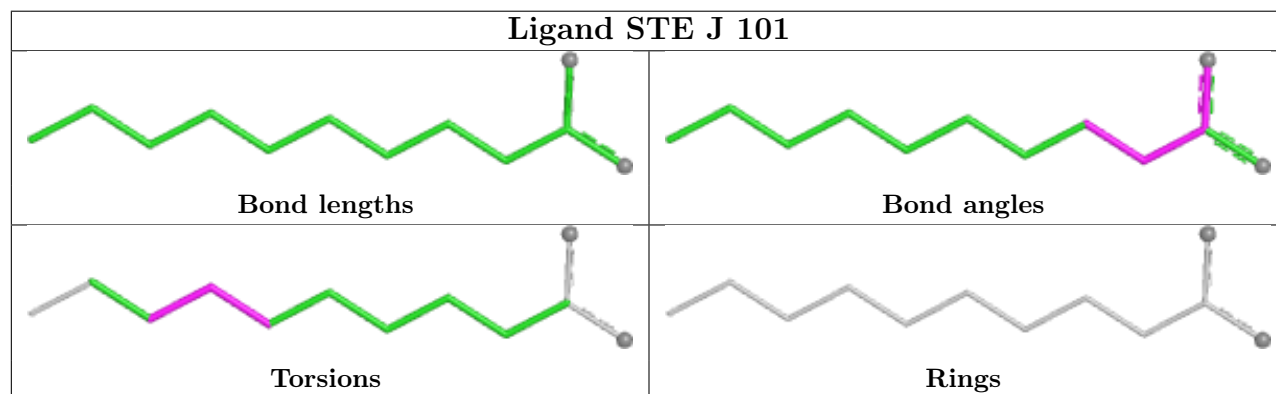
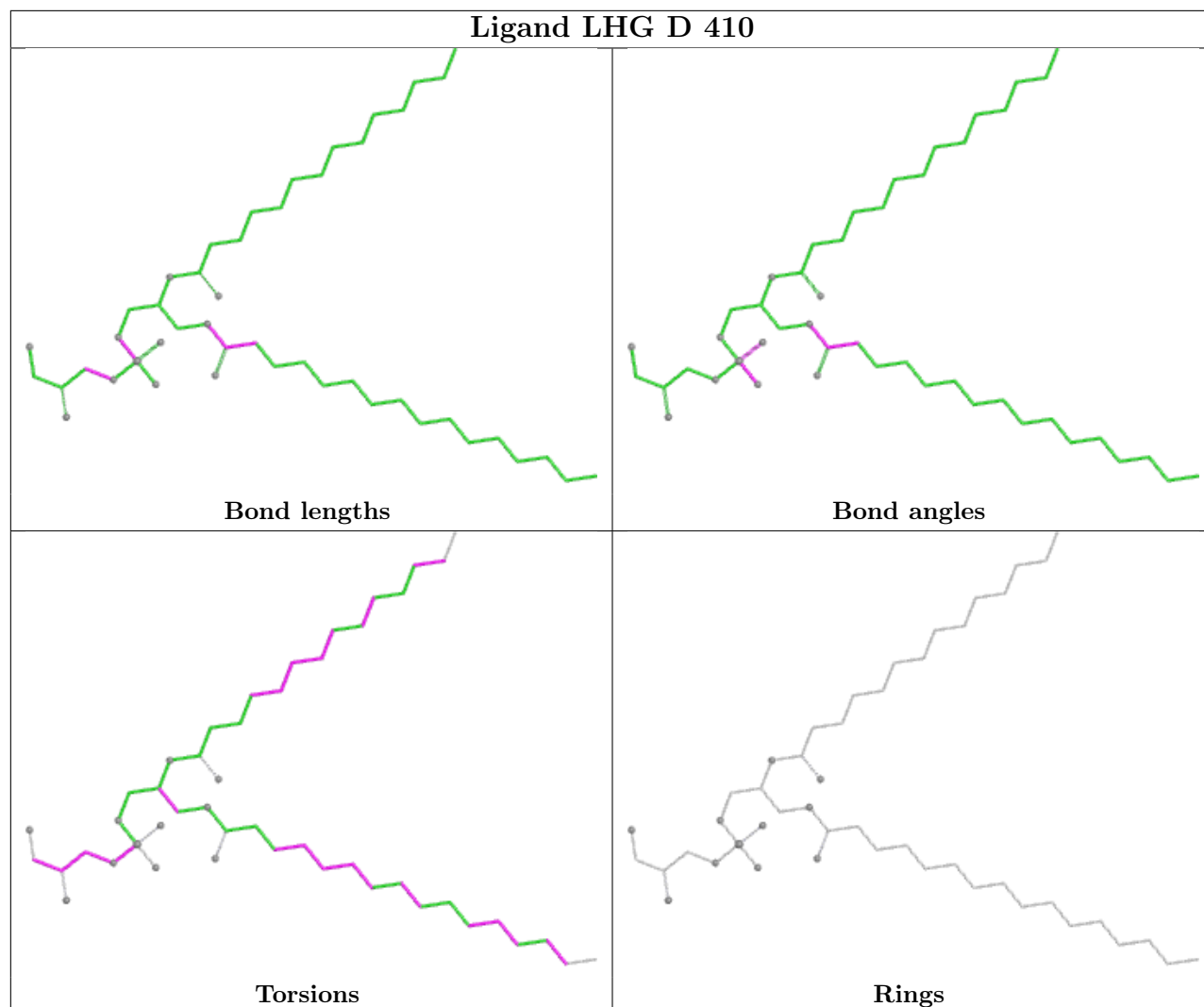




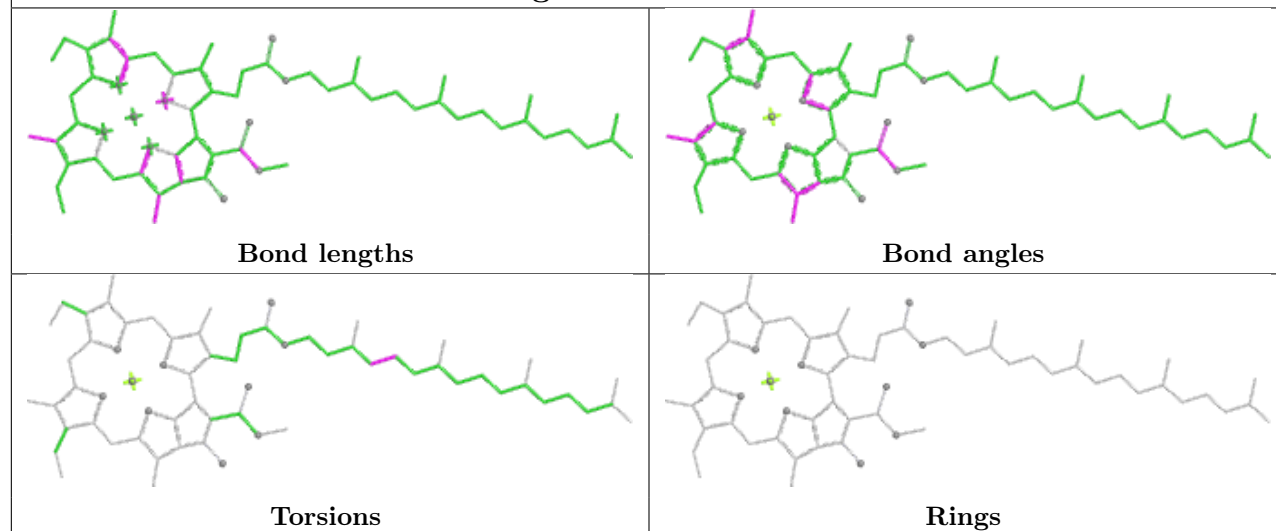




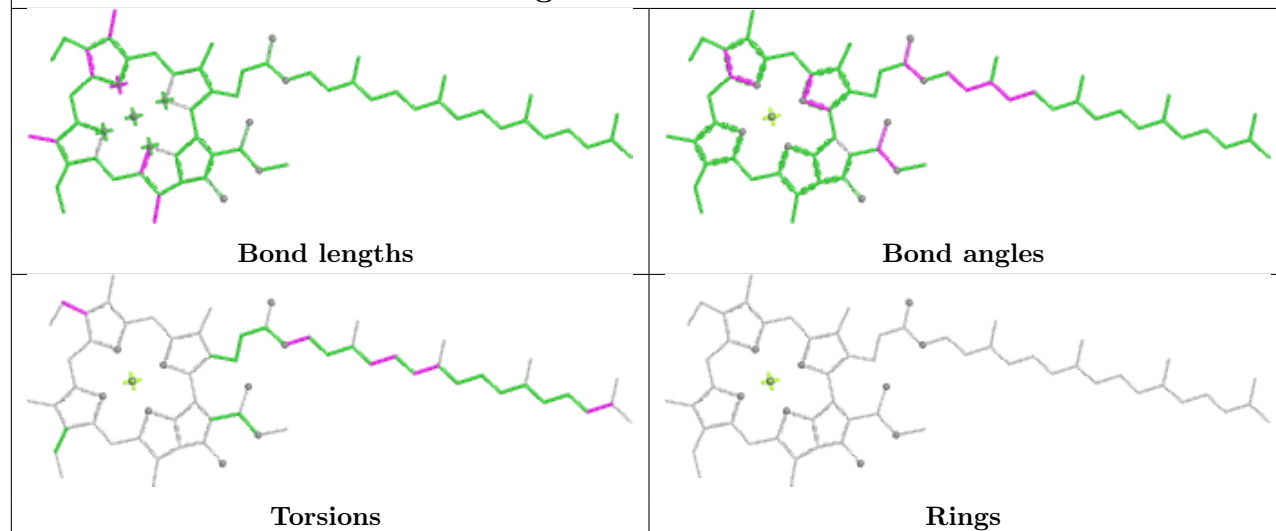




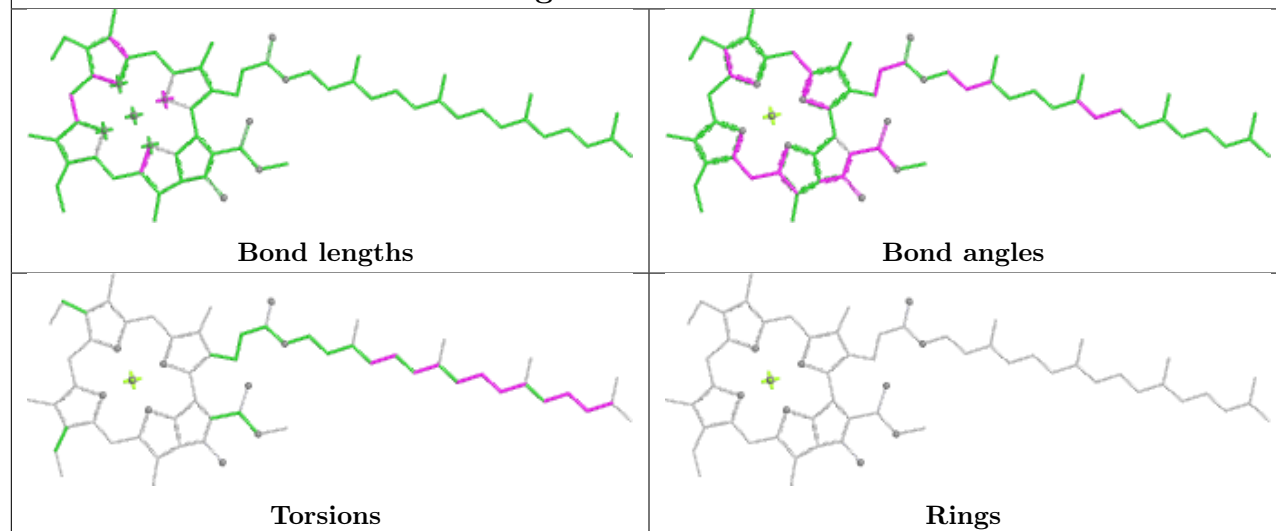
Ligand CLA B 608



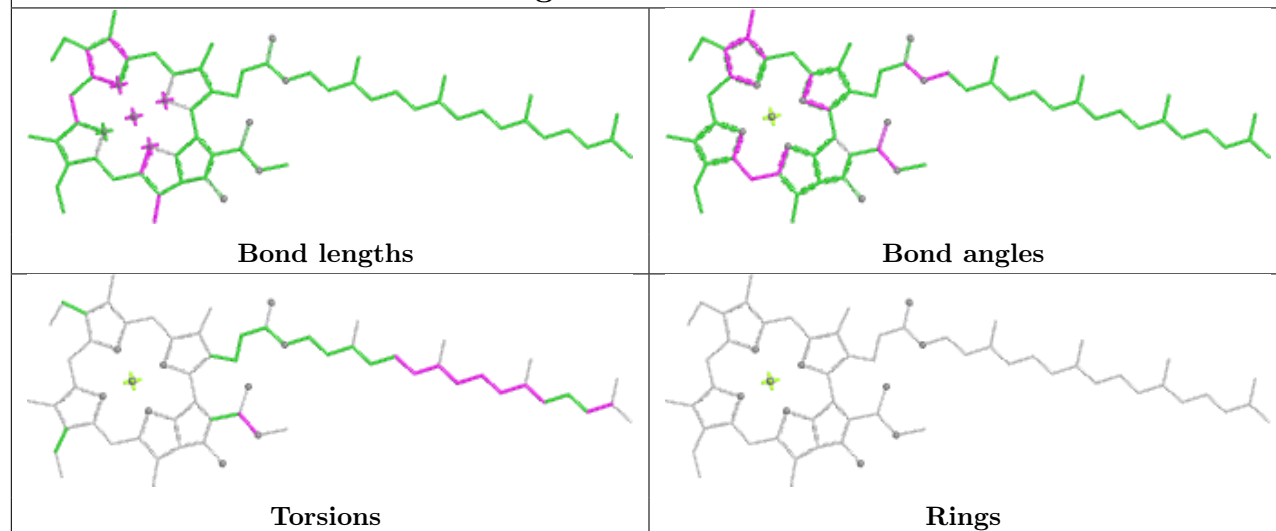
Ligand CLA d 402



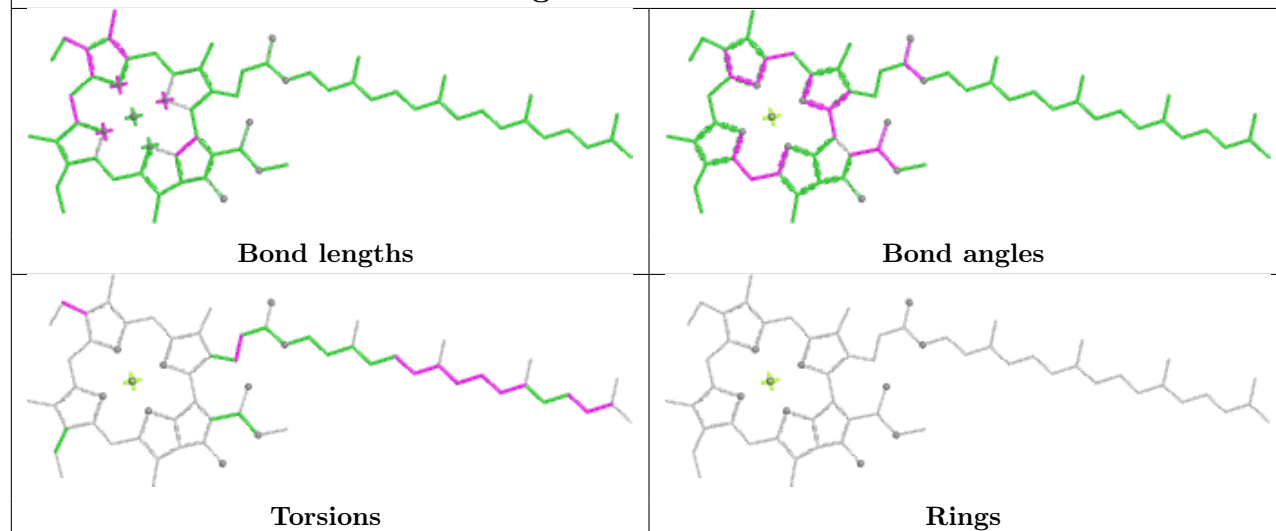
Ligand CLA b 604

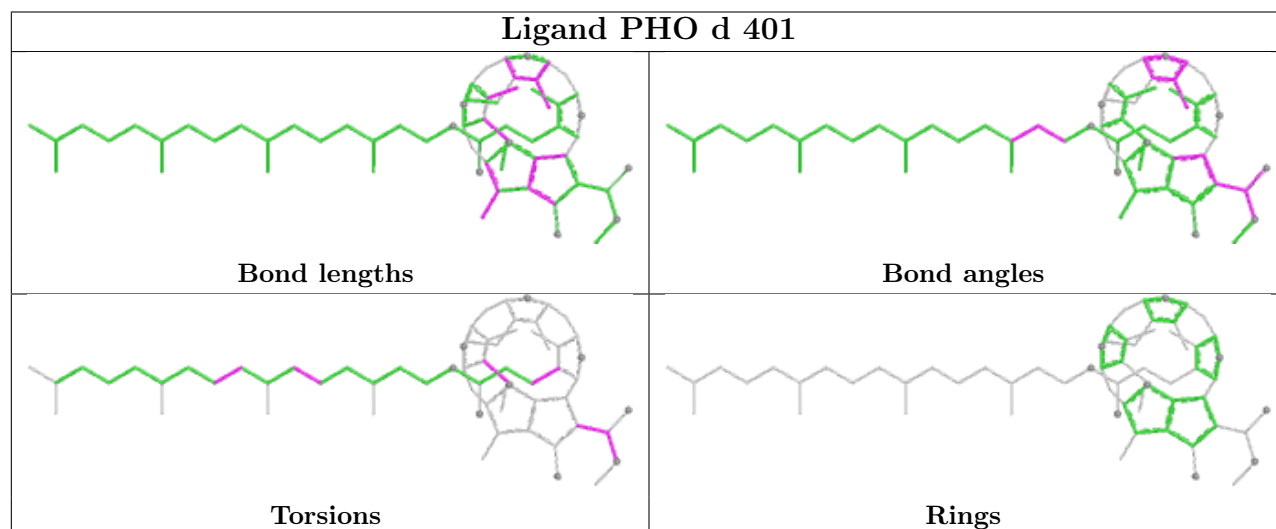
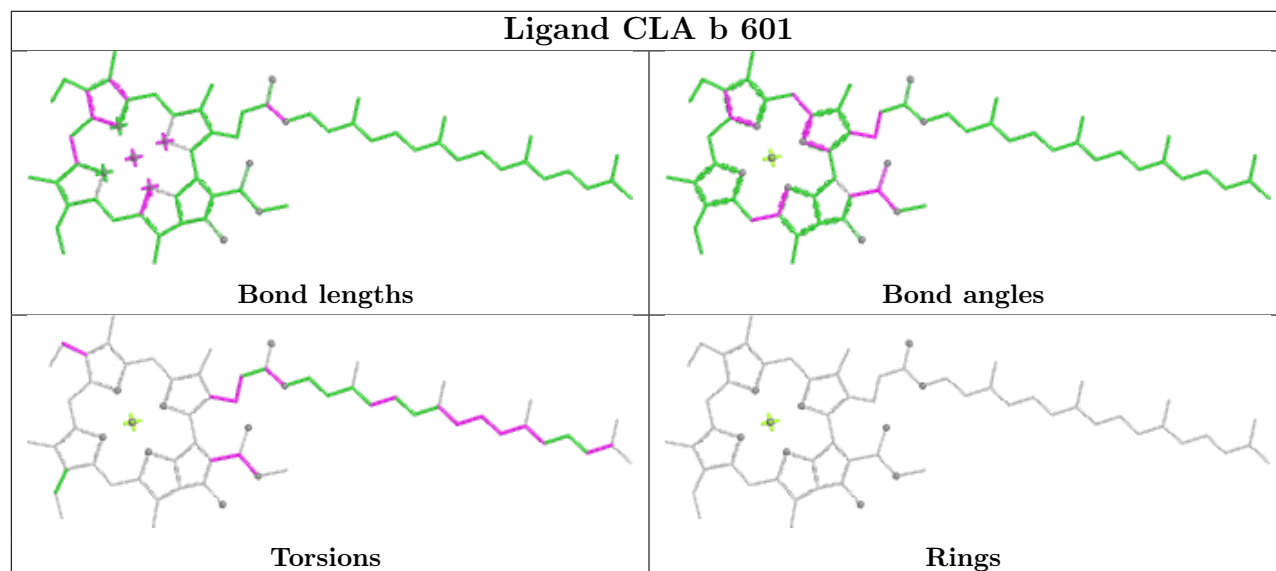
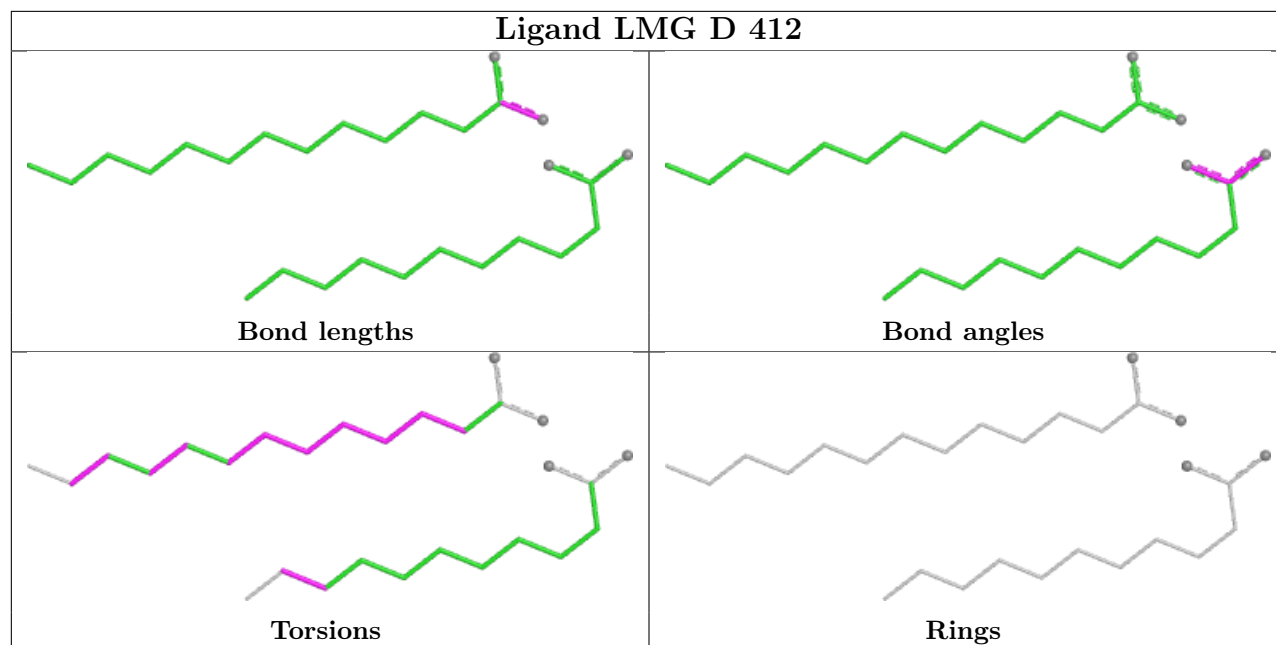


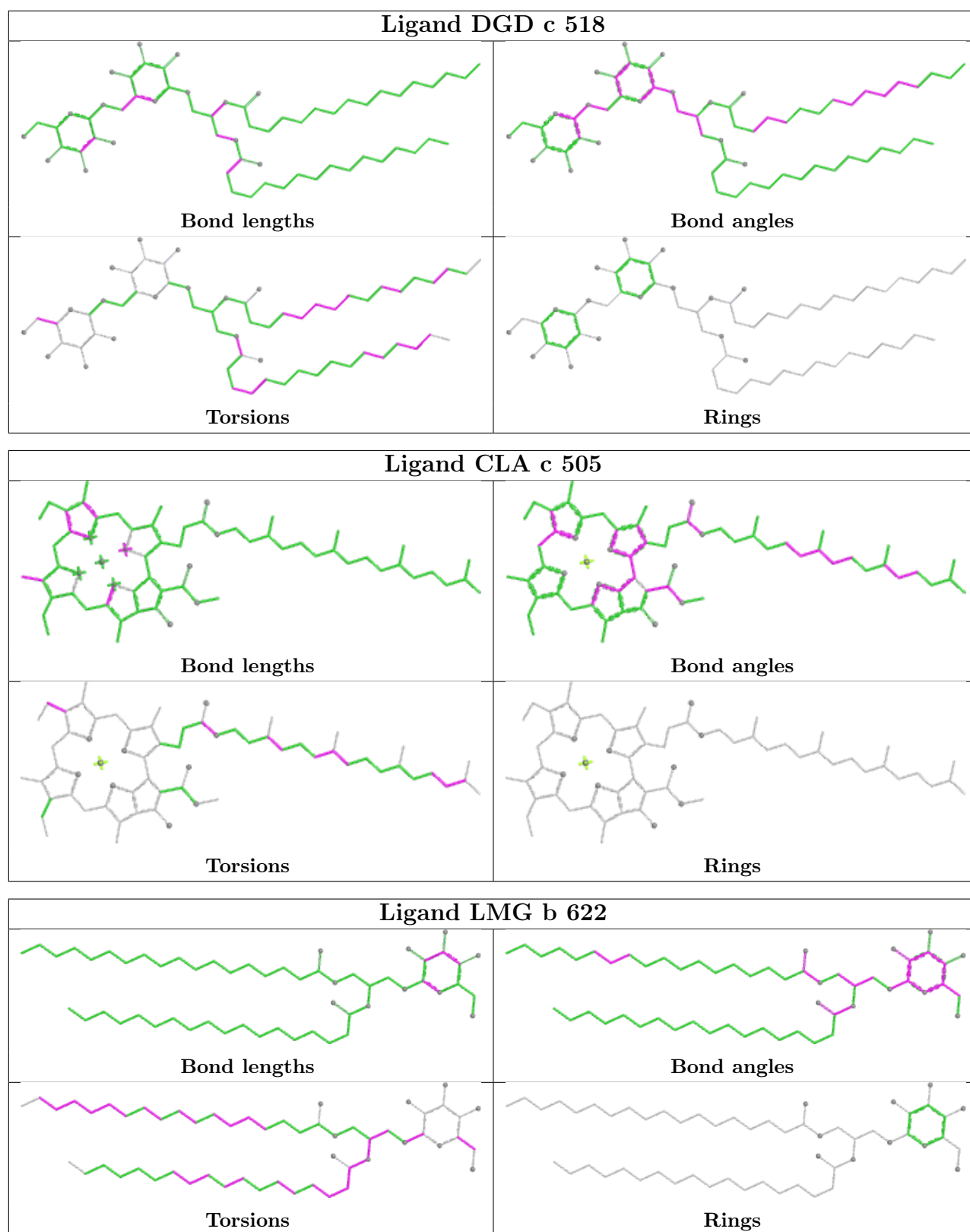
Ligand CLA b 607

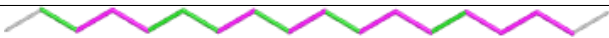


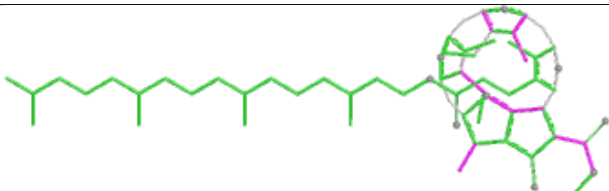
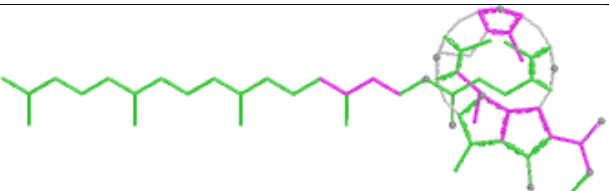
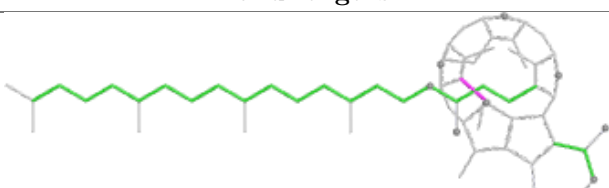
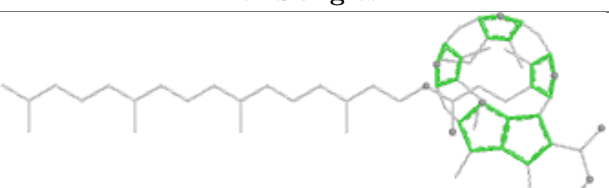
Ligand CLA B 605

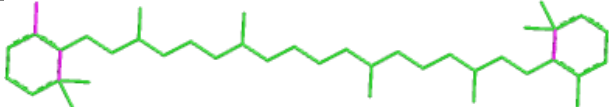
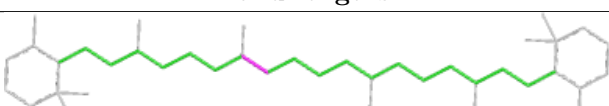
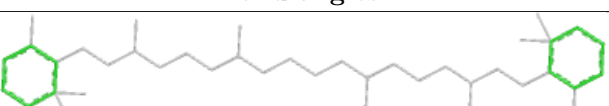


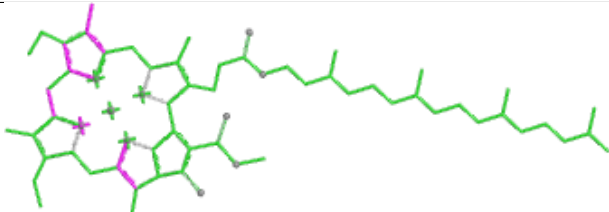
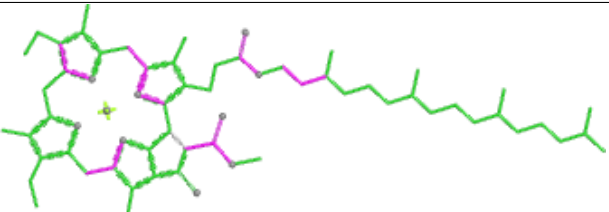
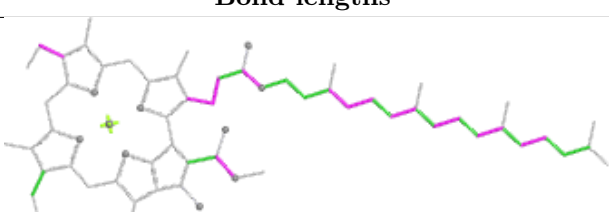
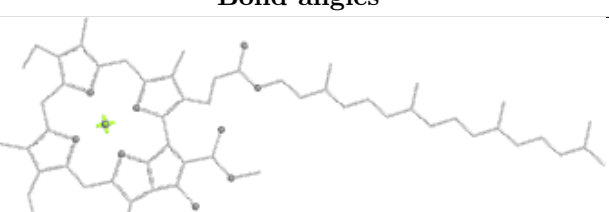


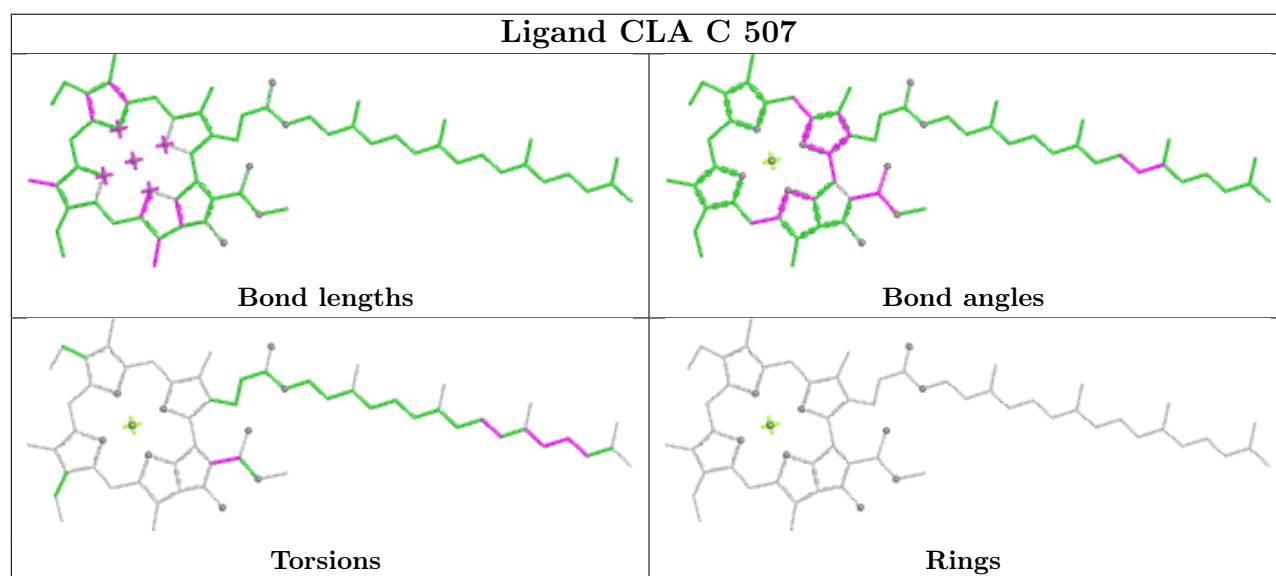
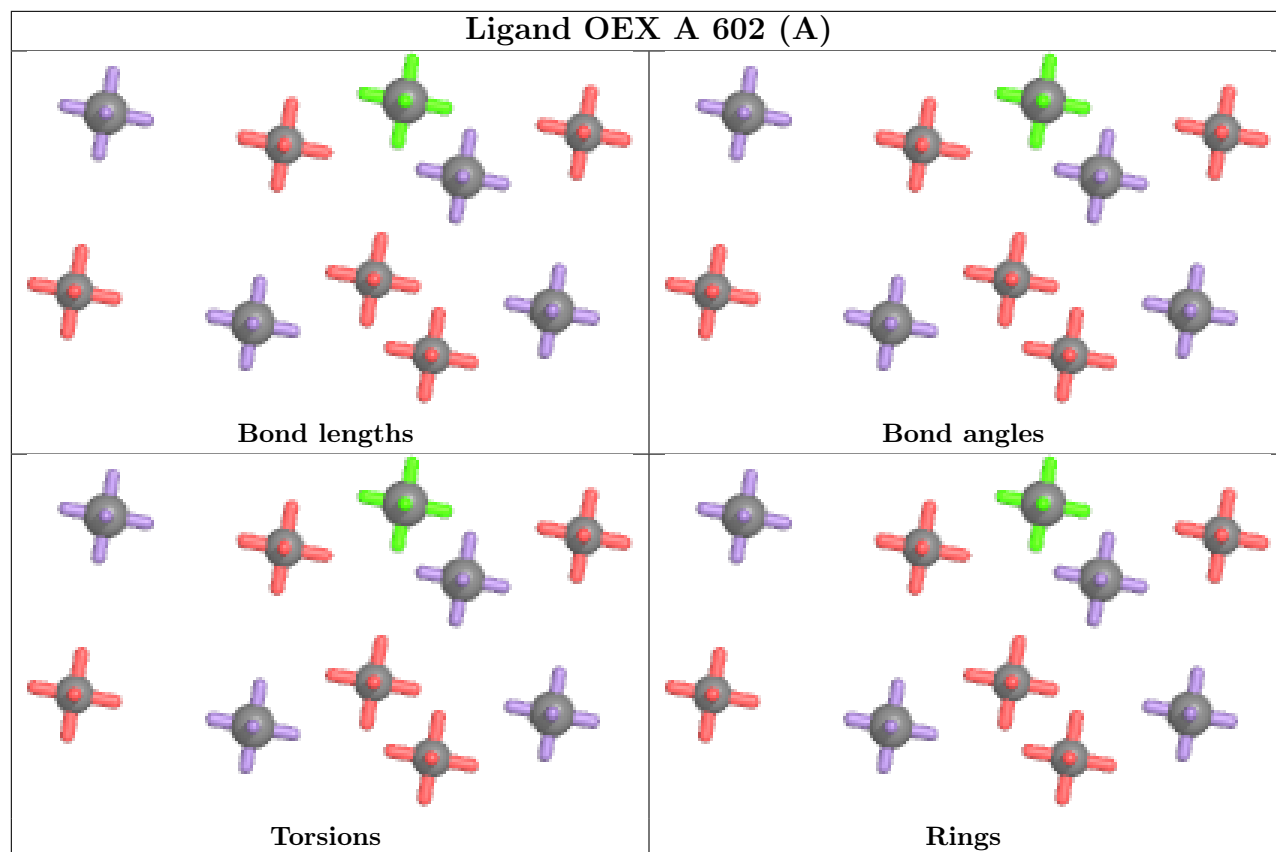


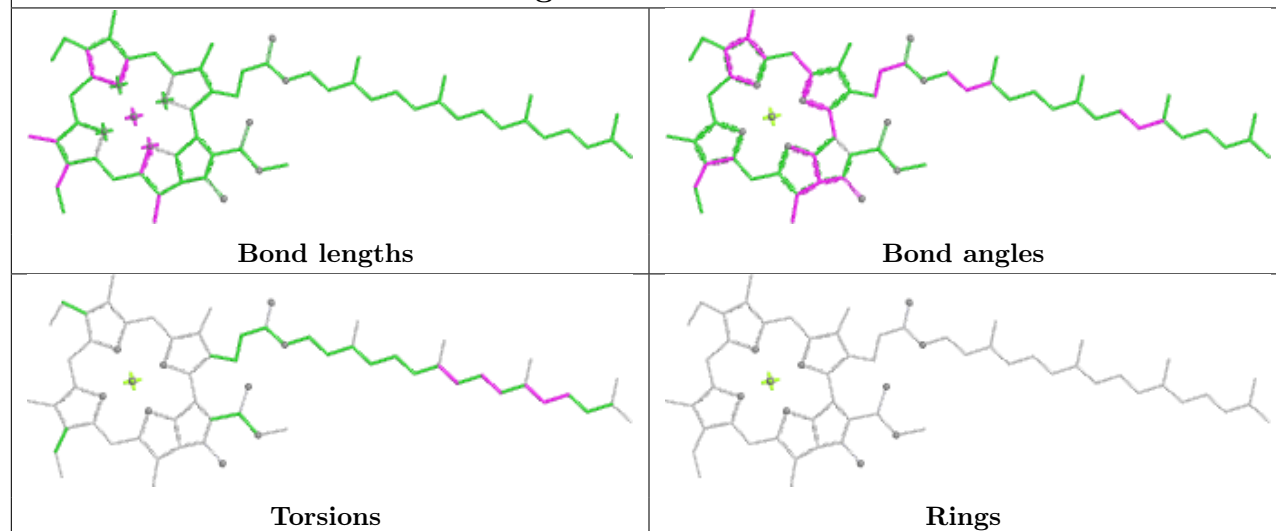
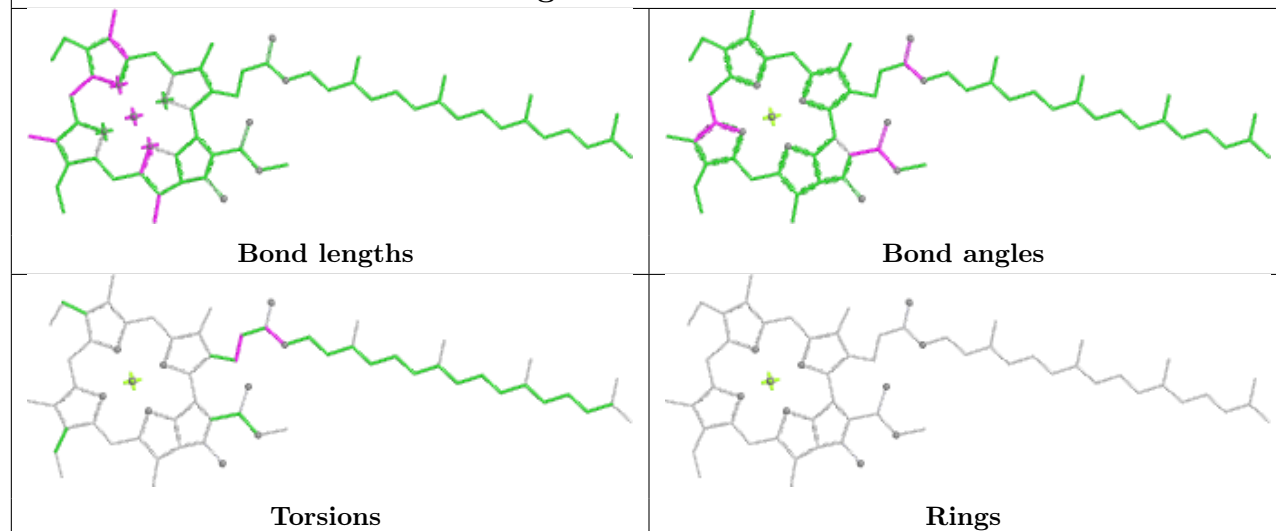
Ligand STE B 623	
 Bond lengths	 Bond angles
 Torsions	 Rings

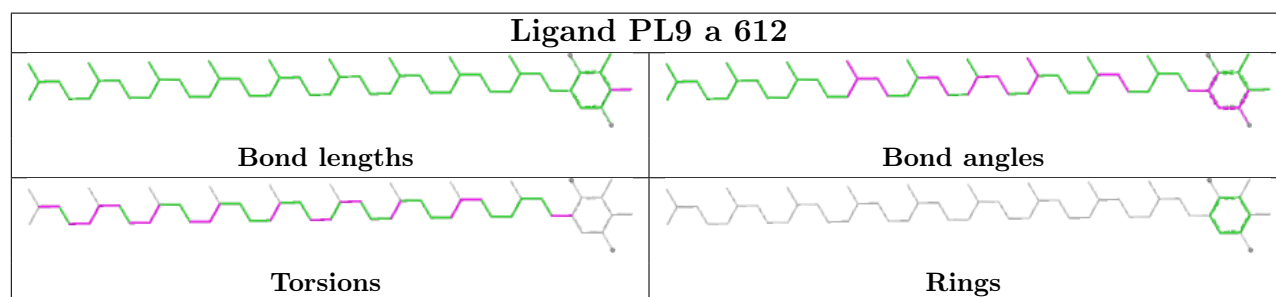
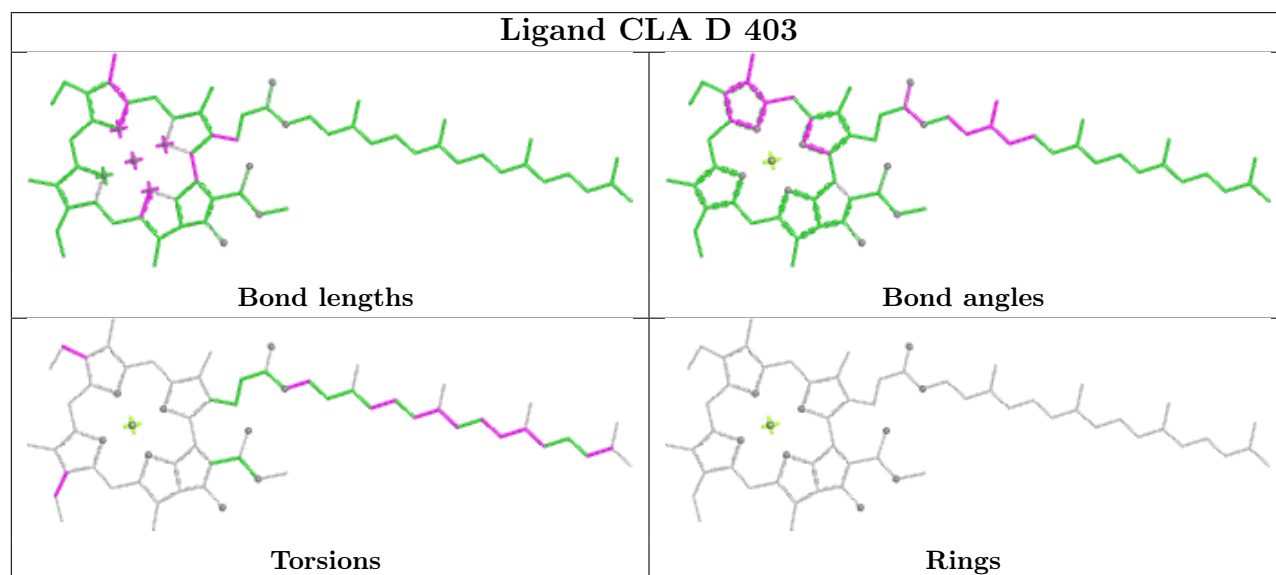
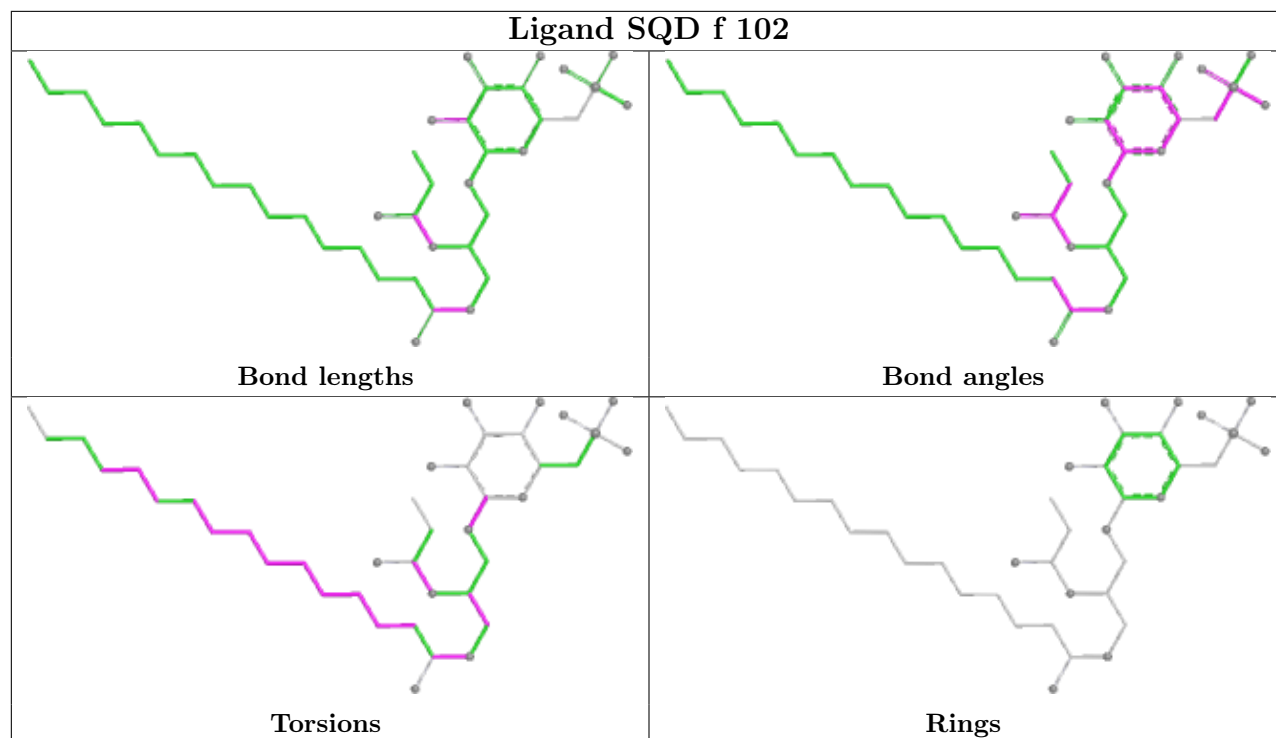
Ligand PHO A 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

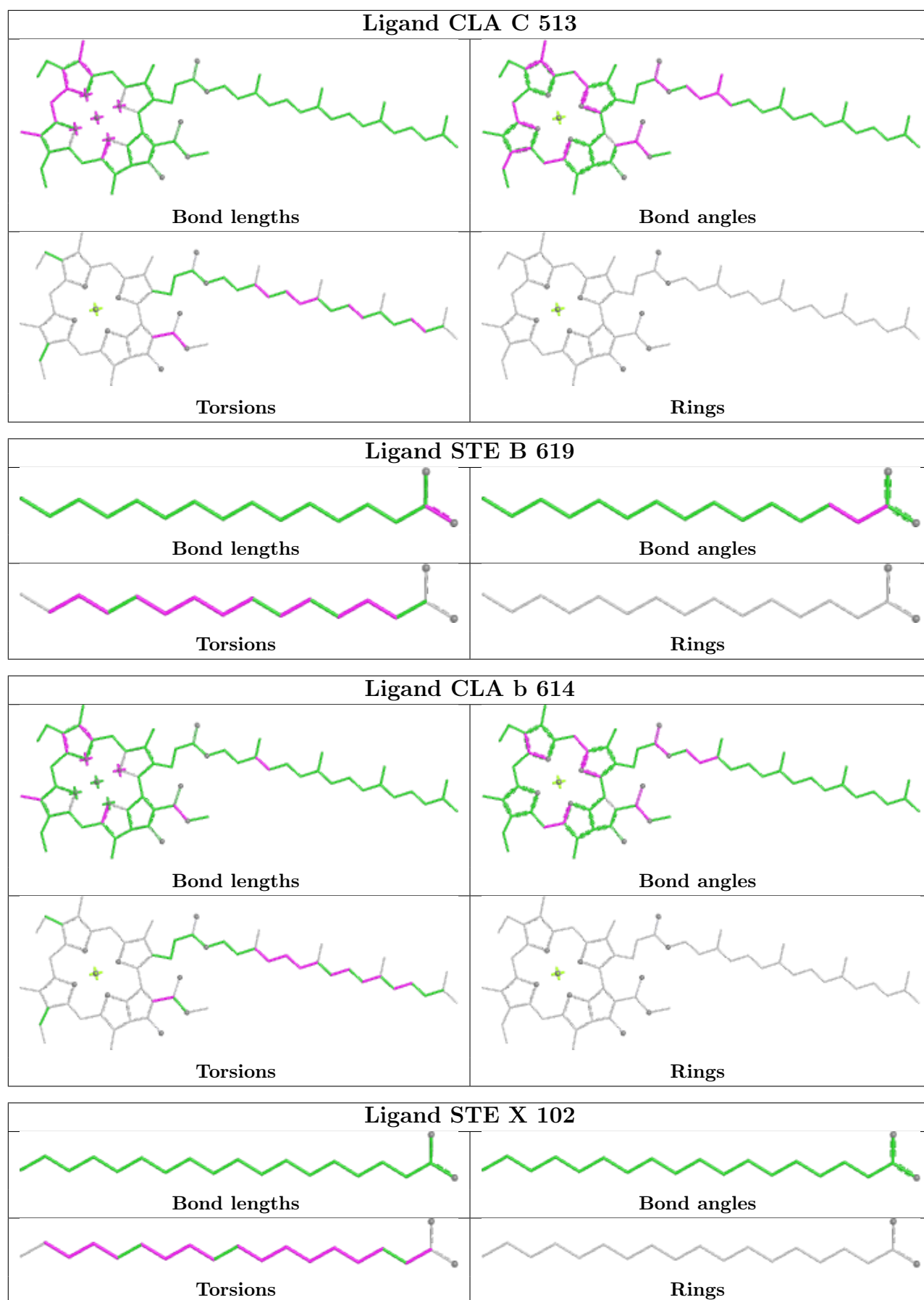
Ligand BCR b 618	
 Bond lengths	 Bond angles
 Torsions	 Rings

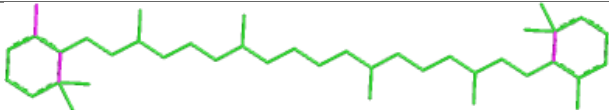
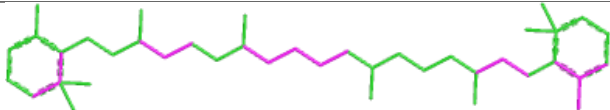
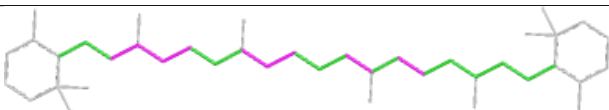
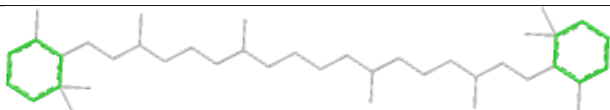
Ligand CLA c 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

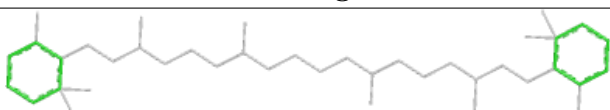


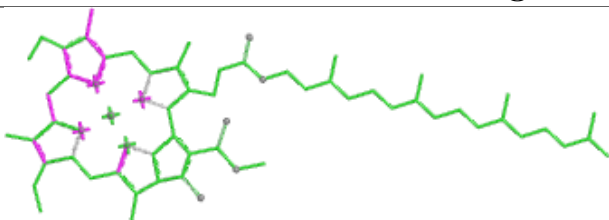
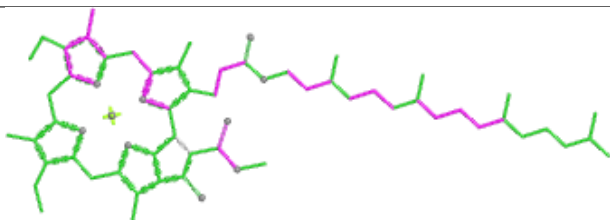
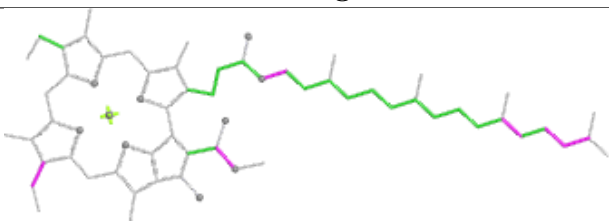
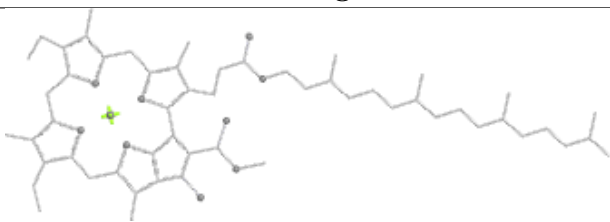
Ligand CLA b 612**Ligand CLA c 501**



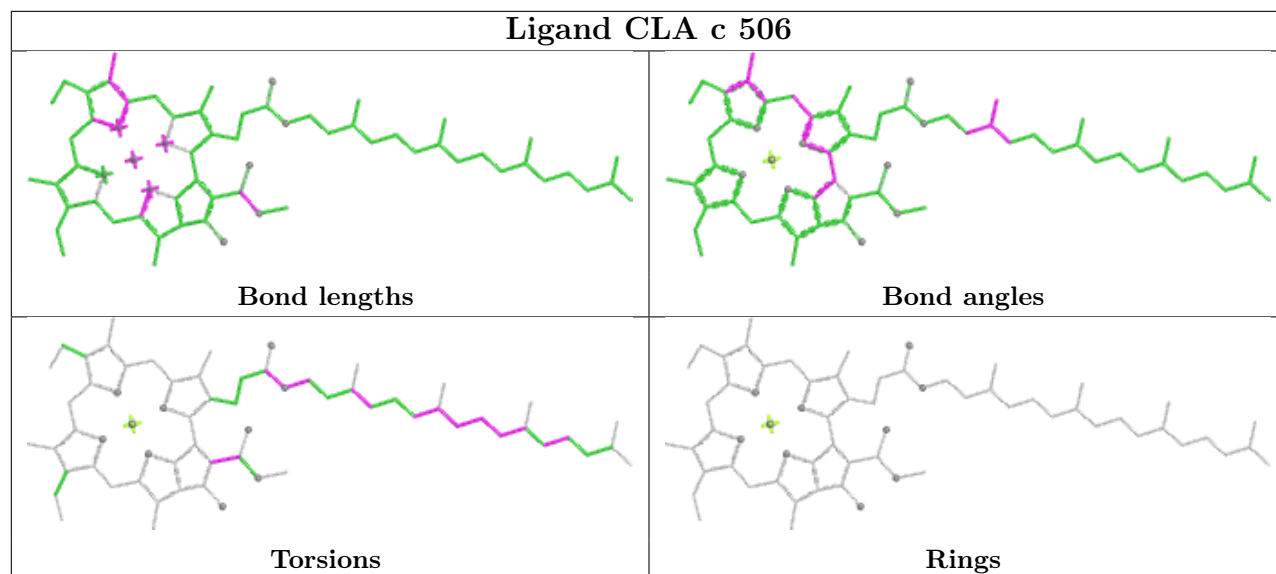


Ligand BCR K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

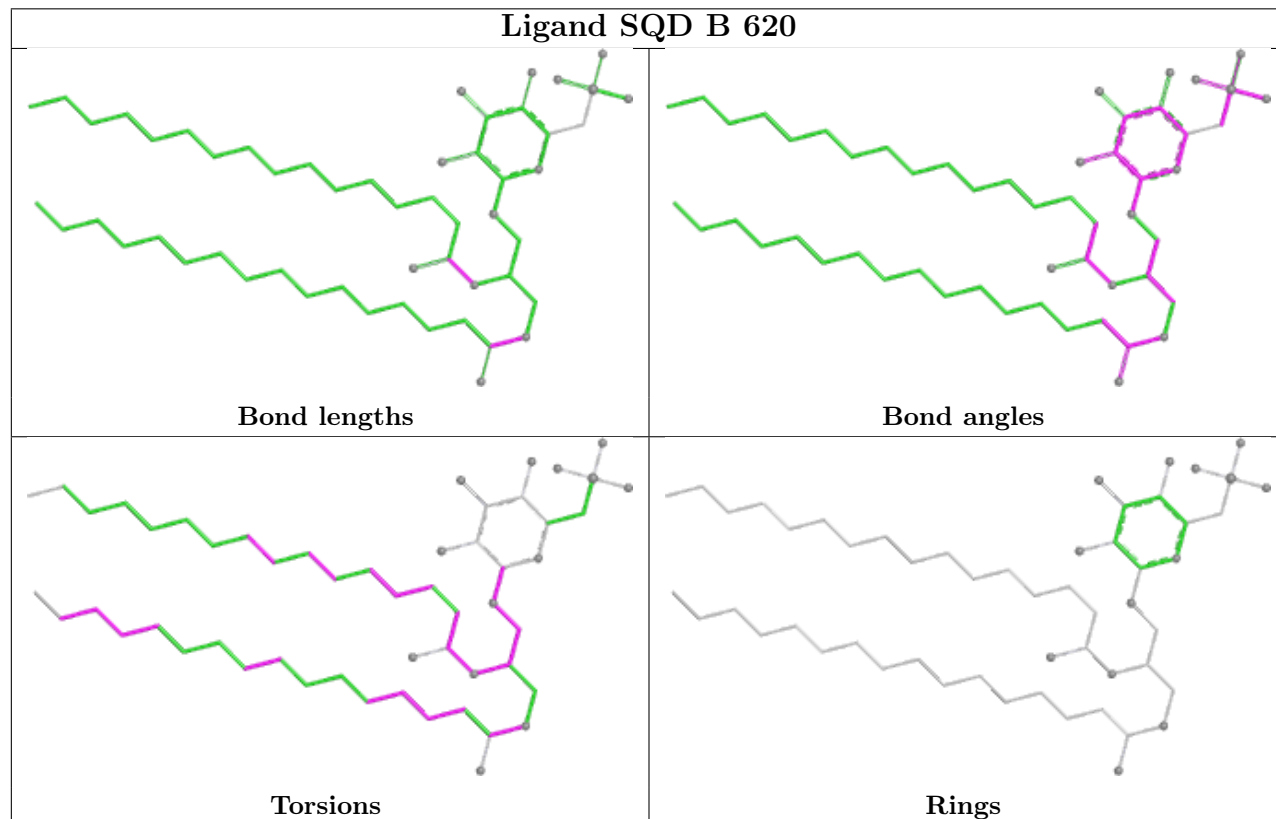
Ligand BCR k 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

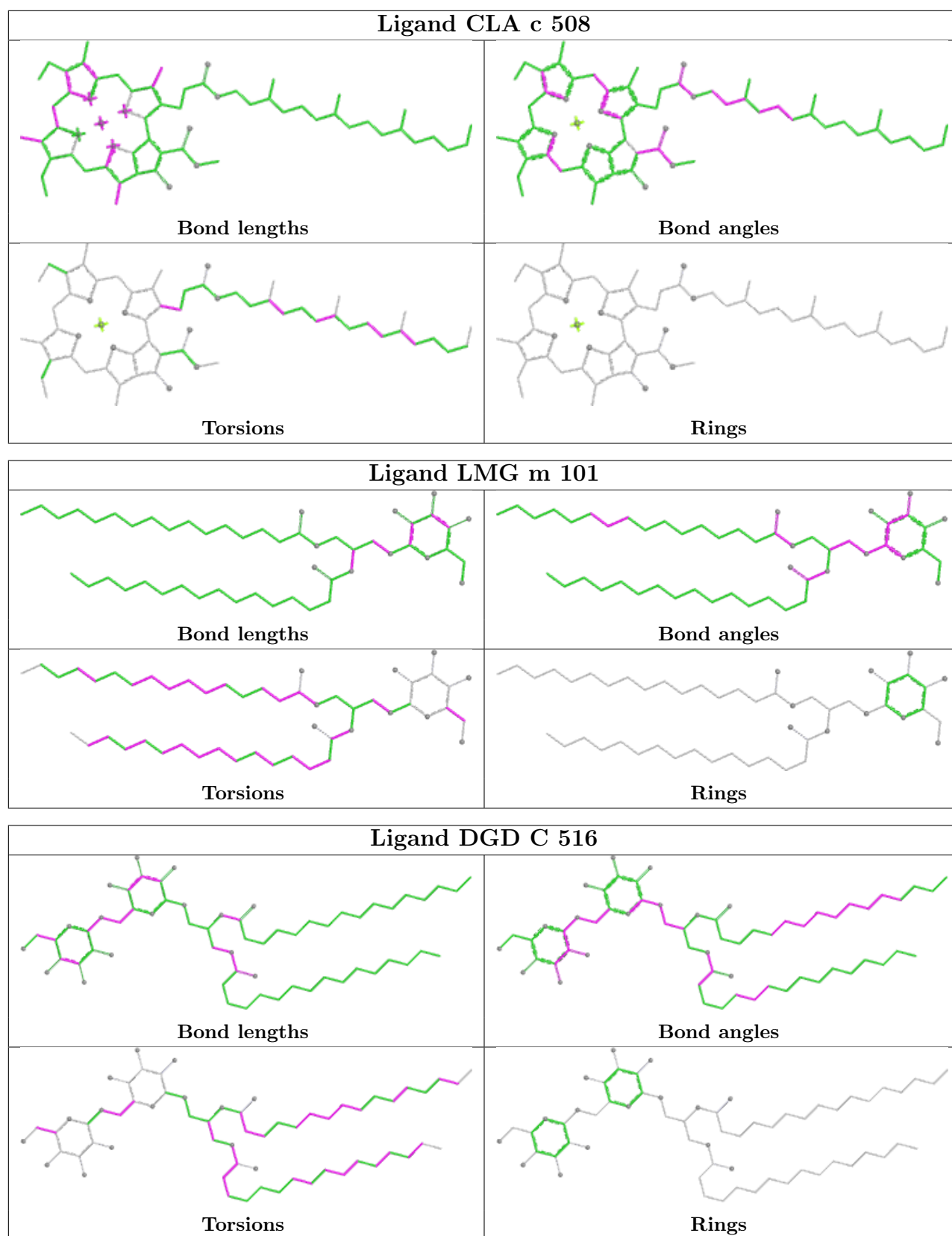
Ligand CLA A 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 506

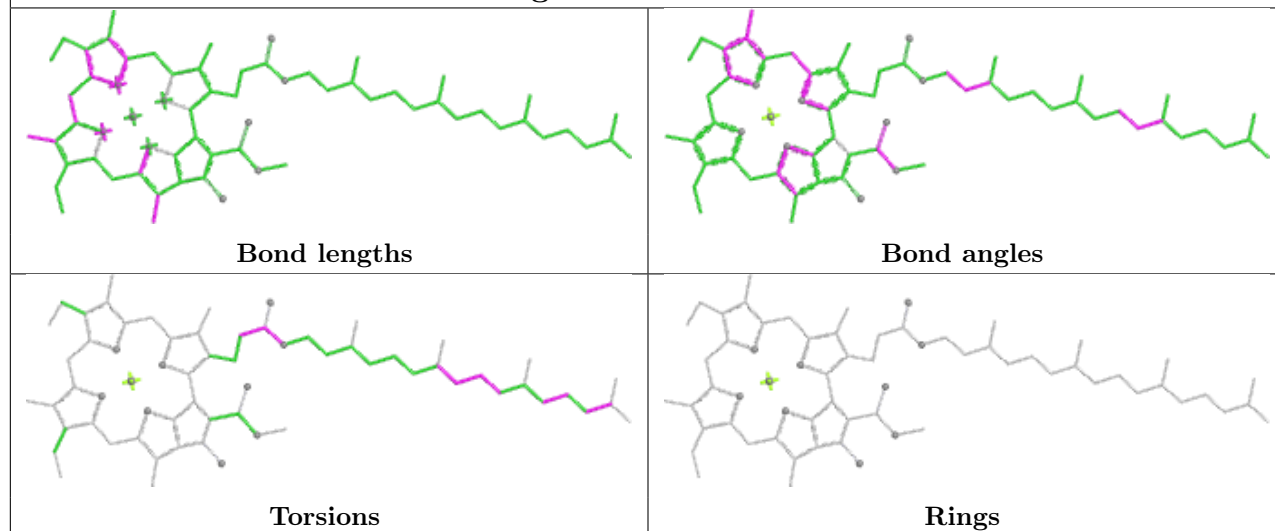


Ligand SQD B 620

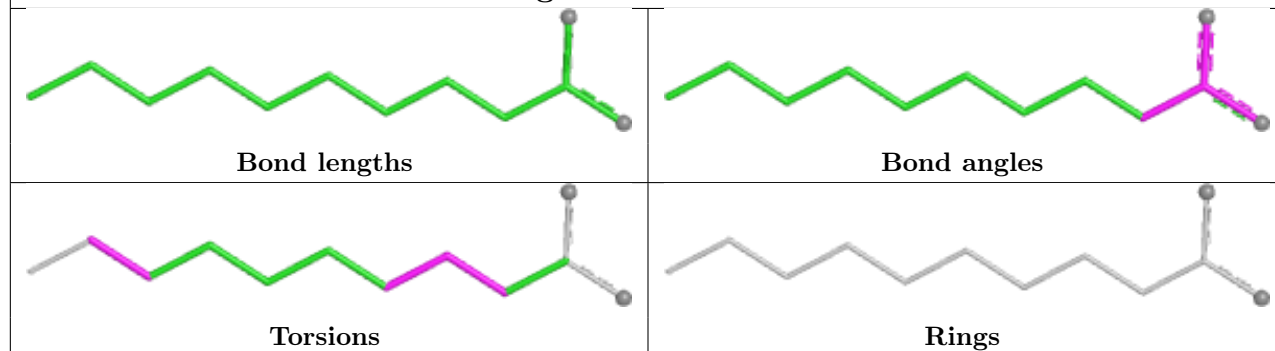




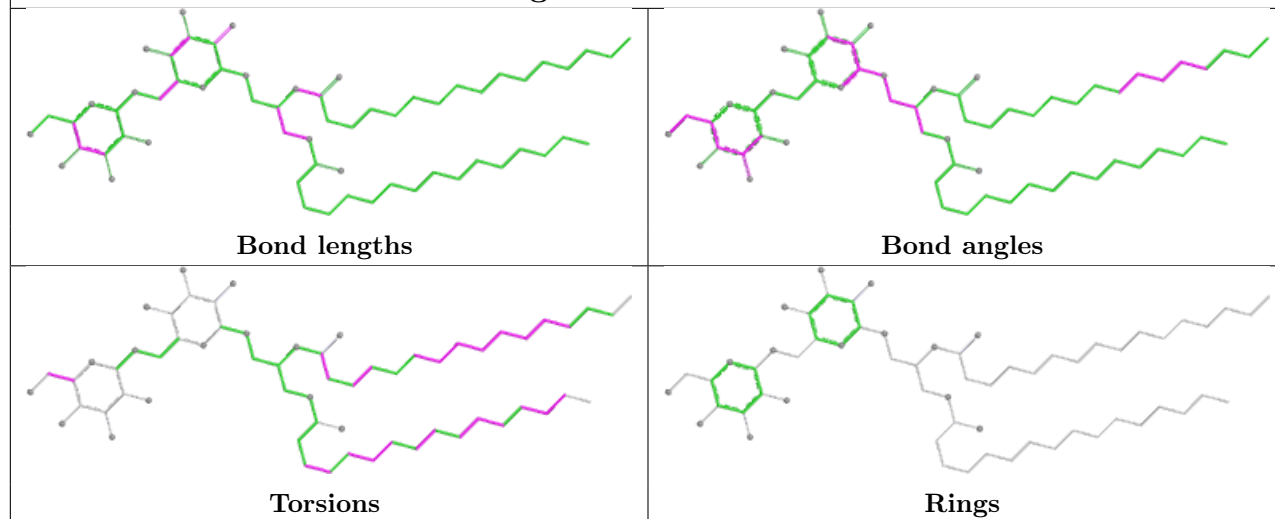
Ligand CLA B 611



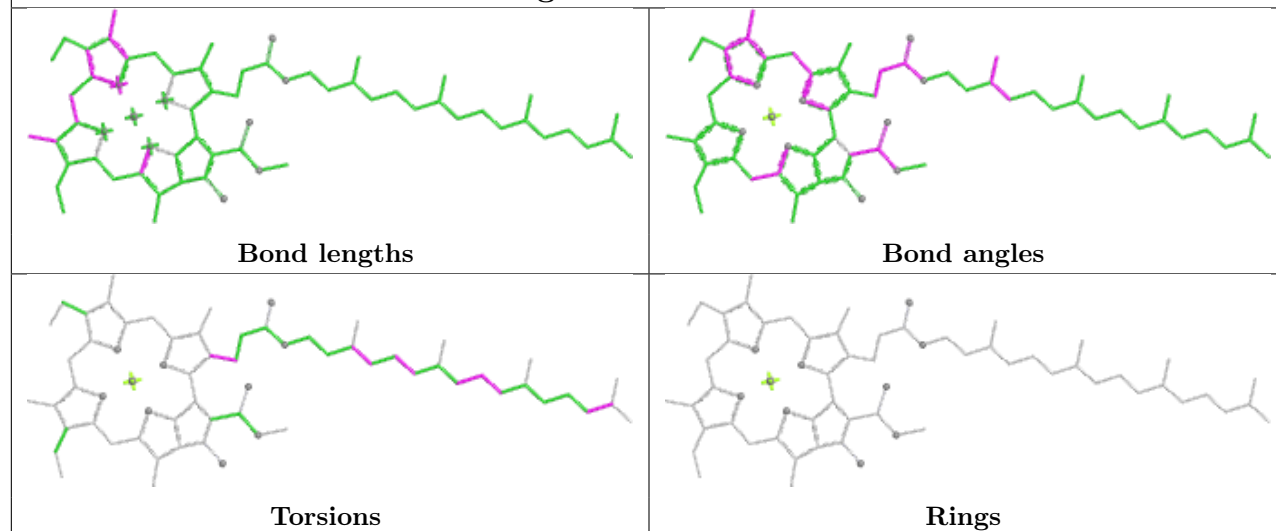
Ligand STE L 102



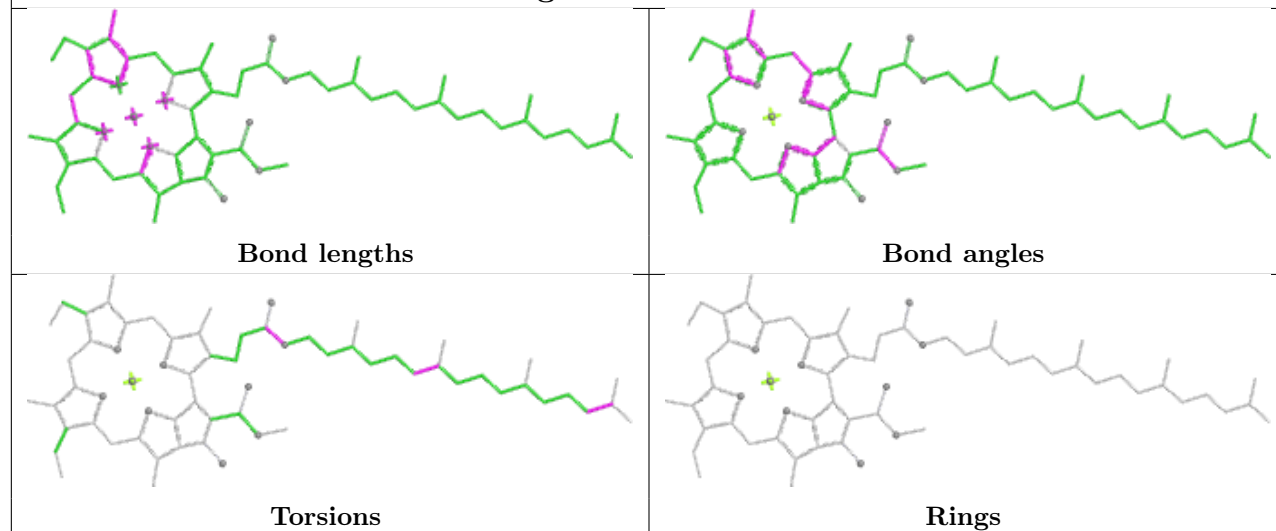
Ligand DGD h 102



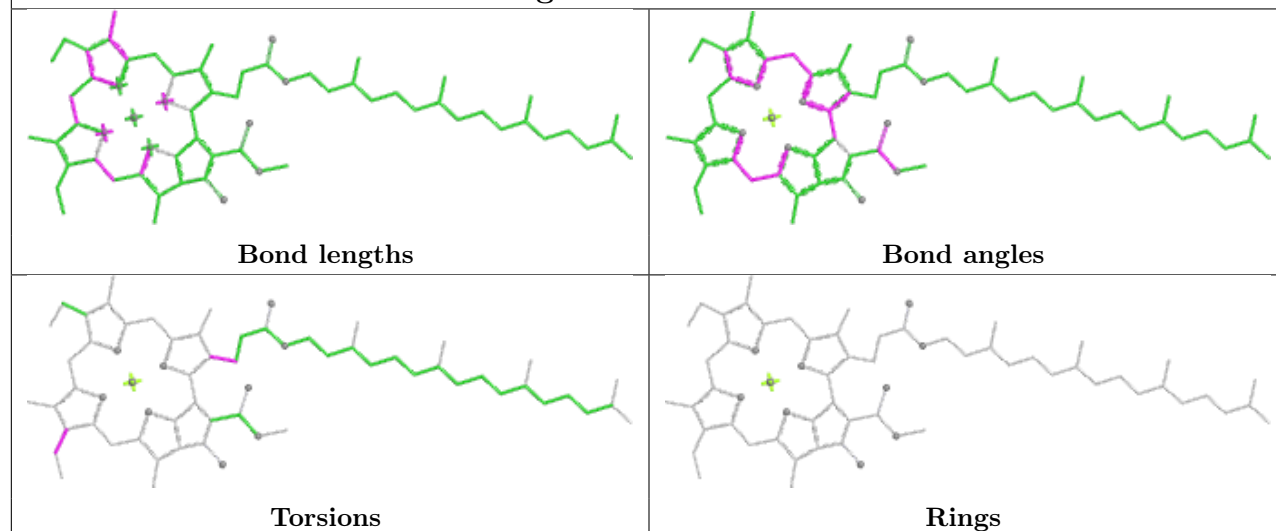
Ligand CLA c 513



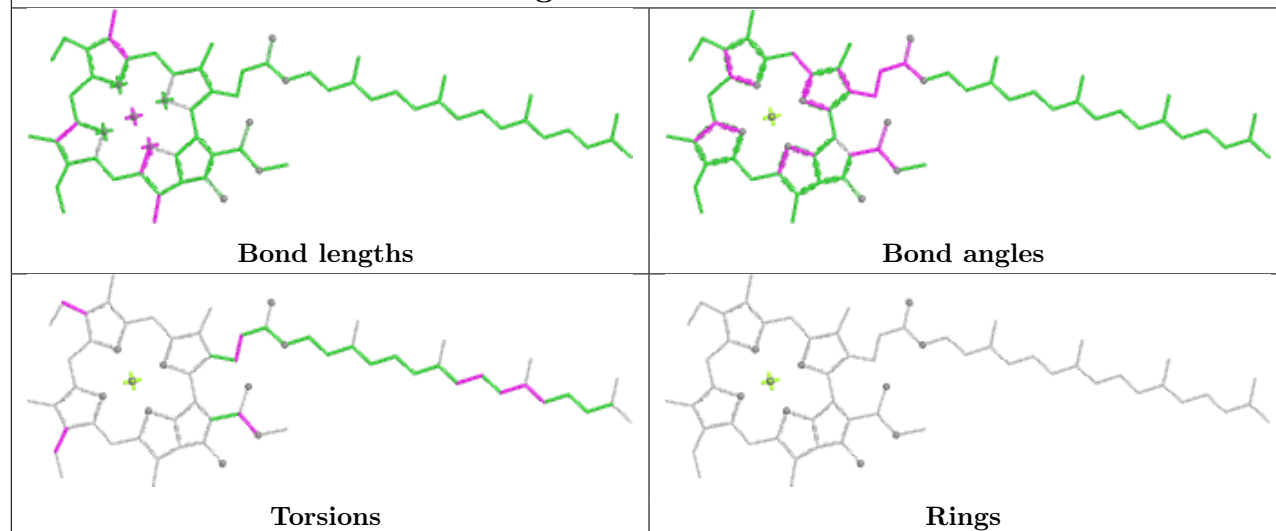
Ligand CLA c 511



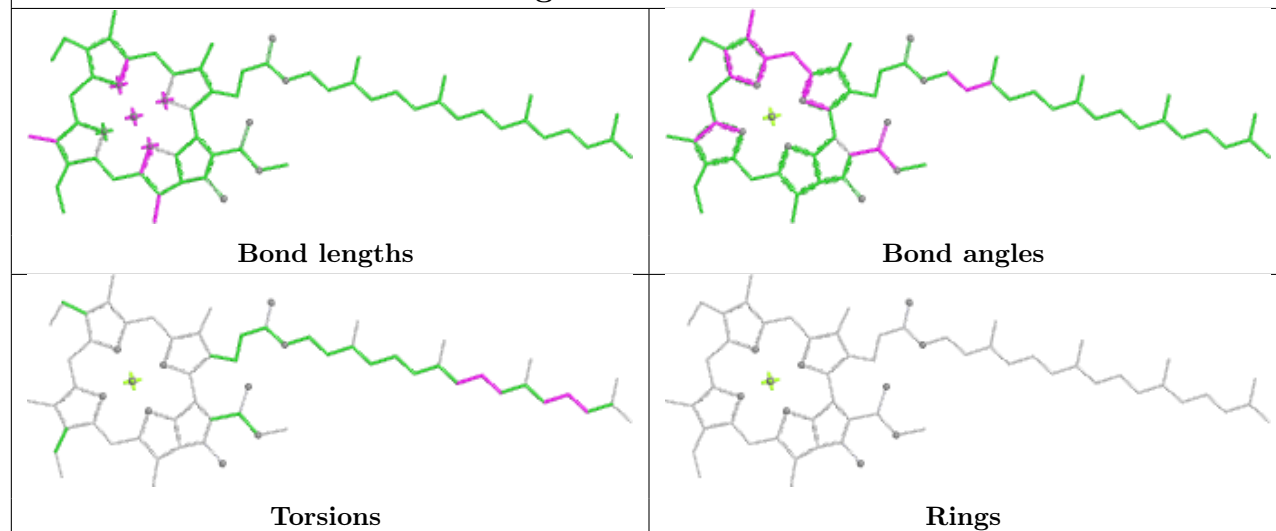
Ligand CLA a 613



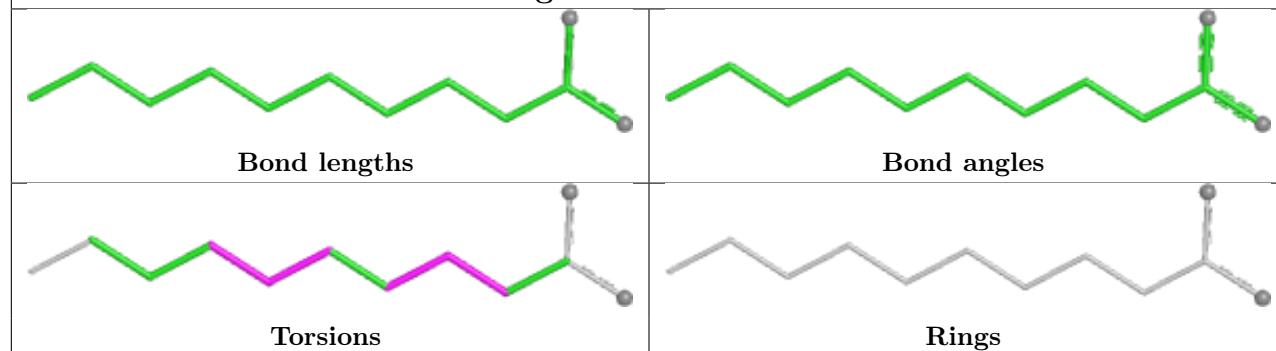
Ligand CLA b 610



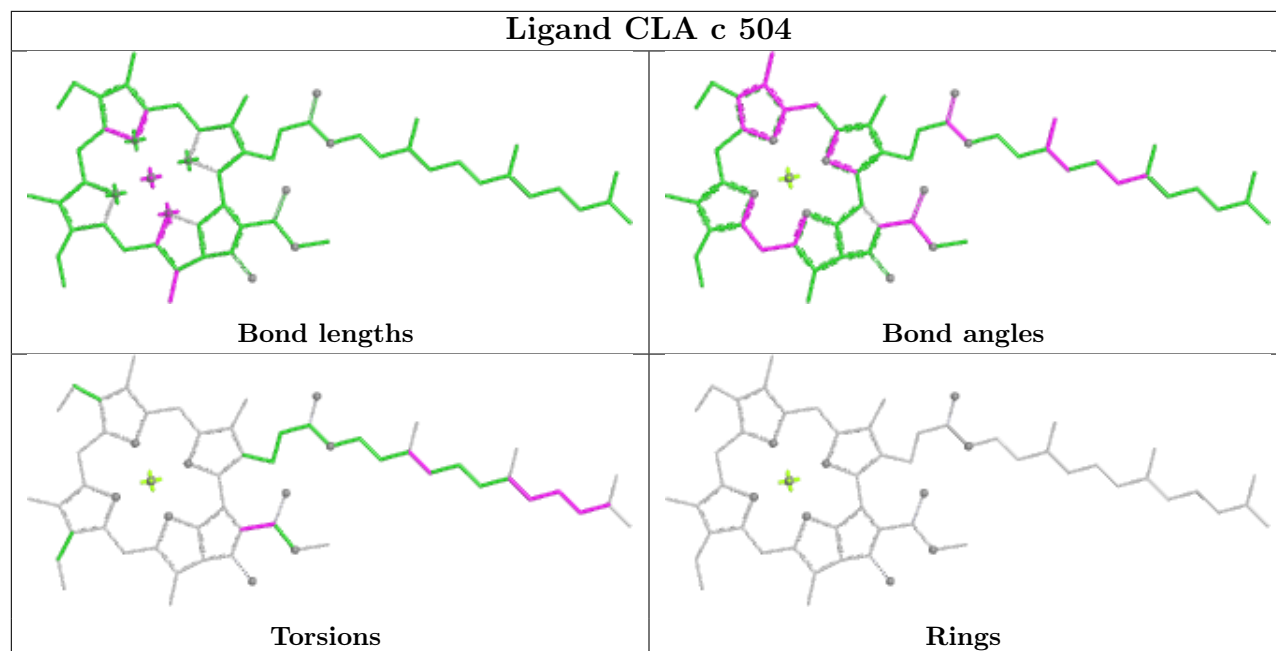
Ligand CLA b 611



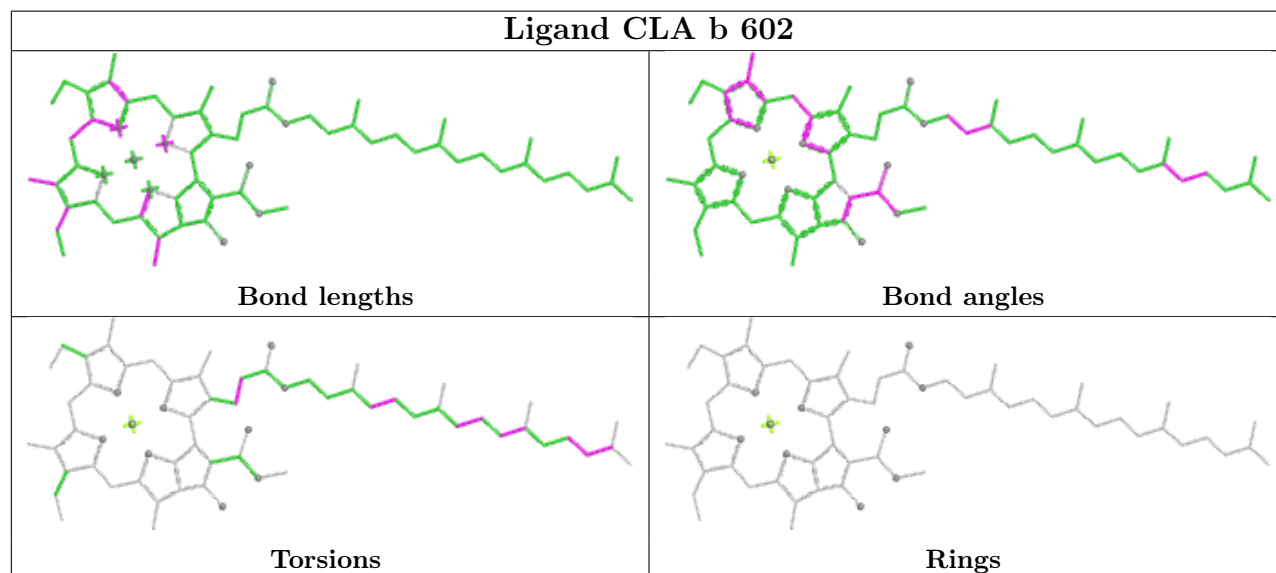
Ligand STE B 626

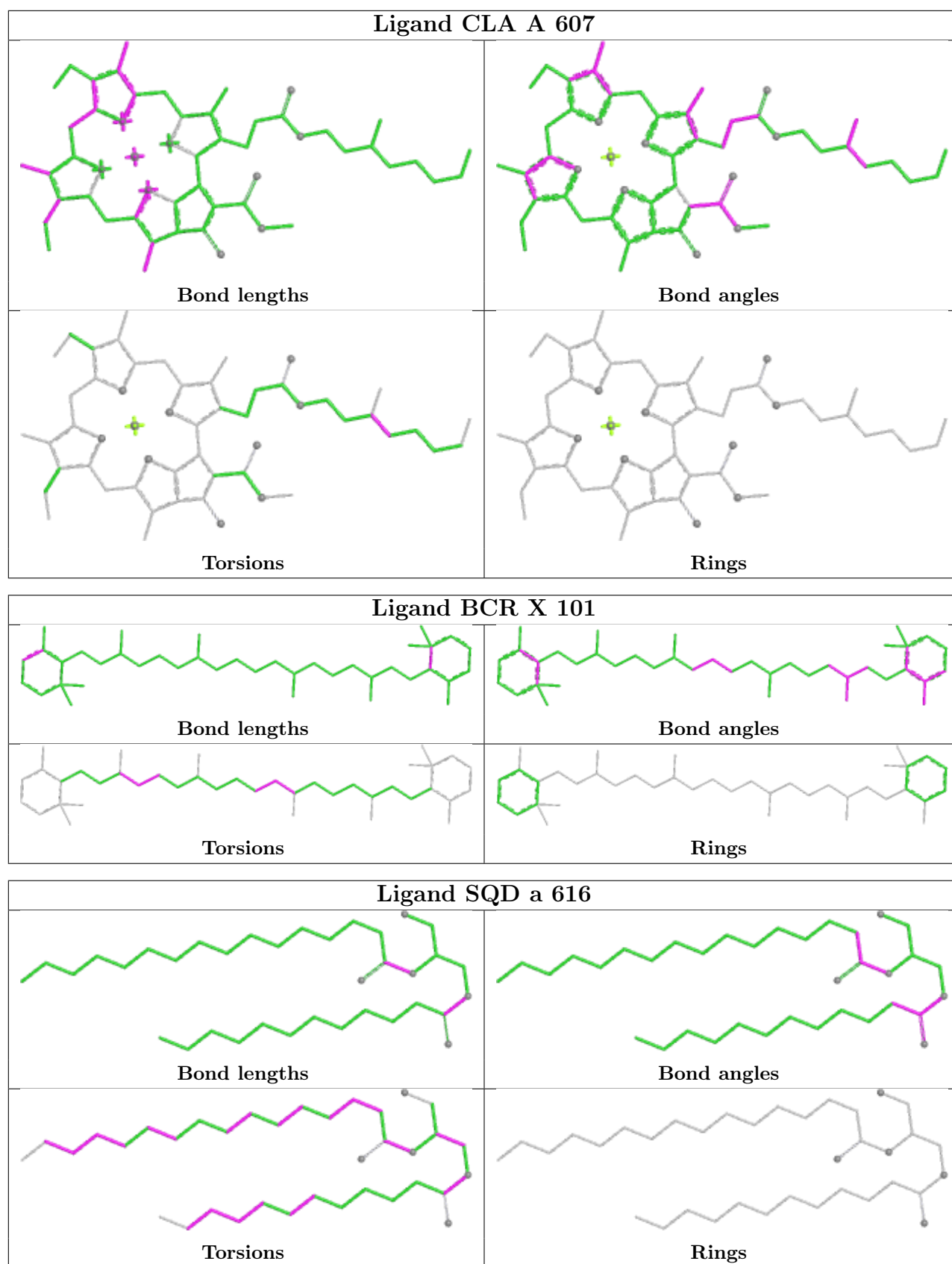


Ligand CLA c 504

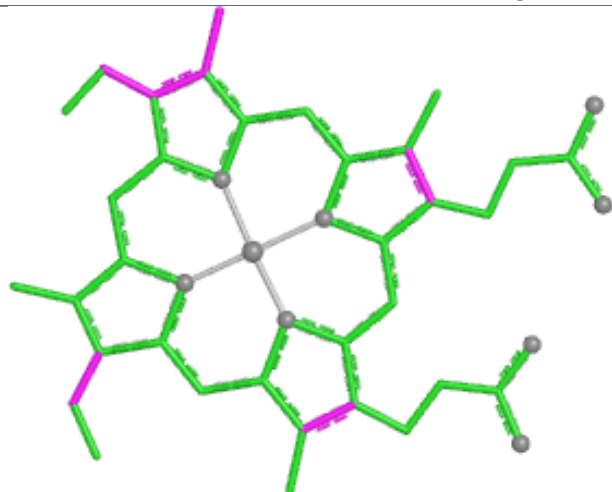


Ligand CLA b 602

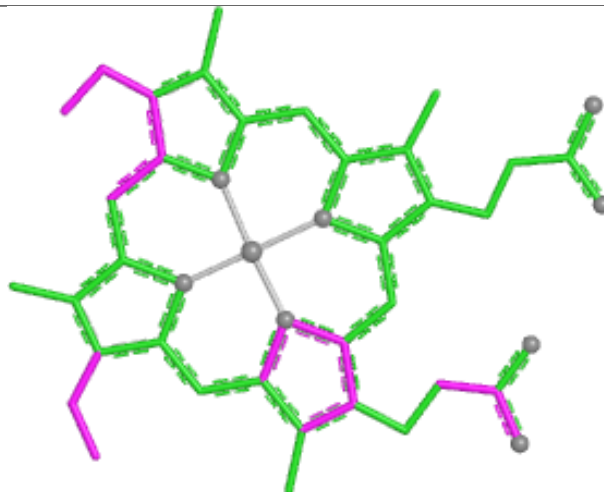




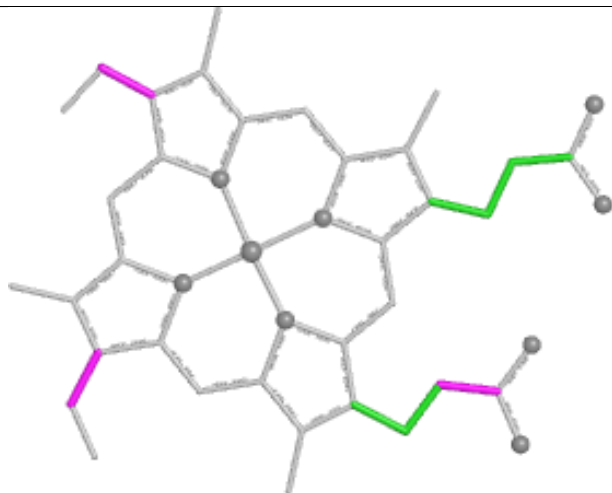
Ligand HEC V 201



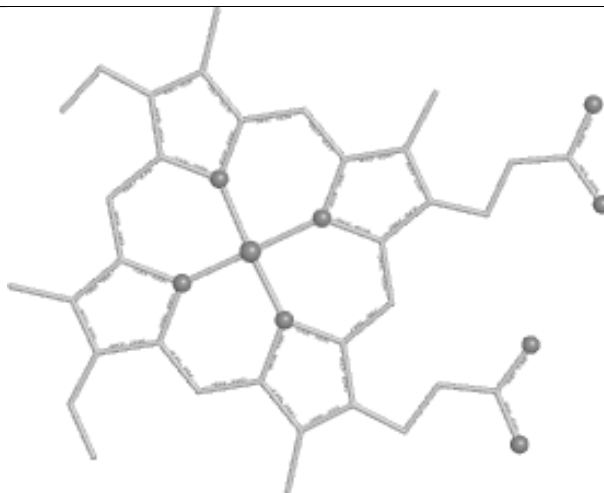
Bond lengths



Bond angles

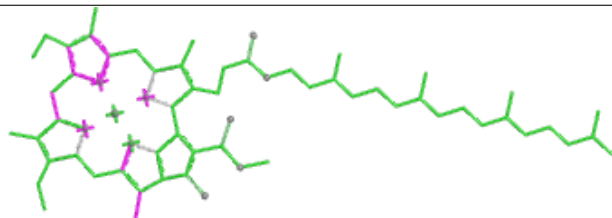


Torsions

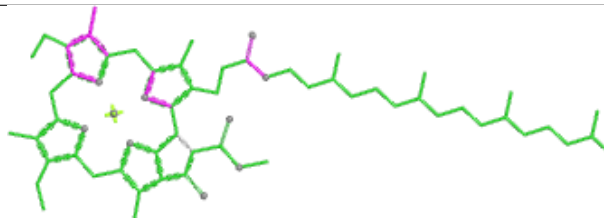


Rings

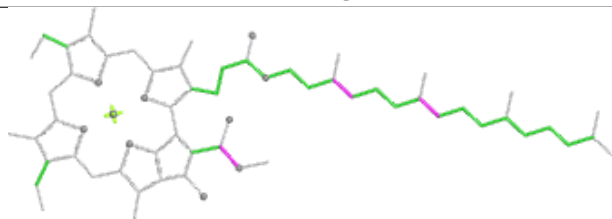
Ligand CLA C 510



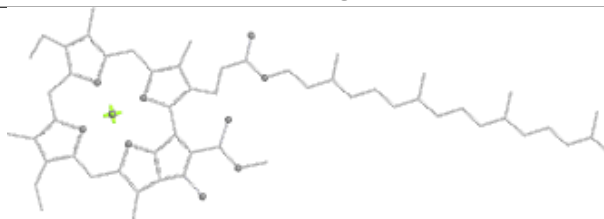
Bond lengths



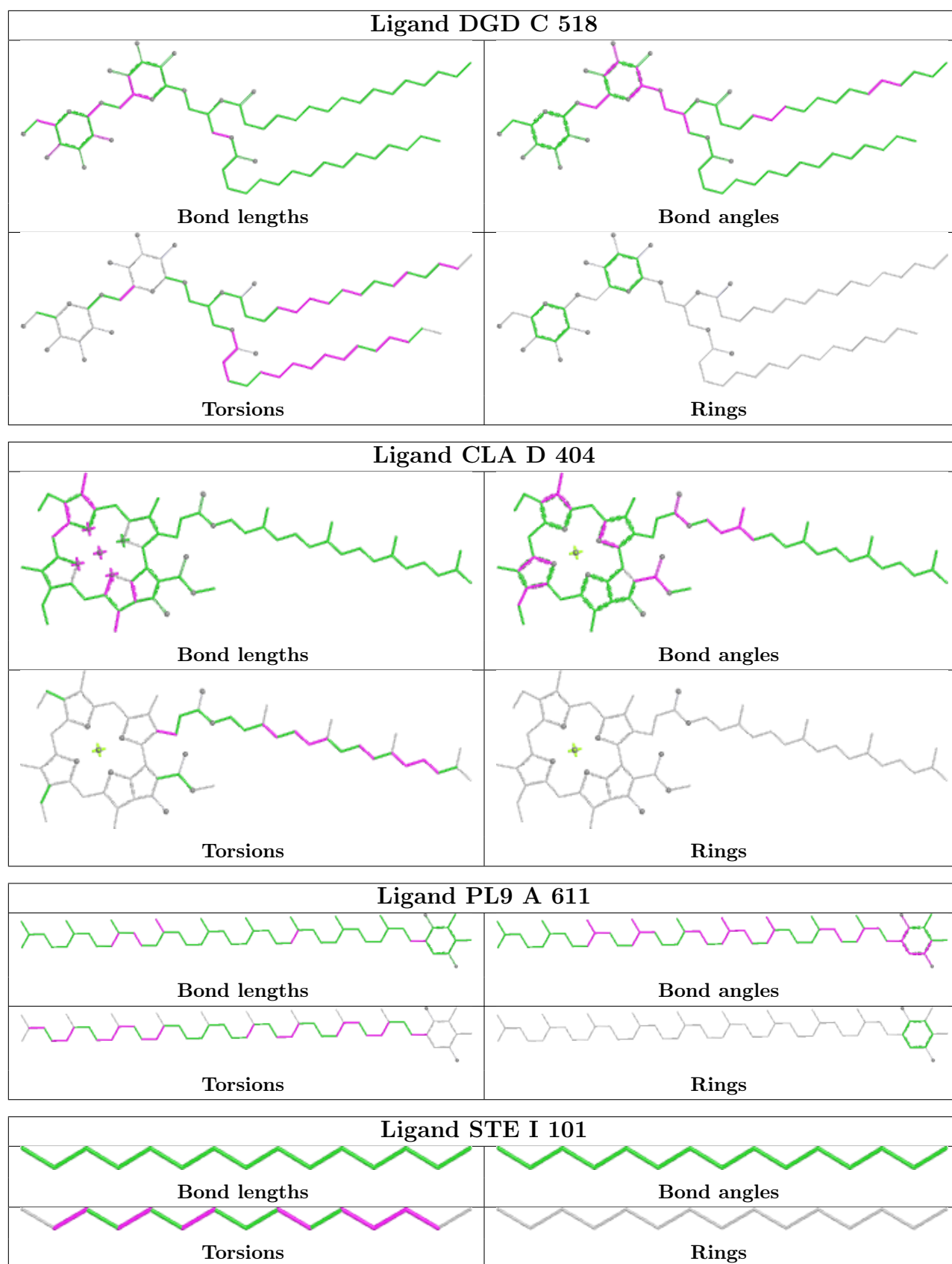
Bond angles

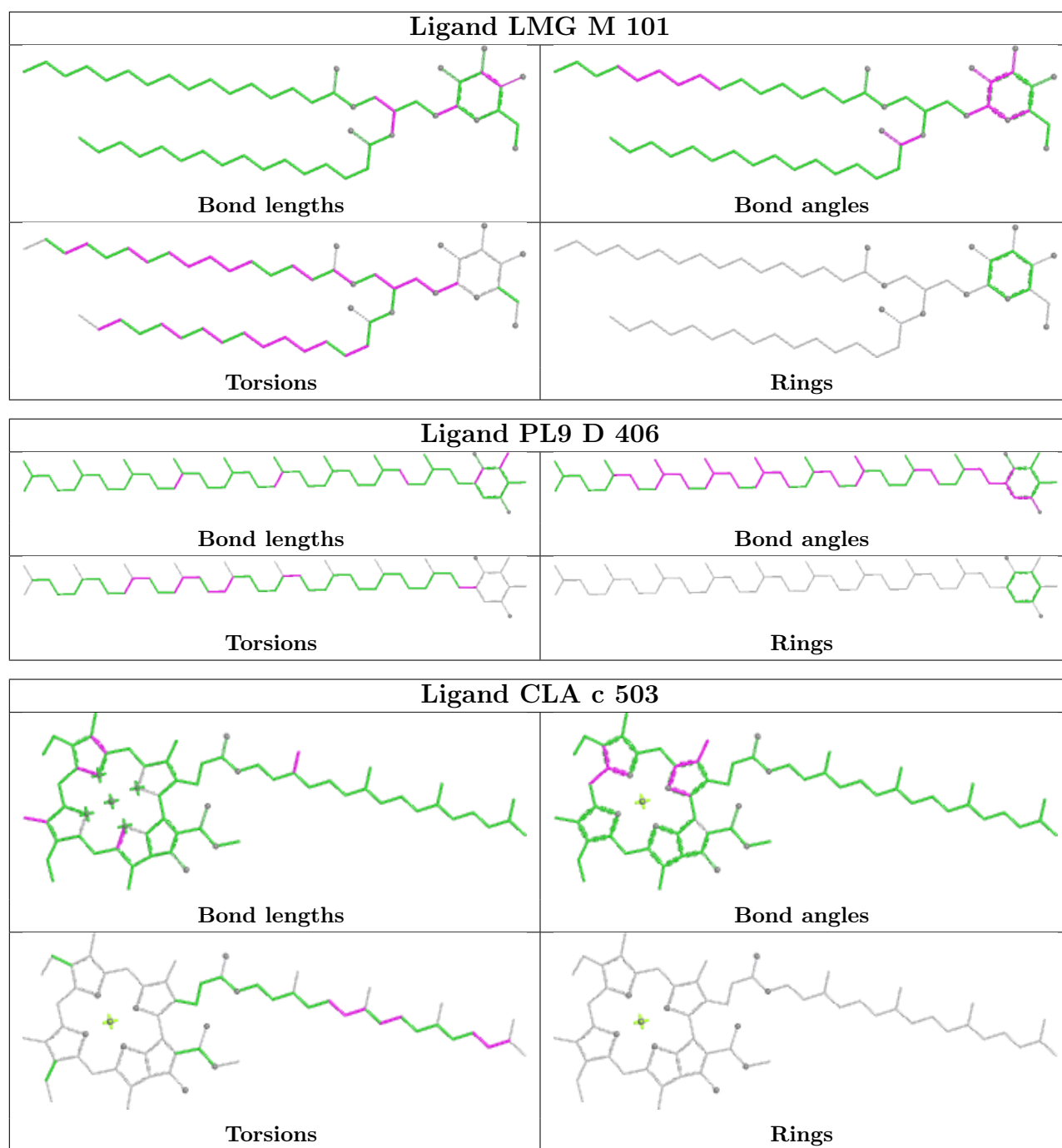


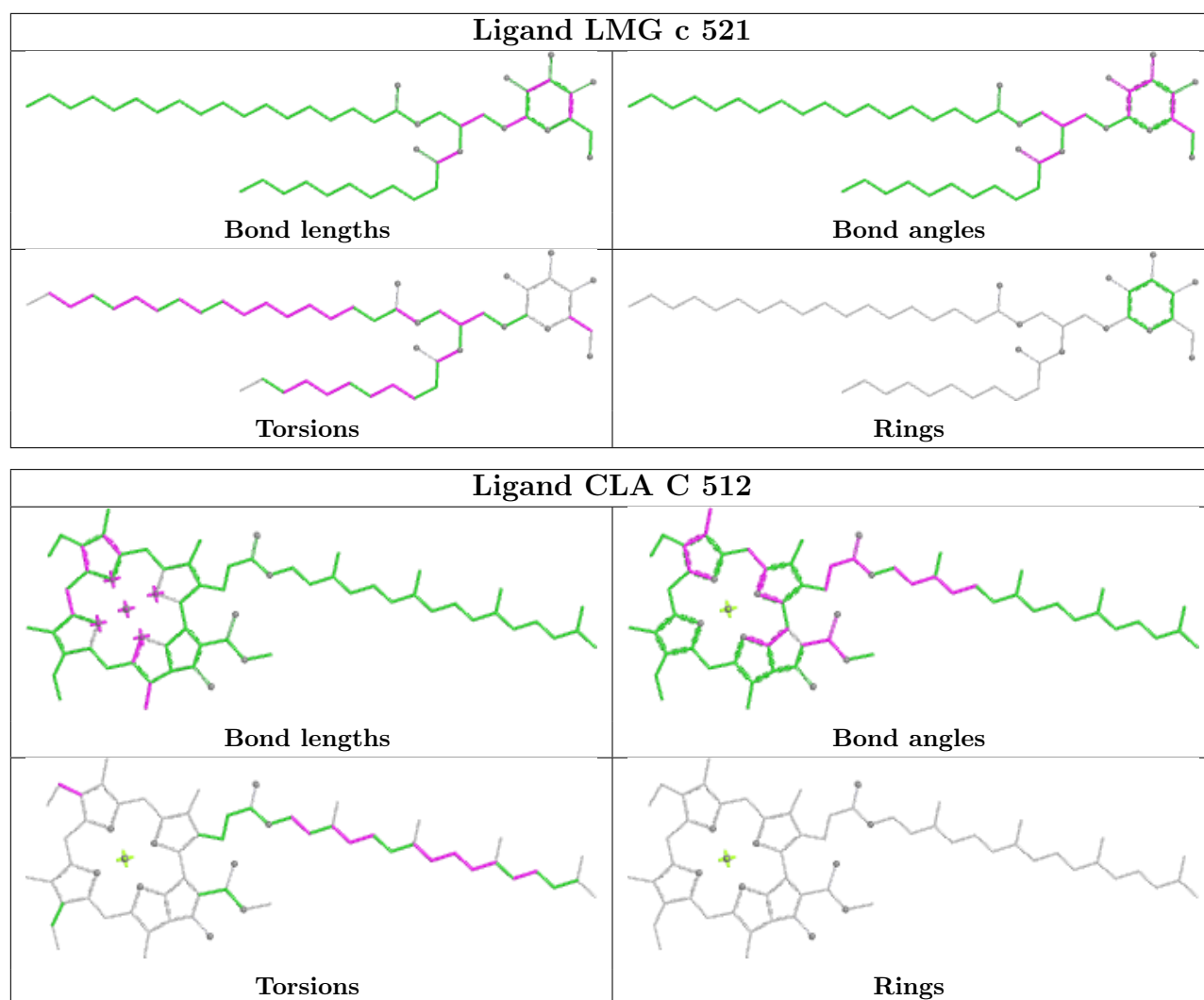
Torsions



Rings







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%)	-0.51	1 (0%) 90 91	16, 36, 59, 92	64 (19%)
1	a	334/344 (97%)	-0.41	5 (1%) 72 73	16, 38, 67, 90	64 (19%)
2	B	505/510 (99%)	-0.45	1 (0%) 91 92	22, 41, 69, 104	4 (0%)
2	b	505/510 (99%)	-0.35	5 (0%) 79 81	32, 44, 80, 119	0
3	C	442/461 (95%)	-0.41	0 100 100	18, 45, 62, 90	11 (2%)
3	c	451/461 (97%)	-0.31	3 (0%) 84 85	18, 48, 70, 106	12 (2%)
4	D	341/352 (96%)	-0.57	0 100 100	19, 38, 58, 92	2 (0%)
4	d	341/352 (96%)	-0.47	0 100 100	19, 41, 68, 94	3 (0%)
5	E	82/84 (97%)	0.10	3 (3%) 45 45	39, 60, 81, 94	1 (1%)
5	e	82/84 (97%)	0.28	3 (3%) 45 45	43, 71, 92, 101	0
6	F	34/45 (75%)	-0.09	1 (2%) 53 54	45, 53, 80, 106	0
6	f	34/45 (75%)	0.06	1 (2%) 53 54	49, 60, 100, 119	0
7	H	65/66 (98%)	-0.25	2 (3%) 51 51	39, 50, 67, 83	0
7	h	63/66 (95%)	0.01	1 (1%) 70 72	47, 61, 72, 79	0
8	I	35/38 (92%)	-0.37	2 (5%) 29 27	39, 47, 76, 95	0
8	i	35/38 (92%)	-0.23	0 100 100	39, 48, 80, 86	0
9	J	36/40 (90%)	-0.01	1 (2%) 55 55	44, 60, 92, 103	0
9	j	36/40 (90%)	0.00	1 (2%) 55 55	46, 63, 100, 114	0
10	K	37/46 (80%)	0.01	0 100 100	53, 63, 87, 92	0
10	k	37/46 (80%)	0.10	0 100 100	55, 66, 85, 92	0
11	L	37/37 (100%)	-0.63	0 100 100	33, 37, 70, 75	0
11	l	36/37 (97%)	-0.52	1 (2%) 55 55	29, 39, 73, 96	0
12	M	32/36 (88%)	-0.42	1 (3%) 51 51	32, 42, 65, 79	0
12	m	31/36 (86%)	-0.48	0 100 100	33, 42, 62, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.21	2 (0%) 82 84	32, 50, 89, 135	1 (0%)
13	o	244/272 (89%)	-0.26	2 (0%) 82 84	31, 48, 87, 133	0
14	R	28/41 (68%)	1.53	9 (32%) 1 1	81, 97, 111, 119	0
14	r	28/41 (68%)	2.22	15 (53%) 0 0	90, 127, 142, 149	0
15	T	29/32 (90%)	-0.52	0 100 100	33, 39, 66, 86	0
15	t	29/32 (90%)	-0.40	1 (3%) 48 48	35, 40, 76, 84	0
16	U	97/134 (72%)	-0.30	0 100 100	39, 52, 76, 96	0
16	u	97/134 (72%)	-0.37	0 100 100	37, 48, 63, 91	0
17	V	137/163 (84%)	-0.41	0 100 100	34, 48, 65, 79	0
17	v	137/163 (84%)	-0.17	0 100 100	40, 56, 78, 87	0
18	X	38/41 (92%)	-0.07	0 100 100	48, 61, 83, 86	0
18	x	39/41 (95%)	0.30	1 (2%) 57 58	54, 72, 99, 115	0
19	Y	27/46 (58%)	0.92	2 (7%) 20 18	64, 85, 99, 105	0
19	y	30/46 (65%)	0.65	0 100 100	68, 84, 103, 109	0
20	Z	62/62 (100%)	0.60	4 (6%) 25 23	65, 81, 128, 135	0
20	z	62/62 (100%)	0.67	5 (8%) 18 16	68, 79, 118, 135	0
All	All	5293/5700 (92%)	-0.28	73 (1%) 73 75	16, 46, 85, 149	162 (3%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
18	x	40	SER	6.4
14	r	14	LEU	5.0
13	o	58	ASN	4.7
20	z	33	TRP	3.9
14	r	20	VAL	3.8
20	Z	62	VAL	3.8
15	t	30	THR	3.8
19	Y	20	ALA	3.7
13	O	60	ARG	3.7
20	Z	41	PHE	3.6
3	c	23	ALA	3.5
14	R	13	LEU	3.4
14	r	29	LYS	3.4
20	z	30	PRO	3.2
14	r	3	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
14	r	9	LEU	3.2
1	a	249	VAL	3.1
19	Y	22	LEU	3.1
1	a	11	ALA	3.0
5	e	3	GLY	3.0
14	r	5	VAL	2.9
5	e	79	PHE	2.9
14	R	29	LYS	2.9
2	b	495	PHE	2.9
6	f	15	ILE	2.8
9	j	5	GLY	2.8
5	E	79	PHE	2.8
7	H	66	GLY	2.8
13	O	59	LYS	2.7
1	a	248	ILE	2.7
2	b	502	VAL	2.7
14	r	18	TRP	2.7
1	a	250	ALA	2.6
14	r	28	VAL	2.6
6	F	12	SER	2.6
5	E	84	LYS	2.6
14	r	25	PRO	2.5
5	E	3	GLY	2.5
14	R	20	VAL	2.5
13	o	57	LYS	2.5
12	M	33	GLN	2.5
14	r	26	TYR	2.5
1	A	11	ALA	2.4
9	J	5	GLY	2.4
14	r	24	LEU	2.4
20	z	27	TYR	2.4
14	R	7	VAL	2.4
20	Z	30	PRO	2.3
3	c	24	THR	2.3
3	c	134	ILE	2.3
14	r	12	VAL	2.3
14	r	2	ASP	2.3
14	R	3	TRP	2.3
2	b	499	VAL	2.3
14	R	28	VAL	2.3
1	a	251	ALA	2.3
5	e	4	THR	2.3

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Mol	Chain	Res	Type	RSRZ
20	z	60	PHE	2.3
8	I	36	ASP	2.2
14	r	6	LEU	2.2
20	z	62	VAL	2.2
8	I	34	ARG	2.2
14	r	7	VAL	2.2
14	R	12	VAL	2.1
7	H	41	PHE	2.1
14	R	27	ALA	2.1
2	B	499	VAL	2.1
2	b	84	THR	2.1
7	h	64	ALA	2.1
11	l	2	GLU	2.1
2	b	491	VAL	2.1
20	Z	33	TRP	2.1
14	R	6	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	FME	I	1	10/11	0.95	0.08	45,56,68,71	0
12	FME	M	1	10/11	0.95	0.09	45,54,73,74	0
15	FME	T	1	10/11	0.95	0.08	37,46,65,67	0
8	FME	i	1	10/11	0.95	0.08	46,57,67,70	0
15	FME	t	1	10/11	0.95	0.08	34,48,77,77	0
12	FME	m	1	10/11	0.96	0.08	39,54,76,81	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	STE	I	101	15/20	0.70	0.20	45,62,89,90	0
32	STE	d	411	20/20	0.72	0.18	54,78,96,100	0
32	STE	B	623	18/20	0.74	0.19	54,80,90,94	0
30	LHG	e	101	42/49	0.77	0.16	59,92,114,126	0
30	LHG	A	614	49/49	0.77	0.16	51,87,115,118	0
32	STE	a	618	12/20	0.78	0.14	40,72,79,81	0
32	STE	b	623	16/20	0.79	0.17	50,67,85,92	0
32	STE	L	102	12/20	0.79	0.18	54,70,85,93	0
32	STE	b	625	10/20	0.80	0.16	47,58,68,69	0
24	CLA	b	601	65/65	0.80	0.14	54,74,95,108	0
33	LMG	D	411	33/55	0.80	0.15	44,61,84,94	0
33	LMG	b	622	55/55	0.80	0.17	54,76,98,109	0
33	LMG	c	521	48/55	0.80	0.16	43,78,104,111	0
32	STE	h	103	14/20	0.81	0.18	60,77,87,92	0
32	STE	R	101	12/20	0.81	0.19	66,87,95,107	0
32	STE	B	624	16/20	0.82	0.15	38,69,90,91	0
32	STE	a	617	10/20	0.82	0.15	37,70,76,81	0
32	STE	b	624	20/20	0.83	0.14	42,67,87,89	0
28	PL9	A	611	55/55	0.83	0.16	38,69,87,92	0
33	LMG	a	619	55/55	0.83	0.13	39,61,83,85	0
32	STE	c	523	12/20	0.83	0.13	58,75,87,90	0
32	STE	B	625	15/20	0.83	0.20	46,67,82,96	0
32	STE	T	103	15/20	0.84	0.15	46,65,87,88	0
32	STE	B	622	18/20	0.84	0.12	45,66,89,89	0
32	STE	B	626	12/20	0.84	0.15	57,71,88,88	0
32	STE	d	410	20/20	0.84	0.12	50,65,79,81	0
32	STE	C	521	12/20	0.84	0.14	36,54,66,68	0
32	STE	T	102	16/20	0.85	0.14	43,58,78,83	0
31	DGD	A	616	66/66	0.85	0.11	46,68,85,98	0
32	STE	Z	101	8/20	0.85	0.17	50,64,77,77	0
32	STE	C	519	12/20	0.85	0.13	43,63,75,76	0
32	STE	M	103	10/20	0.86	0.14	44,55,60,69	0
32	STE	j	101	12/20	0.86	0.11	49,65,78,78	0
32	STE	c	520	20/20	0.86	0.13	43,68,86,100	0
33	LMG	Y	101	48/55	0.86	0.13	47,75,101,104	0
32	STE	b	621	20/20	0.86	0.13	45,62,80,86	0
29	SQD	A	615	39/54	0.86	0.13	45,65,95,96	0
29	SQD	a	616	36/54	0.86	0.13	31,69,93,98	0
29	SQD	f	102	41/54	0.87	0.13	64,94,114,118	0
28	PL9	a	612	55/55	0.87	0.14	43,77,95,103	0
32	STE	t	102	14/20	0.87	0.12	42,54,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LMG	c	519	37/55	0.87	0.11	48,69,83,87	0
32	STE	C	520	16/20	0.87	0.12	47,59,68,73	0
32	STE	B	619	17/20	0.88	0.11	35,53,73,77	0
33	LMG	C	515	48/55	0.88	0.11	31,61,83,93	0
33	LMG	c	522	49/55	0.88	0.11	36,61,90,107	0
32	STE	B	621	12/20	0.89	0.12	38,62,74,78	0
33	LMG	D	412	28/55	0.89	0.12	39,56,67,75	0
24	CLA	C	513	65/65	0.89	0.11	50,69,101,107	0
24	CLA	H	101	65/65	0.89	0.10	44,68,98,103	0
33	LMG	m	101	51/55	0.89	0.10	37,55,75,85	0
32	STE	d	409	17/20	0.90	0.11	43,58,66,77	0
32	STE	M	102	15/20	0.90	0.11	42,58,67,69	0
26	BCR	h	101	40/40	0.90	0.11	42,63,87,92	0
29	SQD	B	620	54/54	0.90	0.10	41,62,87,95	0
26	BCR	K	101	40/40	0.90	0.12	45,64,76,82	0
29	SQD	b	620	49/54	0.90	0.10	40,62,90,107	0
32	STE	J	101	12/20	0.90	0.10	50,62,78,78	0
26	BCR	c	514	40/40	0.90	0.11	45,65,82,84	0
33	LMG	M	101	51/55	0.91	0.09	34,53,80,85	0
32	STE	M	104	18/20	0.91	0.11	39,52,86,91	0
29	SQD	D	408	36/54	0.91	0.10	57,78,93,96	0
33	LMG	d	408	44/55	0.91	0.11	37,61,93,102	0
32	STE	X	102	20/20	0.91	0.10	38,57,80,83	0
31	DGD	h	102	62/66	0.92	0.09	35,53,66,79	0
24	CLA	c	513	65/65	0.92	0.11	47,75,105,109	0
26	BCR	k	101	40/40	0.92	0.09	40,67,79,81	0
26	BCR	X	101	40/40	0.92	0.09	34,52,70,73	0
29	SQD	a	615	54/54	0.92	0.10	45,70,92,96	0
26	BCR	D	405	40/40	0.92	0.09	35,51,89,97	0
31	DGD	C	517	62/66	0.92	0.09	38,58,106,117	0
31	DGD	c	517	62/66	0.92	0.09	36,56,97,103	0
26	BCR	b	617	40/40	0.93	0.08	33,49,64,65	0
26	BCR	b	618	40/40	0.93	0.07	28,46,61,65	0
29	SQD	A	613	52/54	0.93	0.10	36,63,92,97	0
26	BCR	B	616	40/40	0.93	0.08	31,44,61,67	0
26	BCR	d	404	40/40	0.93	0.10	40,59,99,107	0
26	BCR	K	102	40/40	0.93	0.09	44,62,77,85	0
33	LMG	D	407	51/55	0.93	0.11	31,64,87,89	0
24	CLA	c	512	65/65	0.93	0.10	47,65,93,98	0
31	DGD	H	102	62/66	0.93	0.09	32,49,62,71	0
34	BCT	a	611	4/4	0.93	0.10	35,36,48,53	0
31	DGD	c	518	62/66	0.94	0.09	32,59,84,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	BCR	A	608	40/40	0.94	0.07	29,40,48,49	0
24	CLA	c	506	65/65	0.94	0.09	35,55,90,101	0
26	BCR	B	617	40/40	0.94	0.07	29,44,58,59	0
26	BCR	b	619	40/40	0.94	0.08	33,54,68,72	0
26	BCR	B	618	40/40	0.94	0.07	29,46,61,71	0
26	BCR	C	514	40/40	0.94	0.09	27,47,60,72	0
24	CLA	c	509	65/65	0.94	0.10	34,55,70,75	0
24	CLA	C	512	65/65	0.94	0.10	41,62,97,102	0
30	LHG	D	410	47/49	0.94	0.10	33,53,93,98	0
30	LHG	a	614	49/49	0.94	0.09	33,54,72,75	0
30	LHG	d	407	39/49	0.94	0.09	38,54,74,77	0
26	BCR	k	102	40/40	0.94	0.10	45,61,74,77	0
26	BCR	t	101	40/40	0.94	0.06	29,44,55,58	0
24	CLA	C	511	65/65	0.94	0.08	38,55,72,78	0
26	BCR	K	103	40/40	0.94	0.09	42,59,74,83	0
26	BCR	T	101	40/40	0.94	0.07	26,47,62,63	0
24	CLA	b	616	60/65	0.95	0.09	33,50,93,101	0
30	LHG	l	101	49/49	0.95	0.08	34,51,61,71	0
26	BCR	a	608	40/40	0.95	0.06	26,39,47,55	0
31	DGD	C	516	62/66	0.95	0.09	27,43,82,94	0
24	CLA	c	502	65/65	0.95	0.07	33,48,67,71	0
31	DGD	C	518	62/66	0.95	0.08	28,53,75,87	0
24	CLA	c	503	65/65	0.95	0.08	36,50,65,65	0
31	DGD	c	516	62/66	0.95	0.09	28,45,75,84	0
24	CLA	c	504	60/65	0.95	0.07	36,52,83,88	0
24	CLA	c	505	65/65	0.95	0.08	30,48,69,76	0
26	BCR	c	515	40/40	0.95	0.09	32,50,72,73	0
24	CLA	C	506	65/65	0.95	0.09	28,47,91,95	0
24	CLA	c	508	64/65	0.95	0.09	36,53,99,120	0
24	CLA	C	508	65/65	0.95	0.09	31,49,105,118	0
24	CLA	c	510	65/65	0.95	0.08	38,54,70,72	0
24	CLA	c	511	65/65	0.95	0.09	41,60,78,81	0
24	CLA	C	510	65/65	0.95	0.07	33,51,68,70	0
24	CLA	B	605	65/65	0.95	0.07	22,41,70,73	0
24	CLA	d	403	65/65	0.95	0.09	31,55,98,106	0
25	PHO	d	401	64/64	0.95	0.07	27,43,53,64	0
24	CLA	B	614	65/65	0.95	0.08	28,43,63,67	0
24	CLA	B	615	60/65	0.95	0.09	27,46,103,111	0
24	CLA	C	503	65/65	0.95	0.07	36,49,61,63	0
24	CLA	a	607	65/65	0.95	0.08	23,41,90,102	0
24	CLA	C	504	59/65	0.95	0.08	34,47,85,97	0
24	CLA	b	602	65/65	0.95	0.08	29,48,67,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	b	605	65/65	0.95	0.07	28,42,56,59	0
24	CLA	b	606	65/65	0.95	0.07	29,46,76,85	0
24	CLA	b	608	65/65	0.95	0.07	30,48,71,80	0
24	CLA	b	609	65/65	0.95	0.08	34,51,74,79	0
24	CLA	c	507	65/65	0.96	0.07	32,49,62,74	0
28	PL9	D	406	55/55	0.96	0.07	25,39,50,65	0
24	CLA	B	611	65/65	0.96	0.06	23,37,51,60	0
28	PL9	d	405	55/55	0.96	0.07	27,41,52,54	0
24	CLA	B	612	65/65	0.96	0.07	22,39,78,86	0
24	CLA	D	403	65/65	0.96	0.07	19,33,57,66	0
24	CLA	D	404	65/65	0.96	0.08	24,47,107,122	0
24	CLA	B	613	65/65	0.96	0.08	25,42,82,92	0
24	CLA	a	604	65/65	0.96	0.06	24,35,49,57	0
24	CLA	d	402	65/65	0.96	0.07	25,40,67,76	0
24	CLA	a	605	65/65	0.96	0.09	30,45,99,110	0
25	PHO	A	606	64/64	0.96	0.06	25,37,46,48	0
25	PHO	D	401	64/64	0.96	0.06	21,34,45,47	0
30	LHG	D	409	49/49	0.96	0.07	29,42,55,71	0
24	CLA	A	612	65/65	0.96	0.06	22,34,54,58	0
30	LHG	D	413	49/49	0.96	0.08	34,47,70,76	0
30	LHG	L	101	49/49	0.96	0.07	32,46,60,67	0
24	CLA	a	613	65/65	0.96	0.07	23,37,48,53	0
30	LHG	d	406	49/49	0.96	0.07	28,45,61,66	0
24	CLA	B	601	65/65	0.96	0.07	27,41,63,71	0
24	CLA	C	501	65/65	0.96	0.07	29,41,55,61	0
24	CLA	b	604	65/65	0.96	0.07	26,41,79,98	0
24	CLA	C	502	65/65	0.96	0.07	32,47,64,67	0
24	CLA	B	602	65/65	0.96	0.07	22,38,61,72	0
24	CLA	b	607	65/65	0.96	0.07	22,43,71,75	0
24	CLA	B	603	65/65	0.96	0.07	23,38,77,86	0
24	CLA	C	505	65/65	0.96	0.08	25,48,71,77	0
24	CLA	b	610	65/65	0.96	0.07	27,43,54,62	0
24	CLA	b	611	65/65	0.96	0.07	25,38,62,75	0
24	CLA	b	612	65/65	0.96	0.07	23,39,55,56	0
24	CLA	b	613	65/65	0.96	0.07	23,41,81,88	0
24	CLA	b	614	65/65	0.96	0.07	29,44,78,91	0
24	CLA	b	615	65/65	0.96	0.08	30,46,69,80	0
24	CLA	B	604	65/65	0.96	0.07	25,38,51,54	0
24	CLA	c	501	65/65	0.96	0.07	31,45,60,63	0
24	CLA	C	507	65/65	0.96	0.07	31,47,67,70	0
24	CLA	A	604	65/65	0.96	0.06	19,33,50,61	0
24	CLA	C	509	65/65	0.96	0.08	30,50,66,77	0

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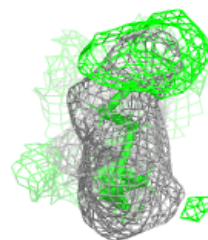
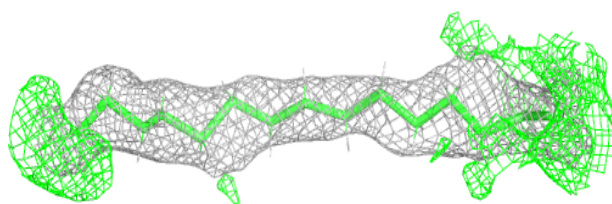
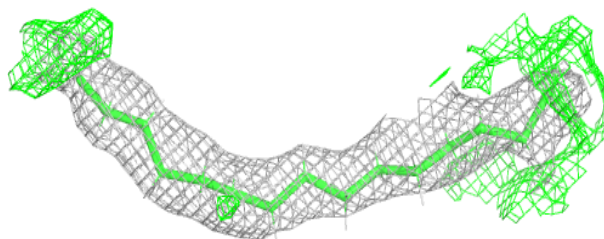
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	B	608	65/65	0.96	0.08	27,45,63,72	0
24	CLA	B	609	65/65	0.96	0.06	22,36,48,51	0
24	CLA	b	603	65/65	0.97	0.07	26,42,74,82	0
25	PHO	a	606	64/64	0.97	0.06	23,35,43,45	0
24	CLA	A	605	65/65	0.97	0.08	24,39,100,106	0
24	CLA	A	607	54/65	0.97	0.06	20,36,69,78	0
24	CLA	B	610	65/65	0.97	0.06	21,35,51,55	0
24	CLA	B	606	65/65	0.97	0.07	22,37,71,79	0
34	BCT	D	402	4/4	0.97	0.07	34,36,43,47	0
24	CLA	B	607	65/65	0.97	0.06	24,40,63,68	0
35	HEM	F	101	43/43	0.97	0.08	42,58,73,76	0
35	HEM	f	101	43/43	0.97	0.09	49,67,93,97	0
36	HEC	V	201	43/43	0.98	0.06	28,38,45,53	0
36	HEC	v	201	43/43	0.98	0.07	32,41,54,58	0
27	CL	A	610	1/1	0.99	0.06	37,37,37,37	0
27	CL	a	609	1/1	0.99	0.04	32,32,32,32	0
27	CL	a	610	1/1	0.99	0.08	35,35,35,35	0
21	OEY	A	601[B]	11/11	0.99	0.04	21,25,29,31	11
21	OEY	a	601[B]	11/11	0.99	0.03	21,26,32,32	11
22	OEX	A	602[A]	10/10	0.99	0.03	33,36,40,40	10
22	OEX	a	602[A]	10/10	0.99	0.03	31,36,39,40	10
27	CL	A	609	1/1	0.99	0.05	34,34,34,34	0
23	FE2	a	603	1/1	1.00	0.03	32,32,32,32	0
23	FE2	A	603	1/1	1.00	0.01	31,31,31,31	0

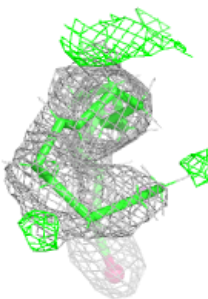
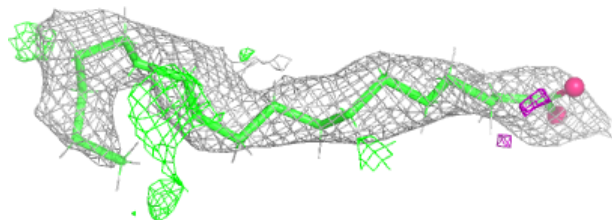
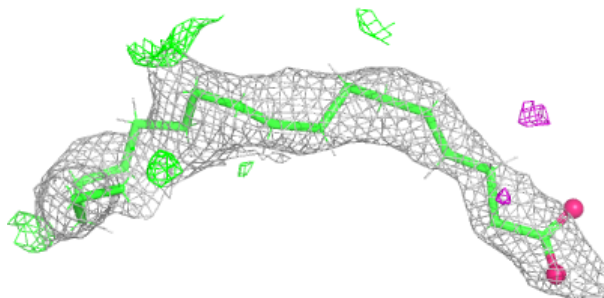
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

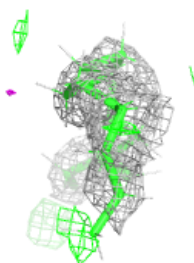
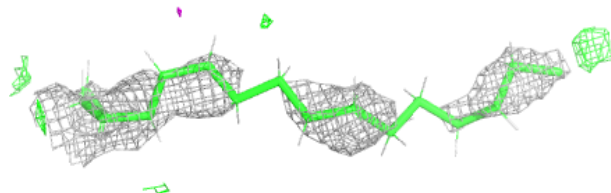
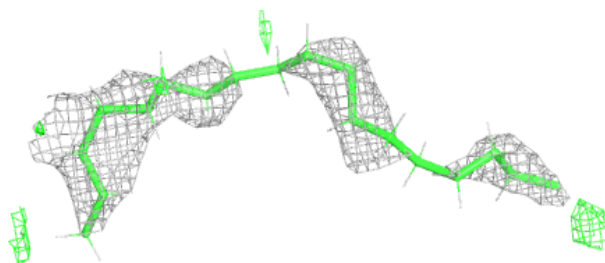
**Electron density around STE d 411:**

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

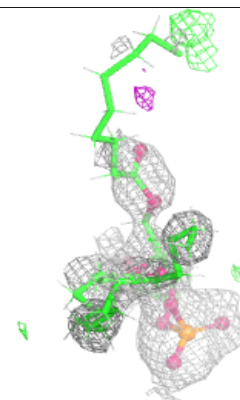
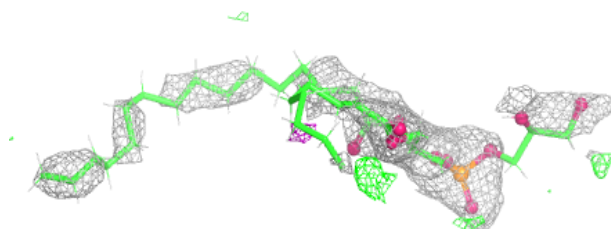
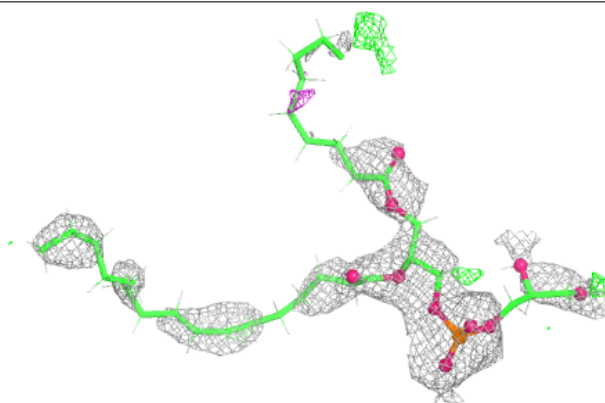


Electron density around STE B 623:

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

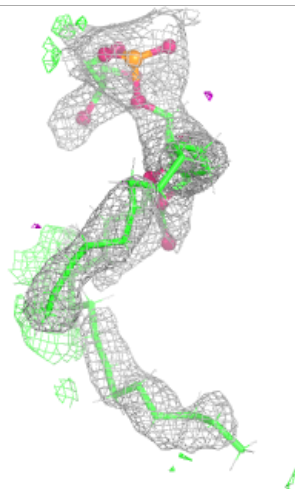
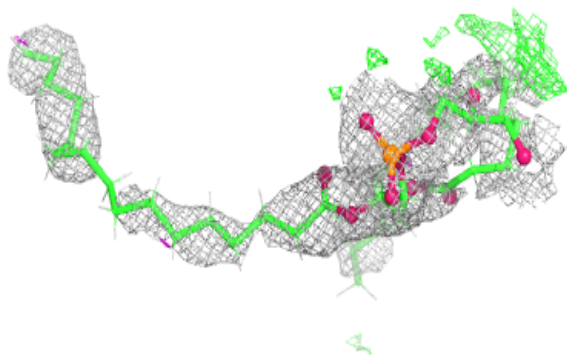
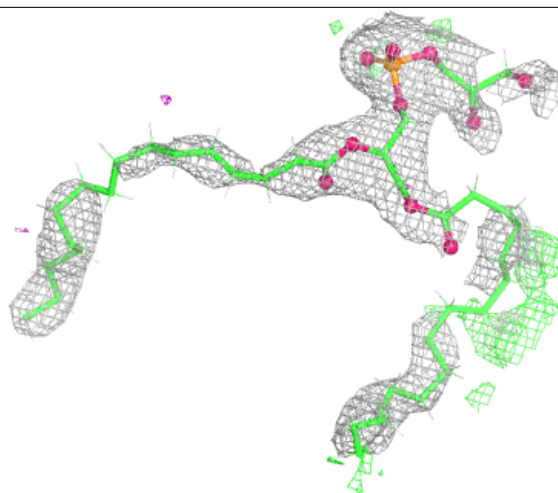
**Electron density around LHG e 101:**

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



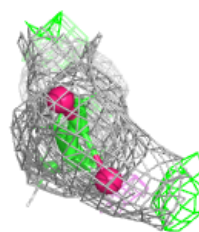
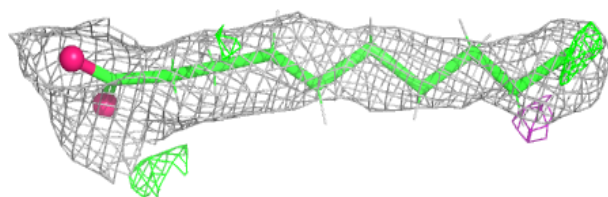
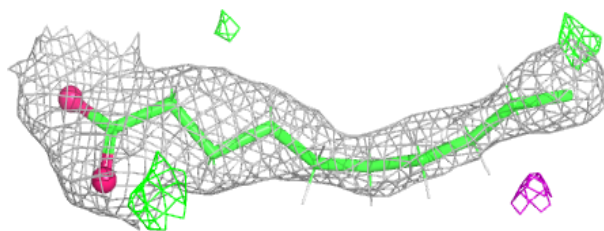
Electron density around LHG A 614:

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

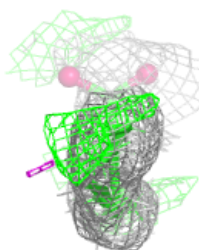
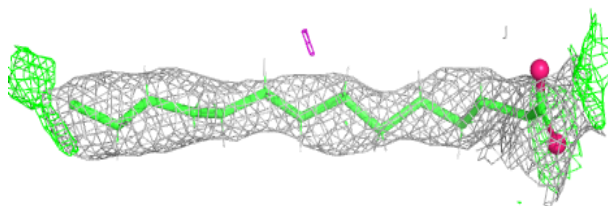


Electron density around STE a 618:

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

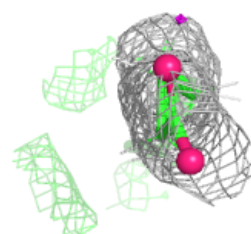
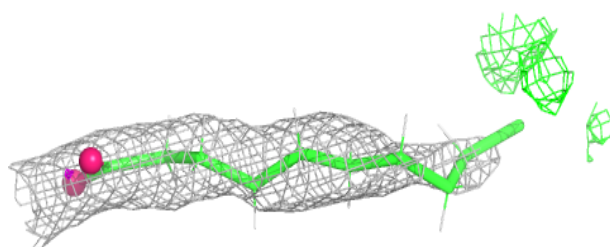
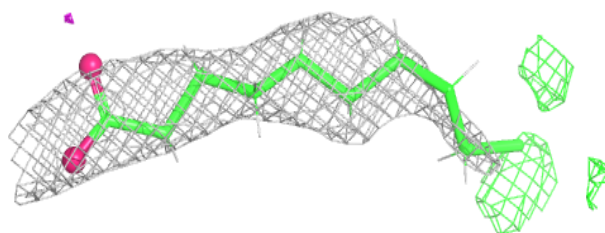
**Electron density around STE b 623:**

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

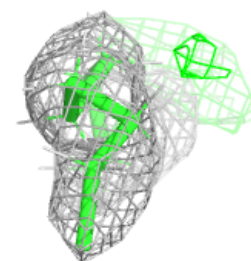
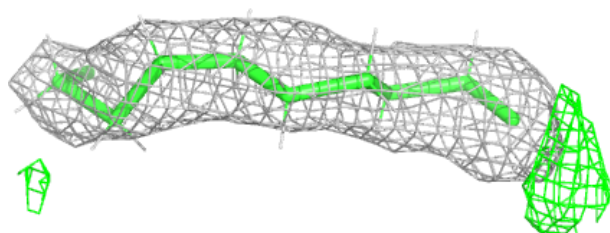
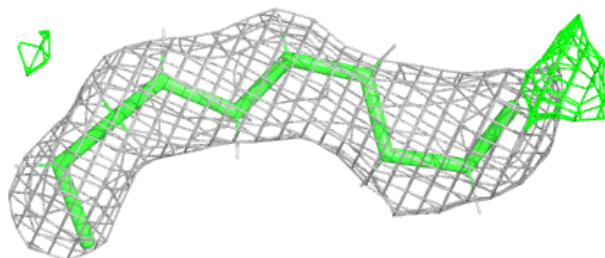


Electron density around STE L 102:

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

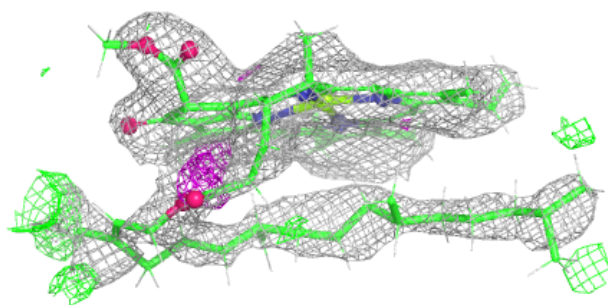
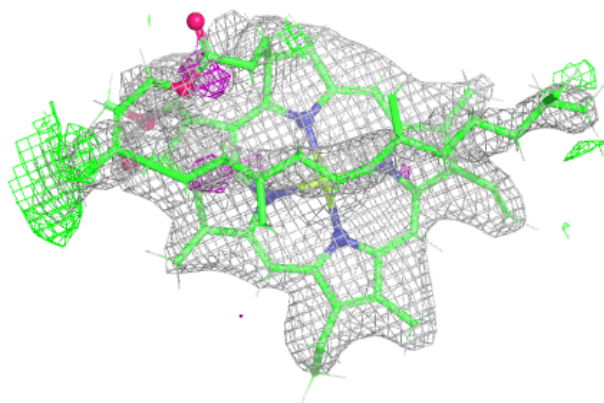
**Electron density around STE b 625:**

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

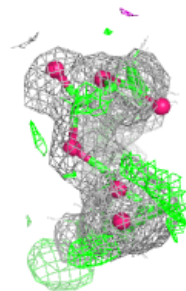
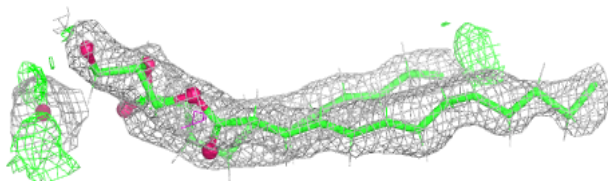
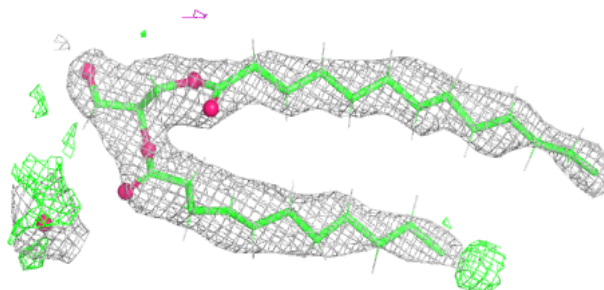


Electron density around CLA b 601:

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

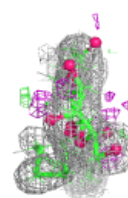
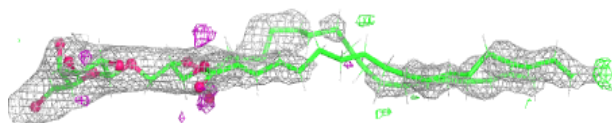
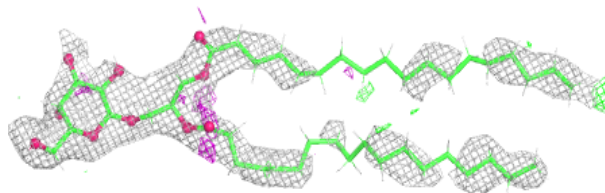
**Electron density around LMG D 411:**

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

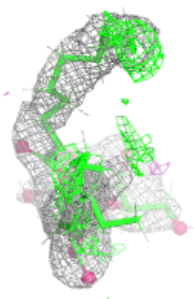
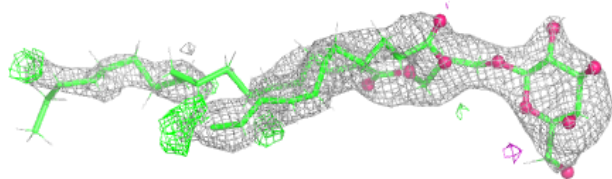
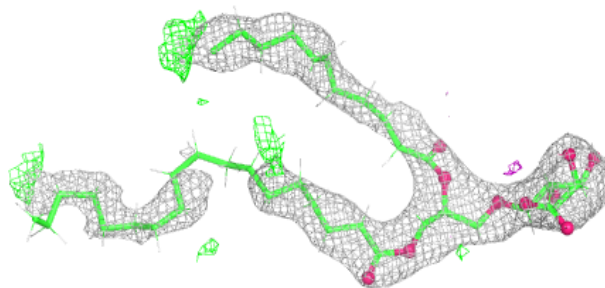


Electron density around LMG b 622:

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

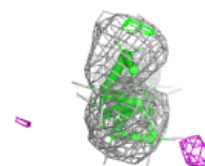
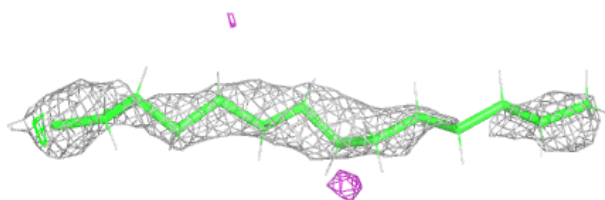
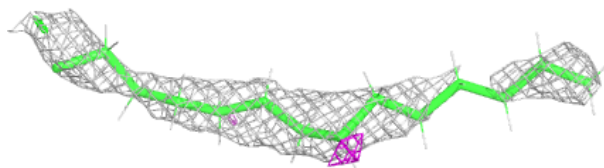
**Electron density around LMG c 521:**

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

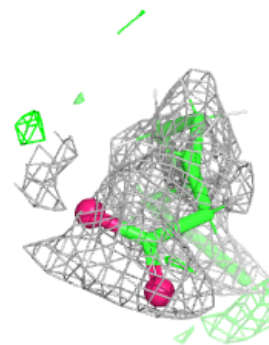
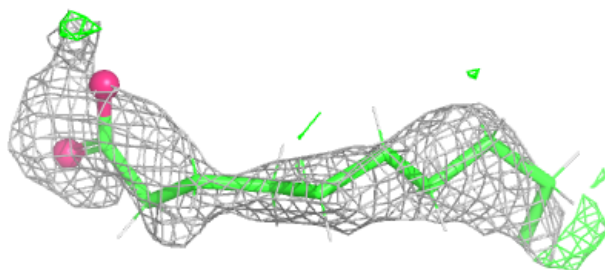
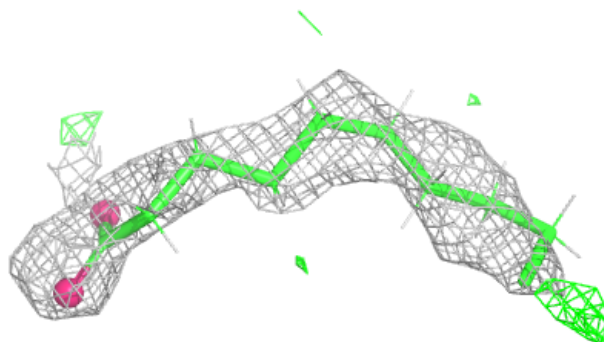


Electron density around STE h 103:

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

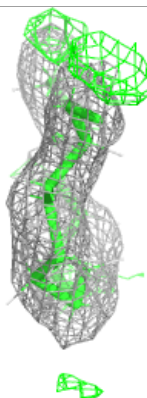
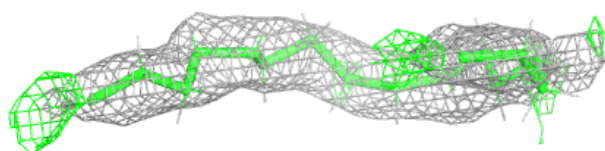
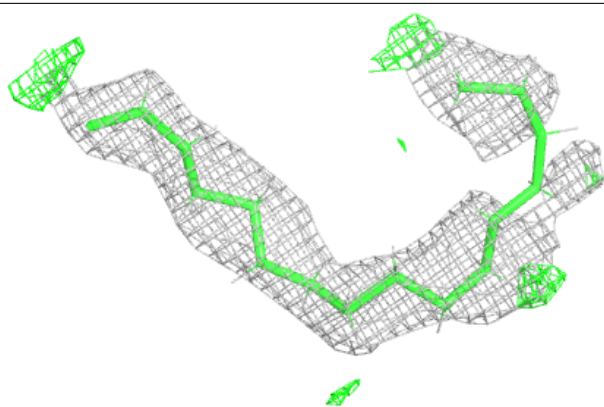
**Electron density around STE R 101:**

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

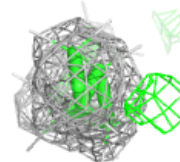
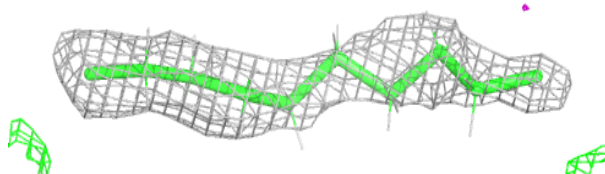
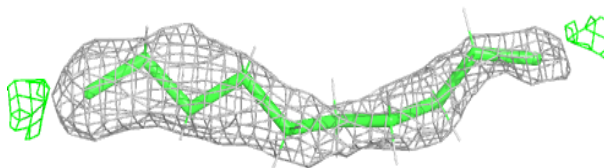


Electron density around STE B 624:

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

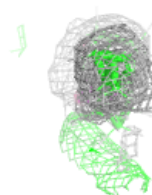
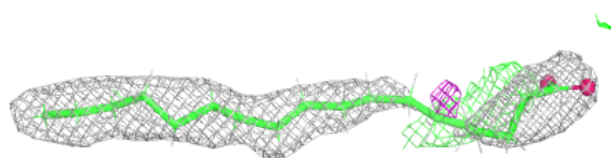
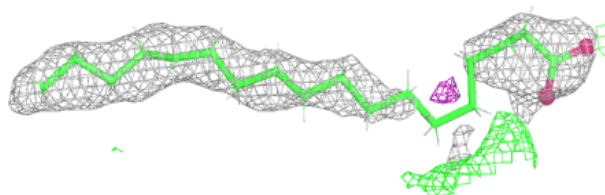
**Electron density around STE a 617:**

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

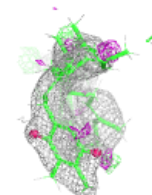
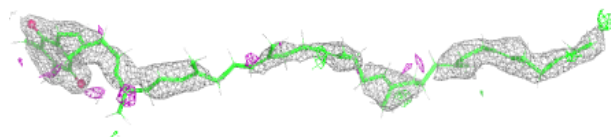
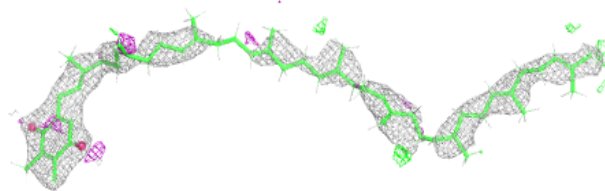


Electron density around STE b 624:

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

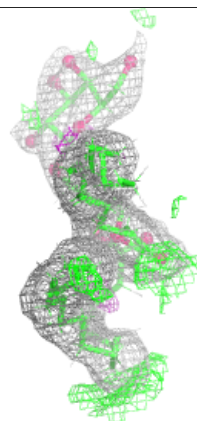
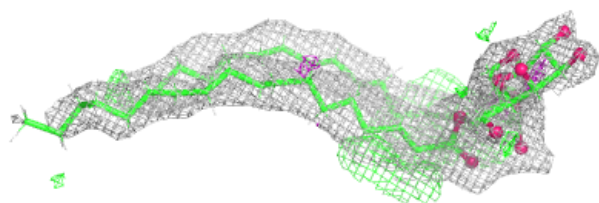
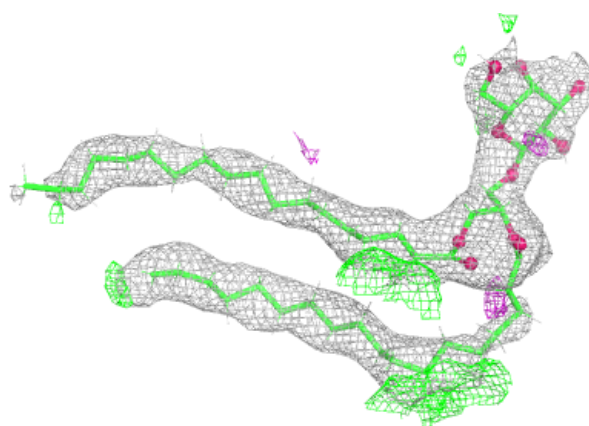
**Electron density around PL9 A 611:**

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

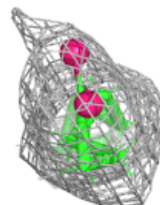
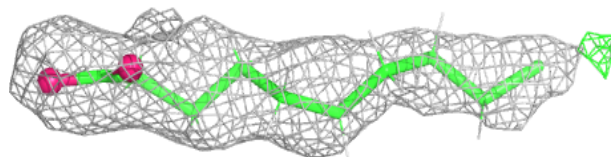
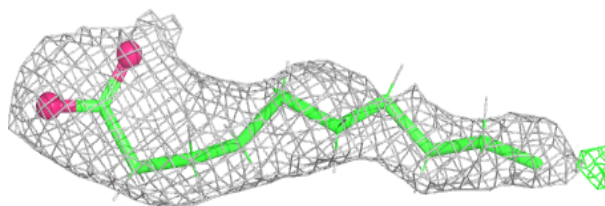


Electron density around LMG a 619:

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

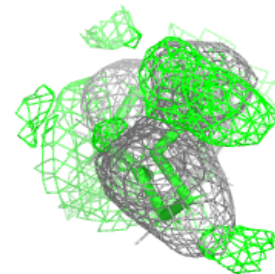
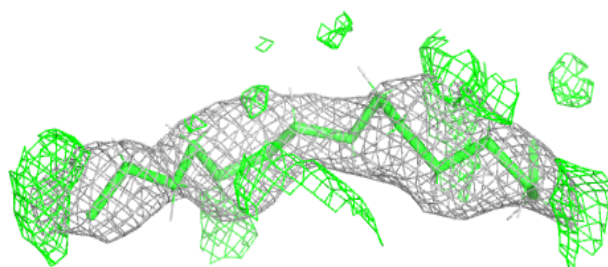
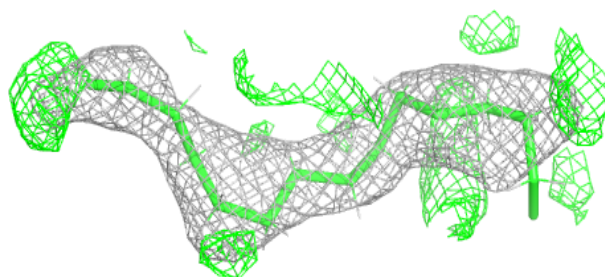
**Electron density around STE c 523:**

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

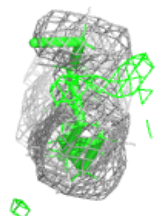
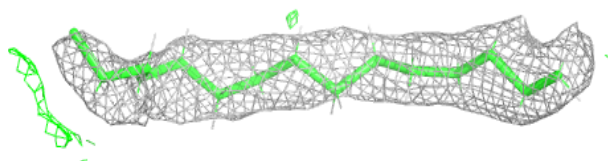
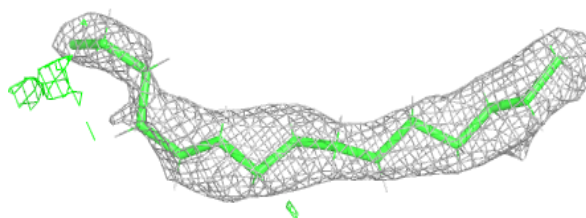


Electron density around STE B 625:

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

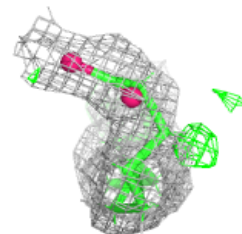
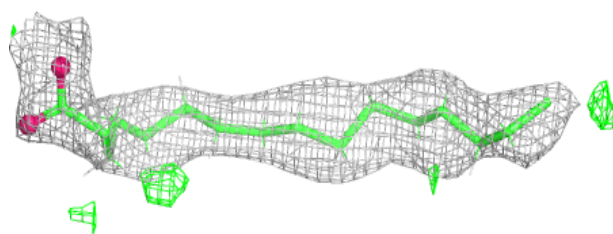
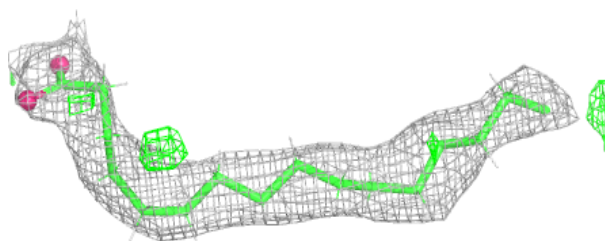
**Electron density around STE T 103:**

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

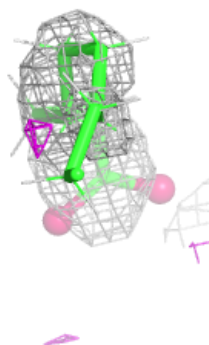
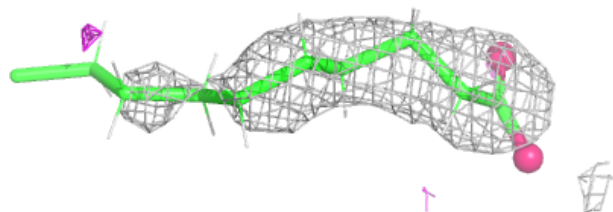
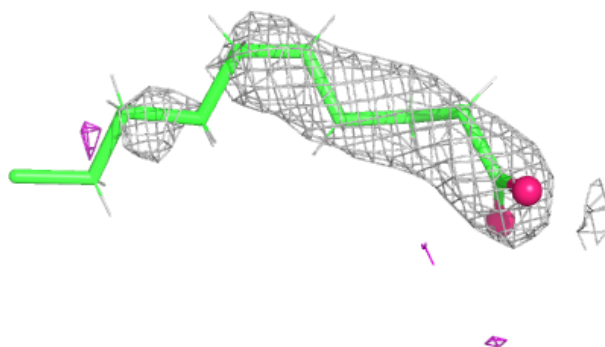


Electron density around STE B 622:

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

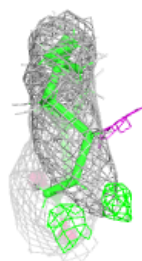
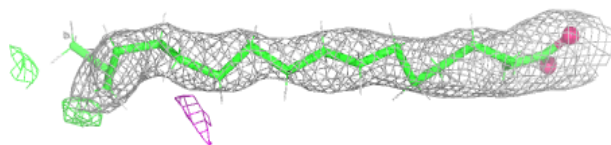
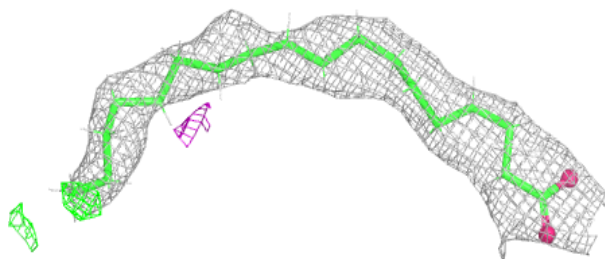
**Electron density around STE B 626:**

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

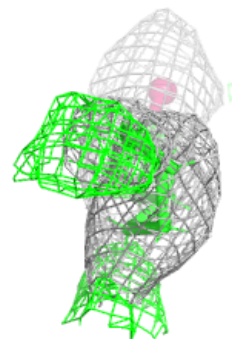
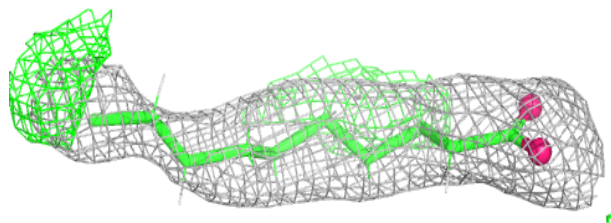
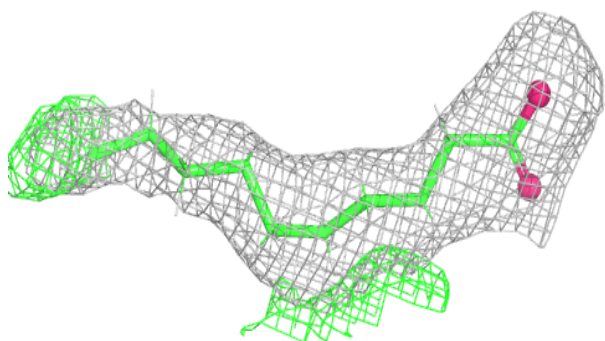


Electron density around STE d 410:

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

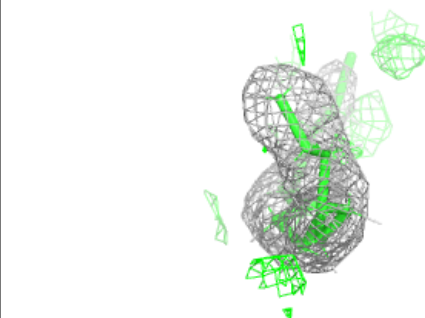
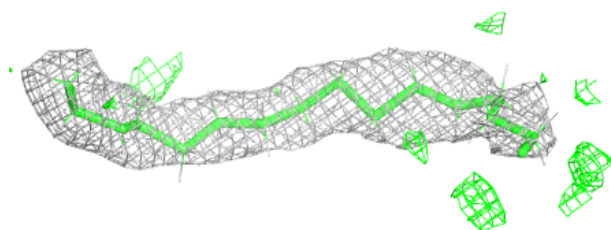
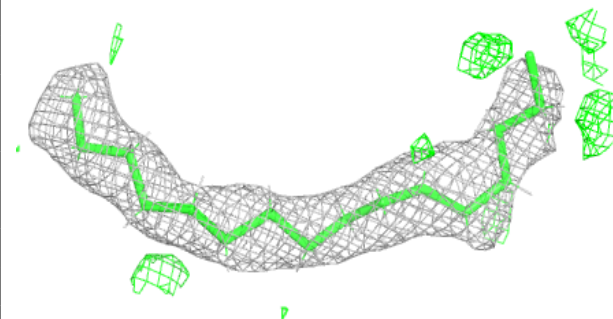
**Electron density around STE C 521:**

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

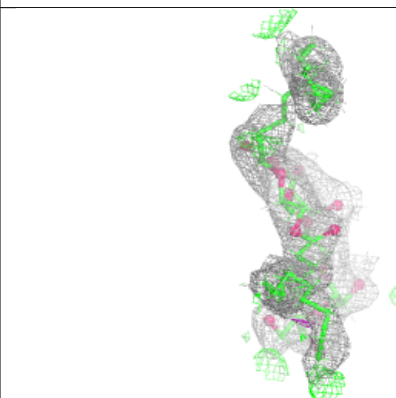
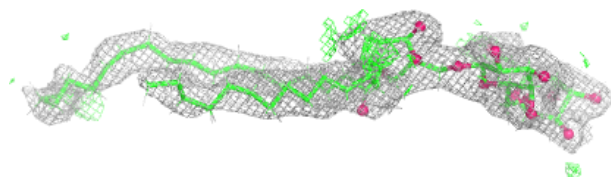
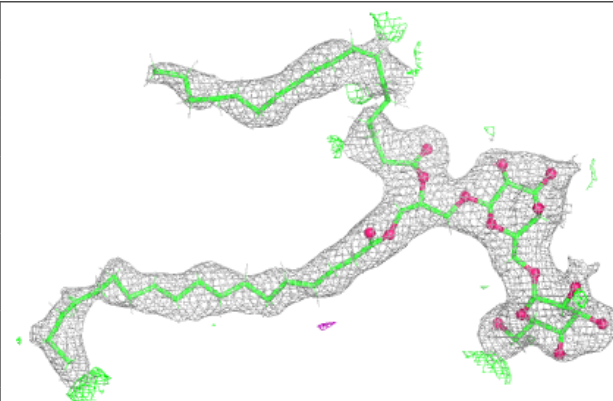


Electron density around STE T 102:

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

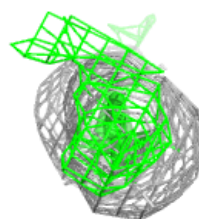
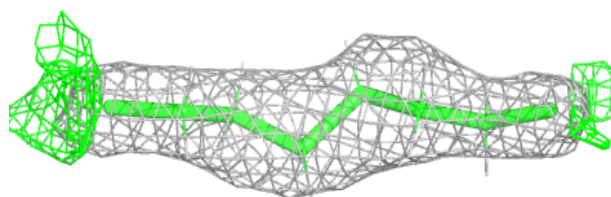
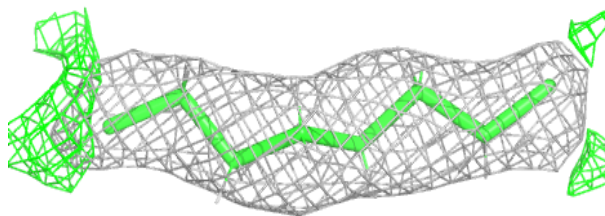
**Electron density around DGD A 616:**

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

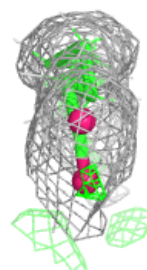
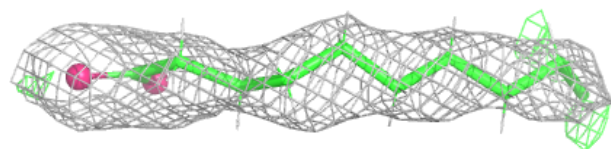
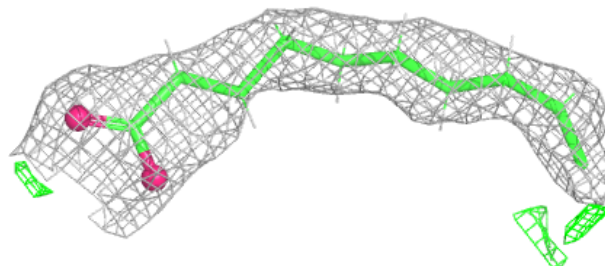


Electron density around STE Z 101:

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

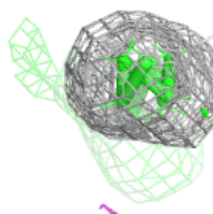
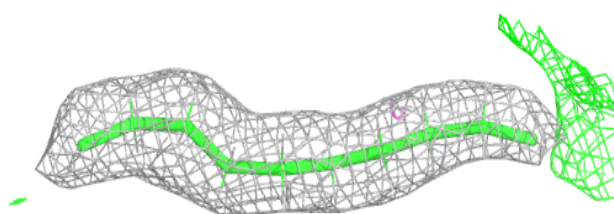
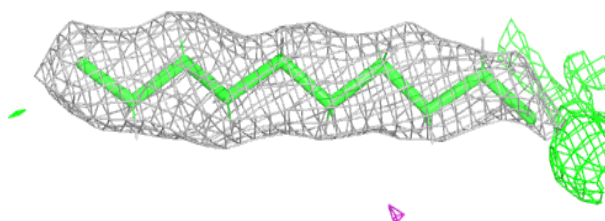
**Electron density around STE C 519:**

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

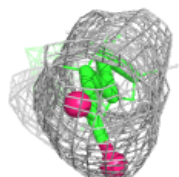
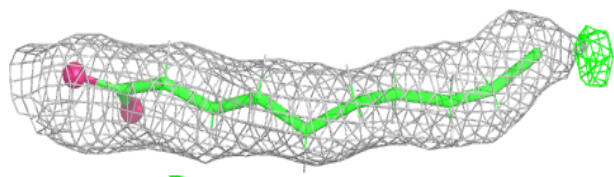
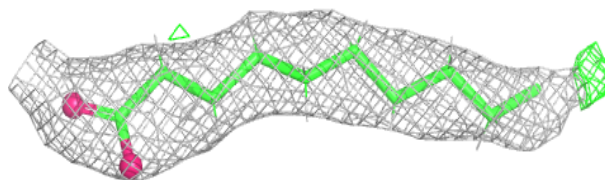


Electron density around STE M 103:

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

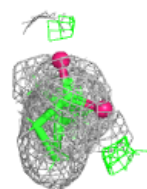
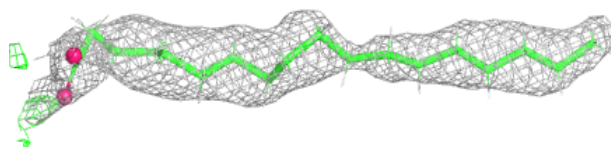
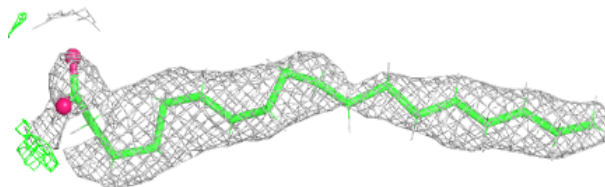
**Electron density around STE j 101:**

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



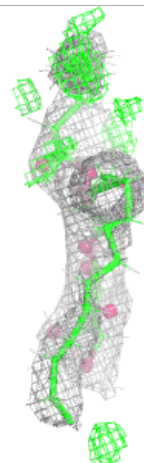
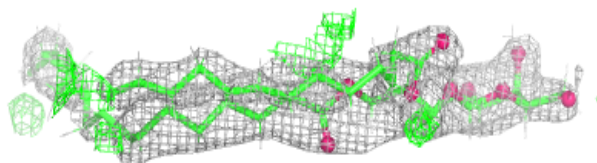
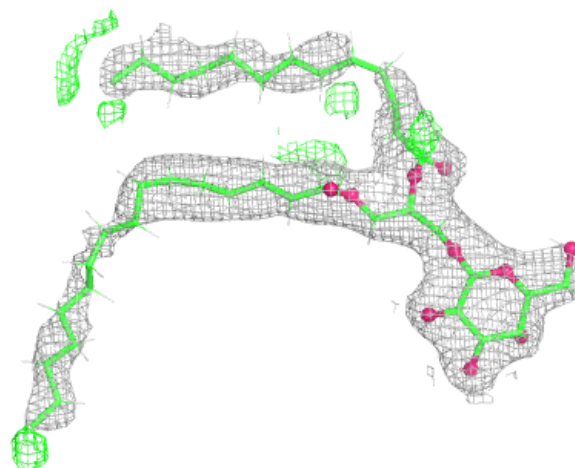
Electron density around STE c 520:

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



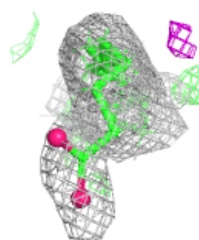
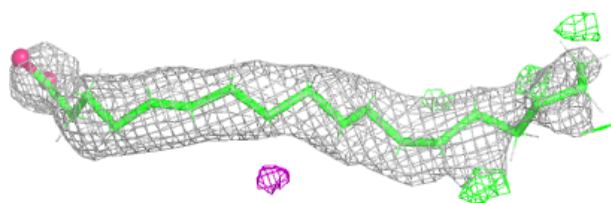
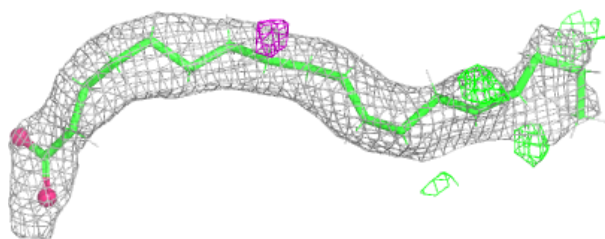
Electron density around LMG Y 101:

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

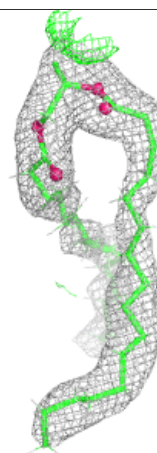
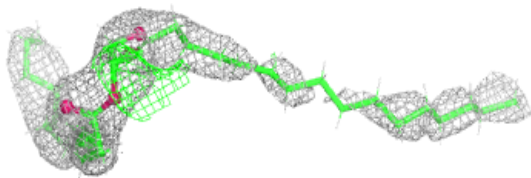
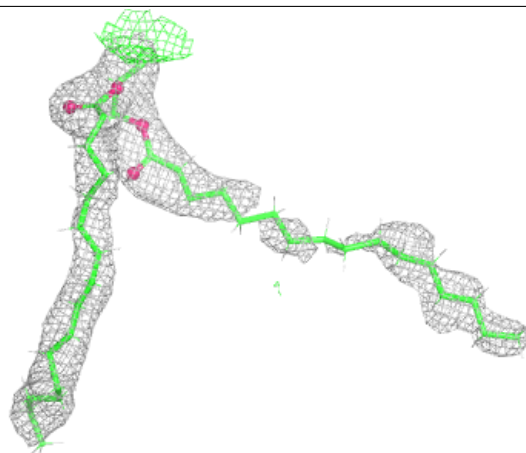


Electron density around STE b 621:

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

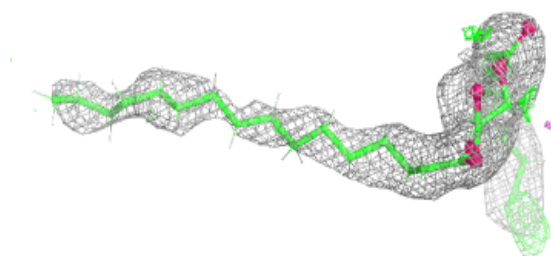
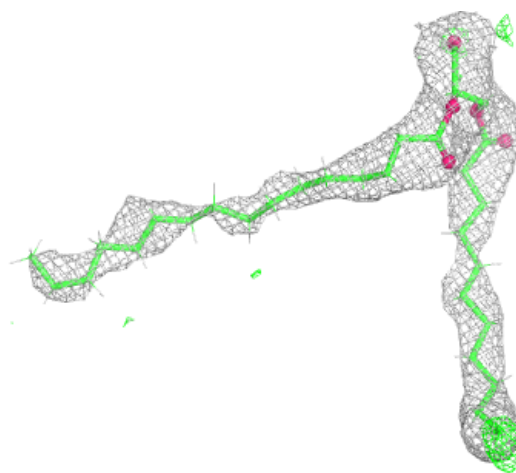
**Electron density around SQD A 615:**

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



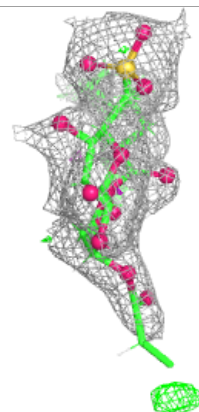
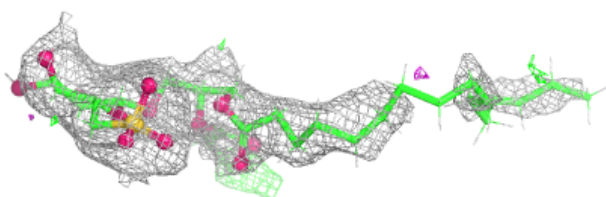
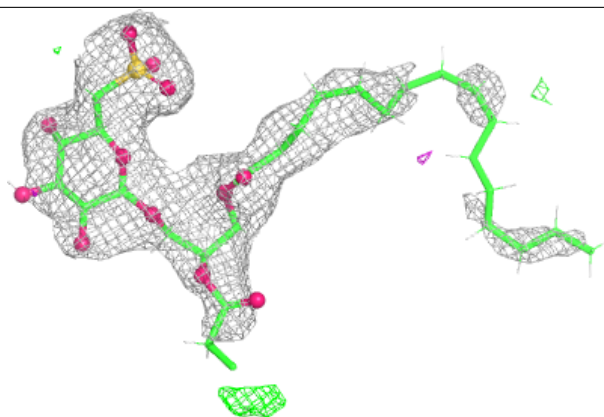
Electron density around SQD a 616:

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

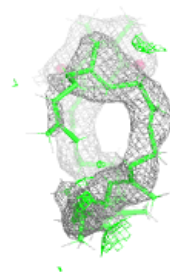
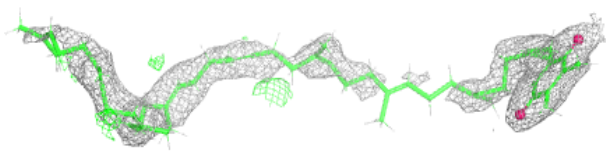
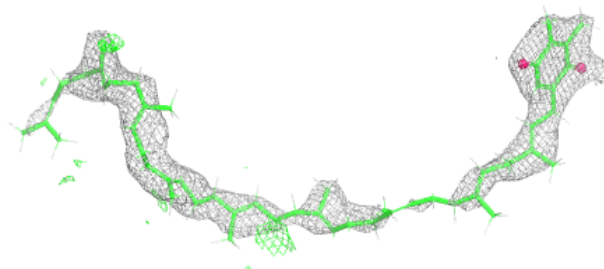


Electron density around SQD f 102:

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

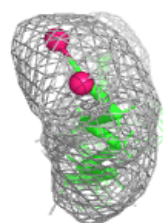
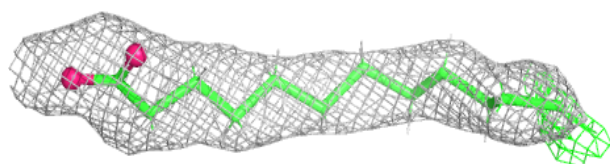
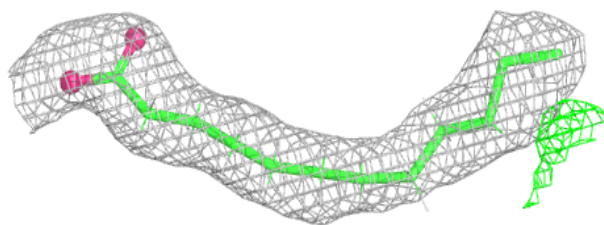
**Electron density around PL9 a 612:**

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

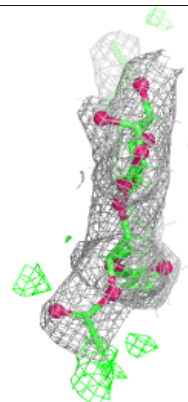
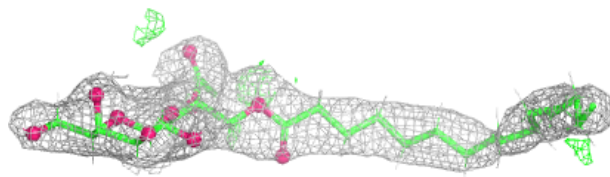
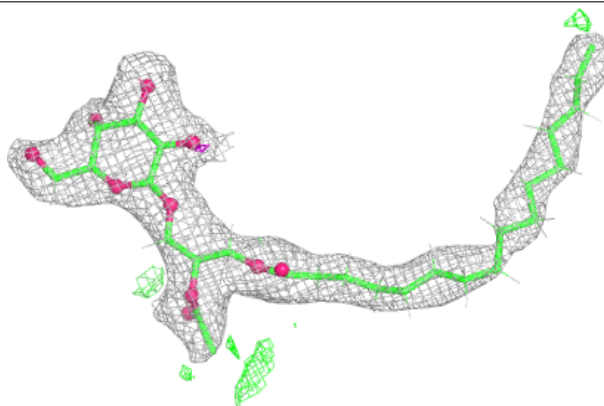


Electron density around STE t 102:

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

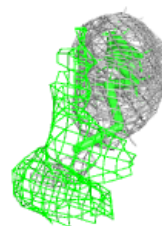
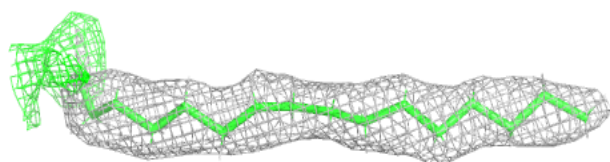
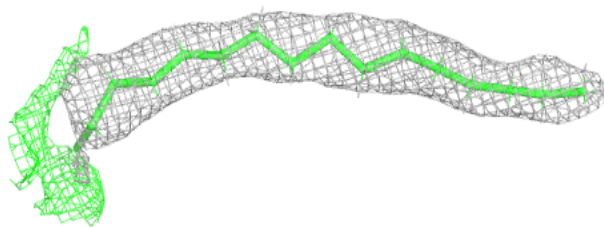
**Electron density around LMG c 519:**

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

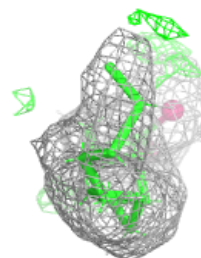
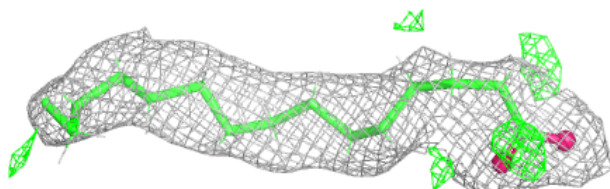
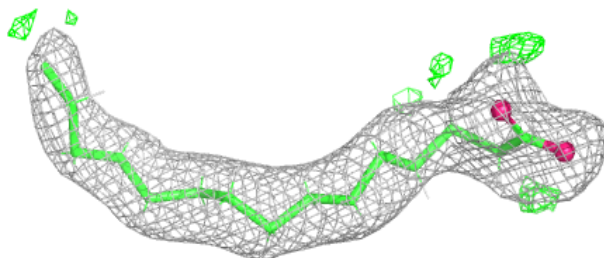


Electron density around STE C 520:

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

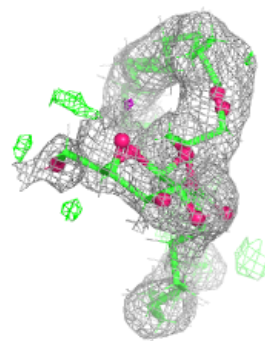
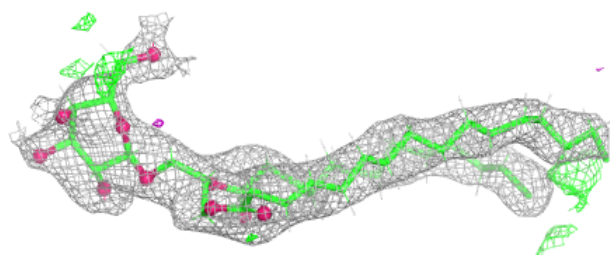
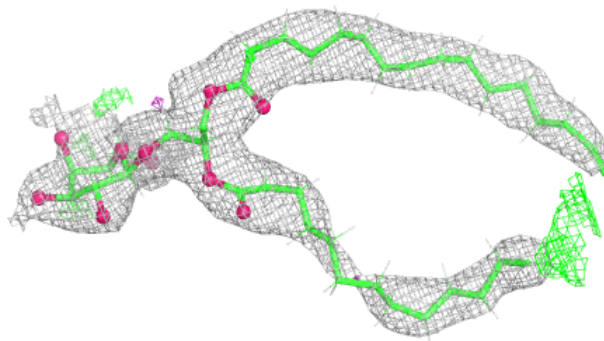
**Electron density around STE B 619:**

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

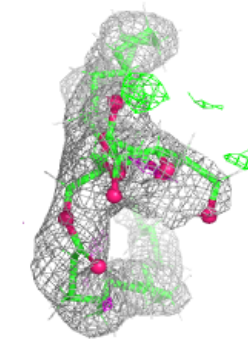
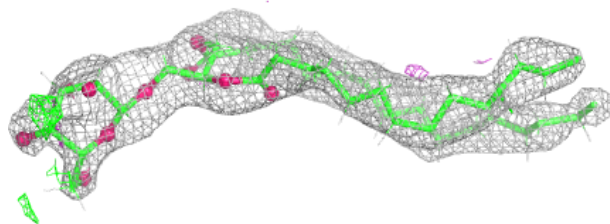
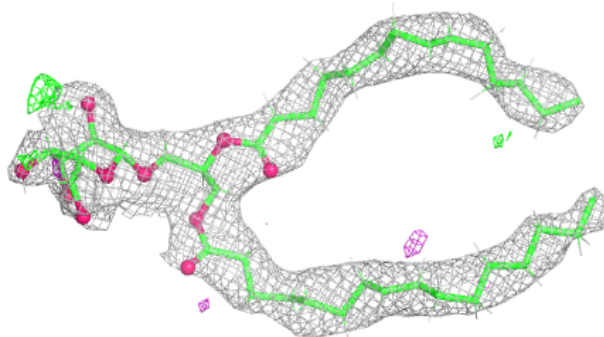


Electron density around LMG C 515:

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

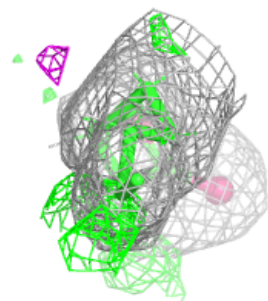
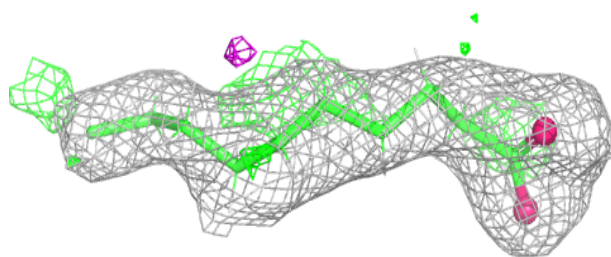
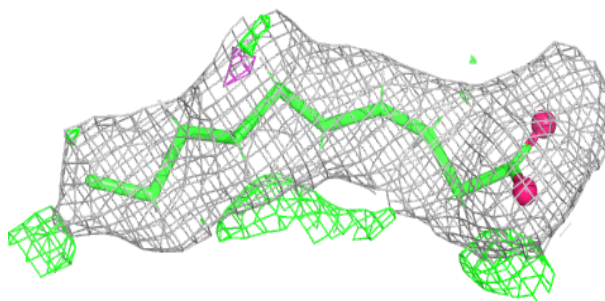
**Electron density around LMG c 522:**

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

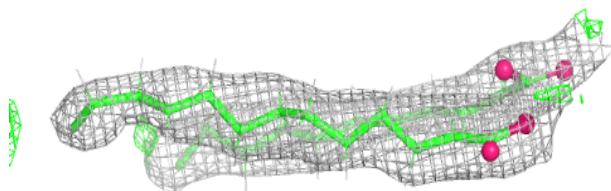
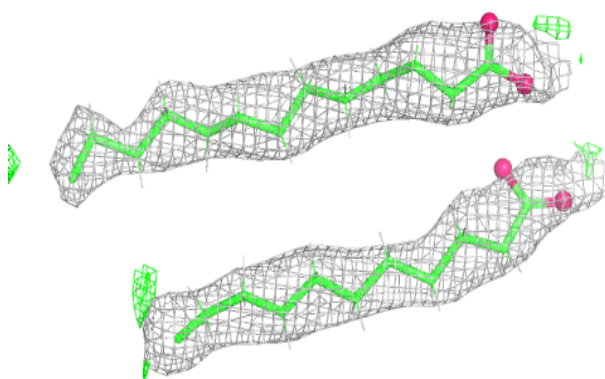


Electron density around STE B 621:

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

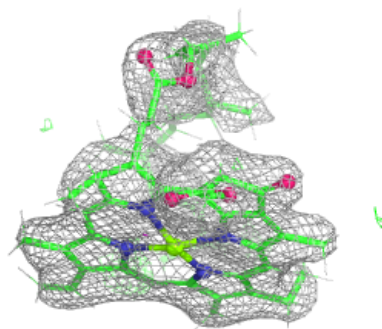
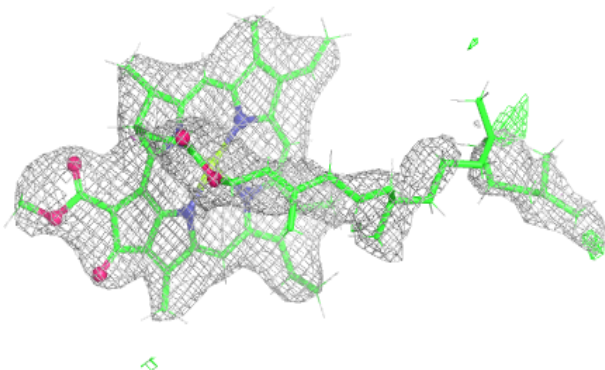
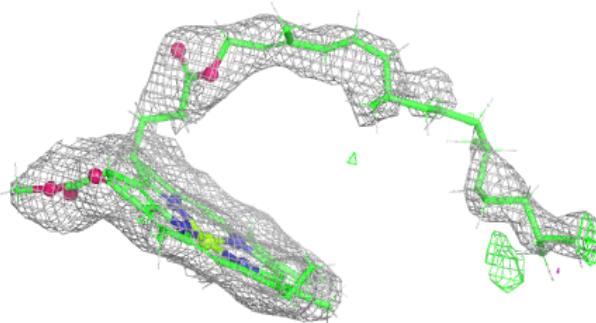
**Electron density around LMG D 412:**

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



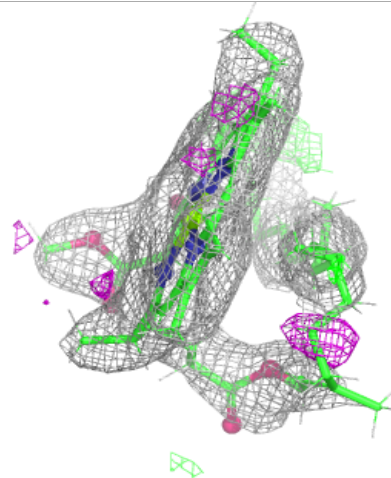
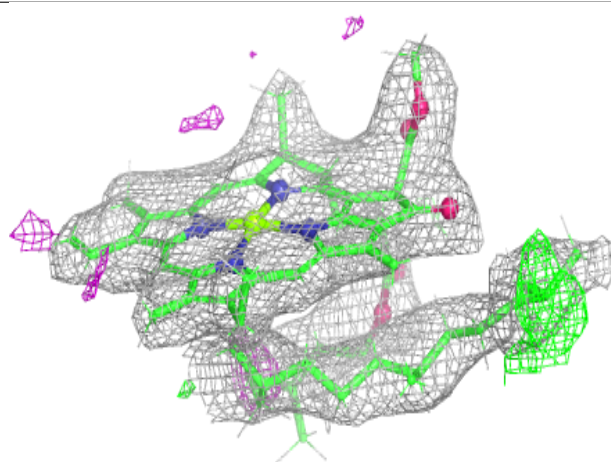
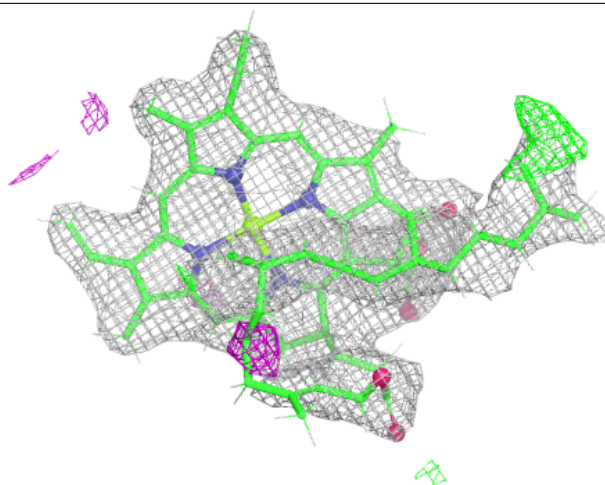
Electron density around CLA C 513:

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



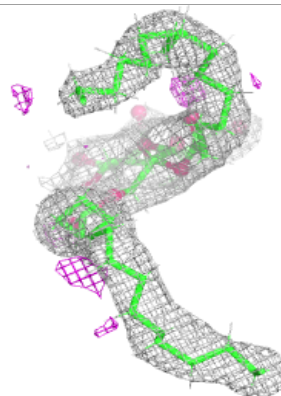
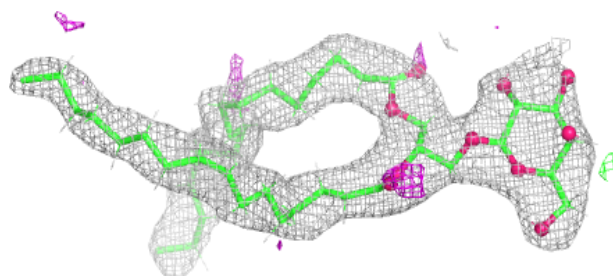
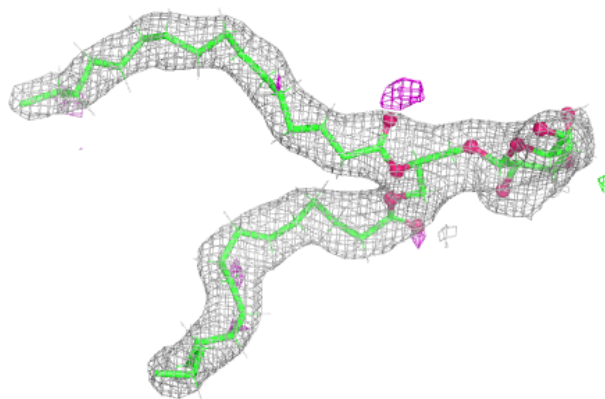
Electron density around CLA H 101:

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

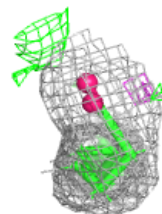
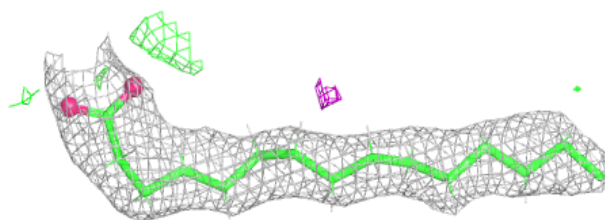


Electron density around LMG m 101:

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

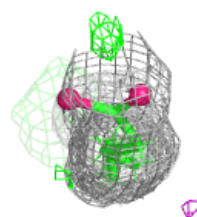
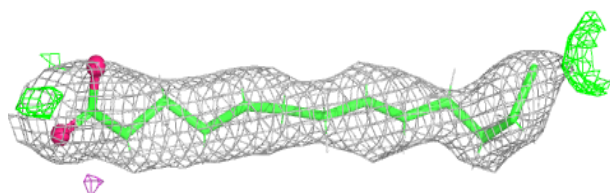
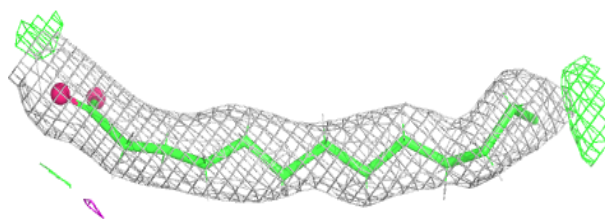
**Electron density around STE d 409:**

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

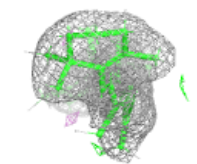
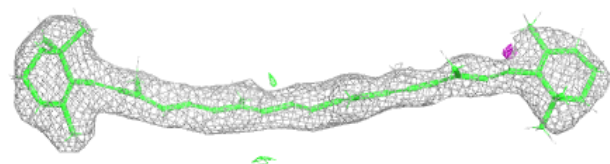
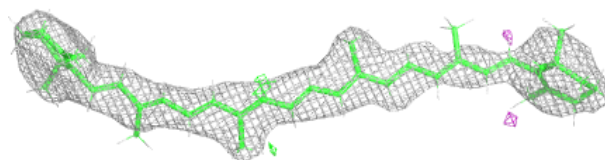


Electron density around STE M 102:

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

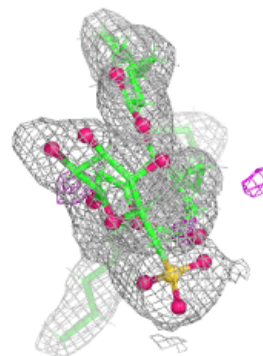
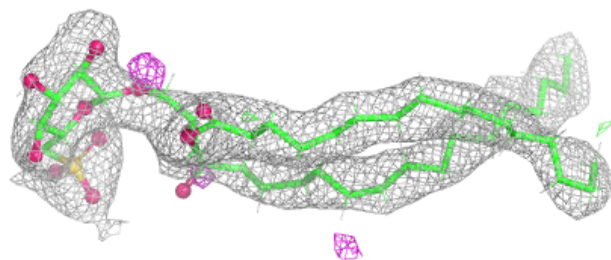
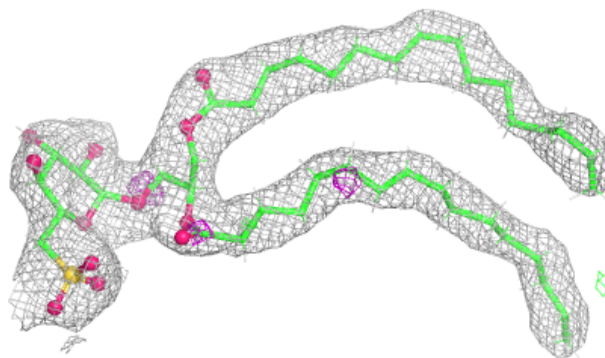
**Electron density around BCR h 101:**

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

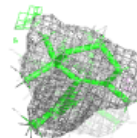


Electron density around SQD B 620:

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

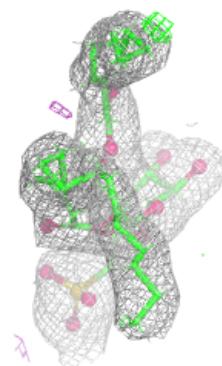
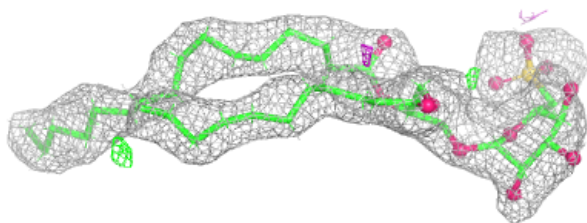
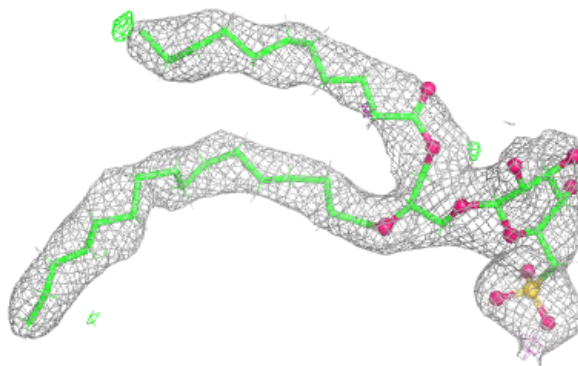
**Electron density around BCR K 101:**

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

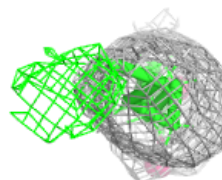
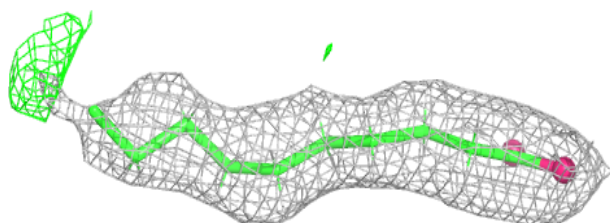
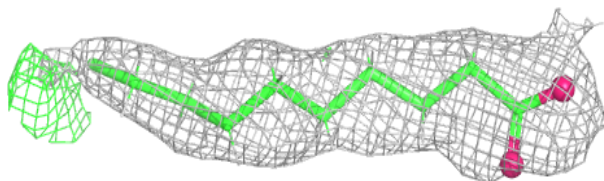


Electron density around SQD b 620:

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

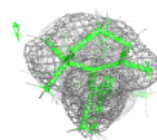
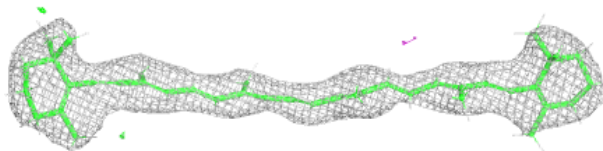
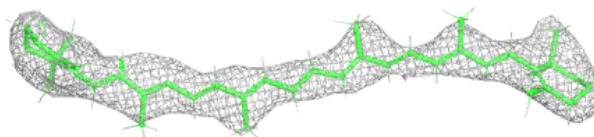
**Electron density around STE J 101:**

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

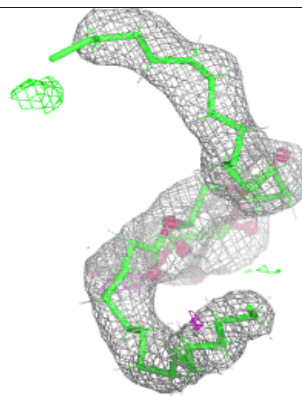
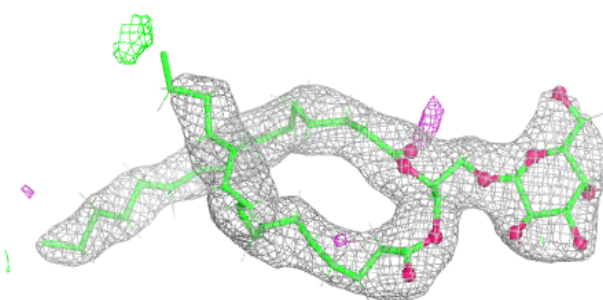
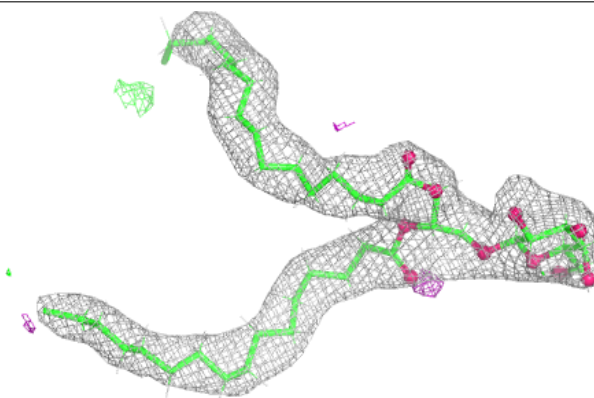


Electron density around BCR c 514:

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

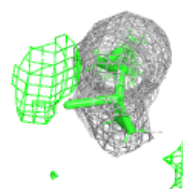
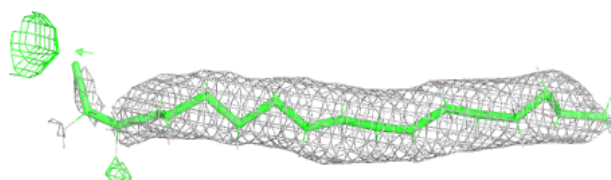
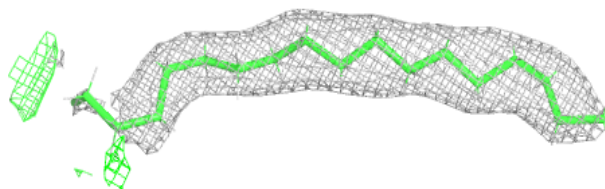
**Electron density around LMG M 101:**

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

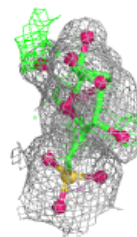
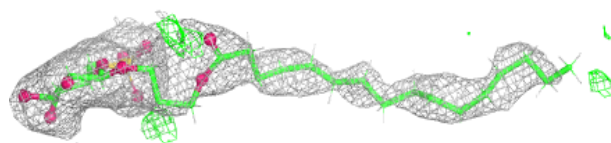
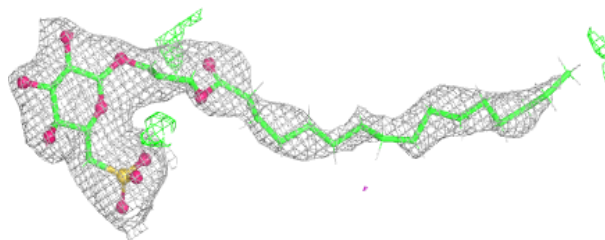


Electron density around STE M 104:

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

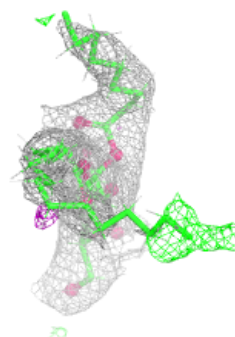
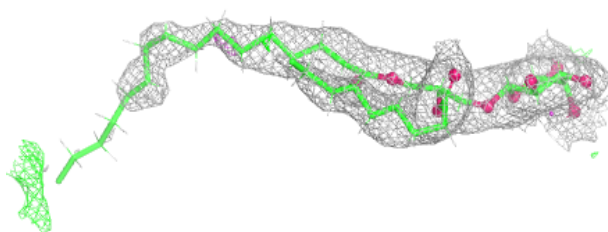
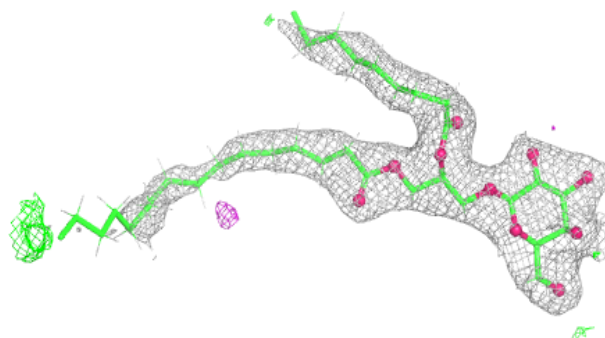
**Electron density around SQD D 408:**

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

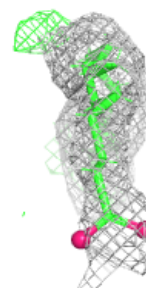
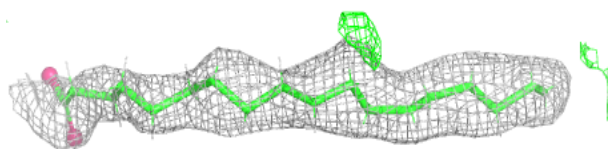
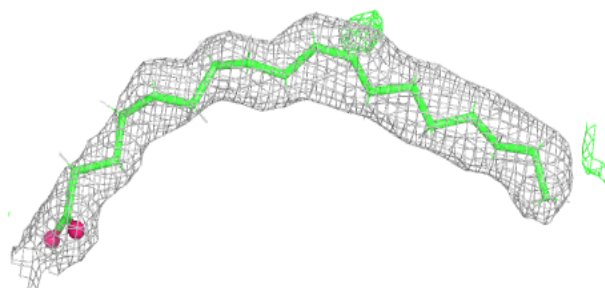


Electron density around LMG d 408:

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

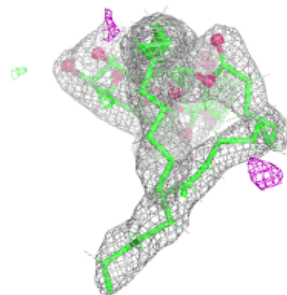
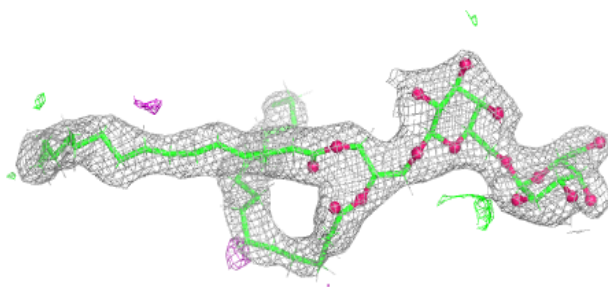
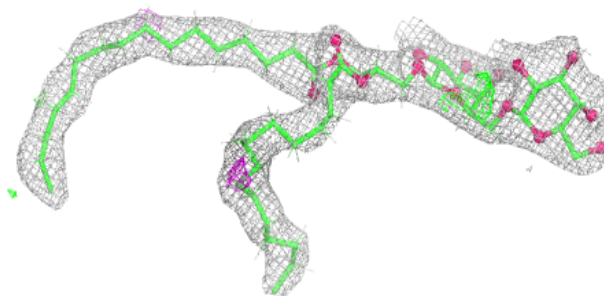
**Electron density around STE X 102:**

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

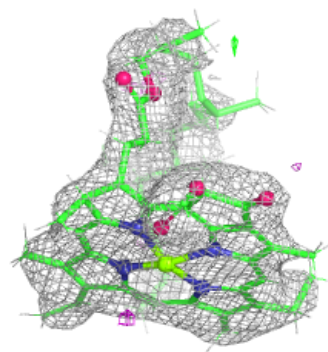
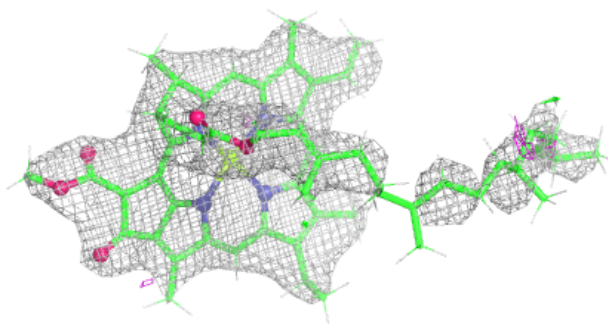
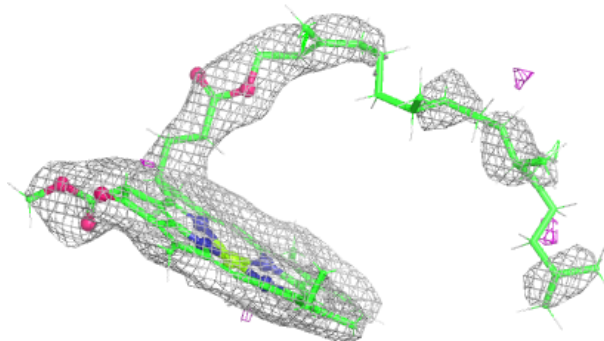


Electron density around DGD h 102:

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

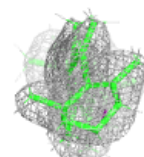
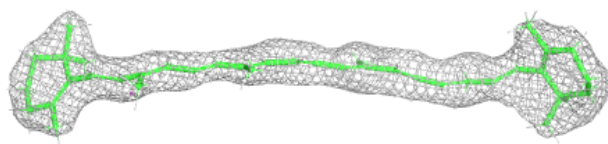
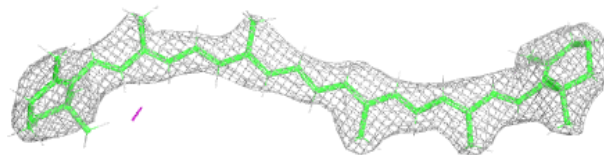
**Electron density around CLA c 513:**

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

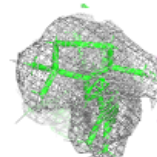
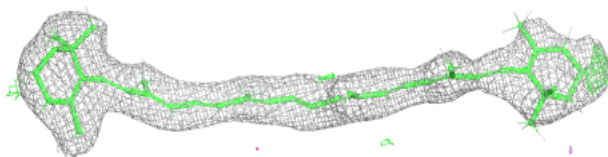
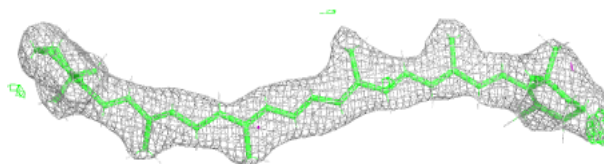


Electron density around BCR k 101:

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

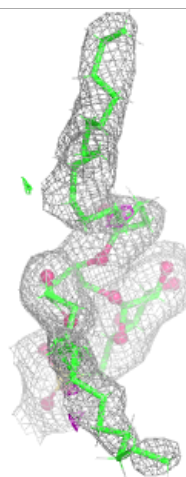
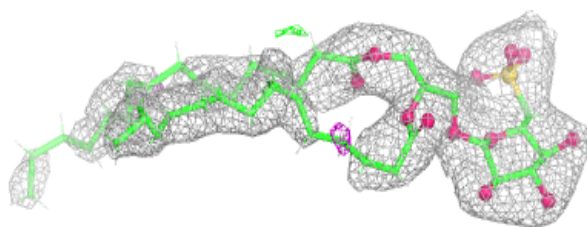
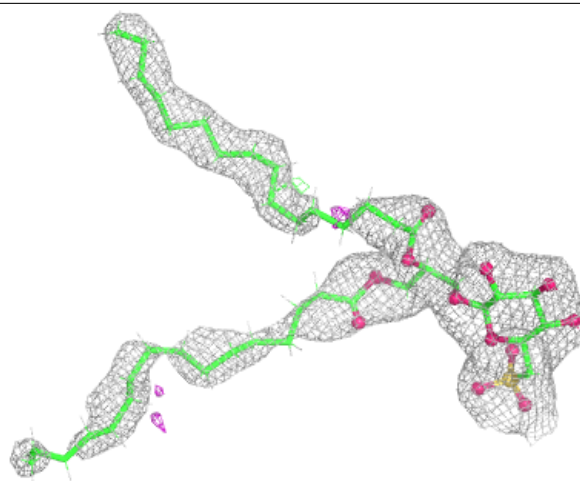
**Electron density around BCR X 101:**

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



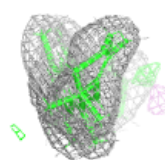
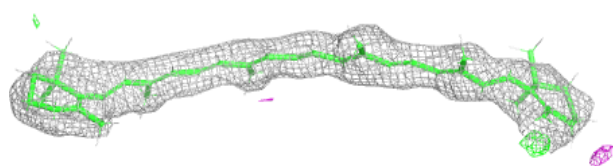
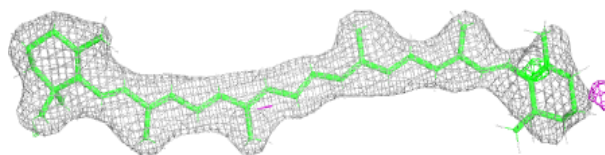
Electron density around SQD a 615:

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

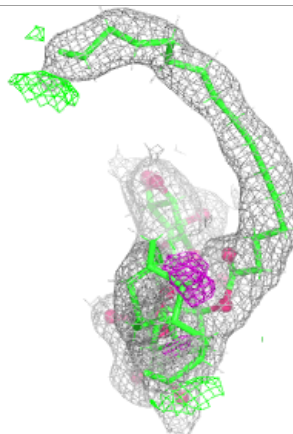
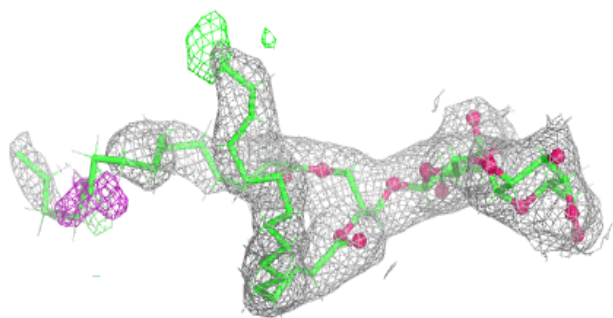
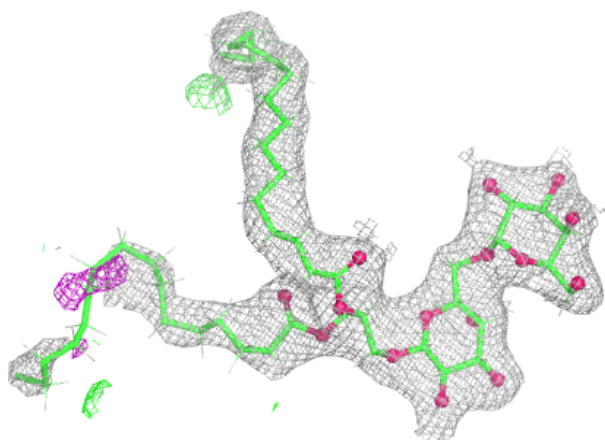


Electron density around BCR D 405:

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

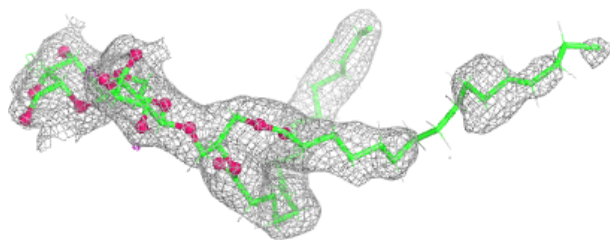
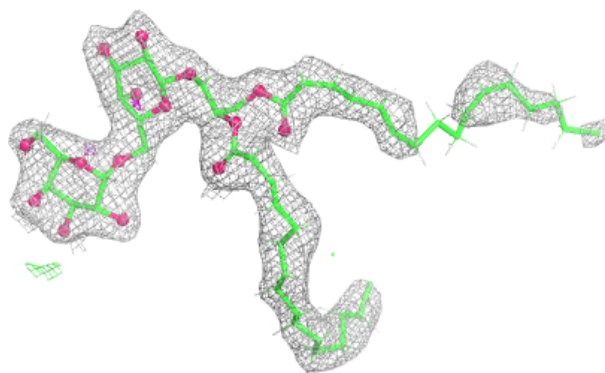
**Electron density around DGD C 517:**

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

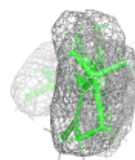
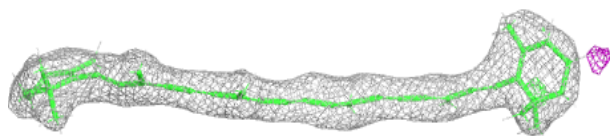
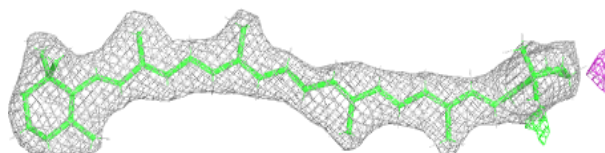


Electron density around DGD c 517:

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

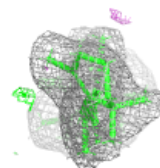
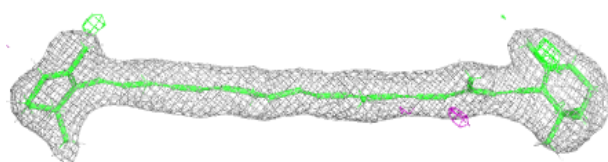
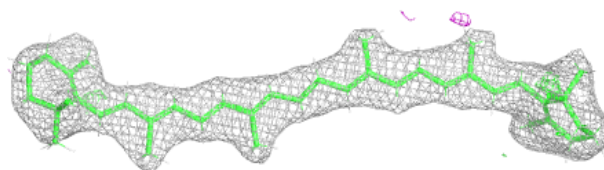
**Electron density around BCR b 617:**

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

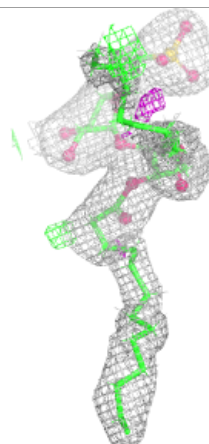
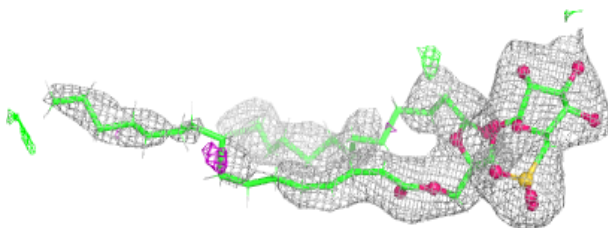
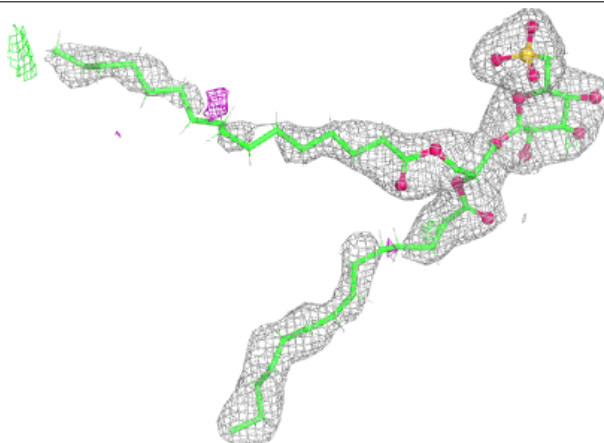


Electron density around BCR b 618:

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

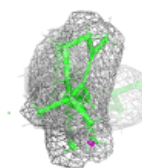
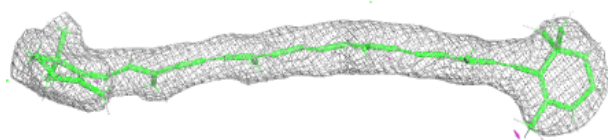
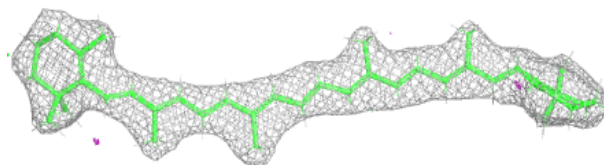
**Electron density around SQD A 613:**

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

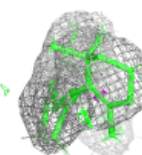
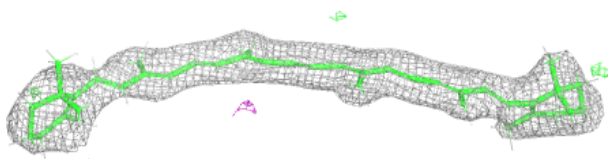


Electron density around BCR B 616:

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

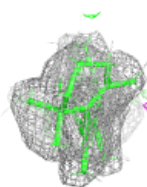
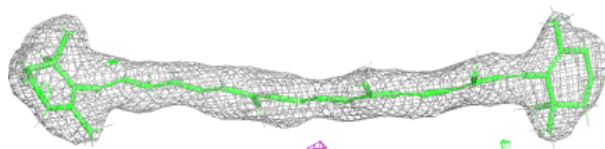
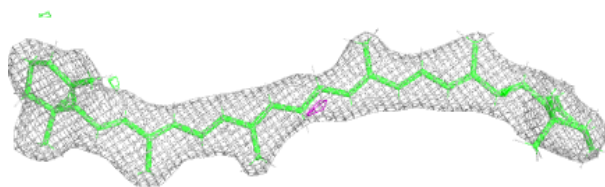
**Electron density around BCR d 404:**

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

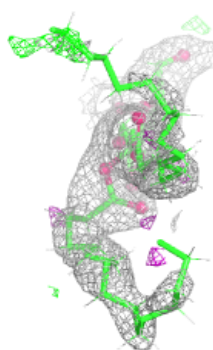
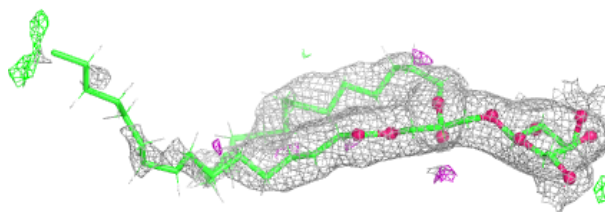
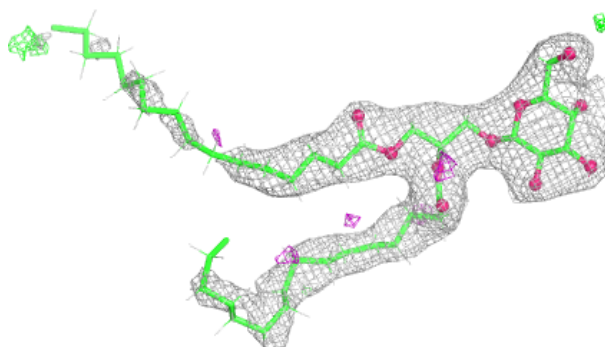


Electron density around BCR K 102:

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

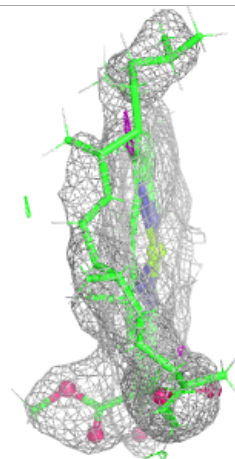
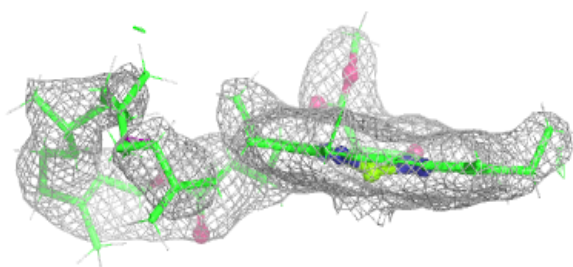
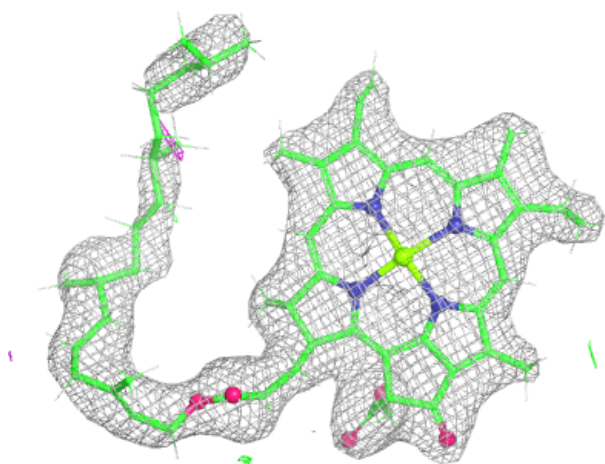
**Electron density around LMG D 407:**

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



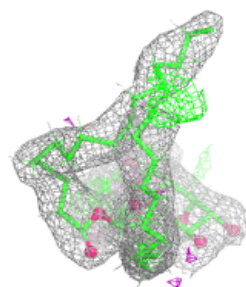
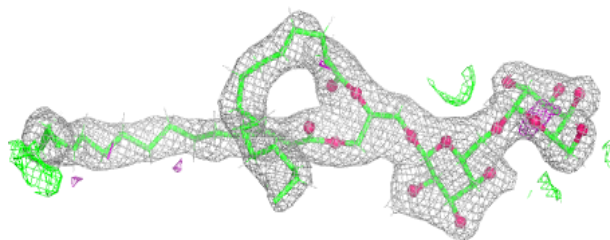
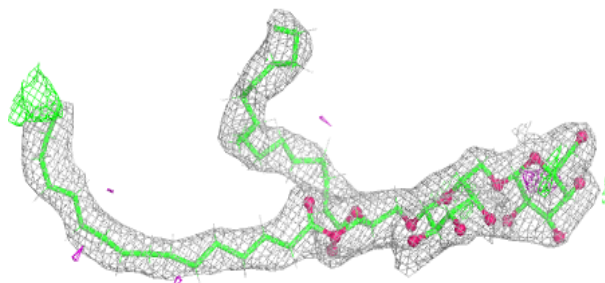
Electron density around CLA c 512:

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

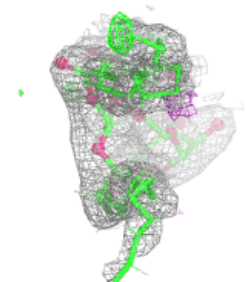
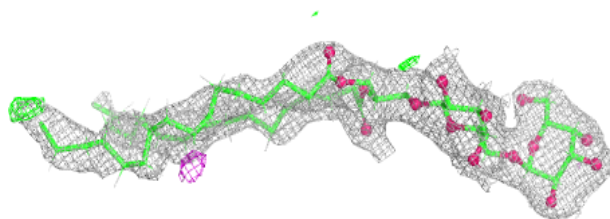
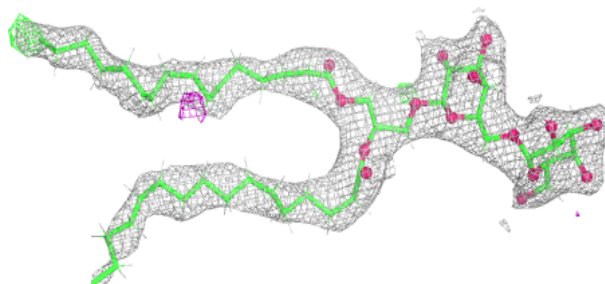


Electron density around DGD H 102:

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

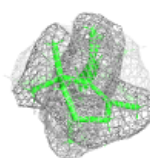
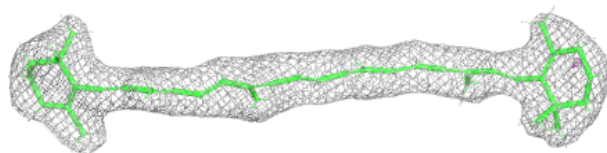
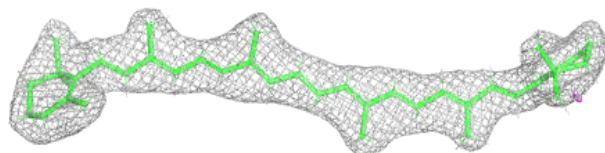
**Electron density around DGD c 518:**

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

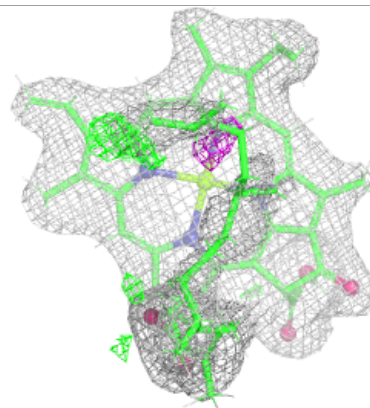
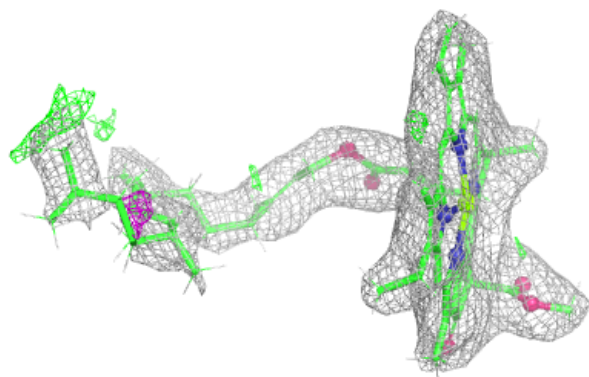
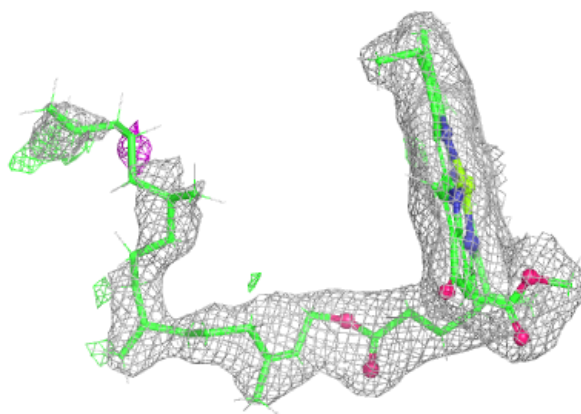


Electron density around BCR A 608:

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

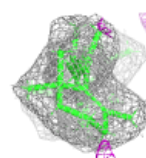
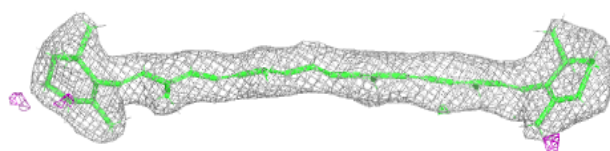
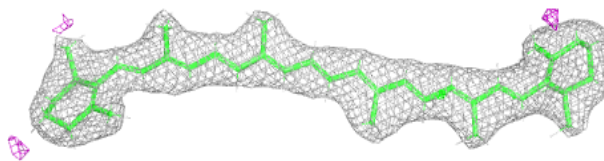
**Electron density around CLA c 506:**

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

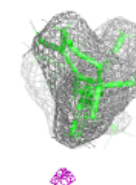
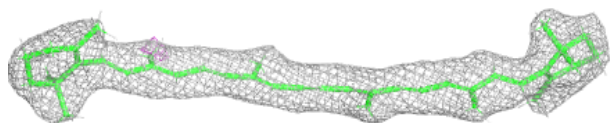
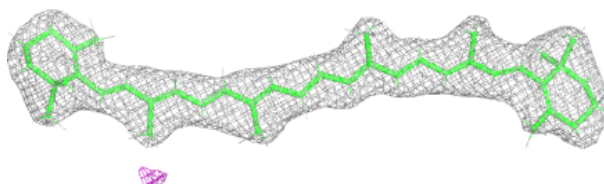


Electron density around BCR B 617:

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

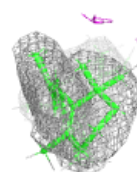
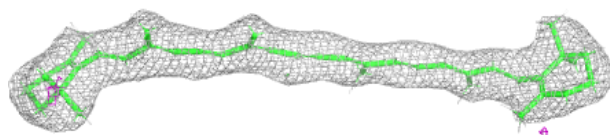
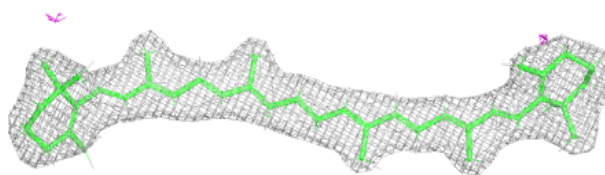
**Electron density around BCR b 619:**

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

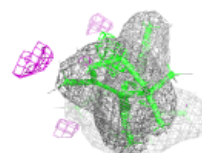
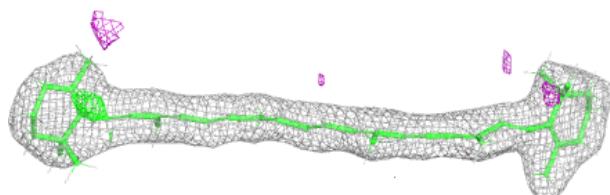
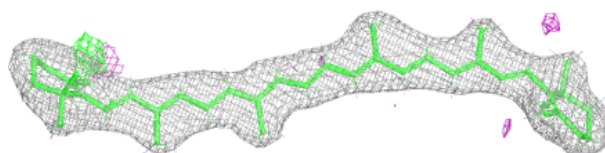


Electron density around BCR B 618:

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

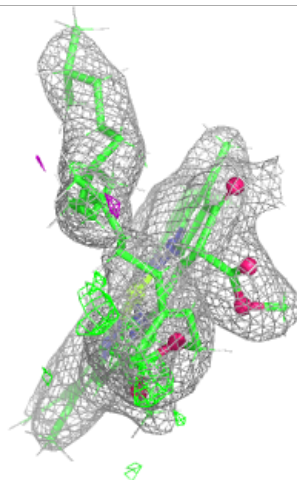
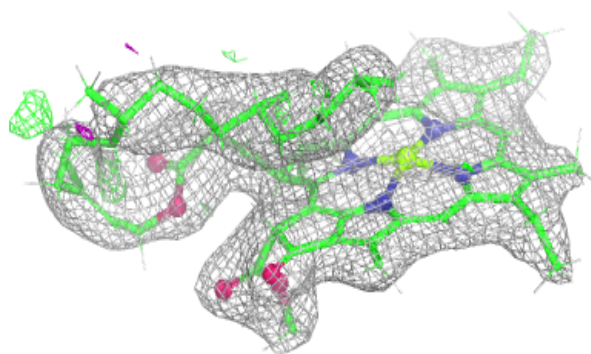
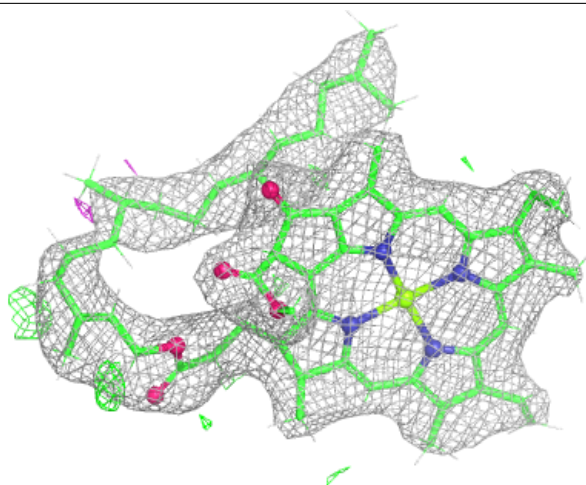
**Electron density around BCR C 514:**

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



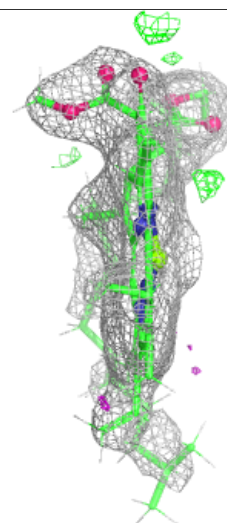
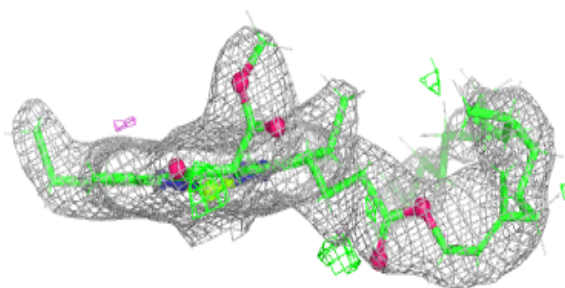
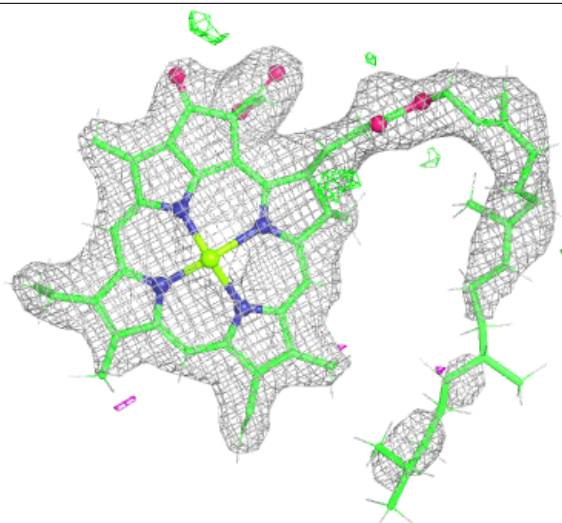
Electron density around CLA c 509:

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



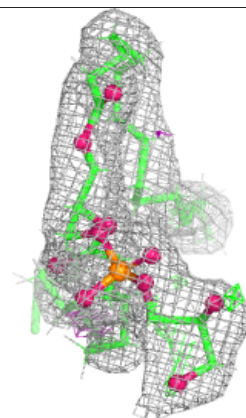
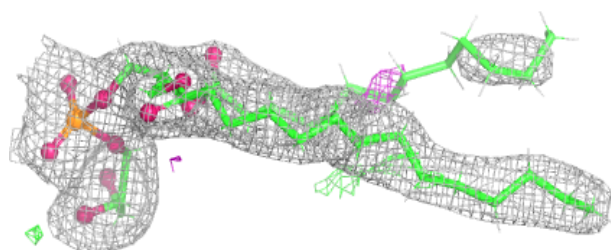
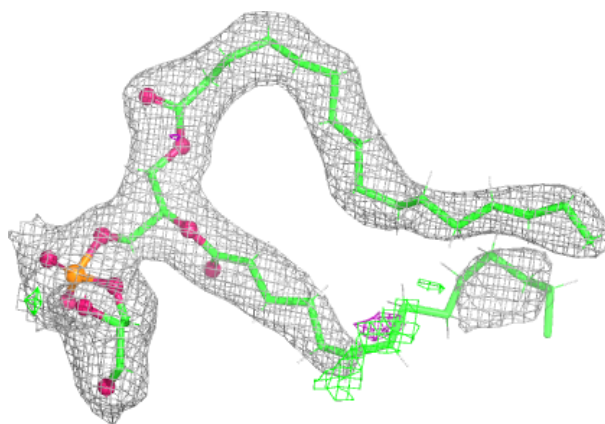
Electron density around CLA C 512:

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

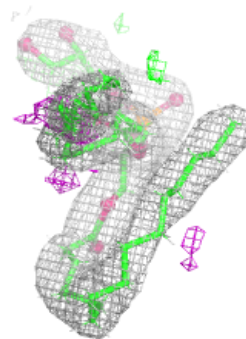
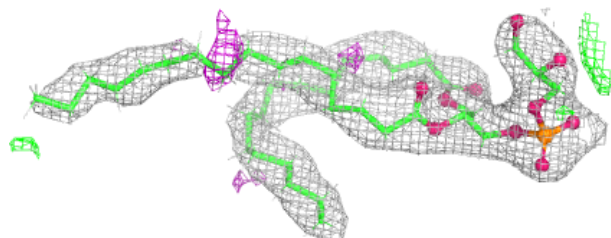
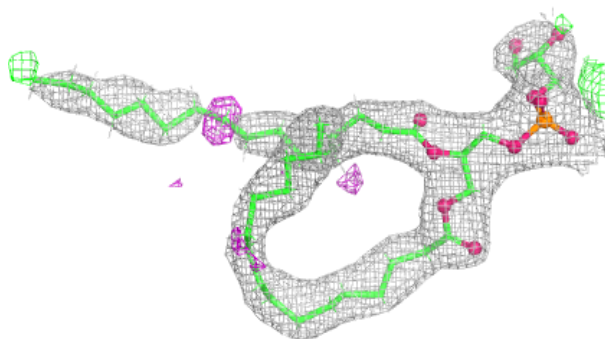


Electron density around LHG D 410:

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

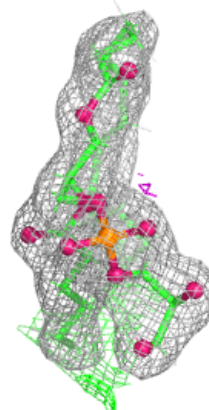
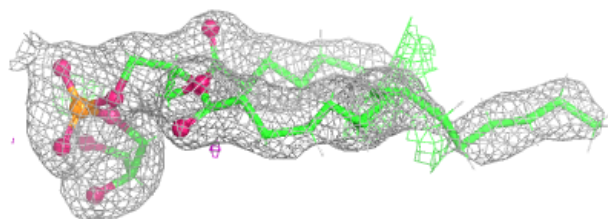
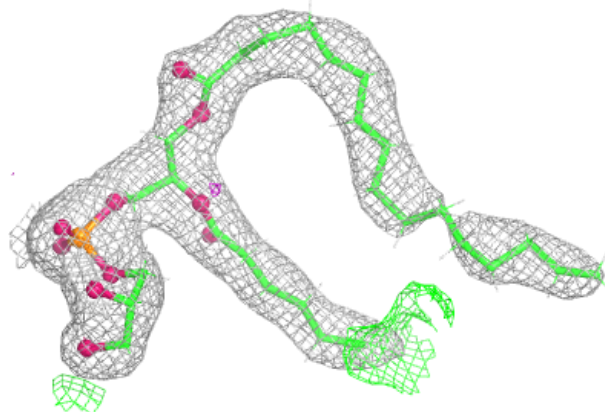
**Electron density around LHG a 614:**

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

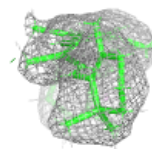
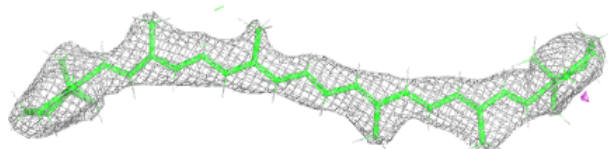
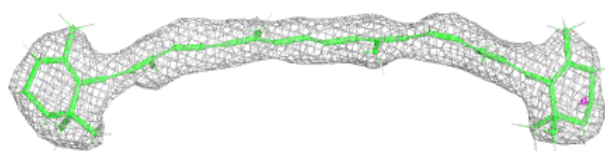


Electron density around LHG d 407:

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

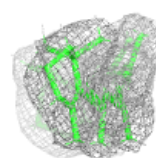
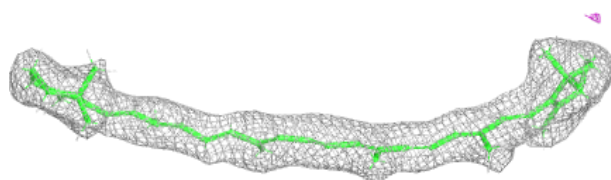
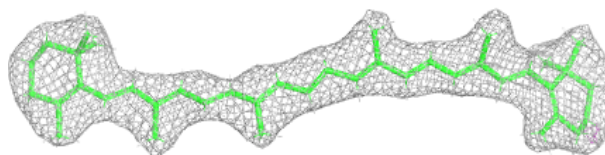
**Electron density around BCR k 102:**

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

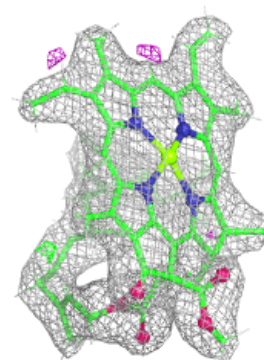
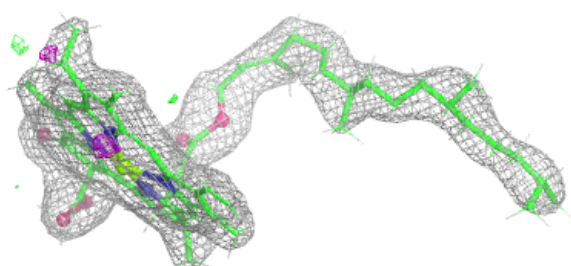
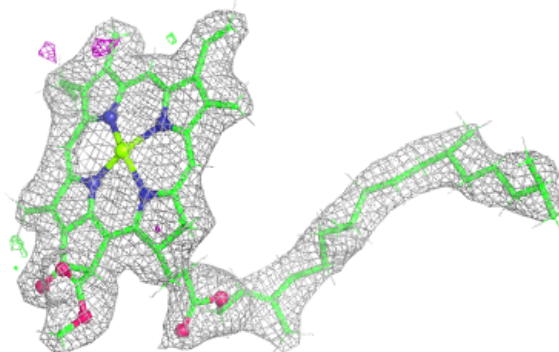


Electron density around BCR t 101:

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

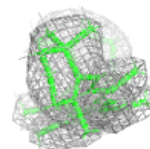
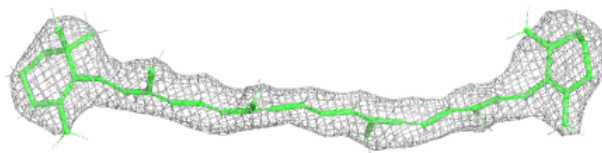
**Electron density around CLA C 511:**

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

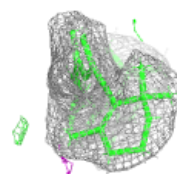
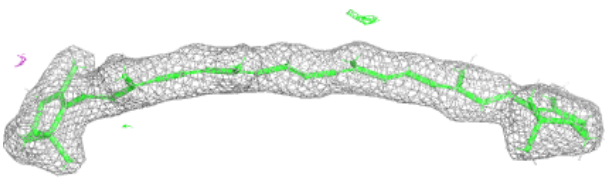
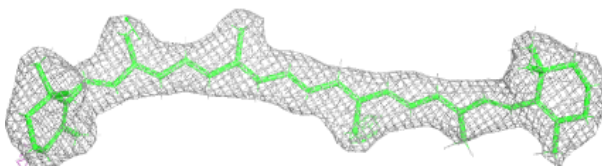


Electron density around BCR K 103:

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

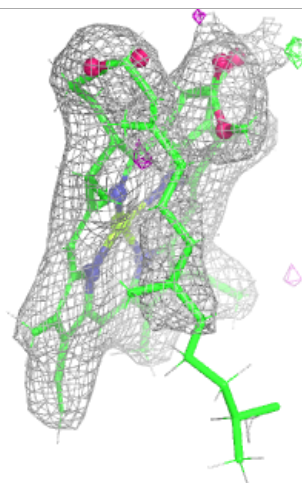
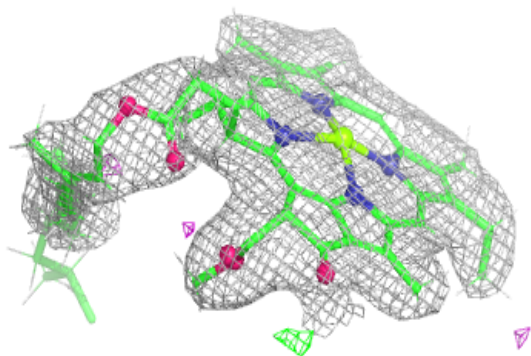
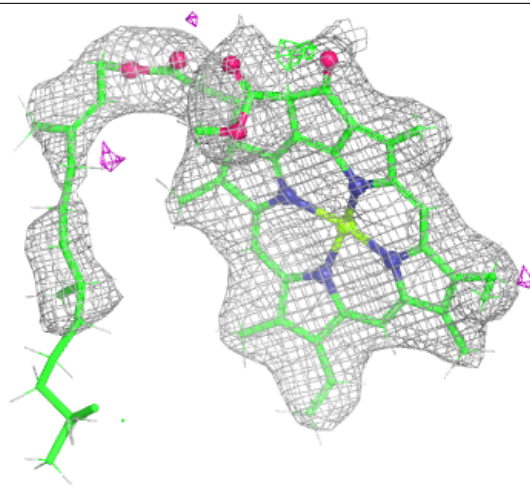
**Electron density around BCR T 101:**

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



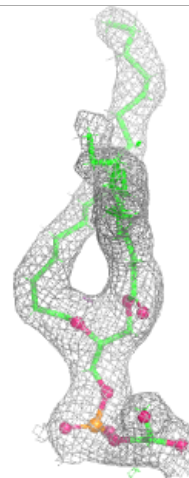
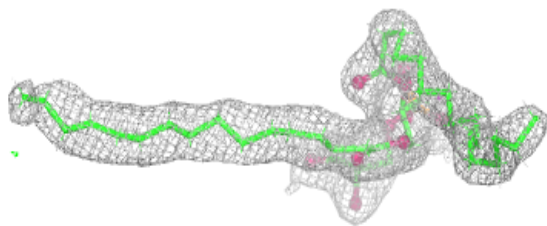
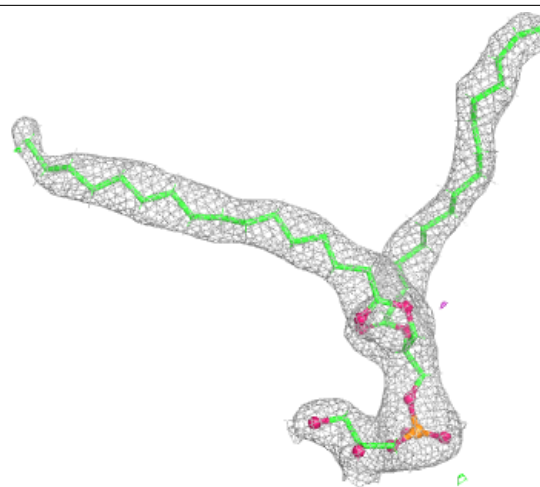
Electron density around CLA b 616:

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



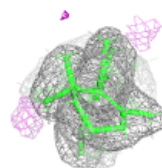
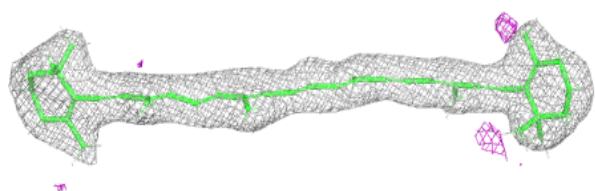
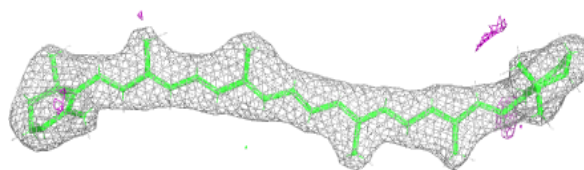
Electron density around LHG 1 101:

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

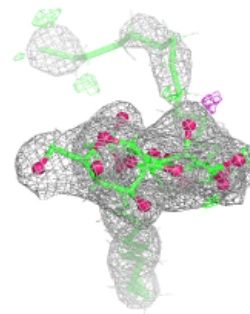
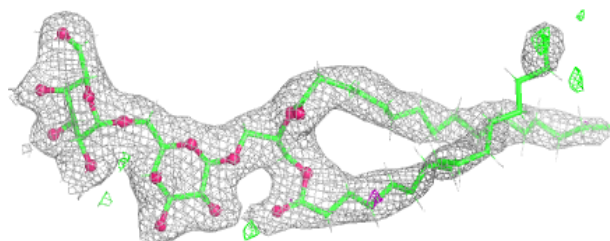
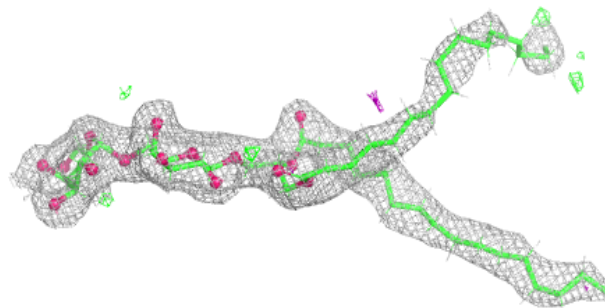


Electron density around BCR a 608:

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

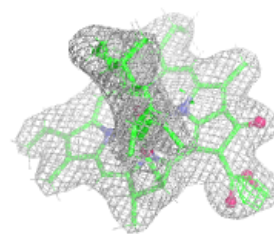
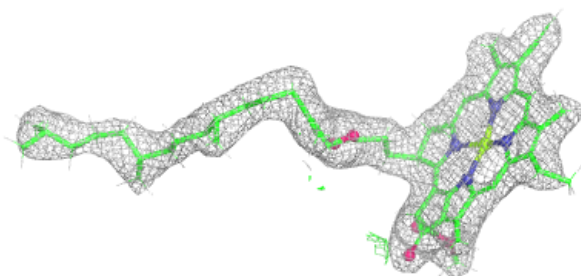
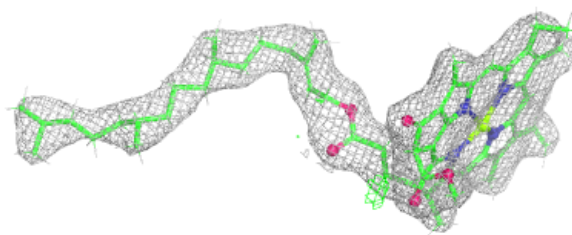
**Electron density around DGD C 516:**

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

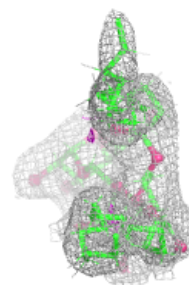
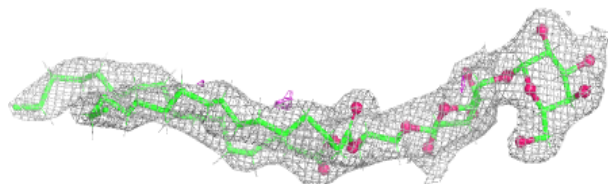
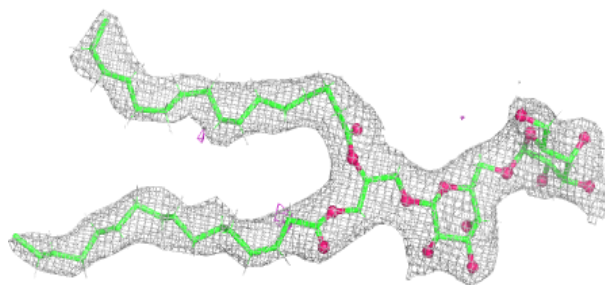


Electron density around CLA c 502:

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

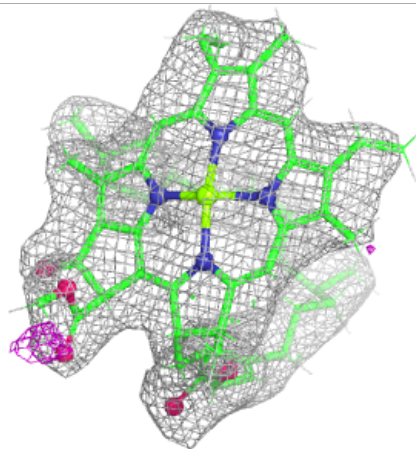
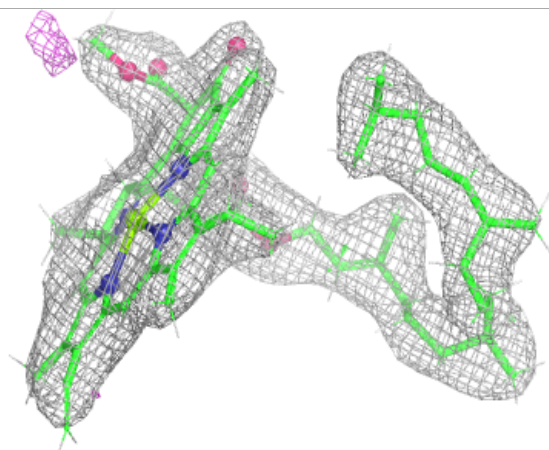
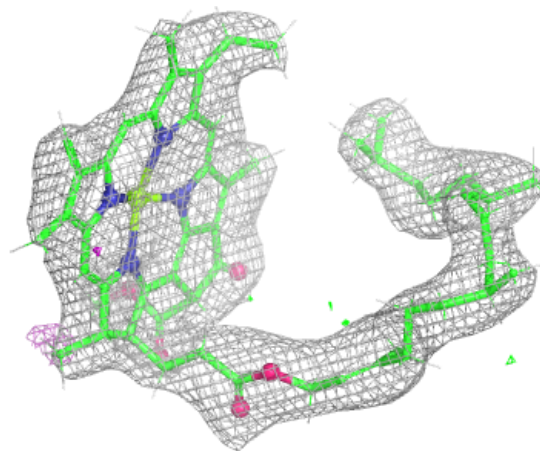
**Electron density around DGD C 518:**

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



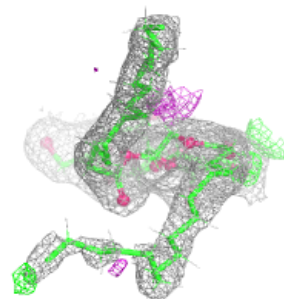
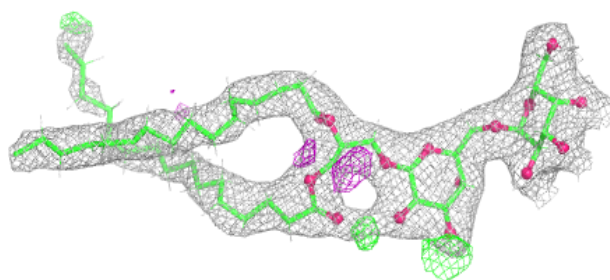
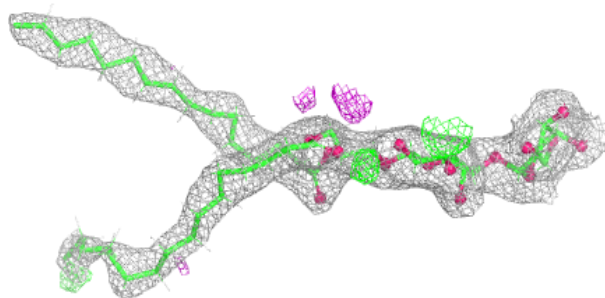
Electron density around CLA c 503:

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

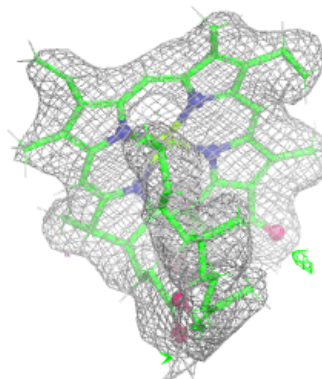
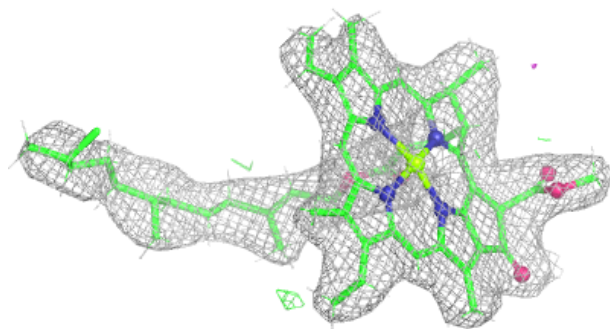
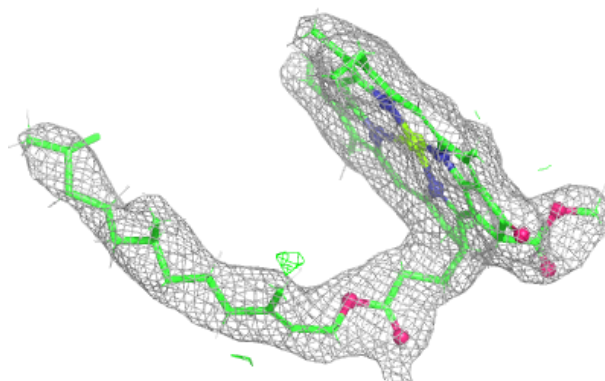


Electron density around DGD c 516:

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

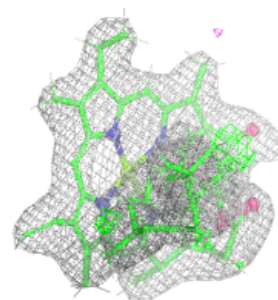
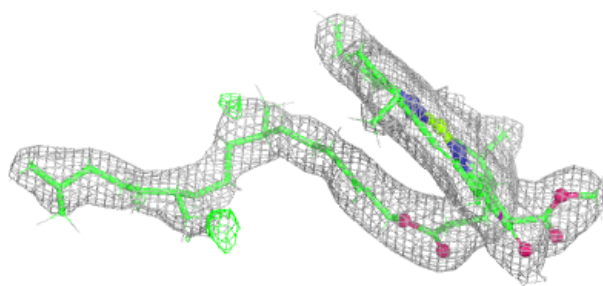
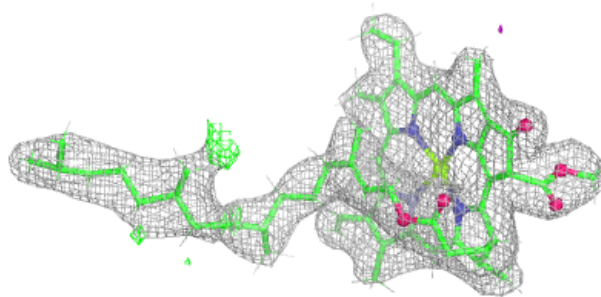
**Electron density around CLA c 504:**

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

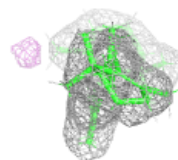
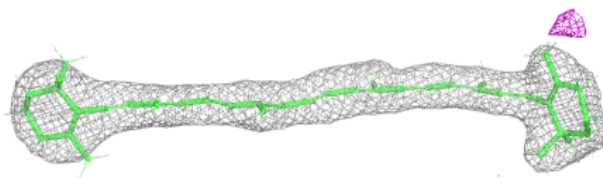
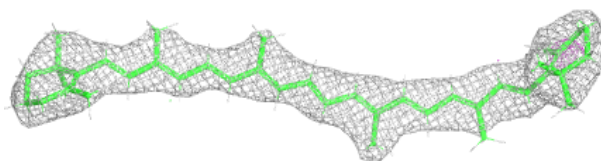


Electron density around CLA c 505:

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

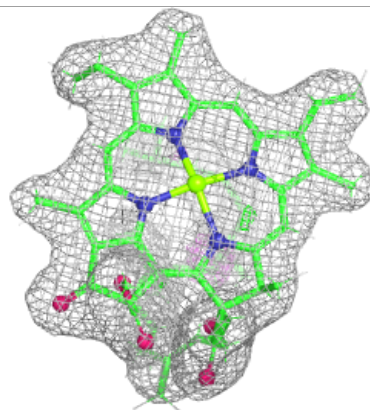
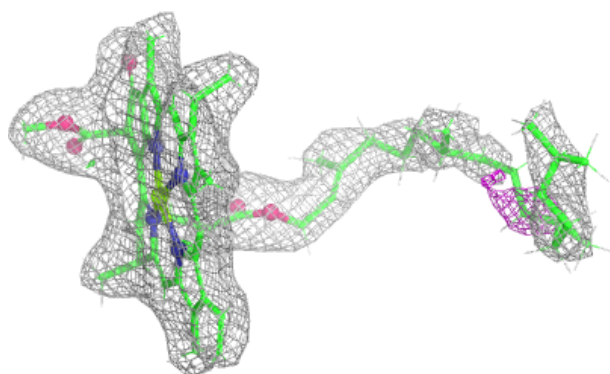
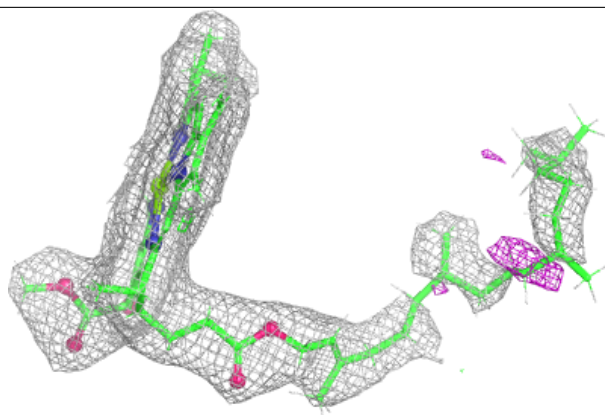
**Electron density around BCR c 515:**

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

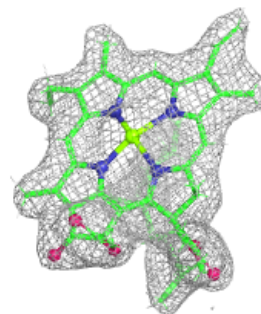
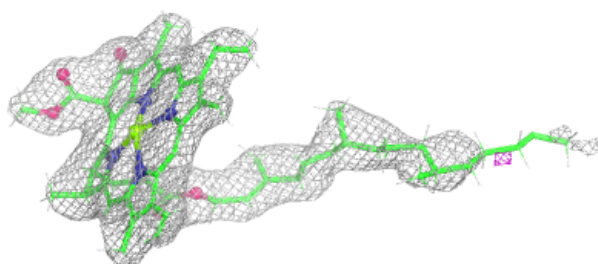
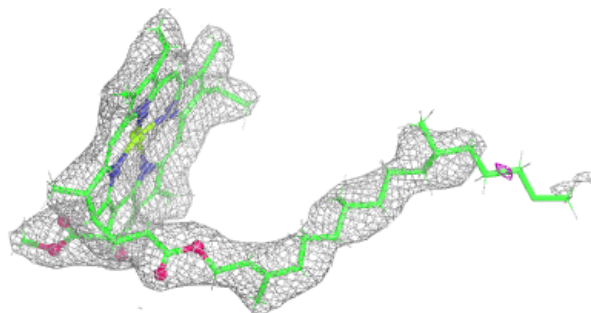


Electron density around CLA C 506:

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

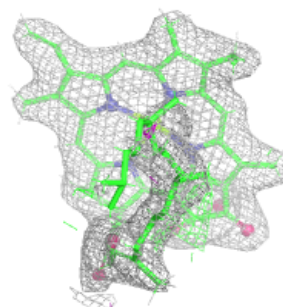
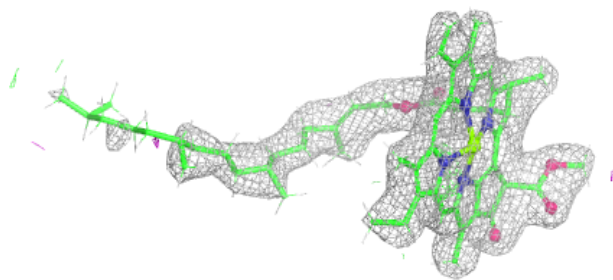
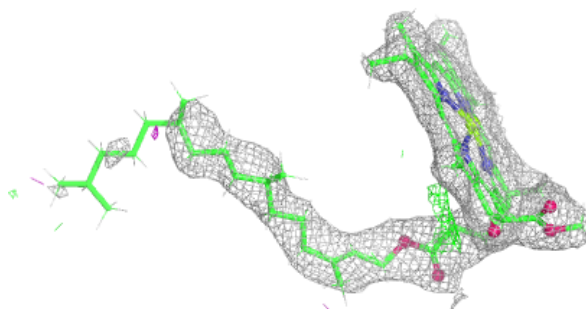
**Electron density around CLA c 508:**

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



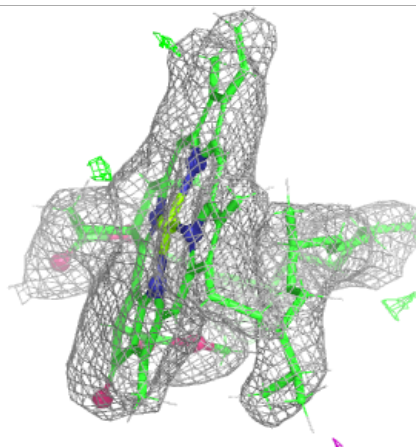
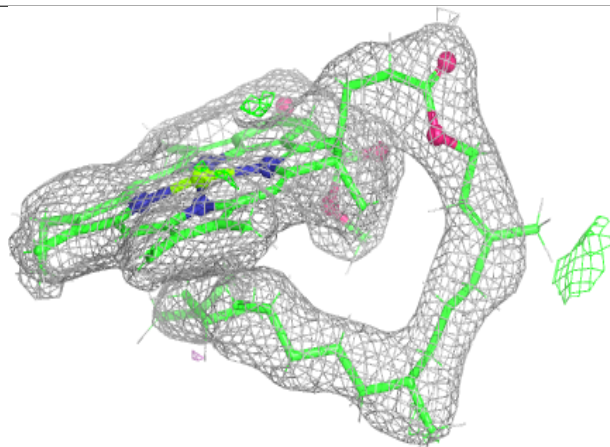
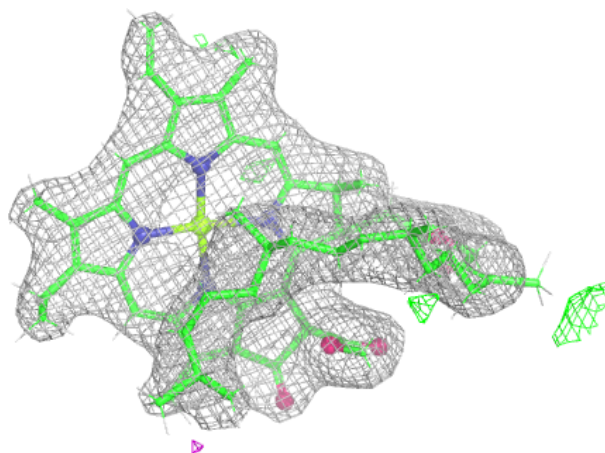
Electron density around CLA C 508:

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



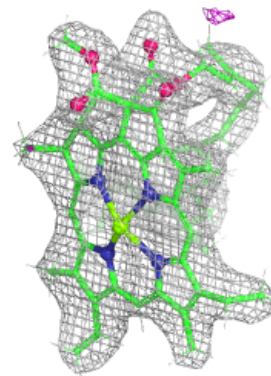
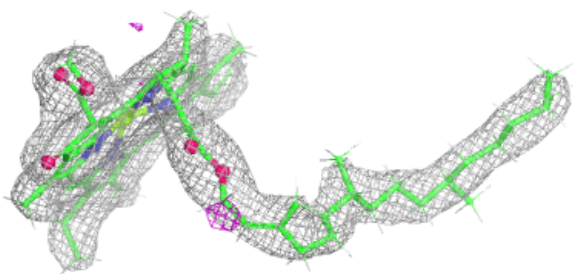
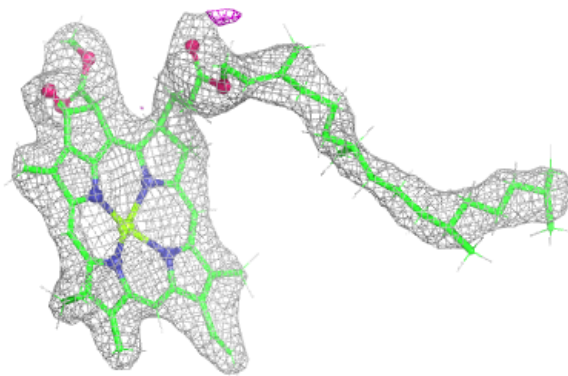
Electron density around CLA c 510:

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



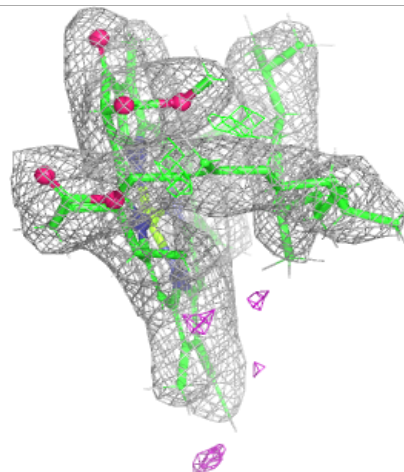
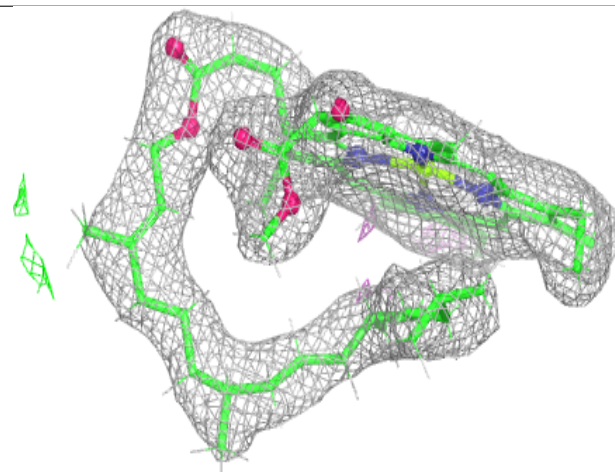
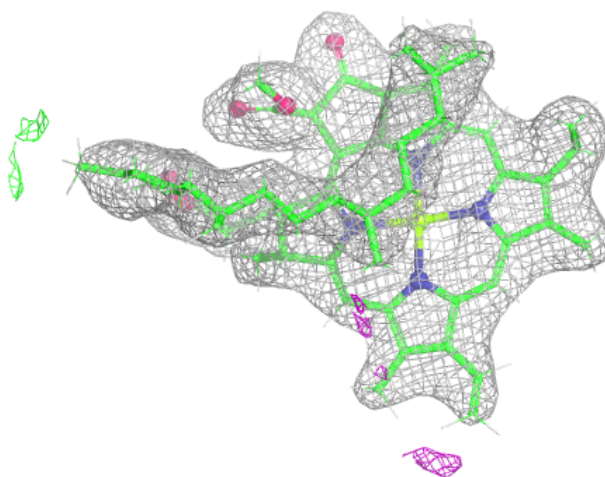
Electron density around CLA c 511:

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



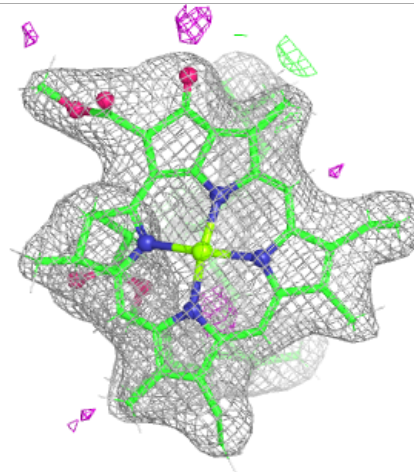
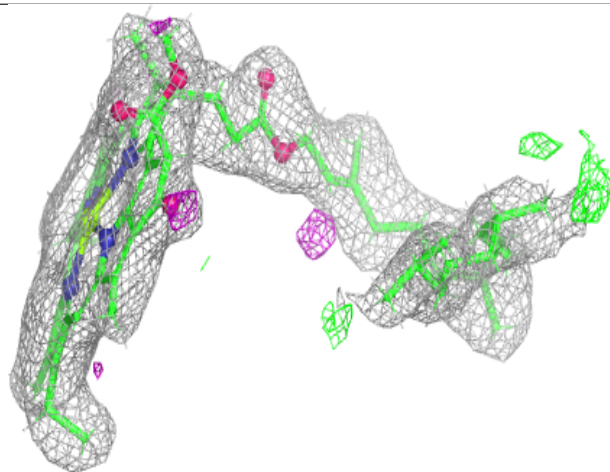
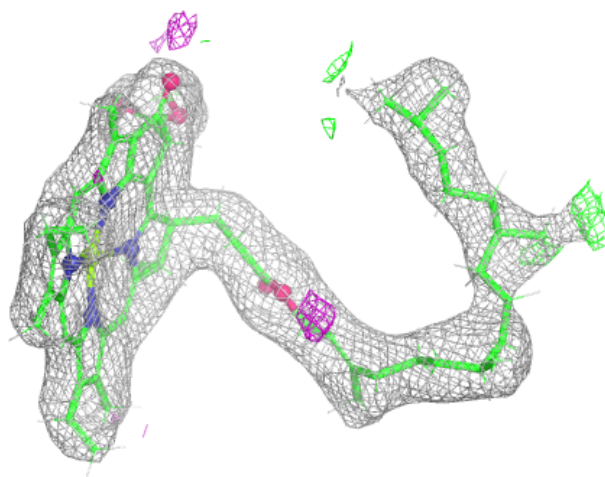
Electron density around CLA C 510:

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



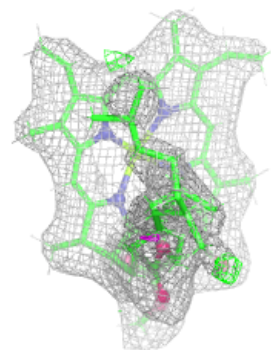
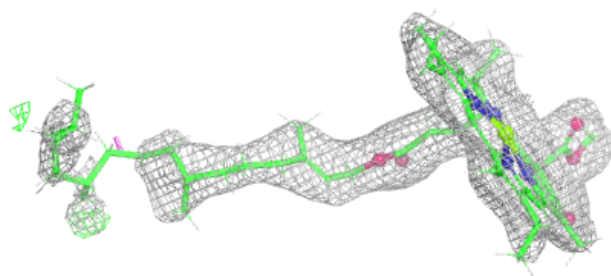
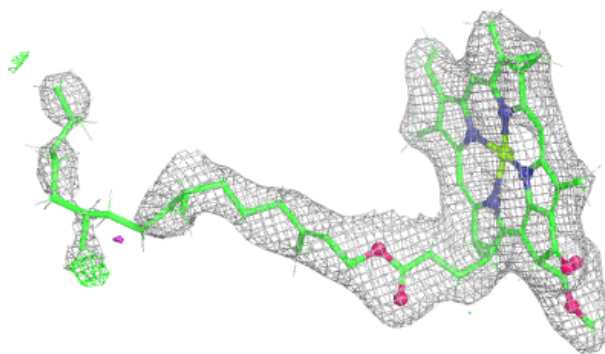
Electron density around CLA B 605:

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



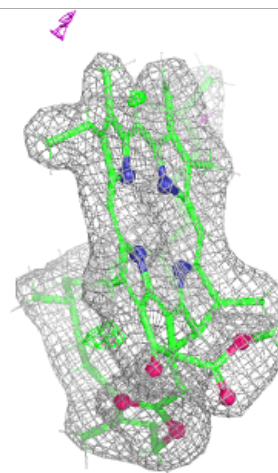
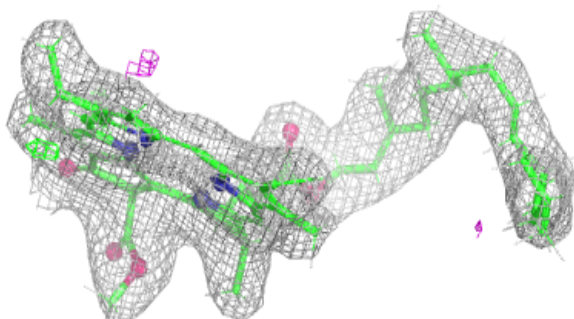
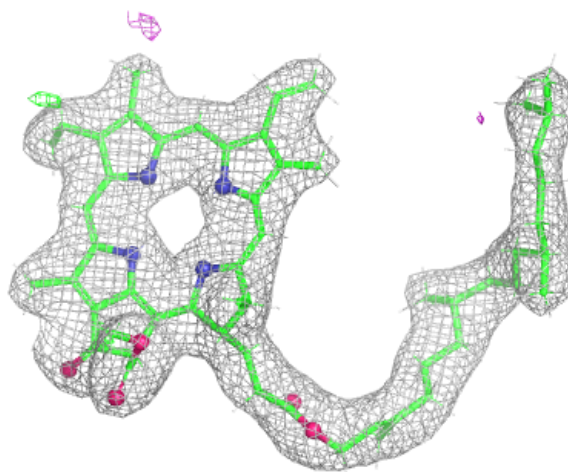
Electron density around CLA d 403:

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



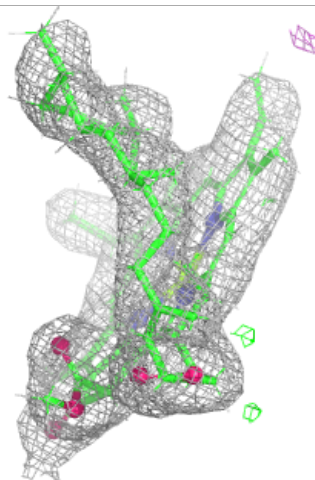
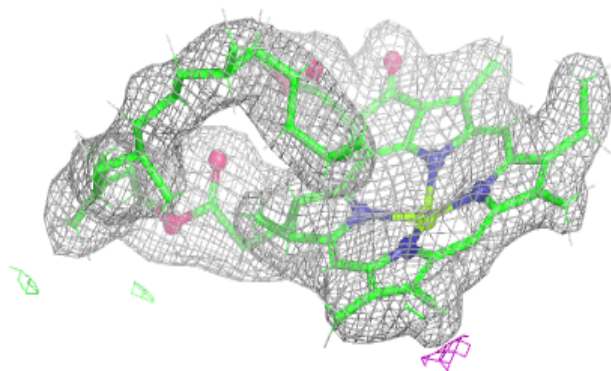
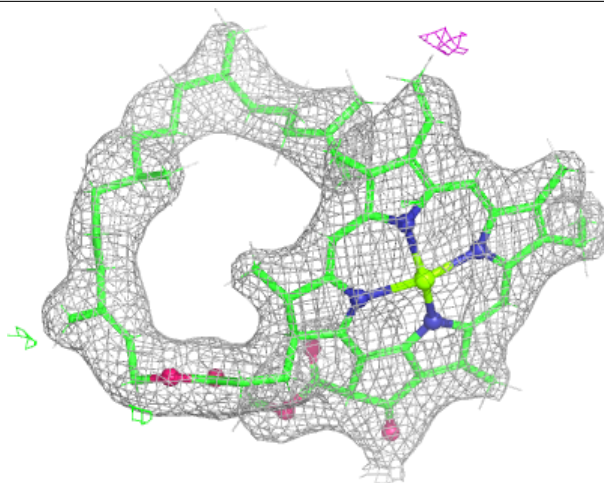
Electron density around PHO d 401:

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



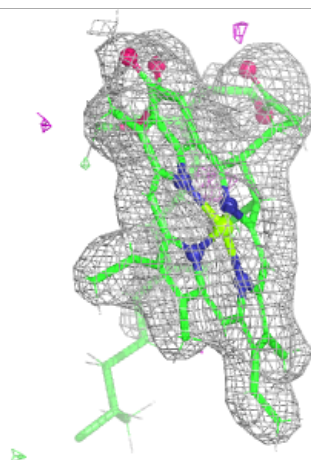
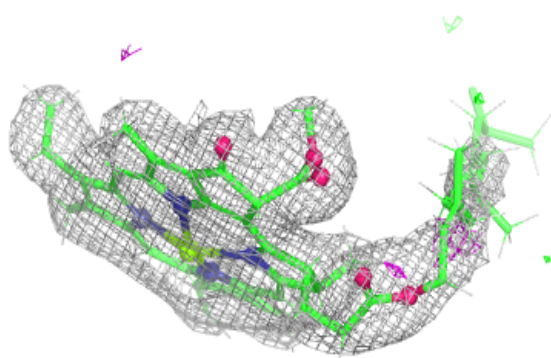
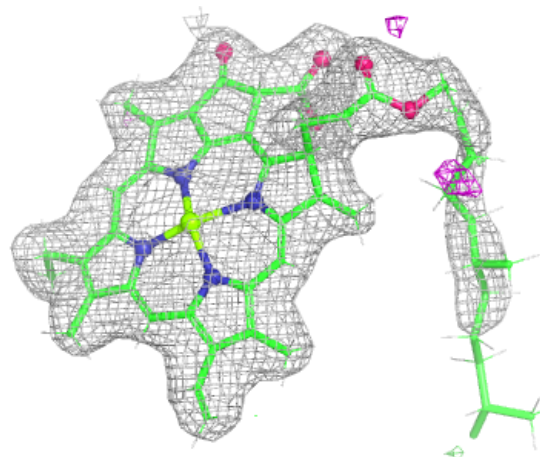
Electron density around CLA B 614:

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



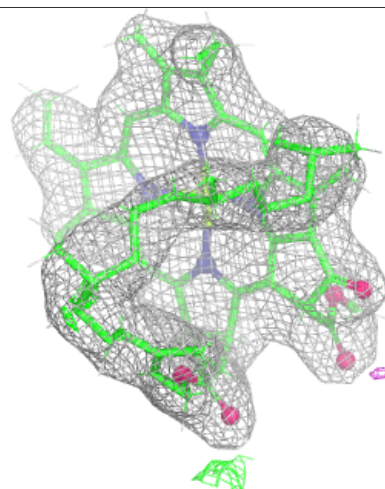
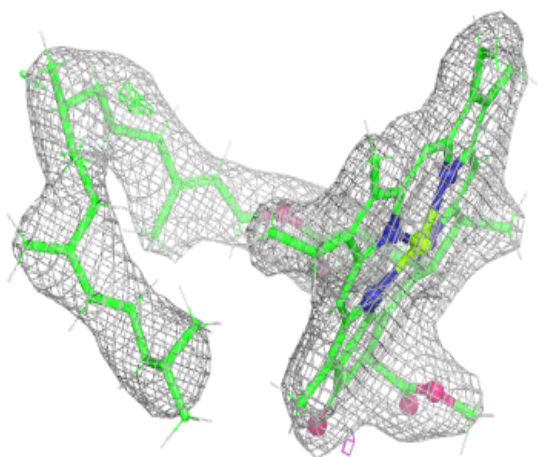
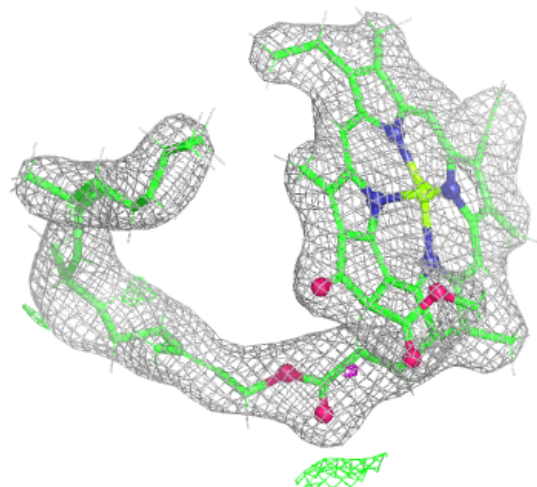
Electron density around CLA B 615:

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



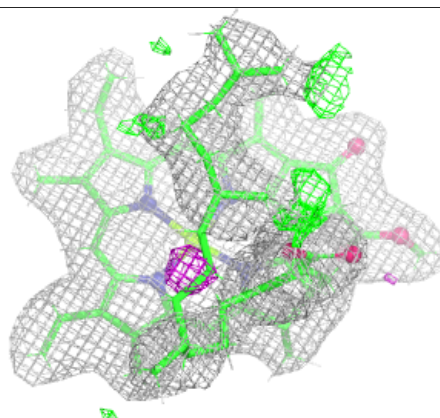
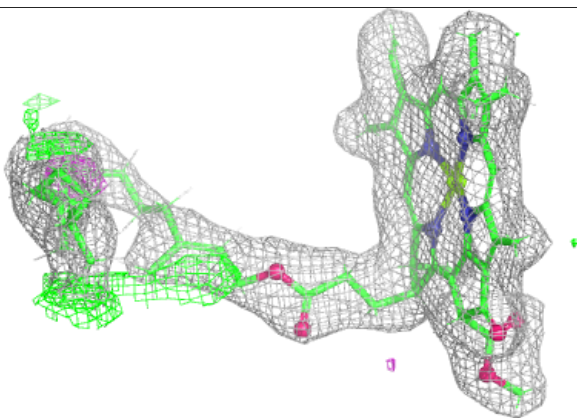
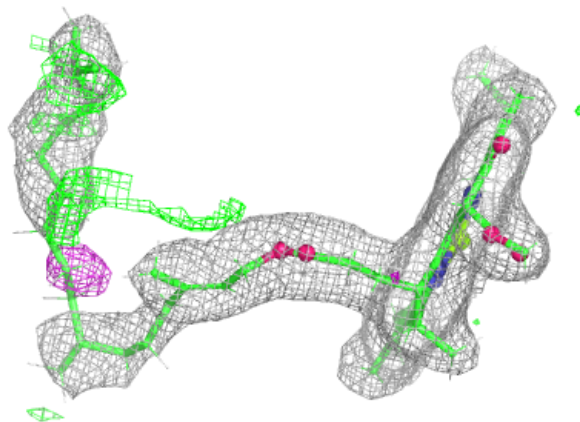
Electron density around CLA C 503:

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

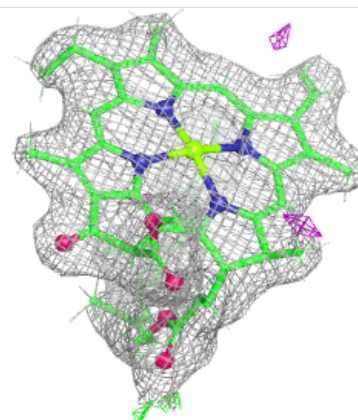
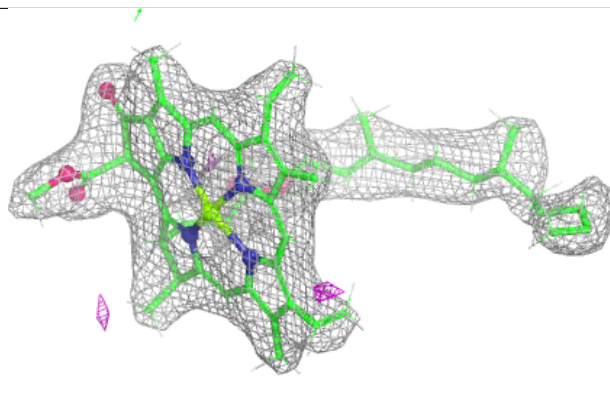
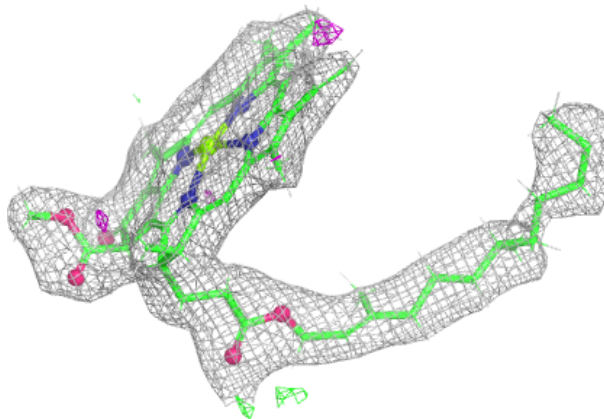


Electron density around CLA a 607:

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

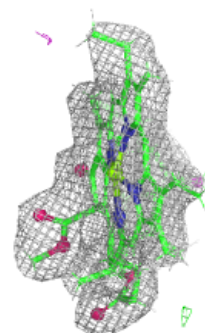
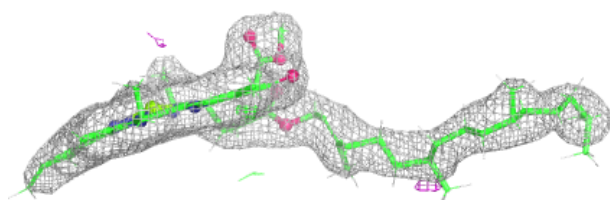
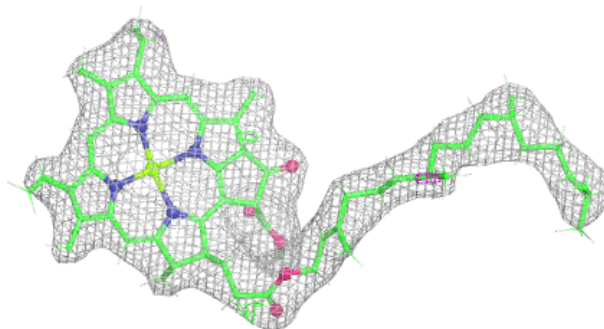
**Electron density around CLA C 504:**

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

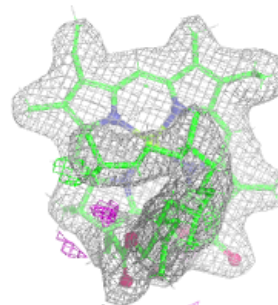
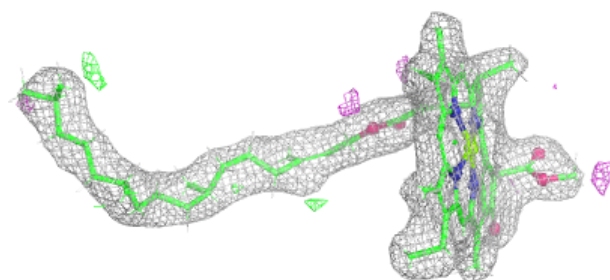
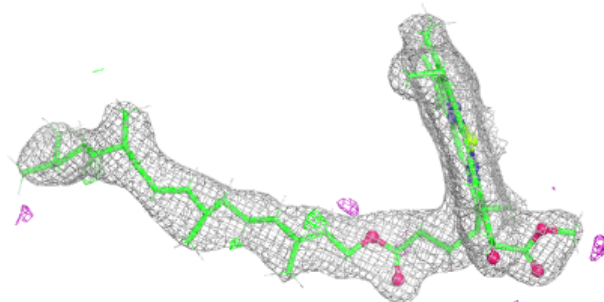


Electron density around CLA b 602:

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

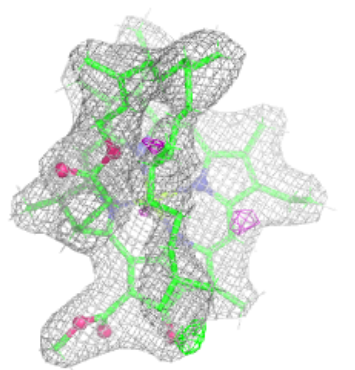
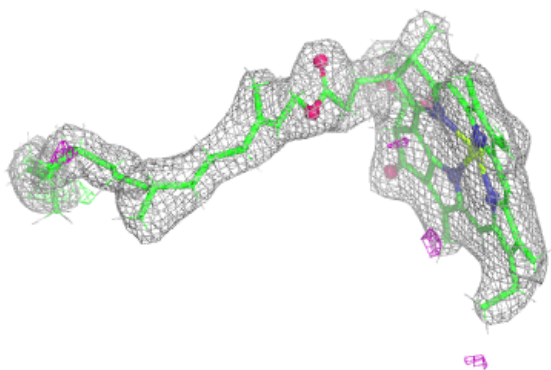
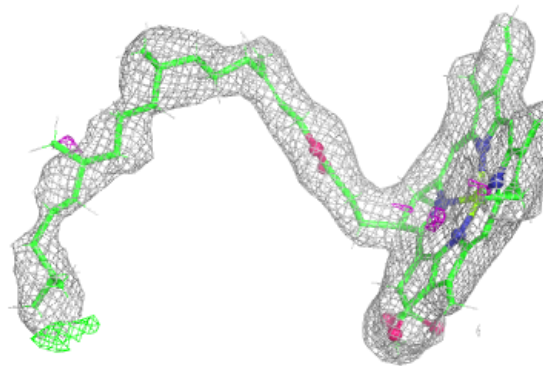
**Electron density around CLA b 605:**

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

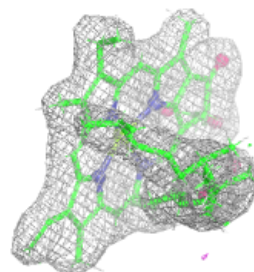
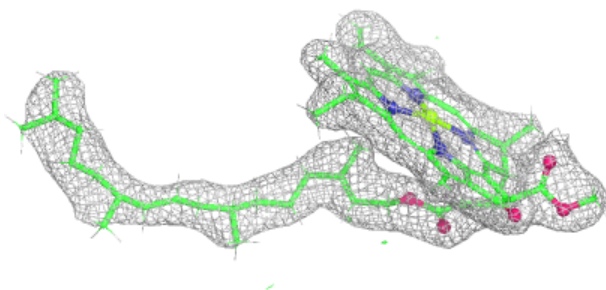
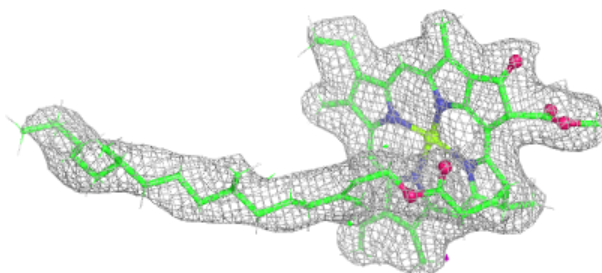


Electron density around CLA b 606:

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

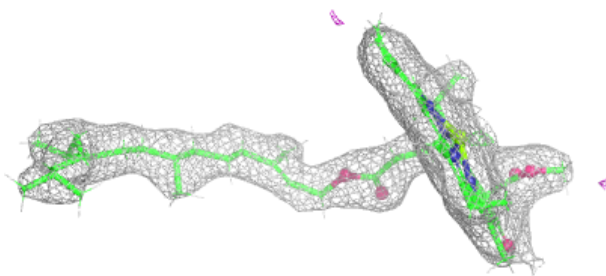
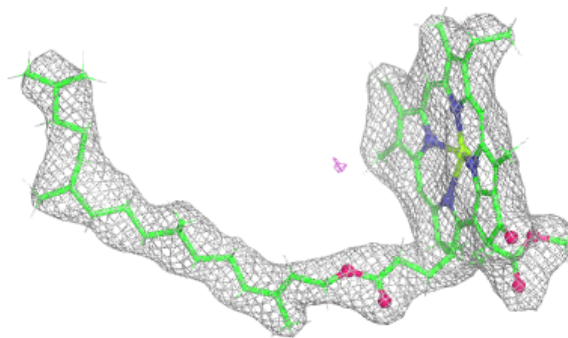
**Electron density around CLA b 608:**

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



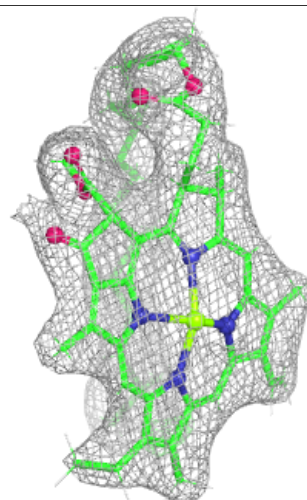
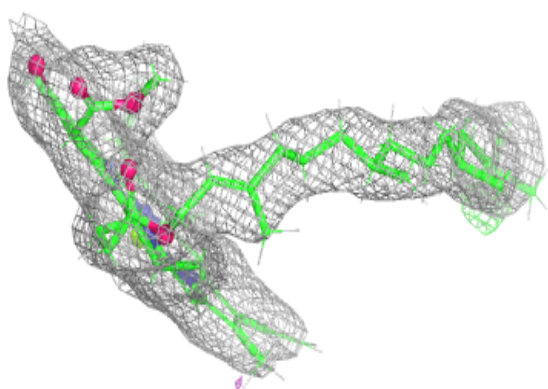
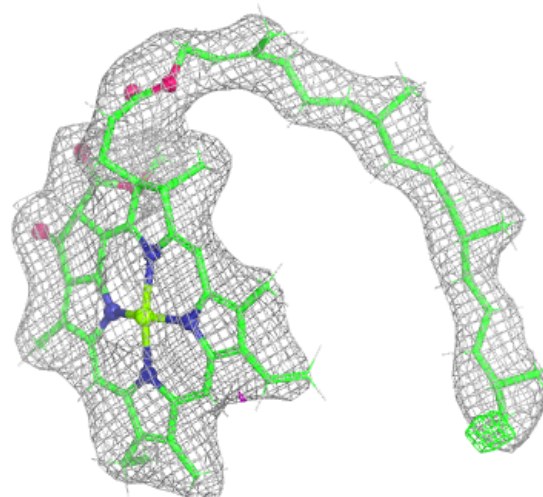
Electron density around CLA b 609:

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



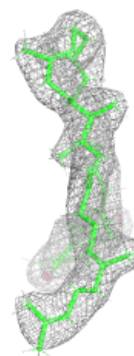
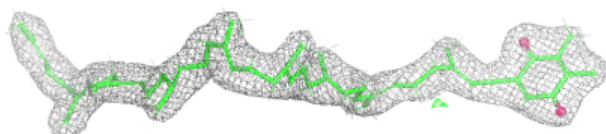
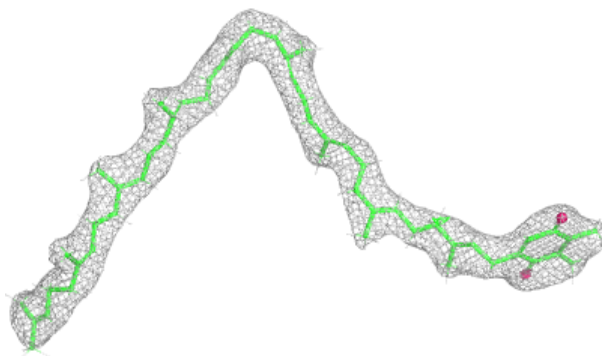
Electron density around CLA c 507:

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

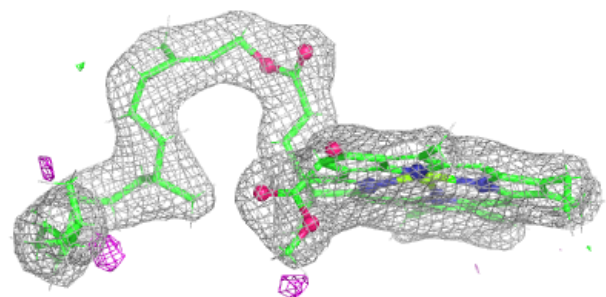
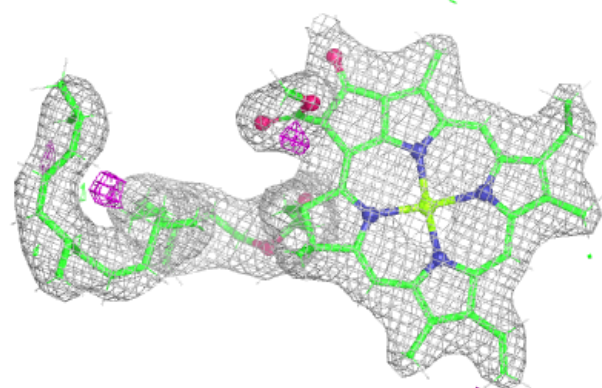


Electron density around PL9 D 406:

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

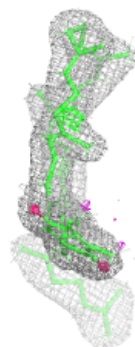
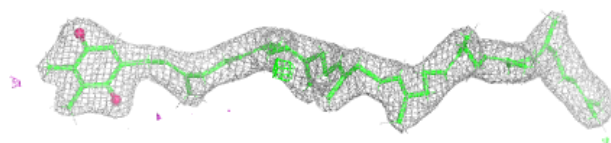
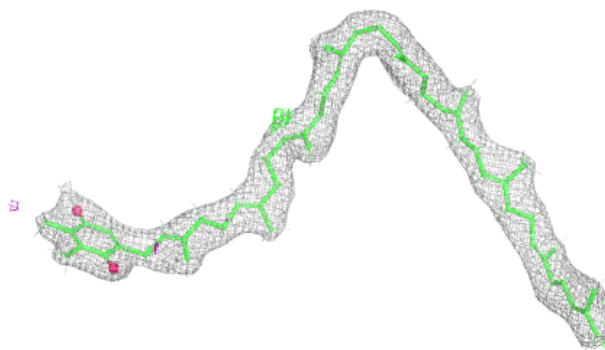
**Electron density around CLA B 611:**

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



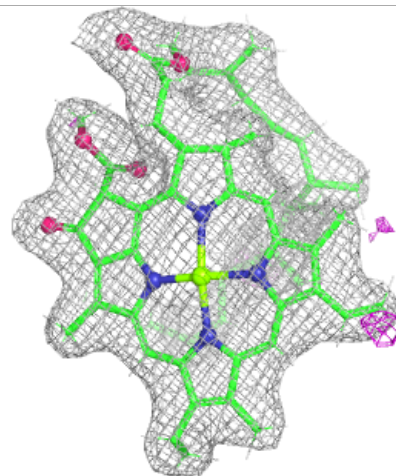
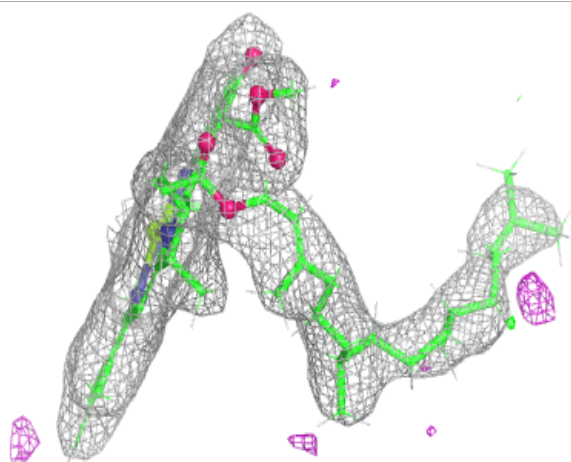
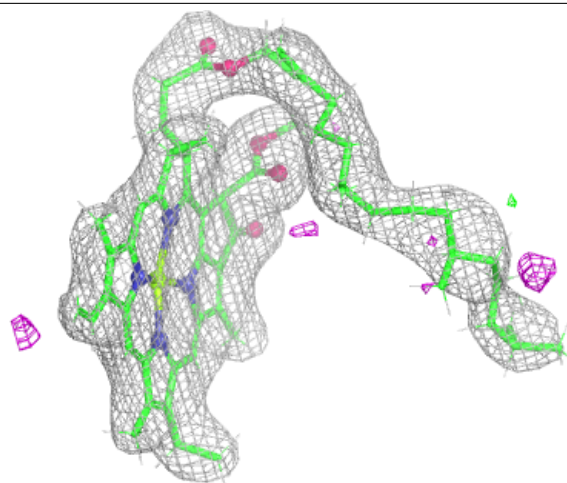
Electron density around PL9 d 405:

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



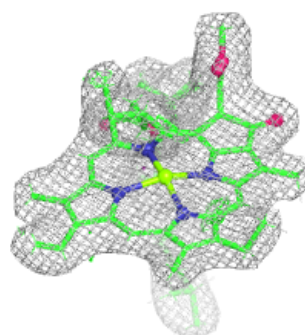
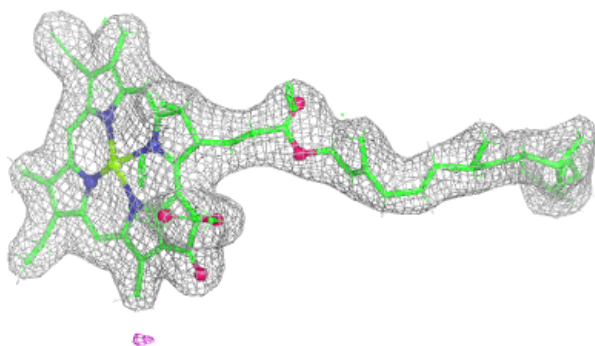
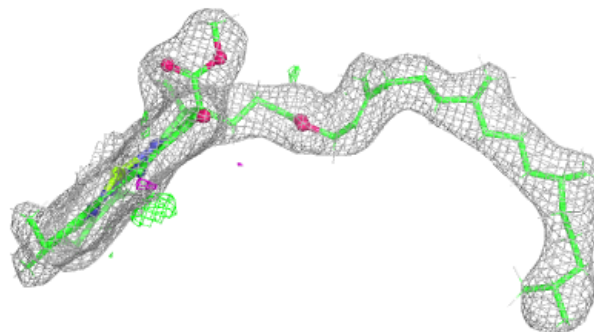
Electron density around CLA B 612:

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

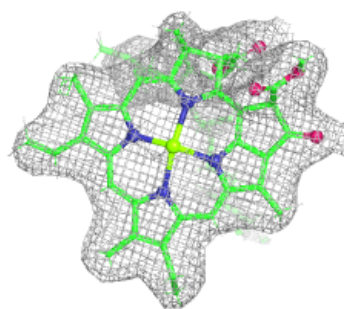
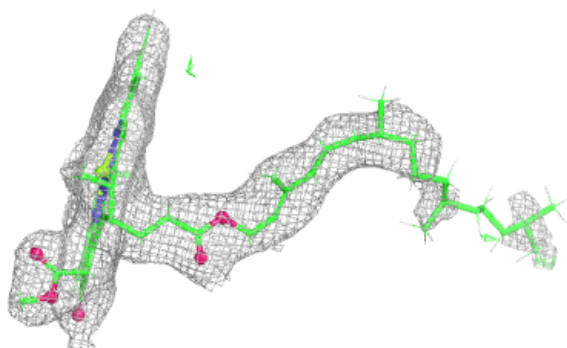
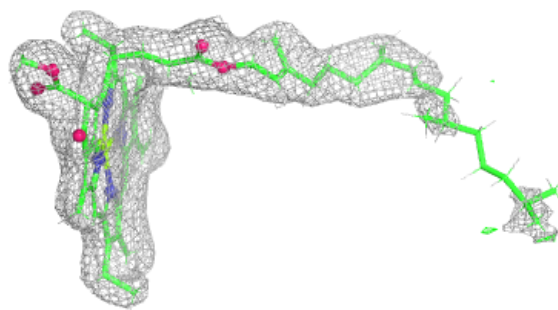


Electron density around CLA D 403:

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

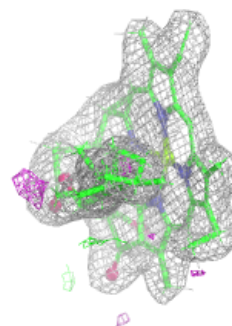
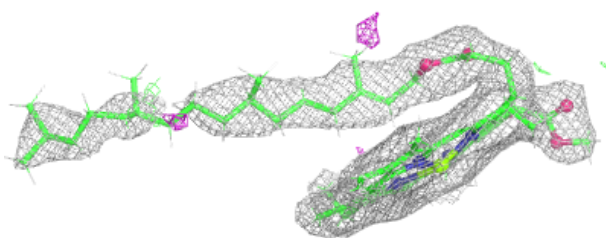
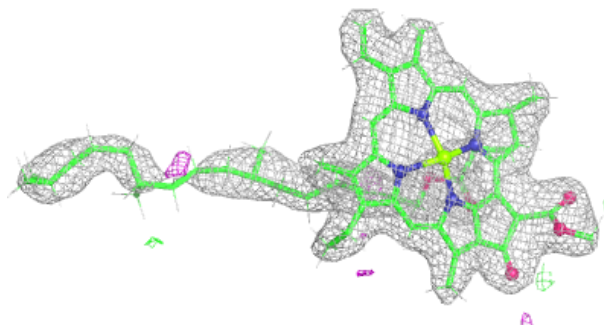
**Electron density around CLA D 404:**

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

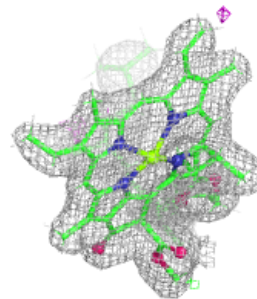
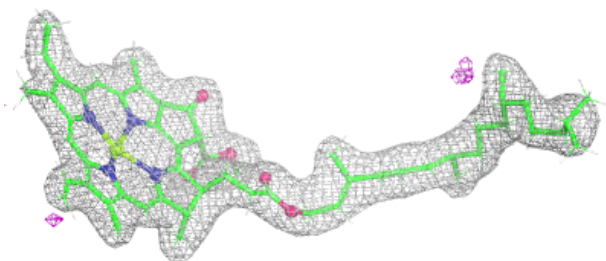
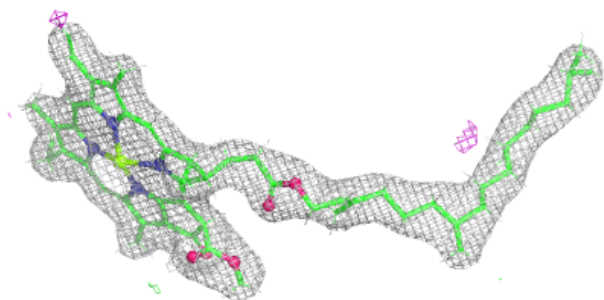


Electron density around CLA B 613:

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

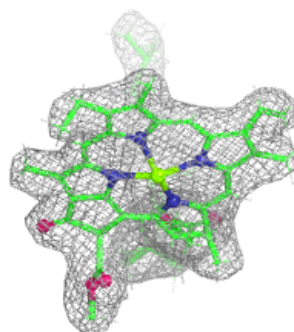
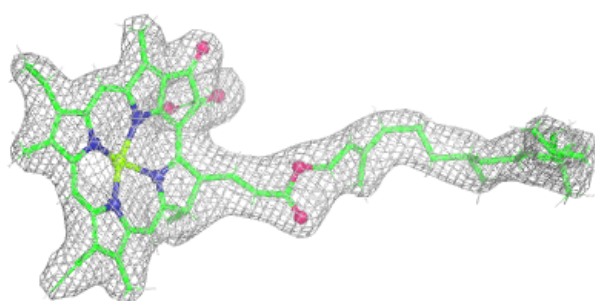
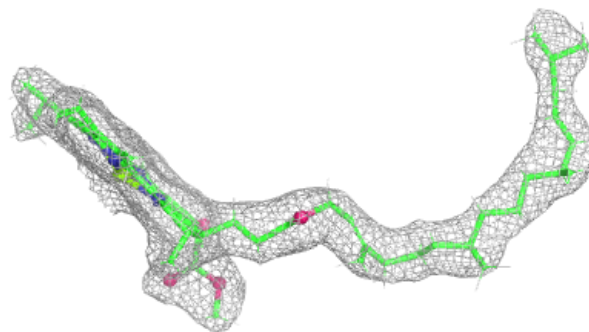
**Electron density around CLA a 604:**

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

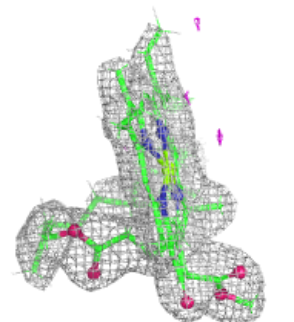
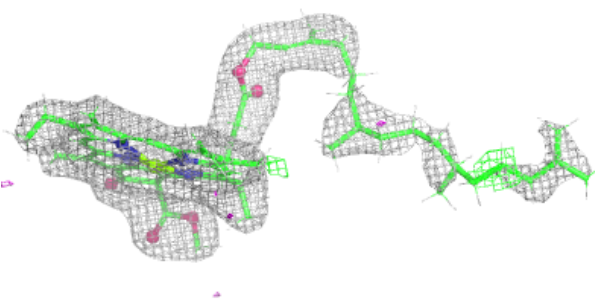
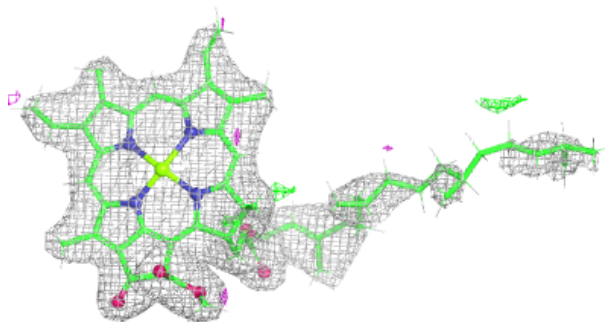


Electron density around CLA d 402:

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

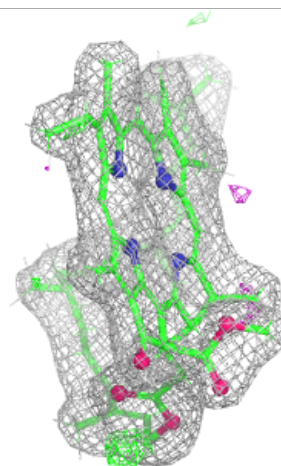
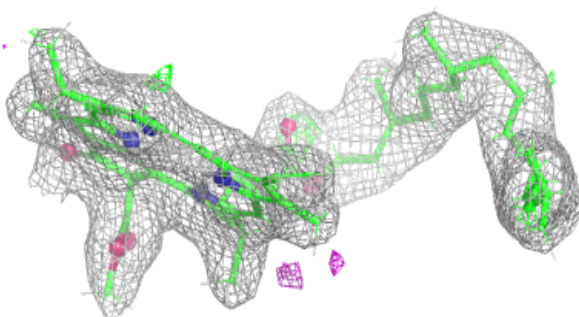
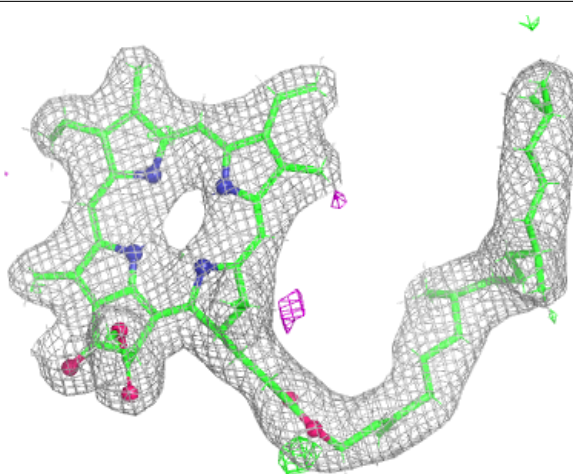
**Electron density around CLA a 605:**

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



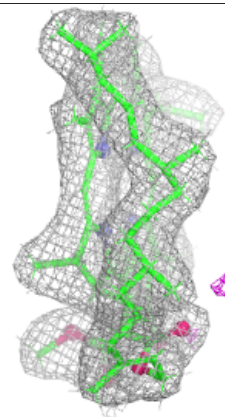
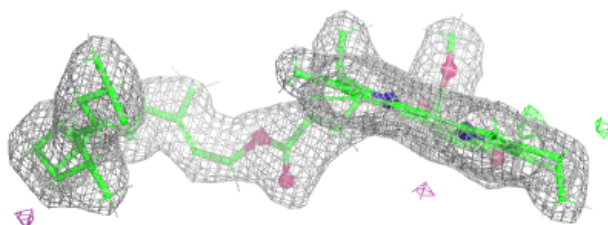
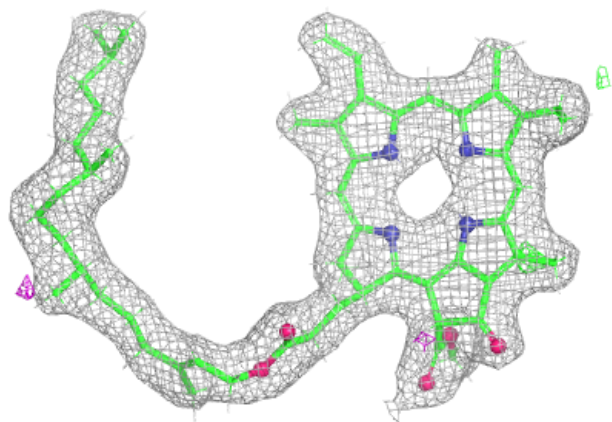
Electron density around PHO A 606:

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



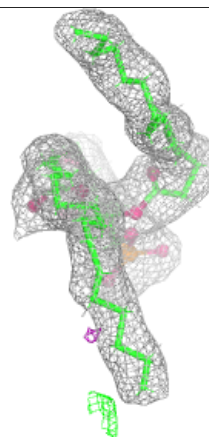
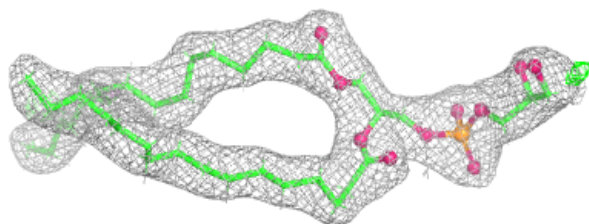
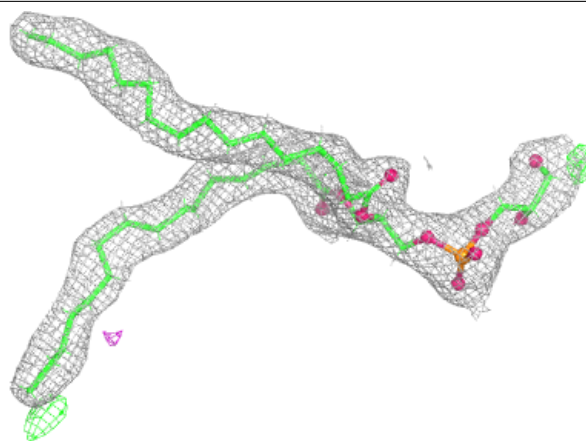
Electron density around PHO D 401:

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

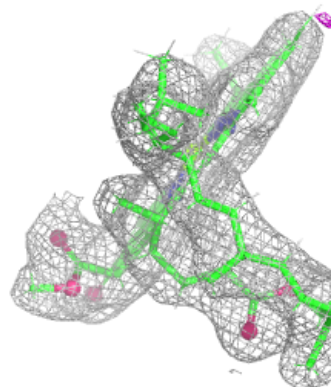
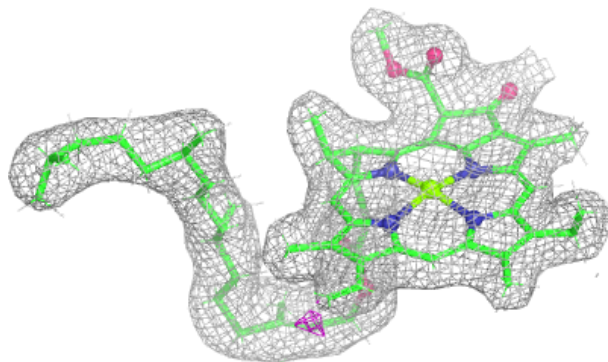
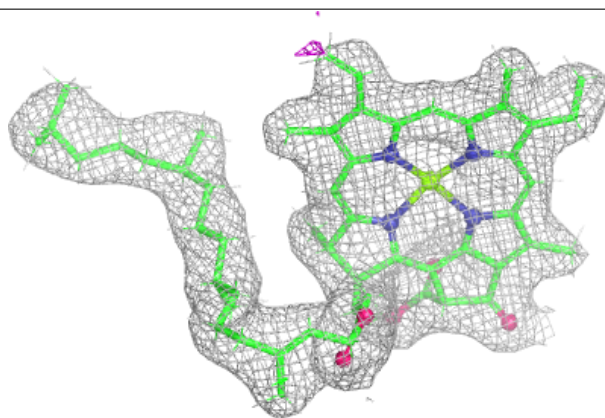


Electron density around LHG D 409:

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

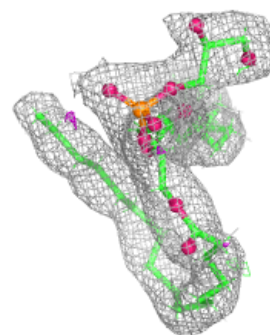
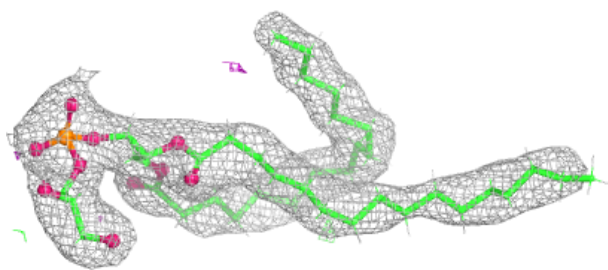
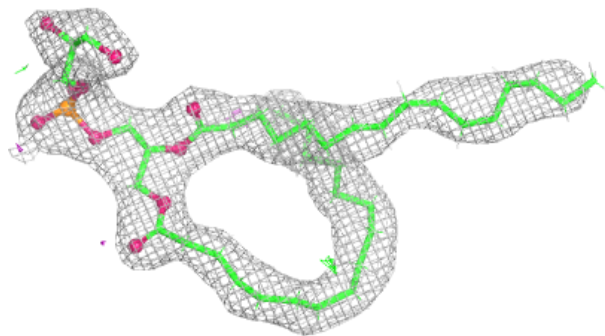
**Electron density around CLA A 612:**

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



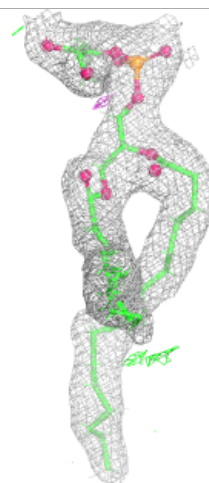
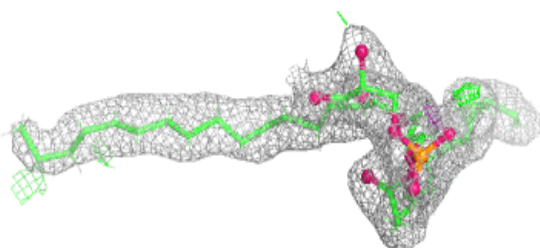
Electron density around LHG D 413:

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



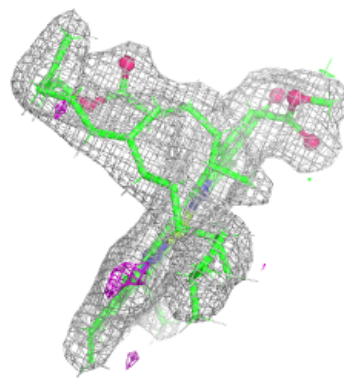
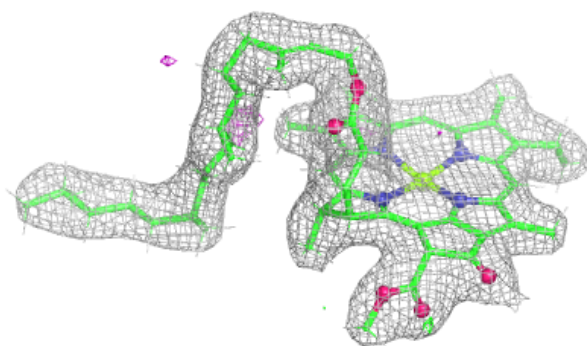
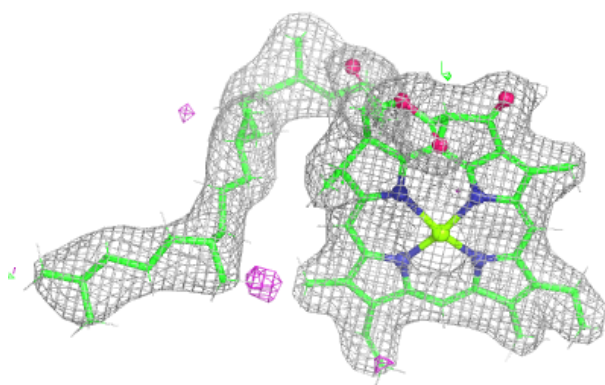
Electron density around LHG L 101:

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

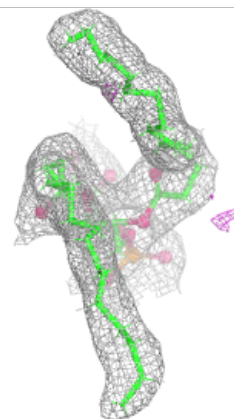
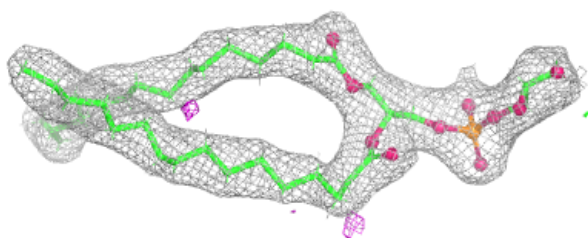
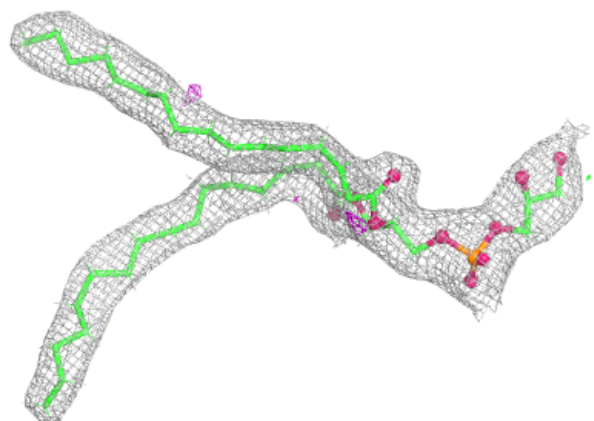


Electron density around CLA a 613:

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

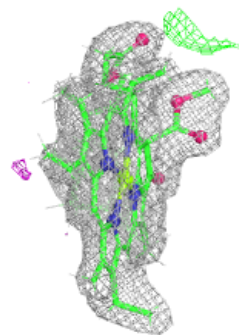
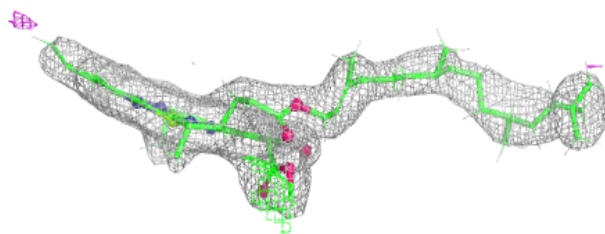
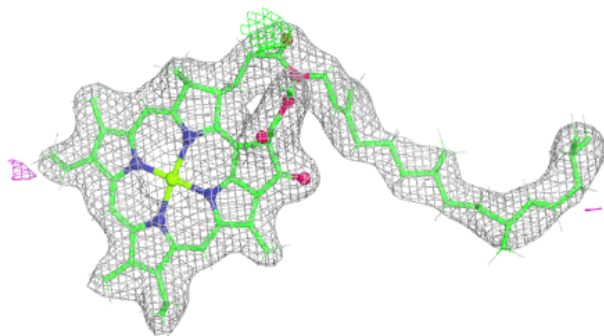
**Electron density around LHG d 406:**

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

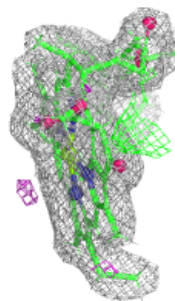
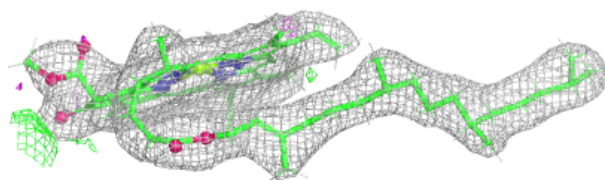
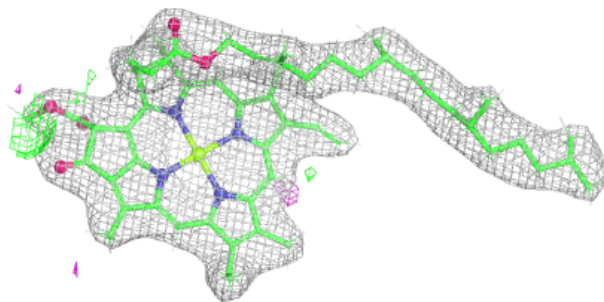


Electron density around CLA B 601:

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

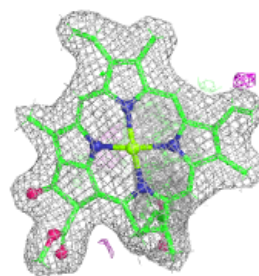
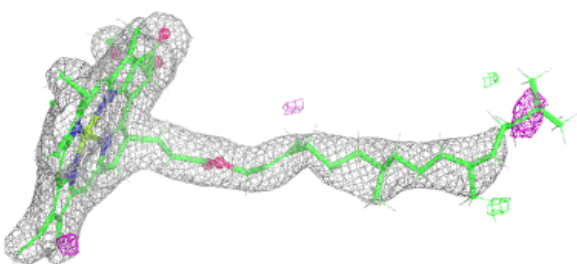
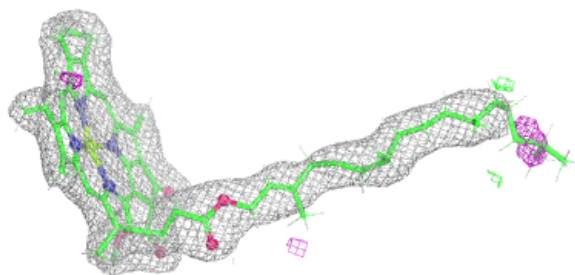
**Electron density around CLA C 501:**

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

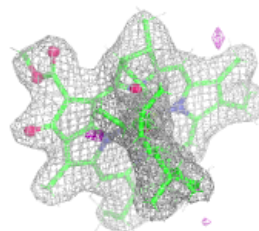
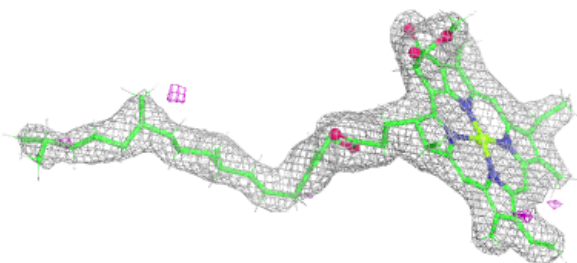
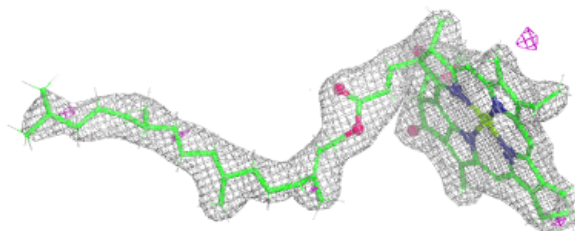


Electron density around CLA b 604:

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

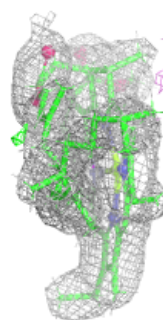
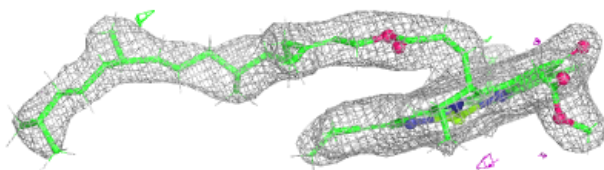
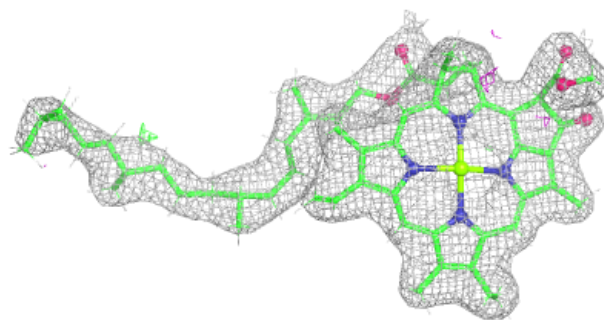
**Electron density around CLA C 502:**

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

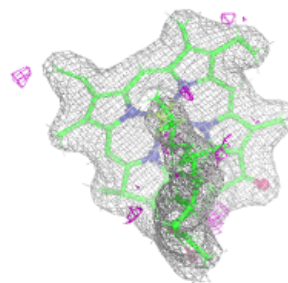
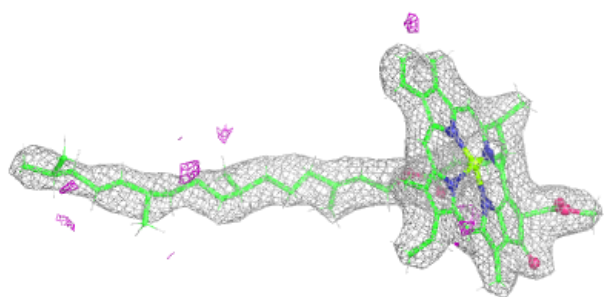
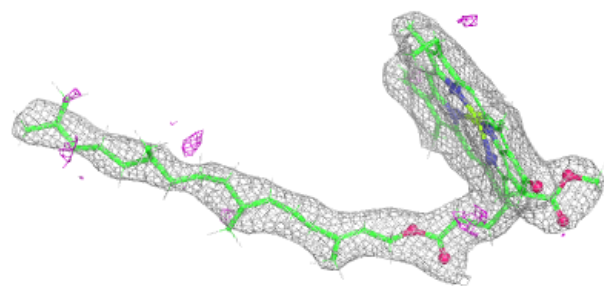


Electron density around CLA B 602:

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

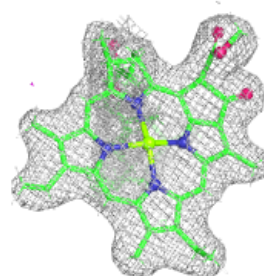
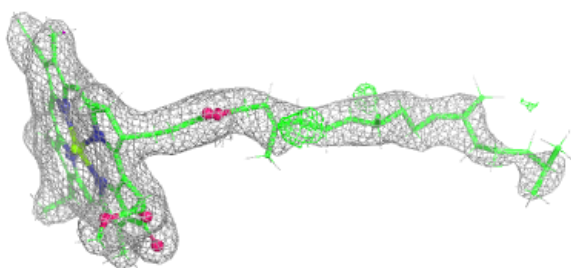
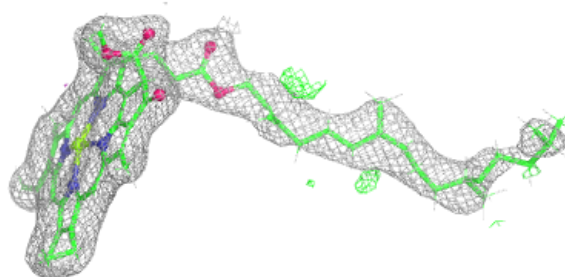
**Electron density around CLA b 607:**

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

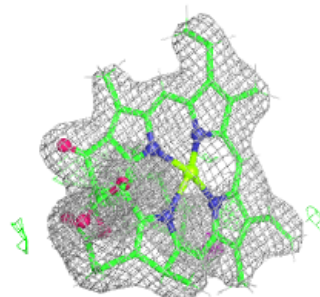
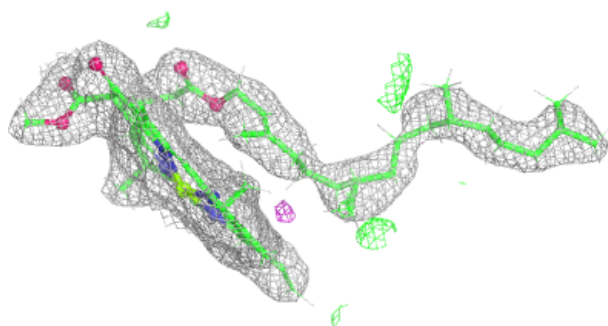
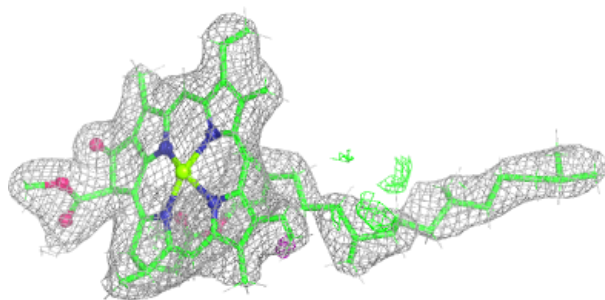


Electron density around CLA B 603:

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

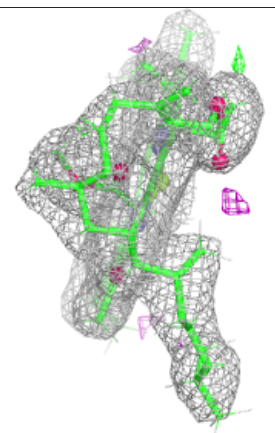
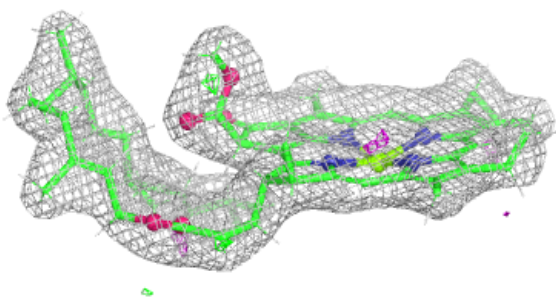
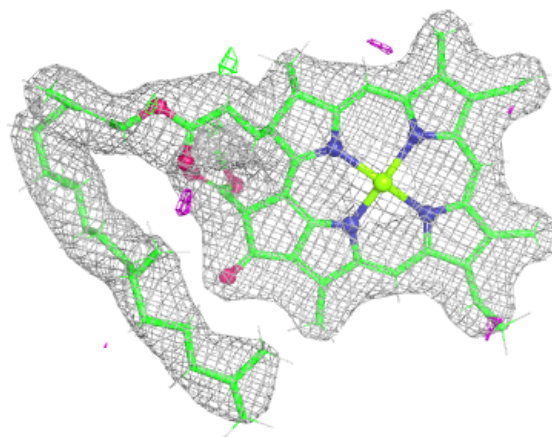
**Electron density around CLA C 505:**

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



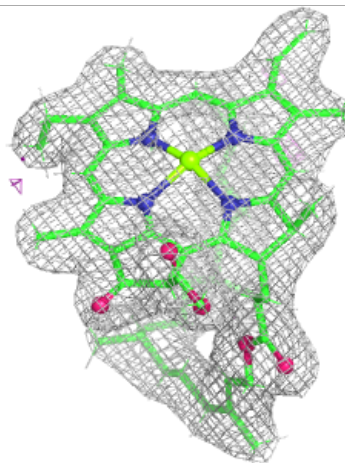
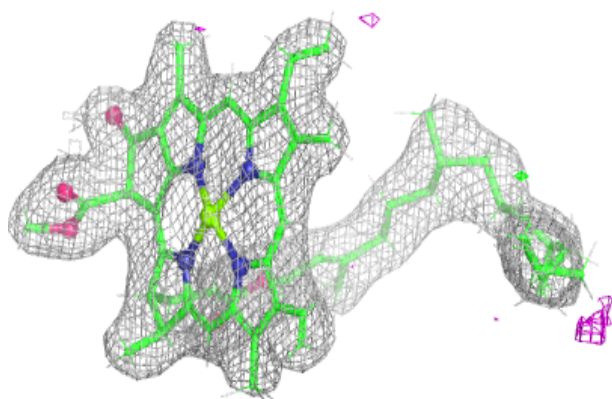
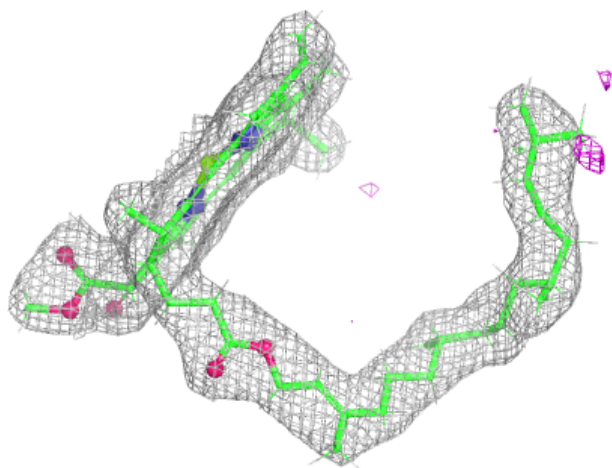
Electron density around CLA b 610:

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



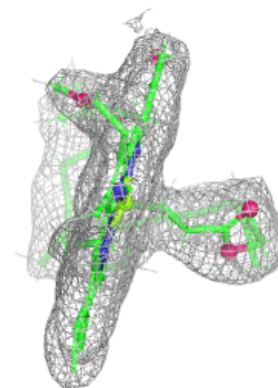
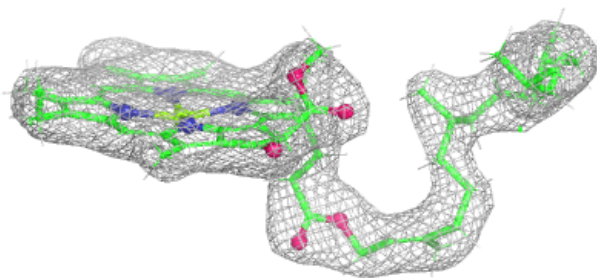
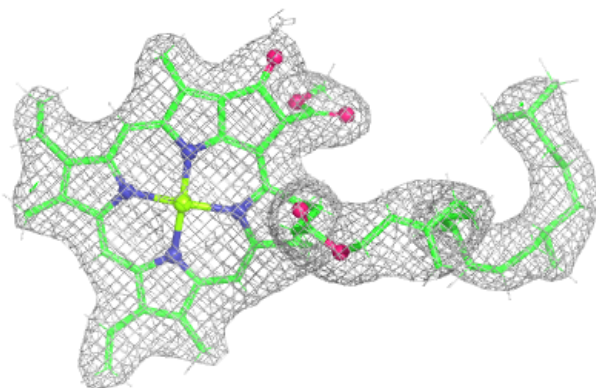
Electron density around CLA b 611:

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



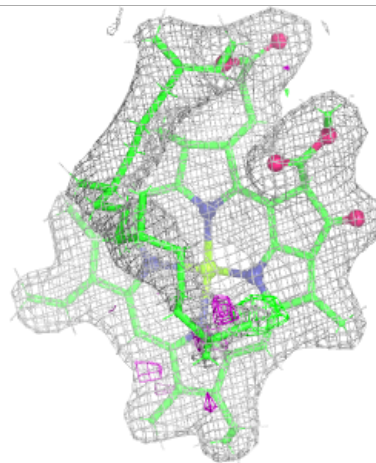
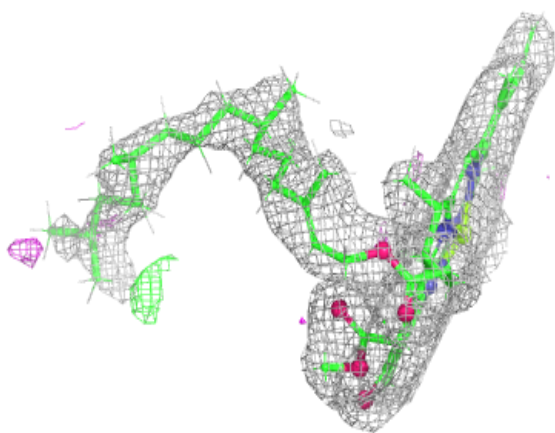
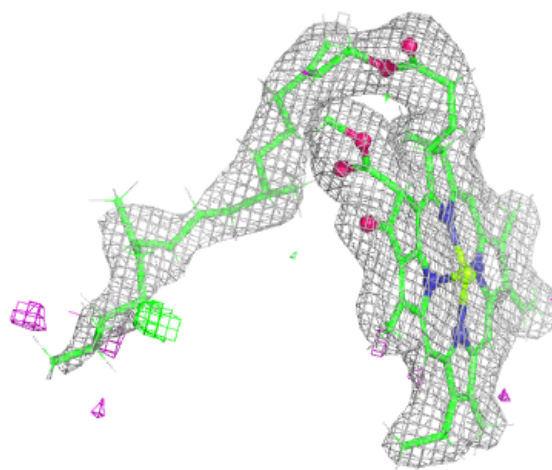
Electron density around CLA b 612:

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



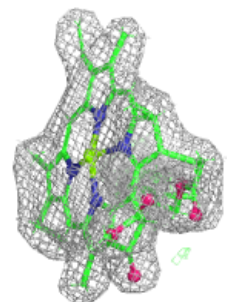
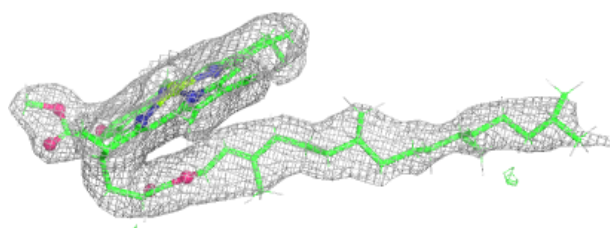
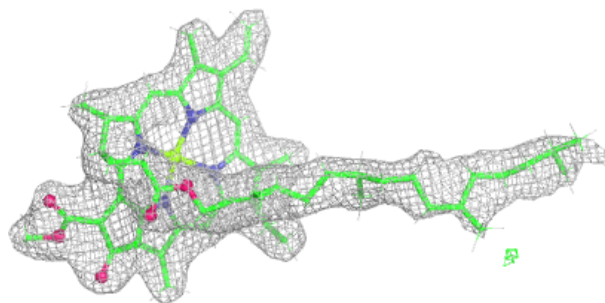
Electron density around CLA b 613:

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



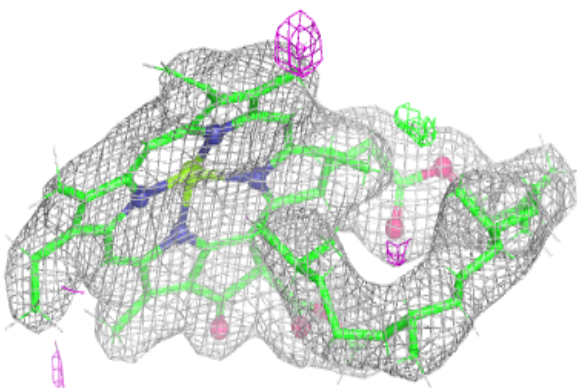
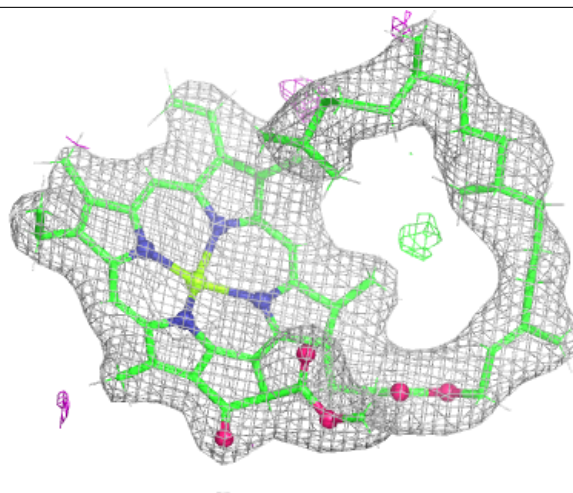
Electron density around CLA b 614:

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



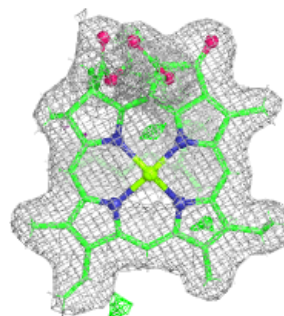
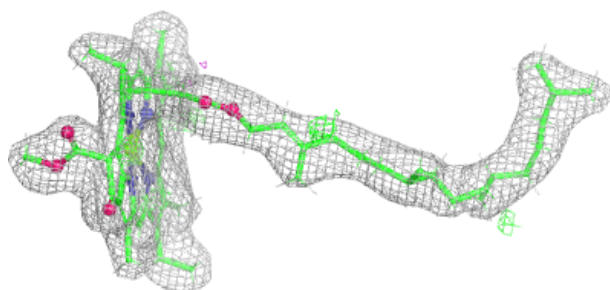
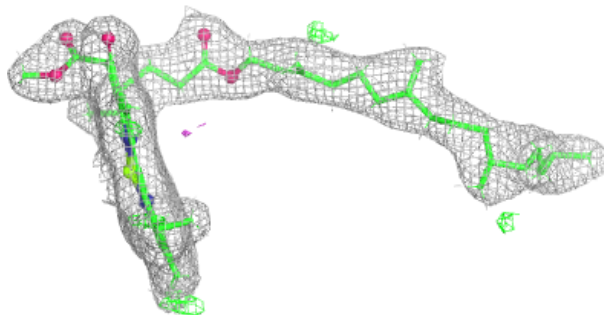
Electron density around CLA b 615:

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

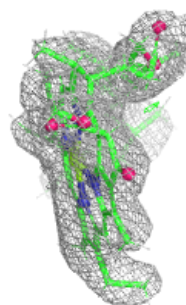
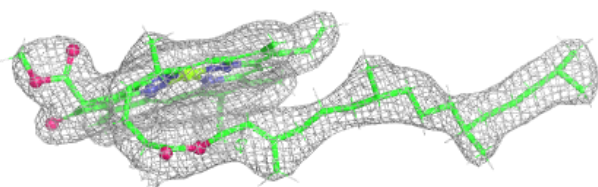
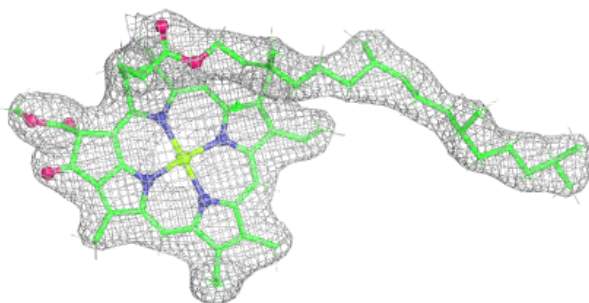


Electron density around CLA B 604:

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

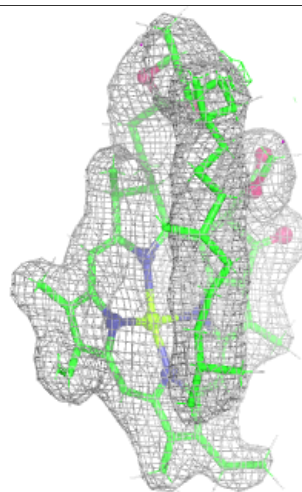
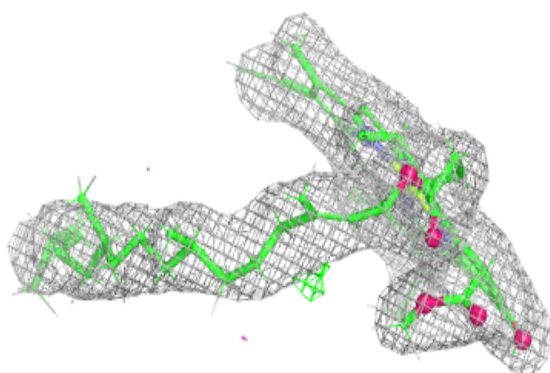
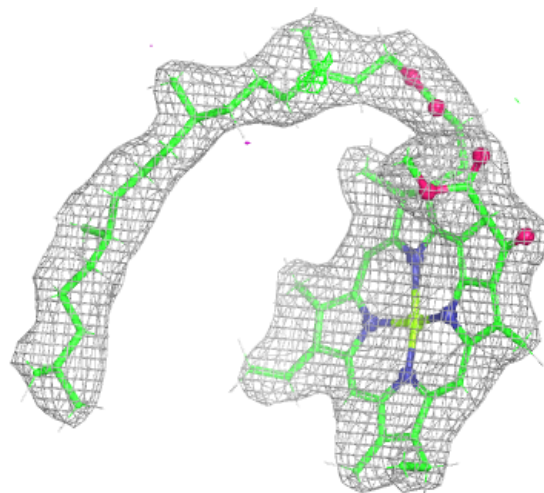
**Electron density around CLA c 501:**

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



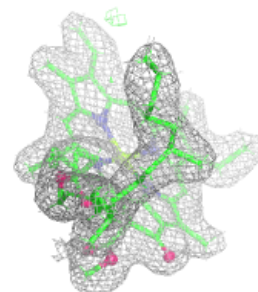
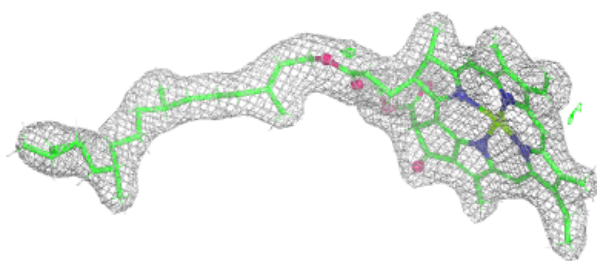
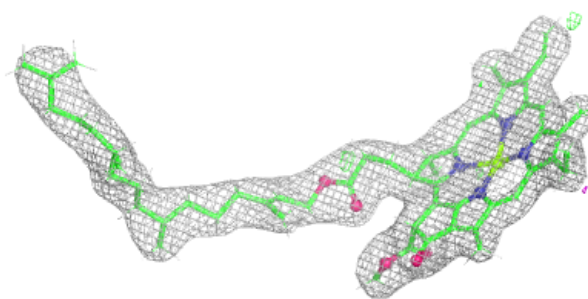
Electron density around CLA C 507:

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



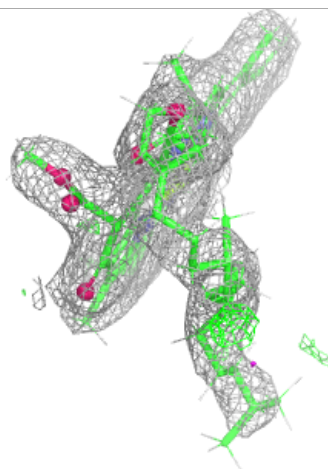
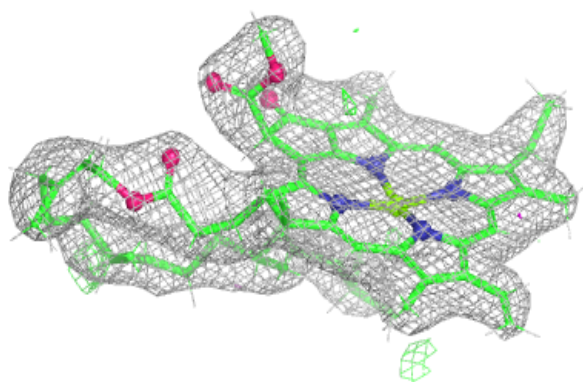
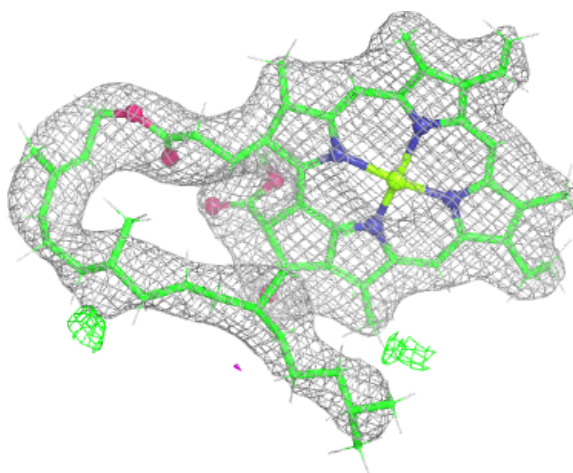
Electron density around CLA A 604:

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



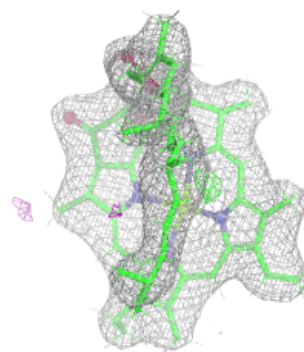
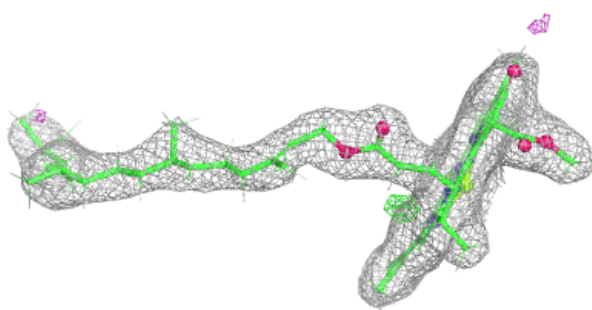
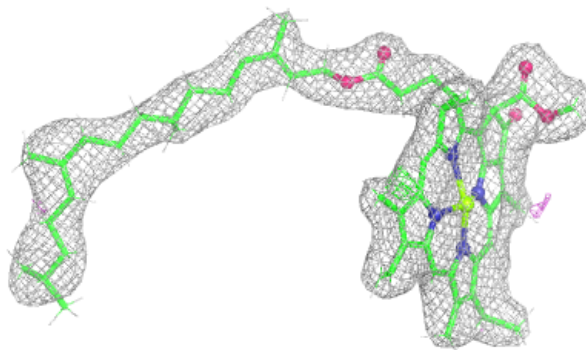
Electron density around CLA C 509:

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

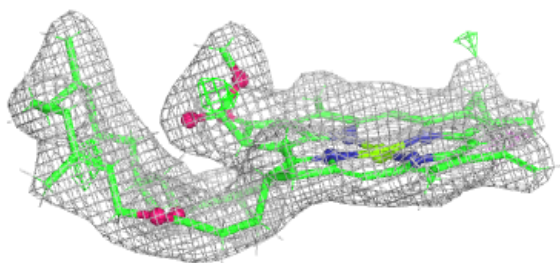
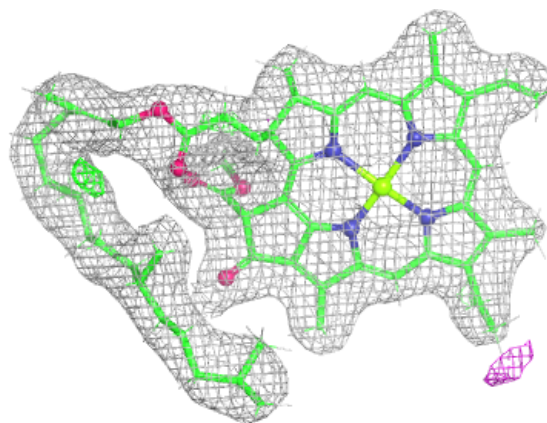


Electron density around CLA B 608:

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

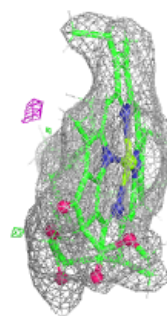
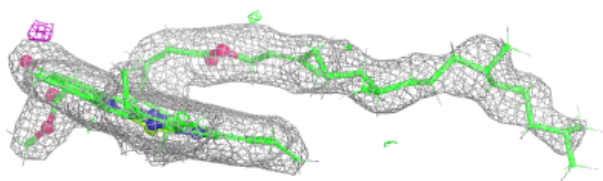
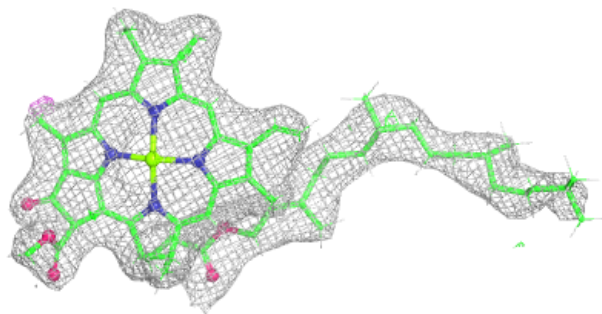
**Electron density around CLA B 609:**

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



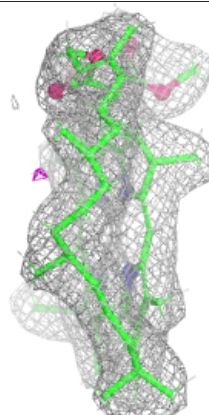
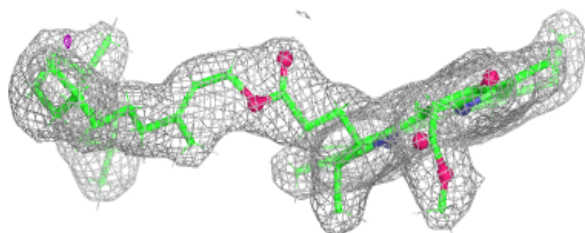
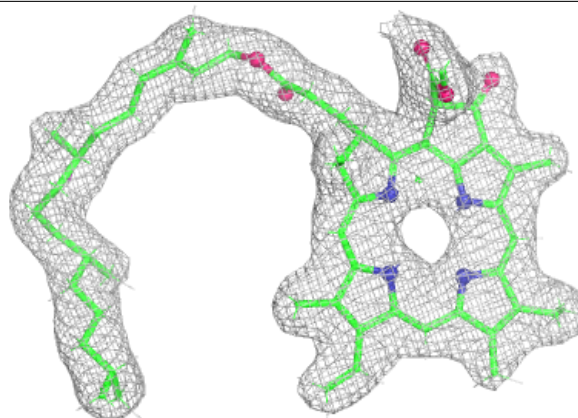
Electron density around CLA b 603:

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

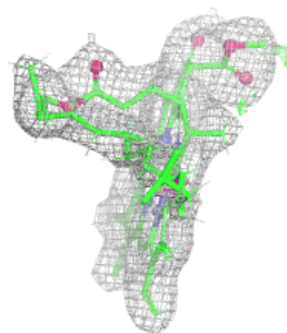
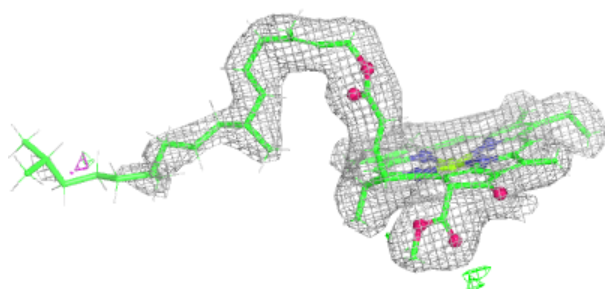
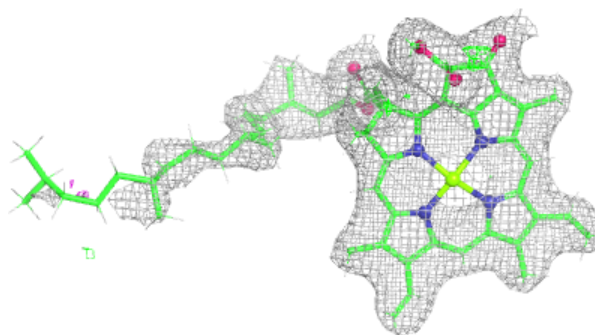


Electron density around PHO a 606:

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

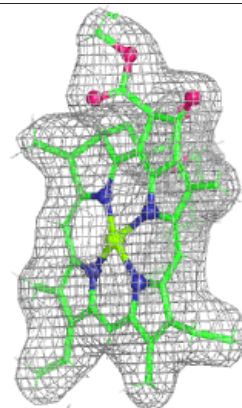
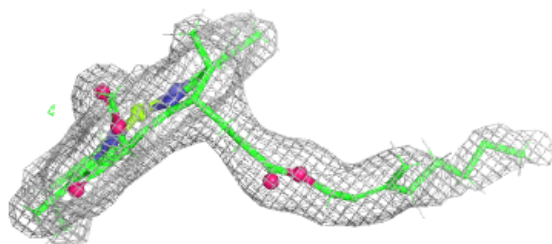
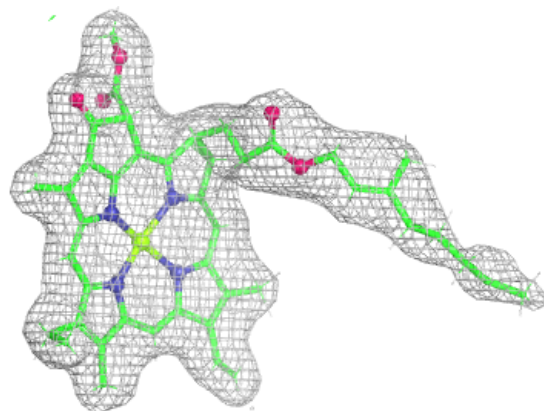
**Electron density around CLA A 605:**

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



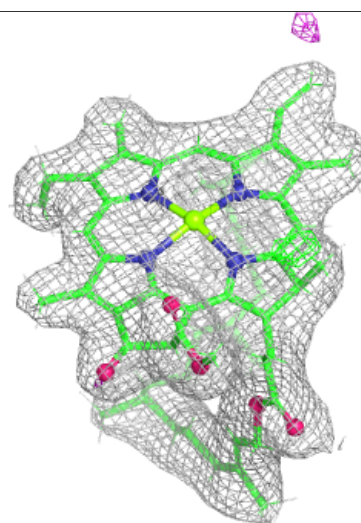
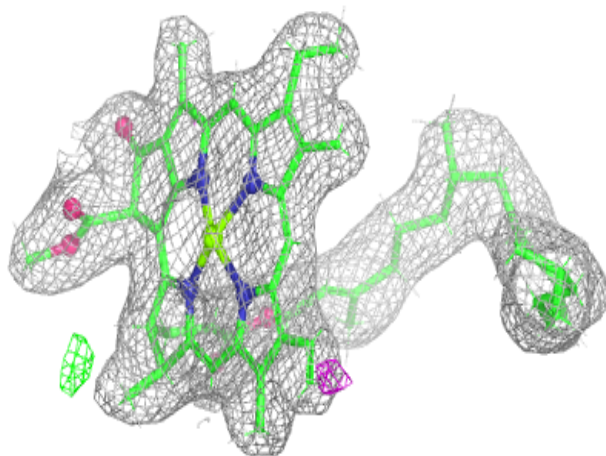
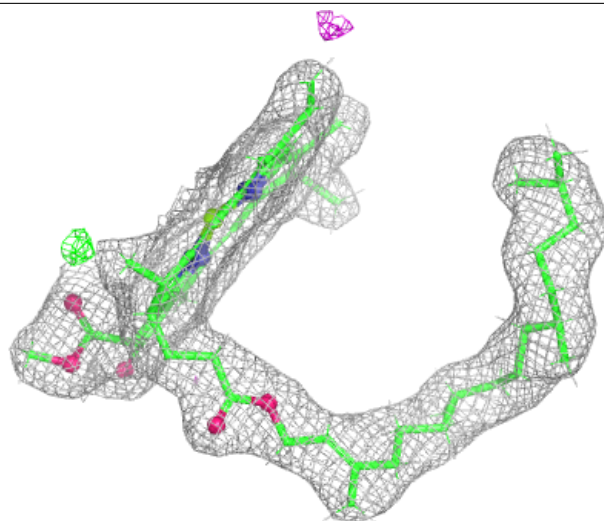
Electron density around CLA A 607:

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



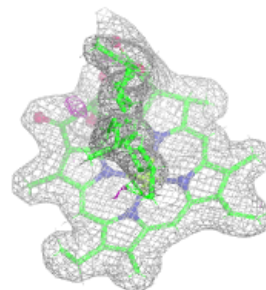
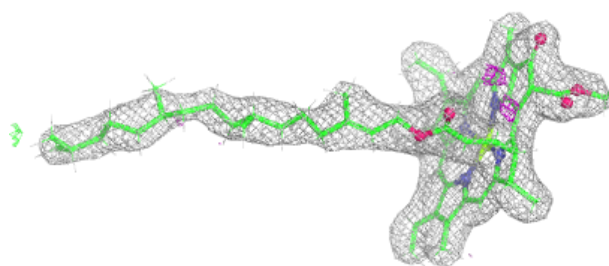
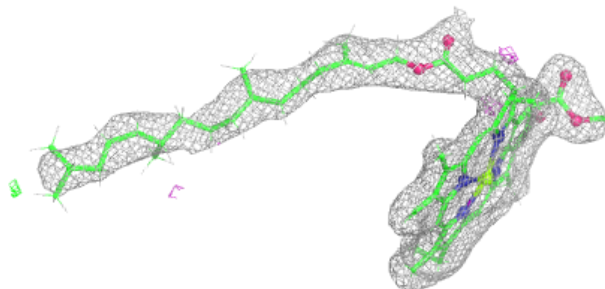
Electron density around CLA B 610:

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

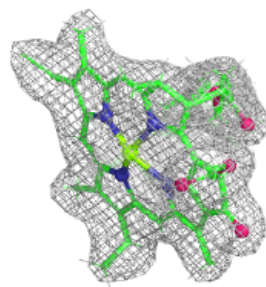
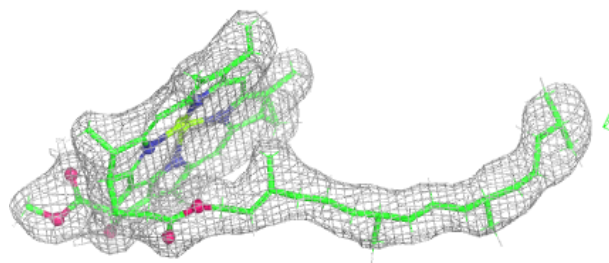
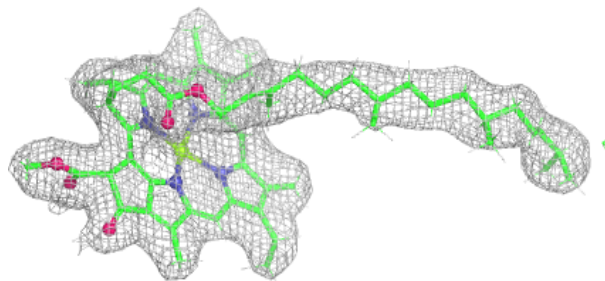


Electron density around CLA B 606:

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

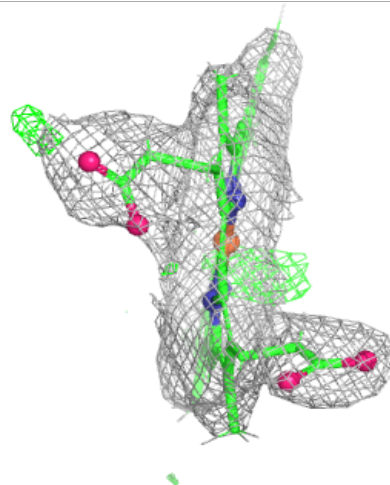
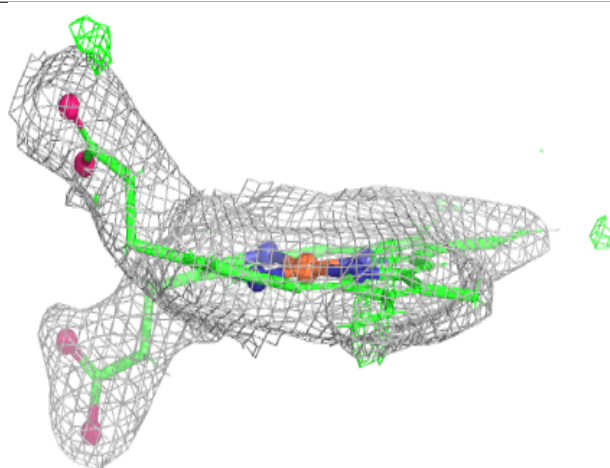
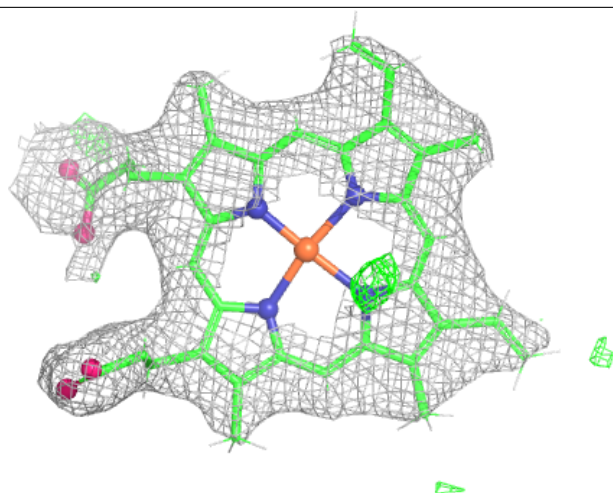
**Electron density around CLA B 607:**

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



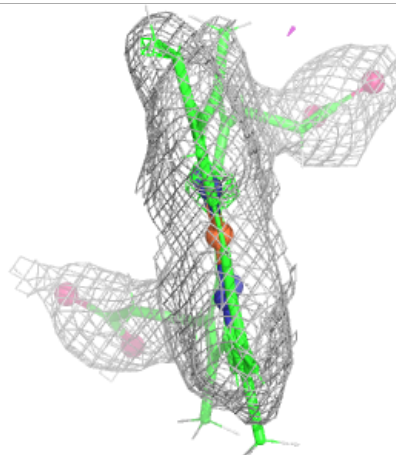
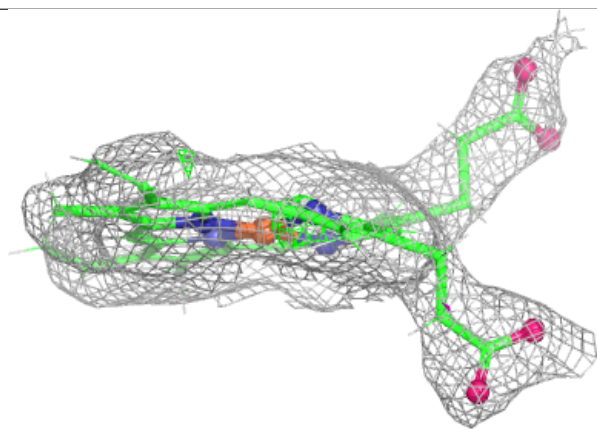
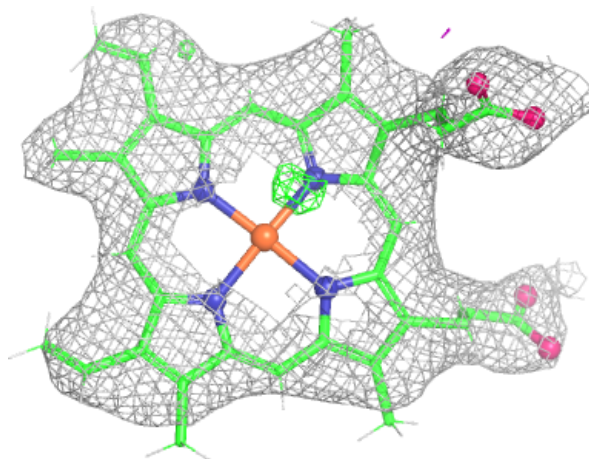
Electron density around HEM F 101:

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



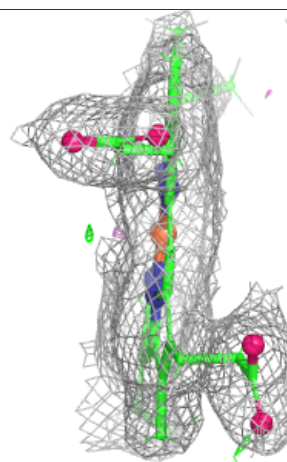
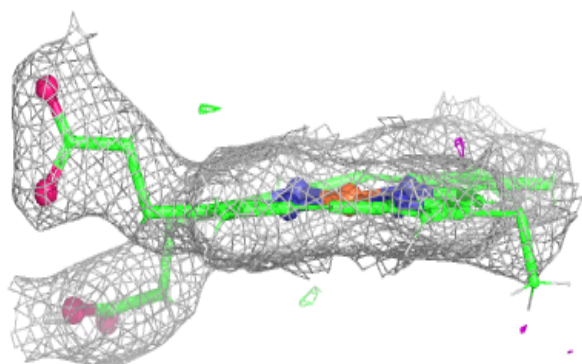
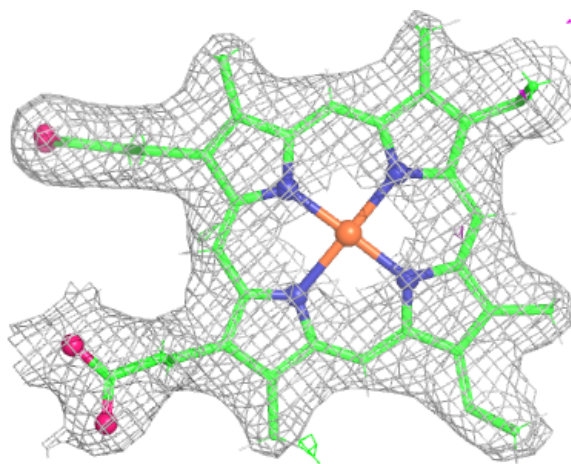
Electron density around HEM f 101:

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



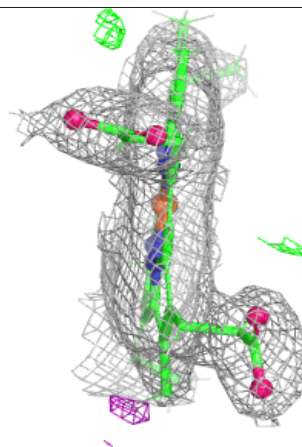
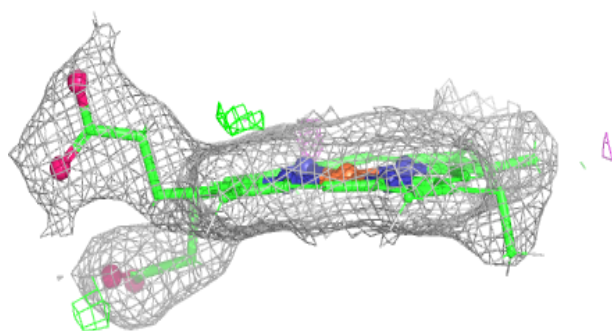
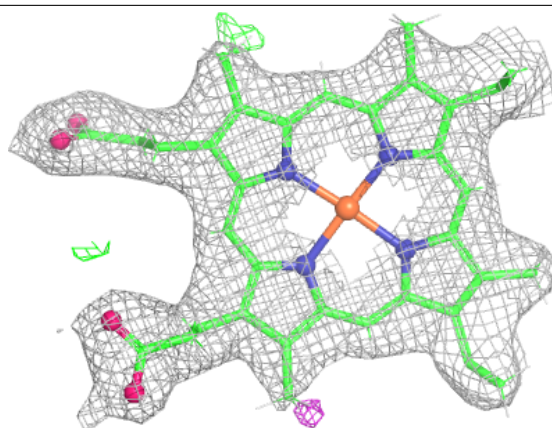
Electron density around HEC V 201:

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



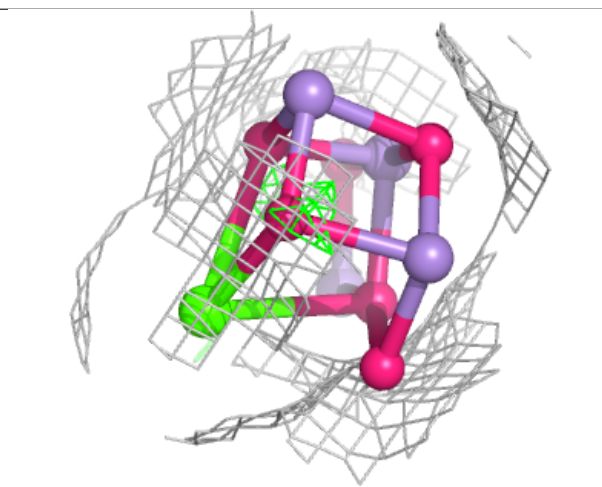
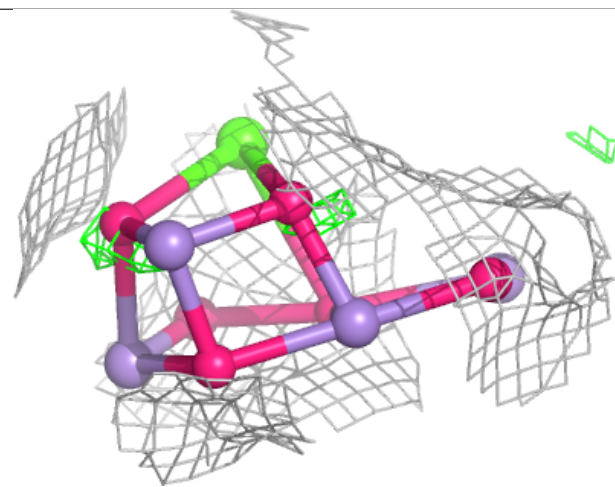
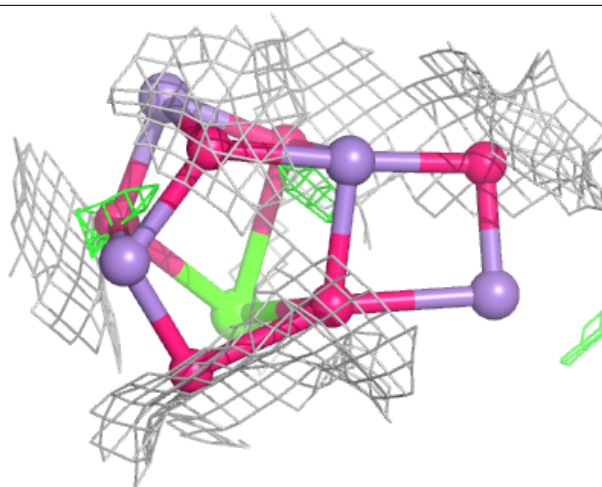
Electron density around HEC v 201:

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



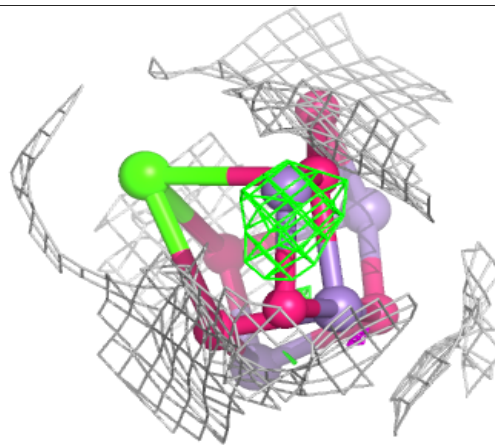
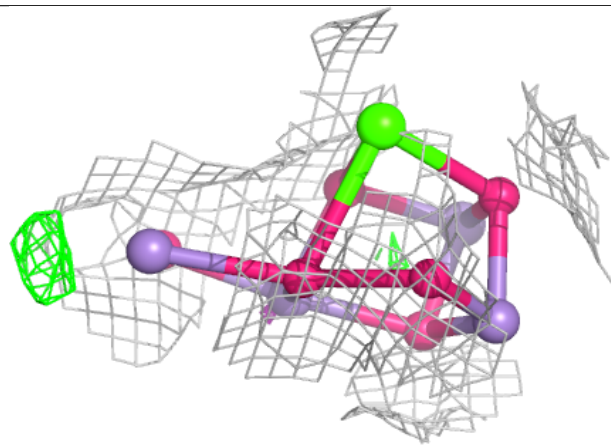
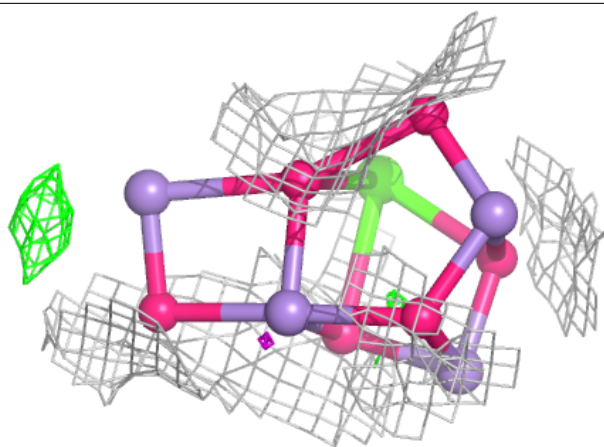
Electron density around OEY A 601 (B):

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



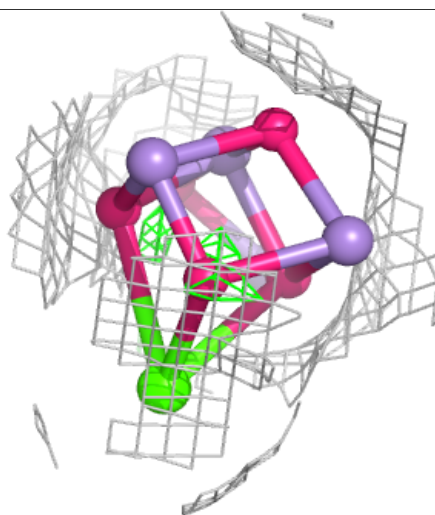
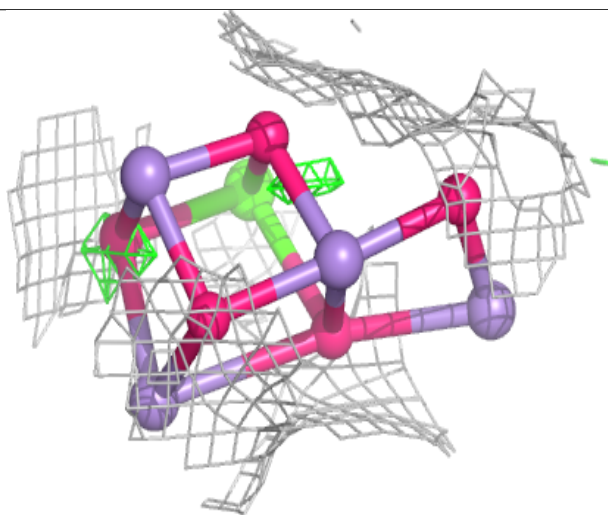
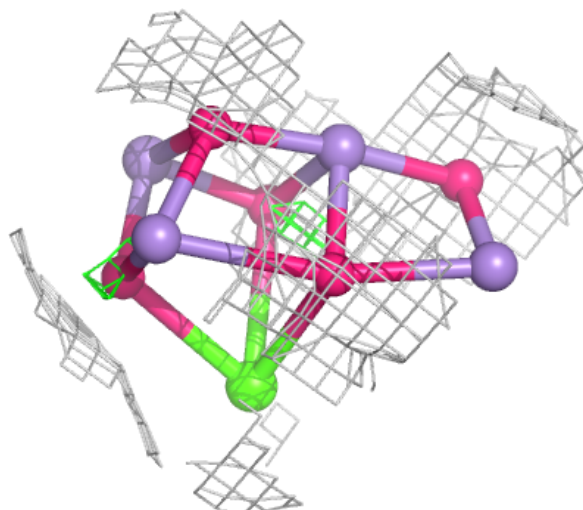
Electron density around OEY a 601 (B):

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



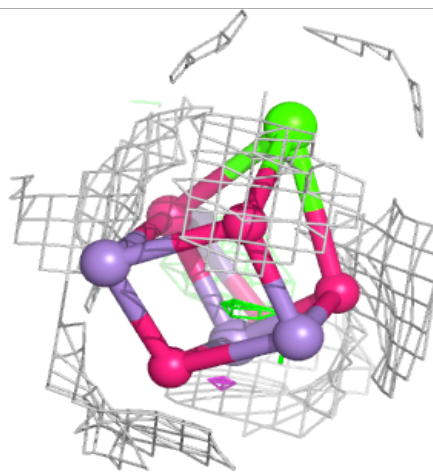
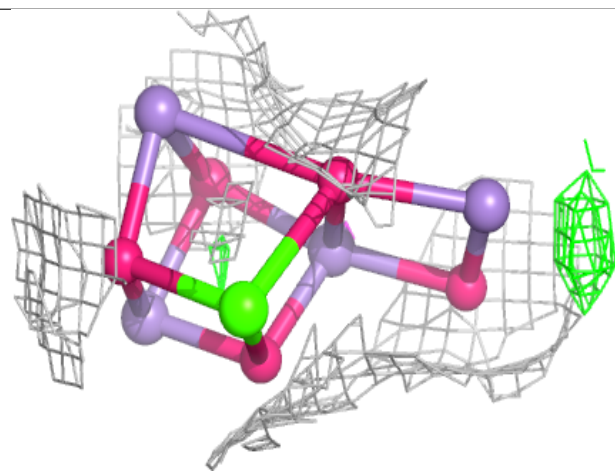
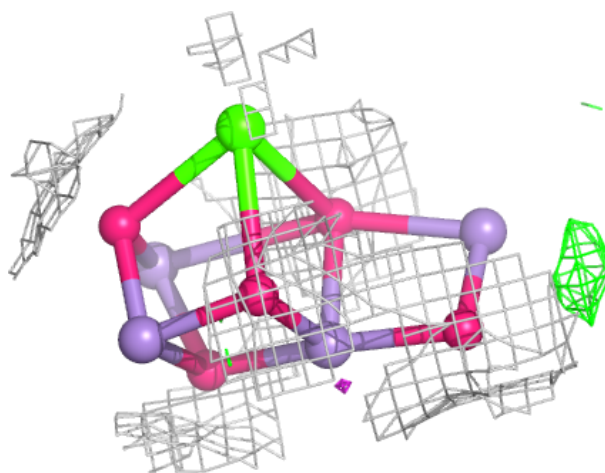
Electron density around OEX A 602 (A):

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



Electron density around OEX a 602 (A):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.