



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:30 PM EDT

PDB ID : 7RF4 / pdb_00007rf4
Title : RT XFEL structure of Photosystem II 50 microseconds after the second illumination at 2.27 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.; Chervnev, 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 : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)

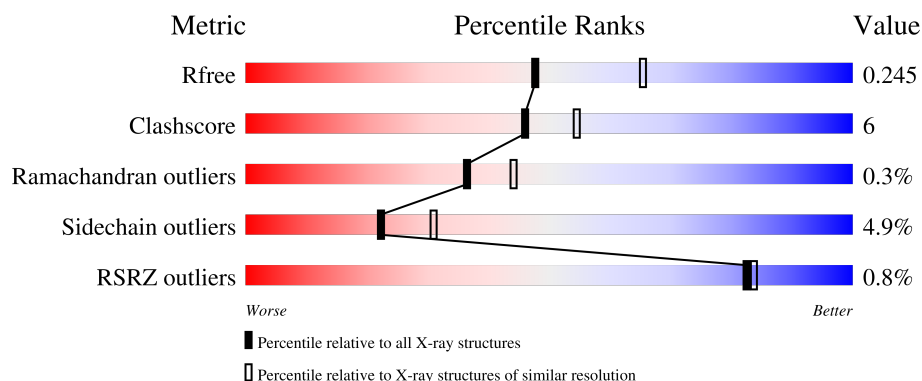
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

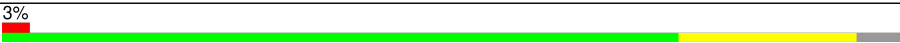
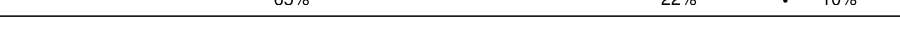
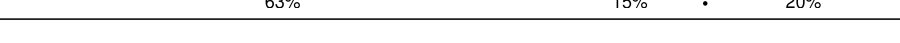
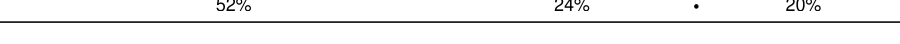
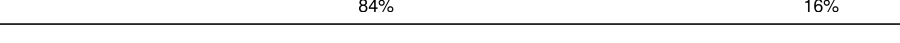
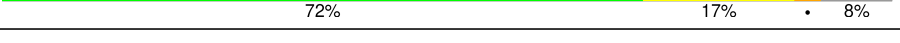
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	 86% 11% •
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) : 2.50

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	HEC	V	201	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 103252 atoms, of which 51649 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	0	0
			5141	1717	2519	431	459	15			
1	a	334	Total	C	H	N	O	S	0	0	0
			5129	1714	2510	431	459	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	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	2	0
			6781	2249	3355	571	593	13			
3	c	451	Total	C	H	N	O	S	0	2	0
			6926	2290	3426	587	610	13			

- 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	0	0
			5338	1800	2621	444	461	12			
4	d	341	Total	C	H	N	O	S	0	1	0
			5350	1804	2627	444	463	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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	FME	-	initiating methionine	UNP Q8DJZ6
i	1	FME	-	initiating methionine	UNP Q8DJZ6

- 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			
10	k	37	Total	C	H	N	O	0	0	0
			598	204	305	43	46			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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		

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	137	Total	C	H	N	O	S	0	0
			2137	675	1073	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2137	675	1073	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			

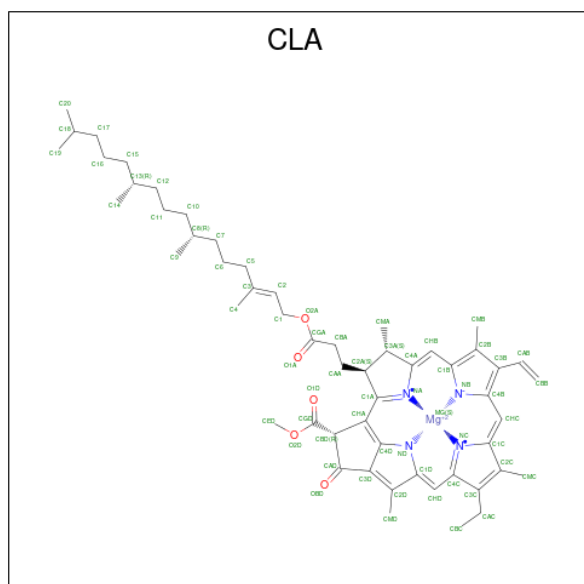
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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 FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	C	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	C	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	D	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	a	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

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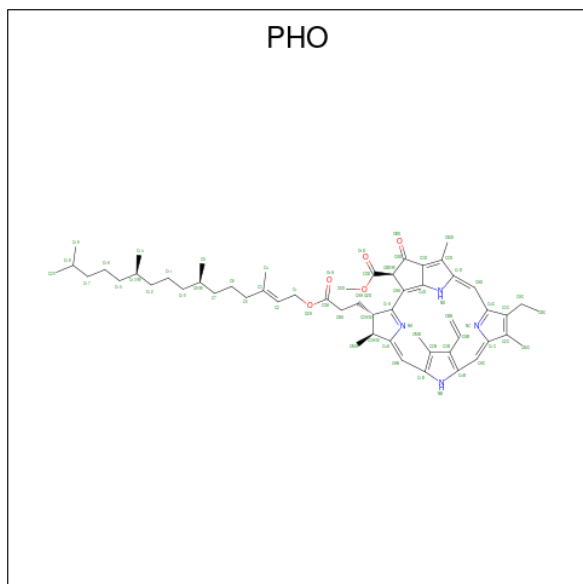
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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

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

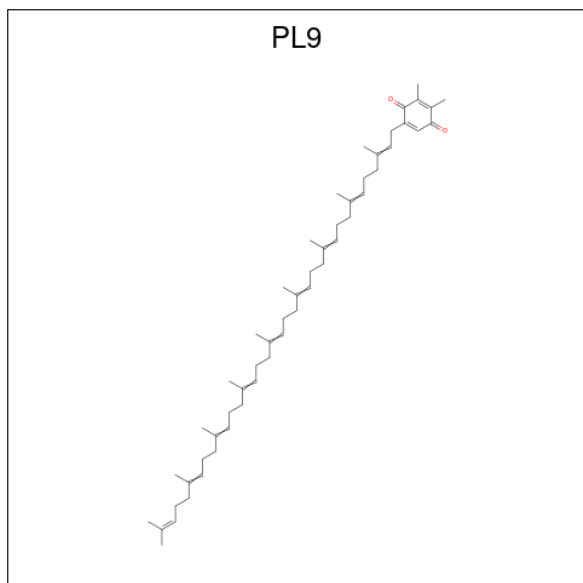


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	D	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	a	1	Total	C	H	N	O	0	0
			138	55	74	4	5		
23	d	1	Total	C	H	N	O	0	0
			138	55	74	4	5		

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

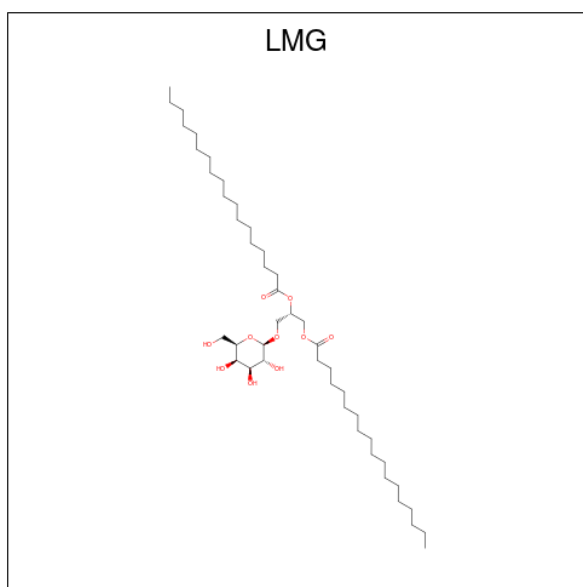
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	2	Total Cl 2 2	0	0
24	a	2	Total Cl 2 2	0	0

- Molecule 25 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: $C_{53}H_{80}O_2$).



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

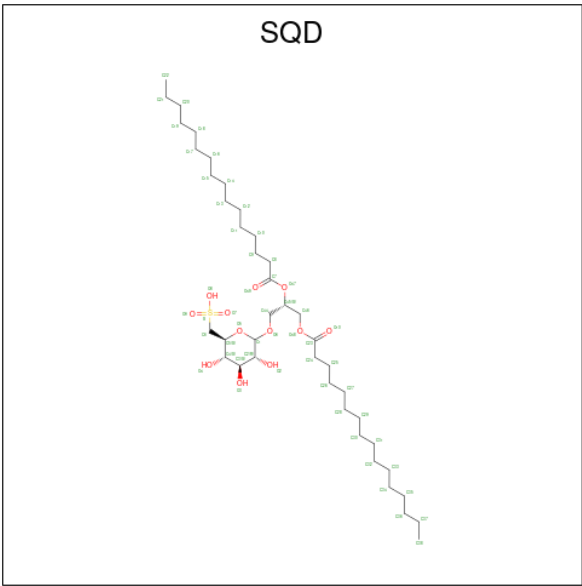
- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

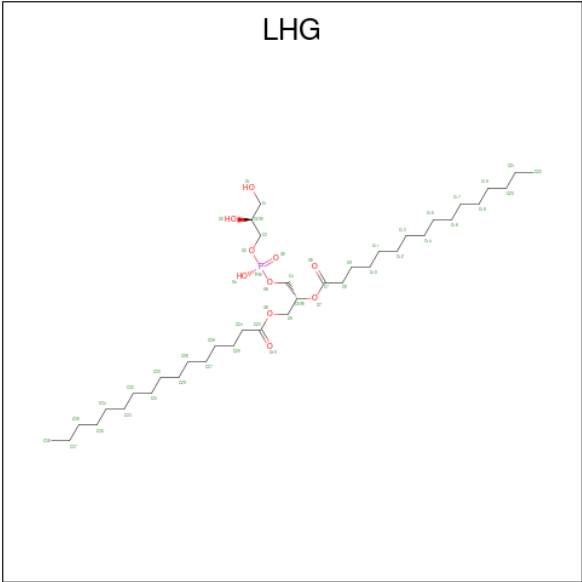
- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



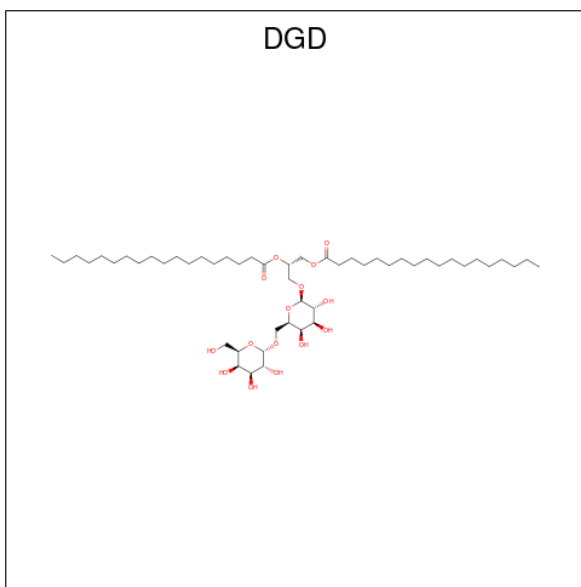
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
27	A	1	Total	C	H	O		0	0
			104	35	65	4			
27	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
27	L	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
27	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
27	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		
27	t	1	Total	C	H	O		0	0
			92	31	56	5			

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



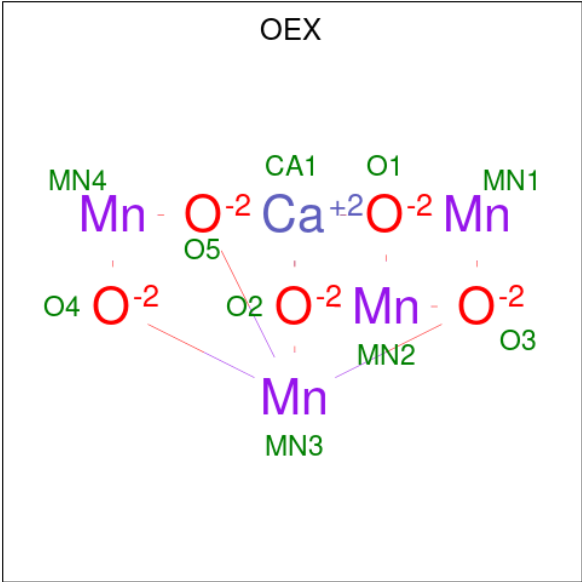
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
28	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	L	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	a	1	Total	C	H	O	P	0	0
			123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

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



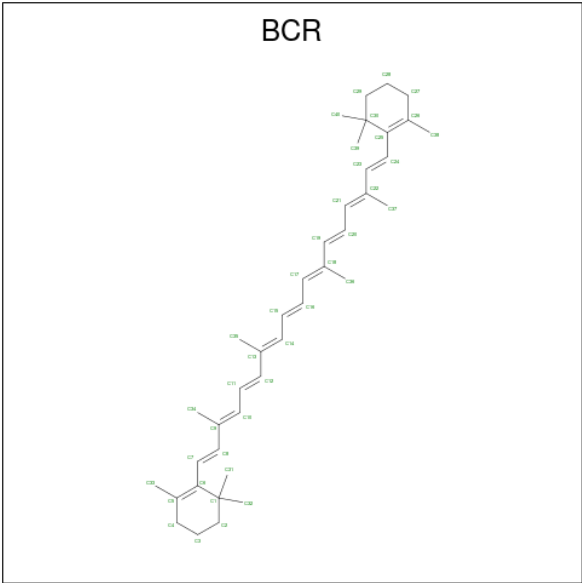
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			162	51	96	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	C	1	Total	C	H	O	0	0
			144	47	82	15		
29	H	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			144	47	82	15		
29	c	1	Total	C	H	O	0	0
			143	47	81	15		
29	h	1	Total	C	H	O	0	0
			144	47	82	15		

- Molecule 30 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
30	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

- Molecule 31 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



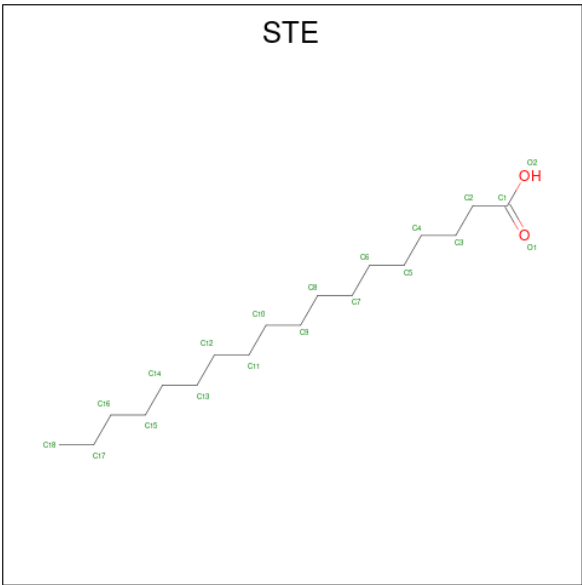
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	B	1	Total	C H	0	0
			96	40 56		
31	B	1	Total	C H	0	0
			96	40 56		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	H	0	0
			96	40	56		
31	C	1	Total	C	H	0	0
			96	40	56		
31	D	1	Total	C	H	0	0
			96	40	56		
31	H	1	Total	C	H	0	0
			96	40	56		
31	I	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	K	1	Total	C	H	0	0
			96	40	56		
31	T	1	Total	C	H	0	0
			96	40	56		
31	Z	1	Total	C	H	0	0
			96	40	56		
31	a	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	b	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	c	1	Total	C	H	0	0
			96	40	56		
31	d	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	k	1	Total	C	H	0	0
			96	40	56		
31	t	1	Total	C	H	0	0
			96	40	56		
31	x	1	Total	C	H	0	0
			96	40	56		

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



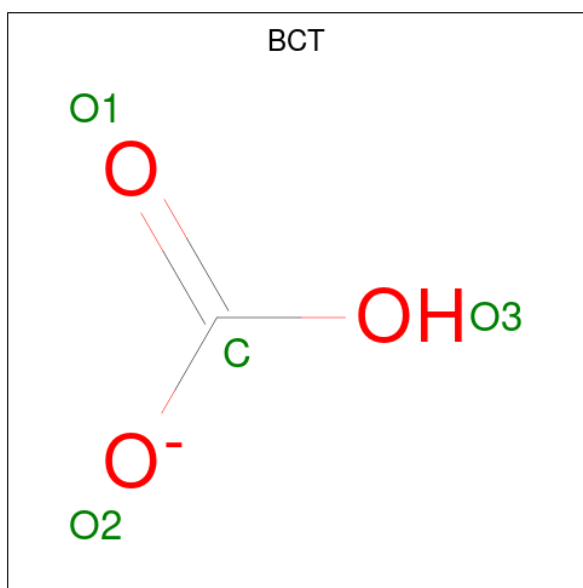
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	B	1	Total C H O 43 15 26 2	0	0
32	B	1	Total C H O 28 10 16 2	0	0
32	B	1	Total C H O 46 16 28 2	0	0
32	B	1	Total C H 47 16 31	0	0
32	B	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	C	1	Total C H 47 16 31	0	0
32	C	1	Total C H O 28 10 16 2	0	0
32	H	1	Total C H 53 18 35	0	0
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	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

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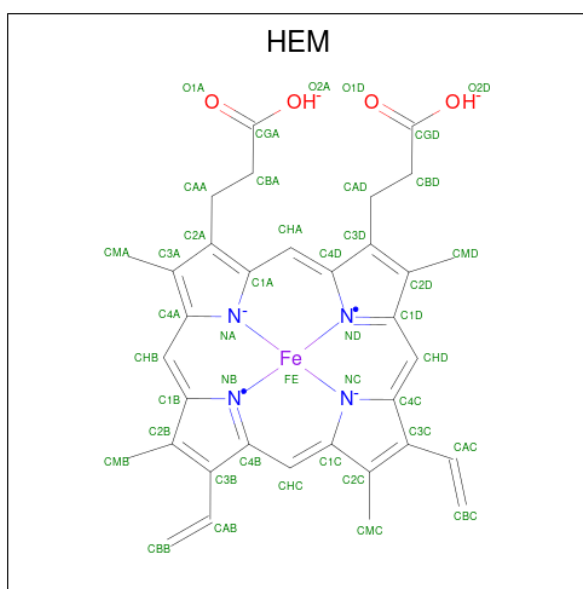
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	R	1	Total C H O 28 10 16 2	0	0
32	X	1	Total C H O 55 18 35 2	0	0
32	Z	1	Total C H 20 8 12	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	a	1	Total C H 41 15 26	0	0
32	b	1	Total C H 47 16 31	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H O 40 14 24 2	0	0
32	b	1	Total C H 44 15 29	0	0
32	b	1	Total C H O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	b	1	Total C H 41 14 27	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	d	1	Total C H O 55 18 35 2	0	0
32	j	1	Total C H O 28 10 16 2	0	0
32	l	1	Total C H 53 18 35	0	0
32	t	1	Total C H O 34 12 20 2	0	0
32	t	1	Total C H 26 10 16	0	0
32	x	1	Total C H O 55 18 35 2	0	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



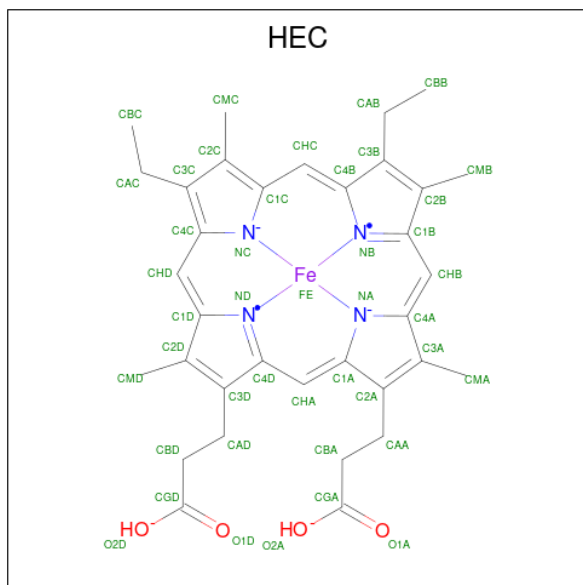
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	D	1	Total	C	H	O	0	0
			5	1	1	3		
33	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 34 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	C	119	Total 119	O 119	0	0
37	D	103	Total 103	O 103	0	0
37	E	20	Total 20	O 20	0	0
37	F	5	Total 5	O 5	0	0
37	H	22	Total 22	O 22	0	0
37	I	12	Total 12	O 12	0	0
37	J	11	Total 11	O 11	0	0
37	K	6	Total 6	O 6	0	0
37	L	9	Total 9	O 9	0	0
37	M	6	Total 6	O 6	0	0
37	O	68	Total 68	O 68	0	0
37	R	8	Total 8	O 8	0	0
37	T	7	Total 7	O 7	0	0
37	U	30	Total 30	O 30	0	0
37	V	49	Total 49	O 49	0	0
37	X	9	Total 9	O 9	0	0
37	Y	3	Total 3	O 3	0	0
37	Z	6	Total 6	O 6	0	0
37	a	99	Total 99	O 99	0	0
37	b	114	Total 114	O 114	0	0
37	c	120	Total 120	O 120	0	0

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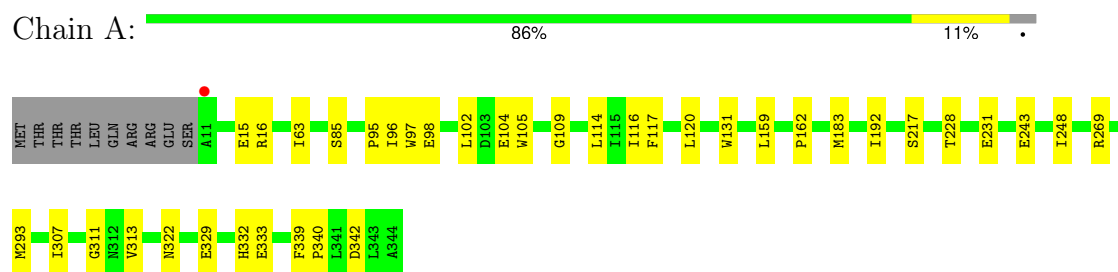
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	d	88	Total 88	O 88	0	0
37	e	18	Total 18	O 18	0	0
37	f	5	Total 5	O 5	0	0
37	h	22	Total 22	O 22	0	0
37	i	8	Total 8	O 8	0	0
37	j	9	Total 9	O 9	0	0
37	k	2	Total 2	O 2	0	0
37	l	11	Total 11	O 11	0	0
37	m	2	Total 2	O 2	0	0
37	o	70	Total 70	O 70	0	0
37	t	11	Total 11	O 11	0	0
37	u	35	Total 35	O 35	0	0
37	v	32	Total 32	O 32	0	0
37	x	7	Total 7	O 7	0	0
37	y	6	Total 6	O 6	0	0
37	z	11	Total 11	O 11	0	0

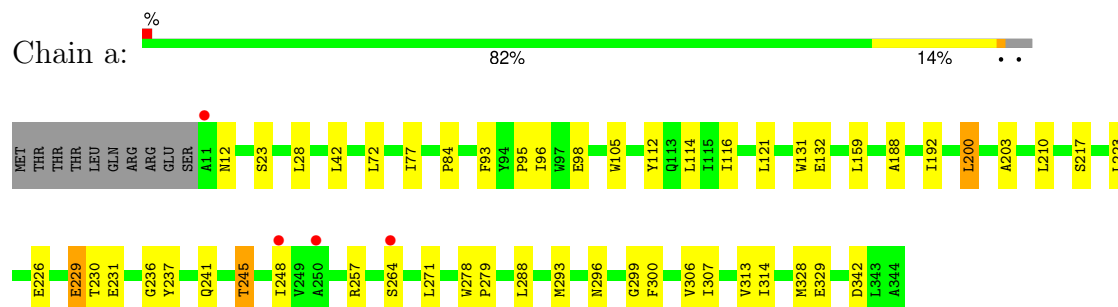
3 Residue-property plots [i](#)

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.

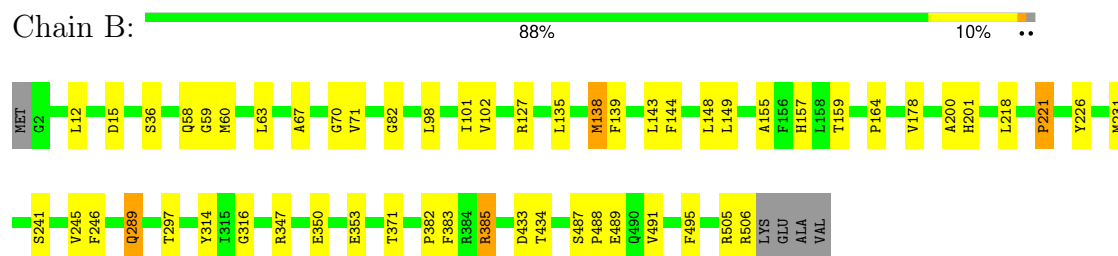
• Molecule 1: Photosystem II protein D1 1



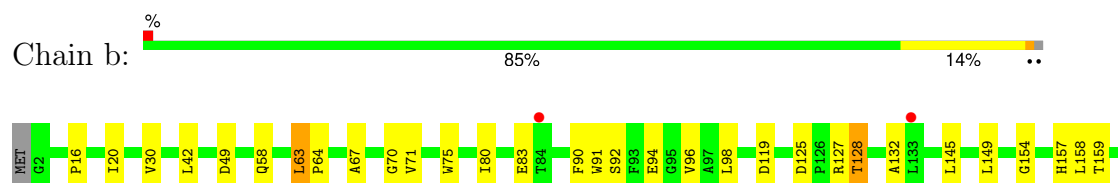
• Molecule 1: Photosystem II protein D1 1

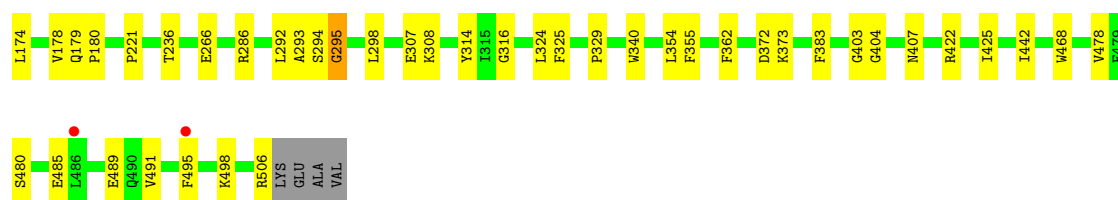


• Molecule 2: Photosystem II CP47 reaction center protein



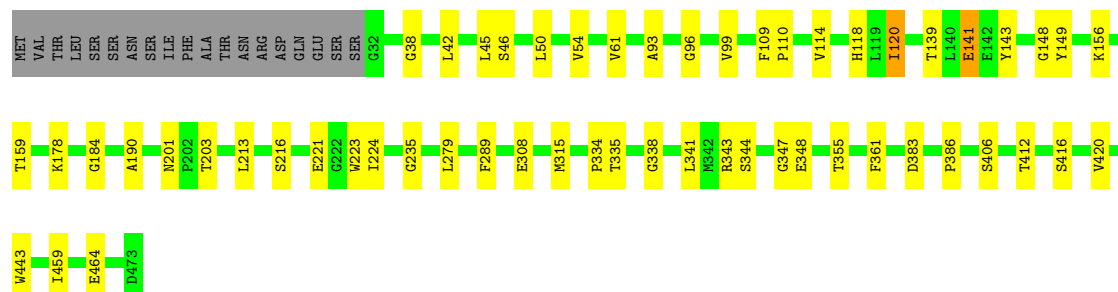
• Molecule 2: Photosystem II CP47 reaction center protein





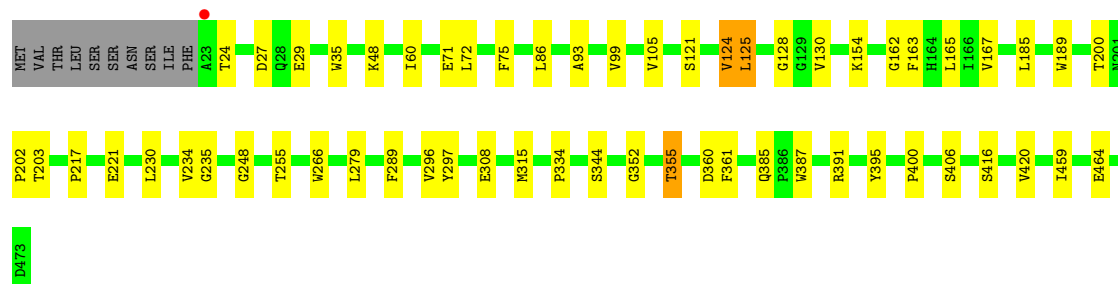
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 84% 12%



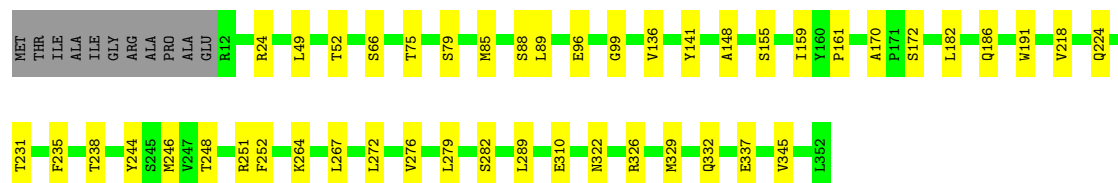
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 85% 12%



• Molecule 4: Photosystem II D2 protein

Chain D: 84% 13%



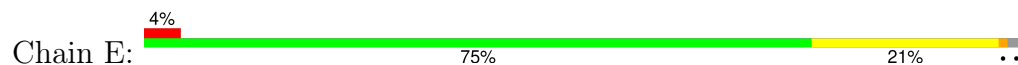
• Molecule 4: Photosystem II D2 protein

Chain d: 82% 14%





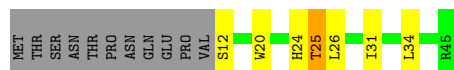
- Molecule 5: Cytochrome b559 subunit alpha



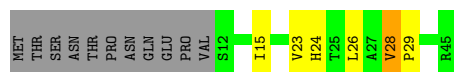
- Molecule 5: Cytochrome b559 subunit alpha



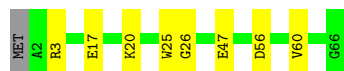
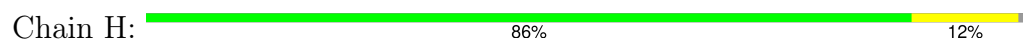
- Molecule 6: Cytochrome b559 subunit beta



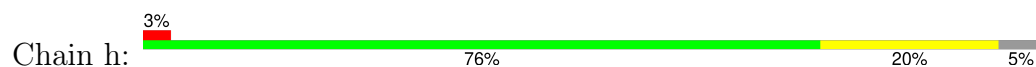
- Molecule 6: Cytochrome b559 subunit beta



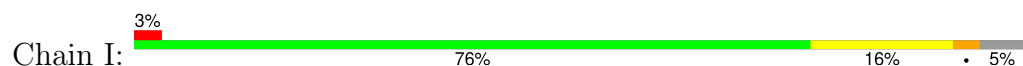
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H



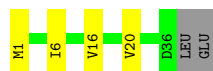
- Molecule 8: Photosystem II reaction center protein I





- Molecule 8: Photosystem II reaction center protein I

Chain i: 84% 11% 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 75% 15% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 65% 22% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 63% 15% 20%



- Molecule 10: Photosystem II reaction center protein K

Chain k: 52% 24% 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 84% 16%

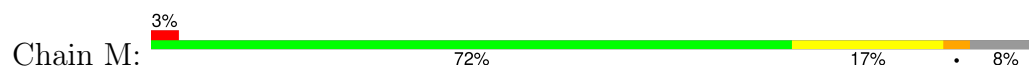


- Molecule 11: Photosystem II reaction center protein L

Chain l: 84% 14%



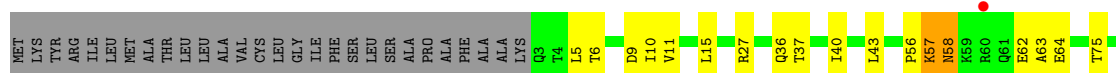
- Molecule 12: Photosystem II reaction center protein M



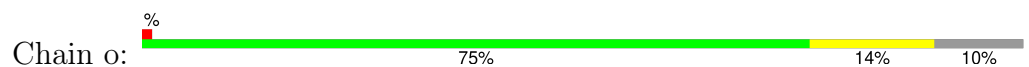
- Molecule 12: Photosystem II reaction center protein M



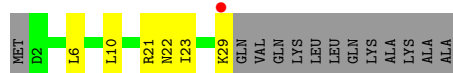
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

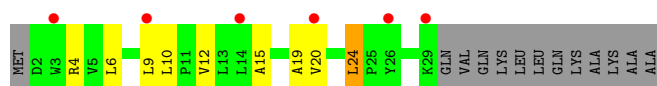


- Molecule 14: Photosystem II protein Y

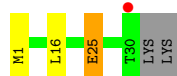
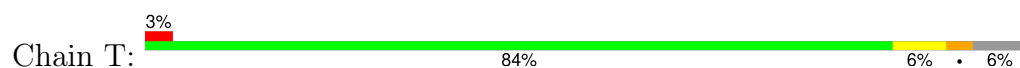


- Molecule 14: Photosystem II protein Y

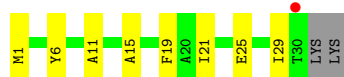




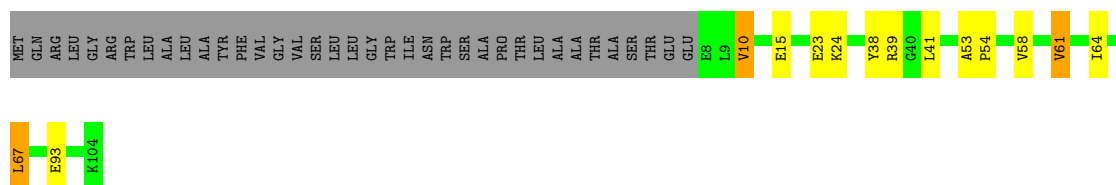
- Molecule 15: Photosystem II reaction center protein T



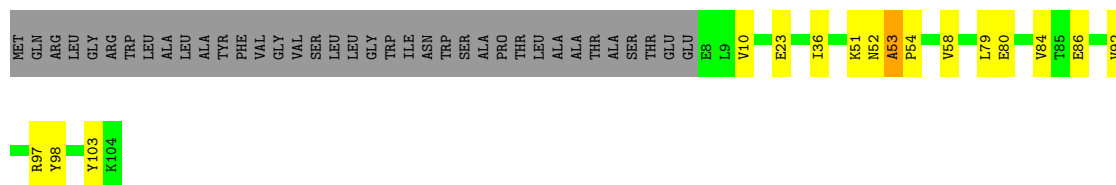
- Molecule 15: Photosystem II reaction center protein T



- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein

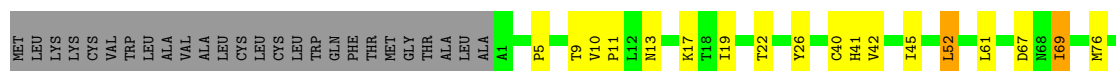


- Molecule 17: Cytochrome c-550



- Molecule 17: Cytochrome c-550

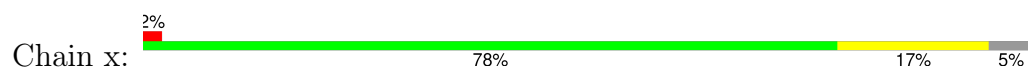




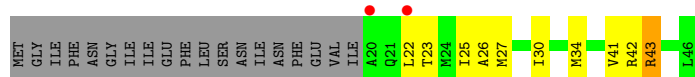
- Molecule 18: Photosystem II reaction center X protein



- Molecule 18: Photosystem II reaction center X protein



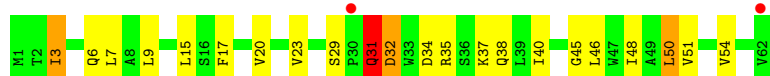
- Molecule 19: Photosystem II reaction center protein Ycf12



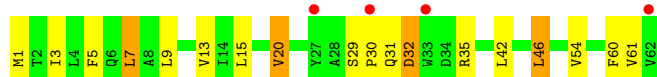
- Molecule 19: Photosystem II reaction center protein Ycf12



- 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	117.07Å 222.05Å 308.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.45 – 2.27 33.45 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.45-2.27) 84.2 (33.45-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.182 , 0.244 0.182 , 0.245	Depositor DCC
R_{free} test set	3275 reflections (0.52%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	103252	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: FME, PL9, OEX, HEM, LMG, PHO, NA, FE2, LHG, STE, DGD, SQD, CL, CLA, HEC, BCT, BCR

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	0.61	0/2707	0.70	0/3692
1	a	0.60	0/2704	0.68	0/3688
2	B	0.59	1/4161 (0.0%)	0.66	1/5669 (0.0%)
2	b	0.57	1/4118 (0.0%)	0.64	1/5611 (0.0%)
3	C	0.56	0/3547	0.64	0/4830
3	c	0.52	0/3619	0.63	0/4926
4	D	0.63	0/2812	0.67	0/3832
4	d	0.58	0/2821	0.66	0/3844
5	E	0.49	0/688	0.54	0/940
5	e	0.44	0/683	0.54	0/932
6	F	0.47	0/284	0.59	0/387
6	f	0.46	0/284	0.59	0/387
7	H	0.57	0/523	0.62	0/713
7	h	0.50	0/511	0.60	0/697
8	I	0.57	0/293	0.70	0/396
8	i	0.56	0/293	0.57	0/396
9	J	0.50	0/263	0.61	0/356
9	j	0.44	0/263	0.59	0/356
10	K	0.44	0/303	0.53	0/416
10	k	0.41	0/303	0.52	0/416
11	L	0.60	0/311	0.59	0/422
11	l	0.63	0/303	0.58	0/412
12	M	0.62	0/249	0.60	0/341
12	m	0.62	0/244	0.74	0/334
13	O	0.55	0/1904	0.64	0/2585
13	o	0.58	0/1905	0.65	0/2583
14	R	0.37	0/227	0.51	0/313
14	r	0.32	0/227	0.44	0/313
15	T	0.66	0/257	0.70	0/349
15	t	0.58	0/255	0.63	0/346
16	U	0.54	0/785	0.61	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.61	1/785 (0.1%)	0.69	0/1064
17	V	0.55	0/1085	0.65	0/1473
17	v	0.49	0/1085	0.59	0/1473
18	X	0.48	0/284	0.53	0/384
18	x	0.43	0/289	0.54	0/391
19	Y	0.41	0/197	0.50	0/264
19	y	0.33	0/219	0.51	0/294
20	Z	0.38	0/490	0.50	0/669
20	z	0.34	0/488	0.45	0/666
All	All	0.56	3/42769 (0.0%)	0.64	2/58224 (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
16	u	0	1
17	V	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	221	PRO	CA-C	-8.47	1.47	1.51
16	u	103	TYR	CA-C	6.27	1.55	1.52
2	B	221	PRO	CA-C	-5.97	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	221	PRO	O-C-N	-6.56	118.29	121.31
2	B	221	PRO	O-C-N	-5.91	118.37	121.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide
16	u	52	ASN	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	2622	2519	2519	25	0
1	a	2619	2510	2510	36	0
2	B	4005	3873	3867	36	0
2	b	3978	3836	3836	41	0
3	C	3426	3355	3343	34	0
3	c	3500	3426	3426	33	0
4	D	2717	2621	2621	35	0
4	d	2723	2627	2627	32	0
5	E	666	651	651	17	0
5	e	664	648	648	16	0
6	F	275	282	282	5	0
6	f	275	282	282	3	0
7	H	510	532	532	4	0
7	h	498	518	518	6	0
8	I	296	311	311	2	0
8	i	296	311	311	1	0
9	J	257	268	268	4	0
9	j	257	268	268	7	0
10	K	293	305	305	6	0
10	k	293	305	305	7	0
11	L	304	316	316	6	0
11	l	296	304	304	1	0
12	M	256	269	269	4	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	30	0
13	o	1874	1846	1846	17	0
14	R	221	238	238	1	0
14	r	221	238	238	5	0
15	T	258	261	261	2	0
15	t	256	256	256	5	0
16	U	774	773	773	7	0
16	u	774	773	773	8	0
17	V	1064	1073	1073	8	0
17	v	1064	1073	1074	21	0
18	X	281	312	312	7	0
18	x	286	316	314	4	0
19	Y	196	217	217	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	y	218	241	241	8	0
20	Z	479	516	516	16	0
20	z	477	509	509	13	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	184	192	192	5	0
22	B	1035	1139	1139	21	0
22	C	839	922	922	18	0
22	D	195	216	216	4	0
22	a	130	144	144	1	0
22	b	1035	1139	1139	23	0
22	c	839	919	919	14	0
22	d	260	288	288	2	0
23	A	64	74	74	0	0
23	D	64	74	74	3	0
23	a	64	74	74	0	0
23	d	64	74	74	2	0
24	A	2	0	0	0	0
24	a	2	0	0	0	0
25	A	55	80	80	2	0
25	D	55	80	80	1	0
25	a	55	80	80	0	0
25	d	55	80	80	1	0
26	A	48	66	66	1	0
26	B	83	126	126	0	0
26	D	84	117	117	2	0
26	M	51	72	72	1	0
26	Y	48	66	66	1	0
26	b	55	86	86	1	0
26	c	134	181	181	4	0
26	d	44	58	58	0	0
26	m	51	72	71	2	0
27	A	91	135	135	3	0
27	B	54	78	77	0	0
27	D	36	45	44	1	0
27	L	49	65	64	4	0
27	a	54	78	78	0	0
27	f	41	48	47	1	0
27	t	36	56	56	1	0
28	A	49	74	74	4	0
28	D	145	215	215	9	0
28	L	49	74	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	a	49	74	74	5	0
28	d	88	125	125	3	0
28	e	42	57	57	0	0
28	l	49	74	74	1	0
29	A	66	96	96	1	0
29	C	186	246	244	6	0
29	H	62	82	81	0	0
29	c	186	245	242	6	0
29	h	62	82	82	2	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	B	120	168	168	7	0
31	C	40	56	56	3	0
31	D	40	56	56	3	0
31	H	40	56	56	0	0
31	I	40	56	56	1	0
31	K	80	112	112	0	0
31	T	40	56	56	1	0
31	Z	40	56	56	0	0
31	a	40	56	56	0	0
31	b	120	168	168	1	0
31	c	80	112	112	1	0
31	d	40	56	56	2	0
31	k	80	112	112	0	0
31	t	40	56	56	2	0
31	x	40	56	56	1	0
32	B	75	117	114	4	0
32	C	40	63	60	2	0
32	H	18	35	35	1	0
32	I	15	26	26	2	0
32	J	12	16	16	2	0
32	L	12	16	16	1	0
32	M	25	38	38	0	0
32	R	12	16	16	0	0
32	X	20	35	35	4	0
32	Z	8	12	12	0	0
32	a	27	42	42	0	0
32	b	111	197	191	7	0
32	c	32	51	51	1	0
32	d	37	61	61	5	0
32	j	12	16	16	2	0
32	l	18	35	35	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	t	24	36	36	1	0
32	x	20	35	35	1	0
33	D	4	1	1	0	0
33	a	4	1	1	0	0
34	F	43	30	30	4	0
34	f	43	30	30	5	0
35	V	43	32	30	0	0
35	v	43	32	31	6	0
36	V	1	0	0	0	0
37	A	125	0	0	5	0
37	B	135	0	0	8	0
37	C	119	0	0	4	0
37	D	103	0	0	5	0
37	E	20	0	0	4	0
37	F	5	0	0	1	0
37	H	22	0	0	2	0
37	I	12	0	0	0	0
37	J	11	0	0	1	0
37	K	6	0	0	1	0
37	L	9	0	0	2	0
37	M	6	0	0	1	0
37	O	68	0	0	5	0
37	R	8	0	0	0	0
37	T	7	0	0	1	0
37	U	30	0	0	1	0
37	V	49	0	0	2	0
37	X	9	0	0	2	0
37	Y	3	0	0	0	0
37	Z	6	0	0	1	0
37	a	99	0	0	7	0
37	b	114	0	0	4	0
37	c	120	0	0	5	0
37	d	88	0	0	2	0
37	e	18	0	0	2	0
37	f	5	0	0	0	0
37	h	22	0	0	4	0
37	i	8	0	0	0	0
37	j	9	0	0	0	0
37	k	2	0	0	0	0
37	l	11	0	0	0	0
37	m	2	0	0	0	0
37	o	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	t	11	0	0	0	0
37	u	35	0	0	2	0
37	v	32	0	0	2	0
37	x	7	0	0	0	0
37	y	6	0	0	3	0
37	z	11	0	0	3	0
All	All	51603	51649	51604	588	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 6.

All (588) 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)
17:v:40:CYS:SG	35:v:201:HEC:CAC	2.10	1.40
16:u:36:ILE:O	37:u:201:HOH:O	1.82	0.97
34:F:101:HEM:O2A	37:F:201:HOH:O	1.82	0.96
17:v:40:CYS:SG	35:v:201:HEC:HAC	2.03	0.96
2:b:372:ASP:OD2	37:b:701:HOH:O	1.82	0.95
2:b:354:LEU:O	37:b:702:HOH:O	1.86	0.94
13:O:145:GLU:OE1	37:O:301:HOH:O	1.85	0.93
7:H:47:GLU:OE2	37:H:201:HOH:O	1.90	0.89
11:L:7:ARG:NH1	37:L:201:HOH:O	2.06	0.89
16:U:93:GLU:OE1	37:U:201:HOH:O	1.94	0.86
7:H:3:ARG:NH2	37:H:202:HOH:O	1.99	0.84
32:B:620:STE:O2	37:B:702:HOH:O	1.93	0.84
15:T:25:GLU:OE1	37:T:201:HOH:O	1.96	0.84
32:X:101:STE:O1	37:X:201:HOH:O	1.96	0.82
28:a:410:LHG:O4	4:d:141:TYR:OH	1.94	0.82
26:D:412:LMG:O1	37:D:502:HOH:O	2.00	0.80
1:a:23:SER:O	37:a:501:HOH:O	1.99	0.80
3:c:387:TRP:NE1	37:c:601:HOH:O	1.93	0.79
17:v:40:CYS:SG	35:v:201:HEC:C3C	2.71	0.78
18:X:39:ARG:O	37:X:202:HOH:O	2.01	0.77
32:c:523:STE:O2	37:c:602:HOH:O	2.01	0.77
17:v:61:LEU:O	37:v:301:HOH:O	2.03	0.76
20:z:32:ASP:N	20:z:32:ASP:OD1	2.17	0.76
9:J:5:GLY:N	37:J:201:HOH:O	2.18	0.76
4:D:75:THR:O	37:D:503:HOH:O	2.04	0.75
2:B:347:ARG:NE	37:B:701:HOH:O	1.80	0.75
4:d:96:GLU:OE1	37:d:501:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:84:GLU:OE1	13:O:86:LYS:NZ	2.21	0.74
13:O:107:THR:HG22	37:O:319:HOH:O	1.88	0.73
2:B:433:ASP:O	37:B:703:HOH:O	2.07	0.72
4:D:337:GLU:OE2	37:D:504:HOH:O	2.07	0.71
3:C:190:ALA:O	37:C:601:HOH:O	2.07	0.71
32:B:627:STE:O1	37:B:704:HOH:O	2.07	0.71
17:v:104:MET:HA	17:v:107:LEU:HD22	1.71	0.71
5:e:7:GLU:OE2	37:e:201:HOH:O	2.07	0.71
13:O:246:ALA:OXT	37:O:302:HOH:O	2.08	0.70
2:B:506:ARG:O	37:B:705:HOH:O	2.08	0.70
5:E:8:ARG:N	37:E:101:HOH:O	2.03	0.70
3:C:143:TYR:OH	37:C:602:HOH:O	2.08	0.69
3:c:360:ASP:OD2	37:c:603:HOH:O	2.09	0.69
16:u:53:ALA:HB1	16:u:54:PRO:HD2	1.72	0.69
2:b:355:PHE:O	37:b:704:HOH:O	2.10	0.69
5:E:61:ARG:NH2	37:E:102:HOH:O	2.26	0.69
10:K:23:ASP:OD2	37:K:201:HOH:O	2.10	0.69
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.75	0.69
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.75	0.69
1:A:311:GLY:O	37:A:501:HOH:O	2.12	0.68
17:v:132:GLY:O	37:v:302:HOH:O	2.10	0.68
1:a:264:SER:O	37:a:502:HOH:O	2.13	0.67
2:B:15:ASP:OD1	37:B:706:HOH:O	2.13	0.67
18:X:17:GLY:HA2	32:X:101:STE:H141	1.77	0.66
20:Z:35:ARG:NH1	20:Z:38:GLN:OE1	2.30	0.65
13:O:218:GLU:OE1	37:O:303:HOH:O	2.14	0.65
5:e:4:THR:OG1	37:e:202:HOH:O	2.14	0.65
4:D:99:GLY:HA3	32:X:101:STE:H21	1.78	0.65
19:y:17:GLU:HB3	37:y:101:HOH:O	1.97	0.65
3:C:406:SER:HA	3:C:420:VAL:HG23	1.78	0.64
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.33	0.63
26:b:622:LMG:O5	37:b:703:HOH:O	1.95	0.63
3:C:148:GLY:O	3:C:156:LYS:NZ	2.29	0.63
19:y:17:GLU:N	37:y:101:HOH:O	2.32	0.62
1:A:342:ASP:O	37:A:502:HOH:O	2.16	0.62
1:A:269:ARG:HD2	4:D:235:PHE:HB2	1.81	0.61
16:U:10:VAL:HG21	16:U:15:GLU:OE2	2.00	0.61
13:o:83:GLY:HA2	13:o:98:GLU:HG3	1.83	0.61
2:b:307:GLU:HG2	2:b:340:TRP:HB2	1.84	0.60
13:o:57:LYS:HB2	13:o:59:LYS:HE2	1.84	0.60
17:v:40:CYS:SG	35:v:201:HEC:CBC	2.87	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:29:SER:O	37:z:101:HOH:O	2.16	0.60
22:C:513:CLA:HHC	22:C:513:CLA:HBB1	1.84	0.60
12:m:4:ASN:ND2	26:m:101:LMG:O10	2.35	0.60
5:E:7:GLU:HA	37:E:101:HOH:O	2.00	0.60
1:a:306:VAL:HG12	1:a:314:ILE:HB	1.84	0.60
3:C:334:PRO:HA	13:O:153:THR:OG1	2.02	0.59
13:O:36:GLN:HE21	13:O:37:THR:H	1.51	0.59
2:b:90:PHE:H	32:b:621:STE:H183	1.68	0.58
22:b:605:CLA:HHC	22:b:605:CLA:HBB1	1.84	0.58
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.85	0.58
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.86	0.58
18:x:3:ILE:HG23	18:x:7:LEU:HD23	1.86	0.58
27:f:102:SQD:H331	18:x:27:VAL:HG21	1.86	0.58
2:b:91:TRP:HE1	32:b:621:STE:H111	1.69	0.58
27:L:101:SQD:H121	22:b:614:CLA:H43	1.86	0.57
3:C:96:GLY:O	37:C:603:HOH:O	2.18	0.57
3:c:391[A]:ARG:HD2	3:c:395:TYR:CZ	2.38	0.57
32:I:102:STE:H131	22:b:606:CLA:H192	1.86	0.57
1:A:97:TRP:HA	8:I:1:FME:HG2	1.86	0.57
19:y:39:LEU:HB3	19:y:46:LEU:HD21	1.87	0.57
3:C:141:GLU:H	3:C:141:GLU:CD	2.13	0.56
3:C:459:ILE:HG21	3:C:464:GLU:HG3	1.86	0.56
7:H:17:GLU:OE2	7:H:20:LYS:HE2	2.05	0.56
20:z:61:VAL:N	37:z:102:HOH:O	2.38	0.56
1:a:12:ASN:OD1	37:a:503:HOH:O	2.18	0.56
2:B:12:LEU:HB2	22:B:612:CLA:HMC2	1.87	0.56
4:D:332:GLN:NE2	37:D:505:HOH:O	2.31	0.56
4:d:126:MET:HE3	4:d:143:ALA:O	2.06	0.56
35:v:201:HEC:HMC1	35:v:201:HEC:HBC3	1.88	0.56
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.88	0.56
22:B:604:CLA:H12	22:B:605:CLA:H42	1.88	0.55
1:a:84:PRO:HA	1:a:112:TYR:CG	2.41	0.55
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.70	0.55
1:a:217:SER:HA	4:d:272:LEU:HD12	1.89	0.55
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.88	0.55
22:B:610:CLA:H111	22:B:615:CLA:HAA1	1.88	0.55
4:d:40:CYS:HB3	4:d:117:HIS:O	2.07	0.55
4:d:126:MET:HA	4:d:129:GLN:OE1	2.06	0.54
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.88	0.54
4:d:267:LEU:C	4:d:267:LEU:HD23	2.32	0.54
5:e:16:SER:HA	9:j:6:GLY:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:101:BCR:H321	31:T:101:BCR:HC8	1.90	0.54
4:d:89:LEU:HD12	7:h:50:ASN:OD1	2.07	0.54
20:z:32:ASP:HA	20:z:35:ARG:HG3	1.90	0.54
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.42	0.54
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.89	0.54
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.90	0.53
34:f:101:HEM:HBC2	34:f:101:HEM:HMC1	1.91	0.53
5:e:14:ILE:O	5:e:20:TRP:NE1	2.40	0.53
25:A:408:PL9:H362	6:F:25:THR:HG21	1.91	0.53
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.09	0.53
2:b:355:PHE:HE2	2:b:373:LYS:HG2	1.74	0.53
32:b:624:STE:H32	26:m:101:LMG:HC5	1.91	0.53
3:c:344:SER:O	13:o:75:THR:HG22	2.09	0.53
12:M:5:GLN:NE2	37:M:202:HOH:O	2.38	0.53
3:c:334:PRO:HA	13:o:153:THR:OG1	2.09	0.53
28:A:411:LHG:HC31	37:A:509:HOH:O	2.08	0.52
3:C:203:THR:O	3:C:235:GLY:HA3	2.09	0.52
13:O:27:ARG:O	13:O:27:ARG:HG2	2.10	0.52
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.91	0.52
23:D:401:PHO:HBA2	22:D:403:CLA:H142	1.91	0.52
32:b:627:STE:H72	32:d:412:STE:H81	1.92	0.52
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.92	0.52
22:B:608:CLA:H172	22:B:609:CLA:H193	1.92	0.52
22:b:601:CLA:H93	31:x:101:BCR:H402	1.92	0.52
22:b:615:CLA:H2	22:b:616:CLA:HBB2	1.92	0.52
4:D:96:GLU:HB2	37:D:519:HOH:O	2.10	0.52
1:a:12:ASN:CG	37:a:503:HOH:O	2.53	0.52
17:v:13:ASN:HD21	17:v:17:LYS:HB3	1.74	0.52
1:A:332:HIS:O	1:A:333:GLU:C	2.53	0.51
34:F:101:HEM:HBB2	34:F:101:HEM:HMB1	1.91	0.51
22:b:608:CLA:H61	22:b:609:CLA:H121	1.93	0.51
9:j:30:TYR:HA	32:j:101:STE:H22	1.92	0.51
20:z:15:LEU:HD22	20:z:46:LEU:HD12	1.91	0.51
2:B:135:LEU:HA	2:B:138:MET:HG3	1.92	0.51
18:X:16:SER:HB3	32:X:101:STE:H92	1.92	0.51
3:c:71:GLU:HB3	3:c:86:LEU:HD22	1.91	0.51
3:c:203:THR:O	3:c:235:GLY:HA3	2.10	0.51
19:y:17:GLU:CD	37:y:102:HOH:O	2.53	0.51
22:B:604:CLA:H93	22:B:605:CLA:HAB	1.93	0.51
20:Z:9:LEU:HD13	20:Z:54:VAL:HG11	1.92	0.51
1:a:229:GLU:CD	1:a:229:GLU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:HA	31:B:618:BCR:C40	2.40	0.51
4:D:267:LEU:C	4:D:267:LEU:HD23	2.35	0.51
13:O:10:ILE:HG23	13:O:15:LEU:HB2	1.91	0.51
16:U:58:VAL:O	16:U:61:VAL:HG22	2.10	0.51
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.92	0.51
18:x:17:GLY:HA2	32:x:102:STE:H31	1.91	0.51
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.41	0.51
4:d:79:SER:HA	4:d:172:SER:HB3	1.92	0.51
20:Z:31:GLN:NE2	20:Z:32:ASP:H	2.08	0.51
22:c:510:CLA:H201	10:k:33:LEU:HD22	1.93	0.51
5:e:26:THR:HA	14:r:15:ALA:HB1	1.91	0.51
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.46	0.51
22:B:606:CLA:H72	31:B:619:BCR:H311	1.92	0.50
5:E:65:LEU:O	5:E:67:THR:HG23	2.11	0.50
4:d:199:MET:HG2	25:d:407:PL9:H321	1.92	0.50
11:L:8:GLN:NE2	37:L:203:HOH:O	2.36	0.50
2:b:422:ARG:O	2:b:425:ILE:HG12	2.10	0.50
4:D:272:LEU:C	4:D:272:LEU:HD23	2.35	0.50
9:j:18:GLY:O	9:j:22:ILE:HD13	2.11	0.50
2:B:149[B]:LEU:HD11	22:B:604:CLA:H162	1.92	0.50
20:z:9:LEU:HD13	20:z:54:VAL:HG11	1.94	0.50
3:C:45:LEU:HA	3:C:139:THR:HG22	1.93	0.50
29:C:516:DGD:O2D	32:J:101:STE:H21	2.12	0.50
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.47	0.50
2:b:324:LEU:HD23	2:b:325:PHE:CE2	2.47	0.50
22:c:501:CLA:C3D	22:c:503:CLA:H2	2.41	0.50
13:o:110:MET:HE2	13:o:116:ILE:HD11	1.94	0.50
2:B:218:LEU:HD12	32:B:627:STE:H22	1.94	0.50
2:b:92:SER:O	2:b:96:VAL:HG23	2.12	0.50
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.94	0.50
3:c:189:TRP:O	37:c:604:HOH:O	2.19	0.50
32:B:620:STE:O1	37:B:707:HOH:O	2.19	0.49
4:D:310:GLU:HG3	13:O:224:ASP:OD2	2.12	0.49
11:L:14:ARG:HH22	27:L:101:SQD:H3	1.76	0.49
13:O:56:PRO:O	13:O:58:ASN:N	2.42	0.49
2:b:292:LEU:HD21	2:b:298:LEU:HD23	1.94	0.49
22:c:511:CLA:H172	20:z:20:VAL:HG22	1.93	0.49
29:C:516:DGD:HO2D	32:J:101:STE:H21	1.77	0.49
26:D:408:LMG:H402	6:F:26:LEU:HB3	1.93	0.49
16:U:23:GLU:HG3	16:U:24:LYS:HG3	1.93	0.49
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:47:GLU:OE2	37:h:201:HOH:O	2.20	0.49
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.47	0.49
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.78	0.49
9:j:15:THR:HG22	9:j:19:MET:HE2	1.94	0.49
27:D:409:SQD:H341	18:X:23:LEU:HD22	1.95	0.49
9:J:19:MET:O	9:J:23:VAL:HG23	2.12	0.49
32:b:624:STE:H42	12:m:6:LEU:HD11	1.94	0.49
4:d:279:LEU:HD22	23:d:402:PHO:HBC3	1.94	0.49
3:C:223:TRP:CG	3:C:224:ILE:H	2.30	0.49
4:D:24:ARG:HD3	18:X:37:VAL:HG12	1.95	0.48
4:D:141:TYR:OH	28:D:413:LHG:O4	2.18	0.48
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.78	0.48
2:B:164:PRO:HG3	22:B:606:CLA:O1D	2.13	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
17:V:63:THR:HG22	17:V:64:PRO:CD	2.43	0.48
19:Y:22:LEU:HA	19:Y:25:ILE:HG22	1.93	0.48
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.48	0.48
3:C:61:VAL:HG12	3:C:118:HIS:O	2.13	0.48
3:C:109:PHE:N	3:C:110:PRO:CD	2.76	0.48
4:d:62:GLY:HA2	5:e:63:ILE:HG21	1.96	0.48
29:A:413:DGD:HD5	2:b:75:TRP:HB3	1.94	0.48
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.48	0.48
3:c:217:PRO:HG3	29:c:516:DGD:HA81	1.95	0.48
4:D:218:VAL:HG22	4:D:244:TYR:CZ	2.48	0.48
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	1.96	0.48
1:a:257:ARG:O	37:a:504:HOH:O	2.19	0.48
1:a:210:LEU:C	1:a:210:LEU:HD23	2.39	0.48
20:Z:51:VAL:O	20:Z:54:VAL:O	2.32	0.48
22:b:608:CLA:HBC2	22:b:609:CLA:H111	1.95	0.48
3:C:383:ASP:OD1	37:C:604:HOH:O	2.20	0.47
5:E:15:THR:HB	9:J:8:ILE:O	2.14	0.47
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.49	0.47
2:B:382:PRO:HG2	2:B:385:ARG:HD2	1.96	0.47
2:b:293:ALA:C	2:b:295:GLY:H	2.22	0.47
1:A:104:GLU:OE1	37:A:503:HOH:O	2.20	0.47
1:a:114:LEU:C	1:a:114:LEU:HD23	2.39	0.47
2:b:145:LEU:HD22	22:b:604:CLA:H161	1.96	0.47
3:c:130:VAL:HG21	22:c:511:CLA:H151	1.96	0.47
22:B:614:CLA:H42	32:L:103:STE:H22	1.97	0.47
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.13	0.47
1:a:278:TRP:HB3	1:a:279:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.15	0.47
26:c:521:LMG:H292	26:c:521:LMG:H112	1.96	0.47
4:d:21:TRP:HA	4:d:24:ARG:HG3	1.96	0.47
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.95	0.47
13:O:5:LEU:HD12	13:O:10:ILE:HD11	1.95	0.47
13:O:64:GLU:OE1	13:O:64:GLU:N	2.47	0.47
2:b:30:VAL:HG12	22:b:605:CLA:HHD	1.96	0.47
22:b:602:CLA:H203	29:h:101:DGD:HBT1	1.96	0.47
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.97	0.47
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.97	0.47
1:a:95:PRO:HD2	1:a:98:GLU:HG3	1.95	0.47
2:b:16:PRO:O	2:b:20:ILE:HD12	2.14	0.47
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.47
13:o:49:THR:HG23	13:o:236:GLN:HB2	1.97	0.47
16:u:53:ALA:HB1	16:u:54:PRO:CD	2.41	0.47
3:C:50:LEU:HD21	22:C:513:CLA:C1B	2.45	0.47
4:D:155:SER:HA	4:D:159:ILE:HB	1.96	0.47
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.50	0.47
17:v:26:TYR:OH	17:v:122:GLU:OE1	2.28	0.47
17:v:67:ASP:OD1	17:v:67:ASP:N	2.41	0.47
20:Z:45:GLY:HA2	20:Z:48:ILE:HD12	1.96	0.46
22:A:402:CLA:C19	28:D:410:LHG:H312	2.44	0.46
4:d:259:ILE:HD13	4:d:259:ILE:H	1.80	0.46
13:o:62:GLU:OE2	13:o:63:ALA:N	2.48	0.46
2:B:241:SER:O	2:B:245:VAL:HG23	2.15	0.46
22:B:601:CLA:HAB	32:H:103:STE:H132	1.97	0.46
22:B:614:CLA:H152	22:B:614:CLA:H18	1.67	0.46
20:Z:3:ILE:HA	20:Z:6:GLN:HG2	1.97	0.46
17:v:10:VAL:HG23	17:v:69:ILE:HD11	1.98	0.46
27:A:410:SQD:H262	28:D:411:LHG:H122	1.97	0.46
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.30	0.46
1:a:77:ILE:HD11	15:t:6:TYR:HB3	1.96	0.46
1:A:114:LEU:C	1:A:114:LEU:HD23	2.41	0.46
1:A:116:ILE:HG13	1:A:117:PHE:N	2.31	0.46
4:D:148:ALA:HB2	4:D:276:VAL:HG13	1.97	0.46
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.98	0.46
16:u:58:VAL:HG23	16:u:84:VAL:HG22	1.97	0.46
2:B:221:PRO:HA	22:B:609:CLA:HED3	1.97	0.46
8:i:16:VAL:O	8:i:20:VAL:HG23	2.16	0.46
13:O:57:LYS:HD3	2:b:49:ASP:OD2	2.15	0.46
5:e:40:THR:HB	14:r:4:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:t:101:BCR:H321	31:t:101:BCR:HC8	1.98	0.46
1:a:237:TYR:HB2	4:d:265:ARG:HG3	1.98	0.46
22:b:607:CLA:H142	22:b:613:CLA:H203	1.98	0.46
20:Z:50:LEU:HD12	20:Z:50:LEU:HA	1.86	0.46
28:a:410:LHG:H351	28:a:410:LHG:H102	1.97	0.46
29:h:101:DGD:O2E	37:h:202:HOH:O	2.21	0.46
26:A:409:LMG:H132	22:C:505:CLA:H203	1.97	0.46
22:B:611:CLA:H203	22:B:613:CLA:H8	1.98	0.46
9:j:19:MET:O	9:j:23:VAL:HG23	2.16	0.46
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.98	0.46
6:F:20:TRP:CE2	6:F:24:HIS:CE1	3.05	0.45
20:Z:34:ASP:O	20:Z:37:LYS:HG2	2.16	0.45
1:a:329:GLU:CD	37:a:506:HOH:O	2.58	0.45
28:d:408:LHG:H321	15:t:21:ILE:HD11	1.97	0.45
2:b:442:ILE:HD11	13:o:174:LEU:HD23	1.97	0.45
10:K:24:VAL:HG21	19:Y:25:ILE:HB	1.97	0.45
5:e:25:ILE:O	5:e:28:PRO:HD2	2.16	0.45
16:u:86:GLU:H	16:u:86:GLU:CD	2.23	0.45
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.97	0.45
2:b:67:ALA:HA	2:b:71:VAL:O	2.17	0.45
14:r:20:VAL:O	14:r:24:LEU:HB2	2.16	0.45
20:z:3:ILE:HG22	20:z:7:LEU:HD22	1.97	0.45
13:O:215:PHE:CD1	13:O:215:PHE:C	2.95	0.45
2:b:154:GLY:HA2	2:b:158:LEU:HD12	1.98	0.45
6:f:24:HIS:O	6:f:28:VAL:HG13	2.16	0.45
17:v:52:LEU:HD12	17:v:52:LEU:HA	1.83	0.45
2:B:139:PHE:CZ	2:B:143:LEU:HD22	2.51	0.45
3:C:216:SER:HB3	3:C:221:GLU:HG3	1.98	0.45
3:c:154:LYS:HG2	3:c:266:TRP:CE3	2.51	0.45
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.98	0.45
17:v:99:ASP:OD1	17:v:99:ASP:N	2.49	0.45
17:V:99:ASP:OD1	17:V:99:ASP:N	2.50	0.45
28:a:410:LHG:HC91	28:l:101:LHG:HC81	1.99	0.45
1:A:269:ARG:HD3	4:D:231:THR:O	2.17	0.45
22:C:504:CLA:H143	22:C:508:CLA:H141	1.98	0.45
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.45
20:z:60:PHE:C	37:z:102:HOH:O	2.60	0.45
2:B:487:SER:OG	2:B:488:PRO:HD2	2.17	0.44
27:L:101:SQD:H102	22:b:614:CLA:H43	1.99	0.44
10:k:26:PRO:O	10:k:29:PRO:HD2	2.17	0.44
28:D:413:LHG:H211	12:M:18:PRO:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:92:HIS:ND1	17:v:93:PRO:HD2	2.32	0.44
2:B:433:ASP:OD1	2:B:433:ASP:C	2.60	0.44
19:Y:42:ARG:HH22	20:Z:31:GLN:HE22	1.64	0.44
22:c:509:CLA:H142	22:c:509:CLA:H111	1.85	0.44
2:B:246:PHE:CD1	2:B:246:PHE:C	2.95	0.44
18:x:3:ILE:HA	18:x:7:LEU:HD23	2.00	0.44
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.99	0.44
2:b:159:THR:O	2:b:180:PRO:HB3	2.18	0.44
2:b:383:PHE:O	13:o:166:SER:HA	2.18	0.44
16:u:98:TYR:O	37:u:202:HOH:O	2.21	0.44
16:U:64:ILE:HB	16:U:67:LEU:HD22	1.98	0.44
1:a:112:TYR:O	1:a:116:ILE:HG12	2.18	0.44
29:c:516:DGD:HA82	26:c:522:LMG:H352	1.99	0.44
28:A:411:LHG:O4	5:E:10:PHE:HB2	2.17	0.44
22:B:604:CLA:H41	22:B:604:CLA:H61	1.68	0.44
5:E:7:GLU:CA	37:E:101:HOH:O	2.64	0.44
1:a:203:ALA:HB2	29:c:518:DGD:HAN1	1.99	0.44
22:c:508:CLA:H91	28:d:409:LHG:H361	1.99	0.44
4:d:192:THR:HG23	22:d:403:CLA:HBC2	2.00	0.44
28:A:411:LHG:HC32	5:E:11:SER:OG	2.17	0.44
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.44
2:b:403:GLY:O	2:b:407:ASN:HB2	2.17	0.44
3:C:178:LYS:NZ	3:C:184:GLY:O	2.47	0.43
28:D:413:LHG:H342	28:D:413:LHG:H312	1.83	0.43
18:X:19:VAL:O	18:X:23:LEU:HB2	2.18	0.43
22:b:605:CLA:H142	22:b:610:CLA:C2	2.48	0.43
22:b:608:CLA:H141	22:b:608:CLA:H161	1.81	0.43
3:c:163:PHE:CG	22:c:512:CLA:HAB	2.53	0.43
22:C:506:CLA:H8	31:C:514:BCR:H12C	2.00	0.43
8:I:17:LEU:HD22	8:I:21:PHE:HE2	1.83	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.53	0.43
16:U:53:ALA:HB1	16:U:54:PRO:HA	2.00	0.43
2:b:119:ASP:HB3	37:h:208:HOH:O	2.18	0.43
2:b:266:GLU:OE2	2:b:308:LYS:NZ	2.51	0.43
7:h:3:ARG:NH2	37:h:205:HOH:O	2.51	0.43
7:h:61:SER:C	7:h:63:LYS:N	2.76	0.43
19:y:41:VAL:C	19:y:43:ARG:H	2.25	0.43
3:C:93:ALA:HB1	3:C:99:VAL:HG11	1.99	0.43
4:D:85:MET:HE1	5:E:72:ALA:HB2	2.00	0.43
26:M:101:LMG:O9	26:M:101:LMG:HC71	2.18	0.43
3:c:27:ASP:HB3	10:k:46:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:501:CLA:C4D	22:c:503:CLA:H2	2.48	0.43
5:e:22:ILE:HG23	14:r:19:ALA:HB2	2.00	0.43
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.00	0.43
2:B:489:GLU:HG3	2:B:495:PHE:CE2	2.54	0.43
25:D:407:PL9:H412	11:L:29:LEU:HD23	2.00	0.43
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.54	0.43
22:d:404:CLA:H43	22:d:404:CLA:O1A	2.19	0.43
17:v:11:PRO:O	17:v:69:ILE:HD12	2.19	0.43
22:C:509:CLA:H92	22:C:509:CLA:H62	1.90	0.43
4:D:186:GLN:HB2	22:D:403:CLA:HBC1	2.01	0.43
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.00	0.43
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.33	0.43
2:b:127:ARG:NH1	7:h:18:TYR:O	2.51	0.43
5:e:30:LEU:HD11	34:f:101:HEM:CBB	2.48	0.43
2:B:144:PHE:CE2	2:B:148:LEU:HD11	2.54	0.43
23:D:401:PHO:HBA2	23:D:401:PHO:H3A	1.81	0.43
22:D:403:CLA:H193	22:D:403:CLA:H162	1.87	0.43
4:d:96:GLU:HB2	37:d:501:HOH:O	2.17	0.43
32:d:411:STE:H81	32:d:412:STE:H51	2.01	0.43
13:o:41:ALA:O	13:o:82:GLN:HG2	2.18	0.43
17:v:108:THR:N	17:v:111:ASP:OD2	2.40	0.43
31:B:619:BCR:H382	27:t:102:SQD:H82	2.00	0.43
4:D:282:SER:HB2	22:D:403:CLA:O1D	2.18	0.43
28:D:411:LHG:H141	28:D:411:LHG:H322	2.01	0.43
5:E:18:ARG:HE	14:R:23:ILE:HD12	1.84	0.43
13:O:78:LEU:HB3	13:O:81:ILE:HD11	2.01	0.43
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.01	0.43
1:a:299:GLY:O	1:a:300:PHE:C	2.61	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.01	0.43
2:B:200:ALA:O	2:B:201:HIS:C	2.60	0.43
22:B:610:CLA:HBD	22:B:610:CLA:H143	2.01	0.43
4:D:322:ASN:O	4:D:326:ARG:HG3	2.19	0.43
22:c:506:CLA:H12	22:c:506:CLA:H51	1.90	0.43
4:d:209:LEU:HD23	4:d:209:LEU:C	2.43	0.43
17:v:41:HIS:O	17:v:42:VAL:C	2.61	0.43
20:z:42:LEU:O	20:z:46:LEU:HB2	2.19	0.43
1:A:322:ASN:OD1	3:C:412:THR:HA	2.19	0.43
2:B:36:SER:OG	31:B:618:BCR:H362	2.18	0.43
3:C:50:LEU:O	3:C:54:VAL:HG23	2.19	0.43
22:C:510:CLA:H193	22:C:510:CLA:HBC3	2.01	0.43
1:a:307:ILE:HG22	1:a:313:VAL:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:49:LEU:HD13	31:d:406:BCR:C15	2.49	0.43
3:c:125:LEU:HD13	31:c:514:BCR:H361	2.00	0.43
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.01	0.43
1:A:131:TRP:CD2	1:A:131:TRP:C	2.94	0.42
22:A:402:CLA:H203	22:A:402:CLA:H162	1.90	0.42
22:B:613:CLA:H161	28:D:413:LHG:H192	2.00	0.42
22:C:513:CLA:H201	32:C:519:STE:H151	2.01	0.42
9:J:15:THR:O	9:J:19:MET:HG3	2.19	0.42
19:Y:42:ARG:HH22	20:Z:31:GLN:NE2	2.16	0.42
1:a:342:ASP:O	37:a:505:HOH:O	2.21	0.42
15:t:15:ALA:O	15:t:19:PHE:HD1	2.03	0.42
17:V:67:ASP:OD1	17:V:67:ASP:N	2.43	0.42
10:k:18:PHE:CE2	20:z:13:VAL:HG21	2.54	0.42
13:o:127:ALA:HB1	13:o:142:PHE:HB3	2.00	0.42
22:B:608:CLA:H191	4:D:89:LEU:HD13	2.00	0.42
31:B:618:BCR:C8	31:B:618:BCR:H331	2.49	0.42
3:C:443:TRP:CZ2	22:C:508:CLA:HMD1	2.54	0.42
13:O:145:GLU:CD	37:O:301:HOH:O	2.49	0.42
34:f:101:HEM:HMB3	14:r:19:ALA:HB3	2.00	0.42
1:A:329:GLU:OE2	17:V:134:LYS:NZ	2.48	0.42
2:B:495:PHE:HD2	2:B:505:ARG:HH12	1.66	0.42
22:C:507:CLA:H61	22:C:507:CLA:H41	1.84	0.42
4:D:218:VAL:HG22	4:D:244:TYR:CE1	2.54	0.42
13:O:93:LEU:O	13:O:128:SER:HA	2.19	0.42
22:b:611:CLA:H72	22:b:611:CLA:H112	1.85	0.42
13:O:123:LYS:O	13:O:124:ASN:HB2	2.19	0.42
17:V:3:LEU:HD23	17:V:3:LEU:HA	1.82	0.42
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.42
2:b:372:ASP:OD1	2:b:372:ASP:C	2.61	0.42
17:v:41:HIS:HA	17:v:45:ILE:O	2.19	0.42
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.00	0.42
22:b:605:CLA:HMC3	22:b:615:CLA:H43	2.00	0.42
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.53	0.42
15:t:11:ALA:HB1	31:t:101:BCR:H16C	2.02	0.42
2:B:226:TYR:CD2	2:B:231:MET:HB2	2.54	0.42
3:C:120:ILE:HD13	3:C:120:ILE:HA	1.91	0.42
13:O:56:PRO:HG3	13:O:63:ALA:N	2.34	0.42
1:A:16:ARG:NH1	37:A:520:HOH:O	2.52	0.42
3:C:213:LEU:HD21	31:C:514:BCR:C20	2.49	0.42
22:C:505:CLA:H43	31:C:514:BCR:HC7	2.01	0.42
1:a:231:GLU:H	1:a:231:GLU:HG2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:627:STE:C5	32:d:412:STE:H122	2.50	0.42
3:c:121:SER:O	3:c:124:VAL:HG13	2.20	0.42
22:c:509:CLA:H3A	22:c:509:CLA:HBA1	1.87	0.42
26:c:521:LMG:H402	26:c:521:LMG:H372	1.79	0.42
17:v:40:CYS:SG	35:v:201:HEC:C2C	3.06	0.42
19:y:42:ARG:O	19:y:43:ARG:C	2.62	0.42
2:B:82:GLY:HA2	37:B:790:HOH:O	2.19	0.42
22:B:614:CLA:H61	22:B:614:CLA:H41	1.70	0.42
3:C:344:SER:O	13:O:75:THR:HG22	2.20	0.42
6:F:34:LEU:HD23	6:F:34:LEU:HA	1.89	0.42
18:X:29:ILE:O	18:X:33:GLN:HG2	2.19	0.42
28:a:410:LHG:H161	22:b:607:CLA:H18	2.02	0.42
2:b:355:PHE:CE2	2:b:373:LYS:HG2	2.53	0.42
3:c:163:PHE:O	3:c:167:VAL:HG23	2.19	0.42
16:u:92:VAL:HG12	16:u:97:ARG:HD2	2.01	0.42
29:C:516:DGD:HB22	26:Y:101:LMG:H302	2.01	0.42
5:E:35:TRP:CD1	5:E:35:TRP:C	2.97	0.42
1:a:300:PHE:HZ	29:c:518:DGD:HB72	1.85	0.42
2:b:42:LEU:HD13	2:b:94:GLU:HG3	2.01	0.42
22:c:504:CLA:H91	22:c:508:CLA:H172	2.02	0.42
5:e:68:ASP:OD2	5:e:71:GLU:HG2	2.20	0.42
19:y:17:GLU:O	19:y:20:ALA:HB3	2.20	0.42
22:B:603:CLA:C3D	22:B:605:CLA:H2	2.49	0.41
3:C:46:SER:HB2	3:C:149:TYR:CE2	2.55	0.41
31:D:406:BCR:H392	31:D:406:BCR:H23C	2.01	0.41
34:f:101:HEM:HBC2	34:f:101:HEM:CMC	2.48	0.41
13:o:178:LYS:HD3	13:o:178:LYS:HA	1.75	0.41
1:A:217:SER:HA	4:D:272:LEU:HD12	2.01	0.41
3:C:343:ARG:NH1	3:C:347:GLY:O	2.50	0.41
22:C:511:CLA:H143	20:Z:20:VAL:HG13	2.02	0.41
3:c:202:PRO:HB3	3:c:234:VAL:HG12	2.02	0.41
20:z:31:GLN:HG3	20:z:32:ASP:OD1	2.20	0.41
22:A:403:CLA:HMB1	22:A:403:CLA:HBB1	2.03	0.41
20:Z:32:ASP:CB	37:Z:202:HOH:O	2.68	0.41
2:b:174:LEU:HA	2:b:308:LYS:HD3	2.02	0.41
22:b:608:CLA:HAB	4:d:123:ILE:HG12	2.02	0.41
29:c:517:DGD:HA42	32:j:101:STE:H91	2.03	0.41
4:d:53:THR:HA	4:d:67:TYR:CD2	2.56	0.41
6:f:26:LEU:O	6:f:29:PRO:HD2	2.20	0.41
1:A:120:LEU:HD23	1:A:120:LEU:HA	1.82	0.41
5:E:64:PRO:HB2	5:E:79:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:I:101:BCR:H24C	31:I:101:BCR:H371	1.94	0.41
28:L:102:LHG:H262	28:L:102:LHG:H291	1.76	0.41
17:V:2:GLU:HB2	37:V:326:HOH:O	2.19	0.41
17:V:63:THR:HB	17:V:83:ASP:C	2.45	0.41
1:a:131:TRP:CE3	1:a:132:GLU:HA	2.56	0.41
1:a:200:LEU:HD12	1:a:200:LEU:HA	1.87	0.41
2:b:63:LEU:N	2:b:64:PRO:HD2	2.34	0.41
3:c:93:ALA:HB1	3:c:99:VAL:HG21	2.01	0.41
13:o:93:LEU:O	13:o:128:SER:HA	2.20	0.41
1:A:95:PRO:HD2	1:A:98:GLU:HG3	2.03	0.41
22:C:507:CLA:H61	22:C:507:CLA:H92	1.85	0.41
4:D:79:SER:HA	4:D:172:SER:HB3	2.01	0.41
20:Z:31:GLN:CD	20:Z:32:ASP:H	2.28	0.41
22:b:602:CLA:H43	7:h:45:ILE:HG22	2.03	0.41
4:d:127:LEU:HD22	32:d:411:STE:H52	2.00	0.41
4:d:346:LEU:HD23	4:d:346:LEU:HA	1.87	0.41
28:d:409:LHG:H242	28:d:409:LHG:H272	1.77	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.03	0.41
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.55	0.41
1:a:236:GLY:HA3	4:d:265:ARG:NH1	2.36	0.41
2:b:157:HIS:CD2	2:b:157:HIS:C	2.98	0.41
22:b:616:CLA:HAA2	22:b:616:CLA:HBD	2.01	0.41
3:c:128:GLY:HA3	22:c:513:CLA:C3C	2.50	0.41
13:o:45:LEU:HD23	13:o:215:PHE:CD2	2.54	0.41
19:y:22:LEU:HA	19:y:25:ILE:HG22	2.03	0.41
1:A:63:ILE:HB	3:C:335:THR:HG21	2.02	0.41
31:B:617:BCR:H11C	31:B:617:BCR:H341	1.96	0.41
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.56	0.41
10:K:25:LEU:N	10:K:26:PRO:HD2	2.36	0.41
10:K:28:ILE:N	10:K:29:PRO:CD	2.84	0.41
22:a:402:CLA:H161	22:a:402:CLA:H122	1.81	0.41
2:b:125:ASP:HB2	2:b:132:ALA:HB3	2.03	0.41
3:c:60:ILE:HG22	22:c:503:CLA:HHD	2.01	0.41
3:c:352:GLY:O	3:c:355:THR:HG22	2.20	0.41
9:j:18:GLY:O	9:j:21:VAL:HG13	2.20	0.41
1:A:159:LEU:C	1:A:162:PRO:HD2	2.46	0.41
22:A:403:CLA:HMD2	4:D:182:LEU:HD11	2.03	0.41
27:A:410:SQD:H122	28:D:411:LHG:C16	2.50	0.41
28:A:411:LHG:HC81	5:E:10:PHE:CD2	2.55	0.41
4:D:88:SER:HB2	5:E:69:ARG:NH2	2.35	0.41
5:E:19:TYR:CE1	5:E:23:HIS:CE1	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:ILE:HG13	34:F:101:HEM:HMC2	2.02	0.41
7:H:25:TRP:O	7:H:26:GLY:C	2.64	0.41
20:Z:29:SER:HB3	20:Z:31:GLN:HE21	1.86	0.41
4:d:330:ALA:HB3	4:d:331:PRO:HD3	2.03	0.41
10:k:25:LEU:N	10:k:26:PRO:CD	2.83	0.41
13:o:32:ILE:HG21	13:o:93:LEU:HD21	2.03	0.41
1:A:192:ILE:HG13	1:A:293:MET:HE1	2.02	0.41
27:A:410:SQD:H122	28:D:411:LHG:H162	2.03	0.41
2:B:157:HIS:CD2	2:B:157:HIS:C	2.99	0.41
2:B:434:THR:OG1	13:O:178:LYS:HD3	2.21	0.41
22:B:616:CLA:H41	22:B:616:CLA:H61	1.89	0.41
3:C:38:GLY:HA3	22:C:511:CLA:HMD2	2.02	0.41
27:L:101:SQD:H121	22:b:614:CLA:C4	2.51	0.41
13:O:83:GLY:HA3	13:O:96:VAL:O	2.21	0.41
19:Y:26:ALA:O	19:Y:30:ILE:HG22	2.21	0.41
1:a:72:LEU:HD23	1:a:72:LEU:HA	1.89	0.41
1:a:296:ASN:HB2	3:c:400:PRO:O	2.21	0.41
28:a:410:LHG:HC42	2:b:468:TRP:CH2	2.55	0.41
2:b:489:GLU:HG2	2:b:495:PHE:CD2	2.56	0.41
32:b:627:STE:H61	32:d:412:STE:H102	2.03	0.41
3:c:387:TRP:CE2	37:c:601:HOH:O	2.56	0.41
22:c:512:CLA:H203	26:c:521:LMG:H452	2.03	0.41
4:d:218:VAL:HG22	4:d:244:TYR:CZ	2.56	0.41
23:d:402:PHO:H122	23:d:402:PHO:H161	1.83	0.41
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.38	0.41
17:v:5:PRO:O	17:v:9:THR:OG1	2.27	0.41
4:D:49:LEU:HD13	31:D:406:BCR:C15	2.51	0.41
4:D:52:THR:O	4:D:66:SER:HA	2.21	0.41
29:c:517:DGD:HB32	29:c:517:DGD:HB61	1.64	0.41
4:d:194:ASN:HA	4:d:295:SER:OG	2.21	0.41
31:d:406:BCR:H402	9:j:21:VAL:HG21	2.03	0.41
1:A:183:MET:HA	22:A:402:CLA:HMD1	2.03	0.40
2:B:58:GLN:O	2:B:60:MET:HE2	2.21	0.40
2:B:67:ALA:HA	2:B:71:VAL:O	2.21	0.40
2:B:102:VAL:HA	31:B:618:BCR:H401	2.03	0.40
22:C:509:CLA:H93	22:C:509:CLA:H112	1.89	0.40
17:V:55:ARG:HD2	37:V:328:HOH:O	2.21	0.40
1:a:278:TRP:HB3	1:a:279:PRO:CD	2.51	0.40
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.51	0.40
1:A:102:LEU:HD11	32:I:102:STE:H61	2.04	0.40
25:A:408:PL9:H251	25:A:408:PL9:H272	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:C:508:CLA:H203	29:C:516:DGD:HAE1	2.04	0.40
29:C:516:DGD:HAE2	29:C:516:DGD:HA61	2.04	0.40
4:D:251:ARG:O	4:D:252:PHE:C	2.65	0.40
11:L:22:LEU:HB2	15:T:16:LEU:HD21	2.04	0.40
11:L:36:PHE:HB3	12:M:3:VAL:HB	2.03	0.40
22:b:609:CLA:H91	22:b:609:CLA:H112	1.94	0.40
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.55	0.40
2:B:59:GLY:O	22:B:607:CLA:HED2	2.21	0.40
2:B:155:ALA:O	2:B:159:THR:OG1	2.32	0.40
22:b:615:CLA:H3A	22:b:615:CLA:HBA1	1.86	0.40
31:b:618:BCR:H15C	31:b:618:BCR:H351	1.93	0.40
13:o:44:CYS:O	13:o:239:PHE:HA	2.21	0.40
2:B:289:GLN:HE21	2:B:289:GLN:HA	1.85	0.40
3:C:338:GLY:HA3	3:C:341:LEU:O	2.21	0.40
22:C:510:CLA:OBD	10:K:33:LEU:HD13	2.20	0.40
29:C:515:DGD:O2E	29:C:515:DGD:HD4	2.21	0.40
4:D:279:LEU:HD22	23:D:401:PHO:HBC3	2.04	0.40
31:D:406:BCR:H20C	31:D:406:BCR:H361	1.93	0.40
1:a:72:LEU:HD21	32:t:103:STE:H41	2.03	0.40
3:c:459:ILE:HG21	3:c:464:GLU:HG3	2.04	0.40
3:C:114:VAL:HG22	32:C:519:STE:H82	2.03	0.40
13:O:81:ILE:HA	13:O:100:GLY:HA3	2.04	0.40
19:Y:42:ARG:O	19:Y:43:ARG:C	2.65	0.40
2:b:58:GLN:C	2:b:329:PRO:HB3	2.46	0.40
3:c:296:VAL:HG23	3:c:297:TYR:CD2	2.56	0.40
4:d:210:LEU:HA	4:d:213:ILE:HG22	2.02	0.40
11:l:14:ARG:HB3	15:t:25:GLU:HG3	2.03	0.40
12:m:9:ILE:HG13	12:m:13:LEU:HD22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
1	a	332/344 (96%)	323 (97%)	9 (3%)	0	100	100
2	B	508/510 (100%)	500 (98%)	8 (2%)	0	100	100
2	b	503/510 (99%)	487 (97%)	13 (3%)	3 (1%)	21	25
3	C	442/461 (96%)	424 (96%)	17 (4%)	1 (0%)	43	53
3	c	451/461 (98%)	437 (97%)	13 (3%)	1 (0%)	43	53
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
5	E	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
5	e	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	61 (97%)	1 (2%)	1 (2%)	7	6
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
10	K	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
10	k	35/46 (76%)	32 (91%)	3 (9%)	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%)	228 (94%)	12 (5%)	3 (1%)	10	10
13	o	242/272 (89%)	228 (94%)	13 (5%)	1 (0%)	30	36
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	91 (96%)	4 (4%)	0	100	100
16	u	95/134 (71%)	91 (96%)	3 (3%)	1 (1%)	11	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	21
17	v	135/163 (83%)	131 (97%)	4 (3%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	1
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	1
20	Z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	1
20	z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	7	6
All	All	5231/5700 (92%)	5049 (96%)	165 (3%)	17 (0%)	36	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
20	Z	31	GLN
3	c	416	SER
16	u	53	ALA
13	O	58	ASN
13	O	62	GLU
13	o	61	GLN
19	Y	43	ARG
20	Z	32	ASP
2	b	294	SER
19	y	43	ARG
2	b	295	GLY
13	O	57	LYS
2	b	404	GLY
20	z	30	PRO
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	270/280 (96%)	265 (98%)	5 (2%)	50	66
1	a	269/280 (96%)	256 (95%)	13 (5%)	23	32
2	B	408/407 (100%)	397 (97%)	11 (3%)	39	55
2	b	402/407 (99%)	387 (96%)	15 (4%)	30	43
3	C	346/362 (96%)	337 (97%)	9 (3%)	40	56
3	c	354/362 (98%)	340 (96%)	14 (4%)	28	40
4	D	276/283 (98%)	271 (98%)	5 (2%)	51	68
4	d	277/283 (98%)	264 (95%)	13 (5%)	23	33
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	37
5	e	71/73 (97%)	66 (93%)	5 (7%)	14	17
6	F	28/39 (72%)	26 (93%)	2 (7%)	13	17
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	7
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	66
7	h	53/55 (96%)	47 (89%)	6 (11%)	5	6
8	I	32/34 (94%)	28 (88%)	4 (12%)	4	4
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	50
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	37
9	j	24/28 (86%)	21 (88%)	3 (12%)	4	4
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	19
10	k	30/37 (81%)	23 (77%)	7 (23%)	1	0
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	5
12	M	28/32 (88%)	25 (89%)	3 (11%)	6	7
12	m	28/32 (88%)	25 (89%)	3 (11%)	6	7
13	O	206/228 (90%)	196 (95%)	10 (5%)	22	31
13	o	207/228 (91%)	196 (95%)	11 (5%)	20	28
14	R	22/33 (67%)	17 (77%)	5 (23%)	1	1
14	r	22/33 (67%)	17 (77%)	5 (23%)	1	1
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	42
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	40
16	U	84/112 (75%)	80 (95%)	4 (5%)	23	32
16	u	84/112 (75%)	80 (95%)	4 (5%)	23	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	V	117/138 (85%)	109 (93%)	8 (7%)	14	18
17	v	117/138 (85%)	110 (94%)	7 (6%)	17	23
18	X	31/34 (91%)	28 (90%)	3 (10%)	8	8
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	8
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	7
19	y	22/37 (60%)	20 (91%)	2 (9%)	9	10
20	Z	52/52 (100%)	45 (86%)	7 (14%)	4	3
20	z	51/52 (98%)	46 (90%)	5 (10%)	7	8
All	All	4321/4654 (93%)	4110 (95%)	211 (5%)	22	31

All (211) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	228	THR
1	A	231	GLU
1	A	243	GLU
1	A	248	ILE
2	B	63	LEU
2	B	98	LEU
2	B	101	ILE
2	B	127	ARG
2	B	138	MET
2	B	289	GLN
2	B	297	THR
2	B	350	GLU
2	B	353	GLU
2	B	371	THR
2	B	385	ARG
3	C	120	ILE
3	C	141	GLU
3	C	159	THR
3	C	201	ASN
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
3	C	355	THR
3	C	386	PRO
4	D	224	GLN

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Mol	Chain	Res	Type
4	D	238	THR
4	D	248	THR
4	D	329	MET
4	D	345	VAL
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
6	F	12	SER
6	F	25	THR
7	H	56	ASP
8	I	2	GLU
8	I	4	LEU
8	I	11	VAL
8	I	35	LYS
9	J	24	ILE
10	K	13	GLU
10	K	25	LEU
12	M	16	LEU
12	M	20	VAL
12	M	25	LEU
13	O	78	LEU
13	O	86	LYS
13	O	89	SER
13	O	107	THR
13	O	118	LEU
13	O	133	VAL
13	O	191	SER
13	O	214	THR
13	O	218	GLU
13	O	225	MET
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	22	ASN
14	R	29	LYS
15	T	25	GLU
16	U	10	VAL
16	U	39	ARG
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL

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Mol	Chain	Res	Type
17	V	17	LYS
17	V	19	ILE
17	V	21	LEU
17	V	27	LEU
17	V	42	VAL
17	V	90	GLU
18	X	3	ILE
18	X	29	ILE
18	X	37	VAL
19	Y	34	MET
19	Y	41	VAL
20	Z	3	ILE
20	Z	7	LEU
20	Z	15	LEU
20	Z	17	PHE
20	Z	31	GLN
20	Z	46	LEU
20	Z	50	LEU
1	a	28	LEU
1	a	42	LEU
1	a	121	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	226	GLU
1	a	229	GLU
1	a	230	THR
1	a	245	THR
1	a	248	ILE
1	a	271	LEU
1	a	288	LEU
2	b	63	LEU
2	b	80	ILE
2	b	83	GLU
2	b	98	LEU
2	b	128	THR
2	b	149	LEU
2	b	179	GLN
2	b	236	THR
2	b	286	ARG
2	b	362	PHE
2	b	478	VAL

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Mol	Chain	Res	Type
2	b	480	SER
2	b	485	GLU
2	b	491	VAL
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	48	LYS
3	c	72	LEU
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	200	THR
3	c	221	GLU
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	315	MET
3	c	355	THR
4	d	90	LEU
4	d	150	ILE
4	d	182	LEU
4	d	227[A]	GLU
4	d	227[B]	GLU
4	d	230	SER
4	d	233	ARG
4	d	256	ILE
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
5	e	4	THR
5	e	65	LEU
5	e	66	VAL
5	e	75	GLN
5	e	84	LYS
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL
7	h	7	LEU
7	h	12	ARG
7	h	27	THR

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Mol	Chain	Res	Type
7	h	30	LEU
7	h	37	LEU
7	h	43	LEU
8	i	6	ILE
9	j	7	ARG
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	17	ILE
10	k	25	LEU
10	k	30	VAL
10	k	35	LEU
10	k	46	ARG
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
12	m	20	VAL
13	o	49	THR
13	o	55	GLU
13	o	58	ASN
13	o	64	GLU
13	o	72	THR
13	o	87	VAL
13	o	118	LEU
13	o	135	SER
13	o	191	SER
13	o	198	SER
13	o	207	ARG
14	r	6	LEU
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
14	r	24	LEU
15	t	29	ILE
16	u	10	VAL
16	u	23	GLU
16	u	51	LYS
16	u	80	GLU

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Mol	Chain	Res	Type
17	v	19	ILE
17	v	22	THR
17	v	52	LEU
17	v	69	ILE
17	v	90	GLU
17	v	107	LEU
17	v	112	LEU
18	x	8	LYS
18	x	15	LEU
18	x	21	LEU
19	y	19	ILE
19	y	23	THR
20	z	1	MET
20	z	7	LEU
20	z	20	VAL
20	z	32	ASP
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	165	GLN
1	A	199	GLN
1	A	261	GLN
1	A	338	ASN
2	B	216	HIS
2	B	289	GLN
3	C	56	HIS
3	C	155	ASN
3	C	327	ASN
3	C	385	GLN
13	O	36	GLN
13	O	124	ASN
13	O	231	HIS
16	U	37	GLN
16	U	78	ASN
17	V	86	GLN
18	X	38	GLN
19	Y	45	ASN
20	Z	6	GLN
20	Z	31	GLN

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Mol	Chain	Res	Type
1	a	181	ASN
1	a	199	GLN
1	a	234	ASN
2	b	338	GLN
2	b	409	GLN
2	b	490	GLN
3	c	378	ASN
3	c	415	ASN
13	o	61	GLN
13	o	219	GLN
18	x	33	GLN
18	x	38	GLN
20	z	31	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	FME	t	1	15	8,9,10	1.49	1 (12%)	8,9,11	1.16	1 (12%)
12	FME	m	1	12	8,9,10	1.07	0	8,9,11	1.52	2 (25%)
8	FME	I	1	8	8,9,10	1.12	1 (12%)	8,9,11	0.76	0
8	FME	i	1	8	8,9,10	1.10	1 (12%)	8,9,11	1.13	0
15	FME	T	1	15	8,9,10	0.99	0	8,9,11	1.02	1 (12%)
12	FME	M	1	12	8,9,10	1.07	1 (12%)	8,9,11	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	FME	t	1	15	-	3/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
8	FME	I	1	8	-	4/7/9/11	-
8	FME	i	1	8	-	2/7/9/11	-
15	FME	T	1	15	-	4/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.87	1.40	1.46
12	M	1	FME	CA-N	-2.24	1.43	1.46
8	I	1	FME	CA-N	-2.13	1.43	1.46
8	i	1	FME	CA-N	-2.13	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	m	1	FME	CA-N-CN	2.98	127.41	122.82
12	m	1	FME	CB-CA-N	2.42	114.92	110.52
15	t	1	FME	CA-N-CN	-2.26	119.35	122.82
15	T	1	FME	CG-CB-CA	2.04	119.09	112.87

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
8	i	1	FME	CB-CA-N-CN
12	M	1	FME	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 190 ligands modelled in this entry, 7 are monoatomic - leaving 183 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	$\# Z > 2$
32	STE	B	623	-	11,11,19	0.76	0	11,11,19	1.17	1 (9%)
32	STE	R	101	-	11,11,19	0.86	0	11,11,19	0.89	0
22	CLA	c	511	3	69,73,73	1.41	8 (11%)	82,113,113	1.49	5 (6%)
22	CLA	b	615	2	69,73,73	1.88	11 (15%)	82,113,113	1.29	9 (10%)
32	STE	C	518	-	11,11,19	0.98	1 (9%)	11,11,19	1.23	1 (9%)
27	SQD	f	102	-	39,41,54	1.14	4 (10%)	49,52,65	1.79	10 (20%)
31	BCR	b	619	-	41,41,41	1.19	2 (4%)	56,56,56	1.31	10 (17%)
32	STE	b	627	-	13,13,19	0.47	0	12,12,19	0.56	0
22	CLA	d	405	4	69,73,73	1.52	11 (15%)	82,113,113	1.22	6 (7%)
22	CLA	c	513	3	69,73,73	1.31	9 (13%)	82,113,113	1.20	7 (8%)
31	BCR	a	405	-	41,41,41	1.23	5 (12%)	56,56,56	1.44	9 (16%)
22	CLA	A	402	1	69,73,73	1.22	7 (10%)	82,113,113	1.48	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	BCR	K	101	-	41,41,41	1.30	3 (7%)	56,56,56	1.23	6 (10%)
31	BCR	Z	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.34	5 (8%)
23	PHO	D	401	-	58,69,69	2.05	9 (15%)	55,99,99	1.46	8 (14%)
22	CLA	b	612	2	69,73,73	1.35	8 (11%)	82,113,113	1.52	13 (15%)
29	DGD	A	413	-	67,67,67	1.26	8 (11%)	81,81,81	1.37	11 (13%)
32	STE	X	101	-	19,19,19	0.71	1 (5%)	19,19,19	1.11	0
32	STE	d	411	-	16,16,19	0.78	0	16,16,19	1.01	0
26	LMG	c	522	-	49,49,55	1.20	5 (10%)	57,57,63	1.42	7 (12%)
22	CLA	c	505	3	69,73,73	1.11	6 (8%)	82,113,113	1.30	7 (8%)
32	STE	t	104	-	9,9,19	0.58	0	8,8,19	0.45	0
22	CLA	B	609	2	69,73,73	1.27	7 (10%)	82,113,113	1.46	11 (13%)
31	BCR	b	618	-	41,41,41	1.56	4 (9%)	56,56,56	1.28	7 (12%)
31	BCR	I	101	-	41,41,41	1.24	5 (12%)	56,56,56	1.40	9 (16%)
22	CLA	a	404	1	69,73,73	1.38	10 (14%)	82,113,113	1.26	9 (10%)
32	STE	L	103	-	11,11,19	0.72	0	11,11,19	1.33	2 (18%)
22	CLA	A	403	37	69,73,73	1.45	11 (15%)	82,113,113	1.31	10 (12%)
22	CLA	C	507	37	69,73,73	1.19	5 (7%)	82,113,113	1.49	10 (12%)
32	STE	d	412	-	19,19,19	0.76	1 (5%)	19,19,19	0.93	0
26	LMG	A	409	-	48,48,55	1.19	3 (6%)	56,56,63	1.44	10 (17%)
22	CLA	b	602	2	69,73,73	1.34	9 (13%)	82,113,113	1.42	8 (9%)
31	BCR	b	617	-	41,41,41	1.16	3 (7%)	56,56,56	1.29	5 (8%)
22	CLA	b	614	2	69,73,73	1.42	11 (15%)	82,113,113	1.42	11 (13%)
27	SQD	A	412	-	38,38,54	1.07	3 (7%)	40,40,65	1.39	4 (10%)
32	STE	b	624	-	14,14,19	0.35	0	13,13,19	1.01	0
22	CLA	B	607	37	69,73,73	1.43	10 (14%)	82,113,113	1.26	6 (7%)
32	STE	Z	102	-	7,7,19	0.52	0	6,6,19	0.29	0
22	CLA	C	503	3	69,73,73	1.40	10 (14%)	82,113,113	1.64	11 (13%)
32	STE	c	520	-	19,19,19	0.79	1 (5%)	19,19,19	0.89	0
26	LMG	c	521	-	48,48,55	1.08	4 (8%)	56,56,63	1.35	7 (12%)
29	DGD	C	515	-	63,63,67	1.37	9 (14%)	77,77,81	1.35	11 (14%)
31	BCR	H	101	-	41,41,41	1.11	1 (2%)	56,56,56	1.17	5 (8%)
23	PHO	a	403	-	58,69,69	1.95	11 (18%)	55,99,99	1.53	9 (16%)
22	CLA	C	501	3	69,73,73	1.63	11 (15%)	82,113,113	1.43	6 (7%)
29	DGD	h	101	-	63,63,67	1.11	4 (6%)	77,77,81	1.41	14 (18%)
32	STE	b	623	-	15,15,19	0.84	1 (6%)	15,15,19	0.87	0
32	STE	I	102	-	14,14,19	0.54	0	13,13,19	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OEX	A	414	37,3,1	0,14,14	-	-	-		
27	SQD	a	411	-	52,54,54	1.04	4 (7%)	62,65,65	1.68	11 (17%)
28	LHG	l	101	-	48,48,48	0.82	2 (4%)	51,54,54	1.14	3 (5%)
26	LMG	M	101	-	51,51,55	1.04	4 (7%)	59,59,63	1.39	8 (13%)
22	CLA	B	605	2	69,73,73	1.07	4 (5%)	82,113,113	1.33	10 (12%)
22	CLA	B	613	2	69,73,73	1.82	11 (15%)	82,113,113	1.21	8 (9%)
22	CLA	b	605	2	69,73,73	1.17	10 (14%)	82,113,113	1.50	14 (17%)
22	CLA	c	512	3	69,73,73	1.37	11 (15%)	82,113,113	1.38	9 (10%)
22	CLA	b	604	2	69,73,73	1.21	7 (10%)	82,113,113	1.46	11 (13%)
22	CLA	B	610	37	69,73,73	1.34	9 (13%)	82,113,113	1.49	11 (13%)
22	CLA	b	609	2	69,73,73	1.49	10 (14%)	82,113,113	1.41	11 (13%)
32	STE	H	103	-	17,17,19	0.47	0	16,16,19	0.68	0
35	HEC	V	201	17	50,50,50	1.63	5 (10%)	68,82,82	1.52	15 (22%)
28	LHG	A	411	-	48,48,48	0.88	3 (6%)	51,54,54	1.26	6 (11%)
32	STE	b	626	-	9,9,19	0.52	0	8,8,19	0.52	0
26	LMG	d	410	-	44,44,55	1.27	5 (11%)	52,52,63	1.29	5 (9%)
32	STE	J	101	-	11,11,19	0.72	0	11,11,19	1.30	1 (9%)
23	PHO	d	402	-	58,69,69	2.15	11 (18%)	55,99,99	1.73	11 (20%)
26	LMG	b	622	-	55,55,55	1.15	6 (10%)	63,63,63	1.38	7 (11%)
31	BCR	T	101	-	41,41,41	1.17	4 (9%)	56,56,56	1.30	6 (10%)
29	DGD	H	102	-	63,63,67	1.33	8 (12%)	77,77,81	1.53	12 (15%)
22	CLA	B	616	2	64,68,73	1.62	10 (15%)	76,107,113	1.43	8 (10%)
22	CLA	c	507	37	69,73,73	1.76	11 (15%)	82,113,113	1.48	12 (14%)
22	CLA	d	401	37	69,73,73	1.25	10 (14%)	82,113,113	1.33	11 (13%)
22	CLA	d	404	37	69,73,73	1.44	8 (11%)	82,113,113	1.66	13 (15%)
25	PL9	A	408	-	55,55,55	1.59	4 (7%)	68,69,69	1.53	11 (16%)
22	CLA	b	601	37	69,73,73	1.41	10 (14%)	82,113,113	1.39	9 (10%)
32	STE	l	102	-	17,17,19	0.44	0	16,16,19	0.83	0
27	SQD	t	102	-	35,35,54	1.13	2 (5%)	37,37,65	1.38	4 (10%)
32	STE	a	412	-	11,11,19	0.85	0	11,11,19	0.92	0
31	BCR	B	617	-	41,41,41	1.19	3 (7%)	56,56,56	1.42	8 (14%)
22	CLA	C	505	3	69,73,73	1.19	7 (10%)	82,113,113	1.32	12 (14%)
32	STE	t	103	-	13,13,19	0.77	0	13,13,19	1.36	3 (23%)
27	SQD	L	101	-	47,49,54	0.97	2 (4%)	57,60,65	2.16	16 (28%)
26	LMG	B	626	-	55,55,55	1.23	7 (12%)	63,63,63	1.31	5 (7%)
32	STE	j	101	-	11,11,19	0.95	1 (9%)	11,11,19	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	PL9	D	407	-	55,55,55	1.46	8 (14%)	68,69,69	1.54	13 (19%)
26	LMG	c	519	-	37,37,55	1.41	7 (18%)	45,45,63	1.37	5 (11%)
27	SQD	B	622	-	52,54,54	1.01	3 (5%)	62,65,65	1.92	13 (20%)
33	BCT	D	402	21	3,3,3	1.03	0	2,3,3	3.61	2 (100%)
30	OEX	a	414	37,3,1	0,14,14	-	-	-	-	-
22	CLA	b	608	2	69,73,73	1.12	7 (10%)	82,113,113	1.33	7 (8%)
33	BCT	a	408	21	3,3,3	1.16	0	2,3,3	3.37	2 (100%)
34	HEM	f	101	6,5	50,50,50	1.37	7 (14%)	67,82,82	1.25	5 (7%)
29	DGD	c	517	-	63,63,67	1.07	6 (9%)	77,77,81	1.53	13 (16%)
28	LHG	D	411	-	46,46,48	1.02	3 (6%)	49,52,54	1.23	4 (8%)
29	DGD	c	518	-	63,63,67	1.22	10 (15%)	77,77,81	1.40	10 (12%)
32	STE	a	413	-	14,14,19	0.48	0	13,13,19	0.69	0
31	BCR	c	514	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	9 (16%)
22	CLA	C	509	3	69,73,73	1.29	8 (11%)	82,113,113	1.32	9 (10%)
22	CLA	B	602	2	69,73,73	1.41	10 (14%)	82,113,113	1.38	11 (13%)
22	CLA	B	614	2	69,73,73	1.17	5 (7%)	82,113,113	1.28	9 (10%)
35	HEC	v	201	17	50,50,50	1.59	6 (12%)	68,82,82	1.59	13 (19%)
22	CLA	d	403	4	69,73,73	1.47	12 (17%)	82,113,113	1.24	8 (9%)
22	CLA	b	616	2	64,68,73	1.15	7 (10%)	76,107,113	1.53	11 (14%)
32	STE	b	621	-	19,19,19	0.72	0	19,19,19	0.99	1 (5%)
31	BCR	t	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.37	7 (12%)
31	BCR	d	406	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	8 (14%)
31	BCR	D	406	-	41,41,41	1.26	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	D	404	37	69,73,73	1.49	9 (13%)	82,113,113	1.26	7 (8%)
22	CLA	c	506	3	69,73,73	1.49	7 (10%)	82,113,113	1.36	9 (10%)
22	CLA	c	510	3	69,73,73	1.14	7 (10%)	82,113,113	1.23	8 (9%)
32	STE	B	620	-	16,16,19	0.78	0	16,16,19	0.96	0
32	STE	b	625	-	19,19,19	0.74	0	19,19,19	0.74	0
32	STE	x	102	-	19,19,19	0.71	0	19,19,19	1.13	2 (10%)
32	STE	M	103	-	9,9,19	0.65	0	8,8,19	0.46	0
29	DGD	C	516	-	63,63,67	1.25	9 (14%)	77,77,81	1.48	16 (20%)
31	BCR	k	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.23	5 (8%)
22	CLA	B	601	37	69,73,73	1.49	9 (13%)	82,113,113	1.32	6 (7%)
25	PL9	a	409	-	55,55,55	1.05	3 (5%)	68,69,69	1.65	15 (22%)
32	STE	B	624	-	17,17,19	0.68	0	17,17,19	0.99	0
27	SQD	D	409	-	34,36,54	1.02	3 (8%)	42,45,65	1.90	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	b	603	2	69,73,73	1.32	8 (11%)	82,113,113	1.65	13 (15%)
31	BCR	C	514	-	41,41,41	1.28	2 (4%)	56,56,56	1.34	9 (16%)
28	LHG	a	410	-	48,48,48	0.91	1 (2%)	51,54,54	1.29	6 (11%)
22	CLA	A	405	1	58,62,73	1.31	9 (15%)	68,99,113	1.50	10 (14%)
34	HEM	F	101	6,5	50,50,50	1.45	4 (8%)	67,82,82	1.25	8 (11%)
22	CLA	B	604	2	69,73,73	1.46	9 (13%)	82,113,113	1.79	18 (21%)
26	LMG	D	412	-	31,31,55	1.03	3 (9%)	33,33,63	1.18	4 (12%)
32	STE	B	625	-	15,15,19	0.49	0	14,14,19	0.84	0
22	CLA	C	506	3	69,73,73	1.60	12 (17%)	82,113,113	1.24	8 (9%)
22	CLA	c	504	37	64,68,73	1.23	7 (10%)	76,107,113	1.21	8 (10%)
22	CLA	C	502	3	69,73,73	1.60	8 (11%)	82,113,113	1.36	10 (12%)
28	LHG	D	413	-	48,48,48	1.02	3 (6%)	51,54,54	1.37	6 (11%)
22	CLA	B	611	2	69,73,73	1.42	9 (13%)	82,113,113	1.63	12 (14%)
22	CLA	B	606	2	69,73,73	1.76	10 (14%)	82,113,113	1.26	10 (12%)
22	CLA	B	612	2	69,73,73	1.20	9 (13%)	82,113,113	1.45	9 (10%)
22	CLA	D	403	4	69,73,73	1.17	4 (5%)	82,113,113	1.17	5 (6%)
28	LHG	D	410	-	48,48,48	0.95	3 (6%)	51,54,54	1.24	6 (11%)
22	CLA	c	508	3	68,72,73	1.22	9 (13%)	80,111,113	1.26	10 (12%)
22	CLA	C	508	3	69,73,73	1.31	8 (11%)	82,113,113	1.44	14 (17%)
32	STE	c	523	-	11,11,19	0.84	0	11,11,19	1.23	1 (9%)
22	CLA	C	513	3	69,73,73	1.33	10 (14%)	82,113,113	1.50	10 (12%)
26	LMG	D	408	-	51,51,55	0.88	2 (3%)	59,59,63	1.28	6 (10%)
27	SQD	A	410	-	50,52,54	1.09	4 (8%)	60,63,65	2.04	15 (25%)
29	DGD	C	517	-	63,63,67	1.19	8 (12%)	77,77,81	1.56	12 (15%)
22	CLA	c	501	3	69,73,73	1.46	11 (15%)	82,113,113	1.49	8 (9%)
31	BCR	K	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.22	5 (8%)
22	CLA	b	610	37	69,73,73	1.71	9 (13%)	82,113,113	1.27	10 (12%)
25	PL9	d	407	-	55,55,55	1.56	10 (18%)	68,69,69	1.58	15 (22%)
22	CLA	b	611	2	69,73,73	1.20	5 (7%)	82,113,113	1.49	14 (17%)
22	CLA	b	607	37	69,73,73	1.33	13 (18%)	82,113,113	1.27	9 (10%)
22	CLA	B	603	2	69,73,73	1.21	9 (13%)	82,113,113	1.41	14 (17%)
22	CLA	c	509	3	69,73,73	1.40	9 (13%)	82,113,113	1.43	11 (13%)
22	CLA	C	510	3	69,73,73	1.33	12 (17%)	82,113,113	1.56	10 (12%)
26	LMG	Y	101	-	48,48,55	1.08	7 (14%)	56,56,63	1.25	6 (10%)
22	CLA	D	405	4	69,73,73	1.68	11 (15%)	82,113,113	1.22	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMG	m	101	-	51,51,55	1.31	6 (11%)	59,59,63	1.39	8 (13%)
31	BCR	B	618	-	41,41,41	1.19	6 (14%)	56,56,56	1.32	6 (10%)
32	STE	M	102	-	14,14,19	0.86	0	14,14,19	0.93	0
22	CLA	C	512	3	69,73,73	1.29	7 (10%)	82,113,113	1.37	7 (8%)
22	CLA	b	613	2	69,73,73	1.45	11 (15%)	82,113,113	1.46	10 (12%)
23	PHO	A	404	-	58,69,69	1.77	11 (18%)	55,99,99	1.68	12 (21%)
29	DGD	c	516	-	63,63,67	1.30	8 (12%)	77,77,81	1.45	13 (16%)
31	BCR	x	101	-	41,41,41	1.10	3 (7%)	56,56,56	1.41	10 (17%)
32	STE	B	627	-	11,11,19	0.90	0	11,11,19	0.93	0
22	CLA	c	502	3	69,73,73	1.27	12 (17%)	82,113,113	1.40	13 (15%)
31	BCR	k	101	-	41,41,41	1.16	3 (7%)	56,56,56	1.08	3 (5%)
32	STE	C	519	-	15,15,19	0.52	0	14,14,19	0.66	0
28	LHG	d	408	-	48,48,48	0.73	1 (2%)	51,54,54	1.21	4 (7%)
31	BCR	c	515	-	41,41,41	1.20	6 (14%)	56,56,56	1.31	8 (14%)
32	STE	C	520	-	11,11,19	0.75	0	11,11,19	1.22	0
22	CLA	a	402	1	69,73,73	1.36	9 (13%)	82,113,113	1.53	9 (10%)
26	LMG	B	621	-	26,26,55	1.09	2 (7%)	26,26,63	1.08	1 (3%)
32	STE	b	620	-	15,15,19	0.46	0	14,14,19	0.80	0
22	CLA	B	615	2	69,73,73	1.20	9 (13%)	82,113,113	1.31	5 (6%)
22	CLA	C	511	3	69,73,73	1.44	9 (13%)	82,113,113	1.41	3 (3%)
28	LHG	L	102	-	48,48,48	0.84	2 (4%)	51,54,54	1.18	4 (7%)
28	LHG	d	409	-	38,38,48	0.93	2 (5%)	41,44,54	1.23	5 (12%)
28	LHG	e	101	-	41,41,48	1.05	3 (7%)	44,47,54	1.31	4 (9%)
31	BCR	B	619	-	41,41,41	1.28	3 (7%)	56,56,56	1.51	11 (19%)
22	CLA	B	608	2	69,73,73	1.59	10 (14%)	82,113,113	1.16	11 (13%)
22	CLA	c	503	3	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
22	CLA	C	504	37	63,67,73	1.27	8 (12%)	74,105,113	1.30	8 (10%)
22	CLA	b	606	2	69,73,73	1.50	9 (13%)	82,113,113	1.54	6 (7%)

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
32	STE	B	623	-	-	6/9/9/17	-
32	STE	R	101	-	-	4/9/9/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	511	3	-	14/39/115/115	-
22	CLA	b	615	2	-	11/39/115/115	-
32	STE	C	518	-	-	4/9/9/17	-
27	SQD	f	102	-	-	14/36/56/69	0/1/1/1
31	BCR	b	619	-	-	7/29/63/63	0/2/2/2
32	STE	b	627	-	-	7/11/11/17	-
22	CLA	d	405	4	-	11/39/115/115	-
22	CLA	c	513	3	-	9/39/115/115	-
31	BCR	a	405	-	-	3/29/63/63	0/2/2/2
22	CLA	A	402	1	-	5/39/115/115	-
31	BCR	K	101	-	-	12/29/63/63	0/2/2/2
31	BCR	Z	101	-	-	11/29/63/63	0/2/2/2
23	PHO	D	401	-	-	2/37/103/103	0/5/6/6
22	CLA	b	612	2	-	5/39/115/115	-
29	DGD	A	413	-	-	32/55/95/95	0/2/2/2
32	STE	X	101	-	-	13/17/17/17	-
32	STE	d	411	-	-	8/14/14/17	-
26	LMG	c	522	-	-	25/44/64/70	0/1/1/1
22	CLA	c	505	3	-	11/39/115/115	-
32	STE	t	104	-	-	3/7/7/17	-
22	CLA	B	609	2	-	6/39/115/115	-
31	BCR	b	618	-	-	1/29/63/63	0/2/2/2
31	BCR	I	101	-	-	5/29/63/63	0/2/2/2
22	CLA	a	404	1	-	8/39/115/115	-
32	STE	L	103	-	-	5/9/9/17	-
22	CLA	A	403	37	-	10/39/115/115	-
22	CLA	C	507	37	-	7/39/115/115	-
32	STE	d	412	-	-	9/17/17/17	-
26	LMG	A	409	-	-	18/43/63/70	0/1/1/1
22	CLA	b	602	2	-	13/39/115/115	-
31	BCR	b	617	-	-	9/29/63/63	0/2/2/2
22	CLA	b	614	2	-	16/39/115/115	-
27	SQD	A	412	-	-	19/39/39/69	-
32	STE	b	624	-	-	7/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	607	37	-	12/39/115/115	-
32	STE	Z	102	-	-	4/5/5/17	-
22	CLA	C	503	3	-	9/39/115/115	-
32	STE	c	520	-	-	7/17/17/17	-
26	LMG	c	521	-	-	22/43/63/70	0/1/1/1
29	DGD	C	515	-	-	23/51/91/95	0/2/2/2
31	BCR	H	101	-	-	10/29/63/63	0/2/2/2
23	PHO	a	403	-	-	4/37/103/103	0/5/6/6
22	CLA	C	501	3	-	2/39/115/115	-
29	DGD	h	101	-	-	17/51/91/95	0/2/2/2
32	STE	b	623	-	-	9/13/13/17	-
32	STE	I	102	-	-	4/12/12/17	-
27	SQD	a	411	-	-	21/49/69/69	0/1/1/1
28	LHG	l	101	-	-	16/53/53/53	-
26	LMG	M	101	-	-	20/46/66/70	0/1/1/1
22	CLA	B	605	2	-	13/39/115/115	-
22	CLA	B	613	2	-	11/39/115/115	-
22	CLA	b	605	2	-	15/39/115/115	-
22	CLA	c	512	3	-	20/39/115/115	-
22	CLA	b	604	2	-	10/39/115/115	-
22	CLA	B	610	37	-	10/39/115/115	-
22	CLA	b	609	2	-	14/39/115/115	-
32	STE	H	103	-	-	8/15/15/17	-
35	HEC	V	201	17	1/1/7/7	6/14/54/54	-
28	LHG	A	411	-	-	22/53/53/53	-
32	STE	b	626	-	-	4/7/7/17	-
26	LMG	d	410	-	-	10/39/59/70	0/1/1/1
32	STE	J	101	-	-	8/9/9/17	-
23	PHO	d	402	-	-	8/37/103/103	0/5/6/6
26	LMG	b	622	-	-	30/50/70/70	0/1/1/1
31	BCR	T	101	-	-	12/29/63/63	0/2/2/2
29	DGD	H	102	-	-	18/51/91/95	0/2/2/2
22	CLA	B	616	2	-	8/33/109/115	-
22	CLA	c	507	37	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	d	401	37	-	13/39/115/115	-
22	CLA	d	404	37	-	4/39/115/115	-
25	PL9	A	408	-	-	18/53/73/73	0/1/1/1
22	CLA	b	601	37	-	22/39/115/115	-
32	STE	l	102	-	-	7/15/15/17	-
27	SQD	t	102	-	-	15/37/37/69	-
32	STE	a	412	-	-	6/9/9/17	-
31	BCR	B	617	-	-	7/29/63/63	0/2/2/2
22	CLA	C	505	3	-	8/39/115/115	-
32	STE	t	103	-	-	4/11/11/17	-
27	SQD	L	101	-	-	29/44/64/69	0/1/1/1
26	LMG	B	626	-	-	35/50/70/70	0/1/1/1
32	STE	j	101	-	-	3/9/9/17	-
25	PL9	D	407	-	-	13/53/73/73	0/1/1/1
26	LMG	c	519	-	-	12/31/51/70	0/1/1/1
27	SQD	B	622	-	-	25/49/69/69	0/1/1/1
22	CLA	b	608	2	-	7/39/115/115	-
34	HEM	f	101	6,5	-	4/14/54/54	-
29	DGD	c	517	-	-	19/51/91/95	0/2/2/2
28	LHG	D	411	-	-	19/51/51/53	-
29	DGD	c	518	-	-	16/51/91/95	0/2/2/2
32	STE	a	413	-	-	8/12/12/17	-
31	BCR	c	514	-	-	8/29/63/63	0/2/2/2
22	CLA	C	509	3	-	15/39/115/115	-
22	CLA	B	614	2	-	19/39/115/115	-
22	CLA	B	602	2	-	9/39/115/115	-
35	HEC	v	201	17	1/1/7/7	6/14/54/54	-
22	CLA	d	403	4	-	11/39/115/115	-
22	CLA	b	616	2	-	10/33/109/115	-
32	STE	b	621	-	-	10/17/17/17	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
31	BCR	d	406	-	-	8/29/63/63	0/2/2/2
31	BCR	D	406	-	-	7/29/63/63	0/2/2/2
22	CLA	D	404	37	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	c	506	3	-	13/39/115/115	-
22	CLA	c	510	3	-	14/39/115/115	-
32	STE	B	620	-	-	5/14/14/17	-
32	STE	b	625	-	-	9/17/17/17	-
32	STE	x	102	-	-	13/17/17/17	-
32	STE	M	103	-	-	2/7/7/17	-
29	DGD	C	516	-	-	25/51/91/95	0/2/2/2
31	BCR	k	102	-	-	3/29/63/63	0/2/2/2
22	CLA	B	601	37	-	16/39/115/115	-
25	PL9	a	409	-	-	28/53/73/73	0/1/1/1
32	STE	B	624	-	-	11/15/15/17	-
27	SQD	D	409	-	-	13/28/48/69	0/1/1/1
22	CLA	b	603	2	-	10/39/115/115	-
31	BCR	C	514	-	-	6/29/63/63	0/2/2/2
28	LHG	a	410	-	-	21/53/53/53	-
22	CLA	A	405	1	-	5/26/102/115	-
34	HEM	F	101	6,5	-	3/14/54/54	-
22	CLA	B	604	2	-	14/39/115/115	-
26	LMG	D	412	-	-	19/33/33/70	-
32	STE	B	625	-	-	7/13/13/17	-
22	CLA	C	506	3	-	20/39/115/115	-
22	CLA	c	504	37	-	4/33/109/115	-
22	CLA	C	502	3	-	11/39/115/115	-
28	LHG	D	413	-	-	20/53/53/53	-
22	CLA	B	611	2	-	6/39/115/115	-
22	CLA	B	606	2	-	12/39/115/115	-
22	CLA	B	612	2	-	9/39/115/115	-
22	CLA	D	403	4	-	6/39/115/115	-
28	LHG	D	410	-	-	23/53/53/53	-
22	CLA	c	508	3	-	10/38/114/115	-
22	CLA	C	508	3	-	8/39/115/115	-
32	STE	c	523	-	-	6/9/9/17	-
22	CLA	C	513	3	-	9/39/115/115	-
26	LMG	D	408	-	-	15/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SQD	A	410	-	-	20/47/67/69	0/1/1/1
29	DGD	C	517	-	-	14/51/91/95	0/2/2/2
22	CLA	c	501	3	-	10/39/115/115	-
31	BCR	K	102	-	-	9/29/63/63	0/2/2/2
22	CLA	b	610	37	-	6/39/115/115	-
25	PL9	d	407	-	-	16/53/73/73	0/1/1/1
22	CLA	b	611	2	-	8/39/115/115	-
22	CLA	b	607	37	-	15/39/115/115	-
22	CLA	B	603	2	-	16/39/115/115	-
22	CLA	c	509	3	-	8/39/115/115	-
22	CLA	C	510	3	-	8/39/115/115	-
26	LMG	Y	101	-	-	22/43/63/70	0/1/1/1
22	CLA	D	405	4	-	13/39/115/115	-
26	LMG	m	101	-	-	24/46/66/70	0/1/1/1
31	BCR	B	618	-	-	10/29/63/63	0/2/2/2
32	STE	M	102	-	-	6/12/12/17	-
22	CLA	C	512	3	-	14/39/115/115	-
22	CLA	b	613	2	-	10/39/115/115	-
23	PHO	A	404	-	-	7/37/103/103	0/5/6/6
29	DGD	c	516	-	-	20/51/91/95	0/2/2/2
31	BCR	x	101	-	-	6/29/63/63	0/2/2/2
32	STE	B	627	-	-	6/9/9/17	-
22	CLA	c	502	3	-	10/39/115/115	-
31	BCR	k	101	-	-	12/29/63/63	0/2/2/2
32	STE	C	519	-	-	5/13/13/17	-
28	LHG	d	408	-	-	24/53/53/53	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
32	STE	C	520	-	-	4/9/9/17	-
22	CLA	a	402	1	-	2/39/115/115	-
26	LMG	B	621	-	-	12/22/22/70	-
32	STE	b	620	-	-	7/13/13/17	-
22	CLA	B	615	2	-	8/39/115/115	-
22	CLA	C	511	3	-	6/39/115/115	-
28	LHG	L	102	-	-	23/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	409	-	-	10/43/43/53	-
28	LHG	e	101	-	-	24/46/46/53	-
31	BCR	B	619	-	-	6/29/63/63	0/2/2/2
22	CLA	B	608	2	-	11/39/115/115	-
22	CLA	c	503	3	-	7/39/115/115	-
22	CLA	C	504	37	-	8/32/108/115	-
22	CLA	b	606	2	-	5/39/115/115	-

All (971) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	MG-ND	-10.84	1.84	2.05
22	b	610	CLA	MG-NB	-10.06	1.85	2.05
22	B	606	CLA	MG-NA	9.77	2.29	2.06
23	d	402	PHO	C1B-C2B	9.34	1.49	1.39
22	C	502	CLA	MG-NB	-8.85	1.88	2.05
23	D	401	PHO	C3B-C4B	8.75	1.50	1.41
22	b	615	CLA	MG-ND	-8.40	1.89	2.05
23	d	402	PHO	C3B-C4B	8.37	1.50	1.41
23	a	403	PHO	C1B-C2B	8.27	1.48	1.39
23	D	401	PHO	C1B-C2B	8.18	1.48	1.39
22	c	507	CLA	MG-NB	-7.76	1.90	2.05
22	C	506	CLA	MG-ND	-7.73	1.90	2.05
22	b	606	CLA	MG-NA	7.55	2.24	2.06
23	a	403	PHO	C3B-C4B	7.49	1.49	1.41
25	A	408	PL9	C7-C3	-7.48	1.41	1.51
22	B	616	CLA	MG-NC	7.40	2.23	2.06
22	B	601	CLA	MG-NA	7.27	2.23	2.06
22	D	404	CLA	MG-NA	7.24	2.23	2.06
22	B	608	CLA	MG-NA	7.11	2.23	2.06
35	v	201	HEC	C3D-C2D	6.91	1.51	1.36
22	d	404	CLA	MG-NA	6.77	2.22	2.06
22	b	615	CLA	MG-NA	6.77	2.22	2.06
22	C	501	CLA	MG-NB	-6.71	1.92	2.05
23	A	404	PHO	C1B-C2B	6.23	1.46	1.39
35	V	201	HEC	FE-ND	6.23	2.14	1.94
22	C	501	CLA	MG-NA	6.21	2.21	2.06
22	c	507	CLA	MG-NA	6.17	2.20	2.06
22	D	405	CLA	MG-NB	-6.14	1.93	2.05
23	A	404	PHO	C3B-C4B	6.13	1.47	1.41
22	c	501	CLA	MG-NB	-6.12	1.93	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	MG-ND	-6.00	1.93	2.05
22	b	609	CLA	MG-NC	5.93	2.20	2.06
31	b	618	BCR	C30-C25	-5.89	1.46	1.53
22	d	405	CLA	MG-NA	5.88	2.20	2.06
22	B	611	CLA	MG-NA	5.84	2.20	2.06
35	V	201	HEC	C3D-C2D	5.80	1.49	1.36
22	b	603	CLA	MG-NA	5.55	2.19	2.06
22	B	608	CLA	MG-NC	-5.50	1.93	2.06
29	c	516	DGD	O5D-C6D	-5.44	1.34	1.43
22	C	511	CLA	MG-NA	5.41	2.19	2.06
22	b	613	CLA	MG-NB	-5.38	1.95	2.05
22	c	511	CLA	MG-NA	5.36	2.19	2.06
22	c	509	CLA	MG-NC	-5.28	1.93	2.06
31	C	514	BCR	C1-C6	-5.26	1.47	1.53
22	D	405	CLA	MG-NC	5.17	2.18	2.06
22	a	402	CLA	MG-NA	5.17	2.18	2.06
29	C	515	DGD	O5D-C6D	-5.16	1.34	1.43
22	D	405	CLA	MG-ND	-5.08	1.95	2.05
22	a	404	CLA	MG-ND	-5.08	1.95	2.05
22	A	403	CLA	C4B-NB	5.07	1.44	1.37
26	m	101	LMG	C4-C3	5.07	1.65	1.52
22	c	513	CLA	MG-ND	-5.01	1.95	2.05
26	A	409	LMG	O1-C7	-4.96	1.35	1.43
22	c	507	CLA	MG-NC	-4.89	1.94	2.06
25	d	407	PL9	C3-C4	-4.88	1.41	1.49
23	d	402	PHO	C1D-C2D	4.86	1.44	1.39
22	C	503	CLA	MG-NC	4.84	2.17	2.06
31	K	101	BCR	C30-C25	-4.84	1.47	1.53
22	B	607	CLA	MG-NA	4.82	2.17	2.06
34	F	101	HEM	FE-NB	4.80	2.09	1.94
22	C	507	CLA	C1B-NB	-4.74	1.31	1.37
22	D	405	CLA	C1D-ND	4.68	1.44	1.37
22	C	508	CLA	MG-ND	4.66	2.15	2.05
22	B	602	CLA	C1D-ND	4.62	1.43	1.37
22	b	601	CLA	MG-NA	4.61	2.17	2.06
22	B	606	CLA	MG-NC	-4.58	1.95	2.06
25	d	407	PL9	C53-C6	-4.55	1.41	1.50
22	C	512	CLA	MG-NA	4.52	2.17	2.06
22	B	604	CLA	MG-NA	4.46	2.16	2.06
22	b	614	CLA	MG-NC	4.42	2.16	2.06
25	A	408	PL9	C3-C4	-4.41	1.42	1.49
22	C	508	CLA	MG-NA	4.39	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	MG-NC	4.32	2.16	2.06
22	b	601	CLA	MG-NC	-4.30	1.96	2.06
22	a	404	CLA	C1D-ND	4.29	1.43	1.37
22	C	509	CLA	MG-NA	4.28	2.16	2.06
31	H	101	BCR	C30-C25	-4.28	1.48	1.53
22	B	614	CLA	C4B-NB	4.23	1.43	1.37
31	D	406	BCR	C30-C25	-4.23	1.48	1.53
22	c	509	CLA	MG-NB	-4.18	1.97	2.05
22	b	615	CLA	MG-NB	4.18	2.14	2.05
26	B	626	LMG	C4-C5	4.17	1.61	1.53
22	b	614	CLA	MG-ND	4.17	2.14	2.05
31	K	101	BCR	C1-C6	-4.15	1.48	1.53
22	b	612	CLA	MG-NC	4.15	2.16	2.06
22	b	609	CLA	MG-ND	-4.15	1.97	2.05
22	C	513	CLA	C1D-ND	4.14	1.43	1.37
31	b	619	BCR	C1-C6	-4.13	1.48	1.53
31	b	617	BCR	C1-C6	-4.13	1.48	1.53
22	d	405	CLA	MG-NC	-4.13	1.96	2.06
22	c	501	CLA	MG-NA	4.12	2.16	2.06
22	B	607	CLA	MG-NC	-4.11	1.96	2.06
26	d	410	LMG	C4-C5	4.11	1.61	1.53
22	A	402	CLA	C4B-NB	4.11	1.43	1.37
22	b	602	CLA	MG-NA	4.10	2.16	2.06
22	b	613	CLA	MG-NC	4.10	2.16	2.06
25	D	407	PL9	C52-C5	-4.09	1.42	1.50
31	t	101	BCR	C30-C25	-4.08	1.48	1.53
22	c	509	CLA	MG-ND	4.08	2.13	2.05
22	C	510	CLA	MG-NB	4.08	2.13	2.05
31	k	102	BCR	C30-C25	-4.08	1.48	1.53
22	B	607	CLA	MG-NB	-4.07	1.97	2.05
31	c	514	BCR	C1-C6	-4.07	1.48	1.53
25	A	408	PL9	C7-C8	-4.05	1.44	1.50
31	k	101	BCR	C30-C25	-4.05	1.48	1.53
22	C	511	CLA	MG-NB	-4.04	1.97	2.05
22	c	512	CLA	C4B-NB	4.04	1.43	1.37
22	b	607	CLA	MG-NB	-4.02	1.97	2.05
31	a	405	BCR	C30-C25	-3.99	1.48	1.53
22	C	512	CLA	MG-NB	3.96	2.13	2.05
22	b	609	CLA	C1D-ND	3.93	1.43	1.37
23	D	401	PHO	C4D-ND	-3.89	1.32	1.38
22	b	602	CLA	C1D-ND	3.89	1.43	1.37
22	B	604	CLA	MG-ND	-3.87	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	413	LHG	O7-C5	-3.86	1.37	1.46
26	m	101	LMG	O1-C7	-3.86	1.37	1.43
22	B	602	CLA	MG-NB	-3.84	1.98	2.05
31	b	618	BCR	C1-C6	-3.83	1.48	1.53
22	C	505	CLA	CHC-C1C	3.82	1.46	1.38
29	A	413	DGD	C4D-C5D	3.81	1.61	1.53
22	d	403	CLA	C1D-ND	3.80	1.42	1.37
31	Z	101	BCR	C30-C25	-3.80	1.48	1.53
31	B	619	BCR	C1-C6	-3.78	1.48	1.53
31	T	101	BCR	C30-C25	-3.78	1.48	1.53
22	B	604	CLA	C1D-ND	3.77	1.42	1.37
22	C	501	CLA	C1D-ND	3.77	1.42	1.37
22	b	610	CLA	MG-ND	3.77	2.13	2.05
22	B	611	CLA	MG-ND	3.77	2.13	2.05
22	c	506	CLA	C1D-ND	3.76	1.42	1.37
26	c	519	LMG	C4-C5	3.76	1.61	1.53
22	B	604	CLA	MG-NC	3.76	2.15	2.06
22	d	405	CLA	MG-NB	-3.75	1.98	2.05
22	B	602	CLA	C4B-NB	3.75	1.42	1.37
26	d	410	LMG	O1-C7	-3.74	1.37	1.43
22	b	602	CLA	MG-NB	-3.71	1.98	2.05
22	B	612	CLA	MG-NA	3.70	2.15	2.06
22	b	615	CLA	C1D-ND	3.70	1.42	1.37
22	B	613	CLA	C4B-NB	3.70	1.42	1.37
22	B	610	CLA	MG-NA	3.69	2.15	2.06
22	D	404	CLA	C1D-ND	3.68	1.42	1.37
22	c	503	CLA	MG-NA	3.68	2.15	2.06
22	b	610	CLA	MG-NC	-3.68	1.97	2.06
22	c	511	CLA	C1B-C2B	3.68	1.51	1.43
29	A	413	DGD	C4E-C5E	3.67	1.60	1.53
27	a	411	SQD	O48-C23	3.65	1.44	1.33
25	a	409	PL9	C53-C6	-3.64	1.43	1.50
27	t	102	SQD	O47-C7	3.64	1.44	1.34
22	c	506	CLA	MG-NA	3.64	2.14	2.06
22	B	610	CLA	C1D-ND	3.64	1.42	1.37
22	c	510	CLA	C1D-ND	3.63	1.42	1.37
31	I	101	BCR	C1-C6	-3.62	1.49	1.53
22	b	613	CLA	MG-ND	3.62	2.13	2.05
27	L	101	SQD	O48-C23	3.62	1.43	1.33
22	c	512	CLA	MG-NC	3.61	2.14	2.06
27	A	412	SQD	O47-C7	3.60	1.44	1.34
26	Y	101	LMG	C4-C5	3.60	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	522	LMG	C3-C2	3.60	1.61	1.52
26	D	412	LMG	C7-C8	3.60	1.59	1.51
22	b	612	CLA	MG-ND	-3.59	1.98	2.05
22	b	609	CLA	C4B-NB	3.59	1.42	1.37
23	A	404	PHO	C4D-CHA	3.58	1.44	1.39
22	A	403	CLA	C1B-C2B	3.58	1.51	1.43
22	b	611	CLA	MG-NA	3.57	2.14	2.06
22	c	512	CLA	MG-ND	3.57	2.12	2.05
27	B	622	SQD	O47-C7	3.57	1.44	1.34
27	A	412	SQD	O48-C23	3.56	1.43	1.33
28	D	411	LHG	P-O6	3.56	1.73	1.59
23	a	403	PHO	C1D-C2D	3.56	1.43	1.39
22	B	609	CLA	MG-NB	-3.56	1.98	2.05
26	b	622	LMG	O1-C7	-3.55	1.37	1.43
25	D	407	PL9	C6-C1	-3.54	1.42	1.48
31	c	515	BCR	C1-C6	-3.54	1.49	1.53
22	B	615	CLA	CMB-C2B	-3.52	1.43	1.50
26	B	621	LMG	O8-C28	3.51	1.42	1.30
31	Z	101	BCR	C1-C6	-3.51	1.49	1.53
26	c	522	LMG	C1-C2	3.50	1.62	1.52
31	d	406	BCR	C30-C25	-3.50	1.49	1.53
27	A	410	SQD	O47-C7	3.50	1.44	1.34
22	c	511	CLA	C1D-ND	3.49	1.42	1.37
22	c	507	CLA	MG-ND	3.48	2.12	2.05
27	A	410	SQD	O48-C23	3.47	1.43	1.33
22	B	616	CLA	C1D-ND	3.47	1.42	1.37
31	c	514	BCR	C30-C25	-3.47	1.49	1.53
22	c	511	CLA	C4B-NB	3.46	1.42	1.37
22	A	403	CLA	MG-NA	3.44	2.14	2.06
22	b	614	CLA	C1B-NB	-3.44	1.33	1.37
22	b	612	CLA	C1D-ND	3.43	1.42	1.37
22	a	402	CLA	C1B-C2B	3.43	1.51	1.43
25	D	407	PL9	C11-C9	-3.42	1.44	1.51
35	V	201	HEC	FE-NA	3.42	2.06	1.95
29	C	517	DGD	O1G-C1G	-3.42	1.37	1.45
22	b	605	CLA	CMC-C2C	-3.42	1.43	1.50
31	D	406	BCR	C1-C6	-3.42	1.49	1.53
23	D	401	PHO	CAC-C3C	-3.40	1.45	1.51
29	C	515	DGD	O1G-C1A	3.40	1.43	1.33
31	x	101	BCR	C30-C25	-3.39	1.49	1.53
27	B	622	SQD	O48-C23	3.38	1.43	1.33
31	B	617	BCR	C30-C25	-3.38	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	604	CLA	MG-NC	3.38	2.14	2.06
22	A	402	CLA	C1B-C2B	3.37	1.51	1.43
23	D	401	PHO	CMD-C2D	-3.36	1.44	1.51
22	B	602	CLA	C1B-C2B	3.36	1.51	1.43
31	d	406	BCR	C1-C6	-3.36	1.49	1.53
22	d	404	CLA	C4B-NB	3.36	1.42	1.37
22	c	502	CLA	MG-NC	-3.35	1.98	2.06
29	H	102	DGD	C1E-C2E	3.35	1.62	1.52
22	d	405	CLA	C1D-ND	3.35	1.42	1.37
23	A	404	PHO	C4D-ND	-3.34	1.33	1.38
29	H	102	DGD	C6D-C5D	3.33	1.61	1.51
22	B	609	CLA	CMD-C2D	-3.31	1.44	1.50
29	h	101	DGD	O5D-C6D	-3.31	1.38	1.43
29	H	102	DGD	O2D-C2D	-3.31	1.34	1.43
31	B	617	BCR	C1-C6	-3.31	1.49	1.53
26	c	521	LMG	O1-C1	3.30	1.45	1.40
22	C	504	CLA	C1B-NB	-3.30	1.33	1.37
26	d	410	LMG	O7-C8	-3.30	1.38	1.46
29	C	517	DGD	O3G-C3G	-3.30	1.38	1.43
22	c	508	CLA	C1D-ND	3.29	1.42	1.37
22	B	608	CLA	MG-ND	3.27	2.12	2.05
23	A	404	PHO	CMD-C2D	-3.26	1.45	1.51
22	b	611	CLA	C1B-C2B	3.25	1.50	1.43
22	C	513	CLA	MG-NB	-3.24	1.99	2.05
22	c	501	CLA	C1D-ND	3.24	1.42	1.37
26	b	622	LMG	C4-C3	3.22	1.60	1.52
25	A	408	PL9	C6-C1	-3.21	1.43	1.48
22	B	603	CLA	MG-NA	3.21	2.13	2.06
22	b	606	CLA	C1D-ND	3.21	1.42	1.37
22	B	601	CLA	C1D-ND	3.21	1.42	1.37
22	B	613	CLA	C1D-ND	3.21	1.42	1.37
35	v	201	HEC	FE-NC	3.21	2.05	1.95
34	F	101	HEM	CAB-C3B	3.20	1.55	1.47
22	b	606	CLA	C4B-NB	3.20	1.42	1.37
22	b	608	CLA	CHC-C1C	3.20	1.44	1.38
22	c	511	CLA	MG-ND	-3.20	1.99	2.05
22	B	604	CLA	MG-NB	3.19	2.12	2.05
22	d	403	CLA	C1B-NB	-3.18	1.33	1.37
22	C	505	CLA	MG-NC	3.18	2.13	2.06
27	D	409	SQD	O48-C23	3.16	1.42	1.33
22	A	402	CLA	MG-NC	-3.16	1.98	2.06
22	b	615	CLA	C4B-NB	3.16	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	410	LHG	O7-C5	-3.16	1.39	1.46
22	C	507	CLA	C1D-ND	3.16	1.42	1.37
22	B	613	CLA	CMD-C2D	-3.15	1.44	1.50
22	B	616	CLA	MG-ND	3.15	2.12	2.05
27	t	102	SQD	O48-C23	3.15	1.42	1.33
23	d	402	PHO	CMC-C2C	-3.15	1.45	1.50
22	c	501	CLA	CMC-C2C	-3.15	1.44	1.50
31	t	101	BCR	C1-C6	-3.15	1.49	1.53
22	B	610	CLA	MG-ND	-3.15	1.99	2.05
22	c	513	CLA	C4B-NB	3.14	1.42	1.37
22	B	611	CLA	C1B-NB	-3.14	1.33	1.37
22	b	602	CLA	CMD-C2D	-3.13	1.44	1.50
22	A	403	CLA	C1D-ND	3.12	1.42	1.37
22	C	506	CLA	C1D-ND	3.12	1.42	1.37
29	H	102	DGD	O5D-C1E	3.12	1.45	1.40
29	C	517	DGD	O2G-C2G	-3.12	1.39	1.46
22	C	510	CLA	MG-NA	3.12	2.13	2.06
22	b	604	CLA	C1B-NB	-3.12	1.33	1.37
26	M	101	LMG	C1-C2	3.11	1.61	1.52
22	C	502	CLA	MG-NA	3.11	2.13	2.06
22	c	503	CLA	C1D-ND	3.10	1.41	1.37
31	K	102	BCR	C30-C25	-3.10	1.49	1.53
29	C	516	DGD	C1E-C2E	3.10	1.61	1.52
29	h	101	DGD	O5D-C1E	3.10	1.45	1.40
29	c	516	DGD	O2G-C2G	-3.09	1.39	1.46
35	v	201	HEC	FE-NB	3.09	2.04	1.94
22	D	404	CLA	MG-ND	3.08	2.11	2.05
22	c	512	CLA	CHC-C1C	3.08	1.44	1.38
27	L	101	SQD	O47-C7	3.08	1.43	1.34
22	B	606	CLA	MG-NB	3.08	2.11	2.05
29	C	516	DGD	O3G-C3G	-3.08	1.38	1.43
22	c	509	CLA	C1B-C2B	3.07	1.50	1.43
23	d	402	PHO	CAC-C3C	-3.06	1.46	1.51
22	B	602	CLA	CMB-C2B	-3.06	1.44	1.50
22	D	403	CLA	MG-NA	3.06	2.13	2.06
31	b	619	BCR	C30-C25	-3.05	1.49	1.53
26	c	519	LMG	C1-C2	3.05	1.61	1.52
22	C	503	CLA	MG-NA	3.05	2.13	2.06
22	b	611	CLA	CMD-C2D	-3.04	1.44	1.50
29	A	413	DGD	O5D-C6D	-3.03	1.38	1.43
22	a	404	CLA	C1B-C2B	3.03	1.50	1.43
22	b	601	CLA	C1B-C2B	3.03	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	502	CLA	C1D-ND	3.02	1.41	1.37
22	C	506	CLA	MG-NB	3.02	2.11	2.05
22	a	402	CLA	MG-NB	3.02	2.11	2.05
26	c	522	LMG	C4-C5	3.02	1.59	1.53
22	B	610	CLA	MG-NB	3.02	2.11	2.05
31	K	102	BCR	C1-C6	-3.02	1.49	1.53
29	c	518	DGD	O4E-C4E	-3.02	1.35	1.43
22	B	609	CLA	MG-ND	3.01	2.11	2.05
22	d	405	CLA	CMD-C2D	-3.01	1.44	1.50
22	b	610	CLA	CHC-C4B	-2.99	1.32	1.39
22	A	403	CLA	MG-NB	-2.98	1.99	2.05
22	B	611	CLA	CMD-C2D	-2.98	1.44	1.50
23	a	403	PHO	C3D-C4D	2.97	1.45	1.41
22	C	505	CLA	C1B-NB	-2.97	1.34	1.37
22	b	612	CLA	CMB-C2B	-2.97	1.44	1.50
22	c	504	CLA	MG-ND	-2.97	1.99	2.05
27	f	102	SQD	O48-C23	2.97	1.42	1.33
22	B	607	CLA	C1B-C2B	2.97	1.50	1.43
28	D	410	LHG	O8-C6	-2.96	1.38	1.45
22	B	610	CLA	CMB-C2B	-2.96	1.44	1.50
22	B	616	CLA	CMD-C2D	-2.96	1.44	1.50
29	H	102	DGD	C4E-C5E	2.96	1.59	1.53
22	C	511	CLA	C1B-C2B	2.96	1.50	1.43
22	B	612	CLA	C1D-ND	2.95	1.41	1.37
29	c	518	DGD	C2A-C1A	-2.94	1.42	1.50
31	a	405	BCR	C1-C6	-2.94	1.50	1.53
22	D	405	CLA	CMD-C2D	-2.94	1.44	1.50
22	B	605	CLA	C1B-NB	-2.93	1.34	1.37
22	C	506	CLA	MG-NC	2.93	2.13	2.06
28	L	102	LHG	O7-C5	-2.93	1.39	1.46
27	f	102	SQD	O47-C7	2.93	1.42	1.34
22	C	504	CLA	C4B-NB	2.93	1.41	1.37
22	B	616	CLA	MG-NB	-2.93	2.00	2.05
26	c	519	LMG	C7-C8	2.93	1.60	1.50
22	C	503	CLA	C1B-C2B	2.93	1.50	1.43
22	C	504	CLA	C1D-ND	2.92	1.41	1.37
22	b	603	CLA	CMC-C2C	-2.92	1.44	1.50
22	c	512	CLA	C1D-ND	2.91	1.41	1.37
22	C	509	CLA	CMD-C2D	-2.91	1.44	1.50
22	c	513	CLA	CMD-C2D	-2.91	1.44	1.50
25	d	407	PL9	C16-C14	-2.91	1.45	1.51
22	d	401	CLA	CMD-C2D	-2.91	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	409	LMG	C4-C3	2.91	1.59	1.52
29	c	516	DGD	C4D-C3D	2.90	1.59	1.52
26	c	521	LMG	C3-C2	2.90	1.59	1.52
22	C	501	CLA	MG-ND	2.90	2.11	2.05
29	C	516	DGD	C6D-C5D	2.90	1.60	1.51
22	B	608	CLA	MG-NB	-2.89	2.00	2.05
22	b	615	CLA	CMD-C2D	-2.89	1.44	1.50
22	B	603	CLA	C1B-C2B	2.89	1.49	1.43
27	a	411	SQD	O47-C7	2.89	1.42	1.34
29	C	516	DGD	C4D-C3D	2.89	1.59	1.52
22	A	405	CLA	C1B-C2B	2.88	1.49	1.43
22	b	604	CLA	C1D-ND	2.88	1.41	1.37
31	k	102	BCR	C1-C6	-2.88	1.50	1.53
25	d	407	PL9	C7-C8	-2.87	1.46	1.50
22	D	403	CLA	C1D-ND	2.87	1.41	1.37
23	a	403	PHO	CMB-C2B	-2.87	1.45	1.51
31	B	617	BCR	C33-C5	-2.87	1.46	1.50
22	c	513	CLA	C1B-C2B	2.86	1.49	1.43
22	B	615	CLA	C4B-NB	2.86	1.41	1.37
22	a	404	CLA	C1B-NB	-2.86	1.34	1.37
22	c	505	CLA	C4B-NB	2.85	1.41	1.37
22	c	507	CLA	C1B-C2B	2.85	1.49	1.43
22	d	403	CLA	C1B-C2B	2.85	1.49	1.43
26	c	519	LMG	C3-C2	2.84	1.59	1.52
22	d	404	CLA	C1B-C2B	2.84	1.49	1.43
22	C	503	CLA	C1D-ND	2.84	1.41	1.37
31	I	101	BCR	C33-C5	-2.84	1.46	1.50
22	B	607	CLA	C1D-ND	2.84	1.41	1.37
26	m	101	LMG	C1-C2	2.83	1.60	1.52
31	B	618	BCR	C30-C25	-2.83	1.50	1.53
26	b	622	LMG	O8-C28	2.82	1.41	1.33
28	l	101	LHG	O7-C5	-2.81	1.40	1.46
22	C	513	CLA	C3B-C4B	2.81	1.50	1.42
22	d	403	CLA	CMB-C2B	-2.81	1.45	1.50
22	B	614	CLA	C1D-ND	2.81	1.41	1.37
22	b	616	CLA	C1D-ND	2.81	1.41	1.37
29	C	515	DGD	C3G-C2G	2.80	1.59	1.50
22	b	615	CLA	C3B-C4B	2.80	1.50	1.42
22	B	606	CLA	C1B-C2B	2.79	1.49	1.43
22	C	513	CLA	C4B-NB	2.79	1.41	1.37
22	B	610	CLA	C3B-C4B	2.79	1.50	1.42
22	d	401	CLA	C4B-NB	2.79	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	405	CLA	C1D-ND	2.79	1.41	1.37
25	D	407	PL9	C26-C24	-2.79	1.45	1.51
22	b	602	CLA	C4B-NB	2.79	1.41	1.37
22	C	511	CLA	C3B-C4B	2.78	1.50	1.42
22	B	601	CLA	C1B-C2B	2.78	1.49	1.43
28	D	411	LHG	O3-C3	-2.78	1.34	1.44
22	c	510	CLA	CMB-C2B	-2.78	1.45	1.50
22	C	509	CLA	MG-NC	-2.77	1.99	2.06
22	b	613	CLA	C1D-ND	2.77	1.41	1.37
22	c	504	CLA	C1B-C2B	2.77	1.49	1.43
28	e	101	LHG	P-O6	2.77	1.70	1.59
26	B	626	LMG	C3-C2	2.76	1.59	1.52
22	c	501	CLA	C4B-NB	2.76	1.41	1.37
22	B	606	CLA	MG-ND	-2.76	2.00	2.05
22	C	510	CLA	C1B-NB	-2.76	1.34	1.37
29	C	516	DGD	O2G-C2G	-2.76	1.40	1.46
22	b	616	CLA	CMD-C2D	-2.76	1.45	1.50
22	c	508	CLA	C1B-NB	-2.75	1.34	1.37
22	b	612	CLA	C3B-C4B	2.75	1.50	1.42
22	b	614	CLA	CHC-C1C	2.75	1.44	1.38
22	b	614	CLA	MG-NB	-2.75	2.00	2.05
22	A	405	CLA	C4B-NB	2.75	1.41	1.37
25	a	409	PL9	C3-C4	-2.75	1.45	1.49
22	C	504	CLA	MG-ND	-2.75	2.00	2.05
22	B	605	CLA	C1B-C2B	2.74	1.49	1.43
26	b	622	LMG	C3-C2	2.74	1.59	1.52
22	B	601	CLA	CHC-C1C	2.74	1.44	1.38
22	B	602	CLA	MG-NA	2.74	2.12	2.06
28	l	101	LHG	P-O6	2.74	1.70	1.59
22	b	605	CLA	C1D-ND	2.74	1.41	1.37
22	A	403	CLA	CMD-C2D	-2.73	1.45	1.50
22	c	510	CLA	C1B-NB	-2.73	1.34	1.37
22	A	405	CLA	MG-NB	-2.73	2.00	2.05
22	C	509	CLA	C1D-ND	2.73	1.41	1.37
22	b	603	CLA	CMD-C2D	-2.73	1.45	1.50
22	B	610	CLA	MG-NC	-2.73	1.99	2.06
22	c	505	CLA	MG-NC	-2.73	1.99	2.06
22	c	504	CLA	C4B-NB	2.72	1.41	1.37
22	b	612	CLA	C4B-NB	2.72	1.41	1.37
22	b	611	CLA	C4B-NB	2.72	1.41	1.37
22	B	604	CLA	C3B-C4B	2.72	1.50	1.42
29	A	413	DGD	C3G-C2G	2.72	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	412	LMG	C9-C8	2.72	1.59	1.50
22	b	614	CLA	C4B-NB	2.72	1.41	1.37
22	C	505	CLA	CMB-C2B	-2.72	1.45	1.50
34	f	101	HEM	C3B-C2B	-2.71	1.31	1.37
22	B	612	CLA	C1B-C2B	2.71	1.49	1.43
29	c	518	DGD	O2E-C2E	-2.71	1.36	1.43
22	c	506	CLA	MG-NB	2.71	2.11	2.05
26	Y	101	LMG	O7-C8	-2.71	1.40	1.46
22	c	513	CLA	C1D-ND	2.70	1.41	1.37
22	c	504	CLA	CMD-C2D	-2.70	1.45	1.50
34	F	101	HEM	CAC-C3C	2.70	1.54	1.47
28	e	101	LHG	O8-C23	2.70	1.41	1.33
29	h	101	DGD	C4D-C3D	2.70	1.59	1.52
22	d	404	CLA	CMB-C2B	-2.69	1.45	1.50
22	c	501	CLA	C1B-C2B	2.69	1.49	1.43
31	B	619	BCR	C30-C25	-2.69	1.50	1.53
22	C	510	CLA	C1B-C2B	2.68	1.49	1.43
22	C	501	CLA	CMD-C2D	-2.68	1.45	1.50
27	D	409	SQD	O2-C2	-2.68	1.36	1.43
28	A	411	LHG	P-O6	2.68	1.69	1.59
22	b	605	CLA	CMD-C2D	-2.67	1.45	1.50
22	C	505	CLA	C4B-NB	2.67	1.41	1.37
22	c	502	CLA	CMD-C2D	-2.67	1.45	1.50
28	d	409	LHG	P-O6	2.67	1.69	1.59
31	b	618	BCR	C33-C5	-2.67	1.46	1.50
26	m	101	LMG	O4-C4	-2.67	1.36	1.43
22	d	401	CLA	CHC-C1C	2.67	1.43	1.38
29	C	515	DGD	C4E-C3E	2.67	1.59	1.52
22	c	507	CLA	C1D-ND	2.66	1.41	1.37
23	d	402	PHO	C4D-ND	-2.66	1.34	1.38
22	c	506	CLA	CMB-C2B	-2.66	1.45	1.50
22	B	609	CLA	C1B-C2B	2.66	1.49	1.43
34	f	101	HEM	FE-ND	2.66	2.03	1.94
22	B	612	CLA	C1C-NC	-2.66	1.33	1.37
22	B	610	CLA	C1B-C2B	2.66	1.49	1.43
28	D	410	LHG	O7-C5	-2.65	1.40	1.46
22	B	612	CLA	C3B-C4B	2.65	1.50	1.42
22	C	511	CLA	C1D-ND	2.64	1.41	1.37
25	d	407	PL9	C40-C39	-2.64	1.44	1.50
22	b	601	CLA	C1D-ND	2.64	1.41	1.37
22	a	402	CLA	CMB-C2B	-2.64	1.45	1.50
22	B	611	CLA	MG-NC	-2.64	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	512	CLA	C1B-C2B	2.64	1.49	1.43
22	b	614	CLA	C1D-ND	2.64	1.41	1.37
22	b	603	CLA	CMB-C2B	-2.64	1.45	1.50
22	D	405	CLA	CMB-C2B	-2.64	1.45	1.50
22	b	613	CLA	C4B-NB	2.64	1.41	1.37
22	b	615	CLA	C1B-C2B	2.64	1.49	1.43
22	b	601	CLA	C4B-NB	2.64	1.41	1.37
22	b	607	CLA	C1B-NB	-2.63	1.34	1.37
22	C	506	CLA	C4B-NB	2.63	1.41	1.37
22	b	606	CLA	C3B-C4B	2.63	1.50	1.42
22	d	401	CLA	C1B-C2B	2.63	1.49	1.43
22	c	501	CLA	CMB-C2B	-2.62	1.45	1.50
22	b	604	CLA	C4B-NB	2.61	1.41	1.37
31	b	617	BCR	C30-C25	-2.61	1.50	1.53
29	C	517	DGD	O2D-C2D	-2.61	1.36	1.43
22	B	601	CLA	MG-ND	-2.61	2.00	2.05
22	b	607	CLA	C1D-ND	2.61	1.41	1.37
29	c	518	DGD	O2G-C2G	-2.60	1.40	1.46
22	b	605	CLA	C4B-NB	2.60	1.41	1.37
22	c	513	CLA	CHC-C1C	2.60	1.43	1.38
22	A	403	CLA	CMB-C2B	-2.60	1.45	1.50
22	C	511	CLA	CMB-C2B	-2.59	1.45	1.50
22	b	613	CLA	C1B-NB	-2.59	1.34	1.37
22	C	507	CLA	MG-NC	-2.59	2.00	2.06
22	b	613	CLA	CMD-C2D	-2.59	1.45	1.50
28	A	411	LHG	C24-C23	2.59	1.58	1.50
22	C	513	CLA	CMB-C2B	-2.59	1.45	1.50
22	B	613	CLA	C1B-C2B	2.59	1.49	1.43
26	c	521	LMG	C4-C3	2.59	1.59	1.52
22	D	405	CLA	C4B-NB	2.58	1.41	1.37
31	k	101	BCR	C1-C6	-2.58	1.50	1.53
22	c	508	CLA	MG-NB	2.58	2.10	2.05
22	B	606	CLA	C1D-ND	2.58	1.41	1.37
22	C	503	CLA	C4B-NB	2.58	1.41	1.37
22	b	615	CLA	CMB-C2B	-2.58	1.45	1.50
29	H	102	DGD	O6E-C1E	2.58	1.48	1.41
22	C	508	CLA	C1B-C2B	2.58	1.49	1.43
22	b	616	CLA	C1B-C2B	2.58	1.49	1.43
22	C	503	CLA	CMB-C2B	-2.57	1.45	1.50
22	b	607	CLA	C1B-C2B	2.57	1.49	1.43
22	d	403	CLA	MG-NB	-2.57	2.00	2.05
22	c	509	CLA	C1D-ND	2.57	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	PHO	CMB-C2B	-2.57	1.46	1.51
22	c	502	CLA	CMC-C2C	-2.57	1.45	1.50
28	L	102	LHG	P-O6	2.56	1.69	1.59
22	B	601	CLA	CMB-C2B	-2.56	1.45	1.50
22	D	405	CLA	C1B-C2B	2.56	1.49	1.43
22	b	604	CLA	C1B-C2B	2.56	1.49	1.43
22	b	602	CLA	C1B-C2B	2.56	1.49	1.43
22	b	605	CLA	C1B-C2B	2.56	1.49	1.43
22	C	511	CLA	MG-NC	2.55	2.12	2.06
22	B	601	CLA	C4B-NB	2.55	1.41	1.37
22	a	402	CLA	C1D-ND	2.55	1.41	1.37
22	c	506	CLA	C4B-NB	2.55	1.41	1.37
22	B	615	CLA	CHC-C4B	-2.55	1.33	1.39
22	B	606	CLA	CMA-C3A	-2.54	1.47	1.53
22	d	405	CLA	CMB-C2B	-2.54	1.45	1.50
27	f	102	SQD	O2-C2	-2.54	1.36	1.43
29	C	517	DGD	O2E-C2E	-2.54	1.36	1.43
22	B	609	CLA	C1D-ND	2.54	1.41	1.37
22	b	608	CLA	MG-NB	2.54	2.10	2.05
22	c	513	CLA	C3B-C4B	2.54	1.50	1.42
22	b	603	CLA	C3B-C4B	2.53	1.50	1.42
22	B	609	CLA	CMC-C2C	-2.53	1.45	1.50
22	b	610	CLA	C1B-C2B	2.53	1.49	1.43
22	B	603	CLA	C1D-ND	2.53	1.41	1.37
22	C	509	CLA	MG-NB	-2.53	2.00	2.05
25	D	407	PL9	C53-C6	-2.53	1.45	1.50
28	D	411	LHG	O7-C7	2.53	1.41	1.34
22	B	616	CLA	C4B-NB	2.53	1.41	1.37
22	C	506	CLA	C1B-C2B	2.53	1.49	1.43
22	C	503	CLA	CHC-C1C	2.52	1.43	1.38
22	a	402	CLA	C3B-C4B	2.52	1.50	1.42
22	c	512	CLA	C1B-C2B	2.52	1.49	1.43
29	A	413	DGD	C1E-C2E	2.52	1.59	1.52
29	c	518	DGD	O3D-C3D	-2.52	1.36	1.43
22	B	616	CLA	CMB-C2B	-2.52	1.45	1.50
34	f	101	HEM	C2A-C3A	-2.52	1.32	1.38
22	c	508	CLA	CMD-C2D	-2.52	1.45	1.50
22	B	615	CLA	C1D-ND	2.51	1.41	1.37
22	C	502	CLA	C1D-ND	2.51	1.41	1.37
22	B	608	CLA	CMC-C2C	-2.50	1.45	1.50
22	D	404	CLA	C1B-C2B	2.50	1.49	1.43
22	b	601	CLA	O2A-CGA	2.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	CMB-C2B	-2.50	1.45	1.50
22	D	403	CLA	C1B-C2B	2.50	1.49	1.43
29	A	413	DGD	O1G-C1A	2.50	1.40	1.33
23	D	401	PHO	C1D-C2D	2.50	1.42	1.39
22	c	504	CLA	C1D-ND	2.49	1.41	1.37
22	c	507	CLA	CHC-C4B	-2.49	1.33	1.39
23	a	403	PHO	C4D-ND	-2.49	1.34	1.38
22	c	502	CLA	C1B-C2B	2.49	1.49	1.43
22	d	403	CLA	C4B-NB	2.49	1.41	1.37
22	c	508	CLA	CHC-C1C	2.49	1.43	1.38
31	C	514	BCR	C33-C5	-2.49	1.47	1.50
22	C	512	CLA	CMD-C2D	-2.49	1.45	1.50
22	b	614	CLA	C1B-C2B	2.49	1.49	1.43
22	b	604	CLA	CMC-C2C	-2.48	1.45	1.50
22	B	613	CLA	CMC-C2C	-2.48	1.45	1.50
22	d	403	CLA	CMD-C2D	-2.48	1.45	1.50
26	M	101	LMG	O7-C8	-2.48	1.40	1.46
28	D	413	LHG	O8-C23	2.48	1.40	1.33
22	B	616	CLA	CMC-C2C	-2.48	1.45	1.50
22	b	616	CLA	MG-ND	-2.48	2.00	2.05
22	B	603	CLA	CHC-C4B	-2.48	1.33	1.39
22	d	401	CLA	MG-ND	-2.48	2.00	2.05
22	b	602	CLA	CMB-C2B	-2.47	1.45	1.50
22	B	606	CLA	CHC-C1C	2.47	1.43	1.38
29	c	517	DGD	O3D-C3D	-2.47	1.36	1.43
22	B	608	CLA	CMD-C2D	-2.47	1.45	1.50
22	C	509	CLA	C3B-C4B	2.47	1.49	1.42
29	c	516	DGD	C4E-C3E	2.47	1.58	1.52
22	c	511	CLA	C3B-C4B	2.47	1.49	1.42
22	b	614	CLA	CMC-C2C	-2.46	1.45	1.50
22	B	611	CLA	CHC-C4B	-2.46	1.33	1.39
22	B	615	CLA	C1B-C2B	2.46	1.48	1.43
22	A	405	CLA	CMD-C2D	-2.46	1.45	1.50
23	A	404	PHO	CMC-C2C	-2.46	1.46	1.50
29	C	515	DGD	O5D-C1E	2.46	1.44	1.40
29	c	516	DGD	O3E-C3E	-2.45	1.36	1.43
27	A	410	SQD	O2-C2	-2.45	1.36	1.43
26	d	410	LMG	O6-C5	-2.45	1.38	1.44
22	C	510	CLA	C4B-NB	2.45	1.41	1.37
22	b	609	CLA	CMB-C2B	-2.45	1.45	1.50
22	C	501	CLA	CHC-C1C	2.45	1.43	1.38
29	c	517	DGD	O6D-C5D	-2.44	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	517	DGD	O2E-C2E	-2.44	1.36	1.43
22	b	615	CLA	CHC-C1C	2.44	1.43	1.38
23	A	404	PHO	C3B-C2B	-2.43	1.37	1.40
22	a	402	CLA	CMC-C2C	-2.43	1.45	1.50
22	b	610	CLA	CMD-C2D	-2.43	1.45	1.50
31	b	617	BCR	C33-C5	-2.43	1.47	1.50
22	B	607	CLA	C3B-C4B	2.43	1.49	1.42
29	C	516	DGD	C4E-C5E	2.43	1.58	1.53
29	C	515	DGD	O2G-C2G	-2.43	1.40	1.46
22	B	605	CLA	CMD-C2D	-2.42	1.45	1.50
22	a	404	CLA	CHC-C4B	-2.42	1.34	1.39
23	D	401	PHO	CMB-C2B	-2.42	1.46	1.51
23	d	402	PHO	CMD-C2D	-2.42	1.46	1.51
26	c	519	LMG	O7-C10	2.42	1.40	1.35
22	d	401	CLA	MG-NB	2.42	2.10	2.05
22	d	404	CLA	CHC-C1C	2.42	1.43	1.38
28	D	413	LHG	P-O6	2.42	1.68	1.59
22	C	513	CLA	CHC-C1C	2.42	1.43	1.38
22	C	501	CLA	CAC-C3C	-2.42	1.44	1.51
22	b	612	CLA	CMC-C2C	-2.41	1.45	1.50
22	c	503	CLA	CMC-C2C	-2.41	1.45	1.50
23	A	404	PHO	C1C-NC	-2.41	1.30	1.37
22	b	616	CLA	C4B-NB	2.41	1.41	1.37
22	c	505	CLA	C1B-C2B	2.41	1.48	1.43
22	B	616	CLA	C1B-C2B	2.41	1.48	1.43
22	C	509	CLA	CMB-C2B	-2.41	1.45	1.50
22	b	609	CLA	CHC-C1C	2.40	1.43	1.38
22	c	505	CLA	C3B-C4B	2.40	1.49	1.42
26	A	409	LMG	C4-C5	2.40	1.58	1.53
22	b	609	CLA	CMD-C2D	-2.40	1.45	1.50
22	c	501	CLA	C1B-NB	-2.40	1.34	1.37
22	b	615	CLA	MG-NC	-2.40	2.00	2.06
27	a	411	SQD	O2-C2	-2.40	1.37	1.43
31	B	618	BCR	C1-C6	-2.39	1.50	1.53
23	d	402	PHO	C3D-C4D	2.39	1.44	1.41
23	d	402	PHO	CBD-CGD	-2.39	1.49	1.52
22	b	607	CLA	CMD-C2D	-2.39	1.45	1.50
22	C	508	CLA	CMD-C2D	-2.39	1.45	1.50
26	Y	101	LMG	C3-C2	2.39	1.58	1.52
22	b	606	CLA	C1B-C2B	2.39	1.48	1.43
22	D	404	CLA	CMB-C2B	-2.39	1.45	1.50
22	b	607	CLA	CHC-C4B	-2.39	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	515	BCR	C30-C25	-2.38	1.50	1.53
22	C	503	CLA	C3B-C4B	2.38	1.49	1.42
22	c	507	CLA	CMC-C2C	-2.38	1.45	1.50
22	b	601	CLA	CMB-C2B	-2.38	1.45	1.50
22	B	602	CLA	C3B-C4B	2.38	1.49	1.42
22	d	403	CLA	C3D-C4D	2.38	1.49	1.44
22	b	602	CLA	C3B-C4B	2.37	1.49	1.42
29	c	518	DGD	C4D-C5D	2.37	1.58	1.53
22	b	611	CLA	CHC-C4B	-2.37	1.34	1.39
29	c	517	DGD	C4E-C5E	2.37	1.58	1.53
22	C	506	CLA	CHC-C1C	2.37	1.43	1.38
22	b	607	CLA	MG-NC	-2.37	2.00	2.06
34	f	101	HEM	CAC-C3C	2.37	1.53	1.47
23	D	401	PHO	CBD-CGD	-2.37	1.49	1.52
23	d	402	PHO	C4D-CHA	2.37	1.43	1.39
22	B	606	CLA	C3B-C4B	2.37	1.49	1.42
22	c	503	CLA	C1B-C2B	2.37	1.48	1.43
22	D	404	CLA	C4B-NB	2.36	1.41	1.37
22	d	403	CLA	CHC-C1C	2.36	1.43	1.38
31	a	405	BCR	C38-C26	-2.36	1.47	1.50
22	A	402	CLA	C3B-C4B	2.36	1.49	1.42
22	B	602	CLA	CAC-C3C	-2.36	1.45	1.51
22	b	613	CLA	CMB-C2B	-2.35	1.46	1.50
22	d	401	CLA	CMB-C2B	-2.35	1.46	1.50
26	Y	101	LMG	O8-C9	-2.35	1.39	1.45
26	B	621	LMG	O7-C10	2.35	1.38	1.30
23	a	403	PHO	C1C-NC	-2.34	1.30	1.37
22	C	501	CLA	C1B-C2B	2.34	1.48	1.43
26	m	101	LMG	C4-C5	2.34	1.58	1.53
22	b	606	CLA	O2D-CED	-2.34	1.40	1.45
26	b	622	LMG	O6-C1	2.33	1.47	1.41
31	k	101	BCR	C33-C5	-2.33	1.47	1.50
22	c	507	CLA	C3D-C4D	2.33	1.49	1.44
22	B	614	CLA	MG-NA	2.33	2.11	2.06
22	c	508	CLA	CMC-C2C	-2.33	1.46	1.50
22	b	616	CLA	MG-NA	2.33	2.11	2.06
22	C	510	CLA	C3B-C4B	2.32	1.49	1.42
22	B	612	CLA	C4B-NB	2.32	1.40	1.37
26	c	522	LMG	O6-C5	-2.32	1.38	1.44
27	a	411	SQD	O3-C3	-2.32	1.37	1.43
22	C	507	CLA	CMB-C2B	-2.32	1.46	1.50
22	b	607	CLA	CMB-C2B	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	CHC-C1C	2.32	1.43	1.38
22	c	512	CLA	C3B-C4B	2.32	1.49	1.42
22	B	604	CLA	CHC-C1C	2.31	1.43	1.38
22	B	615	CLA	CAB-C3B	-2.31	1.41	1.47
25	D	407	PL9	C51-C49	-2.31	1.44	1.50
22	B	611	CLA	CHC-C1C	2.31	1.43	1.38
26	c	521	LMG	C7-C8	2.31	1.58	1.50
34	f	101	HEM	CMC-C2C	2.31	1.55	1.50
22	c	510	CLA	CMC-C2C	-2.31	1.46	1.50
32	c	520	STE	C2-C1	2.30	1.55	1.50
22	B	611	CLA	C1B-C2B	2.30	1.48	1.43
22	c	502	CLA	C1B-NB	-2.30	1.34	1.37
22	C	506	CLA	C3B-C4B	2.30	1.49	1.42
29	c	516	DGD	C3G-C2G	2.30	1.58	1.50
22	C	513	CLA	MG-NA	2.30	2.11	2.06
22	B	602	CLA	CHC-C4B	-2.30	1.34	1.39
22	A	402	CLA	C3C-C2C	2.30	1.41	1.36
22	b	609	CLA	C3B-C4B	2.29	1.49	1.42
22	b	606	CLA	CMD-C2D	-2.29	1.46	1.50
25	d	407	PL9	C10-C9	-2.29	1.45	1.50
22	B	608	CLA	C1B-NB	-2.29	1.34	1.37
22	C	512	CLA	C3B-C4B	2.29	1.49	1.42
22	b	607	CLA	CMC-C2C	-2.29	1.46	1.50
31	x	101	BCR	C1-C6	-2.29	1.50	1.53
22	C	510	CLA	CMD-C2D	-2.29	1.46	1.50
31	I	101	BCR	C34-C9	-2.29	1.46	1.50
22	C	502	CLA	C1B-C2B	2.28	1.48	1.43
35	v	201	HEC	FE-NA	2.28	2.02	1.95
27	f	102	SQD	O3-C3	-2.28	1.37	1.43
31	K	102	BCR	C27-C26	-2.28	1.46	1.51
22	C	505	CLA	CMC-C2C	-2.28	1.46	1.50
22	c	512	CLA	CMB-C2B	-2.28	1.46	1.50
22	b	610	CLA	C1B-NB	-2.28	1.34	1.37
23	a	403	PHO	C4D-CHA	2.28	1.43	1.39
22	B	604	CLA	C1D-C2D	2.28	1.49	1.45
22	C	506	CLA	CAC-C3C	-2.28	1.45	1.51
34	f	101	HEM	CAB-C3B	2.28	1.53	1.47
22	D	404	CLA	CHC-C1C	2.28	1.43	1.38
22	D	405	CLA	CMC-C2C	-2.27	1.46	1.50
22	c	506	CLA	C1B-NB	-2.27	1.34	1.37
22	c	512	CLA	C3D-C4D	2.27	1.49	1.44
31	T	101	BCR	C1-C6	-2.27	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	413	DGD	O5D-C1E	2.27	1.44	1.40
22	B	601	CLA	C3B-C4B	2.27	1.49	1.42
25	d	407	PL9	C26-C24	-2.27	1.46	1.51
22	B	612	CLA	CMC-C2C	-2.27	1.46	1.50
22	C	510	CLA	C3C-C2C	2.27	1.41	1.36
22	d	401	CLA	CAB-C3B	-2.27	1.41	1.47
31	I	101	BCR	C38-C26	-2.27	1.47	1.50
22	b	614	CLA	C3B-C4B	2.26	1.49	1.42
22	A	405	CLA	CHC-C4B	-2.26	1.34	1.39
22	A	402	CLA	MG-NA	2.26	2.11	2.06
22	C	513	CLA	C1B-C2B	2.26	1.48	1.43
22	b	601	CLA	C3B-C4B	2.26	1.49	1.42
27	A	412	SQD	O47-C45	-2.26	1.43	1.47
22	c	503	CLA	C4B-NB	2.26	1.40	1.37
28	e	101	LHG	C24-C23	2.26	1.57	1.50
25	d	407	PL9	C16-C17	2.26	1.61	1.53
22	c	512	CLA	CMC-C2C	-2.26	1.46	1.50
22	C	501	CLA	CMC-C2C	-2.25	1.46	1.50
22	a	404	CLA	C3B-C4B	2.25	1.49	1.42
31	t	101	BCR	C33-C5	-2.25	1.47	1.50
22	b	607	CLA	C4B-NB	2.25	1.40	1.37
34	f	101	HEM	FE-NA	2.25	2.02	1.95
22	D	403	CLA	C4B-NB	2.25	1.40	1.37
22	b	602	CLA	CAC-C3C	-2.25	1.45	1.51
25	D	407	PL9	C46-C44	-2.25	1.46	1.51
22	b	608	CLA	C3B-C4B	2.25	1.49	1.42
26	d	410	LMG	O2-C2	-2.24	1.37	1.43
31	t	101	BCR	C27-C26	-2.24	1.46	1.51
22	A	405	CLA	CMC-C2C	-2.24	1.46	1.50
26	Y	101	LMG	O1-C1	2.24	1.43	1.40
29	c	518	DGD	C1D-C2D	2.24	1.59	1.52
22	B	614	CLA	C1B-C2B	2.24	1.48	1.43
22	C	508	CLA	C4B-NB	2.24	1.40	1.37
22	d	401	CLA	C1D-ND	2.24	1.40	1.37
29	C	517	DGD	C2B-C1B	-2.24	1.44	1.50
28	A	411	LHG	O7-C5	-2.24	1.41	1.46
22	c	513	CLA	C1B-NB	-2.24	1.34	1.37
22	B	608	CLA	C1B-C2B	2.24	1.48	1.43
22	B	613	CLA	MG-NB	2.24	2.10	2.05
29	c	517	DGD	O2G-C2G	-2.24	1.41	1.46
22	d	405	CLA	C1B-C2B	2.24	1.48	1.43
22	a	402	CLA	C3D-C4D	2.24	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	CMD-C2D	-2.23	1.46	1.50
31	x	101	BCR	C33-C5	-2.23	1.47	1.50
22	B	607	CLA	CMB-C2B	-2.23	1.46	1.50
22	B	611	CLA	CMB-C2B	-2.23	1.46	1.50
29	c	516	DGD	O5D-C1E	2.23	1.43	1.40
23	D	401	PHO	C3B-C2B	-2.23	1.37	1.40
22	C	504	CLA	CMB-C2B	-2.23	1.46	1.50
29	C	517	DGD	O6D-C5D	-2.23	1.38	1.44
29	C	515	DGD	C2A-C1A	-2.23	1.44	1.50
22	b	606	CLA	CHC-C1C	2.23	1.43	1.38
22	B	607	CLA	CMC-C2C	-2.23	1.46	1.50
26	c	522	LMG	C4-C3	2.23	1.58	1.52
22	c	509	CLA	MG-NA	2.23	2.11	2.06
22	D	405	CLA	C3B-C4B	2.23	1.49	1.42
22	C	512	CLA	CHC-C1C	2.22	1.42	1.38
22	C	508	CLA	C3B-C4B	2.22	1.49	1.42
22	c	505	CLA	CHC-C1C	2.22	1.42	1.38
22	c	508	CLA	C3B-C4B	2.22	1.49	1.42
22	d	405	CLA	O1D-CGD	2.22	1.26	1.21
22	C	506	CLA	CMC-C2C	-2.22	1.46	1.50
22	c	505	CLA	MG-NA	2.21	2.11	2.06
22	C	510	CLA	CHC-C1C	2.21	1.42	1.38
22	c	508	CLA	C4B-NB	2.21	1.40	1.37
29	C	516	DGD	O1G-C1G	-2.21	1.40	1.45
25	a	409	PL9	C6-C1	-2.21	1.44	1.48
27	B	622	SQD	O2-C2	-2.21	1.37	1.43
22	C	502	CLA	C4B-NB	2.20	1.40	1.37
22	C	501	CLA	C3B-C4B	2.20	1.49	1.42
22	c	502	CLA	C3B-C4B	2.20	1.49	1.42
22	B	615	CLA	O2A-CGA	2.20	1.39	1.33
22	C	512	CLA	CMC-C2C	-2.20	1.46	1.50
23	d	402	PHO	CMB-C2B	-2.20	1.47	1.51
22	B	616	CLA	CAA-C2A	-2.20	1.50	1.54
29	c	518	DGD	C3G-C2G	2.20	1.57	1.50
22	C	502	CLA	C1B-NB	-2.20	1.35	1.37
22	A	403	CLA	CMC-C2C	-2.20	1.46	1.50
27	A	410	SQD	O3-C3	-2.20	1.37	1.43
22	b	616	CLA	CMC-C2C	-2.19	1.46	1.50
34	F	101	HEM	C3B-C2B	-2.19	1.32	1.37
22	C	504	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	603	CLA	C1B-C2B	2.19	1.48	1.43
22	c	501	CLA	CHC-C4B	-2.19	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	510	CLA	CMD-C2D	-2.19	1.46	1.50
22	C	507	CLA	CMD-C2D	-2.18	1.46	1.50
22	c	509	CLA	CHC-C4B	-2.18	1.34	1.39
22	A	402	CLA	CHC-C1C	2.18	1.42	1.38
22	B	608	CLA	O2A-CGA	2.18	1.39	1.33
25	d	407	PL9	C6-C1	-2.18	1.45	1.48
26	B	626	LMG	C14-C13	2.18	1.62	1.51
22	d	405	CLA	C3B-C4B	2.18	1.49	1.42
22	B	612	CLA	MG-NC	2.18	2.11	2.06
22	C	503	CLA	MG-ND	2.18	2.10	2.05
31	a	405	BCR	C33-C5	-2.17	1.47	1.50
29	C	515	DGD	O1A-C1A	2.17	1.29	1.22
22	b	609	CLA	CMC-C2C	-2.17	1.46	1.50
22	C	510	CLA	C1D-ND	2.17	1.40	1.37
22	B	603	CLA	C1B-NB	-2.17	1.35	1.37
22	B	608	CLA	CHC-C1C	2.17	1.42	1.38
22	C	503	CLA	CMC-C2C	-2.17	1.46	1.50
22	C	504	CLA	O2D-CGD	2.17	1.38	1.33
31	T	101	BCR	C38-C26	-2.16	1.47	1.50
22	c	508	CLA	C1B-C2B	2.16	1.48	1.43
22	C	502	CLA	CMB-C2B	-2.16	1.46	1.50
23	a	403	PHO	CMC-C2C	-2.16	1.47	1.50
26	D	412	LMG	O8-C28	2.16	1.39	1.33
22	D	404	CLA	O2D-CED	-2.16	1.40	1.45
26	b	622	LMG	C4-C5	2.16	1.57	1.53
31	c	515	BCR	C27-C26	-2.16	1.47	1.51
22	b	608	CLA	C1C-C2C	2.16	1.48	1.44
22	b	607	CLA	O2D-CGD	2.15	1.38	1.33
26	c	519	LMG	O1-C1	2.15	1.43	1.40
35	V	201	HEC	CAC-C3C	2.15	1.56	1.51
29	H	102	DGD	C4D-C3D	2.15	1.57	1.52
22	c	502	CLA	C4B-NB	2.15	1.40	1.37
22	b	605	CLA	CAC-C3C	-2.15	1.45	1.51
22	c	502	CLA	MG-NB	-2.14	2.01	2.05
28	d	408	LHG	P-O3	2.14	1.67	1.59
31	K	101	BCR	C33-C5	-2.14	1.47	1.50
26	Y	101	LMG	C1-C2	2.14	1.58	1.52
22	d	405	CLA	CHC-C4B	-2.14	1.34	1.39
29	c	517	DGD	C3E-C2E	2.14	1.57	1.52
26	m	101	LMG	C6-C5	2.14	1.59	1.51
22	C	513	CLA	CMC-C2C	-2.14	1.46	1.50
22	b	608	CLA	O2A-CGA	2.14	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	CMB-C2B	-2.13	1.46	1.50
29	C	516	DGD	C2B-C1B	-2.13	1.44	1.50
31	B	619	BCR	C33-C5	-2.13	1.47	1.50
22	b	605	CLA	C3B-C4B	2.13	1.49	1.42
23	a	403	PHO	O2D-CGD	2.13	1.38	1.33
22	a	404	CLA	CMD-C2D	-2.13	1.46	1.50
22	C	511	CLA	C4B-NB	2.13	1.40	1.37
22	d	401	CLA	C1B-NB	-2.13	1.35	1.37
22	c	512	CLA	CMD-C2D	-2.12	1.46	1.50
22	B	613	CLA	C3B-C4B	2.12	1.48	1.42
26	B	626	LMG	O1-C7	2.12	1.47	1.43
22	C	505	CLA	C1B-C2B	2.12	1.48	1.43
22	c	507	CLA	CMB-C2B	-2.12	1.46	1.50
28	d	409	LHG	C6-C5	2.12	1.57	1.50
31	k	102	BCR	C33-C5	-2.12	1.47	1.50
22	a	402	CLA	C1B-NB	-2.12	1.35	1.37
25	D	407	PL9	C2-C1	2.12	1.50	1.44
22	B	602	CLA	CMD-C2D	-2.12	1.46	1.50
26	D	408	LMG	C7-C8	2.11	1.57	1.50
26	M	101	LMG	O6-C1	2.11	1.47	1.41
31	c	515	BCR	C35-C13	-2.11	1.46	1.50
22	b	613	CLA	CMC-C2C	-2.11	1.46	1.50
22	d	405	CLA	CAB-C3B	-2.11	1.41	1.47
29	h	101	DGD	C4E-C5E	2.11	1.57	1.53
22	C	504	CLA	MG-NA	-2.11	2.01	2.06
29	C	515	DGD	C1D-C2D	2.11	1.58	1.52
22	B	604	CLA	C1B-NB	-2.11	1.35	1.37
31	I	101	BCR	C4-C5	-2.10	1.47	1.51
22	B	614	CLA	MG-NB	-2.10	2.01	2.05
35	v	201	HEC	CMD-C2D	2.10	1.55	1.50
22	c	501	CLA	CMD-C2D	-2.10	1.46	1.50
22	A	405	CLA	CMA-C3A	-2.10	1.48	1.53
22	D	404	CLA	MG-NC	-2.10	2.01	2.06
22	C	506	CLA	CAA-C2A	-2.10	1.50	1.54
22	b	612	CLA	CMD-C2D	-2.10	1.46	1.50
22	b	607	CLA	C3B-C4B	2.09	1.48	1.42
22	b	610	CLA	C1A-CHA	-2.09	1.34	1.43
22	B	605	CLA	C5-C3	-2.09	1.47	1.51
22	b	608	CLA	CMA-C3A	-2.09	1.48	1.53
22	c	501	CLA	C3B-C4B	2.09	1.48	1.42
32	X	101	STE	O1-C1	2.09	1.28	1.22
26	M	101	LMG	C7-C8	2.09	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	T	101	BCR	C27-C26	-2.09	1.47	1.51
22	B	603	CLA	CAB-C3B	-2.09	1.41	1.47
22	B	607	CLA	CAC-C3C	-2.09	1.45	1.51
22	A	403	CLA	CHC-C1C	2.08	1.42	1.38
25	d	407	PL9	C46-C44	-2.08	1.47	1.51
22	B	610	CLA	CMC-C2C	-2.08	1.46	1.50
22	b	603	CLA	C4B-NB	2.08	1.40	1.37
22	c	504	CLA	C3B-C4B	2.08	1.48	1.42
22	b	603	CLA	C1D-ND	2.08	1.40	1.37
22	a	404	CLA	CMC-C2C	-2.08	1.46	1.50
29	C	516	DGD	C1G-C2G	2.08	1.57	1.50
22	b	606	CLA	CMB-C2B	-2.08	1.46	1.50
22	c	503	CLA	CAC-C3C	-2.08	1.45	1.51
22	b	605	CLA	C3D-C4D	2.08	1.48	1.44
31	B	618	BCR	C35-C13	-2.08	1.46	1.50
22	C	508	CLA	CMB-C2B	-2.08	1.46	1.50
22	c	504	CLA	CAC-C3C	-2.08	1.45	1.51
22	B	607	CLA	CHC-C4B	-2.08	1.34	1.39
26	B	626	LMG	O7-C10	2.07	1.40	1.34
22	b	613	CLA	CAA-C2A	-2.07	1.50	1.54
22	C	513	CLA	MG-ND	2.07	2.09	2.05
22	b	609	CLA	C1B-C2B	2.07	1.48	1.43
22	B	603	CLA	CMB-C2B	-2.07	1.46	1.50
26	B	626	LMG	O8-C9	-2.07	1.40	1.45
22	B	603	CLA	CMC-C2C	-2.07	1.46	1.50
23	A	404	PHO	O2D-CGD	2.06	1.38	1.33
22	c	509	CLA	CMB-C2B	-2.06	1.46	1.50
31	B	618	BCR	C27-C26	-2.06	1.47	1.51
22	b	601	CLA	CMC-C2C	-2.06	1.46	1.50
22	b	613	CLA	C1B-C2B	2.06	1.48	1.43
22	C	506	CLA	C1B-NB	-2.06	1.35	1.37
22	b	610	CLA	CMC-C2C	-2.06	1.46	1.50
22	c	507	CLA	CMD-C2D	-2.05	1.46	1.50
22	d	404	CLA	CMD-C2D	-2.05	1.46	1.50
22	C	501	CLA	C1B-NB	-2.05	1.35	1.37
22	D	405	CLA	C1B-NB	-2.05	1.35	1.37
32	d	412	STE	O1-C1	2.05	1.28	1.22
35	v	201	HEC	CHD-C4C	-2.04	1.34	1.39
22	c	509	CLA	C3B-C4B	2.04	1.48	1.42
22	C	502	CLA	MG-NC	2.04	2.11	2.06
22	B	613	CLA	C4-C3	-2.04	1.45	1.50
29	c	516	DGD	O4D-C4D	-2.04	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	511	CLA	CMB-C2B	-2.04	1.46	1.50
22	b	614	CLA	C1A-CHA	-2.04	1.34	1.43
31	B	618	BCR	C4-C5	-2.04	1.47	1.51
31	a	405	BCR	C27-C26	-2.04	1.47	1.51
22	c	502	CLA	CHC-C4B	-2.04	1.34	1.39
29	H	102	DGD	C1G-C2G	2.04	1.57	1.50
22	A	403	CLA	MG-NC	-2.04	2.01	2.06
22	c	502	CLA	CHC-C1C	2.03	1.42	1.38
22	b	601	CLA	CMD-C2D	-2.03	1.46	1.50
22	B	615	CLA	C1B-NB	-2.03	1.35	1.37
22	d	404	CLA	MG-NB	2.03	2.09	2.05
31	c	515	BCR	C33-C5	-2.03	1.47	1.50
22	c	503	CLA	C1B-NB	-2.03	1.35	1.37
22	d	403	CLA	MG-NA	-2.03	2.01	2.06
22	C	510	CLA	MG-NC	2.03	2.11	2.06
22	b	607	CLA	MG-NA	2.03	2.11	2.06
22	b	605	CLA	MG-ND	2.03	2.09	2.05
22	a	404	CLA	MG-NB	-2.03	2.01	2.05
22	B	612	CLA	MG-ND	-2.03	2.01	2.05
22	B	609	CLA	C4B-NB	2.03	1.40	1.37
26	Y	101	LMG	C6-C5	2.03	1.58	1.51
22	d	404	CLA	CMA-C3A	-2.03	1.48	1.53
22	B	606	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	608	CLA	CMC-C2C	-2.03	1.46	1.50
26	D	408	LMG	O7-C8	-2.03	1.41	1.46
29	C	517	DGD	C2A-C1A	-2.02	1.44	1.50
31	c	515	BCR	C38-C26	-2.02	1.47	1.50
22	d	403	CLA	CMC-C2C	-2.02	1.46	1.50
22	B	603	CLA	C3B-C4B	2.02	1.48	1.42
26	B	626	LMG	O1-C1	2.02	1.43	1.40
22	C	511	CLA	CMD-C2D	-2.02	1.46	1.50
22	A	405	CLA	CAB-C3B	-2.02	1.42	1.47
29	A	413	DGD	C3D-C2D	2.02	1.57	1.52
28	D	410	LHG	C8-C7	-2.02	1.44	1.50
23	a	403	PHO	CMD-C2D	-2.02	1.47	1.51
35	V	201	HEC	C3C-C2C	-2.02	1.33	1.38
26	c	519	LMG	O2-C2	-2.02	1.38	1.43
22	b	605	CLA	C1A-CHA	-2.02	1.34	1.43
32	C	518	STE	O2-C1	-2.02	1.24	1.30
32	b	623	STE	C2-C1	2.01	1.55	1.50
22	C	508	CLA	CMC-C2C	-2.01	1.46	1.50
31	B	618	BCR	C33-C5	-2.01	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	618	BCR	C36-C18	-2.01	1.46	1.50
22	A	403	CLA	C1B-NB	-2.01	1.35	1.37
31	d	406	BCR	C33-C5	-2.01	1.47	1.50
22	C	510	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	510	CLA	CHC-C1C	2.01	1.42	1.38
27	D	409	SQD	O3-C3	-2.01	1.38	1.43
22	c	510	CLA	O2D-CGD	2.01	1.38	1.33
22	a	404	CLA	CMB-C2B	-2.01	1.46	1.50
22	C	509	CLA	O2D-CGD	2.01	1.38	1.33
29	c	518	DGD	O2G-C1B	2.01	1.39	1.34
22	B	613	CLA	C1B-NB	-2.01	1.35	1.37
32	j	101	STE	O1-C1	2.00	1.28	1.22
22	b	604	CLA	MG-NB	-2.00	2.01	2.05
22	c	502	CLA	MG-NA	2.00	2.11	2.06
22	B	601	CLA	CMC-C2C	-2.00	1.46	1.50
23	A	404	PHO	CAC-C3C	-2.00	1.48	1.51
29	c	518	DGD	O4D-C4D	-2.00	1.38	1.43

All (1294) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	9.53	111.03	106.68
22	c	511	CLA	C4A-NA-C1A	9.38	110.96	106.68
27	L	101	SQD	O6-C1-C2	9.32	122.43	108.27
22	C	511	CLA	C4A-NA-C1A	8.57	110.59	106.68
22	C	510	CLA	C4A-NA-C1A	8.41	110.52	106.68
22	a	402	CLA	C4A-NA-C1A	8.16	110.40	106.68
22	B	604	CLA	C4A-NA-C1A	7.99	110.32	106.68
22	c	501	CLA	C4A-NA-C1A	7.68	110.18	106.68
27	A	410	SQD	O6-C1-C2	7.20	119.21	108.27
22	C	507	CLA	C4A-NA-C1A	7.19	109.96	106.68
22	d	404	CLA	C4A-NA-C1A	7.08	109.91	106.68
27	B	622	SQD	O6-C1-C2	7.05	118.98	108.27
22	B	609	CLA	C4A-NA-C1A	6.98	109.86	106.68
22	C	501	CLA	C4A-NA-C1A	6.96	109.85	106.68
22	B	601	CLA	C4A-NA-C1A	6.94	109.84	106.68
22	B	616	CLA	C4A-NA-C1A	6.83	109.80	106.68
22	b	606	CLA	C4A-NA-C1A	6.71	109.74	106.68
22	B	612	CLA	C4A-NA-C1A	6.45	109.62	106.68
22	b	601	CLA	C4A-NA-C1A	6.41	109.61	106.68
22	C	502	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	A	402	CLA	C4A-NA-C1A	6.37	109.59	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	615	CLA	C4A-NA-C1A	6.35	109.58	106.68
22	b	603	CLA	O2D-CGD-O1D	-6.26	111.66	123.85
22	b	612	CLA	C4A-NA-C1A	6.24	109.53	106.68
22	c	507	CLA	C4A-NA-C1A	6.14	109.48	106.68
22	B	610	CLA	C4A-NA-C1A	6.11	109.47	106.68
22	C	513	CLA	C4A-NA-C1A	6.03	109.43	106.68
22	B	606	CLA	C4A-NA-C1A	5.99	109.41	106.68
27	a	411	SQD	O6-C1-C2	5.90	117.23	108.27
22	B	607	CLA	C4A-NA-C1A	5.87	109.36	106.68
25	a	409	PL9	C7-C3-C4	5.81	121.69	116.91
22	C	512	CLA	C4A-NA-C1A	5.75	109.30	106.68
22	C	508	CLA	C4A-NA-C1A	5.71	109.28	106.68
22	b	608	CLA	C3B-C4B-NB	-5.68	105.46	110.53
22	b	613	CLA	C4A-NA-C1A	5.67	109.27	106.68
27	D	409	SQD	O6-C1-C2	5.67	116.89	108.27
22	c	506	CLA	C4A-NA-C1A	5.57	109.22	106.68
22	b	606	CLA	O2D-CGD-O1D	-5.57	113.01	123.85
22	b	603	CLA	C4A-NA-C1A	5.53	109.20	106.68
22	b	615	CLA	C4A-NA-C1A	5.51	109.19	106.68
27	f	102	SQD	O6-C1-C2	5.43	116.51	108.27
22	b	616	CLA	O2D-CGD-O1D	-5.41	113.32	123.85
22	d	404	CLA	C1D-ND-C4D	5.40	110.10	106.31
22	b	614	CLA	C4A-NA-C1A	5.38	109.13	106.68
27	A	410	SQD	O7-S-C6	5.37	114.77	106.76
27	B	622	SQD	O7-S-C6	5.34	114.73	106.76
22	B	602	CLA	O2D-CGD-CBD	5.29	120.48	111.23
29	H	102	DGD	O3G-C3G-C2G	-5.20	98.17	110.82
27	D	409	SQD	O8-S-C6	5.19	115.99	105.97
22	B	610	CLA	O2D-CGD-O1D	-5.12	113.89	123.85
22	D	404	CLA	C4A-NA-C1A	5.08	109.00	106.68
22	b	605	CLA	C4A-NA-C1A	5.08	109.00	106.68
22	c	509	CLA	C4A-NA-C1A	5.06	108.99	106.68
22	B	611	CLA	C4A-NA-C1A	5.05	108.98	106.68
22	b	611	CLA	C4A-NA-C1A	5.02	108.97	106.68
23	A	404	PHO	C2B-C1B-NB	-5.00	105.81	109.43
22	b	616	CLA	C4A-NA-C1A	4.99	108.96	106.68
22	B	611	CLA	CMB-C2B-C1B	-4.94	117.90	125.42
27	f	102	SQD	O7-S-C6	4.89	114.06	106.76
29	C	517	DGD	O3G-C3G-C2G	-4.88	98.95	110.82
22	B	605	CLA	O2D-CGD-O1D	-4.87	114.37	123.85
25	A	408	PL9	C7-C3-C4	4.80	120.86	116.91
22	b	609	CLA	C4A-NA-C1A	4.80	108.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	403	CLA	C4A-NA-C1A	4.80	108.87	106.68
23	a	403	PHO	C2B-C1B-NB	-4.79	105.97	109.43
22	c	505	CLA	O2D-CGD-O1D	-4.74	114.63	123.85
27	B	622	SQD	O47-C7-C8	4.72	121.68	111.48
22	c	501	CLA	O2D-CGD-O1D	-4.72	114.67	123.85
22	b	603	CLA	O2D-CGD-CBD	4.69	119.44	111.23
22	b	602	CLA	C4A-NA-C1A	4.68	108.81	106.68
27	D	409	SQD	O9-S-C6	4.68	113.74	106.76
22	b	604	CLA	C4A-NA-C1A	4.67	108.81	106.68
23	d	402	PHO	C4D-CHA-CBD	-4.66	106.22	108.45
22	C	513	CLA	O2D-CGD-O1D	-4.65	114.79	123.85
22	B	603	CLA	O2D-CGD-O1D	-4.62	114.86	123.85
22	c	509	CLA	O2A-CGA-O1A	-4.60	112.13	123.63
22	C	509	CLA	C4A-NA-C1A	4.58	108.77	106.68
28	D	413	LHG	O4-P-O5	4.55	133.60	112.44
35	v	201	HEC	C1D-ND-C4D	4.51	110.55	105.21
27	f	102	SQD	O9-S-C6	4.50	113.48	106.76
25	a	409	PL9	C7-C3-C2	-4.49	118.10	123.39
28	A	411	LHG	O4-P-O5	4.48	133.29	112.44
25	D	407	PL9	C7-C3-C4	4.48	120.60	116.91
23	d	402	PHO	C2B-C1B-NB	-4.46	106.20	109.43
22	c	512	CLA	C3B-C4B-NB	-4.44	106.57	110.53
22	B	611	CLA	O2D-CGD-O1D	-4.43	115.23	123.85
28	d	408	LHG	O4-P-O5	4.40	132.89	112.44
28	D	411	LHG	O4-P-O5	4.39	132.88	112.44
28	e	101	LHG	O4-P-O5	4.36	132.75	112.44
22	b	602	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
33	D	402	BCT	O2-C-O1	4.35	130.81	119.68
28	d	409	LHG	O4-P-O5	4.35	132.69	112.44
27	t	102	SQD	O47-C7-C8	4.35	120.89	111.48
27	B	622	SQD	C3-C4-C5	4.34	118.09	110.23
27	A	410	SQD	O9-S-O7	-4.33	99.75	113.82
22	b	604	CLA	C1-C2-C3	-4.29	119.17	126.20
22	B	604	CLA	O2A-CGA-O1A	-4.28	112.92	123.63
27	A	410	SQD	O47-C7-C8	4.28	120.74	111.48
22	b	606	CLA	O2D-CGD-CBD	4.27	118.69	111.23
23	A	404	PHO	C3B-C4B-NB	-4.22	104.71	107.46
28	D	410	LHG	O4-P-O5	4.21	132.03	112.44
25	A	408	PL9	O1-C4-C3	-4.20	116.30	120.73
22	A	405	CLA	C4A-NA-C1A	4.19	108.59	106.68
27	A	412	SQD	C45-O47-C7	4.18	123.82	117.78
22	b	607	CLA	C4A-NA-C1A	4.18	108.58	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	617	BCR	C2-C1-C6	4.16	116.48	110.44
28	a	410	LHG	O4-P-O5	4.15	131.74	112.44
23	D	401	PHO	C4D-CHA-CBD	-4.14	106.47	108.45
29	C	516	DGD	O3G-C3G-C2G	-4.14	100.74	110.82
29	h	101	DGD	C3D-C4D-C5D	-4.13	102.75	110.23
22	c	513	CLA	C4A-NA-C1A	4.12	108.56	106.68
27	L	101	SQD	C1-C2-C3	-4.12	101.35	110.01
22	D	405	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
22	C	506	CLA	C4A-NA-C1A	4.07	108.54	106.68
23	A	404	PHO	C4D-CHA-CBD	-4.07	106.50	108.45
27	f	102	SQD	O9-S-O7	-4.05	100.64	113.82
23	D	401	PHO	CMB-C2B-C3B	4.04	132.75	124.68
22	b	605	CLA	O2D-CGD-O1D	-4.02	116.02	123.85
29	C	517	DGD	C4D-C3D-C2D	-4.02	103.78	110.83
22	c	505	CLA	O2D-CGD-CBD	4.00	118.23	111.23
22	c	512	CLA	C4A-NA-C1A	4.00	108.50	106.68
22	c	510	CLA	C4A-NA-C1A	3.97	108.49	106.68
22	C	505	CLA	C3B-C4B-NB	-3.96	107.00	110.53
28	l	101	LHG	O4-P-O5	3.95	130.81	112.44
22	c	512	CLA	C1-C2-C3	-3.94	119.74	126.20
31	B	618	BCR	C29-C30-C25	3.94	116.16	110.44
27	L	101	SQD	O7-S-C6	3.93	112.62	106.76
25	d	407	PL9	C40-C39-C41	3.93	122.05	115.23
22	C	510	CLA	O2D-CGD-O1D	-3.93	116.21	123.85
28	L	102	LHG	O4-P-O5	3.92	130.69	112.44
31	b	617	BCR	C2-C1-C6	3.92	116.13	110.44
22	C	512	CLA	CHB-C4A-NA	3.91	130.04	124.40
22	c	507	CLA	O2A-CGA-O1A	-3.90	113.87	123.63
29	c	517	DGD	O3G-C3G-C2G	-3.89	101.36	110.82
27	a	411	SQD	O8-S-C6	3.86	113.42	105.97
22	a	404	CLA	CHB-C4A-NA	3.85	129.96	124.40
23	a	403	PHO	C4D-CHA-CBD	-3.85	106.61	108.45
22	a	402	CLA	O1D-CGD-CBD	3.84	132.09	124.52
35	V	201	HEC	C1D-ND-C4D	3.84	109.75	105.21
22	b	613	CLA	CMB-C2B-C1B	-3.83	119.59	125.42
22	C	507	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
27	L	101	SQD	O48-C23-C24	3.82	123.49	111.83
22	b	609	CLA	C3B-C4B-NB	-3.82	107.12	110.53
35	v	201	HEC	CHA-C4D-ND	3.82	128.53	124.42
22	b	602	CLA	O2D-CGD-CBD	3.81	117.89	111.23
27	A	412	SQD	O47-C7-C8	3.81	119.72	111.48
22	b	616	CLA	O1D-CGD-CBD	3.80	132.01	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Z	101	BCR	C15-C16-C17	-3.79	115.77	123.52
22	B	604	CLA	O2D-CGD-O1D	-3.78	116.48	123.85
31	x	101	BCR	C27-C26-C25	3.78	127.82	122.70
31	d	406	BCR	C38-C26-C25	-3.78	120.36	124.48
25	d	407	PL9	C22-C23-C24	-3.78	118.98	127.62
22	C	502	CLA	O1D-CGD-CBD	3.77	131.95	124.52
22	c	509	CLA	O2D-CGD-O1D	-3.76	116.52	123.85
22	C	513	CLA	CAC-C3C-C4C	3.76	129.68	124.79
26	c	519	LMG	O6-C1-O1	-3.75	101.17	110.04
22	c	507	CLA	O2D-CGD-O1D	-3.75	116.54	123.85
27	L	101	SQD	O5-C5-C4	3.75	116.46	109.70
26	c	522	LMG	C1-C2-C3	3.75	117.90	110.01
26	b	622	LMG	C1-O6-C5	-3.75	106.41	113.72
22	A	405	CLA	O2D-CGD-CBD	3.74	117.77	111.23
22	A	403	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
22	c	508	CLA	C4A-NA-C1A	3.74	108.39	106.68
22	C	512	CLA	O2D-CGD-O1D	-3.72	116.60	123.85
22	A	403	CLA	C4A-NA-C1A	3.72	108.38	106.68
22	b	615	CLA	CHB-C1B-NB	3.71	129.61	124.05
23	d	402	PHO	O1D-CGD-CBD	3.71	130.35	124.72
22	b	612	CLA	O2A-CGA-O1A	-3.69	114.39	123.63
22	A	402	CLA	CHB-C4A-NA	3.69	129.73	124.40
25	A	408	PL9	C7-C3-C2	-3.68	119.05	123.39
23	d	402	PHO	CMB-C2B-C3B	3.68	132.04	124.68
27	A	410	SQD	O5-C1-C2	-3.67	102.83	110.37
35	v	201	HEC	CMC-C2C-C1C	-3.67	119.84	125.42
22	C	507	CLA	C4-C3-C5	3.67	121.59	115.23
29	h	101	DGD	C4D-C3D-C2D	-3.66	104.40	110.83
29	c	517	DGD	C3E-C4E-C5E	-3.66	103.59	110.23
22	B	615	CLA	CHC-C4B-NB	3.66	129.54	124.05
27	B	622	SQD	O48-C23-C24	3.66	122.99	111.83
22	b	601	CLA	CHB-C4A-NA	3.65	129.67	124.40
22	C	513	CLA	O1D-CGD-CBD	3.65	131.72	124.52
22	B	611	CLA	CMB-C2B-C3B	3.65	135.14	126.55
22	B	611	CLA	O2D-CGD-CBD	3.65	117.61	111.23
31	B	619	BCR	C2-C1-C6	3.64	115.73	110.44
33	a	408	BCT	O2-C-O1	3.64	128.99	119.68
23	a	403	PHO	CMB-C2B-C3B	3.63	131.93	124.68
22	b	613	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
22	B	602	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
26	m	101	LMG	O3-C3-C2	-3.60	101.89	110.38
22	D	403	CLA	O2A-CGA-O1A	-3.60	114.62	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	611	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
22	d	405	CLA	CMB-C2B-C1B	-3.59	119.96	125.42
22	c	512	CLA	O2D-CGD-O1D	-3.58	116.87	123.85
29	c	517	DGD	O6D-C1D-O3G	-3.58	101.59	110.04
22	C	501	CLA	O2D-CGD-CBD	3.58	117.48	111.23
22	C	505	CLA	CMB-C2B-C1B	-3.56	120.00	125.42
22	d	404	CLA	C2D-C1D-ND	-3.55	106.61	110.13
22	c	502	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
22	B	614	CLA	C4A-NA-C1A	3.55	108.30	106.68
25	D	407	PL9	C36-C34-C33	-3.55	113.20	121.17
26	B	626	LMG	C1-C2-C3	-3.54	102.56	110.01
23	A	404	PHO	C1-C2-C3	-3.54	120.40	126.20
22	d	401	CLA	CHB-C4A-NA	3.54	129.51	124.40
22	B	605	CLA	O1D-CGD-CBD	3.54	131.49	124.52
25	A	408	PL9	C36-C34-C33	-3.54	113.23	121.17
27	t	102	SQD	O48-C23-O10	-3.54	114.78	123.63
22	b	613	CLA	CHB-C4A-NA	3.53	129.50	124.40
22	c	502	CLA	C4A-NA-C1A	3.52	108.29	106.68
22	B	610	CLA	O2A-CGA-O1A	-3.52	114.82	123.63
22	B	604	CLA	CHB-C4A-NA	3.51	129.47	124.40
29	A	413	DGD	O5D-C1E-C2E	3.50	113.59	108.27
22	c	503	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
34	f	101	HEM	CBD-CAD-C3D	-3.50	102.85	112.53
22	B	615	CLA	CHB-C4A-NA	3.50	129.45	124.40
31	B	619	BCR	C29-C30-C25	3.50	115.52	110.44
22	A	405	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
26	m	101	LMG	O1-C7-C8	-3.48	102.36	110.82
22	b	612	CLA	CAC-C3C-C4C	3.47	129.30	124.79
26	d	410	LMG	O6-C1-O1	-3.46	101.86	110.04
29	c	517	DGD	O6E-C1E-O5D	-3.46	101.87	110.04
29	c	518	DGD	O6D-C1D-O3G	-3.46	101.87	110.04
22	d	404	CLA	C3B-C4B-NB	-3.45	107.45	110.53
31	T	101	BCR	C27-C26-C25	3.44	127.35	122.70
22	B	603	CLA	C4A-NA-C1A	3.43	108.25	106.68
29	c	518	DGD	O3G-C3G-C2G	-3.43	102.49	110.82
22	B	604	CLA	C6-C7-C8	-3.42	104.58	115.97
22	c	508	CLA	O2A-CGA-O1A	-3.42	115.06	123.63
31	B	618	BCR	C37-C22-C21	-3.42	117.27	122.82
22	B	612	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
29	C	516	DGD	C1D-C2D-C3D	-3.42	102.82	110.01
31	C	514	BCR	C15-C16-C17	-3.41	116.54	123.52
22	d	401	CLA	C1D-ND-C4D	3.41	108.70	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	C1-C2-C3	-3.40	120.62	126.20
29	H	102	DGD	O2D-C2D-C1D	-3.40	101.98	110.08
27	D	409	SQD	O8-S-O9	-3.39	102.92	111.40
22	d	405	CLA	O2A-CGA-O1A	-3.38	115.17	123.63
35	V	201	HEC	CAD-CBD-CGD	-3.38	104.70	113.67
26	c	522	LMG	C1-O6-C5	-3.38	107.12	113.72
35	v	201	HEC	CBD-CAD-C3D	-3.37	103.20	112.53
22	c	509	CLA	CHB-C4A-NA	3.37	129.26	124.40
22	d	401	CLA	C2D-C1D-ND	-3.37	106.79	110.13
22	D	403	CLA	C4-C3-C5	3.37	121.07	115.23
22	b	605	CLA	C4-C3-C5	3.36	121.06	115.23
22	c	513	CLA	C1-C2-C3	-3.36	120.69	126.20
23	d	402	PHO	C3D-C4D-ND	3.36	112.01	107.71
22	b	609	CLA	O1D-CGD-CBD	3.35	131.13	124.52
35	V	201	HEC	CHA-C4D-ND	3.35	128.03	124.42
22	C	502	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
22	c	501	CLA	CED-O2D-CGD	-3.35	108.31	115.92
22	B	614	CLA	CHC-C4B-NB	3.34	129.07	124.05
26	A	409	LMG	O6-C1-O1	-3.34	102.15	110.04
22	a	404	CLA	O2A-CGA-O1A	-3.34	115.27	123.63
31	B	619	BCR	C38-C26-C25	-3.34	120.84	124.48
31	B	617	BCR	C37-C22-C23	3.33	123.18	118.09
22	b	602	CLA	CHB-C4A-NA	3.33	129.20	124.40
29	C	515	DGD	O6D-C1D-O3G	-3.32	102.19	110.04
22	B	614	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
27	a	411	SQD	O9-S-O7	-3.32	103.03	113.82
27	a	411	SQD	C1-C2-C3	-3.32	103.03	110.01
31	T	101	BCR	C7-C8-C9	-3.31	121.34	126.23
27	t	102	SQD	O48-C23-C24	3.31	121.92	111.83
22	b	601	CLA	CHD-C1D-ND	-3.30	120.15	124.80
23	D	401	PHO	C2B-C1B-NB	-3.30	107.04	109.43
22	b	611	CLA	O2D-CGD-CBD	3.30	117.00	111.23
27	a	411	SQD	O48-C23-C24	3.29	121.87	111.83
32	x	102	STE	O2-C1-C2	3.29	124.38	114.00
22	c	510	CLA	C3B-C4B-NB	-3.28	107.60	110.53
22	C	501	CLA	C3B-C4B-NB	-3.27	107.61	110.53
22	B	601	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
22	C	509	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
25	D	407	PL9	C22-C23-C24	-3.25	120.18	127.62
22	B	602	CLA	CHB-C4A-NA	3.24	129.08	124.40
26	c	522	LMG	O6-C1-O1	-3.24	102.40	110.04
22	b	614	CLA	O2A-CGA-O1A	-3.24	115.53	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	407	PL9	C40-C39-C41	3.22	120.83	115.23
27	a	411	SQD	C1-O5-C5	-3.22	107.43	113.72
29	C	517	DGD	O6D-C1D-O3G	-3.22	102.45	110.04
22	C	507	CLA	CHB-C4A-NA	3.21	129.03	124.40
22	C	513	CLA	C3B-C4B-NB	-3.20	107.67	110.53
25	d	407	PL9	C37-C38-C39	-3.20	120.31	127.62
22	b	614	CLA	C1-C2-C3	-3.20	120.96	126.20
29	A	413	DGD	O6D-C1D-O3G	-3.20	102.49	110.04
31	D	406	BCR	C27-C26-C25	3.19	127.02	122.70
31	b	618	BCR	C36-C18-C17	-3.18	117.66	122.82
29	A	413	DGD	O6E-C5E-C4E	3.18	115.42	109.70
22	c	505	CLA	C3B-C4B-NB	-3.17	107.70	110.53
22	B	613	CLA	CHB-C4A-NA	3.17	128.98	124.40
27	L	101	SQD	C3-C4-C5	3.16	115.96	110.23
31	D	406	BCR	C2-C1-C6	3.16	115.03	110.44
27	L	101	SQD	C45-O47-C7	3.16	125.35	117.80
31	H	101	BCR	C24-C23-C22	-3.15	121.58	126.23
22	B	604	CLA	C4-C3-C5	3.15	120.69	115.23
29	C	515	DGD	O1G-C1A-C2A	-3.14	102.25	111.83
31	c	514	BCR	C15-C16-C17	-3.14	117.10	123.52
31	I	101	BCR	C27-C26-C25	3.13	126.94	122.70
22	B	603	CLA	C4-C3-C5	3.13	120.66	115.23
35	v	201	HEC	CHB-C1B-NB	3.13	127.79	124.42
22	b	610	CLA	CHB-C4A-NA	3.13	128.91	124.40
26	b	622	LMG	O1-C1-C2	-3.13	103.53	108.27
31	K	101	BCR	C27-C26-C25	3.12	126.92	122.70
22	C	501	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
22	d	401	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
22	b	616	CLA	CHB-C4A-NA	3.11	128.89	124.40
25	d	407	PL9	C32-C33-C34	-3.11	120.50	127.62
22	C	508	CLA	CHD-C1D-ND	-3.11	120.42	124.80
22	B	601	CLA	C3B-C4B-NB	-3.11	107.75	110.53
22	C	503	CLA	C4-C3-C5	3.11	120.62	115.23
22	c	513	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
22	b	614	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
28	e	101	LHG	O8-C23-C24	3.11	121.30	111.83
34	F	101	HEM	CBD-CAD-C3D	-3.10	103.96	112.53
22	c	506	CLA	C2D-C1D-ND	-3.09	107.06	110.13
22	d	404	CLA	O2D-CGD-CBD	3.09	116.64	111.23
27	A	410	SQD	C1-O5-C5	-3.09	107.68	113.72
22	b	614	CLA	C3B-C4B-NB	-3.09	107.77	110.53
31	Z	101	BCR	C27-C26-C25	3.08	126.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	610	CLA	CHB-C4A-NA	3.08	128.84	124.40
33	a	408	BCT	O3-C-O1	-3.07	111.81	119.68
31	a	405	BCR	C27-C26-C25	3.07	126.85	122.70
31	B	617	BCR	C15-C16-C17	-3.06	117.25	123.52
26	c	521	LMG	O2-C2-C1	-3.06	102.78	110.08
22	B	611	CLA	C1-C2-C3	-3.06	121.18	126.20
22	b	604	CLA	C4-C3-C5	3.06	120.54	115.23
31	B	617	BCR	C27-C26-C25	3.06	126.84	122.70
26	m	101	LMG	O6-C1-O1	-3.05	102.83	110.04
22	d	401	CLA	C4A-NA-C1A	3.05	108.07	106.68
27	A	410	SQD	O5-C1-O6	3.05	117.26	110.04
29	C	515	DGD	O3G-C3G-C2G	-3.05	103.40	110.82
28	D	413	LHG	O8-C23-O10	-3.05	116.01	123.63
31	D	406	BCR	C7-C8-C9	-3.04	121.73	126.23
31	K	102	BCR	C15-C16-C17	-3.04	117.29	123.52
22	a	402	CLA	CHB-C4A-NA	3.04	128.79	124.40
22	c	504	CLA	C4A-NA-C1A	3.04	108.07	106.68
22	D	405	CLA	C4A-NA-C1A	3.04	108.06	106.68
27	f	102	SQD	O48-C23-O10	-3.04	116.03	123.63
27	L	101	SQD	O47-C7-C8	3.03	118.05	111.48
31	d	406	BCR	C3-C4-C5	-3.03	108.65	114.06
22	C	512	CLA	C3B-C4B-NB	-3.03	107.82	110.53
22	b	612	CLA	CHB-C4A-NA	3.03	128.77	124.40
22	b	612	CLA	CMB-C2B-C1B	-3.03	120.81	125.42
22	c	511	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
22	c	510	CLA	CHB-C4A-NA	3.02	128.75	124.40
22	b	614	CLA	C4-C3-C5	3.02	120.46	115.23
27	a	411	SQD	O9-S-C6	3.02	111.26	106.76
22	D	405	CLA	O1D-CGD-CBD	3.01	130.46	124.52
22	d	405	CLA	CMB-C2B-C3B	3.01	133.63	126.55
32	C	518	STE	O2-C1-O1	-3.01	115.59	123.33
23	D	401	PHO	C3B-C4B-NB	-3.01	105.50	107.46
22	C	504	CLA	C4A-NA-C1A	3.01	108.05	106.68
22	c	506	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
22	A	403	CLA	CED-O2D-CGD	-3.00	109.10	115.92
26	c	521	LMG	O1-C1-C2	-3.00	103.71	108.27
22	B	603	CLA	C6-C7-C8	-3.00	105.99	115.97
31	b	617	BCR	C27-C26-C25	3.00	126.76	122.70
22	B	610	CLA	O2D-CGD-CBD	3.00	116.47	111.23
25	A	408	PL9	C22-C23-C24	-2.99	120.77	127.62
22	C	509	CLA	CHB-C4A-NA	2.99	128.72	124.40
26	M	101	LMG	O6-C1-O1	-2.99	102.97	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	PHO	C1-C2-C3	-2.99	121.30	126.20
27	D	409	SQD	O48-C23-C24	2.99	120.94	111.83
22	d	401	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	C	508	CLA	C3B-C4B-NB	-2.98	107.87	110.53
22	D	403	CLA	C1-C2-C3	-2.98	121.32	126.20
22	b	601	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
27	a	411	SQD	O5-C1-O6	2.97	117.06	110.04
22	B	614	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	C	504	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
22	c	508	CLA	C3B-C4B-NB	-2.97	107.88	110.53
22	b	604	CLA	CHB-C4A-NA	2.96	128.68	124.40
27	B	622	SQD	O9-S-O7	-2.96	104.19	113.82
25	a	409	PL9	C32-C33-C34	-2.96	120.85	127.62
31	d	406	BCR	C27-C26-C25	2.96	126.70	122.70
22	b	609	CLA	CHB-C4A-NA	2.96	128.66	124.40
22	A	405	CLA	CHD-C1D-ND	-2.95	120.64	124.80
22	C	506	CLA	C3B-C4B-NB	-2.95	107.89	110.53
22	C	510	CLA	C3B-C4B-NB	-2.95	107.89	110.53
22	b	605	CLA	O1D-CGD-CBD	2.95	130.34	124.52
32	t	103	STE	O2-C1-C2	2.95	123.31	114.00
22	c	502	CLA	CHD-C1D-ND	-2.95	120.66	124.80
26	c	519	LMG	O2-C2-C3	-2.94	103.44	110.38
27	A	410	SQD	C1-C2-C3	-2.94	103.82	110.01
22	d	404	CLA	CHB-C4A-NA	2.94	128.64	124.40
29	c	516	DGD	C3G-C2G-C1G	-2.94	104.94	111.78
25	A	408	PL9	C27-C28-C29	-2.93	120.91	127.62
22	B	613	CLA	O1D-CGD-CBD	2.93	130.30	124.52
22	B	609	CLA	CHD-C4C-NC	2.93	128.77	124.23
29	C	515	DGD	CDB-CCB-CBB	-2.93	99.56	114.37
22	b	604	CLA	C3B-C4B-NB	-2.93	107.92	110.53
26	c	522	LMG	O2-C2-C1	-2.93	103.10	110.08
22	b	616	CLA	C3B-C4B-NB	-2.93	107.92	110.53
22	d	404	CLA	C1-C2-C3	-2.93	121.40	126.20
31	c	515	BCR	C2-C1-C6	2.93	114.69	110.44
35	V	201	HEC	C4B-NB-C1B	2.92	108.67	105.21
22	C	505	CLA	O2A-CGA-O1A	-2.92	116.33	123.63
26	b	622	LMG	O2-C2-C1	-2.91	103.13	110.08
31	c	515	BCR	C27-C26-C25	2.91	126.64	122.70
29	C	515	DGD	O2D-C2D-C1D	-2.91	103.14	110.08
28	D	413	LHG	O8-C23-C24	2.91	120.71	111.83
29	c	517	DGD	C3D-C4D-C5D	-2.91	104.96	110.23
28	d	408	LHG	O8-C23-C24	2.91	120.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	405	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
25	D	407	PL9	C30-C29-C31	-2.91	110.18	115.23
23	d	402	PHO	O2D-CGD-O1D	-2.90	118.19	123.85
22	b	615	CLA	C3B-C4B-NB	-2.90	107.94	110.53
31	H	101	BCR	C2-C1-C6	2.90	114.65	110.44
31	C	514	BCR	C7-C8-C9	-2.90	121.95	126.23
22	B	612	CLA	C11-C12-C13	-2.90	106.34	115.97
22	c	504	CLA	C4-C3-C5	2.90	120.25	115.23
29	H	102	DGD	C4E-C3E-C2E	-2.89	105.75	110.83
29	H	102	DGD	C1D-C2D-C3D	-2.89	103.92	110.01
35	v	201	HEC	CBA-CAA-C2A	-2.89	104.53	112.53
22	b	610	CLA	CAA-CBA-CGA	-2.89	104.99	113.21
22	B	609	CLA	C2C-C1C-NC	2.89	113.02	109.98
31	a	405	BCR	C7-C8-C9	-2.89	121.96	126.23
22	d	401	CLA	CED-O2D-CGD	-2.89	109.36	115.92
27	L	101	SQD	O47-C45-C46	2.89	118.70	108.34
31	a	405	BCR	C37-C22-C21	-2.89	118.14	122.82
31	Z	101	BCR	C7-C8-C9	-2.88	121.97	126.23
22	B	602	CLA	C4A-NA-C1A	2.88	108.00	106.68
29	c	516	DGD	O2D-C2D-C1D	-2.88	103.20	110.08
22	B	613	CLA	CHA-C1A-NA	-2.88	119.86	126.39
28	D	413	LHG	O3-P-O5	-2.88	97.51	108.94
23	A	404	PHO	C1A-C2A-C3A	-2.88	100.10	102.84
22	d	404	CLA	C2B-C1B-NB	-2.88	107.34	110.33
22	D	404	CLA	C16-C15-C13	-2.87	106.41	115.97
31	x	101	BCR	C38-C26-C25	-2.87	121.35	124.48
23	a	403	PHO	O2D-CGD-CBD	2.87	114.10	110.95
22	b	605	CLA	CHD-C1D-ND	-2.87	120.76	124.80
22	b	612	CLA	C3B-C4B-NB	-2.87	107.97	110.53
22	B	603	CLA	O2A-CGA-O1A	-2.87	116.46	123.63
22	B	616	CLA	C2A-C3A-C4A	2.86	106.50	101.87
22	B	612	CLA	O2A-CGA-O1A	-2.86	116.47	123.63
22	C	511	CLA	CAC-C3C-C4C	2.86	128.51	124.79
29	C	516	DGD	C7B-C6B-C5B	-2.86	99.91	114.37
27	B	622	SQD	C4-C3-C2	2.86	115.85	110.83
32	L	103	STE	O2-C1-C2	2.86	123.03	114.00
27	f	102	SQD	C1-C2-C3	-2.85	104.01	110.01
22	A	402	CLA	C1D-ND-C4D	-2.85	104.31	106.31
22	c	510	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
22	b	608	CLA	CHB-C4A-NA	2.85	128.51	124.40
22	C	504	CLA	C3B-C4B-NB	-2.85	107.99	110.53
22	B	616	CLA	O2D-CGD-O1D	-2.84	118.31	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	410	SQD	O5-C5-C4	2.84	114.82	109.70
22	d	404	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
22	c	510	CLA	C16-C15-C13	-2.84	106.53	115.97
22	c	503	CLA	C4A-NA-C1A	2.84	107.97	106.68
22	c	506	CLA	CHB-C4A-NA	2.84	128.50	124.40
22	c	501	CLA	O2D-CGD-CBD	2.84	116.19	111.23
22	c	502	CLA	C1-C2-C3	-2.84	121.55	126.20
28	l	101	LHG	O8-C23-C24	2.83	120.47	111.83
22	C	508	CLA	CMB-C2B-C1B	-2.83	121.11	125.42
22	C	510	CLA	CMB-C2B-C1B	-2.83	121.12	125.42
27	B	622	SQD	O48-C23-O10	-2.82	116.56	123.63
22	C	510	CLA	C1D-ND-C4D	2.82	108.29	106.31
22	b	610	CLA	C4A-NA-C1A	2.82	107.97	106.68
22	C	504	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
27	L	101	SQD	O2-C2-C1	2.81	116.78	110.08
22	C	509	CLA	CMB-C2B-C1B	-2.81	121.14	125.42
22	A	402	CLA	O1D-CGD-CBD	2.81	130.06	124.52
27	B	622	SQD	O5-C5-C4	2.81	114.76	109.70
31	c	514	BCR	C37-C22-C21	-2.81	118.27	122.82
22	b	602	CLA	O2A-CGA-O1A	-2.81	116.61	123.63
31	b	618	BCR	C15-C16-C17	-2.80	117.78	123.52
22	B	605	CLA	C16-C15-C13	-2.80	106.64	115.97
22	C	503	CLA	C3B-C4B-NB	-2.80	108.03	110.53
22	B	613	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
22	b	612	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
22	b	603	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
22	b	616	CLA	CHC-C4B-NB	2.80	128.25	124.05
31	b	617	BCR	C15-C16-C17	-2.80	117.79	123.52
22	A	403	CLA	O2D-CGD-CBD	2.79	116.11	111.23
22	c	502	CLA	CHD-C1D-C2D	2.79	131.30	125.49
22	b	611	CLA	CHD-C1D-C2D	2.79	131.29	125.49
22	C	508	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	c	505	CLA	C4A-NA-C1A	2.79	107.95	106.68
31	C	514	BCR	C36-C18-C17	-2.78	118.31	122.82
31	b	619	BCR	C37-C22-C21	-2.78	118.31	122.82
22	B	612	CLA	CHB-C4A-NA	2.78	128.41	124.40
22	c	505	CLA	O2A-CGA-O1A	-2.77	116.69	123.63
22	B	608	CLA	CHB-C1B-NB	2.77	128.21	124.05
31	b	619	BCR	C29-C30-C25	2.77	114.47	110.44
22	B	604	CLA	C2D-C1D-ND	-2.77	107.38	110.13
22	b	611	CLA	O2A-CGA-O1A	-2.77	116.69	123.63
22	b	603	CLA	C3B-C4B-NB	-2.77	108.06	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	611	CLA	CHB-C4A-NA	2.77	128.40	124.40
27	L	101	SQD	O9-S-C6	2.77	110.89	106.76
27	L	101	SQD	O8-S-C6	2.77	111.31	105.97
35	V	201	HEC	C2B-C1B-NB	-2.76	106.71	109.90
25	a	409	PL9	C12-C13-C14	-2.76	121.30	127.62
22	b	603	CLA	CHB-C1B-NB	2.76	128.19	124.05
26	A	409	LMG	C9-C8-C7	-2.76	105.35	111.78
22	b	611	CLA	CHB-C4A-NA	2.76	128.38	124.40
22	b	611	CLA	CHD-C1D-ND	-2.75	120.93	124.80
29	c	517	DGD	O5D-C1E-C2E	2.75	112.45	108.27
25	a	409	PL9	C40-C39-C41	2.75	120.00	115.23
35	V	201	HEC	CMD-C2D-C1D	2.75	129.33	125.03
22	c	502	CLA	C6-C5-C3	-2.75	106.78	113.47
31	B	619	BCR	C36-C18-C17	-2.75	118.37	122.82
22	D	404	CLA	C3B-C4B-NB	-2.74	108.08	110.53
22	D	404	CLA	CHB-C4A-NA	2.74	128.36	124.40
23	d	402	PHO	O2A-CGA-O1A	-2.74	116.78	123.63
22	b	613	CLA	CAC-C3C-C4C	2.74	128.35	124.79
29	h	101	DGD	C1D-C2D-C3D	-2.74	104.25	110.01
35	v	201	HEC	CMD-C2D-C1D	2.74	129.31	125.03
22	B	608	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
22	c	512	CLA	CHB-C4A-NA	2.73	128.35	124.40
22	c	512	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
22	C	509	CLA	C3B-C4B-NB	-2.73	108.09	110.53
22	B	611	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
22	B	616	CLA	CHB-C4A-NA	2.73	128.34	124.40
26	d	410	LMG	O1-C1-C2	-2.72	104.14	108.27
31	k	101	BCR	C38-C26-C25	-2.72	121.51	124.48
31	b	618	BCR	C8-C7-C6	-2.72	119.73	127.00
22	A	403	CLA	CHB-C4A-NA	2.72	128.32	124.40
22	B	612	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
22	c	502	CLA	C4D-C3D-CAD	-2.72	105.15	108.11
22	C	510	CLA	O2D-CGD-CBD	2.72	115.98	111.23
29	c	516	DGD	O6D-C1D-O3G	-2.72	103.62	110.04
22	b	604	CLA	C11-C12-C13	-2.72	106.94	115.97
28	d	409	LHG	C26-C25-C24	2.72	123.11	113.13
22	c	512	CLA	CHD-C1D-ND	-2.72	120.98	124.80
31	D	406	BCR	C24-C23-C22	-2.71	122.22	126.23
31	t	101	BCR	C1-C6-C5	-2.71	118.93	122.64
22	C	503	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
22	c	512	CLA	CHD-C4C-NC	2.71	128.43	124.23
26	M	101	LMG	C38-C37-C36	-2.71	100.69	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CAB-C3B-C4B	2.71	128.31	124.79
22	b	605	CLA	CHB-C4A-NA	2.70	128.30	124.40
22	B	602	CLA	C1-C2-C3	-2.70	121.78	126.20
35	v	201	HEC	C1D-C2D-C3D	-2.70	104.14	106.98
34	F	101	HEM	CHC-C1C-NC	2.69	127.39	124.45
34	f	101	HEM	CHD-C4C-NC	2.69	127.39	124.45
29	c	516	DGD	O4D-C4D-C5D	-2.69	102.69	109.32
29	h	101	DGD	O6E-C5E-C4E	2.69	114.55	109.70
31	k	102	BCR	C27-C26-C25	2.69	126.34	122.70
23	A	404	PHO	C5-C3-C2	2.69	127.20	121.17
31	H	101	BCR	C27-C26-C25	2.69	126.34	122.70
22	b	601	CLA	CHD-C4C-NC	2.69	128.40	124.23
26	m	101	LMG	O7-C10-O9	-2.69	117.42	123.70
31	t	101	BCR	C7-C8-C9	-2.68	122.26	126.23
22	d	403	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
31	k	102	BCR	C39-C30-C25	-2.68	106.04	110.24
29	H	102	DGD	O6D-C1D-O3G	-2.68	103.71	110.04
22	B	616	CLA	O1D-CGD-CBD	2.68	129.81	124.52
22	c	509	CLA	CHD-C1D-ND	-2.68	121.03	124.80
34	f	101	HEM	CBA-CAA-C2A	-2.67	105.14	112.53
31	K	101	BCR	C8-C7-C6	-2.67	119.85	127.00
27	L	101	SQD	O47-C7-O49	-2.67	117.45	123.70
22	c	510	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
22	b	612	CLA	C11-C10-C8	-2.67	107.08	115.97
22	c	501	CLA	CMB-C2B-C1B	-2.67	121.36	125.42
23	d	402	PHO	C1-C2-C3	-2.67	121.83	126.20
22	C	506	CLA	CHB-C4A-NA	2.67	128.25	124.40
31	d	406	BCR	C16-C15-C14	-2.67	118.06	123.52
22	b	605	CLA	CHD-C4C-NC	2.67	128.37	124.23
31	d	406	BCR	C11-C10-C9	-2.67	123.54	127.28
22	B	613	CLA	C1-C2-C3	-2.67	121.83	126.20
25	D	407	PL9	C12-C13-C14	-2.66	121.53	127.62
28	a	410	LHG	C11-C10-C9	-2.66	100.91	114.37
22	A	402	CLA	CMB-C2B-C1B	-2.66	121.36	125.42
33	D	402	BCT	O3-C-O1	-2.66	112.87	119.68
22	C	501	CLA	C4-C3-C5	2.66	119.85	115.23
28	D	410	LHG	O8-C23-C24	2.66	119.94	111.83
29	c	516	DGD	O3G-C3G-C2G	-2.66	104.35	110.82
31	K	102	BCR	C37-C22-C21	-2.66	118.51	122.82
28	D	410	LHG	C11-C10-C9	-2.66	100.94	114.37
22	a	402	CLA	C2A-C1A-CHA	2.65	128.47	123.87
22	b	613	CLA	C3B-C4B-NB	-2.65	108.16	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	408	LMG	O8-C28-O10	-2.65	116.99	123.63
22	b	608	CLA	O2D-CGD-CBD	2.65	115.87	111.23
31	c	514	BCR	C36-C18-C17	-2.65	118.52	122.82
22	C	512	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
22	C	508	CLA	CHD-C1D-C2D	2.64	130.99	125.49
22	B	616	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	a	405	BCR	C39-C30-C25	-2.64	106.10	110.24
22	A	403	CLA	C2D-C1D-ND	-2.64	107.51	110.13
22	C	512	CLA	C1-C2-C3	-2.64	121.87	126.20
22	c	507	CLA	CHD-C1D-ND	-2.64	121.09	124.80
35	v	201	HEC	C3D-C4D-ND	-2.64	107.80	110.35
29	c	518	DGD	CDB-CCB-CBB	-2.64	101.04	114.37
22	c	509	CLA	O1D-CGD-CBD	2.64	129.72	124.52
22	B	604	CLA	O2A-CGA-CBA	2.64	119.87	111.83
31	x	101	BCR	C15-C16-C17	-2.64	118.13	123.52
25	a	409	PL9	C42-C43-C44	-2.64	121.59	127.62
29	A	413	DGD	C3G-C2G-C1G	-2.64	105.64	111.78
22	B	605	CLA	CHD-C1D-ND	-2.63	121.10	124.80
31	C	514	BCR	C2-C1-C6	2.63	114.25	110.44
22	b	604	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
26	c	522	LMG	O3-C3-C2	-2.62	104.19	110.38
22	c	512	CLA	O1D-CGD-CBD	2.62	129.69	124.52
25	d	407	PL9	C42-C43-C44	-2.62	121.62	127.62
22	B	604	CLA	CMB-C2B-C1B	-2.62	121.43	125.42
25	a	409	PL9	C20-C19-C21	2.62	119.77	115.23
27	L	101	SQD	O9-S-O7	-2.62	105.31	113.82
31	t	101	BCR	C15-C16-C17	-2.62	118.16	123.52
29	C	516	DGD	CDB-CCB-CBB	-2.61	101.16	114.37
23	A	404	PHO	C4B-NB-C1B	2.61	112.62	108.82
35	V	201	HEC	CBD-CAD-C3D	-2.61	105.31	112.53
26	c	521	LMG	O8-C28-O10	-2.61	117.10	123.63
25	a	409	PL9	C22-C23-C24	-2.61	121.66	127.62
35	V	201	HEC	CMC-C2C-C1C	-2.61	121.45	125.42
27	a	411	SQD	O47-C7-C8	2.60	117.11	111.48
25	D	407	PL9	C42-C43-C44	-2.60	121.67	127.62
25	a	409	PL9	C7-C8-C9	-2.60	122.35	126.83
22	b	615	CLA	CAA-CBA-CGA	-2.60	105.83	113.21
29	c	517	DGD	C8B-C7B-C6B	-2.60	101.24	114.37
31	c	514	BCR	C15-C14-C13	-2.60	123.64	127.28
35	V	201	HEC	C1D-C2D-C3D	-2.59	104.25	106.98
22	C	505	CLA	CHB-C4A-NA	2.59	128.14	124.40
22	C	504	CLA	CMB-C2B-C1B	-2.59	121.48	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	607	CLA	CMB-C2B-C1B	-2.59	121.48	125.42
31	c	514	BCR	C27-C26-C25	2.59	126.20	122.70
22	C	503	CLA	C4D-CHA-C1A	2.59	124.33	121.24
22	A	402	CLA	CHD-C1D-ND	-2.59	121.16	124.80
22	B	610	CLA	O1D-CGD-CBD	2.59	129.62	124.52
22	C	506	CLA	C2D-C1D-ND	-2.59	107.57	110.13
22	b	603	CLA	CHD-C1D-ND	-2.59	121.16	124.80
22	A	405	CLA	C4-C3-C5	2.58	119.72	115.23
29	c	518	DGD	C3G-C2G-C1G	-2.58	105.76	111.78
28	A	411	LHG	O8-C23-C24	2.58	119.72	111.83
22	B	610	CLA	CHC-C1C-NC	2.58	128.20	124.31
32	c	523	STE	O2-C1-C2	2.58	122.16	114.00
22	b	602	CLA	C1-C2-C3	-2.58	121.98	126.20
28	a	410	LHG	O8-C23-C24	2.57	119.68	111.83
22	B	605	CLA	CHB-C4A-NA	2.57	128.11	124.40
26	A	409	LMG	O3-C3-C2	-2.57	104.32	110.38
31	k	101	BCR	C27-C26-C25	2.57	126.18	122.70
31	a	405	BCR	C16-C17-C18	-2.57	123.67	127.28
27	B	622	SQD	C46-C45-C44	-2.56	105.81	111.78
29	c	516	DGD	C4E-C3E-C2E	-2.56	106.33	110.83
22	C	505	CLA	CMB-C2B-C3B	2.56	132.58	126.55
22	c	502	CLA	C1D-ND-C4D	2.56	108.11	106.31
22	C	513	CLA	CHC-C1C-NC	2.56	128.17	124.31
22	C	502	CLA	CHA-C1A-NA	-2.56	120.59	126.39
22	B	603	CLA	O1D-CGD-CBD	2.56	129.56	124.52
25	a	409	PL9	C30-C29-C28	-2.56	117.06	123.63
22	B	612	CLA	CMB-C2B-C3B	2.55	132.55	126.55
22	B	607	CLA	CHD-C1D-ND	-2.55	121.21	124.80
22	c	503	CLA	C3B-C4B-NB	-2.55	108.25	110.53
22	b	601	CLA	O2D-CGD-CBD	2.55	115.69	111.23
26	c	522	LMG	O2-C2-C3	-2.55	104.37	110.38
22	A	402	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
22	A	402	CLA	C3B-C4B-NB	-2.54	108.26	110.53
27	B	622	SQD	O9-S-C6	2.54	110.55	106.76
29	C	515	DGD	O3E-C3E-C2E	-2.54	104.39	110.38
31	k	102	BCR	C1-C6-C5	-2.54	119.16	122.64
22	b	606	CLA	CHB-C1B-NB	2.54	127.86	124.05
22	c	509	CLA	C1-O2A-CGA	-2.54	110.51	116.65
31	c	514	BCR	C7-C8-C9	-2.54	122.48	126.23
22	A	402	CLA	C7-C6-C5	-2.53	106.51	113.26
27	A	410	SQD	O48-C23-C24	2.53	119.56	111.83
35	v	201	HEC	C2A-C1A-NA	-2.53	107.88	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	521	LMG	O6-C1-O1	-2.53	104.06	110.04
28	e	101	LHG	C11-C10-C9	-2.53	101.58	114.37
22	B	611	CLA	C3B-C4B-NB	-2.53	108.27	110.53
29	A	413	DGD	O3E-C3E-C2E	-2.53	104.41	110.38
22	b	609	CLA	CHB-C1B-NB	2.53	127.84	124.05
31	I	101	BCR	C37-C22-C21	-2.53	118.72	122.82
26	D	412	LMG	O7-C10-O9	-2.52	117.80	123.70
28	D	411	LHG	O8-C23-C24	2.52	119.53	111.83
23	A	404	PHO	O2D-CGD-O1D	-2.52	118.94	123.85
22	c	508	CLA	CHB-C4A-NA	2.52	128.03	124.40
31	B	618	BCR	C7-C8-C9	-2.52	122.51	126.23
22	C	511	CLA	C1-C2-C3	-2.52	122.07	126.20
27	D	409	SQD	O9-S-O7	-2.52	105.64	113.82
22	B	602	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
22	C	508	CLA	CHD-C4C-NC	2.51	128.13	124.23
27	A	410	SQD	O6-C44-C45	2.51	116.93	110.82
31	x	101	BCR	C36-C18-C17	-2.51	118.75	122.82
22	b	613	CLA	CMB-C2B-C3B	2.51	132.45	126.55
29	C	517	DGD	O5D-C6D-C5D	-2.51	103.77	109.42
22	B	616	CLA	CHC-C4B-NB	2.51	127.81	124.05
22	C	508	CLA	C3C-C4C-NC	-2.50	107.22	110.43
22	C	505	CLA	C1D-ND-C4D	2.50	108.07	106.31
22	b	614	CLA	O2D-CGD-CBD	2.50	115.61	111.23
22	D	404	CLA	C1-C2-C3	-2.50	122.10	126.20
34	F	101	HEM	CBA-CAA-C2A	-2.50	105.61	112.53
22	C	510	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	c	504	CLA	C6-C7-C8	-2.50	107.65	115.97
22	b	614	CLA	CHB-C4A-NA	2.50	128.01	124.40
22	A	403	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
22	B	606	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
27	B	622	SQD	O47-C45-C46	2.50	117.30	108.34
26	b	622	LMG	C3-C4-C5	-2.50	105.70	110.23
35	V	201	HEC	C1B-C2B-C3B	2.50	109.61	106.98
29	c	517	DGD	O5D-C6D-C5D	-2.50	103.79	109.42
25	D	407	PL9	C8-C7-C3	2.50	118.48	112.03
22	b	608	CLA	C4A-NA-C1A	2.50	107.82	106.68
22	B	605	CLA	CHD-C4C-NC	2.50	128.10	124.23
31	T	101	BCR	C37-C22-C23	2.49	121.90	118.09
22	c	503	CLA	O1D-CGD-CBD	2.49	129.43	124.52
22	b	615	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
29	c	517	DGD	C4E-C3E-C2E	-2.49	106.46	110.83
22	B	603	CLA	O2D-CGD-CBD	2.49	115.58	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	607	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
29	H	102	DGD	O2G-C1B-O1B	-2.48	117.90	123.70
25	d	407	PL9	C7-C8-C9	-2.48	122.56	126.83
22	b	611	CLA	CED-O2D-CGD	-2.48	110.29	115.92
26	c	522	LMG	O8-C28-O10	-2.48	117.43	123.63
29	h	101	DGD	C4E-C3E-C2E	-2.48	106.48	110.83
31	I	101	BCR	C34-C9-C8	-2.48	114.30	118.09
22	a	404	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
22	d	404	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
31	K	102	BCR	C28-C27-C26	-2.48	109.64	114.06
31	C	514	BCR	C36-C18-C19	2.48	121.87	118.09
22	B	608	CLA	CHD-C4C-NC	2.48	128.07	124.23
25	a	409	PL9	C37-C38-C39	-2.48	121.95	127.62
22	c	506	CLA	C3B-C4B-NB	-2.48	108.32	110.53
22	b	604	CLA	C6-C7-C8	-2.48	107.74	115.97
22	b	611	CLA	C2D-C1D-ND	-2.47	107.68	110.13
22	d	404	CLA	CHC-C4B-NB	2.47	127.76	124.05
22	b	611	CLA	C3A-C2A-C1A	2.47	105.04	101.34
35	V	201	HEC	CHB-C4A-NA	2.47	127.14	124.45
22	a	404	CLA	CHA-C1A-NA	-2.47	120.80	126.39
22	b	607	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
22	b	612	CLA	C11-C12-C13	-2.47	107.76	115.97
22	b	607	CLA	CHD-C1D-ND	-2.47	121.33	124.80
22	c	502	CLA	CMB-C2B-C3B	2.47	132.35	126.55
22	b	610	CLA	CAC-C3C-C4C	2.46	127.99	124.79
25	D	407	PL9	C7-C8-C9	-2.46	122.59	126.83
26	d	410	LMG	O3-C3-C2	-2.46	104.57	110.38
26	Y	101	LMG	O6-C5-C6	2.46	112.54	106.44
22	B	601	CLA	C4-C3-C5	2.46	119.50	115.23
22	c	506	CLA	C1D-ND-C4D	2.46	108.04	106.31
22	D	405	CLA	C2D-C1D-ND	-2.46	107.69	110.13
26	Y	101	LMG	O2-C2-C1	-2.46	104.22	110.08
22	c	507	CLA	O2D-CGD-CBD	2.46	115.52	111.23
22	b	604	CLA	CMB-C2B-C1B	-2.46	121.68	125.42
22	B	605	CLA	CHD-C1D-C2D	2.45	130.59	125.49
25	d	407	PL9	C20-C19-C21	2.45	119.49	115.23
27	A	412	SQD	O47-C45-C44	2.45	113.45	107.96
29	C	517	DGD	C3G-C2G-C1G	-2.45	106.07	111.78
22	a	402	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
31	t	101	BCR	C4-C5-C6	2.45	126.02	122.70
23	a	403	PHO	O2D-CGD-O1D	-2.45	119.08	123.85
31	B	619	BCR	C30-C25-C26	-2.45	119.29	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	409	SQD	O48-C23-O10	-2.45	117.50	123.63
25	a	409	PL9	C27-C28-C29	-2.45	122.02	127.62
29	C	516	DGD	CAB-C9B-C8B	-2.45	101.99	114.37
31	x	101	BCR	C34-C9-C8	-2.45	114.35	118.09
22	B	612	CLA	O1D-CGD-CBD	2.45	129.34	124.52
22	B	608	CLA	C3B-C4B-NB	-2.44	108.35	110.53
22	C	503	CLA	C1-O2A-CGA	2.44	122.56	116.65
22	C	501	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
22	C	503	CLA	CHD-C1D-ND	-2.44	121.37	124.80
29	h	101	DGD	O3G-C3G-C2G	-2.44	104.88	110.82
22	c	507	CLA	C2C-C1C-NC	2.44	112.54	109.98
22	D	405	CLA	CHB-C1B-NB	2.44	127.70	124.05
31	I	101	BCR	C15-C16-C17	-2.44	118.54	123.52
22	B	608	CLA	CHB-C4A-NA	2.44	127.91	124.40
25	d	407	PL9	C27-C28-C29	-2.43	122.06	127.62
22	c	504	CLA	C1-C2-C3	-2.43	122.21	126.20
31	b	618	BCR	C38-C26-C25	-2.43	121.83	124.48
26	c	521	LMG	O7-C10-O9	-2.43	118.02	123.70
22	B	610	CLA	CHD-C1D-ND	-2.43	121.38	124.80
22	b	609	CLA	C6-C5-C3	2.43	119.39	113.47
22	b	605	CLA	C1D-ND-C4D	-2.43	104.61	106.31
22	b	612	CLA	CMB-C2B-C3B	2.43	132.26	126.55
22	c	513	CLA	O1D-CGD-CBD	2.43	129.31	124.52
22	a	402	CLA	O2A-CGA-O1A	-2.43	117.56	123.63
22	b	611	CLA	CGD-CBD-CAD	-2.43	102.99	110.85
22	B	608	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
26	d	410	LMG	O6-C5-C4	2.42	114.06	109.70
27	L	101	SQD	O5-C1-C2	-2.42	105.40	110.37
22	d	403	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
22	b	611	CLA	CAA-CBA-CGA	-2.42	106.35	113.21
22	c	508	CLA	C7-C6-C5	-2.41	106.83	113.26
31	x	101	BCR	C37-C22-C21	-2.41	118.91	122.82
22	c	508	CLA	CHD-C1D-ND	-2.41	121.41	124.80
29	H	102	DGD	C3E-C4E-C5E	-2.41	105.86	110.23
31	I	101	BCR	C11-C10-C9	-2.41	123.90	127.28
27	D	409	SQD	C1-C2-C3	-2.41	104.94	110.01
22	d	401	CLA	CAC-C3C-C4C	2.41	127.92	124.79
34	F	101	HEM	C1D-C2D-C3D	2.41	109.51	106.98
22	A	402	CLA	C16-C15-C13	-2.41	107.97	115.97
31	c	514	BCR	C11-C10-C9	-2.40	123.91	127.28
31	d	406	BCR	C2-C1-C6	2.40	113.93	110.44
31	d	406	BCR	C7-C8-C9	-2.40	122.68	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	606	CLA	C3B-C4B-NB	-2.40	108.39	110.53
31	b	619	BCR	C20-C21-C22	-2.40	123.91	127.28
31	t	101	BCR	C36-C18-C19	2.40	121.75	118.09
22	b	605	CLA	CHD-C4C-C3C	-2.40	121.28	124.77
22	b	605	CLA	C3B-C4B-NB	-2.40	108.39	110.53
26	b	622	LMG	O6-C5-C6	2.39	112.37	106.44
25	d	407	PL9	C50-C49-C48	-2.39	115.47	122.66
29	H	102	DGD	CDB-CCB-CBB	-2.39	102.28	114.37
29	h	101	DGD	O6D-C1D-O3G	-2.39	104.39	110.04
22	C	507	CLA	O1D-CGD-CBD	2.39	129.23	124.52
22	d	403	CLA	C1-C2-C3	-2.39	122.28	126.20
31	B	618	BCR	C35-C13-C14	-2.39	118.94	122.82
35	V	201	HEC	C1C-C2C-C3C	2.39	109.55	106.82
34	f	101	HEM	CAB-C3B-C2B	-2.39	120.67	128.43
23	A	404	PHO	CMB-C2B-C3B	2.39	129.45	124.68
22	B	604	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	x	101	BCR	C7-C8-C9	-2.38	122.71	126.23
22	D	405	CLA	CHC-C4B-NB	2.38	127.62	124.05
29	C	517	DGD	O3E-C3E-C2E	-2.38	104.76	110.38
25	d	407	PL9	C45-C44-C46	-2.38	111.10	115.23
31	x	101	BCR	C2-C1-C6	2.38	113.89	110.44
25	a	409	PL9	O2-C1-C2	-2.38	116.43	121.83
29	C	516	DGD	O6D-C1D-O3G	-2.37	104.43	110.04
22	b	603	CLA	C7-C6-C5	-2.37	106.94	113.26
22	b	605	CLA	CHC-C1C-NC	2.37	127.88	124.31
22	b	605	CLA	C3D-C4D-ND	2.37	113.84	109.99
22	B	609	CLA	CHD-C4C-C3C	-2.37	121.32	124.77
22	b	613	CLA	C7-C6-C5	-2.37	106.94	113.26
22	C	504	CLA	O2D-CGD-CBD	2.37	115.37	111.23
22	C	508	CLA	CHB-C1B-NB	2.37	127.61	124.05
29	A	413	DGD	O3D-C3D-C4D	-2.37	104.80	110.38
22	C	503	CLA	C3A-C2A-C1A	2.36	104.88	101.34
31	a	405	BCR	C38-C26-C27	-2.36	108.55	113.60
22	c	509	CLA	CMB-C2B-C3B	2.36	132.11	126.55
22	B	602	CLA	C16-C15-C13	-2.36	108.11	115.97
31	Z	101	BCR	C36-C18-C17	-2.36	118.99	122.82
31	t	101	BCR	C2-C1-C6	2.36	113.87	110.44
22	b	616	CLA	C2C-C1C-NC	2.36	112.46	109.98
29	c	517	DGD	CDB-CCB-CBB	-2.36	102.43	114.37
22	A	405	CLA	CHB-C4A-NA	2.36	127.81	124.40
31	B	619	BCR	C1-C6-C5	-2.36	119.41	122.64
22	C	503	CLA	O1D-CGD-CBD	2.36	129.18	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	517	DGD	CBB-CAB-C9B	-2.36	102.44	114.37
22	C	512	CLA	O1D-CGD-CBD	2.36	129.17	124.52
22	B	603	CLA	C3B-C4B-NB	-2.36	108.42	110.53
31	b	618	BCR	C37-C22-C21	-2.36	119.00	122.82
23	a	403	PHO	C3B-C4B-NB	-2.36	105.93	107.46
27	A	412	SQD	O49-C7-C8	-2.36	114.57	123.78
22	b	605	CLA	C4-C3-C2	-2.35	117.58	123.63
31	a	405	BCR	C29-C30-C25	2.35	113.85	110.44
26	b	622	LMG	O7-C10-O9	-2.35	118.21	123.70
25	A	408	PL9	C40-C39-C41	2.35	119.31	115.23
22	B	614	CLA	C4-C3-C5	2.35	119.30	115.23
22	c	504	CLA	O2D-CGD-CBD	2.35	115.33	111.23
22	b	610	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
22	c	507	CLA	CHA-C1A-NA	-2.35	121.08	126.39
29	c	518	DGD	O5E-C6E-C5E	-2.35	103.35	111.33
22	b	603	CLA	CHD-C1D-C2D	2.34	130.36	125.49
26	c	519	LMG	C9-C8-C7	-2.34	106.32	111.78
25	d	407	PL9	C12-C13-C14	-2.34	122.26	127.62
22	B	605	CLA	CHD-C4C-C3C	-2.34	121.36	124.77
31	H	101	BCR	C16-C15-C14	-2.34	118.73	123.52
22	B	609	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
22	b	609	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
22	a	404	CLA	C2B-C1B-NB	2.34	112.75	110.33
22	B	608	CLA	CMB-C2B-C3B	2.34	132.05	126.55
29	C	516	DGD	O6E-C5E-C4E	2.34	113.91	109.70
26	m	101	LMG	C1-O6-C5	-2.34	109.16	113.72
27	A	410	SQD	O48-C46-C45	2.34	115.13	108.40
23	A	404	PHO	O2D-CGD-CBD	2.34	113.51	110.95
22	C	502	CLA	C2A-C1A-CHA	2.34	127.92	123.87
27	D	409	SQD	C46-C45-C44	-2.34	106.12	113.67
22	B	606	CLA	CHB-C4A-NA	2.33	127.77	124.40
22	a	404	CLA	C3D-C4D-ND	2.33	113.78	109.99
22	B	610	CLA	C1-C2-C3	-2.33	122.37	126.20
22	c	501	CLA	O1D-CGD-CBD	2.33	129.12	124.52
23	d	402	PHO	C1A-C2A-C3A	-2.33	100.62	102.84
26	A	409	LMG	O5-C6-C5	-2.33	103.41	111.33
22	B	604	CLA	C2A-C1A-CHA	2.33	127.90	123.87
27	A	410	SQD	O8-S-C6	2.33	110.46	105.97
22	b	614	CLA	CMB-C2B-C1B	-2.32	121.88	125.42
22	b	612	CLA	C1-C2-C3	-2.32	122.39	126.20
28	L	102	LHG	C5-O7-C7	-2.32	112.23	117.80
22	C	505	CLA	C2D-C1D-ND	-2.32	107.83	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	516	DGD	O3D-C3D-C4D	-2.32	104.91	110.38
22	c	505	CLA	CHB-C4A-NA	2.32	127.75	124.40
31	k	101	BCR	C2-C1-C6	2.32	113.81	110.44
26	M	101	LMG	O3-C3-C2	-2.32	104.91	110.38
26	D	412	LMG	C38-C37-C36	-2.32	102.65	114.37
31	T	101	BCR	C30-C25-C26	-2.32	119.47	122.64
22	C	505	CLA	C1-O2A-CGA	-2.32	111.04	116.65
22	C	510	CLA	CMB-C2B-C3B	2.32	132.00	126.55
22	C	505	CLA	CHB-C1B-NB	2.32	127.52	124.05
26	B	626	LMG	O6-C5-C4	2.32	113.87	109.70
29	H	102	DGD	C8B-C7B-C6B	-2.32	102.67	114.37
31	I	101	BCR	C37-C22-C23	2.31	121.62	118.09
31	K	101	BCR	C38-C26-C25	-2.31	121.96	124.48
28	D	410	LHG	C20-C19-C18	-2.31	102.68	114.37
26	c	521	LMG	O3-C3-C2	-2.31	104.92	110.38
31	b	618	BCR	C27-C26-C25	2.31	125.83	122.70
22	b	606	CLA	C3C-C4C-NC	-2.31	107.47	110.43
22	c	503	CLA	CHD-C1D-ND	-2.31	121.55	124.80
22	B	613	CLA	C4-C3-C5	2.31	119.24	115.23
25	d	407	PL9	C40-C39-C38	-2.31	117.69	123.63
22	C	504	CLA	C4-C3-C5	2.31	119.24	115.23
26	M	101	LMG	C4-C3-C2	-2.31	106.78	110.83
22	c	513	CLA	CHB-C4A-NA	2.31	127.73	124.40
22	d	405	CLA	CHB-C1B-NB	2.31	127.51	124.05
22	b	609	CLA	CHA-C1A-NA	-2.31	121.17	126.39
22	B	605	CLA	CMC-C2C-C1C	2.31	128.64	125.03
31	c	515	BCR	C37-C22-C23	2.31	121.61	118.09
27	A	410	SQD	O3-C3-C2	2.31	115.81	110.38
22	c	513	CLA	C11-C12-C13	-2.30	108.31	115.97
22	C	509	CLA	CMB-C2B-C3B	2.30	131.96	126.55
22	b	606	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
22	b	611	CLA	C1-O2A-CGA	-2.30	111.08	116.65
31	B	619	BCR	C27-C26-C25	2.30	125.81	122.70
22	b	609	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
22	d	401	CLA	O2D-CGD-CBD	2.29	115.24	111.23
31	B	618	BCR	C15-C16-C17	-2.29	118.83	123.52
22	B	604	CLA	CHA-C1A-NA	-2.29	121.20	126.39
26	Y	101	LMG	O6-C1-O1	-2.29	104.63	110.04
22	B	602	CLA	C4-C3-C5	2.29	119.20	115.23
22	c	507	CLA	C1-C2-C3	-2.29	122.44	126.20
22	c	502	CLA	O1D-CGD-CBD	2.29	129.03	124.52
26	D	408	LMG	C3-C4-C5	-2.29	106.08	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	CMB-C2B-C3B	2.29	131.93	126.55
22	C	506	CLA	CGD-CBD-CAD	-2.29	103.44	110.85
22	c	505	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	b	619	BCR	C31-C1-C6	2.29	113.83	110.24
31	I	101	BCR	C8-C7-C6	-2.28	120.89	127.00
22	d	401	CLA	C3C-C4C-NC	-2.28	107.50	110.43
25	A	408	PL9	O2-C1-C2	-2.28	116.64	121.83
22	B	609	CLA	C2A-C3A-C4A	2.28	105.56	101.87
22	B	604	CLA	O1D-CGD-CBD	2.28	129.02	124.52
31	c	514	BCR	C38-C26-C25	-2.28	122.00	124.48
22	c	508	CLA	C1-C2-C3	-2.28	122.46	126.20
22	B	604	CLA	C1D-ND-C4D	2.28	107.91	106.31
31	b	619	BCR	C7-C8-C9	-2.28	122.87	126.23
22	B	602	CLA	CGD-CBD-CAD	-2.28	103.48	110.85
22	C	509	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
22	b	601	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
22	b	608	CLA	CHD-C1D-ND	-2.27	121.60	124.80
25	D	407	PL9	C27-C28-C29	-2.27	122.42	127.62
35	v	201	HEC	O1D-CGD-CBD	-2.27	115.88	123.09
22	b	603	CLA	OBD-CAD-C3D	2.27	133.73	128.42
28	d	409	LHG	O8-C23-C24	2.27	118.77	111.83
26	A	409	LMG	C40-C39-C38	-2.27	102.88	114.37
29	C	515	DGD	C5B-C4B-C3B	-2.27	102.89	114.37
29	C	516	DGD	C1D-O6D-C5D	-2.27	109.29	113.72
23	a	403	PHO	C4B-NB-C1B	2.27	112.12	108.82
29	h	101	DGD	C1E-O6E-C5E	2.27	118.15	113.72
22	B	603	CLA	CHB-C4A-NA	2.27	127.67	124.40
31	K	101	BCR	C12-C13-C14	-2.27	115.44	119.01
22	a	404	CLA	C4A-NA-C1A	2.27	107.71	106.68
22	A	403	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
22	C	508	CLA	CHB-C4A-NA	2.26	127.67	124.40
28	a	410	LHG	C20-C19-C18	-2.26	102.94	114.37
31	a	405	BCR	C37-C22-C23	2.26	121.54	118.09
29	c	516	DGD	O5E-C6E-C5E	-2.26	103.64	111.33
22	C	502	CLA	CHB-C1B-NB	2.26	127.44	124.05
32	t	103	STE	C3-C2-C1	-2.26	108.61	114.51
29	C	517	DGD	O2D-C2D-C1D	-2.26	104.70	110.08
22	C	502	CLA	C3B-C4B-NB	-2.26	108.52	110.53
22	b	608	CLA	CHD-C4C-C3C	-2.26	121.48	124.77
25	D	407	PL9	C7-C3-C2	-2.26	120.73	123.39
22	B	604	CLA	CMB-C2B-C3B	2.26	131.85	126.55
29	C	516	DGD	O4D-C4D-C3D	2.25	115.69	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	609	CLA	C2D-C1D-ND	-2.25	107.89	110.13
22	B	611	CLA	O1A-CGA-CBA	2.25	132.60	123.78
32	J	101	STE	O2-C1-C2	2.25	121.12	114.00
35	V	201	HEC	CHC-C1C-NC	2.25	127.95	123.86
22	A	403	CLA	CAC-C3C-C4C	2.25	127.72	124.79
22	C	503	CLA	CED-O2D-CGD	-2.25	110.81	115.92
22	c	508	CLA	CHD-C1D-C2D	2.25	130.17	125.49
29	C	516	DGD	O2G-C1B-C2B	-2.25	106.61	111.48
31	K	102	BCR	C2-C1-C6	2.25	113.71	110.44
22	A	402	CLA	CMD-C2D-C1D	2.25	128.69	124.73
26	Y	101	LMG	C3-C4-C5	-2.25	106.15	110.23
25	d	407	PL9	C7-C3-C4	2.25	118.76	116.91
22	c	502	CLA	CHD-C4C-NC	2.25	127.72	124.23
29	c	518	DGD	C5B-C4B-C3B	-2.24	103.02	114.37
22	C	513	CLA	CHB-C4A-NA	2.24	127.64	124.40
22	B	609	CLA	CHB-C4A-NA	2.24	127.64	124.40
31	c	515	BCR	C30-C25-C26	-2.24	119.57	122.64
26	d	410	LMG	C40-C39-C38	-2.24	103.04	114.37
22	b	611	CLA	CAA-C2A-C1A	-2.24	104.64	111.97
26	D	412	LMG	O1-C7-C8	-2.24	106.02	111.77
29	c	517	DGD	O2D-C2D-C1D	-2.24	104.75	110.08
31	b	617	BCR	C3-C4-C5	-2.24	110.07	114.06
31	K	101	BCR	C24-C23-C22	-2.24	122.93	126.23
34	F	101	HEM	C3C-C2C-C1C	2.24	109.16	107.05
29	C	516	DGD	O2D-C2D-C1D	-2.24	104.75	110.08
22	B	608	CLA	C1-O2A-CGA	2.23	122.06	116.65
25	a	409	PL9	O2-C1-C6	2.23	124.03	120.48
22	b	615	CLA	CHB-C4A-NA	2.23	127.62	124.40
22	C	509	CLA	C2A-C3A-C4A	2.23	105.47	101.87
29	C	517	DGD	O3D-C3D-C4D	-2.23	105.12	110.38
31	D	406	BCR	C3-C4-C5	-2.23	110.08	114.06
22	A	403	CLA	CHA-C1A-NA	-2.23	121.34	126.39
22	B	602	CLA	C6-C5-C3	-2.23	108.04	113.47
22	c	502	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
26	c	519	LMG	C38-C37-C36	-2.23	103.11	114.37
22	C	502	CLA	C4D-CHA-C1A	2.23	123.90	121.24
29	c	517	DGD	O3D-C3D-C4D	-2.23	105.13	110.38
31	H	101	BCR	C29-C30-C25	2.22	113.67	110.44
22	a	404	CLA	C4D-CHA-C1A	-2.22	118.59	121.24
22	C	507	CLA	CMB-C2B-C1B	-2.22	122.03	125.42
22	b	613	CLA	C2A-C3A-C4A	2.22	105.46	101.87
29	A	413	DGD	O5E-C6E-C5E	-2.22	103.77	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	619	BCR	C33-C5-C6	-2.22	122.06	124.48
22	b	603	CLA	CHB-C1B-C2B	-2.22	120.99	127.43
22	b	616	CLA	CMB-C2B-C3B	2.22	131.76	126.55
22	B	608	CLA	CHD-C1D-ND	-2.22	121.68	124.80
22	c	504	CLA	OBD-CAD-C3D	2.21	133.59	128.42
28	D	410	LHG	C27-C26-C25	-2.21	103.18	114.37
22	B	604	CLA	C11-C10-C8	-2.21	108.61	115.97
31	B	617	BCR	C3-C4-C5	-2.21	110.11	114.06
31	T	101	BCR	C37-C22-C21	-2.21	119.23	122.82
22	C	510	CLA	C11-C10-C8	-2.21	108.62	115.97
22	b	610	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
26	B	626	LMG	O6-C1-O1	-2.21	104.83	110.04
31	I	101	BCR	C40-C30-C25	2.21	113.70	110.24
22	b	601	CLA	CHD-C1D-C2D	2.21	130.07	125.49
35	V	201	HEC	CHB-C1B-C2B	2.20	128.51	125.03
22	d	401	CLA	CHD-C1D-C2D	2.20	130.07	125.49
22	C	507	CLA	CHD-C1D-ND	-2.20	121.70	124.80
22	c	502	CLA	C2D-C1D-ND	-2.20	107.95	110.13
22	C	502	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
31	d	406	BCR	C30-C25-C26	-2.20	119.63	122.64
22	C	502	CLA	CHC-C4B-NB	2.20	127.35	124.05
25	D	407	PL9	C37-C38-C39	-2.20	122.59	127.62
22	b	616	CLA	C2A-C3A-C4A	2.20	105.42	101.87
22	B	604	CLA	CHA-C4D-ND	2.20	137.08	132.55
31	C	514	BCR	C33-C5-C6	-2.19	122.09	124.48
22	B	606	CLA	O2D-CGD-CBD	2.19	115.07	111.23
31	b	619	BCR	C1-C6-C5	-2.19	119.64	122.64
22	b	603	CLA	O1D-CGD-CBD	2.19	128.84	124.52
28	a	410	LHG	O8-C23-O10	-2.19	118.14	123.63
29	C	516	DGD	C5B-C4B-C3B	-2.19	103.29	114.37
22	B	609	CLA	CHD-C1D-ND	-2.19	121.72	124.80
22	B	615	CLA	C6-C7-C8	-2.19	108.69	115.97
28	A	411	LHG	C20-C19-C18	-2.19	103.32	114.37
31	T	101	BCR	C38-C26-C25	-2.18	122.10	124.48
28	D	410	LHG	O8-C23-O10	-2.18	118.16	123.63
22	c	506	CLA	CAC-C3C-C4C	2.18	127.63	124.79
22	C	507	CLA	CMB-C2B-C3B	2.18	131.69	126.55
22	b	602	CLA	C3B-C4B-NB	-2.18	108.58	110.53
31	I	101	BCR	C36-C18-C17	-2.18	119.28	122.82
26	m	101	LMG	C9-C8-C7	-2.18	106.69	111.78
31	B	617	BCR	C15-C14-C13	-2.18	124.22	127.28
22	C	505	CLA	CAC-C3C-C4C	2.18	127.63	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	L	101	SQD	O8-S-O7	-2.18	105.94	111.40
22	d	403	CLA	C1D-ND-C4D	-2.18	104.78	106.31
22	b	607	CLA	C1-C2-C3	-2.18	122.62	126.20
22	B	605	CLA	CAA-CBA-CGA	-2.18	107.02	113.21
32	B	623	STE	O2-C1-C2	2.18	120.88	114.00
23	D	401	PHO	C4B-NB-C1B	2.18	111.99	108.82
28	A	411	LHG	C11-C10-C9	-2.18	103.36	114.37
31	b	618	BCR	C15-C14-C13	-2.18	124.22	127.28
28	e	101	LHG	C20-C19-C18	-2.18	103.36	114.37
22	C	506	CLA	OBD-CAD-C3D	2.18	133.50	128.42
22	c	513	CLA	C3B-C4B-NB	-2.18	108.59	110.53
29	h	101	DGD	C2G-O2G-C1B	2.18	123.00	117.80
32	b	621	STE	C3-C2-C1	-2.18	108.83	114.51
22	b	608	CLA	CHB-C1B-NB	2.17	127.31	124.05
22	B	609	CLA	C3B-C4B-NB	-2.17	108.59	110.53
35	V	201	HEC	CBC-CAC-C3C	2.17	118.31	112.42
22	B	606	CLA	C2A-C3A-C4A	2.17	105.38	101.87
22	B	606	CLA	CHA-C4D-ND	2.17	137.03	132.55
22	B	611	CLA	CHD-C4C-NC	2.17	127.60	124.23
23	d	402	PHO	C4B-NB-C1B	2.17	111.98	108.82
22	D	404	CLA	O2D-CGD-CBD	2.17	115.02	111.23
22	c	509	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
28	d	408	LHG	C27-C26-C25	-2.17	103.42	114.37
31	b	617	BCR	C38-C26-C25	-2.17	122.12	124.48
22	B	606	CLA	CHA-C1A-NA	-2.16	121.49	126.39
28	D	413	LHG	C11-C10-C9	-2.16	103.43	114.37
25	A	408	PL9	C25-C24-C26	2.16	118.98	115.23
22	C	513	CLA	CHB-C1B-NB	2.16	127.29	124.05
26	A	409	LMG	C3-C4-C5	-2.16	106.31	110.23
29	h	101	DGD	CBB-CAB-C9B	-2.16	103.44	114.37
22	a	402	CLA	CAC-C3C-C4C	2.16	127.60	124.79
22	C	505	CLA	C4A-NA-C1A	2.16	107.67	106.68
29	C	517	DGD	CDB-CCB-CBB	-2.16	103.44	114.37
22	B	610	CLA	C3B-C4B-NB	-2.16	108.60	110.53
29	A	413	DGD	O1G-C1A-O1A	-2.16	118.22	123.63
22	b	610	CLA	C3B-C2B-C1B	-2.16	104.62	107.17
22	b	614	CLA	C4-C3-C2	-2.16	118.08	123.63
22	b	613	CLA	O2D-CGD-CBD	2.16	115.00	111.23
28	d	408	LHG	C20-C19-C18	-2.16	103.47	114.37
22	B	603	CLA	CHC-C1C-NC	2.15	127.56	124.31
31	b	619	BCR	C27-C26-C25	2.15	125.61	122.70
22	d	403	CLA	C3B-C4B-NB	-2.15	108.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	f	102	SQD	C46-C45-C44	-2.15	106.76	111.78
28	D	411	LHG	C18-C17-C16	-2.15	103.49	114.37
22	C	507	CLA	CHD-C4C-NC	2.15	127.57	124.23
22	B	606	CLA	C4-C3-C5	2.15	118.96	115.23
22	D	405	CLA	CHA-C1A-NA	-2.15	121.52	126.39
26	M	101	LMG	O5-C6-C5	-2.15	104.01	111.33
29	c	518	DGD	O6E-C1E-O5D	-2.15	104.96	110.04
28	L	102	LHG	C20-C19-C18	-2.15	103.49	114.37
27	t	102	SQD	O49-C7-C8	-2.15	115.37	123.78
31	c	515	BCR	C35-C13-C14	-2.15	119.33	122.82
26	Y	101	LMG	C38-C37-C36	-2.15	103.50	114.37
26	D	408	LMG	O1-C7-C8	-2.15	105.59	110.82
22	b	615	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
29	c	516	DGD	O3E-C3E-C2E	-2.15	105.32	110.38
22	B	612	CLA	C4C-C3C-C2C	-2.15	103.77	106.89
22	c	511	CLA	O1A-CGA-CBA	2.14	132.17	123.78
22	C	513	CLA	CBC-CAC-C3C	2.14	118.23	112.42
31	D	406	BCR	C30-C25-C26	-2.14	119.71	122.64
29	H	102	DGD	C4D-C3D-C2D	-2.14	107.07	110.83
29	c	516	DGD	O6E-C1E-O5D	-2.14	104.98	110.04
26	M	101	LMG	C1-O6-C5	-2.14	109.54	113.72
22	C	508	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
22	C	509	CLA	C1-O2A-CGA	2.14	121.83	116.65
31	k	102	BCR	C36-C18-C19	2.14	121.36	118.09
22	b	616	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
23	d	402	PHO	OBD-CAD-C3D	2.14	131.23	127.89
29	C	517	DGD	C8B-C7B-C6B	-2.14	103.56	114.37
22	B	610	CLA	O2A-CGA-CBA	2.14	118.35	111.83
29	C	517	DGD	C7A-C6A-C5A	-2.14	103.57	114.37
35	v	201	HEC	C1B-C2B-C3B	2.14	109.23	106.98
22	b	607	CLA	C3B-C4B-NB	-2.14	108.62	110.53
22	b	603	CLA	CED-O2D-CGD	-2.13	111.08	115.92
31	B	619	BCR	C40-C30-C29	-2.13	100.76	108.95
29	C	516	DGD	O6E-C1E-O5D	-2.13	105.00	110.04
26	B	626	LMG	C1-O6-C5	-2.13	109.56	113.72
22	c	511	CLA	CHB-C4A-NA	2.13	127.47	124.40
22	B	601	CLA	O2D-CGD-CBD	2.13	114.95	111.23
22	C	506	CLA	CHA-C1A-NA	-2.13	121.57	126.39
22	b	602	CLA	C16-C15-C13	-2.13	108.89	115.97
22	D	403	CLA	CHB-C4A-NA	2.13	127.47	124.40
27	a	411	SQD	O5-C5-C4	2.13	113.53	109.70
29	c	518	DGD	C7B-C6B-C5B	-2.13	103.62	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	619	BCR	C30-C25-C24	2.13	121.42	115.65
32	x	102	STE	O2-C1-O1	-2.12	117.87	123.33
22	B	611	CLA	C3D-C4D-ND	2.12	113.44	109.99
22	b	616	CLA	C1-C2-C3	-2.12	122.72	126.20
23	A	404	PHO	OBD-CAD-CBD	-2.12	122.71	125.82
29	C	517	DGD	O6E-C1E-O5D	-2.12	105.03	110.04
31	c	515	BCR	C29-C30-C25	2.12	113.52	110.44
29	C	515	DGD	CAB-C9B-C8B	-2.12	103.65	114.37
22	B	613	CLA	CMB-C2B-C3B	2.12	131.54	126.55
22	B	606	CLA	CHD-C4C-NC	2.12	127.52	124.23
26	B	626	LMG	C6-C5-C4	-2.12	107.82	113.02
25	d	407	PL9	O1-C4-C3	-2.12	118.50	120.73
25	A	408	PL9	C12-C13-C14	-2.12	122.78	127.62
31	k	102	BCR	C29-C30-C25	2.11	113.51	110.44
22	d	405	CLA	CHA-C1A-NA	-2.11	121.60	126.39
22	b	610	CLA	C2C-C1C-NC	2.11	112.20	109.98
22	B	603	CLA	C5-C3-C2	-2.11	116.42	121.17
26	A	409	LMG	C36-C35-C34	-2.11	103.69	114.37
29	H	102	DGD	C6D-C5D-C4D	2.11	116.50	112.07
22	C	507	CLA	C3B-C4B-NB	-2.11	108.64	110.53
22	C	508	CLA	CMB-C2B-C3B	2.11	131.52	126.55
22	D	404	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
22	B	607	CLA	C2C-C1C-NC	2.11	112.20	109.98
34	F	101	HEM	O2D-CGD-CBD	2.11	120.66	114.00
28	D	413	LHG	C18-C17-C16	-2.11	103.72	114.37
29	C	516	DGD	O3G-C1D-C2D	-2.11	105.07	108.27
32	t	103	STE	O2-C1-O1	-2.11	117.91	123.33
34	F	101	HEM	C3B-C2B-C1B	2.11	107.99	106.41
29	c	518	DGD	O6E-C5E-C4E	2.10	113.49	109.70
28	l	101	LHG	O8-C23-O10	-2.10	118.36	123.63
29	A	413	DGD	CDB-CCB-CBB	-2.10	103.73	114.37
25	A	408	PL9	C40-C39-C38	-2.10	118.22	123.63
28	A	411	LHG	O8-C23-O10	-2.10	118.37	123.63
27	f	102	SQD	O47-C7-O49	-2.10	118.79	123.70
31	C	514	BCR	C37-C22-C21	-2.10	119.41	122.82
28	A	411	LHG	C18-C17-C16	-2.10	103.73	114.37
31	K	102	BCR	C8-C7-C6	-2.10	121.38	127.00
25	d	407	PL9	C7-C3-C2	-2.10	120.91	123.39
29	c	516	DGD	O6E-C5E-C4E	2.10	113.48	109.70
31	t	101	BCR	C12-C13-C14	-2.10	115.70	119.01
23	A	404	PHO	CAC-C3C-C2C	2.10	131.42	127.56
27	f	102	SQD	O5-C1-O6	2.10	115.00	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	h	101	DGD	O1G-C1A-O1A	-2.10	118.38	123.63
22	b	607	CLA	C3A-C2A-C1A	2.10	104.48	101.34
22	a	402	CLA	C3B-C4B-NB	-2.10	108.66	110.53
22	C	503	CLA	CHB-C1B-NB	2.10	127.19	124.05
22	B	609	CLA	CHA-C1A-NA	-2.10	121.65	126.39
22	c	509	CLA	C16-C15-C13	-2.09	109.00	115.97
22	B	603	CLA	CHD-C4C-NC	2.09	127.48	124.23
31	b	619	BCR	C15-C16-C17	-2.09	119.23	123.52
28	d	409	LHG	C29-C28-C27	-2.09	103.78	114.37
22	B	614	CLA	O2D-CGD-CBD	2.09	114.89	111.23
22	B	616	CLA	C2C-C1C-NC	2.09	112.18	109.98
22	D	403	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
27	a	411	SQD	C45-O47-C7	2.09	122.80	117.80
22	D	405	CLA	CHB-C1B-C2B	-2.09	121.36	127.43
22	b	615	CLA	CHC-C1C-NC	2.09	127.46	124.31
22	B	602	CLA	CHA-C4D-ND	2.09	136.85	132.55
22	B	614	CLA	C2C-C1C-NC	2.09	112.17	109.98
26	m	101	LMG	C38-C37-C36	-2.09	103.83	114.37
22	B	614	CLA	CBC-CAC-C3C	-2.09	106.77	112.42
22	C	508	CLA	O1D-CGD-CBD	2.08	128.63	124.52
26	m	101	LMG	O8-C28-O10	-2.08	118.42	123.63
22	c	510	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
31	B	618	BCR	C2-C1-C6	2.08	113.47	110.44
29	c	518	DGD	C3D-C4D-C5D	-2.08	106.45	110.23
22	a	404	CLA	C2C-C1C-NC	2.08	112.17	109.98
23	a	403	PHO	O2A-CGA-O1A	-2.08	118.42	123.63
26	A	409	LMG	O8-C28-O10	-2.08	118.42	123.63
29	C	515	DGD	O6D-C5D-C4D	2.08	113.45	109.70
23	D	401	PHO	CMD-C2D-C3D	2.08	128.84	124.68
22	d	403	CLA	CHB-C4A-NA	2.08	127.40	124.40
22	b	605	CLA	CHC-C1C-C2C	-2.08	121.04	126.95
22	B	603	CLA	CHD-C4C-C3C	-2.08	121.75	124.77
31	B	617	BCR	C30-C25-C26	-2.08	119.80	122.64
29	h	101	DGD	CDB-CCB-CBB	-2.08	103.88	114.37
22	c	507	CLA	CHC-C4B-NB	2.08	127.16	124.05
22	c	507	CLA	C7-C6-C5	-2.07	107.73	113.26
29	A	413	DGD	O5D-C6D-C5D	-2.07	104.75	109.42
23	D	401	PHO	O1D-CGD-CBD	2.07	127.87	124.72
22	A	405	CLA	CED-O2D-CGD	-2.07	111.21	115.92
32	L	103	STE	O1-C1-C2	-2.07	116.52	123.09
26	D	412	LMG	C35-C34-C33	-2.07	103.90	114.37
22	b	601	CLA	C3B-C4B-NB	-2.07	108.68	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	514	BCR	C33-C5-C6	-2.07	122.22	124.48
22	b	609	CLA	C7-C6-C5	-2.07	107.74	113.26
22	B	607	CLA	CMB-C2B-C3B	2.07	131.42	126.55
31	b	619	BCR	C16-C15-C14	-2.07	119.28	123.52
31	c	515	BCR	C37-C22-C21	-2.07	119.46	122.82
26	A	409	LMG	C38-C37-C36	-2.07	103.91	114.37
27	f	102	SQD	C1-O5-C5	-2.07	109.68	113.72
28	a	410	LHG	O7-C7-C8	-2.07	107.01	111.48
22	B	614	CLA	C6-C7-C8	-2.07	109.09	115.97
22	c	506	CLA	CHB-C1B-NB	2.07	127.15	124.05
28	D	411	LHG	C3-C2-C1	-2.07	104.81	111.77
25	a	409	PL9	C45-C44-C43	-2.07	118.32	123.63
22	b	612	CLA	O2A-CGA-CBA	2.07	118.13	111.83
22	c	507	CLA	C2A-C1A-CHA	2.06	127.45	123.87
29	A	413	DGD	C1D-C2D-C3D	-2.06	105.67	110.01
22	c	507	CLA	CHB-C4A-NA	2.06	127.38	124.40
27	D	409	SQD	C3-C4-C5	2.06	113.97	110.23
22	b	607	CLA	CMB-C2B-C3B	2.06	131.39	126.55
22	A	405	CLA	CHD-C1D-C2D	2.06	129.77	125.49
22	b	604	CLA	CMB-C2B-C3B	2.06	131.39	126.55
31	x	101	BCR	C20-C21-C22	-2.06	124.39	127.28
22	c	504	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
22	d	405	CLA	C4A-NA-C1A	2.05	107.62	106.68
23	a	403	PHO	CMD-C2D-C3D	2.05	128.79	124.68
22	C	506	CLA	O1D-CGD-CBD	2.05	128.56	124.52
22	C	504	CLA	CHA-C4D-ND	2.05	136.78	132.55
29	C	516	DGD	O4D-C4D-C5D	-2.05	104.28	109.32
22	c	501	CLA	CHA-C1A-NA	-2.05	121.75	126.39
22	B	608	CLA	C4A-NA-C1A	2.05	107.61	106.68
22	c	504	CLA	C1C-C2C-C3C	-2.05	104.83	106.98
22	a	402	CLA	C4D-CHA-C1A	2.05	123.69	121.24
22	B	607	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
22	B	609	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
22	c	508	CLA	CHD-C4C-NC	2.05	127.40	124.23
28	L	102	LHG	C27-C26-C25	-2.04	104.04	114.37
28	d	409	LHG	O8-C23-O10	-2.04	118.52	123.63
31	B	617	BCR	C37-C22-C21	-2.04	119.51	122.82
26	B	621	LMG	C38-C37-C36	-2.04	104.06	114.37
22	c	501	CLA	CHB-C4A-NA	2.04	127.34	124.40
29	C	516	DGD	C6D-O5D-C1E	2.04	118.17	113.80
22	B	603	CLA	CHC-C1C-C2C	-2.04	121.16	126.95
22	B	601	CLA	CHA-C4D-ND	2.04	136.75	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	101	LMG	C9-C8-C7	-2.04	107.04	111.78
31	Z	101	BCR	C15-C14-C13	-2.04	124.42	127.28
22	c	509	CLA	O2A-CGA-CBA	2.04	118.04	111.83
25	D	407	PL9	C50-C49-C48	-2.04	116.55	122.66
29	H	102	DGD	O2E-C2E-C3E	-2.04	105.58	110.38
22	b	614	CLA	CHA-C4D-ND	2.03	136.75	132.55
31	C	514	BCR	C15-C14-C13	-2.03	124.43	127.28
26	b	622	LMG	C40-C39-C38	-2.03	104.09	114.37
22	d	404	CLA	C2A-C1A-CHA	2.03	127.39	123.87
31	B	619	BCR	C15-C16-C17	-2.03	119.36	123.52
22	d	403	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
22	D	405	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
22	b	612	CLA	O1D-CGD-CBD	2.03	128.51	124.52
34	F	101	HEM	CAC-C3C-C4C	2.03	129.66	124.82
22	b	610	CLA	CHD-C1D-ND	-2.03	121.95	124.80
26	D	408	LMG	O2-C2-C1	-2.02	105.25	110.08
22	c	511	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	Y	101	LMG	C40-C39-C38	-2.02	104.14	114.37
29	c	516	DGD	O5D-C6D-C5D	-2.02	104.86	109.42
27	A	410	SQD	O47-C45-C46	2.02	115.59	108.34
22	b	615	CLA	C3A-C2A-C1A	2.02	104.36	101.34
26	c	521	LMG	C3-C4-C5	-2.02	106.57	110.23
22	b	610	CLA	CHC-C4B-NB	2.02	127.08	124.05
26	A	409	LMG	C1-O6-C5	-2.02	109.78	113.72
29	c	516	DGD	C5B-C4B-C3B	-2.02	104.17	114.37
22	b	604	CLA	CBA-CAA-C2A	-2.02	107.79	113.79
22	B	615	CLA	C4-C3-C5	2.02	118.73	115.23
29	C	515	DGD	C8B-C7B-C6B	-2.02	104.17	114.37
22	b	607	CLA	CHD-C4C-NC	2.02	127.36	124.23
31	c	515	BCR	C1-C6-C5	-2.02	119.88	122.64
31	K	101	BCR	C1-C6-C5	-2.02	119.88	122.64
22	C	510	CLA	C2D-C1D-ND	-2.01	108.13	110.13
31	C	514	BCR	C27-C26-C25	2.01	125.42	122.70
22	c	506	CLA	CHD-C1D-C2D	2.01	129.67	125.49
29	h	101	DGD	CAB-C9B-C8B	-2.01	104.21	114.37
22	A	402	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
22	B	608	CLA	C3D-C4D-ND	2.01	113.25	109.99
22	A	405	CLA	CHC-C1C-C2C	-2.01	121.24	126.95
22	c	508	CLA	CHA-C1A-NA	-2.01	121.84	126.39
31	x	101	BCR	C36-C18-C19	2.01	121.15	118.09
29	h	101	DGD	C3E-C4E-C5E	-2.01	106.59	110.23
26	D	408	LMG	O7-C10-O9	-2.01	119.02	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	M	101	LMG	C37-C36-C35	-2.00	104.23	114.37
31	a	405	BCR	C33-C5-C6	-2.00	122.30	124.48
22	d	404	CLA	CHD-C1D-C2D	2.00	129.65	125.49
22	C	513	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
22	C	505	CLA	CBA-CAA-C2A	2.00	119.75	113.79
26	D	408	LMG	O6-C1-O1	-2.00	105.31	110.04
34	f	101	HEM	C4C-C3C-C2C	2.00	108.55	106.81
22	B	613	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
29	C	515	DGD	O5D-C6D-C5D	-2.00	104.91	109.42
31	b	619	BCR	C38-C26-C25	-2.00	122.30	124.48
27	B	622	SQD	O8-S-O7	-2.00	106.39	111.40
26	c	519	LMG	C40-C39-C38	-2.00	104.26	114.37
22	C	508	CLA	C7-C6-C5	-2.00	107.93	113.26

All (2) chirality outliers are listed below:

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

All (2040) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	606	CLA	C4B-C3B-CAB-CBB
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	C14-C13-C15-C16
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	C	512	CLA	C1A-C2A-CAA-CBA
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	D	405	CLA	C11-C12-C13-C14
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	609	CLA	C2B-C3B-CAB-CBB
22	b	609	CLA	C4B-C3B-CAB-CBB
22	b	613	CLA	C11-C10-C8-C7
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	c	505	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
22	c	505	CLA	C4B-C3B-CAB-CBB
22	c	506	CLA	C1A-C2A-CAA-CBA
22	c	506	CLA	C3A-C2A-CAA-CBA
22	c	506	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	C6-C7-C8-C9
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
22	c	513	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C3A-C2A-CAA-CBA
22	d	401	CLA	C2B-C3B-CAB-CBB
22	d	401	CLA	C4B-C3B-CAB-CBB
23	d	402	PHO	C6-C7-C8-C9
25	A	408	PL9	C22-C23-C24-C26
25	A	408	PL9	C24-C26-C27-C28
25	A	408	PL9	C32-C33-C34-C36
25	A	408	PL9	C37-C38-C39-C40
25	A	408	PL9	C40-C39-C41-C42
25	D	407	PL9	C32-C33-C34-C36
25	D	407	PL9	C42-C43-C44-C45
25	D	407	PL9	C47-C48-C49-C50
25	a	409	PL9	C12-C13-C14-C15
25	a	409	PL9	C12-C13-C14-C16
25	a	409	PL9	C17-C18-C19-C21
25	a	409	PL9	C22-C23-C24-C25
25	a	409	PL9	C22-C23-C24-C26
25	a	409	PL9	C32-C33-C34-C35
25	a	409	PL9	C37-C38-C39-C40
25	a	409	PL9	C42-C43-C44-C45
25	d	407	PL9	C27-C28-C29-C31
25	d	407	PL9	C40-C39-C41-C42
25	d	407	PL9	C47-C48-C49-C50
26	A	409	LMG	O9-C10-O7-C8
26	D	412	LMG	C11-C10-O7-C8
26	Y	101	LMG	C11-C10-O7-C8
26	b	622	LMG	C11-C10-O7-C8
26	c	521	LMG	C11-C10-O7-C8
26	c	522	LMG	O6-C1-O1-C7
27	A	410	SQD	C2-C1-O6-C44
27	A	412	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
27	B	622	SQD	C2-C1-O6-C44
27	B	622	SQD	O5-C1-O6-C44
27	B	622	SQD	O6-C44-C45-O47
27	B	622	SQD	O49-C7-O47-C45
27	B	622	SQD	C8-C7-O47-C45
27	L	101	SQD	O49-C7-O47-C45
27	L	101	SQD	C8-C7-O47-C45
27	a	411	SQD	O6-C44-C45-O47
27	f	102	SQD	C2-C1-O6-C44
27	t	102	SQD	O47-C45-C46-O48
27	t	102	SQD	C8-C7-O47-C45
28	A	411	LHG	C3-O3-P-O4
28	A	411	LHG	C4-O6-P-O3
28	D	410	LHG	O1-C1-C2-C3
28	D	410	LHG	C3-O3-P-O5
28	D	410	LHG	C3-O3-P-O6
28	D	410	LHG	C4-O6-P-O4
28	D	411	LHG	C3-O3-P-O6
28	D	413	LHG	O1-C1-C2-C3
28	D	413	LHG	C1-C2-C3-O3
28	L	102	LHG	C3-O3-P-O4
28	L	102	LHG	C4-O6-P-O4
28	a	410	LHG	C4-O6-P-O3
28	a	410	LHG	C4-O6-P-O4
28	a	410	LHG	C4-O6-P-O5
28	d	408	LHG	C3-O3-P-O4
28	d	408	LHG	C4-O6-P-O3
28	d	408	LHG	C4-O6-P-O4
28	d	409	LHG	C4-O6-P-O4
28	e	101	LHG	O1-C1-C2-O2
28	e	101	LHG	O1-C1-C2-C3
28	e	101	LHG	C3-O3-P-O4
28	e	101	LHG	C3-O3-P-O6
28	e	101	LHG	O6-C4-C5-O7
28	e	101	LHG	O10-C23-O8-C6
28	e	101	LHG	C24-C23-O8-C6
29	A	413	DGD	O2G-C2G-C3G-O3G
31	B	617	BCR	C35-C13-C14-C15
31	B	618	BCR	C11-C10-C9-C34
31	B	618	BCR	C10-C11-C12-C13
31	B	618	BCR	C37-C22-C23-C24
31	B	619	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
31	C	514	BCR	C7-C8-C9-C34
31	D	406	BCR	C7-C8-C9-C10
31	D	406	BCR	C22-C23-C24-C25
31	D	406	BCR	C23-C24-C25-C26
31	H	101	BCR	C11-C12-C13-C14
31	H	101	BCR	C36-C18-C19-C20
31	I	101	BCR	C16-C17-C18-C19
31	K	101	BCR	C16-C17-C18-C36
31	K	101	BCR	C21-C22-C23-C24
31	K	101	BCR	C37-C22-C23-C24
31	K	102	BCR	C11-C10-C9-C34
31	K	102	BCR	C11-C12-C13-C14
31	K	102	BCR	C11-C12-C13-C35
31	T	101	BCR	C1-C6-C7-C8
31	T	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C9-C10-C11-C12
31	T	101	BCR	C11-C12-C13-C14
31	T	101	BCR	C16-C17-C18-C19
31	T	101	BCR	C16-C17-C18-C36
31	Z	101	BCR	C6-C7-C8-C9
31	Z	101	BCR	C7-C8-C9-C34
31	Z	101	BCR	C14-C15-C16-C17
31	Z	101	BCR	C16-C17-C18-C36
31	b	617	BCR	C21-C22-C23-C24
31	b	619	BCR	C11-C12-C13-C14
31	b	619	BCR	C12-C13-C14-C15
31	b	619	BCR	C35-C13-C14-C15
31	c	514	BCR	C6-C7-C8-C9
31	c	514	BCR	C7-C8-C9-C10
31	c	514	BCR	C18-C19-C20-C21
31	c	514	BCR	C20-C21-C22-C37
31	d	406	BCR	C37-C22-C23-C24
31	d	406	BCR	C22-C23-C24-C25
31	k	101	BCR	C7-C8-C9-C10
31	k	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C11-C10-C9-C34
31	t	101	BCR	C35-C13-C14-C15
31	t	101	BCR	C16-C17-C18-C19
31	t	101	BCR	C16-C17-C18-C36
35	V	201	HEC	C2C-C3C-CAC-CBC
22	C	509	CLA	O1D-CGD-O2D-CED
22	b	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	c	519	LMG	C11-C10-O7-C8
22	B	601	CLA	CBD-CGD-O2D-CED
22	B	612	CLA	CBD-CGD-O2D-CED
22	C	501	CLA	CBD-CGD-O2D-CED
22	C	509	CLA	CBD-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	b	614	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	CBD-CGD-O2D-CED
22	c	513	CLA	CBD-CGD-O2D-CED
22	B	601	CLA	O1A-CGA-O2A-C1
26	c	521	LMG	O10-C28-O8-C9
26	c	522	LMG	O10-C28-O8-C9
22	B	614	CLA	C15-C16-C17-C18
35	V	201	HEC	C4C-C3C-CAC-CBC
35	v	201	HEC	C4C-C3C-CAC-CBC
25	D	407	PL9	C47-C48-C49-C51
25	a	409	PL9	C47-C48-C49-C50
25	d	407	PL9	C47-C48-C49-C51
22	B	601	CLA	CBA-CGA-O2A-C1
22	B	604	CLA	O1A-CGA-O2A-C1
26	M	101	LMG	O10-C28-O8-C9
27	L	101	SQD	O10-C23-O48-C46
22	c	506	CLA	O1D-CGD-O2D-CED
22	c	508	CLA	O1D-CGD-O2D-CED
26	c	519	LMG	O9-C10-O7-C8
26	Y	101	LMG	O9-C10-O7-C8
26	b	622	LMG	O9-C10-O7-C8
27	f	102	SQD	O49-C7-O47-C45
27	t	102	SQD	O49-C7-O47-C45
29	A	413	DGD	O1B-C1B-O2G-C2G
25	a	409	PL9	C47-C48-C49-C51
22	B	604	CLA	C3-C5-C6-C7
22	C	506	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
22	B	604	CLA	CBA-CGA-O2A-C1
27	L	101	SQD	C24-C23-O48-C46
22	B	616	CLA	CBD-CGD-O2D-CED
22	b	607	CLA	CBD-CGD-O2D-CED
22	b	613	CLA	CBD-CGD-O2D-CED
26	A	409	LMG	C11-C10-O7-C8
29	A	413	DGD	C2B-C1B-O2G-C2G
22	b	601	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C4-C3-C5-C6
22	B	614	CLA	C4-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
22	C	507	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
25	A	408	PL9	C23-C24-C26-C27
25	a	409	PL9	C28-C29-C31-C32
25	a	409	PL9	C38-C39-C41-C42
26	A	409	LMG	O6-C5-C6-O5
22	c	512	CLA	C2A-CAA-CBA-CGA
22	c	513	CLA	C2A-CAA-CBA-CGA
22	B	605	CLA	C3-C5-C6-C7
22	b	609	CLA	C3-C5-C6-C7
35	V	201	HEC	C2B-C3B-CAB-CBB
26	c	522	LMG	C29-C28-O8-C9
25	a	409	PL9	C27-C28-C29-C30
25	A	408	PL9	C37-C38-C39-C41
25	a	409	PL9	C37-C38-C39-C41
25	a	409	PL9	C42-C43-C44-C46
26	D	412	LMG	O9-C10-O7-C8
26	c	521	LMG	O9-C10-O7-C8
22	C	512	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	c	510	CLA	C3-C5-C6-C7
22	d	405	CLA	CBD-CGD-O2D-CED
28	D	413	LHG	O2-C2-C3-O3
26	M	101	LMG	C29-C28-O8-C9
27	t	102	SQD	C24-C23-O48-C46
26	c	521	LMG	O6-C5-C6-O5
22	B	601	CLA	O1D-CGD-O2D-CED
29	A	413	DGD	O6E-C5E-C6E-O5E
31	b	619	BCR	C14-C15-C16-C17
22	A	405	CLA	C3-C5-C6-C7
28	d	409	LHG	C24-C25-C26-C27
22	D	405	CLA	CBD-CGD-O2D-CED
22	c	510	CLA	O1D-CGD-O2D-CED
22	c	513	CLA	O1D-CGD-O2D-CED
26	c	521	LMG	C29-C28-O8-C9
27	f	102	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
22	A	405	CLA	C4-C3-C5-C6
25	a	409	PL9	C25-C24-C26-C27
22	B	604	CLA	C2-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
22	b	614	CLA	C2-C3-C5-C6
29	c	518	DGD	O1A-C1A-O1G-C1G
25	A	408	PL9	C34-C36-C37-C38
25	A	408	PL9	C44-C46-C47-C48
25	D	407	PL9	C44-C46-C47-C48
25	a	409	PL9	C9-C11-C12-C13
25	a	409	PL9	C19-C21-C22-C23
25	a	409	PL9	C24-C26-C27-C28
25	d	407	PL9	C44-C46-C47-C48
26	A	409	LMG	C4-C5-C6-O5
35	V	201	HEC	C4B-C3B-CAB-CBB
22	B	612	CLA	O1D-CGD-O2D-CED
27	D	409	SQD	O10-C23-O48-C46
22	d	405	CLA	C3-C5-C6-C7
27	A	410	SQD	O5-C1-O6-C44
27	f	102	SQD	O5-C1-O6-C44
26	Y	101	LMG	O6-C5-C6-O5
22	B	604	CLA	CBD-CGD-O2D-CED
22	b	603	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
25	A	408	PL9	C17-C18-C19-C20
25	a	409	PL9	C17-C18-C19-C20
27	f	102	SQD	C8-C7-O47-C45
22	b	602	CLA	C3-C5-C6-C7
28	e	101	LHG	C1-C2-C3-O3
26	B	626	LMG	C29-C28-O8-C9
27	B	622	SQD	C24-C23-O48-C46
27	D	409	SQD	C24-C23-O48-C46
29	c	518	DGD	C2A-C1A-O1G-C1G
29	C	515	DGD	O6E-C5E-C6E-O5E
22	C	501	CLA	O1D-CGD-O2D-CED
29	h	101	DGD	C4E-C5E-C6E-O5E
22	B	604	CLA	C4-C3-C5-C6
22	C	504	CLA	C4-C3-C5-C6
22	A	405	CLA	C2-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
25	D	407	PL9	C33-C34-C36-C37
25	d	407	PL9	C38-C39-C41-C42

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Mol	Chain	Res	Type	Atoms
22	c	501	CLA	CBD-CGD-O2D-CED
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C11-C12-C13-C14
22	B	606	CLA	C11-C10-C8-C9
22	B	607	CLA	C14-C13-C15-C16
22	B	609	CLA	C14-C13-C15-C16
22	B	610	CLA	C14-C13-C15-C16
22	B	614	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	b	616	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C12-C13-C14
22	c	512	CLA	C6-C7-C8-C9
22	d	405	CLA	C11-C12-C13-C14
23	A	404	PHO	C14-C13-C15-C16
22	B	616	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	d	405	CLA	O1D-CGD-O2D-CED
28	A	411	LHG	O2-C2-C3-O3
28	d	408	LHG	O2-C2-C3-O3
26	B	626	LMG	O6-C5-C6-O5
27	f	102	SQD	O10-C23-O48-C46
31	B	619	BCR	C37-C22-C23-C24
31	D	406	BCR	C37-C22-C23-C24
31	T	101	BCR	C11-C12-C13-C35
31	Z	101	BCR	C36-C18-C19-C20
31	a	405	BCR	C37-C22-C23-C24
31	b	618	BCR	C37-C22-C23-C24
31	c	514	BCR	C7-C8-C9-C34
31	k	102	BCR	C37-C22-C23-C24
31	t	101	BCR	C11-C12-C13-C35
31	t	101	BCR	C36-C18-C19-C20
31	x	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C7-C8-C9-C10
28	d	409	LHG	C23-C24-C25-C26
29	C	516	DGD	C1B-C2B-C3B-C4B

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Mol	Chain	Res	Type	Atoms
26	c	522	LMG	O6-C5-C6-O5
22	c	512	CLA	CBA-CGA-O2A-C1
26	D	408	LMG	C10-C11-C12-C13
32	B	623	STE	C4-C5-C6-C7
22	b	607	CLA	O1D-CGD-O2D-CED
35	v	201	HEC	C2C-C3C-CAC-CBC
22	C	507	CLA	C5-C6-C7-C8
22	c	507	CLA	C5-C6-C7-C8
22	c	511	CLA	C13-C15-C16-C17
22	c	511	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
28	D	410	LHG	O1-C1-C2-O2
27	L	101	SQD	C7-C8-C9-C10
25	a	409	PL9	C27-C28-C29-C31
22	C	506	CLA	C15-C16-C17-C18
22	b	609	CLA	C11-C12-C13-C15
22	b	615	CLA	C11-C12-C13-C15
22	d	405	CLA	C6-C7-C8-C10
32	b	621	STE	C14-C15-C16-C17
22	b	608	CLA	C8-C10-C11-C12
26	B	621	LMG	C28-C29-C30-C31
28	a	410	LHG	C7-C8-C9-C10
25	D	407	PL9	C34-C36-C37-C38
25	a	409	PL9	C14-C16-C17-C18
22	B	614	CLA	C13-C15-C16-C17
32	c	520	STE	C2-C3-C4-C5
26	d	410	LMG	C28-C29-C30-C31
22	c	512	CLA	CBD-CGD-O2D-CED
22	B	603	CLA	C8-C10-C11-C12
22	B	604	CLA	C5-C6-C7-C8
22	B	606	CLA	C8-C10-C11-C12
22	B	609	CLA	C15-C16-C17-C18
22	B	610	CLA	C8-C10-C11-C12
22	C	503	CLA	C5-C6-C7-C8
22	C	509	CLA	C10-C11-C12-C13
22	C	510	CLA	C13-C15-C16-C17
22	a	404	CLA	C5-C6-C7-C8
22	c	507	CLA	C8-C10-C11-C12
22	c	510	CLA	C5-C6-C7-C8
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	C2A-CAA-CBA-CGA
22	b	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	B	618	BCR	C18-C19-C20-C21
31	H	101	BCR	C10-C11-C12-C13
31	K	101	BCR	C10-C11-C12-C13
22	B	607	CLA	C5-C6-C7-C8
22	C	502	CLA	C15-C16-C17-C18
22	C	505	CLA	C10-C11-C12-C13
22	D	404	CLA	C13-C15-C16-C17
22	b	605	CLA	C5-C6-C7-C8
22	b	611	CLA	C10-C11-C12-C13
26	B	626	LMG	C10-C11-C12-C13
26	D	412	LMG	C28-C29-C30-C31
26	M	101	LMG	C10-C11-C12-C13
28	l	101	LHG	C23-C24-C25-C26
32	B	624	STE	C1-C2-C3-C4
32	b	623	STE	C1-C2-C3-C4
32	x	102	STE	C1-C2-C3-C4
26	Y	101	LMG	O6-C1-O1-C7
26	m	101	LMG	O6-C1-O1-C7
29	c	517	DGD	O6E-C1E-O5D-C6D
27	B	622	SQD	C11-C10-C9-C8
28	A	411	LHG	C27-C28-C29-C30
28	A	411	LHG	C32-C33-C34-C35
22	B	613	CLA	C8-C10-C11-C12
22	C	508	CLA	C10-C11-C12-C13
22	b	603	CLA	C10-C11-C12-C13
22	c	505	CLA	C15-C16-C17-C18
32	a	413	STE	C4-C5-C6-C7
28	e	101	LHG	O2-C2-C3-O3
26	B	626	LMG	O10-C28-O8-C9
26	c	521	LMG	C4-C5-C6-O5
27	A	410	SQD	C7-C8-C9-C10
27	B	622	SQD	C23-C24-C25-C26
28	d	408	LHG	C7-C8-C9-C10
22	B	607	CLA	C8-C10-C11-C12
22	D	403	CLA	C15-C16-C17-C18
22	D	405	CLA	C10-C11-C12-C13
22	c	510	CLA	C10-C11-C12-C13
22	C	506	CLA	C8-C10-C11-C12
22	b	606	CLA	C10-C11-C12-C13
22	b	610	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
26	m	101	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	B	622	SQD	C7-C8-C9-C10
32	B	625	STE	C9-C10-C11-C12
22	B	608	CLA	C15-C16-C17-C18
22	B	610	CLA	C15-C16-C17-C18
22	B	611	CLA	C13-C15-C16-C17
22	B	614	CLA	C8-C10-C11-C12
22	b	605	CLA	CBD-CGD-O2D-CED
22	c	502	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	C10-C11-C12-C13
29	h	101	DGD	O6E-C5E-C6E-O5E
27	A	410	SQD	C23-C24-C25-C26
26	Y	101	LMG	C4-C5-C6-O5
28	A	411	LHG	C1-C2-C3-O3
22	b	607	CLA	CBA-CGA-O2A-C1
32	B	627	STE	C5-C6-C7-C8
22	C	509	CLA	C13-C15-C16-C17
22	C	510	CLA	C15-C16-C17-C18
22	d	401	CLA	C13-C15-C16-C17
25	A	408	PL9	C47-C48-C49-C51
22	C	502	CLA	CBD-CGD-O2D-CED
32	b	625	STE	C2-C3-C4-C5
22	B	601	CLA	C13-C15-C16-C17
22	b	607	CLA	C8-C10-C11-C12
22	d	401	CLA	C8-C10-C11-C12
22	C	513	CLA	C13-C15-C16-C17
22	D	404	CLA	C15-C16-C17-C18
22	b	614	CLA	C8-C10-C11-C12
22	b	614	CLA	C13-C15-C16-C17
22	b	615	CLA	C15-C16-C17-C18
22	b	604	CLA	C4-C3-C5-C6
22	C	513	CLA	C15-C16-C17-C18
22	b	604	CLA	C3-C5-C6-C7
26	Y	101	LMG	C2-C1-O1-C7
26	c	522	LMG	C2-C1-O1-C7
26	m	101	LMG	C2-C1-O1-C7
29	c	517	DGD	C2E-C1E-O5D-C6D
22	B	606	CLA	C16-C17-C18-C20
22	C	511	CLA	C8-C10-C11-C12
31	B	617	BCR	C16-C17-C18-C36
31	B	617	BCR	C20-C21-C22-C37
31	B	618	BCR	C20-C21-C22-C37
31	B	619	BCR	C35-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	C	514	BCR	C16-C17-C18-C36
31	D	406	BCR	C11-C10-C9-C34
31	D	406	BCR	C20-C21-C22-C37
31	I	101	BCR	C16-C17-C18-C36
31	I	101	BCR	C20-C21-C22-C37
31	K	101	BCR	C11-C10-C9-C34
31	Z	101	BCR	C20-C21-C22-C37
31	b	617	BCR	C35-C13-C14-C15
31	b	617	BCR	C20-C21-C22-C37
31	c	515	BCR	C16-C17-C18-C36
31	c	515	BCR	C20-C21-C22-C37
31	d	406	BCR	C20-C21-C22-C37
31	t	101	BCR	C20-C21-C22-C37
26	b	622	LMG	C28-C29-C30-C31
31	K	102	BCR	C7-C8-C9-C34
31	b	619	BCR	C37-C22-C23-C24
31	t	101	BCR	C7-C8-C9-C34
27	t	102	SQD	O10-C23-O48-C46
28	d	409	LHG	O1-C1-C2-C3
26	d	410	LMG	C10-C11-C12-C13
27	L	101	SQD	C46-C45-O47-C7
22	B	601	CLA	C16-C17-C18-C19
22	B	603	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
22	B	614	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C20
22	c	512	CLA	O1A-CGA-O2A-C1
22	A	402	CLA	C2C-C3C-CAC-CBC
31	B	617	BCR	C12-C13-C14-C15
31	B	618	BCR	C11-C10-C9-C8
31	B	618	BCR	C12-C13-C14-C15
31	B	619	BCR	C11-C10-C9-C8
31	K	101	BCR	C16-C17-C18-C19
31	K	102	BCR	C11-C10-C9-C8
31	Z	101	BCR	C11-C10-C9-C8
31	Z	101	BCR	C16-C17-C18-C19
31	a	405	BCR	C20-C21-C22-C23
31	b	617	BCR	C11-C10-C9-C8
31	b	617	BCR	C12-C13-C14-C15
31	c	514	BCR	C20-C21-C22-C23
31	c	515	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
31	d	406	BCR	C12-C13-C14-C15
31	t	101	BCR	C11-C10-C9-C8
31	x	101	BCR	C11-C10-C9-C8
31	x	101	BCR	C16-C17-C18-C19
28	D	413	LHG	C31-C32-C33-C34
22	C	509	CLA	C2-C1-O2A-CGA
22	B	602	CLA	C16-C17-C18-C19
22	B	614	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
22	b	605	CLA	C16-C17-C18-C19
22	c	510	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
26	m	101	LMG	O10-C28-O8-C9
26	c	519	LMG	C31-C32-C33-C34
28	a	410	LHG	C32-C33-C34-C35
29	C	517	DGD	C4B-C5B-C6B-C7B
32	d	412	STE	C4-C5-C6-C7
32	d	412	STE	C12-C13-C14-C15
31	I	101	BCR	C14-C15-C16-C17
27	B	622	SQD	C28-C29-C30-C31
27	L	101	SQD	C24-C25-C26-C27
27	t	102	SQD	C30-C31-C32-C33
28	A	411	LHG	C26-C27-C28-C29
28	l	101	LHG	C15-C16-C17-C18
29	A	413	DGD	C2B-C3B-C4B-C5B
29	A	413	DGD	C4B-C5B-C6B-C7B
29	C	516	DGD	C6A-C7A-C8A-C9A
32	B	624	STE	C10-C11-C12-C13
32	C	518	STE	C5-C6-C7-C8
32	Z	102	STE	C13-C14-C15-C16
32	a	413	STE	C7-C8-C9-C10
32	b	625	STE	C4-C5-C6-C7
22	b	615	CLA	C5-C6-C7-C8
26	b	622	LMG	C11-C12-C13-C14
26	b	622	LMG	C19-C20-C21-C22
26	c	521	LMG	C41-C42-C43-C44
27	A	412	SQD	C12-C13-C14-C15
28	d	408	LHG	C11-C12-C13-C14
29	c	516	DGD	C3B-C4B-C5B-C6B
32	b	627	STE	C11-C12-C13-C14
32	b	627	STE	C13-C14-C15-C16
32	d	411	STE	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	A	409	LMG	C13-C14-C15-C16
26	M	101	LMG	C12-C13-C14-C15
26	c	522	LMG	C11-C12-C13-C14
26	c	522	LMG	C30-C31-C32-C33
27	a	411	SQD	C11-C10-C9-C8
27	t	102	SQD	C15-C16-C17-C18
28	a	410	LHG	C15-C16-C17-C18
28	e	101	LHG	C11-C10-C9-C8
29	A	413	DGD	C2A-C3A-C4A-C5A
29	C	516	DGD	C2B-C3B-C4B-C5B
29	C	516	DGD	C9B-CAB-CBB-CCB
29	c	517	DGD	C8A-C9A-CAA-CBA
29	h	101	DGD	C5B-C6B-C7B-C8B
32	b	627	STE	C7-C8-C9-C10
32	x	102	STE	C9-C10-C11-C12
28	D	413	LHG	O1-C1-C2-O2
26	A	409	LMG	C36-C37-C38-C39
26	B	626	LMG	C22-C23-C24-C25
27	f	102	SQD	C30-C31-C32-C33
28	d	409	LHG	C29-C30-C31-C32
28	e	101	LHG	C27-C28-C29-C30
29	A	413	DGD	CBB-CCB-CDB-CEB
32	b	623	STE	C3-C4-C5-C6
22	B	604	CLA	O1D-CGD-O2D-CED
22	B	615	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C4B-C3B-CAB-CBB
26	M	101	LMG	C37-C38-C39-C40
28	D	411	LHG	C14-C15-C16-C17
29	C	517	DGD	C6A-C7A-C8A-C9A
22	B	602	CLA	C16-C17-C18-C20
22	B	603	CLA	C16-C17-C18-C20
22	B	606	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C20
22	D	404	CLA	C16-C17-C18-C20
22	b	604	CLA	C16-C17-C18-C19
22	b	604	CLA	C16-C17-C18-C20
22	b	614	CLA	C16-C17-C18-C19
22	b	614	CLA	C16-C17-C18-C20
26	c	521	LMG	C15-C16-C17-C18
26	c	521	LMG	C34-C35-C36-C37
26	c	522	LMG	C17-C18-C19-C20
29	C	516	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
29	c	516	DGD	C4B-C5B-C6B-C7B
22	b	601	CLA	C8-C10-C11-C12
26	B	626	LMG	C11-C10-O7-C8
22	C	506	CLA	C12-C13-C15-C16
22	c	508	CLA	C12-C13-C15-C16
29	A	413	DGD	CCA-CDA-CEA-CFA
28	D	410	LHG	O2-C2-C3-O3
32	M	102	STE	C1-C2-C3-C4
22	b	616	CLA	C10-C11-C12-C13
26	D	412	LMG	C14-C15-C16-C17
26	c	522	LMG	C32-C33-C34-C35
27	a	411	SQD	C10-C11-C12-C13
28	D	413	LHG	C15-C16-C17-C18
32	J	101	STE	C6-C7-C8-C9
32	b	620	STE	C4-C5-C6-C7
32	x	102	STE	C14-C15-C16-C17
22	b	607	CLA	O1A-CGA-O2A-C1
22	C	512	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
27	A	412	SQD	C10-C11-C12-C13
28	L	102	LHG	C12-C13-C14-C15
32	c	520	STE	C9-C10-C11-C12
22	b	604	CLA	C2-C3-C5-C6
26	B	626	LMG	C12-C13-C14-C15
26	M	101	LMG	C30-C31-C32-C33
28	L	102	LHG	C24-C25-C26-C27
32	B	624	STE	C5-C6-C7-C8
22	c	503	CLA	C5-C6-C7-C8
22	D	405	CLA	O1D-CGD-O2D-CED
32	L	103	STE	C1-C2-C3-C4
32	B	623	STE	C6-C7-C8-C9
31	Z	101	BCR	C15-C16-C17-C18
22	B	601	CLA	C16-C17-C18-C20
22	c	503	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
27	f	102	SQD	C25-C26-C27-C28
22	b	616	CLA	CBD-CGD-O2D-CED
26	m	101	LMG	C33-C34-C35-C36
27	a	411	SQD	C12-C13-C14-C15
27	a	411	SQD	C16-C17-C18-C19
28	d	408	LHG	C14-C15-C16-C17
22	c	511	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	C31-C32-C33-C34
26	c	522	LMG	C12-C13-C14-C15
26	c	522	LMG	C13-C14-C15-C16
26	c	522	LMG	C35-C36-C37-C38
27	t	102	SQD	C11-C12-C13-C14
28	D	411	LHG	C25-C26-C27-C28
29	A	413	DGD	C5A-C6A-C7A-C8A
29	A	413	DGD	CBA-CCA-CDA-CEA
29	c	517	DGD	CCB-CDB-CEB-CFB
26	c	519	LMG	C28-C29-C30-C31
27	A	412	SQD	C7-C8-C9-C10
27	L	101	SQD	C23-C24-C25-C26
26	B	626	LMG	C13-C14-C15-C16
26	B	626	LMG	C33-C34-C35-C36
26	Y	101	LMG	C33-C34-C35-C36
27	A	412	SQD	C15-C16-C17-C18
27	D	409	SQD	C26-C27-C28-C29
27	D	409	SQD	C28-C29-C30-C31
27	L	101	SQD	C14-C15-C16-C17
27	f	102	SQD	C27-C28-C29-C30
28	D	411	LHG	C33-C34-C35-C36
28	L	102	LHG	C32-C33-C34-C35
29	A	413	DGD	CEA-CFA-CGA-CHA
29	H	102	DGD	C4B-C5B-C6B-C7B
29	c	516	DGD	C4A-C5A-C6A-C7A
29	c	517	DGD	C7B-C8B-C9B-CAB
29	h	101	DGD	C2B-C3B-C4B-C5B
32	a	413	STE	C10-C11-C12-C13
32	b	624	STE	C6-C7-C8-C9
29	A	413	DGD	C4E-C5E-C6E-O5E
26	m	101	LMG	C12-C13-C14-C15
28	a	410	LHG	C11-C10-C9-C8
28	d	408	LHG	C33-C34-C35-C36
32	d	411	STE	C11-C12-C13-C14
28	D	410	LHG	C17-C18-C19-C20
29	C	516	DGD	C2A-C3A-C4A-C5A
32	a	413	STE	C6-C7-C8-C9
32	l	102	STE	C4-C5-C6-C7
32	x	102	STE	C13-C14-C15-C16
26	c	521	LMG	C30-C31-C32-C33
26	d	410	LMG	C14-C15-C16-C17
29	C	515	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
32	B	624	STE	C11-C10-C9-C8
32	c	523	STE	C5-C6-C7-C8
32	j	101	STE	C4-C5-C6-C7
22	b	605	CLA	C16-C17-C18-C20
22	c	510	CLA	C16-C17-C18-C20
22	B	606	CLA	C2B-C3B-CAB-CBB
31	C	514	BCR	C5-C6-C7-C8
31	D	406	BCR	C23-C24-C25-C30
31	H	101	BCR	C23-C24-C25-C26
31	K	101	BCR	C1-C6-C7-C8
31	K	101	BCR	C5-C6-C7-C8
31	T	101	BCR	C5-C6-C7-C8
31	t	101	BCR	C1-C6-C7-C8
27	B	622	SQD	C11-C12-C13-C14
28	d	408	LHG	C29-C30-C31-C32
32	X	101	STE	C9-C10-C11-C12
32	Z	102	STE	C11-C12-C13-C14
32	b	627	STE	C10-C11-C12-C13
22	d	401	CLA	CBD-CGD-O2D-CED
26	c	519	LMG	C33-C34-C35-C36
29	c	518	DGD	C6B-C7B-C8B-C9B
26	A	409	LMG	C11-C12-C13-C14
28	D	411	LHG	C24-C25-C26-C27
28	D	413	LHG	C9-C10-C11-C12
29	C	516	DGD	C6B-C7B-C8B-C9B
32	X	101	STE	C3-C4-C5-C6
32	X	101	STE	C14-C15-C16-C17
32	b	625	STE	C10-C11-C12-C13
22	B	605	CLA	C15-C16-C17-C18
22	b	611	CLA	C15-C16-C17-C18
27	A	410	SQD	C12-C13-C14-C15
28	D	410	LHG	C11-C12-C13-C14
29	C	517	DGD	C6B-C7B-C8B-C9B
29	c	516	DGD	CAB-CBB-CCB-CDB
25	d	407	PL9	C4-C3-C7-C8
26	B	626	LMG	C17-C18-C19-C20
27	A	410	SQD	C25-C26-C27-C28
28	D	411	LHG	C12-C13-C14-C15
28	d	408	LHG	C11-C10-C9-C8
32	J	101	STE	C2-C3-C4-C5
28	e	101	LHG	O9-C7-O7-C5
26	B	626	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
26	b	622	LMG	C16-C17-C18-C19
27	L	101	SQD	C11-C12-C13-C14
28	A	411	LHG	C28-C29-C30-C31
28	D	413	LHG	C24-C25-C26-C27
29	c	517	DGD	C2A-C3A-C4A-C5A
32	B	623	STE	C2-C3-C4-C5
32	b	620	STE	C2-C3-C4-C5
32	x	102	STE	C3-C4-C5-C6
31	K	102	BCR	C18-C19-C20-C21
31	T	101	BCR	C18-C19-C20-C21
31	Z	101	BCR	C18-C19-C20-C21
31	c	515	BCR	C18-C19-C20-C21
31	k	101	BCR	C10-C11-C12-C13
22	c	504	CLA	C2-C3-C5-C6
26	B	626	LMG	C30-C31-C32-C33
26	c	522	LMG	C37-C38-C39-C40
28	A	411	LHG	C13-C14-C15-C16
28	D	410	LHG	C15-C16-C17-C18
28	D	411	LHG	C27-C28-C29-C30
29	c	518	DGD	C4B-C5B-C6B-C7B
32	I	102	STE	C10-C11-C12-C13
32	l	102	STE	C13-C14-C15-C16
26	b	622	LMG	C10-C11-C12-C13
22	B	605	CLA	CBA-CGA-O2A-C1
22	d	404	CLA	C14-C13-C15-C16
26	B	626	LMG	C36-C37-C38-C39
26	m	101	LMG	C38-C39-C40-C41
29	C	517	DGD	C5A-C6A-C7A-C8A
29	h	101	DGD	C6B-C7B-C8B-C9B
32	J	101	STE	C5-C6-C7-C8
27	t	102	SQD	C11-C10-C9-C8
27	t	102	SQD	C12-C13-C14-C15
32	X	101	STE	C10-C11-C12-C13
32	b	624	STE	C4-C5-C6-C7
26	b	622	LMG	O6-C1-O1-C7
29	C	516	DGD	O6E-C1E-O5D-C6D
32	B	625	STE	C7-C8-C9-C10
29	C	516	DGD	C2E-C1E-O5D-C6D
22	C	512	CLA	C8-C10-C11-C12
26	b	622	LMG	C30-C31-C32-C33
26	b	622	LMG	C31-C32-C33-C34
26	c	519	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
28	D	410	LHG	C32-C33-C34-C35
26	B	626	LMG	C38-C39-C40-C41
26	m	101	LMG	C18-C19-C20-C21
29	A	413	DGD	C5B-C6B-C7B-C8B
29	H	102	DGD	C7A-C8A-C9A-CAA
29	c	517	DGD	C4A-C5A-C6A-C7A
26	B	626	LMG	C37-C38-C39-C40
26	D	412	LMG	C13-C14-C15-C16
26	Y	101	LMG	C12-C13-C14-C15
26	d	410	LMG	C34-C35-C36-C37
32	B	624	STE	C4-C5-C6-C7
27	a	411	SQD	C34-C35-C36-C37
26	c	522	LMG	C11-C10-O7-C8
27	a	411	SQD	C8-C7-O47-C45
28	a	410	LHG	C23-C24-C25-C26
29	c	518	DGD	C8B-C9B-CAB-CBB
26	B	626	LMG	O9-C10-O7-C8
32	B	624	STE	C3-C4-C5-C6
32	x	102	STE	C4-C5-C6-C7
26	Y	101	LMG	C30-C31-C32-C33
28	l	101	LHG	C34-C35-C36-C37
22	a	404	CLA	C10-C11-C12-C13
31	I	101	BCR	C7-C8-C9-C34
31	b	617	BCR	C7-C8-C9-C34
26	Y	101	LMG	C31-C32-C33-C34
27	A	410	SQD	C14-C15-C16-C17
29	c	517	DGD	C6A-C7A-C8A-C9A
32	a	413	STE	C11-C12-C13-C14
26	m	101	LMG	C20-C21-C22-C23
28	D	413	LHG	C32-C33-C34-C35
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	502	CLA	C16-C17-C18-C19
22	D	405	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C19
22	b	609	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C20
22	b	616	CLA	C11-C12-C13-C15
23	D	401	PHO	C16-C17-C18-C20
22	B	614	CLA	CBD-CGD-O2D-CED
22	C	506	CLA	CBD-CGD-O2D-CED
26	B	621	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	C34-C35-C36-C37
27	D	409	SQD	C25-C26-C27-C28
22	C	505	CLA	C4-C3-C5-C6
22	c	504	CLA	C4-C3-C5-C6
25	d	407	PL9	C15-C14-C16-C17
25	d	407	PL9	C30-C29-C31-C32
25	d	407	PL9	C45-C44-C46-C47
29	c	516	DGD	C1B-C2B-C3B-C4B
26	B	626	LMG	C23-C24-C25-C26
26	D	408	LMG	C17-C18-C19-C20
26	b	622	LMG	C15-C16-C17-C18
26	c	521	LMG	C35-C36-C37-C38
28	D	411	LHG	C11-C12-C13-C14
29	C	517	DGD	C3A-C4A-C5A-C6A
32	B	620	STE	C9-C10-C11-C12
22	B	613	CLA	C5-C6-C7-C8
22	b	601	CLA	C13-C15-C16-C17
22	c	512	CLA	C8-C10-C11-C12
27	D	409	SQD	C27-C28-C29-C30
27	a	411	SQD	C9-C10-C11-C12
22	A	402	CLA	C4C-C3C-CAC-CBC
26	D	408	LMG	C36-C37-C38-C39
26	c	519	LMG	C39-C40-C41-C42
26	c	521	LMG	C33-C34-C35-C36
26	m	101	LMG	C17-C18-C19-C20
28	D	413	LHG	C16-C17-C18-C19
28	L	102	LHG	C10-C11-C12-C13
29	C	517	DGD	CCB-CDB-CEB-CFB
32	B	625	STE	C5-C6-C7-C8
32	H	103	STE	C4-C5-C6-C7
22	B	606	CLA	C5-C6-C7-C8
22	b	601	CLA	C5-C6-C7-C8
22	b	603	CLA	C8-C10-C11-C12
22	c	509	CLA	C13-C15-C16-C17
23	A	404	PHO	C15-C16-C17-C18
35	v	201	HEC	C2B-C3B-CAB-CBB
32	R	101	STE	C1-C2-C3-C4
28	D	410	LHG	O9-C7-O7-C5
27	A	412	SQD	C9-C10-C11-C12
27	D	409	SQD	C30-C31-C32-C33
28	D	410	LHG	C28-C29-C30-C31
28	D	413	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
32	d	411	STE	C3-C4-C5-C6
32	d	412	STE	C2-C3-C4-C5
23	d	402	PHO	CBD-CGD-O2D-CED
22	B	608	CLA	C5-C6-C7-C8
22	C	508	CLA	C15-C16-C17-C18
29	c	518	DGD	CCA-CDA-CEA-CFA
22	C	510	CLA	C8-C10-C11-C12
22	c	507	CLA	C13-C15-C16-C17
26	M	101	LMG	C38-C39-C40-C41
26	M	101	LMG	C39-C40-C41-C42
26	m	101	LMG	C16-C17-C18-C19
29	c	516	DGD	CBA-CCA-CDA-CEA
26	b	622	LMG	O6-C5-C6-O5
26	c	521	LMG	O1-C7-C8-O7
27	D	409	SQD	C29-C30-C31-C32
28	L	102	LHG	C28-C29-C30-C31
28	L	102	LHG	C30-C31-C32-C33
29	C	516	DGD	C4A-C5A-C6A-C7A
29	c	516	DGD	C5B-C6B-C7B-C8B
29	h	101	DGD	C3B-C4B-C5B-C6B
26	c	522	LMG	C4-C5-C6-O5
22	b	603	CLA	O1D-CGD-O2D-CED
26	B	626	LMG	C34-C35-C36-C37
28	l	101	LHG	C24-C25-C26-C27
32	B	620	STE	C11-C12-C13-C14
22	B	605	CLA	C8-C10-C11-C12
27	a	411	SQD	C26-C27-C28-C29
28	e	101	LHG	C17-C18-C19-C20
32	H	103	STE	C5-C6-C7-C8
26	Y	101	LMG	C37-C38-C39-C40
28	L	102	LHG	C31-C32-C33-C34
29	C	517	DGD	CBA-CCA-CDA-CEA
29	c	518	DGD	C3A-C4A-C5A-C6A
27	B	622	SQD	C17-C18-C19-C20
32	b	624	STE	C2-C3-C4-C5
26	D	408	LMG	C30-C31-C32-C33
32	b	627	STE	C6-C7-C8-C9
32	d	411	STE	C2-C3-C4-C5
22	c	505	CLA	C2-C3-C5-C6
22	c	512	CLA	C10-C11-C12-C13
26	A	409	LMG	C18-C19-C20-C21
26	A	409	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
26	D	412	LMG	C12-C13-C14-C15
26	c	522	LMG	C33-C34-C35-C36
28	D	410	LHG	C29-C30-C31-C32
28	D	413	LHG	C17-C18-C19-C20
29	H	102	DGD	C8B-C9B-CAB-CBB
32	b	621	STE	C11-C12-C13-C14
32	b	624	STE	C7-C8-C9-C10
32	c	523	STE	C4-C5-C6-C7
22	b	602	CLA	CBD-CGD-O2D-CED
27	A	412	SQD	C24-C23-O48-C46
27	A	412	SQD	C24-C25-C26-C27
27	L	101	SQD	C16-C17-C18-C19
29	H	102	DGD	C6B-C7B-C8B-C9B
32	R	101	STE	C3-C4-C5-C6
26	c	522	LMG	C31-C32-C33-C34
22	b	602	CLA	C15-C16-C17-C18
22	c	506	CLA	C10-C11-C12-C13
27	A	410	SQD	C8-C7-O47-C45
27	L	101	SQD	C26-C27-C28-C29
28	d	408	LHG	C32-C33-C34-C35
32	R	101	STE	C2-C3-C4-C5
22	b	601	CLA	C16-C17-C18-C19
27	A	412	SQD	C29-C30-C31-C32
29	C	516	DGD	C4B-C5B-C6B-C7B
22	B	601	CLA	C1A-C2A-CAA-CBA
22	c	503	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
28	l	101	LHG	C25-C26-C27-C28
29	c	517	DGD	CAB-CBB-CCB-CDB
28	a	410	LHG	C25-C26-C27-C28
27	B	622	SQD	O10-C23-O48-C46
26	c	522	LMG	C34-C35-C36-C37
28	A	411	LHG	C15-C16-C17-C18
29	h	101	DGD	C9A-CAA-CBA-CCA
26	c	519	LMG	O6-C5-C6-O5
32	H	103	STE	C13-C14-C15-C16
22	A	403	CLA	C6-C7-C8-C10
22	A	403	CLA	C11-C12-C13-C15
22	B	605	CLA	C11-C10-C8-C7
22	B	610	CLA	C11-C12-C13-C15
22	B	614	CLA	C11-C12-C13-C15
22	C	507	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	D	405	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C12-C13-C15
22	b	604	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C12-C13-C15
22	b	606	CLA	C11-C10-C8-C7
22	b	607	CLA	C6-C7-C8-C10
22	b	607	CLA	C11-C12-C13-C15
22	b	615	CLA	C12-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C12-C13-C15
22	c	509	CLA	C6-C7-C8-C10
22	c	512	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
22	B	615	CLA	C16-C17-C18-C20
22	b	614	CLA	CBA-CGA-O2A-C1
22	B	611	CLA	C4-C3-C5-C6
25	d	407	PL9	C13-C14-C16-C17
28	D	410	LHG	C13-C14-C15-C16
28	D	413	LHG	C25-C26-C27-C28
28	l	101	LHG	C32-C33-C34-C35
29	C	517	DGD	C3B-C4B-C5B-C6B
32	d	412	STE	C11-C12-C13-C14
26	D	408	LMG	O6-C5-C6-O5
22	C	508	CLA	C13-C15-C16-C17
22	c	512	CLA	O1D-CGD-O2D-CED
22	b	610	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C6-C7-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	605	CLA	C6-C7-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	B	615	CLA	C11-C12-C13-C14
22	B	616	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	C	513	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C12-C13-C14
22	D	405	CLA	C6-C7-C8-C9
22	D	405	CLA	C11-C10-C8-C9
22	b	601	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C11-C12-C13-C14
22	b	607	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	510	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
22	d	405	CLA	C6-C7-C8-C9
32	B	620	STE	C4-C5-C6-C7
26	c	521	LMG	C16-C17-C18-C19
22	C	510	CLA	C10-C11-C12-C13
23	a	403	PHO	CBD-CGD-O2D-CED
27	a	411	SQD	C14-C15-C16-C17
29	C	516	DGD	CBB-CCB-CDB-CEB
25	A	408	PL9	C47-C48-C49-C50
32	L	103	STE	C3-C4-C5-C6
26	B	626	LMG	O1-C7-C8-C9
26	M	101	LMG	C7-C8-C9-O8
26	Y	101	LMG	O1-C7-C8-C9
26	c	521	LMG	C7-C8-C9-O8
26	c	522	LMG	O1-C7-C8-C9
27	B	622	SQD	O6-C44-C45-C46
27	a	411	SQD	O6-C44-C45-C46
27	t	102	SQD	C44-C45-C46-O48
29	A	413	DGD	O1G-C1G-C2G-C3G
29	A	413	DGD	C1G-C2G-C3G-O3G
29	C	515	DGD	O1G-C1G-C2G-C3G
29	A	413	DGD	C7A-C8A-C9A-CAA
32	c	523	STE	C2-C3-C4-C5
29	C	515	DGD	C8A-C9A-CAA-CBA
32	a	413	STE	C12-C13-C14-C15
22	b	607	CLA	C10-C11-C12-C13
22	b	613	CLA	C13-C15-C16-C17
29	H	102	DGD	C4E-C5E-C6E-O5E
27	B	622	SQD	C9-C10-C11-C12
22	C	506	CLA	CBA-CGA-O2A-C1
26	d	410	LMG	O6-C5-C6-O5
29	c	516	DGD	O6E-C5E-C6E-O5E
22	B	610	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
22	D	405	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C14
26	A	409	LMG	C37-C38-C39-C40
28	a	410	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C13-C15-C16-C17
22	B	605	CLA	O1A-CGA-O2A-C1
27	A	412	SQD	C11-C10-C9-C8
28	l	101	LHG	C30-C31-C32-C33
32	H	103	STE	C12-C13-C14-C15
22	C	504	CLA	C8-C10-C11-C12
28	l	101	LHG	C17-C18-C19-C20
29	h	101	DGD	C7B-C8B-C9B-CAB
22	c	505	CLA	C4-C3-C5-C6
22	B	611	CLA	C2-C3-C5-C6
22	C	505	CLA	C2-C3-C5-C6
22	b	608	CLA	C13-C15-C16-C17
31	H	101	BCR	C37-C22-C23-C24
31	c	514	BCR	C36-C18-C19-C20
28	l	101	LHG	C11-C12-C13-C14
29	c	517	DGD	CBA-CCA-CDA-CEA
26	B	626	LMG	C4-C5-C6-O5
26	b	622	LMG	C34-C35-C36-C37
29	C	516	DGD	CBA-CCA-CDA-CEA
29	H	102	DGD	C9B-CAB-CBB-CCB
22	c	503	CLA	C15-C16-C17-C18
22	c	504	CLA	C10-C11-C12-C13
28	l	101	LHG	C9-C10-C11-C12
28	l	101	LHG	C28-C29-C30-C31
32	b	627	STE	C12-C13-C14-C15
27	t	102	SQD	C10-C11-C12-C13
28	D	411	LHG	C13-C14-C15-C16
32	b	621	STE	C3-C4-C5-C6
26	c	521	LMG	C29-C30-C31-C32
29	C	516	DGD	C5A-C6A-C7A-C8A
32	B	627	STE	C1-C2-C3-C4
27	A	410	SQD	C11-C10-C9-C8
27	A	410	SQD	C16-C17-C18-C19
28	D	410	LHG	C30-C31-C32-C33
32	b	621	STE	C6-C7-C8-C9
32	b	626	STE	C4-C5-C6-C7
26	c	522	LMG	C19-C20-C21-C22
28	D	411	LHG	C32-C33-C34-C35
29	A	413	DGD	O6D-C5D-C6D-O5D
28	A	411	LHG	C11-C10-C9-C8
29	c	516	DGD	CBB-CCB-CDB-CEB
32	d	412	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	D	408	LMG	C35-C36-C37-C38
26	c	522	LMG	C36-C37-C38-C39
28	a	410	LHG	C14-C15-C16-C17
32	b	623	STE	C6-C7-C8-C9
26	Y	101	LMG	C28-C29-C30-C31
31	c	515	BCR	C20-C21-C22-C23
31	k	102	BCR	C20-C21-C22-C23
28	L	102	LHG	C13-C14-C15-C16
29	c	516	DGD	C9B-CAB-CBB-CCB
28	l	101	LHG	O6-C4-C5-O7
22	b	601	CLA	C10-C11-C12-C13
29	C	516	DGD	CCB-CDB-CEB-CFB
26	Y	101	LMG	C29-C28-O8-C9
27	a	411	SQD	C13-C14-C15-C16
29	C	516	DGD	C8B-C9B-CAB-CBB
26	D	412	LMG	C37-C38-C39-C40
32	t	104	STE	C7-C8-C9-C10
26	m	101	LMG	C37-C38-C39-C40
28	D	413	LHG	C18-C19-C20-C21
25	a	409	PL9	C30-C29-C31-C32
23	A	404	PHO	C2-C3-C5-C6
26	D	412	LMG	C16-C17-C18-C19
27	B	622	SQD	C13-C14-C15-C16
28	A	411	LHG	C25-C26-C27-C28
23	D	401	PHO	C16-C17-C18-C19
27	A	410	SQD	C29-C30-C31-C32
32	B	625	STE	C6-C7-C8-C9
32	c	520	STE	C4-C5-C6-C7
26	B	621	LMG	C37-C38-C39-C40
28	e	101	LHG	C14-C15-C16-C17
27	a	411	SQD	O47-C45-C46-O48
29	c	518	DGD	CCB-CDB-CEB-CFB
32	B	620	STE	C12-C13-C14-C15
27	L	101	SQD	C27-C28-C29-C30
29	C	515	DGD	C3B-C4B-C5B-C6B
22	A	403	CLA	C3-C5-C6-C7
26	c	522	LMG	C20-C21-C22-C23
29	C	515	DGD	CDA-CEA-CFA-CGA
29	C	516	DGD	CDA-CEA-CFA-CGA
32	b	623	STE	C11-C12-C13-C14
32	d	412	STE	C15-C16-C17-C18
22	B	607	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	Y	101	LMG	C13-C14-C15-C16
27	A	410	SQD	C17-C18-C19-C20
29	C	515	DGD	C6B-C7B-C8B-C9B
26	Y	101	LMG	C11-C12-C13-C14
26	b	622	LMG	C12-C13-C14-C15
27	A	412	SQD	C34-C35-C36-C37
28	d	408	LHG	C15-C16-C17-C18
27	a	411	SQD	C24-C23-O48-C46
26	b	622	LMG	C18-C19-C20-C21
32	b	623	STE	C4-C5-C6-C7
26	m	101	LMG	C40-C41-C42-C43
32	R	101	STE	C7-C8-C9-C10
26	B	626	LMG	C15-C16-C17-C18
32	a	412	STE	C3-C4-C5-C6
31	B	618	BCR	C14-C15-C16-C17
31	T	101	BCR	C14-C15-C16-C17
28	d	409	LHG	C31-C32-C33-C34
22	c	501	CLA	O1D-CGD-O2D-CED
28	e	101	LHG	C7-C8-C9-C10
22	a	404	CLA	C15-C16-C17-C18
22	b	616	CLA	C8-C10-C11-C12
22	C	506	CLA	O1D-CGD-O2D-CED
22	d	401	CLA	O1D-CGD-O2D-CED
25	D	407	PL9	C30-C29-C31-C32
22	b	611	CLA	C2-C3-C5-C6
27	A	410	SQD	C30-C31-C32-C33
28	D	411	LHG	C29-C30-C31-C32
26	B	626	LMG	C40-C41-C42-C43
28	D	410	LHG	C11-C10-C9-C8
29	C	516	DGD	C8A-C9A-CAA-CBA
32	Z	102	STE	C12-C13-C14-C15
28	a	410	LHG	O1-C1-C2-O2
28	d	408	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
22	A	403	CLA	C11-C12-C13-C14
22	B	603	CLA	C11-C12-C13-C14
22	B	607	CLA	C11-C10-C8-C9
22	B	610	CLA	C11-C12-C13-C14
22	C	504	CLA	C11-C10-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C9
22	C	511	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
22	b	604	CLA	C14-C13-C15-C16
22	b	606	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C10-C8-C9
22	b	615	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	d	401	CLA	C11-C10-C8-C9
22	d	403	CLA	C6-C7-C8-C9
22	B	614	CLA	O1D-CGD-O2D-CED
22	B	608	CLA	C10-C11-C12-C13
22	b	601	CLA	C15-C16-C17-C18
22	b	609	CLA	C15-C16-C17-C18
22	b	603	CLA	C4B-C3B-CAB-CBB
22	d	403	CLA	C4B-C3B-CAB-CBB
26	m	101	LMG	C39-C40-C41-C42
29	c	518	DGD	C7B-C8B-C9B-CAB
32	t	103	STE	C3-C4-C5-C6
22	c	509	CLA	CAA-CBA-CGA-O2A
32	a	412	STE	C7-C8-C9-C10
29	A	413	DGD	CCB-CDB-CEB-CFB
26	b	622	LMG	C2-C1-O1-C7
22	B	607	CLA	C13-C15-C16-C17
22	c	502	CLA	C15-C16-C17-C18
26	D	412	LMG	C36-C37-C38-C39
32	l	102	STE	C3-C4-C5-C6
32	b	620	STE	C1-C2-C3-C4
28	l	101	LHG	O6-C4-C5-C6
32	H	103	STE	C6-C7-C8-C9
28	a	410	LHG	C19-C20-C21-C22
32	b	626	STE	C7-C8-C9-C10
22	B	602	CLA	C11-C12-C13-C15
22	B	607	CLA	C11-C10-C8-C7
22	B	611	CLA	C11-C10-C8-C7
22	B	615	CLA	C11-C12-C13-C15
22	B	616	CLA	C6-C7-C8-C10
22	C	502	CLA	C12-C13-C15-C16
22	C	504	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C12-C13-C15
22	D	404	CLA	C11-C12-C13-C15
22	D	405	CLA	C11-C10-C8-C7
22	b	609	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	b	616	CLA	C11-C10-C8-C7
22	c	501	CLA	C11-C12-C13-C15
22	c	505	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C10
22	d	401	CLA	C11-C10-C8-C7
22	d	401	CLA	C12-C13-C15-C16
22	c	502	CLA	O1D-CGD-O2D-CED
27	L	101	SQD	C19-C20-C21-C22
26	B	626	LMG	C39-C40-C41-C42
26	D	408	LMG	C15-C16-C17-C18
26	b	622	LMG	C38-C39-C40-C41
29	H	102	DGD	C5B-C6B-C7B-C8B
28	L	102	LHG	O10-C23-O8-C6
22	C	506	CLA	C3A-C2A-CAA-CBA
22	B	612	CLA	C10-C11-C12-C13
22	B	616	CLA	C5-C6-C7-C8
22	C	509	CLA	C8-C10-C11-C12
25	D	407	PL9	C13-C14-C16-C17
25	a	409	PL9	C23-C24-C26-C27
25	d	407	PL9	C28-C29-C31-C32
32	C	519	STE	C1-C2-C3-C4
26	A	409	LMG	C14-C15-C16-C17
32	t	103	STE	C6-C7-C8-C9
28	a	410	LHG	C30-C31-C32-C33
22	b	614	CLA	O1A-CGA-O2A-C1
31	t	101	BCR	C15-C16-C17-C18
31	B	617	BCR	C36-C18-C19-C20
27	a	411	SQD	C25-C26-C27-C28
22	C	506	CLA	O1A-CGA-O2A-C1
26	B	621	LMG	C14-C15-C16-C17
29	C	515	DGD	C5A-C6A-C7A-C8A
22	A	403	CLA	C15-C16-C17-C18
22	c	509	CLA	C15-C16-C17-C18
27	f	102	SQD	C28-C29-C30-C31
32	J	101	STE	C7-C8-C9-C10
32	c	523	STE	C7-C8-C9-C10
29	H	102	DGD	CBB-CCB-CDB-CEB
26	D	412	LMG	C7-C8-C9-O8
26	c	521	LMG	O1-C7-C8-C9
27	L	101	SQD	C44-C45-C46-O48
29	h	101	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
32	M	102	STE	C10-C11-C12-C13
26	c	521	LMG	C39-C40-C41-C42
28	D	410	LHG	C25-C26-C27-C28
32	J	101	STE	C1-C2-C3-C4
22	B	614	CLA	C5-C6-C7-C8
22	C	513	CLA	C8-C10-C11-C12
32	b	624	STE	C9-C10-C11-C12
32	c	520	STE	C11-C12-C13-C14
28	D	411	LHG	C30-C31-C32-C33
22	C	506	CLA	C4-C3-C5-C6
22	b	611	CLA	C4-C3-C5-C6
22	c	512	CLA	C4-C3-C5-C6
23	A	404	PHO	C4-C3-C5-C6
28	e	101	LHG	C23-C24-C25-C26
26	Y	101	LMG	C32-C33-C34-C35
28	a	410	LHG	C16-C17-C18-C19
28	L	102	LHG	C17-C18-C19-C20
35	v	201	HEC	C4B-C3B-CAB-CBB
22	b	608	CLA	C2C-C3C-CAC-CBC
27	a	411	SQD	C24-C25-C26-C27
28	A	411	LHG	C10-C11-C12-C13
28	L	102	LHG	C15-C16-C17-C18
22	b	612	CLA	C15-C16-C17-C18
32	b	620	STE	C9-C10-C11-C12
31	B	618	BCR	C23-C24-C25-C30
31	C	514	BCR	C1-C6-C7-C8
31	H	101	BCR	C23-C24-C25-C30
31	d	406	BCR	C23-C24-C25-C30
31	k	101	BCR	C1-C6-C7-C8
31	k	101	BCR	C23-C24-C25-C30
31	t	101	BCR	C5-C6-C7-C8
28	A	411	LHG	C18-C19-C20-C21
32	c	520	STE	C10-C11-C12-C13
27	A	412	SQD	C27-C28-C29-C30
32	H	103	STE	C11-C10-C9-C8
26	D	408	LMG	C31-C32-C33-C34
27	A	412	SQD	C16-C17-C18-C19
29	c	517	DGD	C9B-CAB-CBB-CCB
32	C	520	STE	C5-C6-C7-C8
32	a	412	STE	C6-C7-C8-C9
22	B	611	CLA	C16-C17-C18-C20
22	B	615	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C10-C11-C12-C13
26	M	101	LMG	O7-C8-C9-O8
26	Y	101	LMG	O1-C7-C8-O7
26	c	522	LMG	O1-C7-C8-O7
29	A	413	DGD	O1G-C1G-C2G-O2G
25	D	407	PL9	C4-C3-C7-C8
25	a	409	PL9	C4-C3-C7-C8
28	d	409	LHG	C26-C27-C28-C29
32	b	627	STE	C9-C10-C11-C12
28	L	102	LHG	O9-C7-O7-C5
32	b	626	STE	C5-C6-C7-C8
22	c	512	CLA	C2-C3-C5-C6
28	D	413	LHG	C34-C35-C36-C37
28	e	101	LHG	C25-C26-C27-C28
32	l	102	STE	C5-C6-C7-C8
22	b	608	CLA	C4C-C3C-CAC-CBC
22	b	605	CLA	O1D-CGD-O2D-CED
22	D	404	CLA	C16-C17-C18-C19
28	L	102	LHG	C33-C34-C35-C36
32	B	624	STE	C11-C12-C13-C14
32	x	102	STE	C11-C10-C9-C8
22	b	609	CLA	C8-C10-C11-C12
27	L	101	SQD	C17-C18-C19-C20
29	H	102	DGD	CCA-CDA-CEA-CFA
32	I	102	STE	C11-C10-C9-C8
22	B	614	CLA	C6-C7-C8-C9
22	b	603	CLA	C6-C7-C8-C9
29	h	101	DGD	CAB-CBB-CCB-CDB
22	C	512	CLA	C15-C16-C17-C18
32	C	519	STE	C13-C14-C15-C16
26	d	410	LMG	C30-C31-C32-C33
31	B	617	BCR	C6-C7-C8-C9
31	b	617	BCR	C6-C7-C8-C9
26	d	410	LMG	C15-C16-C17-C18
32	b	620	STE	C13-C14-C15-C16
32	l	102	STE	C12-C13-C14-C15
28	A	411	LHG	C17-C18-C19-C20
32	L	103	STE	C7-C8-C9-C10
22	B	610	CLA	C16-C17-C18-C19
22	B	613	CLA	C16-C17-C18-C19
22	b	602	CLA	C16-C17-C18-C19
22	b	616	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	m	101	LMG	C32-C33-C34-C35
32	I	102	STE	C2-C3-C4-C5
29	A	413	DGD	C8A-C9A-CAA-CBA
29	c	516	DGD	C4D-C5D-C6D-O5D
27	B	622	SQD	C24-C25-C26-C27
29	A	413	DGD	C7B-C8B-C9B-CAB
28	D	411	LHG	C35-C36-C37-C38
29	C	515	DGD	C4E-C5E-C6E-O5E
32	a	413	STE	C1-C2-C3-C4
25	a	409	PL9	C12-C11-C9-C8
22	c	505	CLA	C10-C11-C12-C13
26	B	626	LMG	C32-C33-C34-C35
32	B	624	STE	C12-C13-C14-C15
22	A	402	CLA	C13-C15-C16-C17
26	A	409	LMG	C39-C40-C41-C42
27	B	622	SQD	C32-C33-C34-C35
31	H	101	BCR	C35-C13-C14-C15
31	K	102	BCR	C20-C21-C22-C37
31	c	514	BCR	C35-C13-C14-C15
22	a	404	CLA	CBA-CGA-O2A-C1
22	b	609	CLA	CBA-CGA-O2A-C1
28	d	409	LHG	C24-C23-O8-C6
26	B	621	LMG	C29-C30-C31-C32
22	b	611	CLA	C8-C10-C11-C12
23	a	403	PHO	O1D-CGD-O2D-CED
29	A	413	DGD	C6B-C7B-C8B-C9B
32	X	101	STE	C13-C14-C15-C16
22	b	609	CLA	O1A-CGA-O2A-C1
22	b	604	CLA	C15-C16-C17-C18
22	b	605	CLA	C13-C15-C16-C17
22	B	603	CLA	C11-C12-C13-C15
22	B	604	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	B	606	CLA	C11-C10-C8-C7
22	B	607	CLA	C11-C12-C13-C15
22	B	607	CLA	C12-C13-C15-C16
22	B	610	CLA	C12-C13-C15-C16
22	B	614	CLA	C11-C10-C8-C7
22	D	405	CLA	C11-C12-C13-C15
22	b	603	CLA	C6-C7-C8-C10
22	b	605	CLA	C11-C10-C8-C7
22	b	611	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C11-C12-C13-C15
23	A	404	PHO	C12-C13-C15-C16
27	f	102	SQD	C31-C32-C33-C34
29	c	518	DGD	C2A-C3A-C4A-C5A
32	B	627	STE	C6-C7-C8-C9
32	c	520	STE	C7-C8-C9-C10
22	b	616	CLA	C3-C5-C6-C7
22	c	513	CLA	C5-C6-C7-C8
22	C	513	CLA	C2C-C3C-CAC-CBC
31	C	514	BCR	C7-C8-C9-C10
31	C	514	BCR	C11-C12-C13-C14
31	k	101	BCR	C17-C18-C19-C20
26	D	412	LMG	C30-C31-C32-C33
26	b	622	LMG	C29-C30-C31-C32
26	B	626	LMG	C8-C7-O1-C1
29	C	516	DGD	C2G-C3G-O3G-C1D
29	C	516	DGD	C5D-C6D-O5D-C1E
32	b	626	STE	C1-C2-C3-C4
26	b	622	LMG	C35-C36-C37-C38
29	A	413	DGD	C4A-C5A-C6A-C7A
23	d	402	PHO	O1D-CGD-O2D-CED
29	C	515	DGD	O1B-C1B-O2G-C2G
28	A	411	LHG	C31-C32-C33-C34
22	C	502	CLA	O1D-CGD-O2D-CED
26	D	412	LMG	C9-C8-O7-C10
27	f	102	SQD	C46-C45-O47-C7
26	B	626	LMG	C24-C25-C26-C27
22	c	506	CLA	O1A-CGA-O2A-C1
26	Y	101	LMG	O10-C28-O8-C9
28	D	413	LHG	C27-C28-C29-C30
26	d	410	LMG	C12-C13-C14-C15
32	b	623	STE	C5-C6-C7-C8
22	C	508	CLA	C16-C17-C18-C19
32	H	103	STE	C15-C16-C17-C18
27	D	409	SQD	O6-C44-C45-C46
22	c	506	CLA	CBA-CGA-O2A-C1
31	B	617	BCR	C20-C21-C22-C23
29	C	517	DGD	CAB-CBB-CCB-CDB
26	B	626	LMG	C19-C20-C21-C22
26	M	101	LMG	O6-C1-O1-C7
34	F	101	HEM	C4C-C3C-CAC-CBC
28	A	411	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	m	101	LMG	C19-C20-C21-C22
29	H	102	DGD	CBA-CCA-CDA-CEA
22	C	505	CLA	C5-C6-C7-C8
32	x	102	STE	C15-C16-C17-C18
32	c	523	STE	C6-C7-C8-C9
27	L	101	SQD	C30-C31-C32-C33
28	D	411	LHG	C16-C17-C18-C19
29	C	515	DGD	CAB-CBB-CCB-CDB
32	b	621	STE	C2-C3-C4-C5
26	c	521	LMG	O7-C8-C9-O8
26	m	101	LMG	O7-C8-C9-O8
27	L	101	SQD	O47-C45-C46-O48
22	B	603	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	b	607	CLA	C14-C13-C15-C16
22	b	611	CLA	C11-C12-C13-C14
22	b	613	CLA	C6-C7-C8-C9
22	C	509	CLA	C16-C17-C18-C19
26	b	622	LMG	C13-C14-C15-C16
26	c	519	LMG	C34-C35-C36-C37
26	c	519	LMG	C30-C31-C32-C33
32	C	519	STE	C4-C5-C6-C7
22	a	404	CLA	O1A-CGA-O2A-C1
28	a	410	LHG	O10-C23-O8-C6
29	C	516	DGD	O1A-C1A-O1G-C1G
27	A	412	SQD	C13-C14-C15-C16
32	M	103	STE	C2-C3-C4-C5
22	C	503	CLA	CBD-CGD-O2D-CED
28	L	102	LHG	C18-C19-C20-C21
32	B	627	STE	C2-C3-C4-C5
32	b	625	STE	C12-C13-C14-C15
28	l	101	LHG	C33-C34-C35-C36
22	c	513	CLA	C8-C10-C11-C12
29	A	413	DGD	C4D-C5D-C6D-O5D
27	A	412	SQD	C44-C45-O47-C7
22	B	616	CLA	C2-C1-O2A-CGA
28	A	411	LHG	C34-C35-C36-C37
29	H	102	DGD	C3B-C4B-C5B-C6B
32	t	103	STE	C11-C10-C9-C8
32	Z	102	STE	C14-C15-C16-C17
28	D	411	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
22	C	506	CLA	C2-C3-C5-C6
22	b	611	CLA	C13-C15-C16-C17
22	c	501	CLA	C15-C16-C17-C18
22	C	508	CLA	C16-C17-C18-C20
22	C	513	CLA	C16-C17-C18-C19
32	a	412	STE	C2-C3-C4-C5
22	b	610	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CBD-CGD-O2D-CED
22	B	602	CLA	C10-C11-C12-C13
29	c	517	DGD	C2B-C3B-C4B-C5B
22	A	402	CLA	C15-C16-C17-C18
22	c	511	CLA	C1A-C2A-CAA-CBA
29	h	101	DGD	C6A-C7A-C8A-C9A
32	b	624	STE	C5-C6-C7-C8
22	C	503	CLA	C4-C3-C5-C6
22	B	602	CLA	C15-C16-C17-C18
27	B	622	SQD	C25-C26-C27-C28
26	c	521	LMG	C32-C33-C34-C35
22	b	610	CLA	C16-C17-C18-C19
22	d	404	CLA	C16-C17-C18-C20
22	b	607	CLA	C5-C6-C7-C8
26	B	621	LMG	C36-C37-C38-C39
26	m	101	LMG	C15-C16-C17-C18
26	Y	101	LMG	C34-C35-C36-C37
28	e	101	LHG	O6-C4-C5-C6
26	M	101	LMG	C19-C20-C21-C22
29	C	516	DGD	C3A-C4A-C5A-C6A
29	c	518	DGD	CAA-CBA-CCA-CDA
26	B	621	LMG	C32-C33-C34-C35
22	B	601	CLA	C11-C10-C8-C7
22	B	603	CLA	C6-C7-C8-C10
22	B	609	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C7
22	C	506	CLA	C6-C7-C8-C10
22	D	403	CLA	C11-C12-C13-C15
22	b	601	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C10-C8-C7
22	b	612	CLA	C12-C13-C15-C16
22	c	503	CLA	C11-C12-C13-C15
22	c	505	CLA	C6-C7-C8-C10
22	d	401	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
23	a	403	PHO	C6-C7-C8-C10
29	c	516	DGD	O6D-C5D-C6D-O5D
32	B	625	STE	C11-C10-C9-C8
22	C	509	CLA	C16-C17-C18-C20
22	D	403	CLA	C16-C17-C18-C19
22	b	608	CLA	C16-C17-C18-C19
22	b	610	CLA	C16-C17-C18-C20
27	A	410	SQD	C9-C10-C11-C12
26	D	408	LMG	C37-C38-C39-C40
28	L	102	LHG	C9-C10-C11-C12
32	j	101	STE	C2-C3-C4-C5
25	A	408	PL9	C15-C14-C16-C17
26	m	101	LMG	C34-C35-C36-C37
29	H	102	DGD	CCB-CDB-CEB-CFB
29	C	515	DGD	O6D-C5D-C6D-O5D
28	e	101	LHG	C8-C7-O7-C5
22	B	607	CLA	C11-C12-C13-C14
22	b	615	CLA	C11-C12-C13-C14
22	c	511	CLA	C11-C12-C13-C14
29	C	515	DGD	O1G-C1A-C2A-C3A
22	b	612	CLA	C10-C11-C12-C13
31	k	101	BCR	C19-C20-C21-C22
32	b	621	STE	C7-C8-C9-C10
26	b	622	LMG	C32-C33-C34-C35
27	A	410	SQD	C11-C12-C13-C14
32	l	102	STE	C9-C10-C11-C12
28	D	411	LHG	C11-C10-C9-C8
28	D	410	LHG	C9-C10-C11-C12
26	B	626	LMG	O1-C7-C8-O7
26	D	412	LMG	O7-C8-C9-O8
27	L	101	SQD	O6-C44-C45-O47
29	C	515	DGD	O1G-C1G-C2G-O2G
22	B	603	CLA	C10-C11-C12-C13
22	c	501	CLA	C16-C17-C18-C19
26	m	101	LMG	C7-C8-C9-O8
22	c	507	CLA	C4-C3-C5-C6
25	A	408	PL9	C43-C44-C46-C47
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	607	CLA	CAD-CBD-CGD-O2D
22	B	612	CLA	CAD-CBD-CGD-O2D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	506	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	506	CLA	CAD-CBD-CGD-O2D
26	D	408	LMG	C39-C40-C41-C42
22	A	405	CLA	CBA-CGA-O2A-C1
22	C	513	CLA	C16-C17-C18-C20
27	L	101	SQD	C12-C13-C14-C15
22	C	503	CLA	C10-C11-C12-C13
22	B	608	CLA	O1A-CGA-O2A-C1
32	H	103	STE	C2-C3-C4-C5
26	M	101	LMG	C33-C34-C35-C36
28	d	408	LHG	C9-C10-C11-C12
32	B	625	STE	C11-C12-C13-C14
32	b	625	STE	C14-C15-C16-C17
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	B	612	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	506	CLA	CAD-CBD-CGD-O1D
22	c	502	CLA	CAD-CBD-CGD-O1D
22	c	506	CLA	CAD-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O1D
23	d	402	PHO	CHA-CBD-CGD-O2D
28	A	411	LHG	C4-O6-P-O5
28	D	411	LHG	C3-O3-P-O5
28	L	102	LHG	C3-O3-P-O6
31	H	101	BCR	C13-C14-C15-C16
22	d	404	CLA	C16-C17-C18-C19
27	t	102	SQD	C19-C20-C21-C22
22	B	608	CLA	C4-C3-C5-C6
22	B	615	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
31	K	101	BCR	C23-C24-C25-C30
32	L	103	STE	C6-C7-C8-C9
29	h	101	DGD	O2G-C1B-C2B-C3B
25	a	409	PL9	C43-C44-C46-C47
31	k	101	BCR	C37-C22-C23-C24
29	H	102	DGD	O6E-C5E-C6E-O5E
23	d	402	PHO	C2C-C3C-CAC-CBC
29	c	517	DGD	C3B-C4B-C5B-C6B
32	d	411	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	608	CLA	C16-C17-C18-C20
22	B	612	CLA	C16-C17-C18-C19
22	b	603	CLA	C16-C17-C18-C20
27	L	101	SQD	C9-C10-C11-C12
29	C	515	DGD	CBB-CCB-CDB-CEB
27	L	101	SQD	C29-C30-C31-C32
29	A	413	DGD	CAA-CBA-CCA-CDA
25	A	408	PL9	C4-C3-C7-C8
28	A	411	LHG	C23-C24-C25-C26
22	D	405	CLA	O2A-C1-C2-C3
26	B	626	LMG	C9-C8-O7-C10
29	A	413	DGD	CFB-CGB-CHB-CIB
22	B	613	CLA	C13-C15-C16-C17
22	c	510	CLA	C8-C10-C11-C12
27	B	622	SQD	C31-C32-C33-C34
29	H	102	DGD	CAB-CBB-CCB-CDB
32	x	102	STE	C11-C12-C13-C14
25	D	407	PL9	C2-C3-C7-C8
31	x	101	BCR	C15-C16-C17-C18
22	C	513	CLA	C10-C11-C12-C13
27	A	410	SQD	C24-C23-O48-C46
22	c	501	CLA	C11-C12-C13-C14
22	c	510	CLA	C11-C10-C8-C9
22	B	603	CLA	C11-C10-C8-C7
22	B	614	CLA	C12-C13-C15-C16
31	T	101	BCR	C12-C13-C14-C15
27	A	412	SQD	C23-C24-C25-C26
22	b	602	CLA	O1D-CGD-O2D-CED
27	L	101	SQD	O5-C1-O6-C44
27	a	411	SQD	O10-C23-O48-C46
32	C	519	STE	C2-C3-C4-C5
22	C	503	CLA	C2-C3-C5-C6
32	B	624	STE	C2-C3-C4-C5
22	B	615	CLA	C5-C6-C7-C8
32	C	519	STE	C6-C7-C8-C9
28	e	101	LHG	C16-C17-C18-C19
26	B	626	LMG	O8-C28-C29-C30
32	x	102	STE	C10-C11-C12-C13
31	K	101	BCR	C13-C14-C15-C16
26	c	519	LMG	C32-C33-C34-C35
29	c	516	DGD	CDB-CEB-CFB-CGB
27	A	412	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	CBA-CGA-O2A-C1
32	L	103	STE	C4-C5-C6-C7
32	b	623	STE	C10-C11-C12-C13
26	B	626	LMG	C16-C17-C18-C19
29	H	102	DGD	O2G-C1B-C2B-C3B
27	L	101	SQD	C10-C11-C12-C13
22	C	509	CLA	C3-C5-C6-C7
29	c	516	DGD	O1G-C1A-C2A-C3A
31	d	406	BCR	C11-C12-C13-C35
27	B	622	SQD	C26-C27-C28-C29
27	L	101	SQD	C45-C44-O6-C1
28	a	410	LHG	C33-C34-C35-C36
22	D	403	CLA	C16-C17-C18-C20
22	c	501	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C14
22	c	511	CLA	C2C-C3C-CAC-CBC
27	B	622	SQD	C29-C30-C31-C32
27	L	101	SQD	C15-C16-C17-C18
29	C	516	DGD	CDB-CEB-CFB-CGB
32	b	621	STE	C4-C5-C6-C7
22	A	403	CLA	C10-C11-C12-C13
29	h	101	DGD	C1A-C2A-C3A-C4A
22	c	507	CLA	O1A-CGA-O2A-C1
27	B	622	SQD	C30-C31-C32-C33
27	D	409	SQD	O10-C23-C24-C25
27	D	409	SQD	C45-C44-O6-C1
28	d	408	LHG	C1-C2-C3-O3
26	m	101	LMG	C22-C23-C24-C25
22	B	603	CLA	C11-C10-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	608	CLA	C11-C10-C8-C9
22	b	609	CLA	C6-C7-C8-C9
22	c	505	CLA	C14-C13-C15-C16
22	c	508	CLA	C11-C10-C8-C9
22	d	401	CLA	C14-C13-C15-C16
22	b	602	CLA	C4B-C3B-CAB-CBB
25	D	407	PL9	C32-C33-C34-C35
29	c	518	DGD	CDA-CEA-CFA-CGA
28	d	408	LHG	C12-C13-C14-C15
22	c	507	CLA	CBA-CGA-O2A-C1
22	B	608	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	A	408	PL9	C13-C14-C16-C17
29	C	515	DGD	C2B-C3B-C4B-C5B
32	b	625	STE	C11-C12-C13-C14
22	B	602	CLA	C8-C10-C11-C12
27	A	410	SQD	C28-C29-C30-C31
26	M	101	LMG	C16-C17-C18-C19
28	a	410	LHG	C29-C30-C31-C32
22	C	503	CLA	C6-C7-C8-C10
22	C	508	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	b	614	CLA	C5-C6-C7-C8
22	b	602	CLA	O1A-CGA-O2A-C1
22	A	405	CLA	O1A-CGA-O2A-C1
26	D	412	LMG	C15-C16-C17-C18
22	b	610	CLA	O1D-CGD-O2D-CED
27	D	409	SQD	O48-C23-C24-C25
28	d	408	LHG	C16-C17-C18-C19
22	B	608	CLA	C16-C17-C18-C19
29	c	518	DGD	C9B-CAB-CBB-CCB
25	A	408	PL9	C35-C34-C36-C37
26	D	408	LMG	C28-C29-C30-C31
32	c	520	STE	C11-C10-C9-C8
23	A	404	PHO	C10-C11-C12-C13
26	B	626	LMG	O6-C1-O1-C7
31	a	405	BCR	C35-C13-C14-C15
32	M	102	STE	C2-C3-C4-C5
32	b	624	STE	C11-C10-C9-C8
31	t	101	BCR	C19-C20-C21-C22
32	b	621	STE	C5-C6-C7-C8
22	B	612	CLA	C13-C15-C16-C17
28	d	409	LHG	C2-C3-O3-P
29	A	413	DGD	CAB-CBB-CCB-CDB
32	d	412	STE	C11-C10-C9-C8
31	Z	101	BCR	C7-C8-C9-C10
28	d	408	LHG	C31-C32-C33-C34
26	M	101	LMG	C35-C36-C37-C38
22	B	606	CLA	C15-C16-C17-C18
32	t	104	STE	C4-C5-C6-C7
22	d	405	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C6-C7-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	C	508	CLA	C11-C10-C8-C9
22	b	601	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	b	606	CLA	C14-C13-C15-C16
22	b	609	CLA	C11-C12-C13-C14
22	c	502	CLA	C6-C7-C8-C9
22	c	502	CLA	C14-C13-C15-C16
22	c	508	CLA	C6-C7-C8-C9
22	c	511	CLA	C11-C10-C8-C9
28	a	410	LHG	O1-C1-C2-C3
22	b	603	CLA	C13-C15-C16-C17
22	b	605	CLA	C10-C11-C12-C13
29	H	102	DGD	C5A-C6A-C7A-C8A
26	M	101	LMG	C7-C8-O7-C10
22	B	603	CLA	C13-C15-C16-C17
32	C	518	STE	O2-C1-C2-C3
34	f	101	HEM	CAD-CBD-CGD-O1D
28	d	408	LHG	C28-C29-C30-C31
22	C	505	CLA	CBD-CGD-O2D-CED
32	B	624	STE	C6-C7-C8-C9
32	X	101	STE	O1-C1-C2-C3
28	D	410	LHG	C12-C13-C14-C15
22	B	610	CLA	C2A-CAA-CBA-CGA
28	e	101	LHG	C11-C12-C13-C14
22	c	507	CLA	O1D-CGD-O2D-CED
22	c	501	CLA	C1A-C2A-CAA-CBA
26	c	521	LMG	C36-C37-C38-C39
32	x	102	STE	O1-C1-C2-C3
26	B	626	LMG	C11-C12-C13-C14
28	d	408	LHG	C26-C27-C28-C29
31	b	617	BCR	C1-C6-C7-C8
31	k	101	BCR	C5-C6-C7-C8
31	k	101	BCR	C23-C24-C25-C26
31	x	101	BCR	C23-C24-C25-C30
28	D	410	LHG	C23-C24-C25-C26
22	B	608	CLA	CBA-CGA-O2A-C1
22	D	404	CLA	C8-C10-C11-C12
32	C	518	STE	C7-C8-C9-C10
29	c	516	DGD	C6B-C7B-C8B-C9B
32	b	625	STE	C9-C10-C11-C12
22	d	404	CLA	C15-C16-C17-C18
32	C	518	STE	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	h	101	DGD	C8A-C9A-CAA-CBA
22	B	606	CLA	C12-C13-C15-C16
22	B	613	CLA	C6-C7-C8-C10
22	D	405	CLA	C12-C13-C15-C16
22	c	508	CLA	C11-C10-C8-C7
22	c	511	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C12-C13-C15
29	c	516	DGD	C7A-C8A-C9A-CAA
34	f	101	HEM	CAD-CBD-CGD-O2D
26	D	408	LMG	C32-C33-C34-C35
26	b	622	LMG	C40-C41-C42-C43
26	m	101	LMG	C29-C28-O8-C9
32	M	102	STE	O1-C1-C2-C3
26	A	409	LMG	C32-C33-C34-C35
32	M	103	STE	C1-C2-C3-C4
31	K	101	BCR	C7-C8-C9-C34
31	d	406	BCR	C7-C8-C9-C34
34	F	101	HEM	CAD-CBD-CGD-O1D
22	c	508	CLA	C4-C3-C5-C6
32	b	623	STE	C2-C3-C4-C5
26	B	621	LMG	C31-C32-C33-C34
28	L	102	LHG	C35-C36-C37-C38
31	H	101	BCR	C17-C18-C19-C20
22	A	403	CLA	C16-C17-C18-C20
26	M	101	LMG	C17-C18-C19-C20
29	C	516	DGD	CAA-CBA-CCA-CDA
32	d	411	STE	O2-C1-C2-C3
22	C	510	CLA	C14-C13-C15-C16
22	b	602	CLA	C14-C13-C15-C16
32	X	101	STE	C15-C16-C17-C18
29	C	517	DGD	C7A-C8A-C9A-CAA
26	b	622	LMG	C42-C43-C44-C45
32	M	102	STE	O2-C1-C2-C3
32	X	101	STE	O2-C1-C2-C3
32	b	625	STE	O1-C1-C2-C3
32	B	620	STE	C11-C10-C9-C8
28	l	101	LHG	C14-C15-C16-C17
22	B	616	CLA	C4-C3-C5-C6
32	l	102	STE	C11-C12-C13-C14
22	c	509	CLA	CAA-CBA-CGA-O1A
22	B	605	CLA	C2-C3-C5-C6
26	D	408	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	d	411	STE	O1-C1-C2-C3
32	C	520	STE	C6-C7-C8-C9
26	M	101	LMG	O1-C7-C8-C9
27	a	411	SQD	C44-C45-C46-O48
29	C	517	DGD	O1G-C1G-C2G-C3G
29	c	518	DGD	O1G-C1G-C2G-C3G
32	b	625	STE	O2-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O2D
29	C	515	DGD	C4D-C5D-C6D-O5D
28	D	413	LHG	O10-C23-O8-C6
26	B	621	LMG	C17-C18-C19-C20
29	c	517	DGD	C7A-C8A-C9A-CAA
26	D	412	LMG	C33-C34-C35-C36
32	x	102	STE	O2-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O1D
22	d	403	CLA	C4-C3-C5-C6
32	a	412	STE	O2-C1-C2-C3
28	e	101	LHG	C28-C29-C30-C31
28	D	410	LHG	C7-C8-C9-C10
22	B	605	CLA	C16-C17-C18-C20
28	d	408	LHG	C34-C35-C36-C37
22	B	603	CLA	C4B-C3B-CAB-CBB
22	C	502	CLA	C4B-C3B-CAB-CBB
32	b	621	STE	O1-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O2D
35	V	201	HEC	CAD-CBD-CGD-O2D
22	b	609	CLA	O1D-CGD-O2D-CED
28	L	102	LHG	C29-C30-C31-C32
22	C	512	CLA	C16-C17-C18-C19
23	A	404	PHO	CHA-CBD-CGD-O1D
31	k	101	BCR	C16-C17-C18-C36
26	B	626	LMG	C29-C30-C31-C32
32	X	101	STE	C5-C6-C7-C8
32	X	101	STE	C11-C12-C13-C14
25	A	408	PL9	C25-C24-C26-C27
27	a	411	SQD	C11-C12-C13-C14
26	B	626	LMG	O7-C8-C9-O8
26	b	622	LMG	O1-C7-C8-O7
27	f	102	SQD	O6-C44-C45-O47
26	b	622	LMG	C23-C24-C25-C26
26	c	521	LMG	C38-C39-C40-C41
22	b	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
34	f	101	HEM	CAA-CBA-CGA-O2A
28	A	411	LHG	C29-C30-C31-C32
32	J	101	STE	C3-C4-C5-C6
32	M	102	STE	C11-C10-C9-C8
22	c	508	CLA	C8-C10-C11-C12
31	x	101	BCR	C9-C10-C11-C12
27	L	101	SQD	C11-C10-C9-C8
32	a	412	STE	O1-C1-C2-C3
22	B	601	CLA	C11-C10-C8-C9
22	B	608	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	a	404	CLA	C6-C7-C8-C9
22	b	605	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	b	613	CLA	C14-C13-C15-C16
22	c	512	CLA	C15-C16-C17-C18
27	L	101	SQD	C5-C6-S-O8
28	d	408	LHG	C30-C31-C32-C33
22	B	614	CLA	C2A-CAA-CBA-CGA
22	C	511	CLA	C2-C1-O2A-CGA
22	d	405	CLA	C15-C16-C17-C18
22	b	602	CLA	CBA-CGA-O2A-C1
32	C	520	STE	C1-C2-C3-C4
22	b	601	CLA	C3A-C2A-CAA-CBA
22	d	401	CLA	C3A-C2A-CAA-CBA
22	d	405	CLA	C3A-C2A-CAA-CBA
29	C	515	DGD	CDB-CEB-CFB-CGB
32	I	102	STE	C12-C13-C14-C15
32	B	623	STE	O2-C1-C2-C3
29	c	517	DGD	CBB-CCB-CDB-CEB
22	c	505	CLA	C5-C6-C7-C8
27	D	409	SQD	C44-C45-C46-O48
26	M	101	LMG	C2-C1-O1-C7
26	A	409	LMG	C7-C8-O7-C10
35	V	201	HEC	CAD-CBD-CGD-O1D
32	B	624	STE	C9-C10-C11-C12
32	t	103	STE	C7-C8-C9-C10
26	c	519	LMG	C36-C37-C38-C39
25	D	407	PL9	C28-C29-C31-C32
22	b	612	CLA	C8-C10-C11-C12
22	B	612	CLA	C16-C17-C18-C20
31	b	619	BCR	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	B	623	STE	O1-C1-C2-C3
32	J	101	STE	O2-C1-C2-C3
32	B	625	STE	C12-C13-C14-C15
29	C	515	DGD	O6E-C1E-O5D-C6D
29	c	518	DGD	O6D-C1D-O3G-C3G
23	d	402	PHO	C5-C6-C7-C8
28	a	410	LHG	C24-C25-C26-C27
26	b	622	LMG	O1-C7-C8-C9
26	m	101	LMG	O1-C7-C8-C9
29	h	101	DGD	C1G-C2G-C3G-O3G
22	c	501	CLA	O1A-CGA-O2A-C1
23	d	402	PHO	C8-C10-C11-C12
26	D	412	LMG	C11-C12-C13-C14
32	b	620	STE	C7-C8-C9-C10
26	D	408	LMG	C38-C39-C40-C41
28	D	413	LHG	C19-C20-C21-C22
25	a	409	PL9	C45-C44-C46-C47
32	J	101	STE	O1-C1-C2-C3
32	d	412	STE	O1-C1-C2-C3
31	H	101	BCR	C15-C16-C17-C18
32	b	620	STE	C11-C10-C9-C8
32	X	101	STE	C6-C7-C8-C9
26	D	408	LMG	C40-C41-C42-C43
32	X	101	STE	C1-C2-C3-C4
26	b	622	LMG	O8-C28-C29-C30
29	C	517	DGD	CAA-CBA-CCA-CDA
22	B	613	CLA	C14-C13-C15-C16
22	b	614	CLA	C6-C7-C8-C9
22	c	502	CLA	C11-C12-C13-C14
22	d	401	CLA	C11-C12-C13-C14
22	d	403	CLA	C11-C10-C8-C9
28	e	101	LHG	O8-C23-C24-C25
29	C	515	DGD	C9A-CAA-CBA-CCA
28	a	410	LHG	O6-C4-C5-C6
27	a	411	SQD	C23-C24-C25-C26
26	A	409	LMG	C16-C17-C18-C19
25	d	407	PL9	C27-C28-C29-C30
34	f	101	HEM	CAA-CBA-CGA-O1A
27	L	101	SQD	C13-C14-C15-C16
22	A	403	CLA	C12-C13-C15-C16
22	B	604	CLA	C11-C10-C8-C7
22	B	606	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	B	609	CLA	C11-C12-C13-C15
22	B	610	CLA	C11-C10-C8-C7
22	C	505	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C12-C13-C15
22	C	508	CLA	C11-C10-C8-C7
22	b	602	CLA	C12-C13-C15-C16
22	b	605	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C10-C8-C7
22	c	513	CLA	C12-C13-C15-C16
22	d	403	CLA	C11-C12-C13-C15
29	A	413	DGD	C1A-C2A-C3A-C4A
22	B	603	CLA	C2B-C3B-CAB-CBB
22	C	502	CLA	C2B-C3B-CAB-CBB
22	b	602	CLA	C2B-C3B-CAB-CBB
22	b	603	CLA	C2B-C3B-CAB-CBB
22	d	403	CLA	C2B-C3B-CAB-CBB
31	B	618	BCR	C23-C24-C25-C26
31	B	619	BCR	C1-C6-C7-C8
31	B	619	BCR	C5-C6-C7-C8
31	K	101	BCR	C23-C24-C25-C26
31	K	102	BCR	C1-C6-C7-C8
31	K	102	BCR	C5-C6-C7-C8
31	b	617	BCR	C5-C6-C7-C8
31	d	406	BCR	C23-C24-C25-C26
31	k	102	BCR	C23-C24-C25-C26
29	C	515	DGD	CCB-CDB-CEB-CFB
26	c	522	LMG	O9-C10-O7-C8
26	b	622	LMG	C14-C15-C16-C17
26	c	522	LMG	C16-C17-C18-C19
27	A	412	SQD	C31-C32-C33-C34
32	x	102	STE	C6-C7-C8-C9
27	B	622	SQD	C10-C11-C12-C13
22	d	403	CLA	C3-C5-C6-C7
22	C	512	CLA	C5-C6-C7-C8
22	B	605	CLA	C4-C3-C5-C6
29	C	517	DGD	CCA-CDA-CEA-CFA
29	H	102	DGD	C1B-C2B-C3B-C4B
25	d	407	PL9	C43-C44-C46-C47
28	L	102	LHG	C25-C26-C27-C28
29	A	413	DGD	CDB-CEB-CFB-CGB
22	c	511	CLA	C3-C5-C6-C7
26	M	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
28	d	408	LHG	C13-C14-C15-C16
27	t	102	SQD	O48-C23-C24-C25
26	m	101	LMG	O8-C28-C29-C30
22	a	402	CLA	C15-C16-C17-C18
28	D	411	LHG	C17-C18-C19-C20
32	B	623	STE	C7-C8-C9-C10
29	C	515	DGD	C8B-C9B-CAB-CBB
22	B	613	CLA	C6-C7-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	b	604	CLA	C11-C10-C8-C9
22	c	502	CLA	C13-C15-C16-C17
28	D	411	LHG	C2-C3-O3-P
22	c	511	CLA	O1A-CGA-O2A-C1
26	A	409	LMG	C7-C8-C9-O8
27	A	410	SQD	C44-C45-C46-O48
27	f	102	SQD	O6-C44-C45-C46
29	c	516	DGD	C1G-C2G-C3G-O3G
22	B	601	CLA	C4B-C3B-CAB-CBB
22	B	602	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C4B-C3B-CAB-CBB
22	C	504	CLA	C1A-C2A-CAA-CBA
22	C	504	CLA	C4B-C3B-CAB-CBB
22	C	506	CLA	C1A-C2A-CAA-CBA
22	a	404	CLA	C1A-C2A-CAA-CBA
32	b	621	STE	O2-C1-C2-C3
22	B	616	CLA	C3-C5-C6-C7
29	c	517	DGD	O6D-C1D-O3G-C3G
26	Y	101	LMG	O7-C10-C11-C12
22	c	508	CLA	C2-C3-C5-C6
29	c	518	DGD	O1G-C1G-C2G-O2G
28	A	411	LHG	C35-C36-C37-C38
28	l	101	LHG	C10-C11-C12-C13
31	b	619	BCR	C13-C14-C15-C16
31	c	515	BCR	C13-C14-C15-C16
26	D	412	LMG	O10-C28-O8-C9
26	d	410	LMG	C31-C32-C33-C34
29	h	101	DGD	C5A-C6A-C7A-C8A
32	d	412	STE	O2-C1-C2-C3
28	L	102	LHG	O7-C7-C8-C9
22	c	507	CLA	C2A-CAA-CBA-CGA
22	B	608	CLA	C13-C15-C16-C17
22	b	601	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
29	c	517	DGD	O2G-C1B-C2B-C3B
22	B	604	CLA	C2-C1-O2A-CGA
22	D	403	CLA	C2-C1-O2A-CGA
22	c	512	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
22	B	605	CLA	C6-C7-C8-C10
22	B	615	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	C	509	CLA	C12-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C7
22	a	404	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C10-C8-C7
22	A	402	CLA	C16-C17-C18-C20
32	a	413	STE	C9-C10-C11-C12
26	A	409	LMG	C9-C8-O7-C10
28	L	102	LHG	C14-C15-C16-C17
28	D	413	LHG	C29-C30-C31-C32
22	b	601	CLA	O1A-CGA-O2A-C1
29	h	101	DGD	CBB-CCB-CDB-CEB
22	C	511	CLA	O1A-CGA-O2A-C1
22	c	510	CLA	C15-C16-C17-C18
22	B	601	CLA	C4-C3-C5-C6
22	B	602	CLA	C3A-C2A-CAA-CBA
26	b	622	LMG	O10-C28-C29-C30
22	b	607	CLA	C16-C17-C18-C20
22	B	605	CLA	C10-C11-C12-C13
29	c	517	DGD	O1B-C1B-C2B-C3B
27	B	622	SQD	C14-C15-C16-C17
22	c	511	CLA	CBA-CGA-O2A-C1
28	D	413	LHG	O6-C4-C5-O7
22	B	613	CLA	CAA-CBA-CGA-O2A
25	d	407	PL9	C11-C12-C13-C14
25	d	407	PL9	C31-C32-C33-C34
22	C	511	CLA	CBA-CGA-O2A-C1
22	b	615	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
23	a	403	PHO	C6-C7-C8-C9
22	b	613	CLA	CAA-CBA-CGA-O2A
26	B	621	LMG	O7-C10-C11-C12
27	A	410	SQD	C31-C32-C33-C34
32	d	411	STE	C11-C10-C9-C8
22	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	Y	101	LMG	O9-C10-C11-C12
26	d	410	LMG	O9-C10-C11-C12
28	e	101	LHG	O10-C23-C24-C25
32	X	101	STE	C7-C8-C9-C10
22	B	609	CLA	C2-C3-C5-C6
22	b	604	CLA	C13-C15-C16-C17
22	c	511	CLA	C8-C10-C11-C12
32	B	627	STE	O2-C1-C2-C3
29	H	102	DGD	CDB-CEB-CFB-CGB
27	A	412	SQD	C18-C19-C20-C21
22	c	510	CLA	CAA-CBA-CGA-O2A
31	k	101	BCR	C21-C22-C23-C24
29	C	515	DGD	C5D-C6D-O5D-C1E
28	D	410	LHG	C34-C35-C36-C37
27	a	411	SQD	O49-C7-C8-C9
29	c	516	DGD	O2G-C1B-C2B-C3B
22	b	614	CLA	C2A-CAA-CBA-CGA
32	t	104	STE	C3-C4-C5-C6
32	C	520	STE	O1-C1-C2-C3
32	c	523	STE	O2-C1-C2-C3
27	A	410	SQD	O49-C7-C8-C9
29	A	413	DGD	O1B-C1B-C2B-C3B
29	c	516	DGD	O1B-C1B-C2B-C3B
26	B	621	LMG	C34-C35-C36-C37
22	B	612	CLA	CAA-CBA-CGA-O2A
22	a	402	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	C	512	CLA	C2C-C3C-CAC-CBC
32	b	623	STE	C7-C8-C9-C10
29	C	516	DGD	O2G-C1B-C2B-C3B
29	C	517	DGD	O6D-C5D-C6D-O5D
28	D	410	LHG	C33-C34-C35-C36
22	C	506	CLA	C2-C1-O2A-CGA
22	c	502	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
32	B	627	STE	O1-C1-C2-C3
27	t	102	SQD	O6-C44-C45-C46
29	c	516	DGD	C6A-C7A-C8A-C9A
26	A	409	LMG	C19-C20-C21-C22
29	A	413	DGD	C3B-C4B-C5B-C6B
26	B	621	LMG	O10-C28-C29-C30
26	b	622	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	c	510	CLA	CAA-CBA-CGA-O1A
29	c	517	DGD	CDA-CEA-CFA-CGA
32	j	101	STE	O2-C1-C2-C3
22	B	613	CLA	CAA-CBA-CGA-O1A
28	d	408	LHG	C25-C26-C27-C28

There are no ring outliers.

121 monomers are involved in 193 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	511	CLA	2	0
22	b	615	CLA	3	0
27	f	102	SQD	1	0
32	b	627	STE	3	0
22	c	513	CLA	1	0
22	A	402	CLA	3	0
23	D	401	PHO	3	0
29	A	413	DGD	1	0
32	X	101	STE	4	0
32	d	411	STE	2	0
26	c	522	LMG	1	0
22	B	609	CLA	2	0
31	b	618	BCR	1	0
31	I	101	BCR	1	0
32	L	103	STE	1	0
22	A	403	CLA	2	0
22	C	507	CLA	2	0
32	d	412	STE	4	0
26	A	409	LMG	1	0
22	b	602	CLA	2	0
22	b	614	CLA	3	0
32	b	624	STE	2	0
22	B	607	CLA	1	0
26	c	521	LMG	3	0
29	C	515	DGD	1	0
29	h	101	DGD	2	0
32	I	102	STE	2	0
28	l	101	LHG	1	0
26	M	101	LMG	1	0
22	B	605	CLA	3	0
22	B	613	CLA	2	0
22	b	605	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	c	512	CLA	2	0
22	b	604	CLA	1	0
22	B	610	CLA	2	0
22	b	609	CLA	3	0
32	H	103	STE	1	0
28	A	411	LHG	4	0
32	J	101	STE	2	0
23	d	402	PHO	2	0
26	b	622	LMG	1	0
31	T	101	BCR	1	0
22	B	616	CLA	1	0
22	d	404	CLA	1	0
25	A	408	PL9	2	0
22	b	601	CLA	1	0
27	t	102	SQD	1	0
31	B	617	BCR	1	0
22	C	505	CLA	2	0
32	t	103	STE	1	0
27	L	101	SQD	4	0
32	j	101	STE	2	0
25	D	407	PL9	1	0
22	b	608	CLA	4	0
34	f	101	HEM	5	0
29	c	517	DGD	2	0
28	D	411	LHG	4	0
29	c	518	DGD	2	0
31	c	514	BCR	1	0
22	C	509	CLA	2	0
22	B	614	CLA	3	0
35	v	201	HEC	6	0
22	d	403	CLA	1	0
22	b	616	CLA	2	0
32	b	621	STE	2	0
31	t	101	BCR	2	0
31	d	406	BCR	2	0
31	D	406	BCR	3	0
22	c	506	CLA	1	0
22	c	510	CLA	1	0
32	B	620	STE	2	0
32	x	102	STE	1	0
29	C	516	DGD	5	0
22	B	601	CLA	1	0

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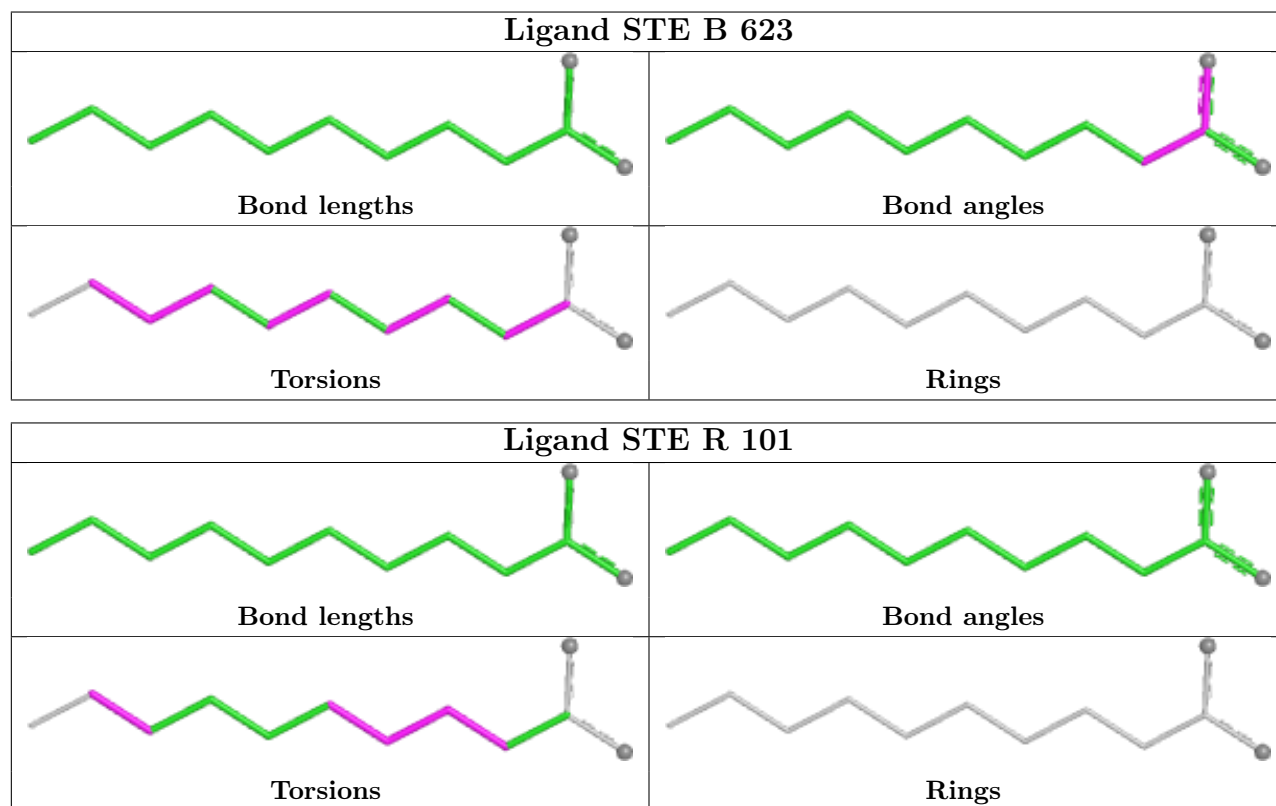
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	409	SQD	1	0
31	C	514	BCR	3	0
28	a	410	LHG	5	0
34	F	101	HEM	4	0
22	B	604	CLA	4	0
26	D	412	LMG	1	0
22	C	506	CLA	1	0
22	c	504	CLA	1	0
28	D	413	LHG	4	0
22	B	611	CLA	1	0
22	B	606	CLA	2	0
22	B	612	CLA	1	0
22	D	403	CLA	4	0
28	D	410	LHG	1	0
22	c	508	CLA	2	0
22	C	508	CLA	3	0
32	c	523	STE	1	0
22	C	513	CLA	3	0
26	D	408	LMG	1	0
27	A	410	SQD	3	0
22	c	501	CLA	2	0
22	b	610	CLA	1	0
25	d	407	PL9	1	0
22	b	611	CLA	1	0
22	b	607	CLA	2	0
22	B	603	CLA	1	0
22	c	509	CLA	2	0
22	C	510	CLA	2	0
26	Y	101	LMG	1	0
26	m	101	LMG	2	0
31	B	618	BCR	4	0
22	b	613	CLA	1	0
29	c	516	DGD	2	0
31	x	101	BCR	1	0
32	B	627	STE	2	0
32	C	519	STE	2	0
28	d	408	LHG	1	0
22	a	402	CLA	1	0
22	B	615	CLA	1	0
22	C	511	CLA	3	0
28	L	102	LHG	1	0
28	d	409	LHG	2	0

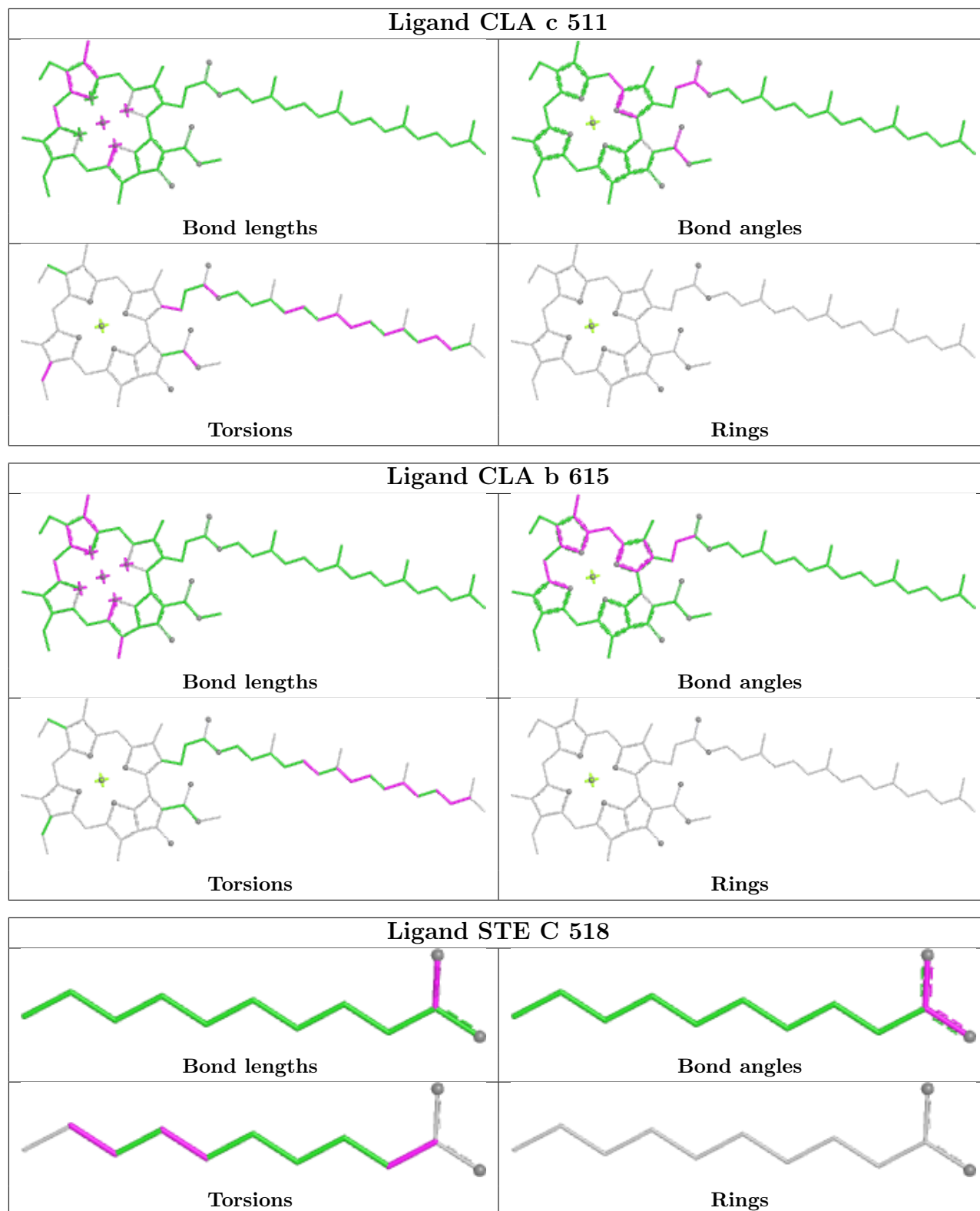
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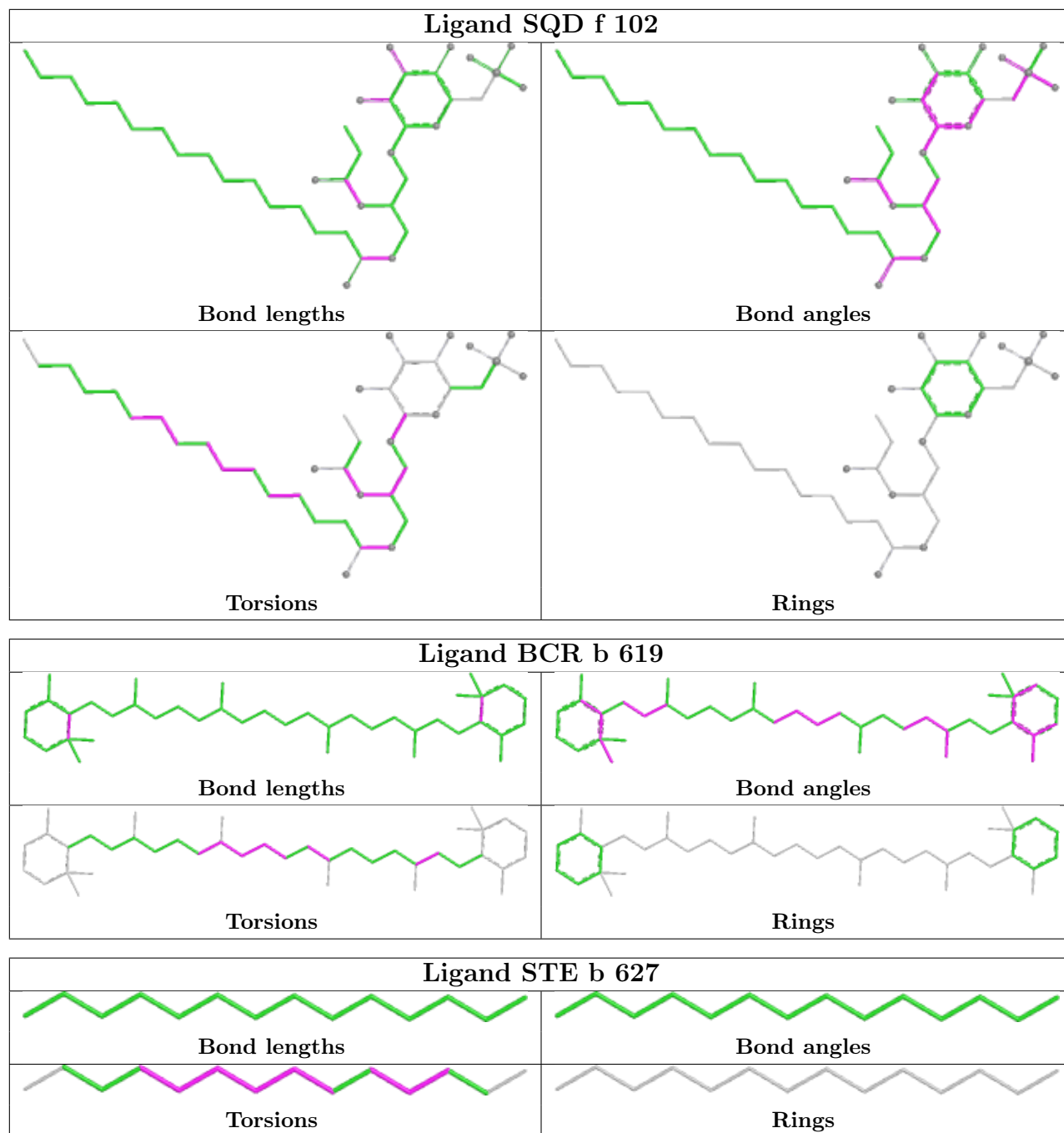
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	619	BCR	2	0
22	B	608	CLA	2	0
22	c	503	CLA	3	0
22	C	504	CLA	1	0
22	b	606	CLA	1	0

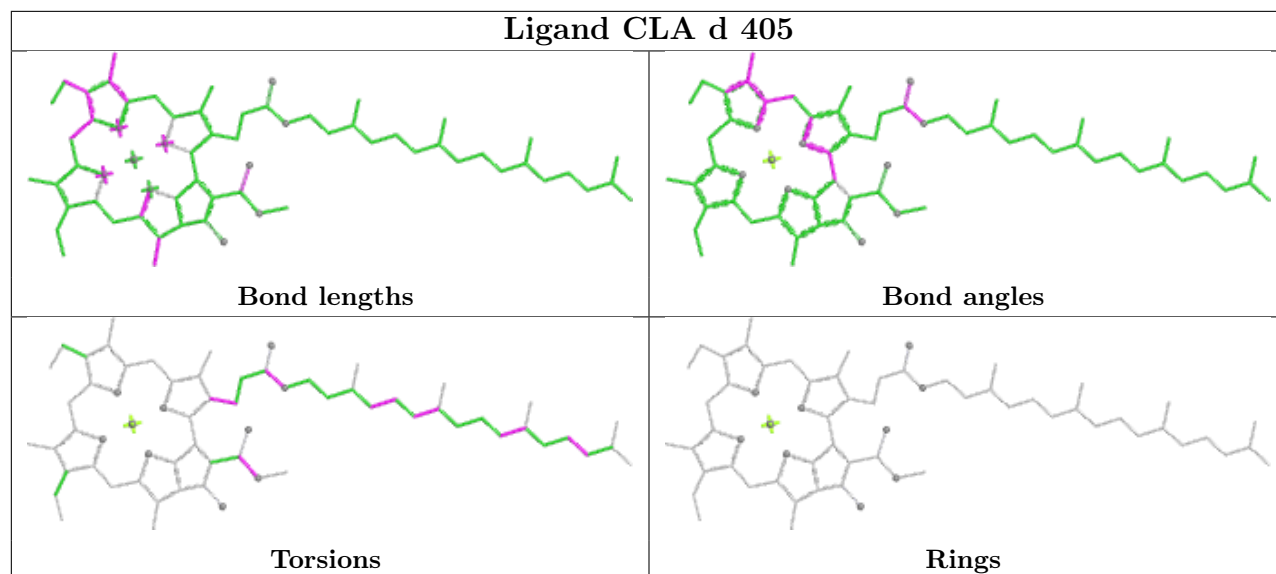
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



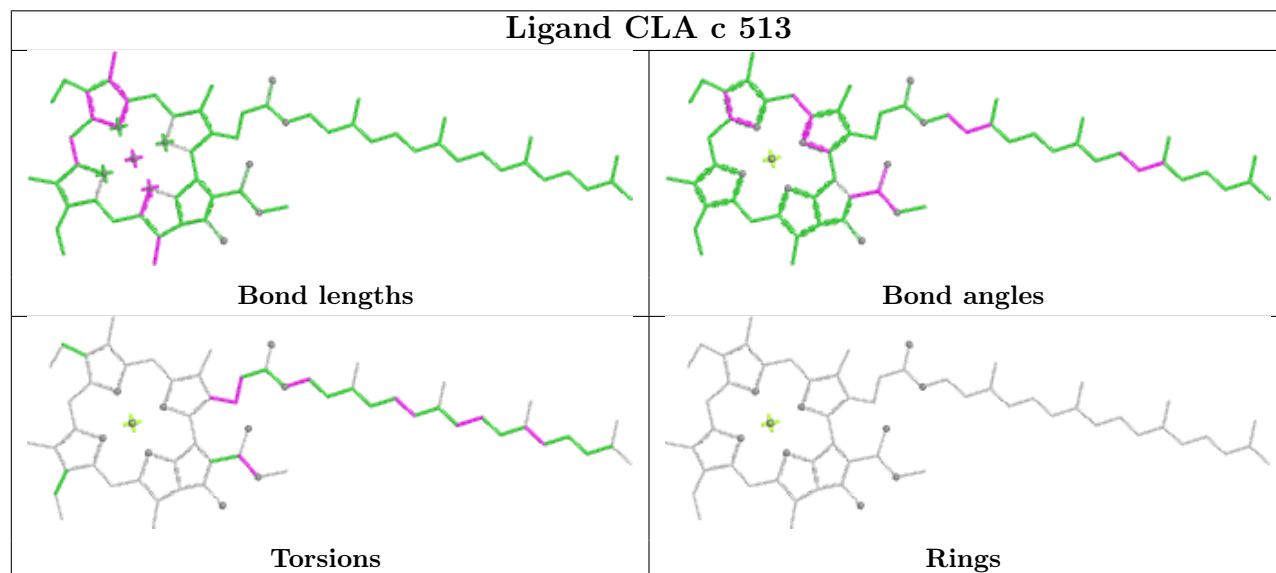




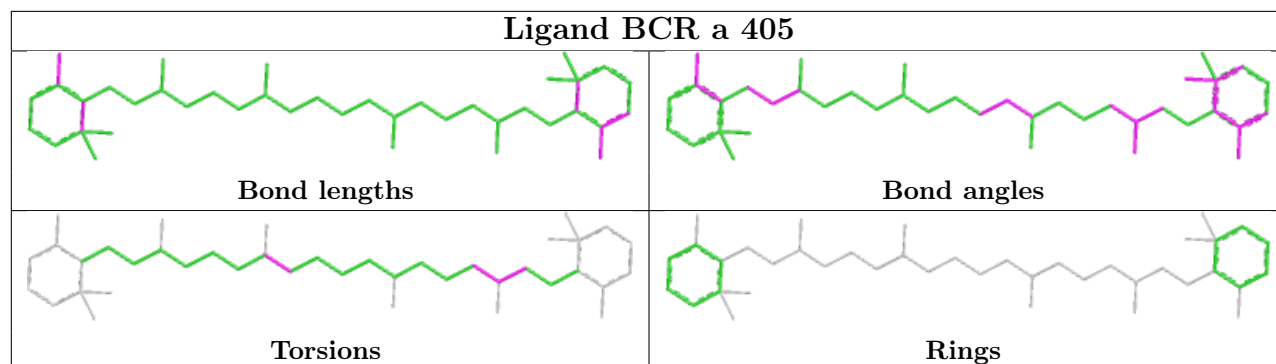
Ligand CLA d 405

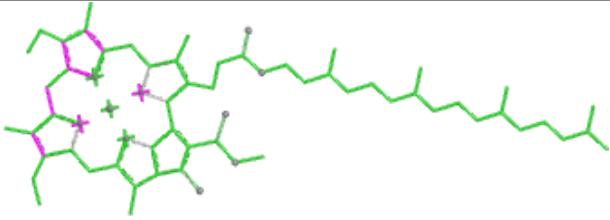
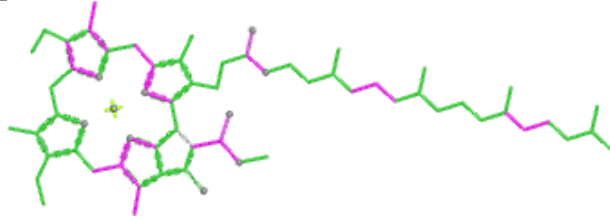
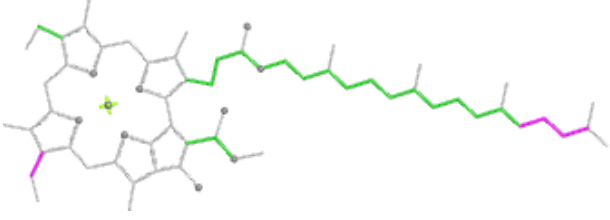
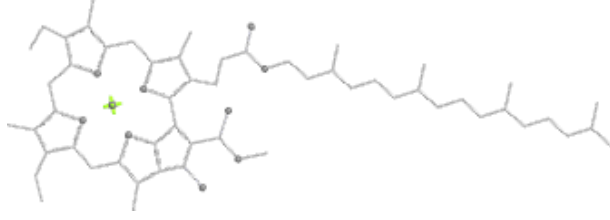
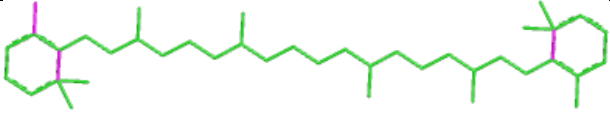
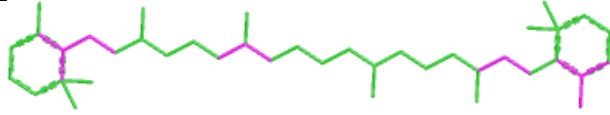
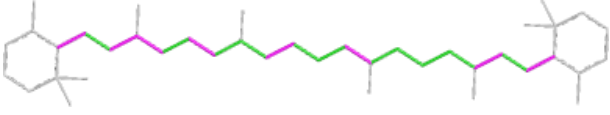
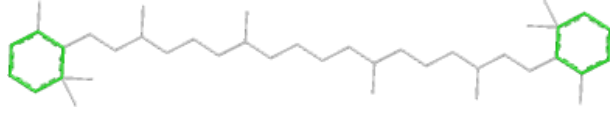
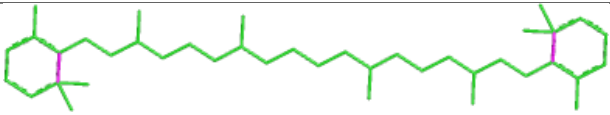
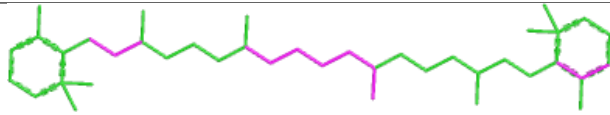
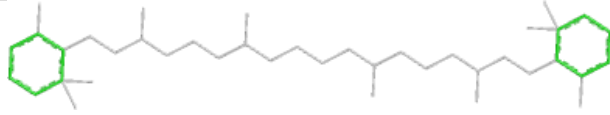


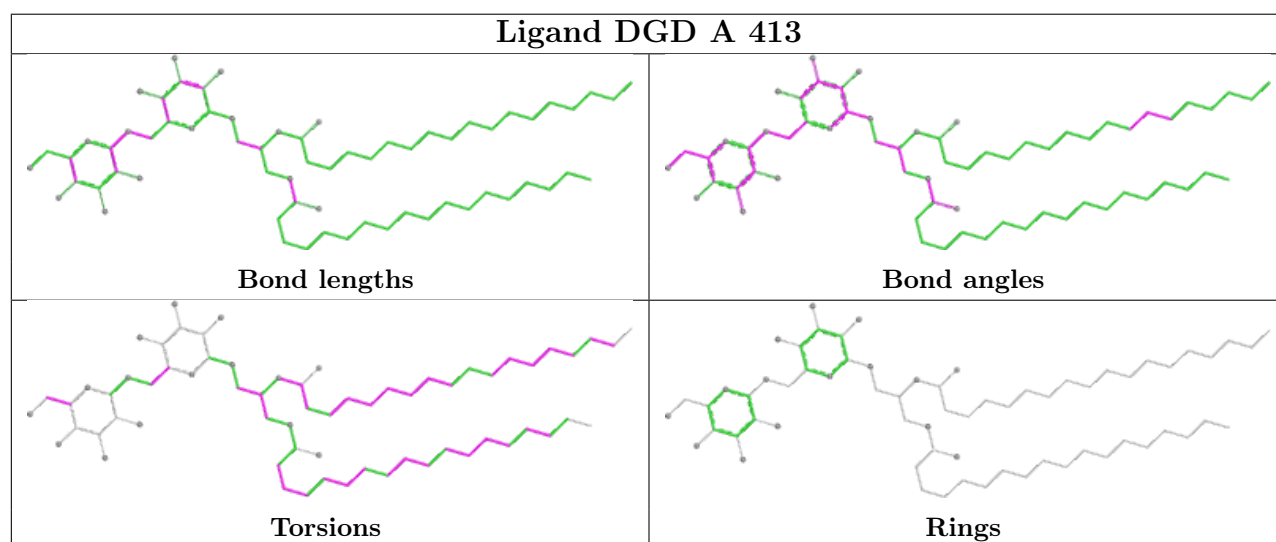
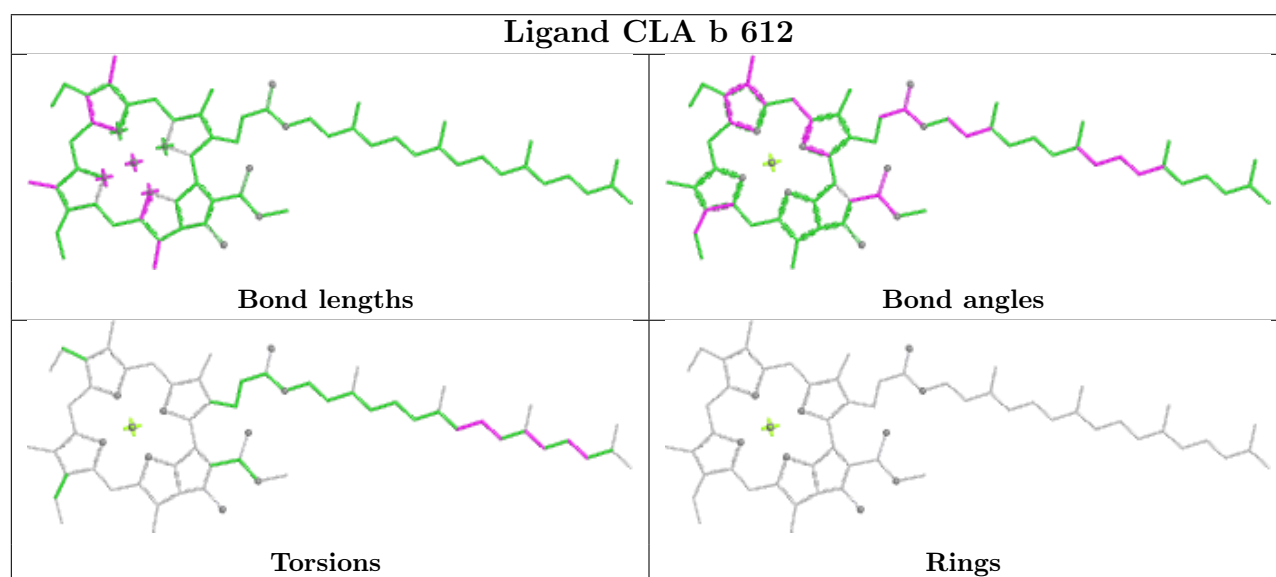
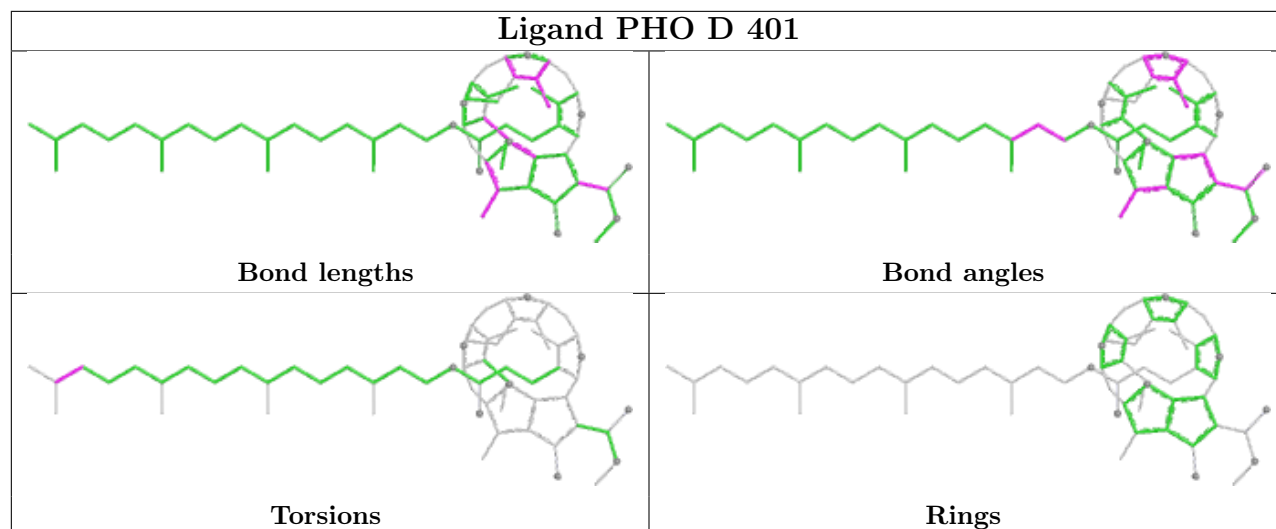
Ligand CLA c 513

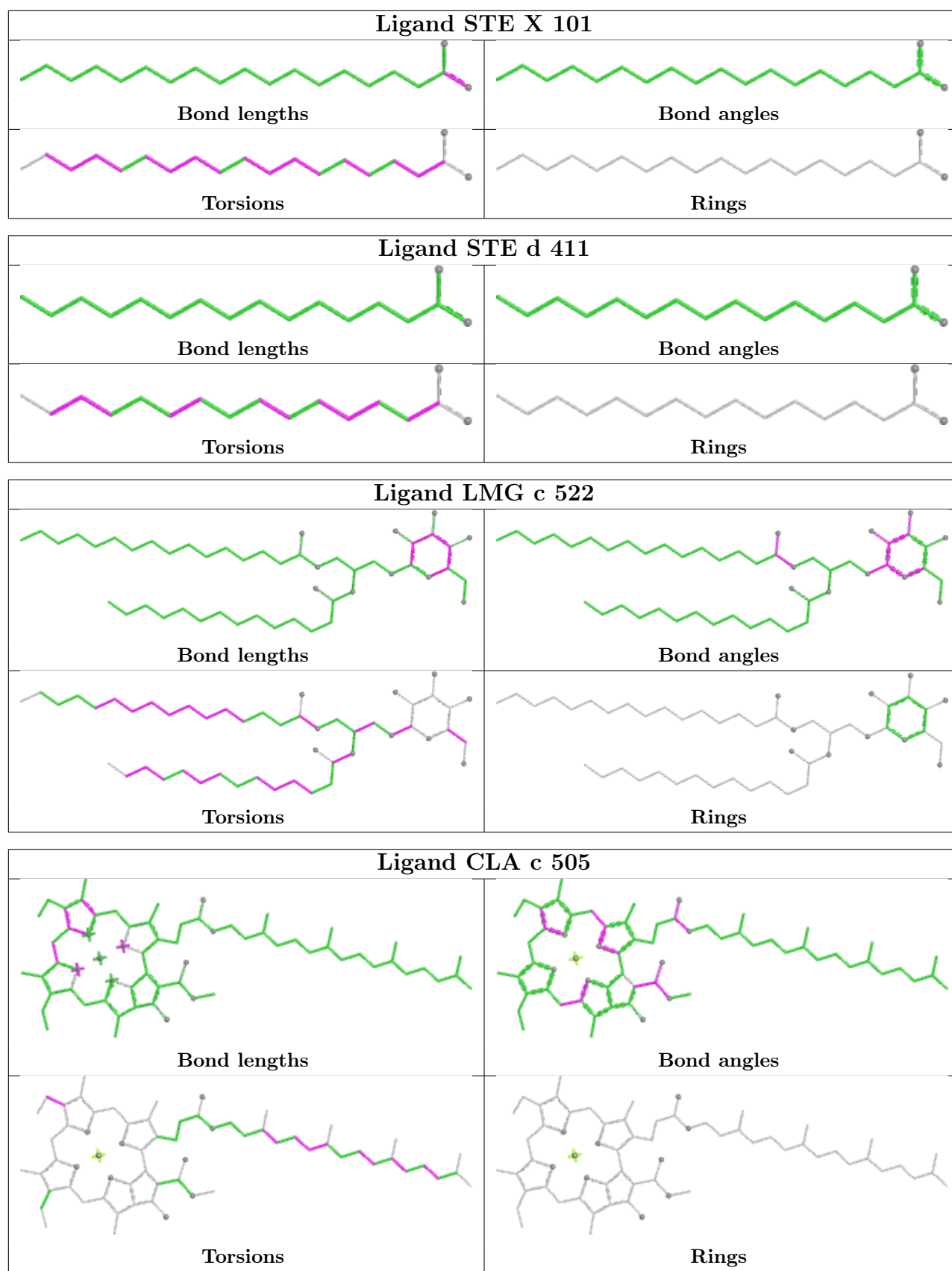


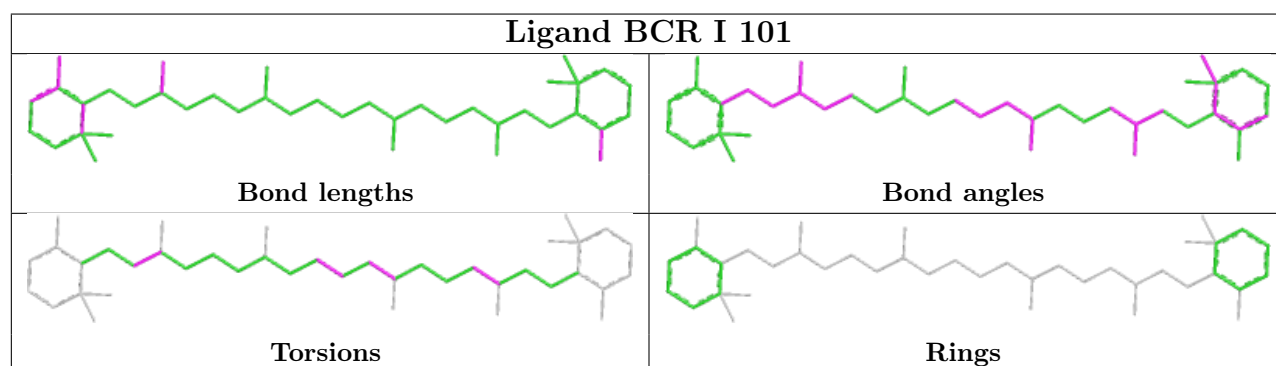
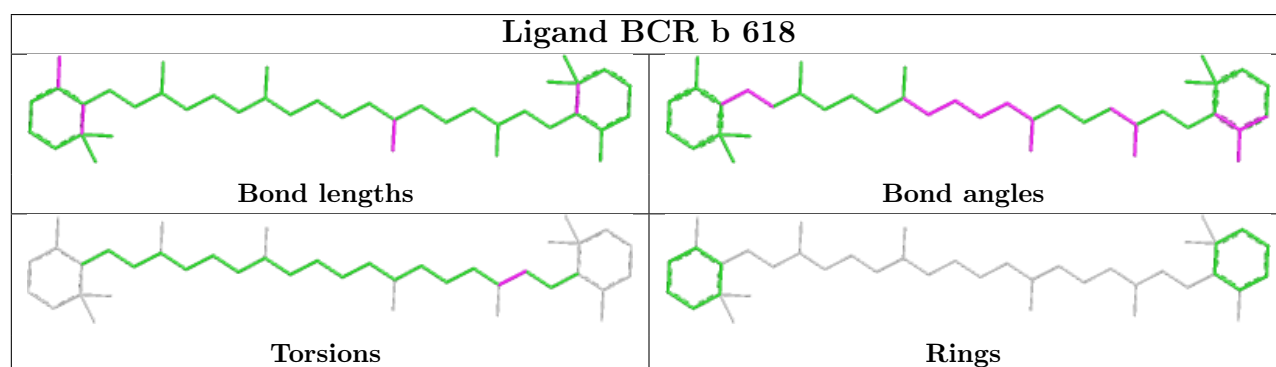
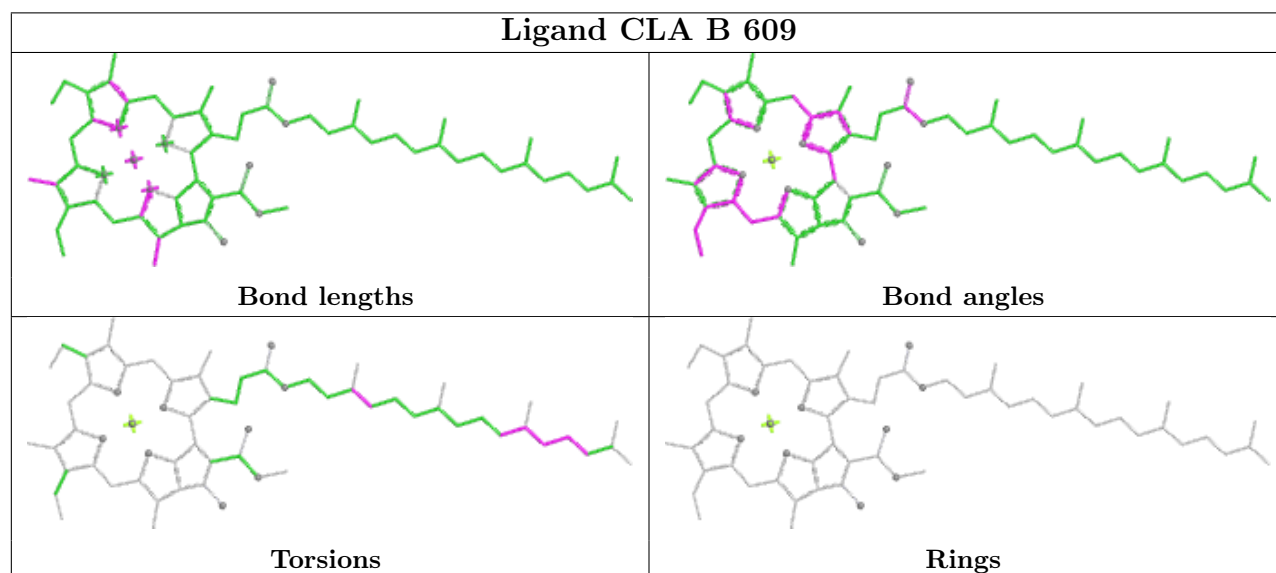
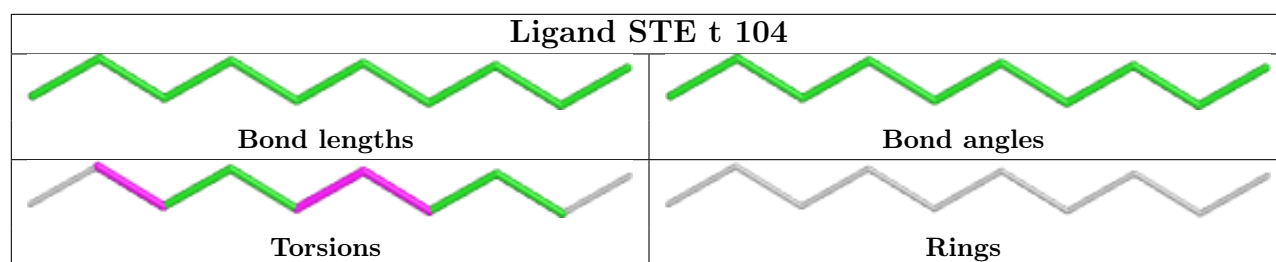
Ligand BCR a 405



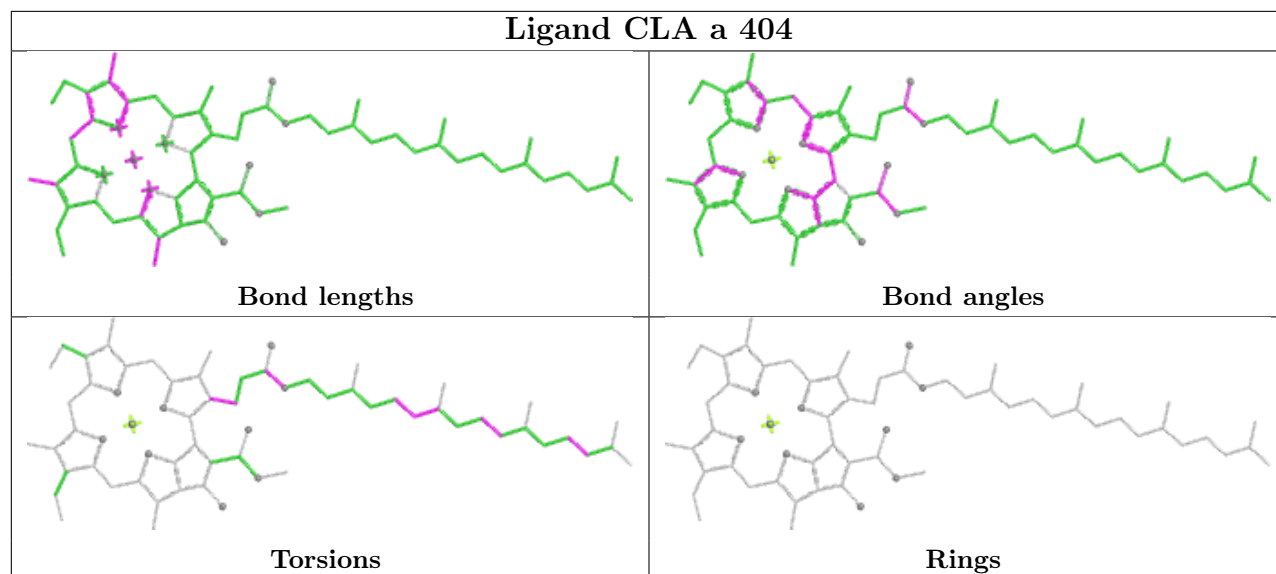
Ligand CLA A 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Z 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



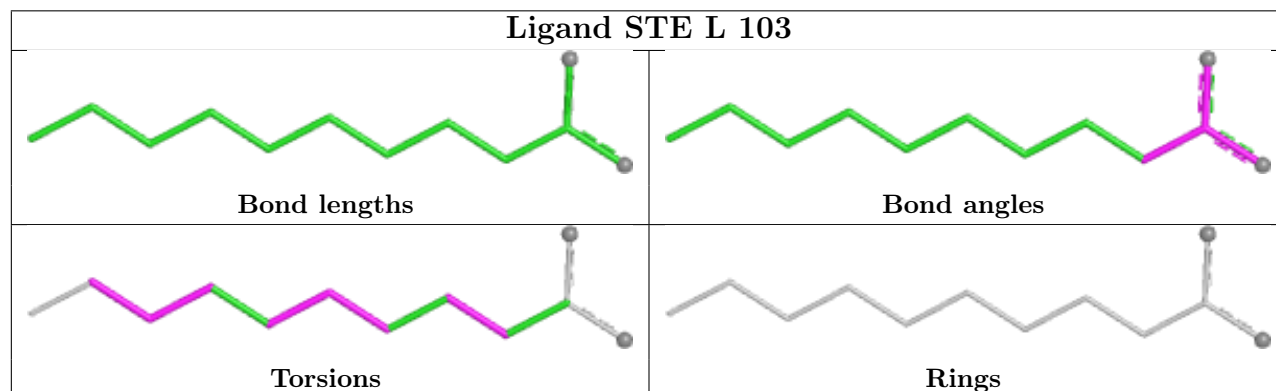




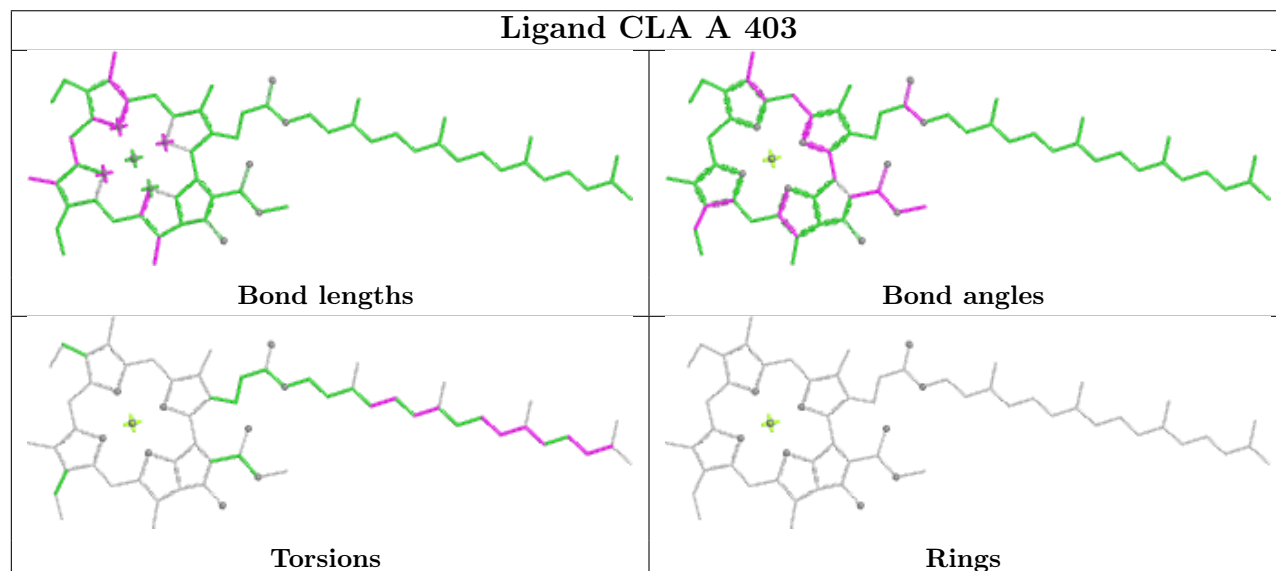
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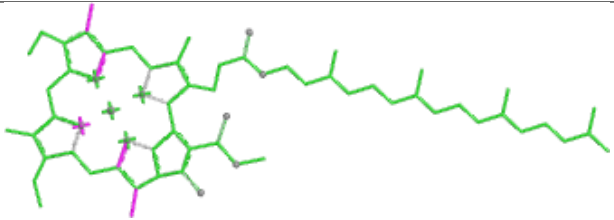
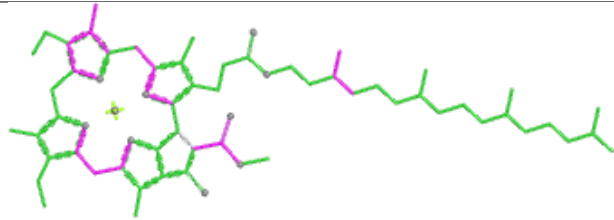
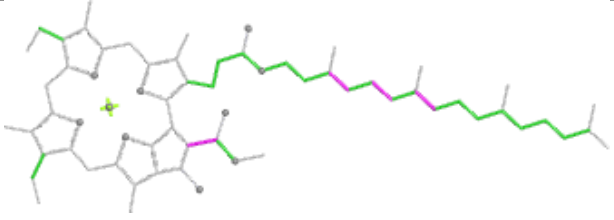
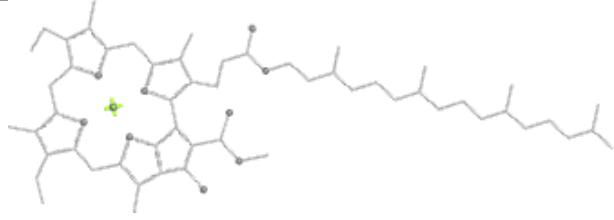


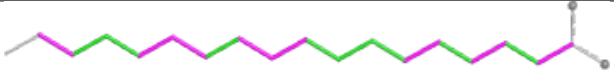
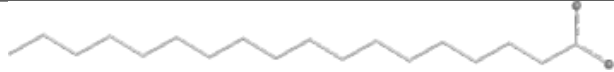
Ligand STE L 103

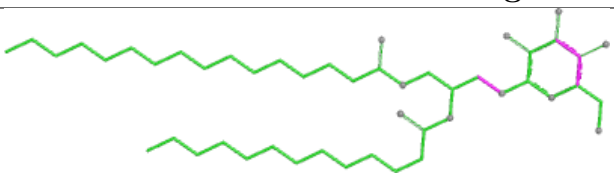
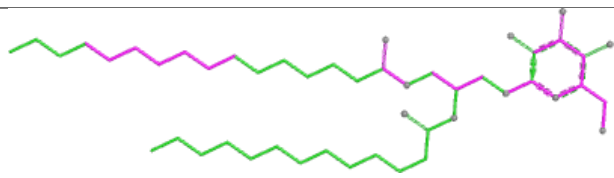
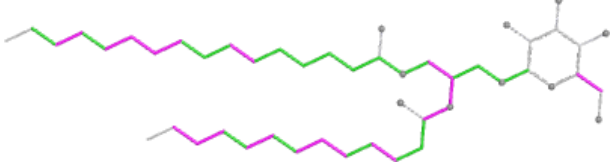
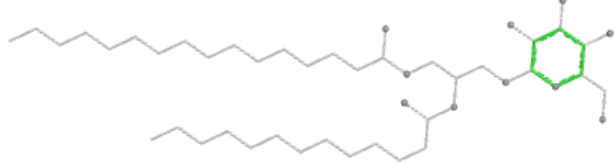


Ligand CLA A 403

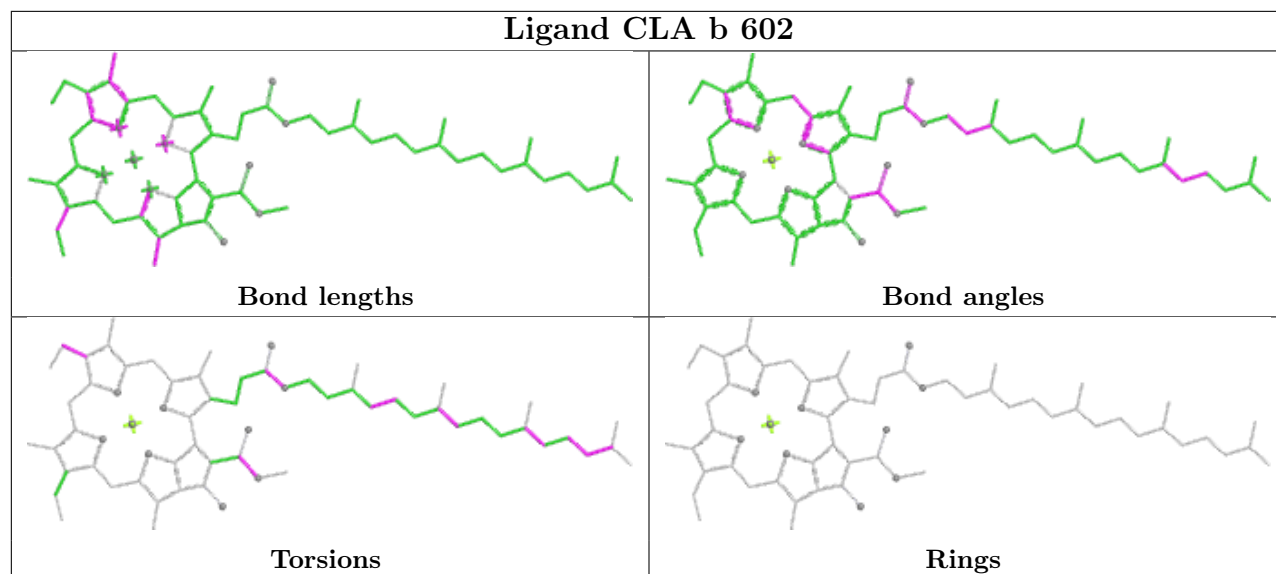


Ligand CLA C 507	
	
Bond lengths	Bond angles
	
Torsions	Rings

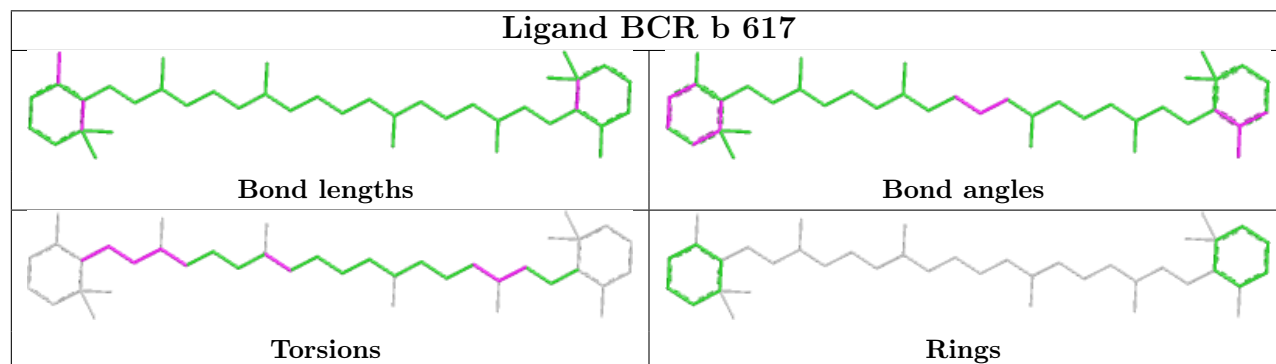
Ligand STE d 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

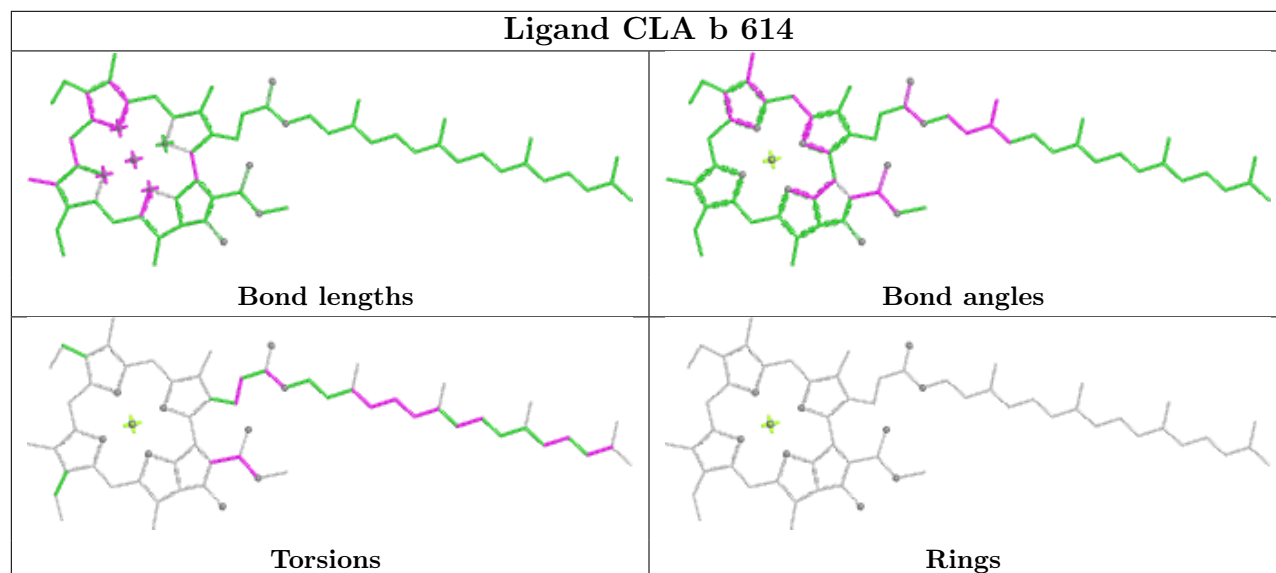
Ligand CLA b 602

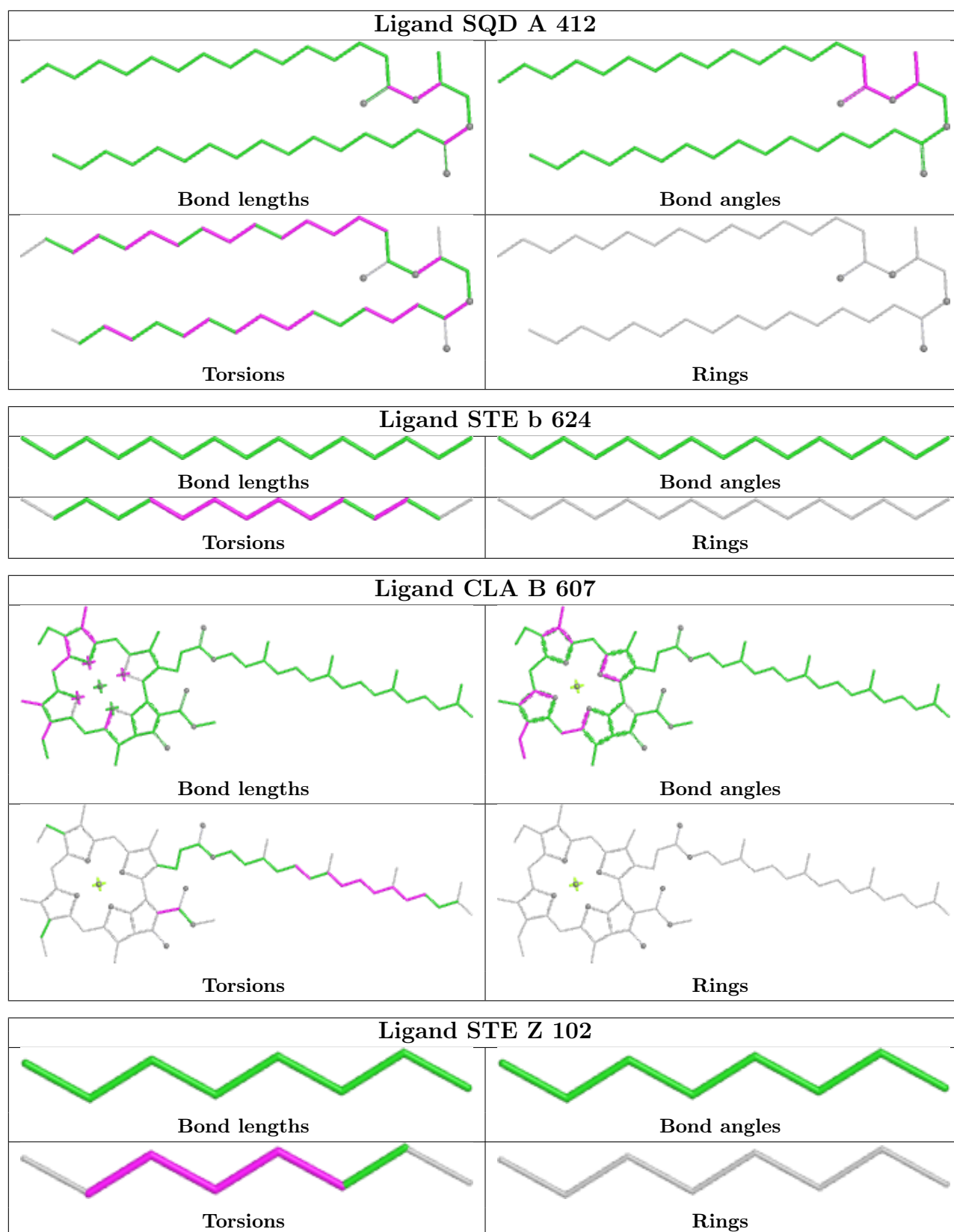


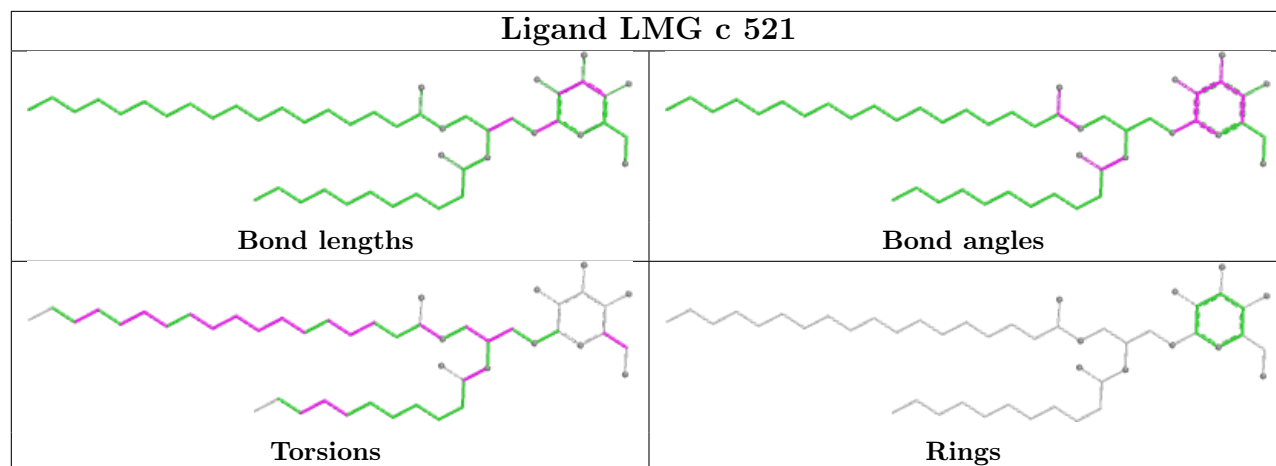
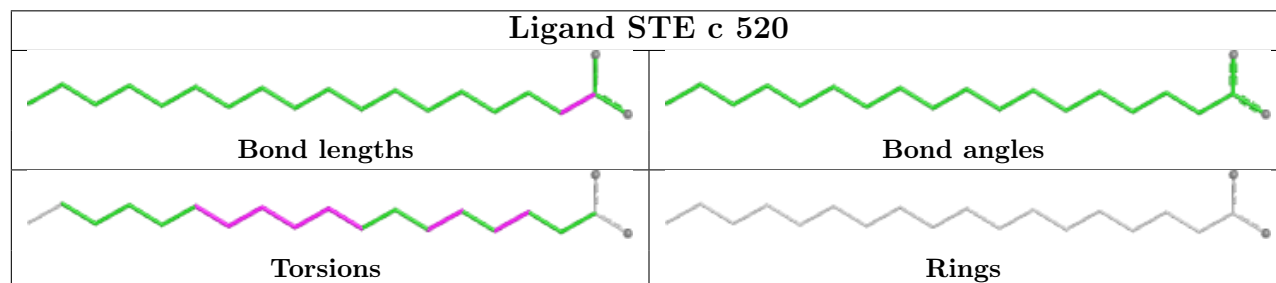
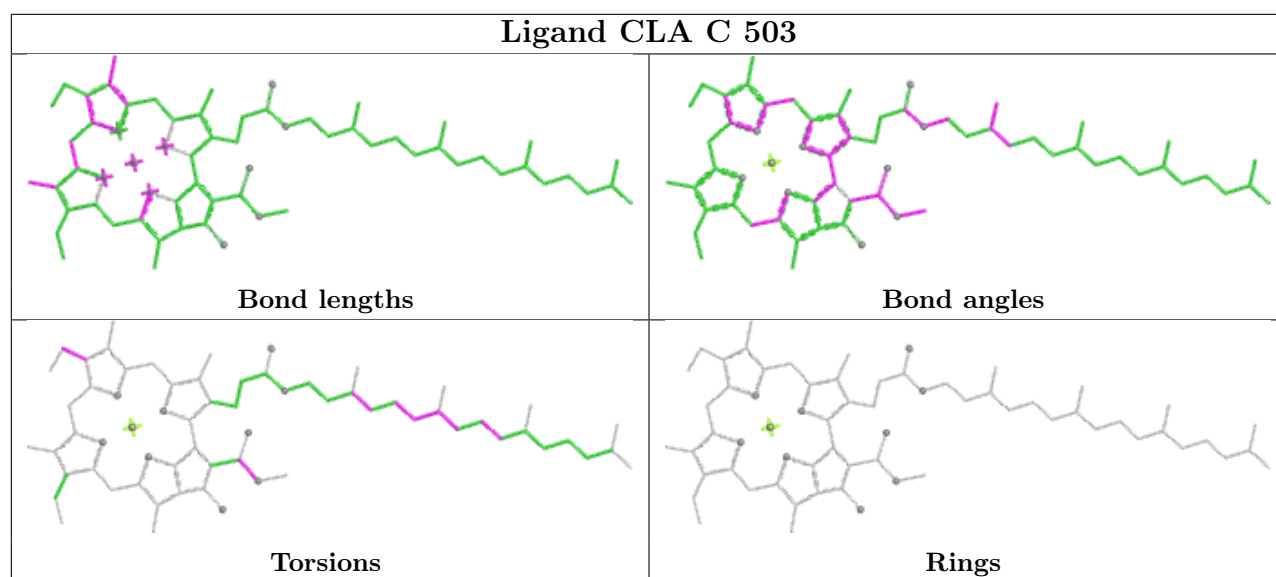
Ligand BCR b 617

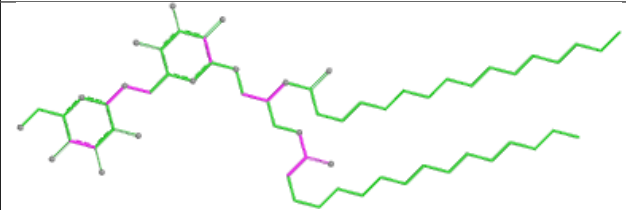
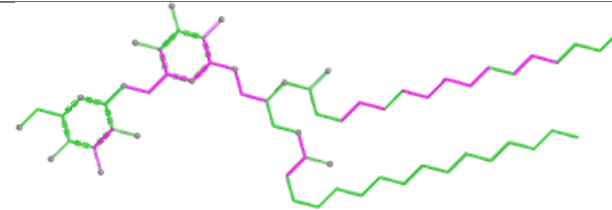
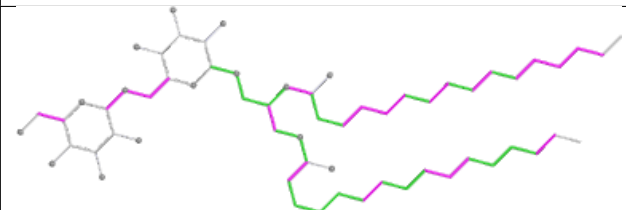
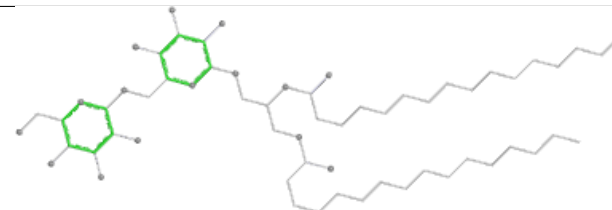


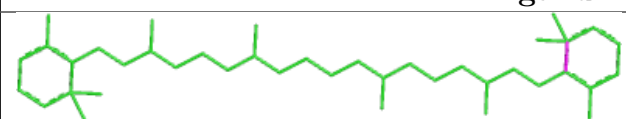
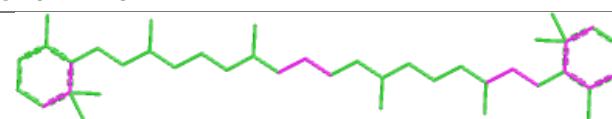
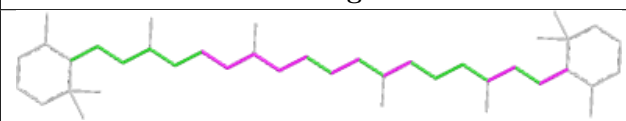
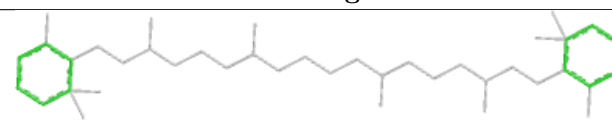
Ligand CLA b 614

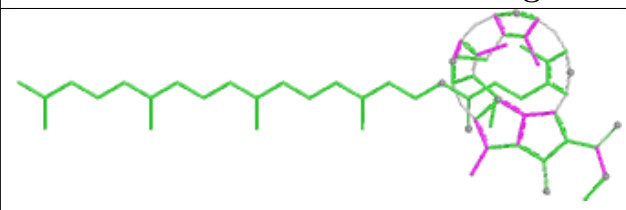
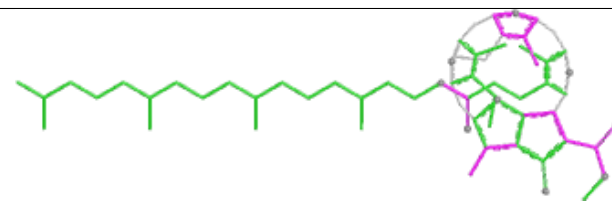
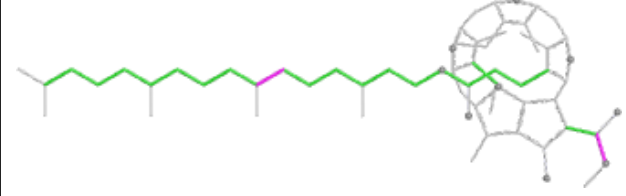
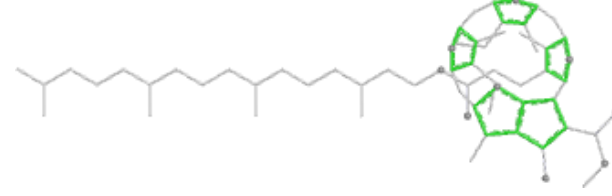


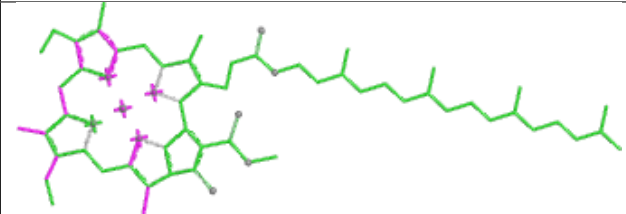
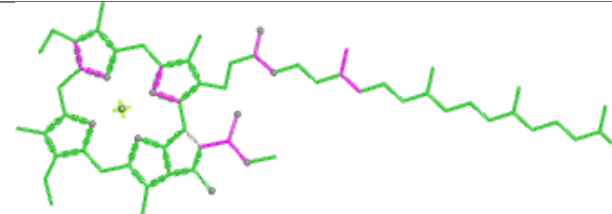
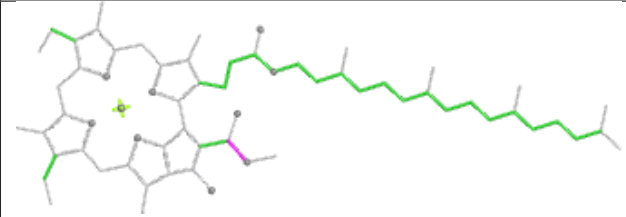
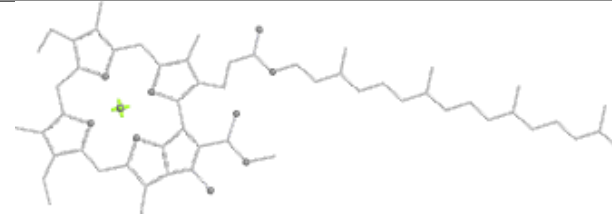


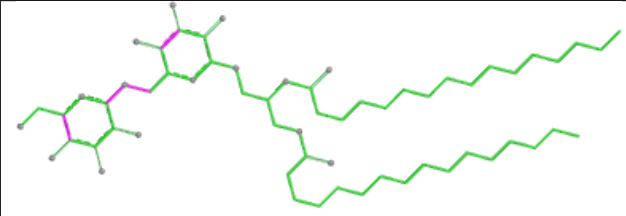
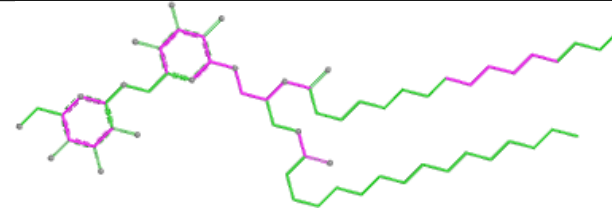
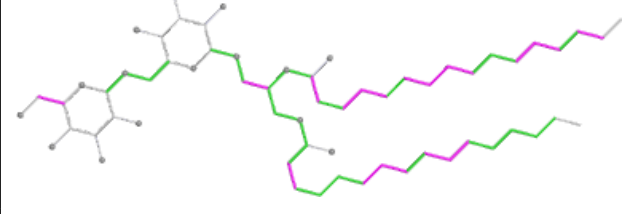
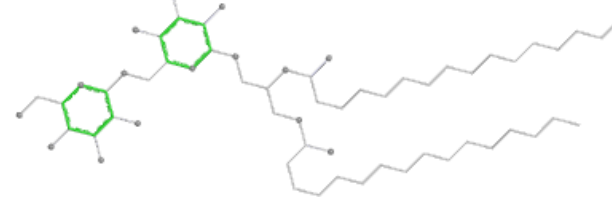


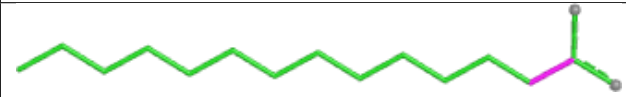
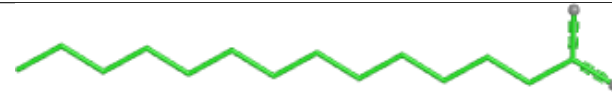
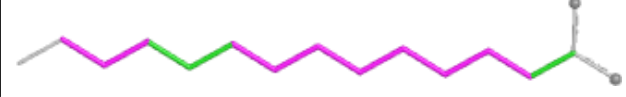
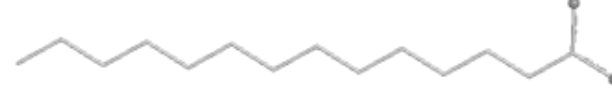
Ligand DGD C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

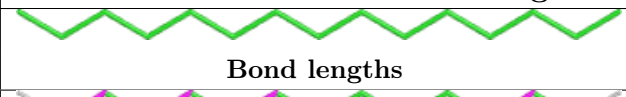
Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

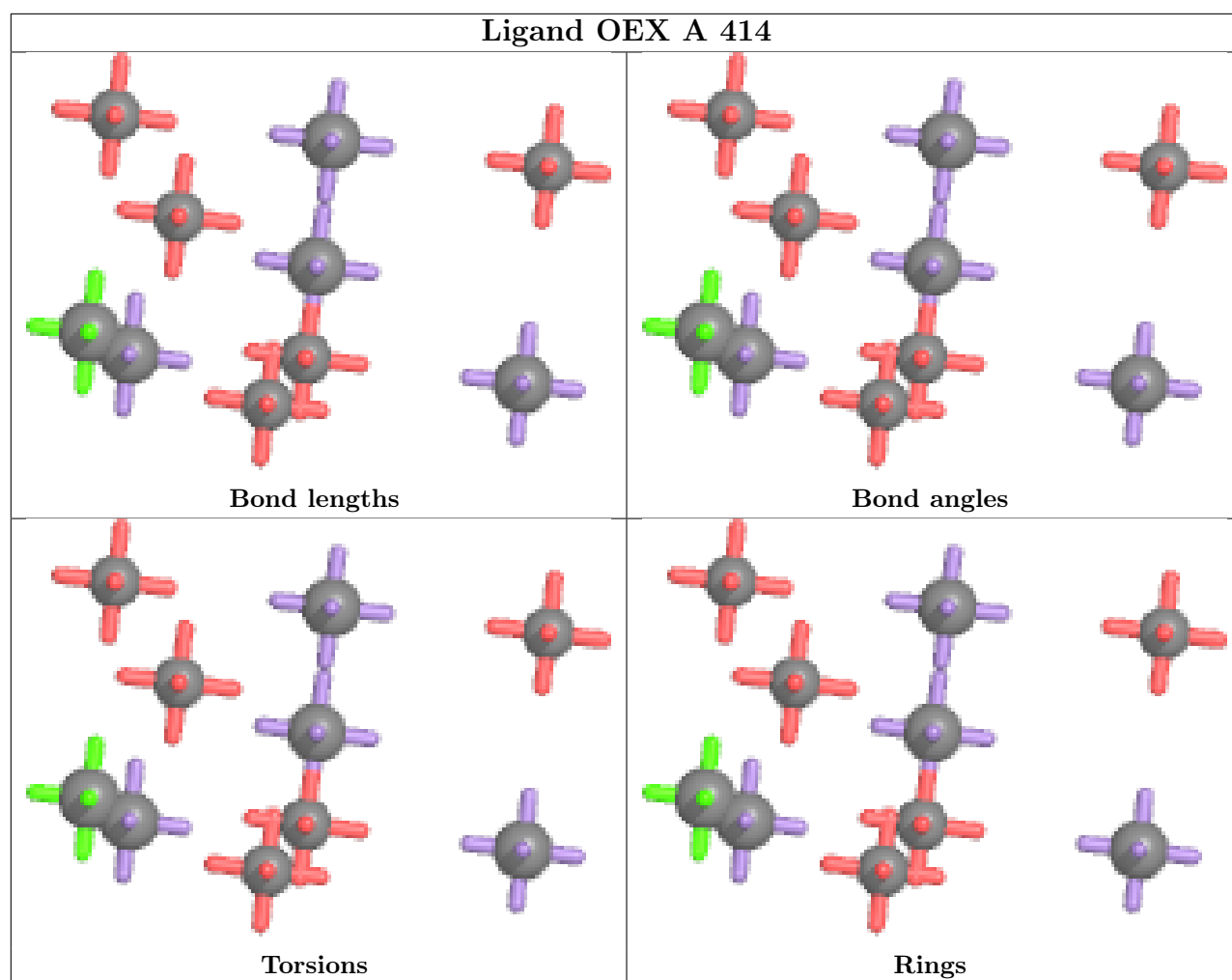
Ligand PHO a 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

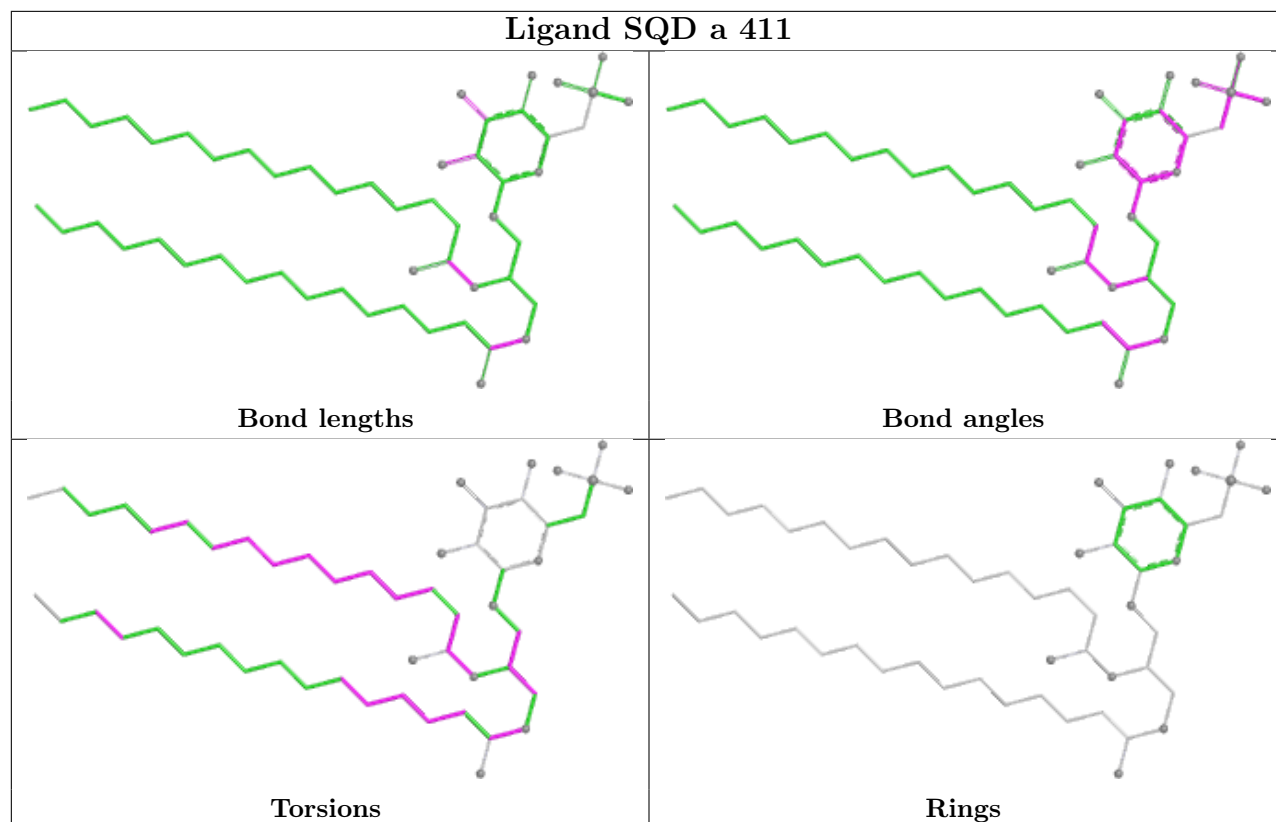
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

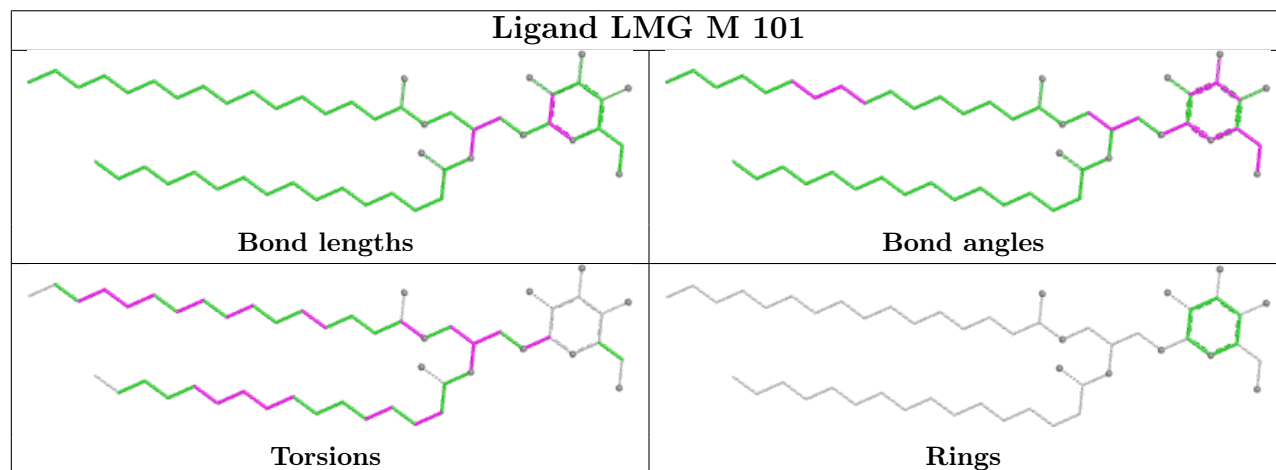
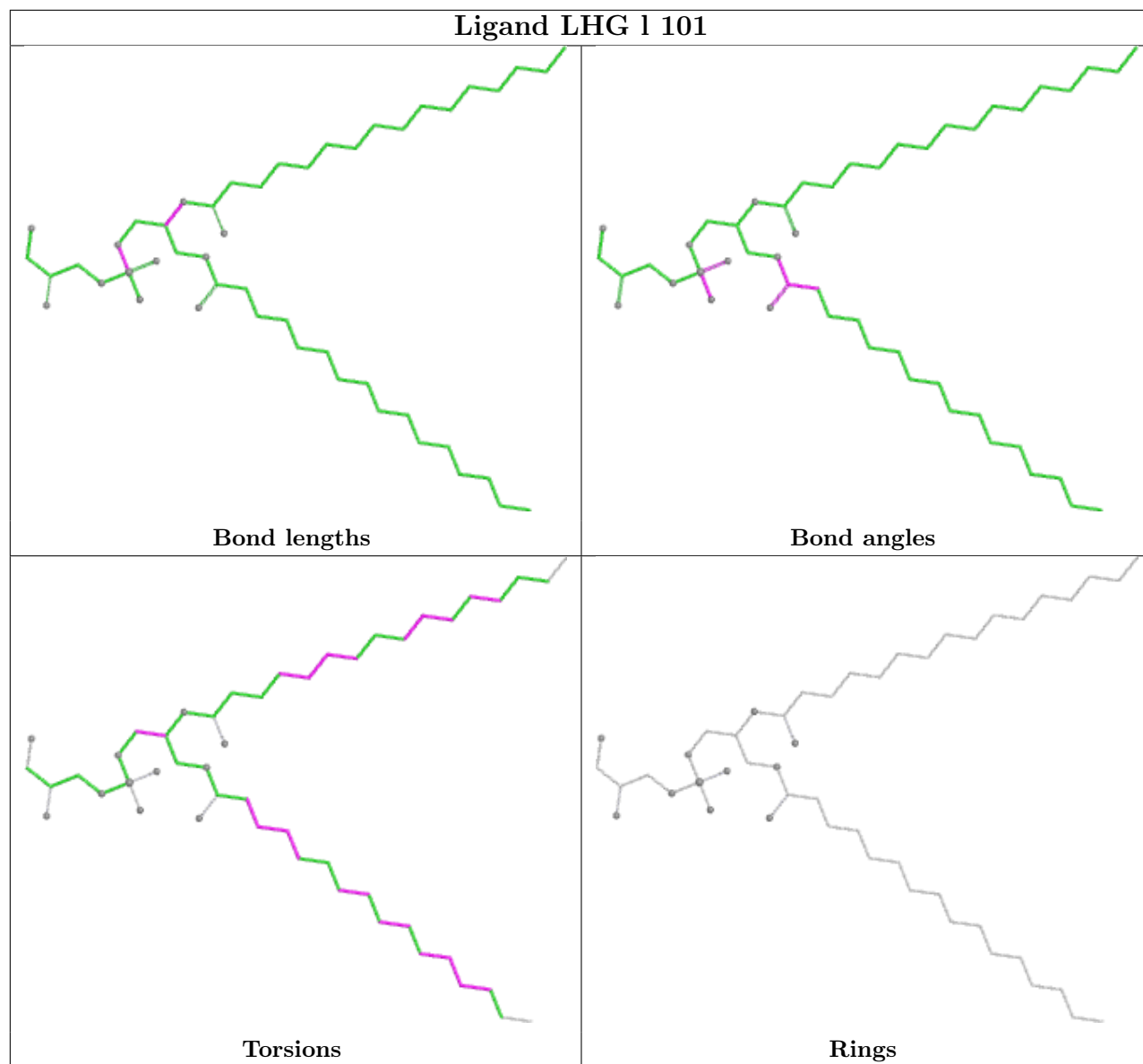
Ligand DGD h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

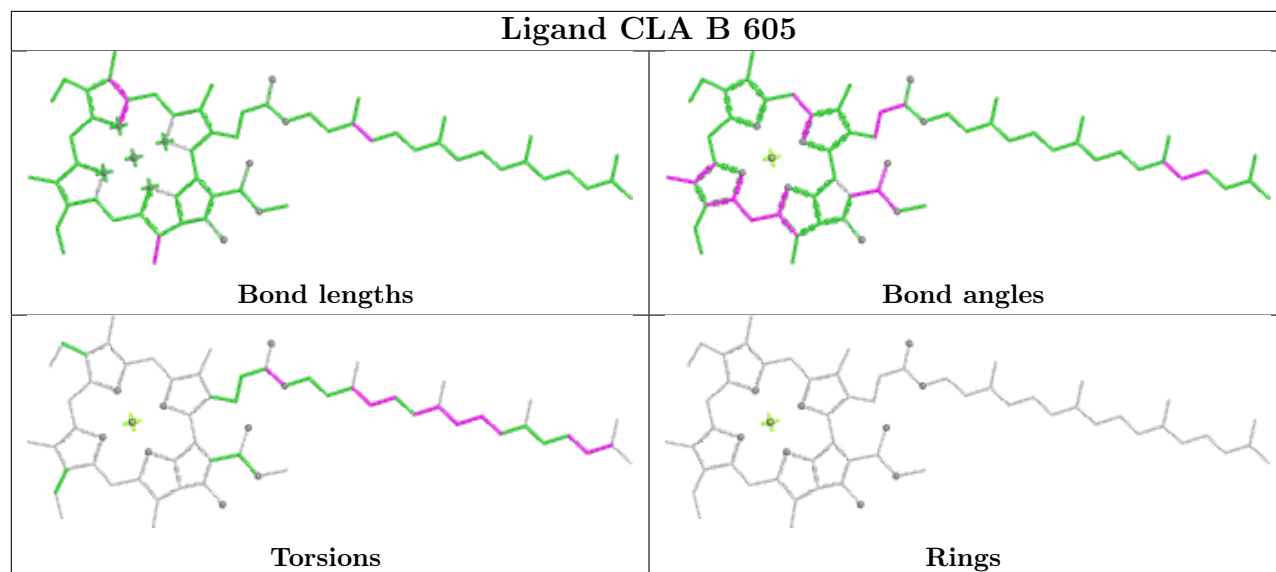
Ligand STE I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings



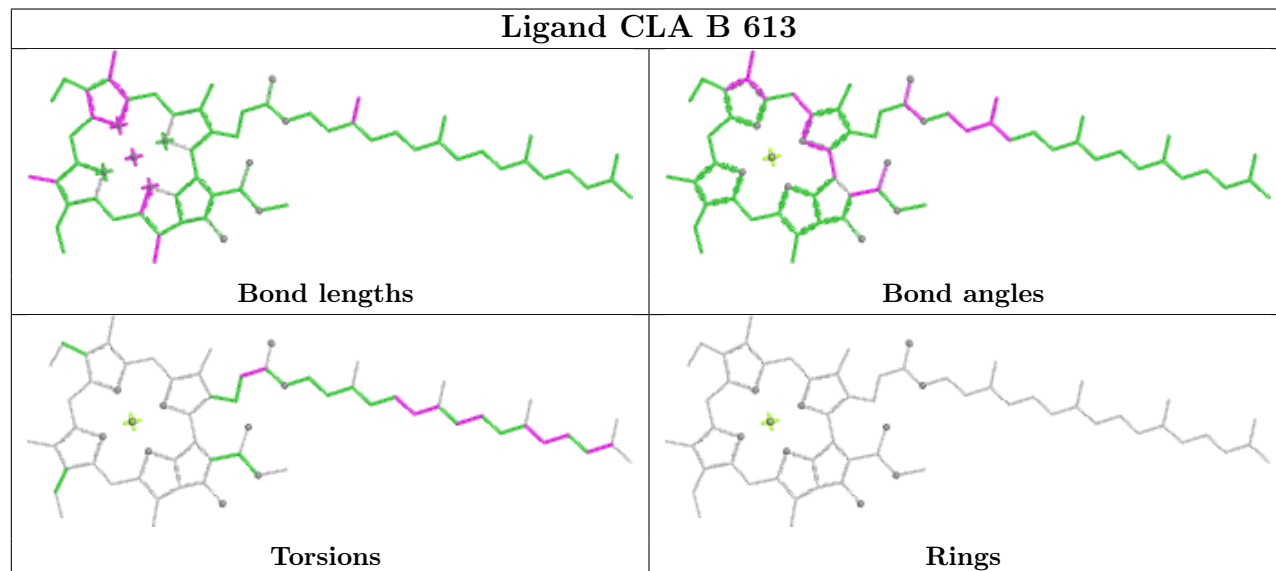




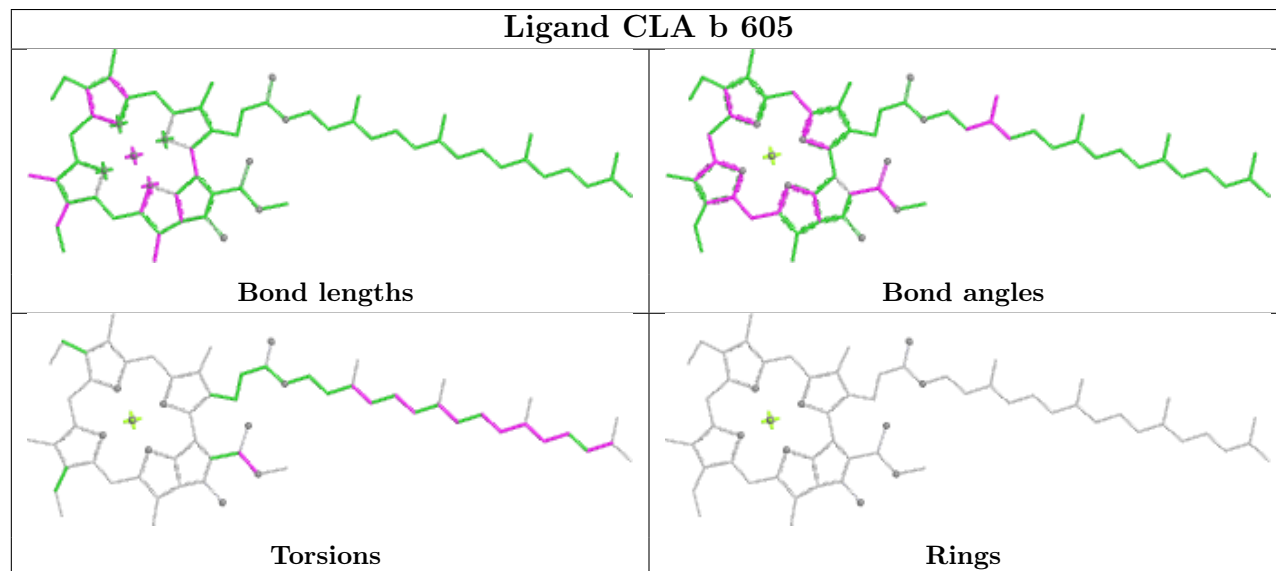
Ligand CLA B 605



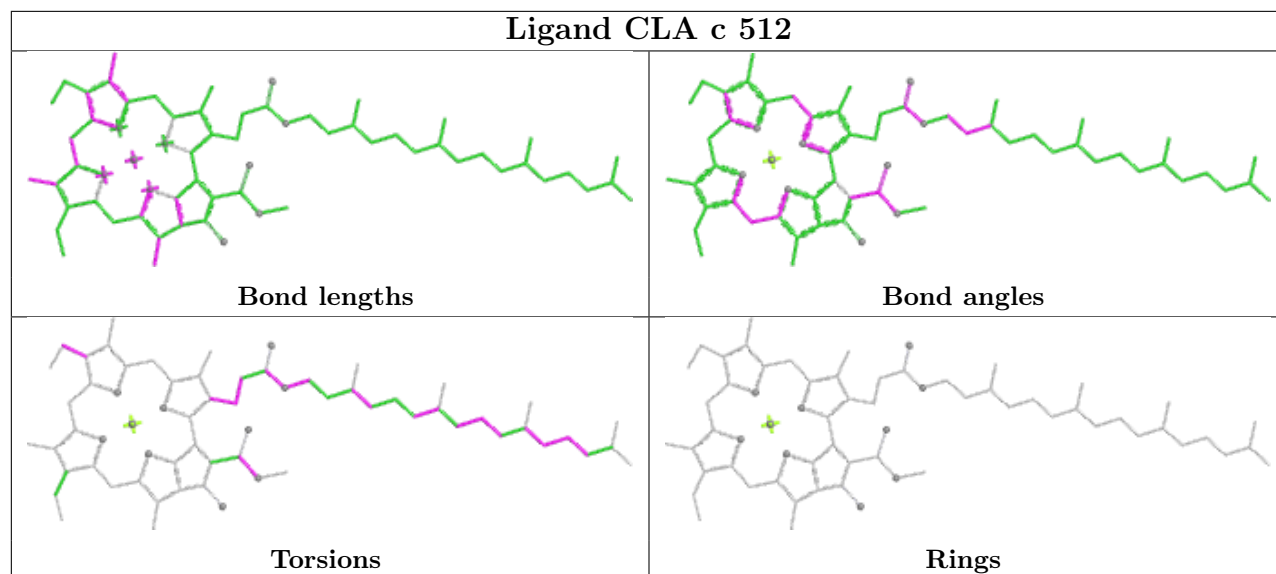
Ligand CLA B 613



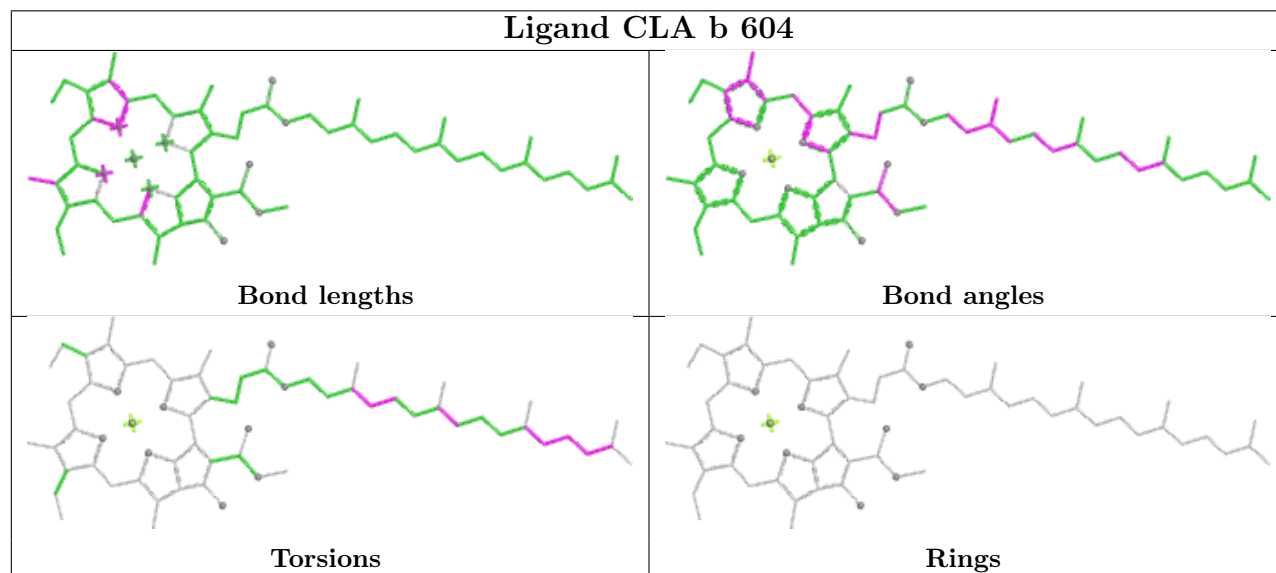
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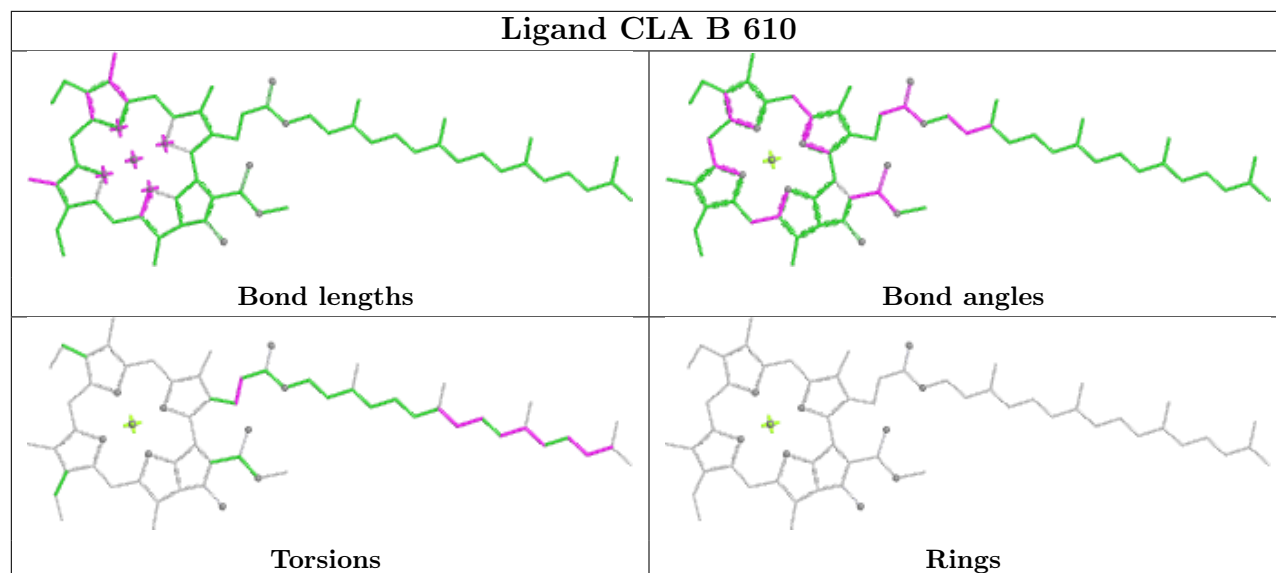
Ligand CLA c 512

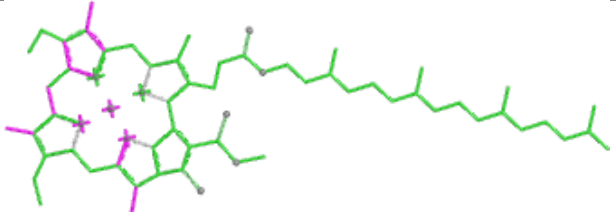
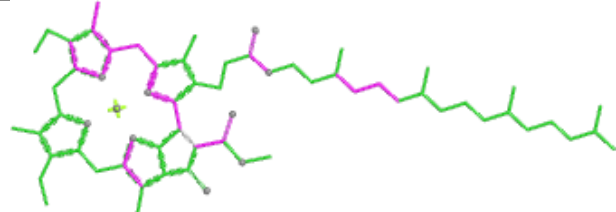
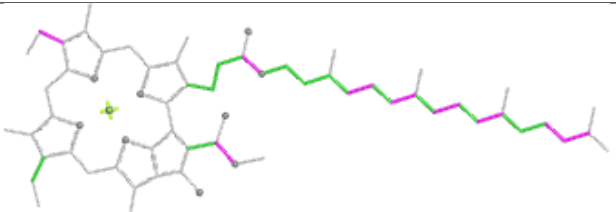
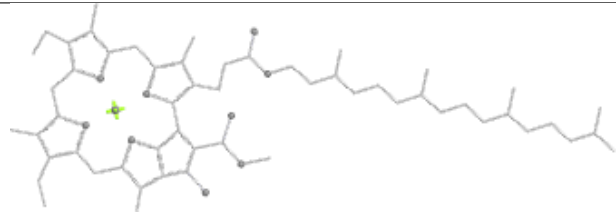


Ligand CLA b 604

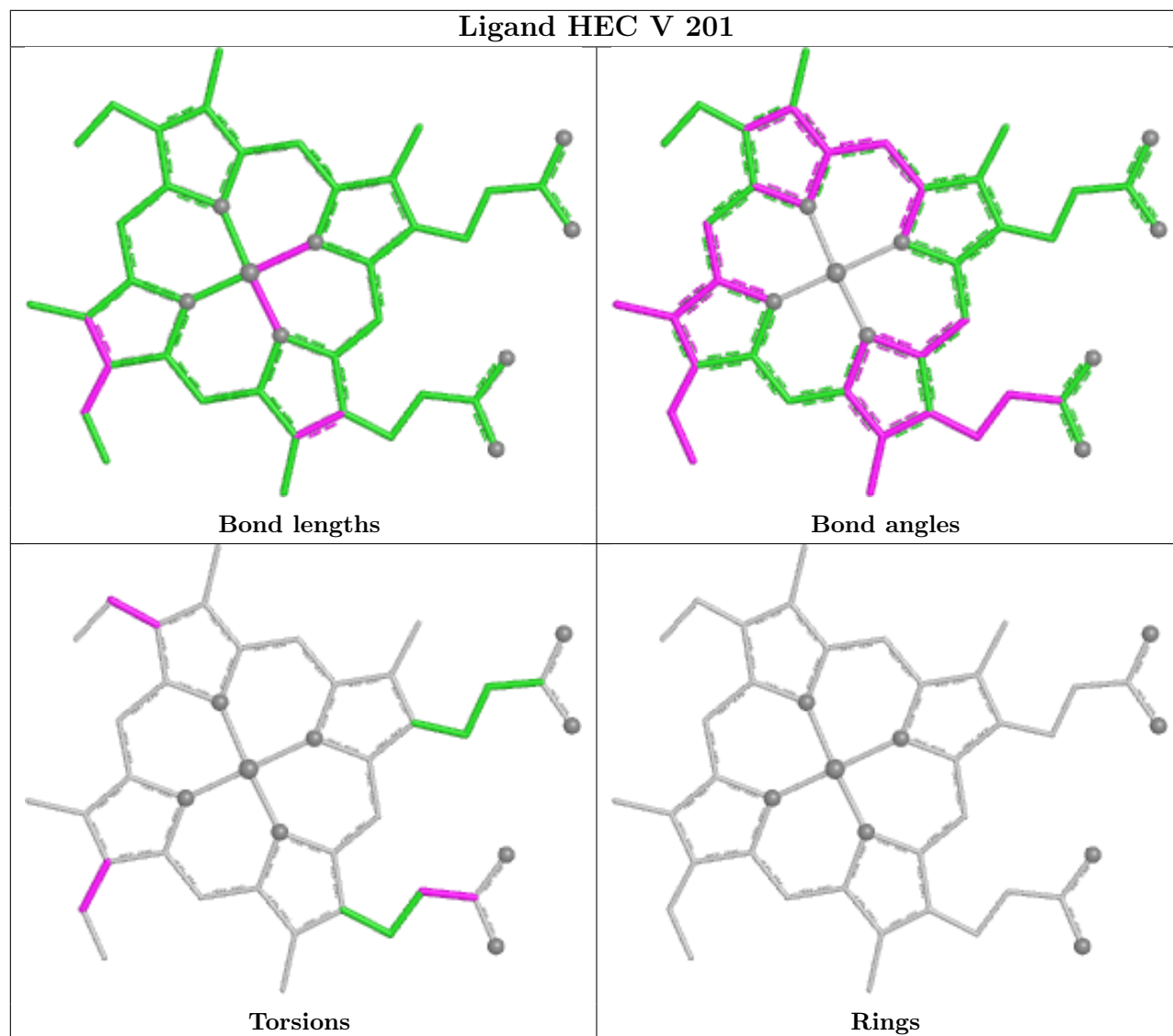


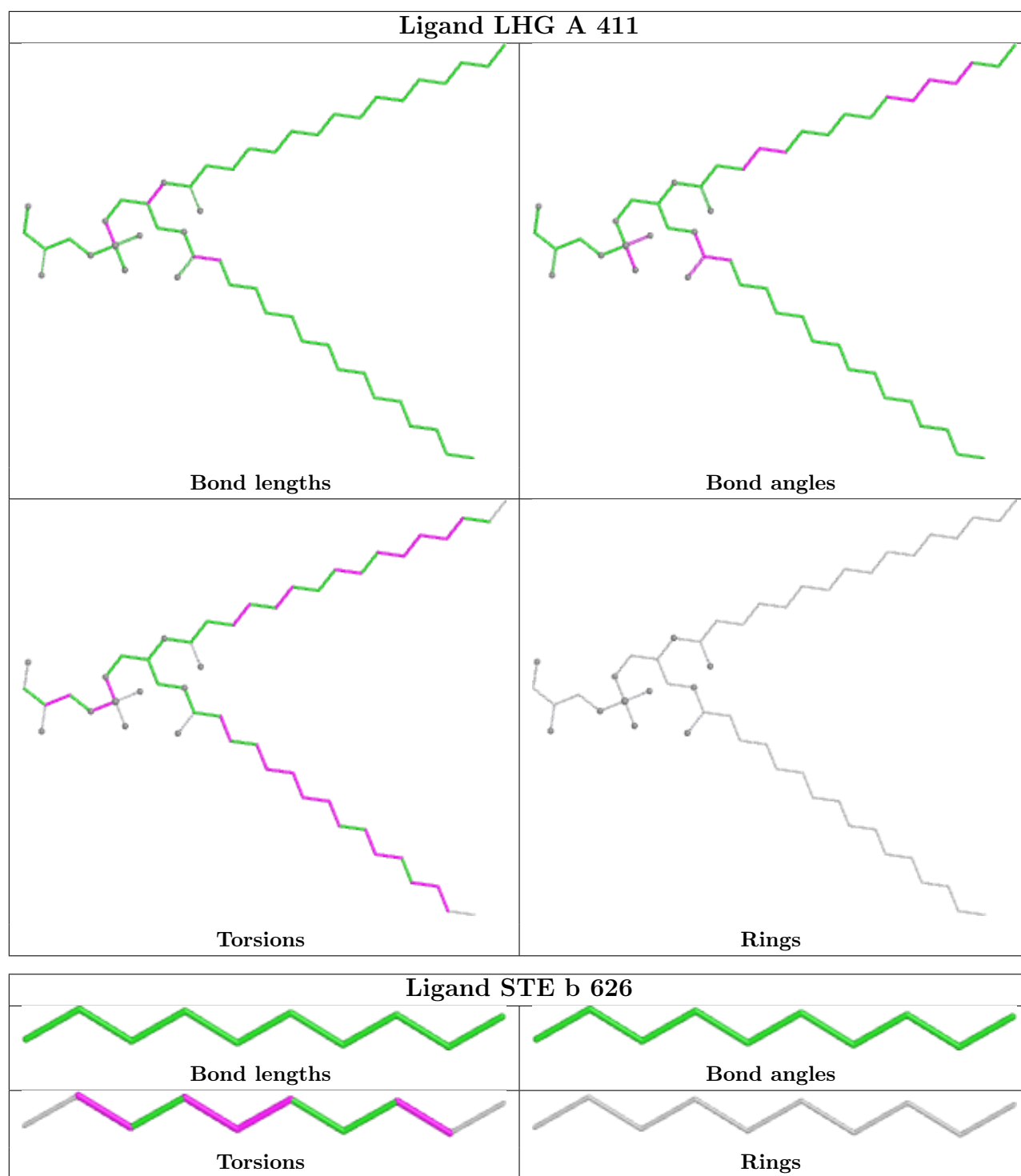
Ligand CLA B 610

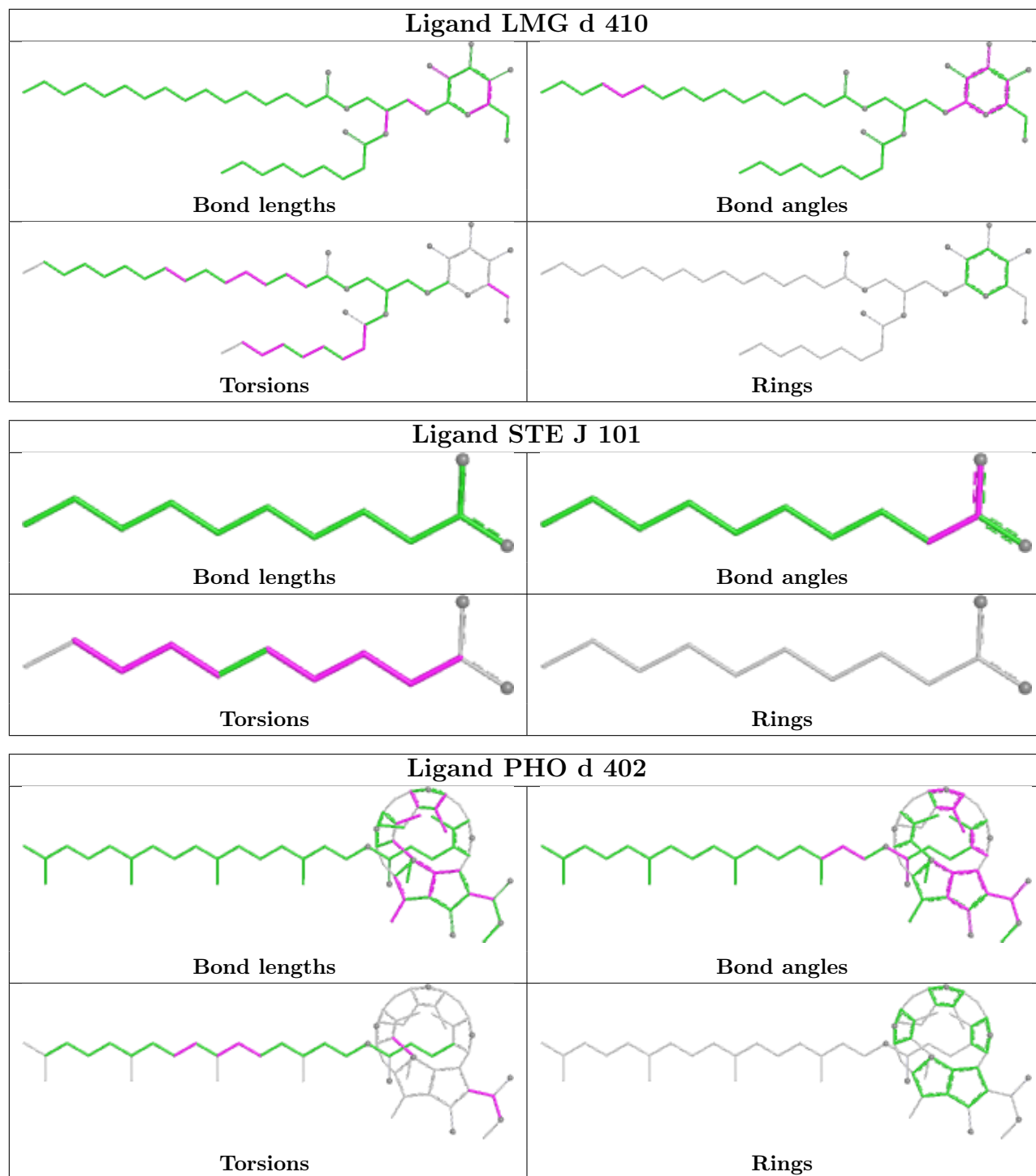


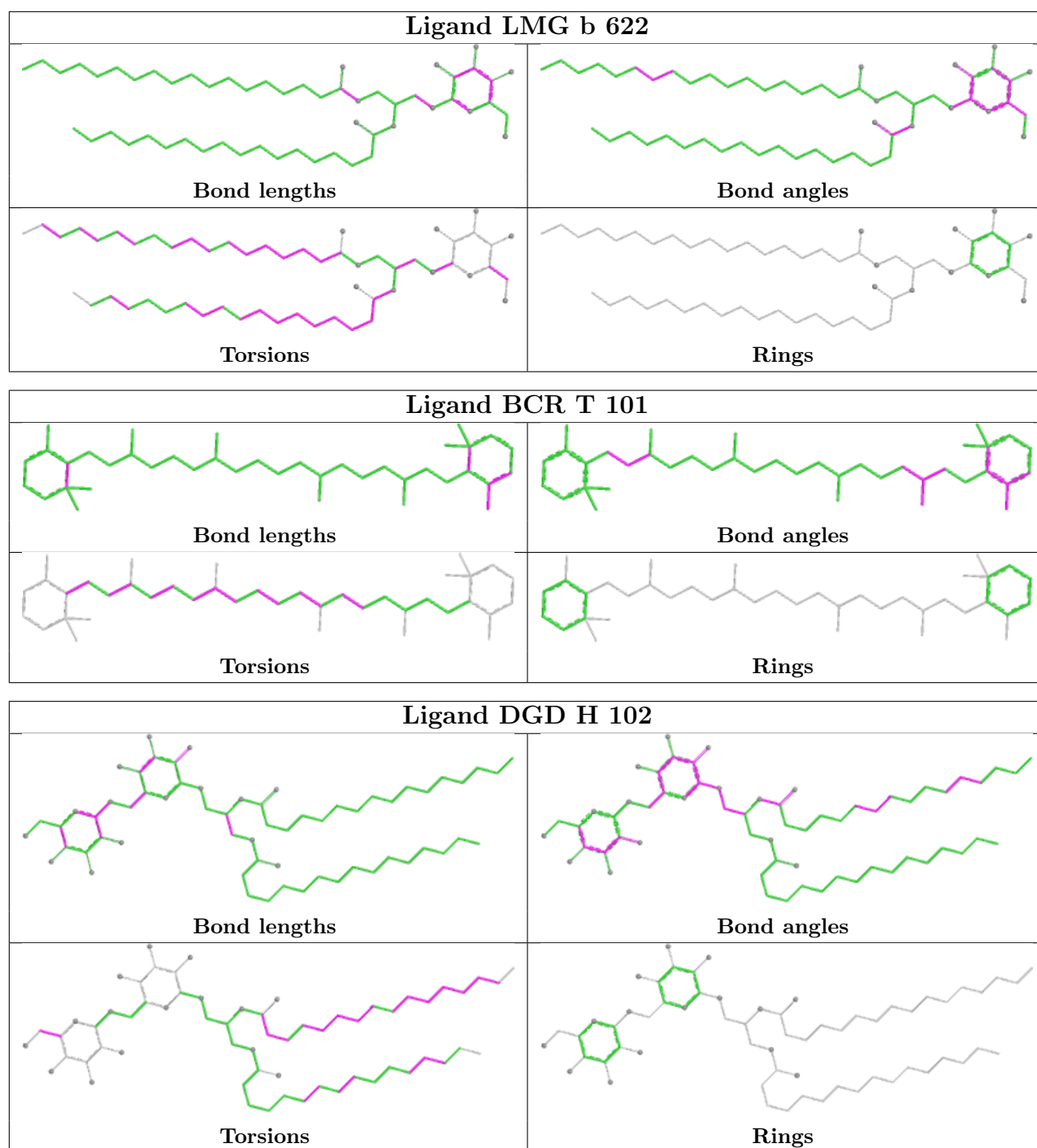
Ligand CLA b 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE H 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

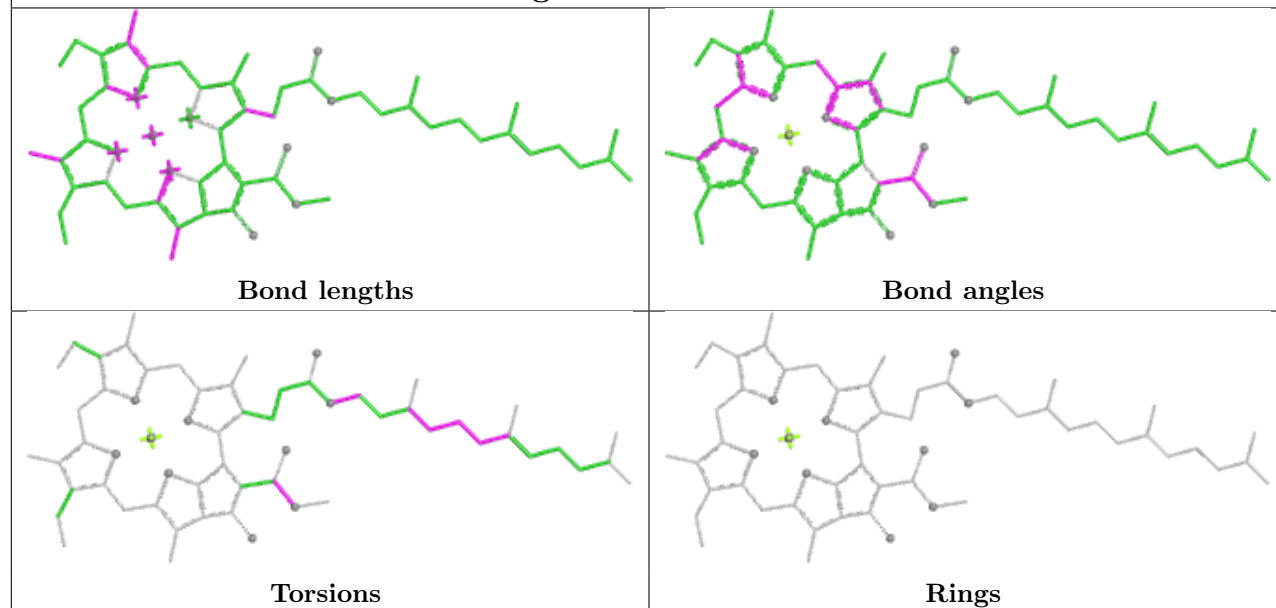




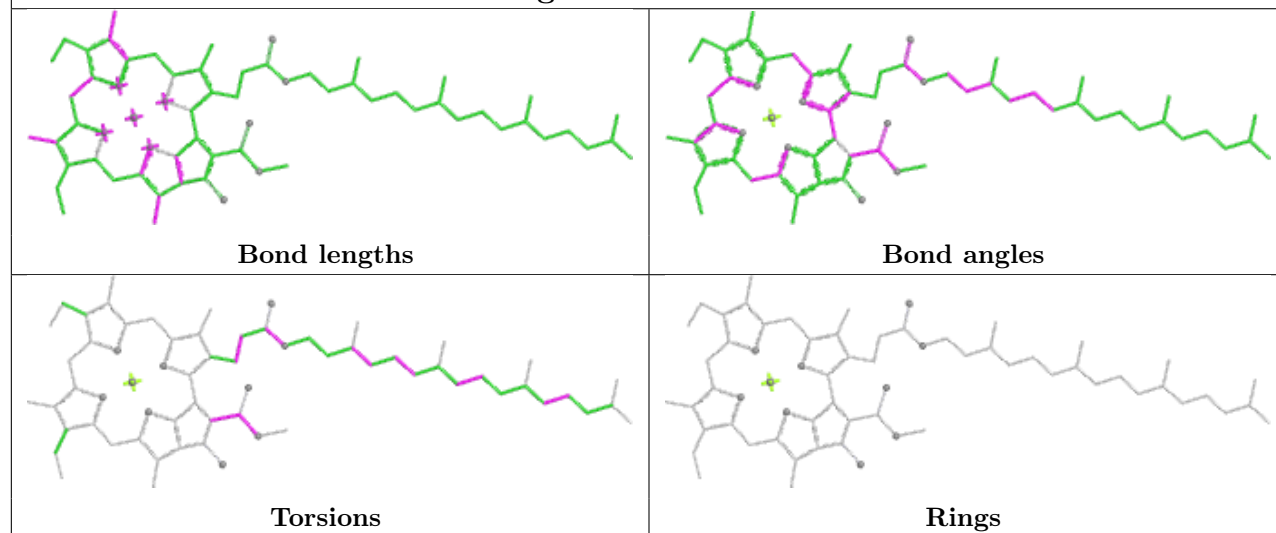


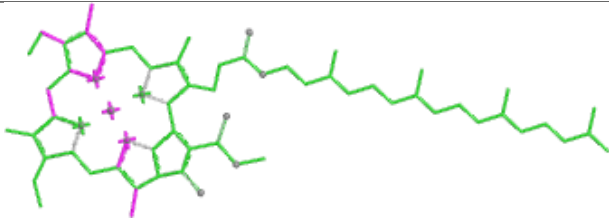
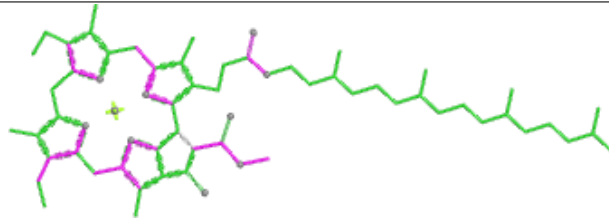
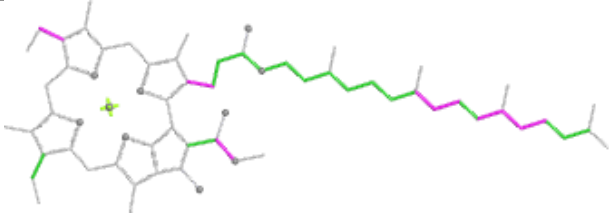
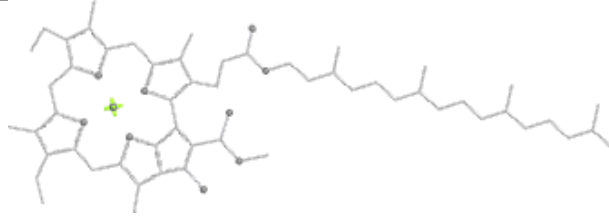


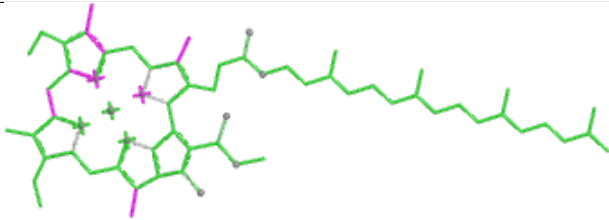
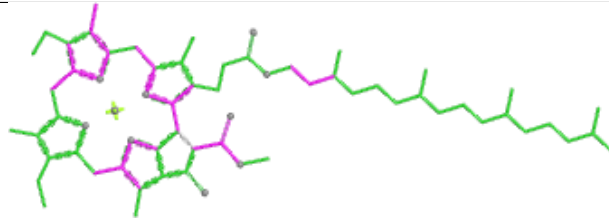
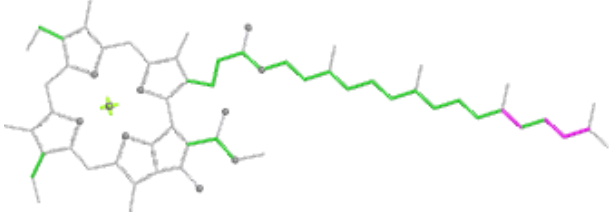
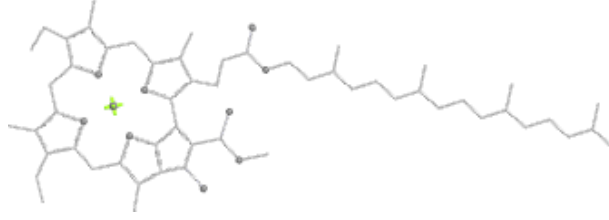
Ligand CLA B 616

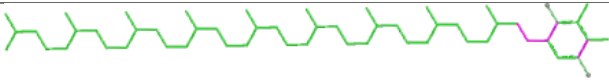
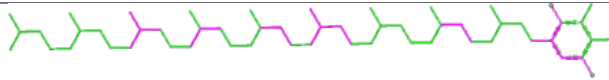
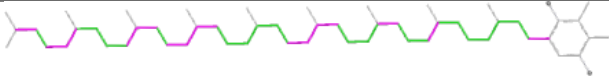
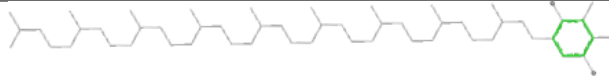


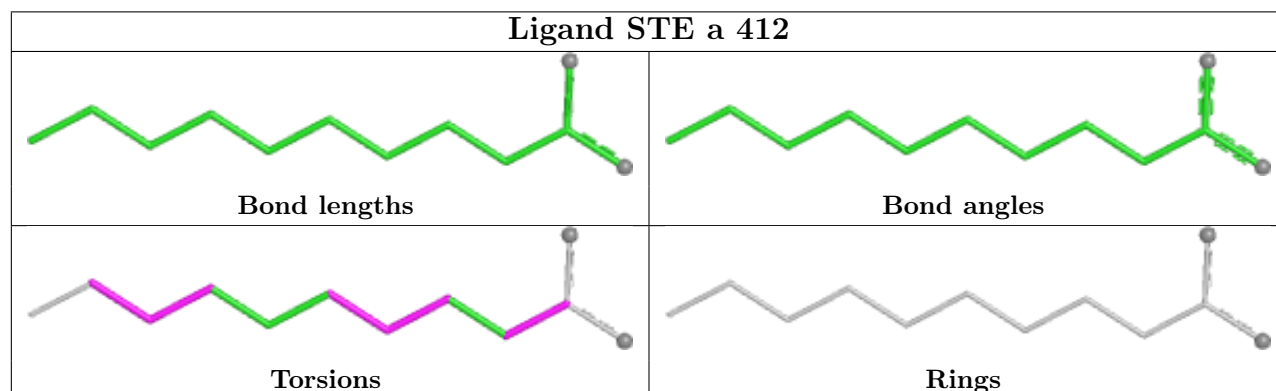
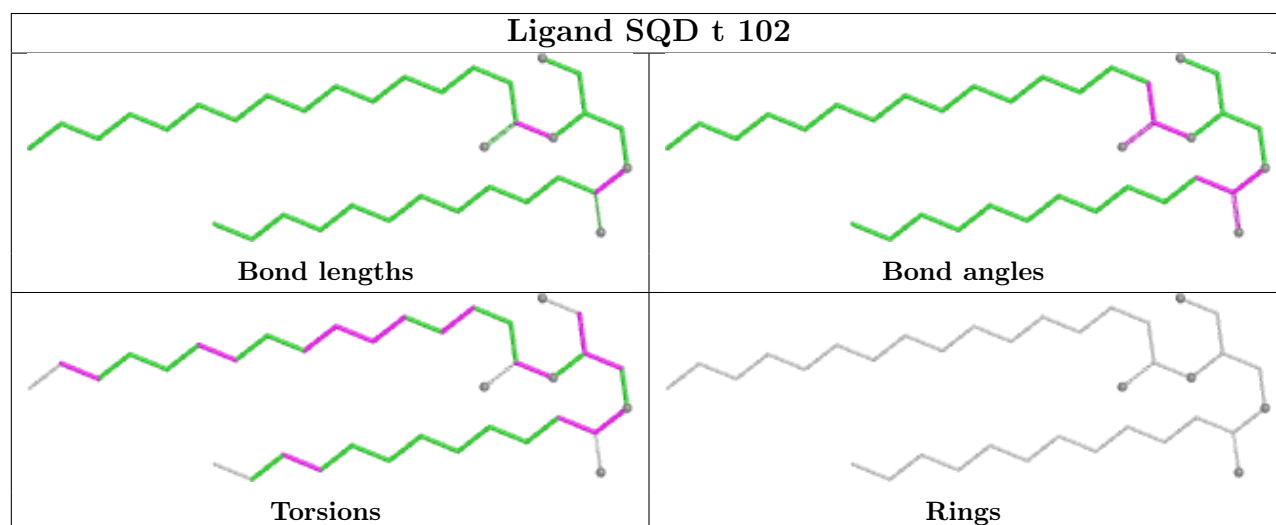
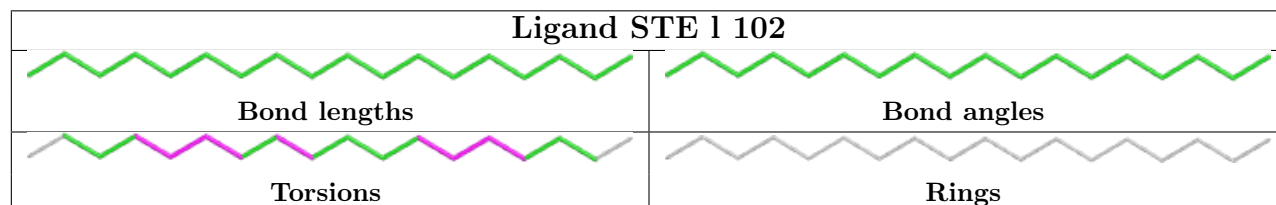
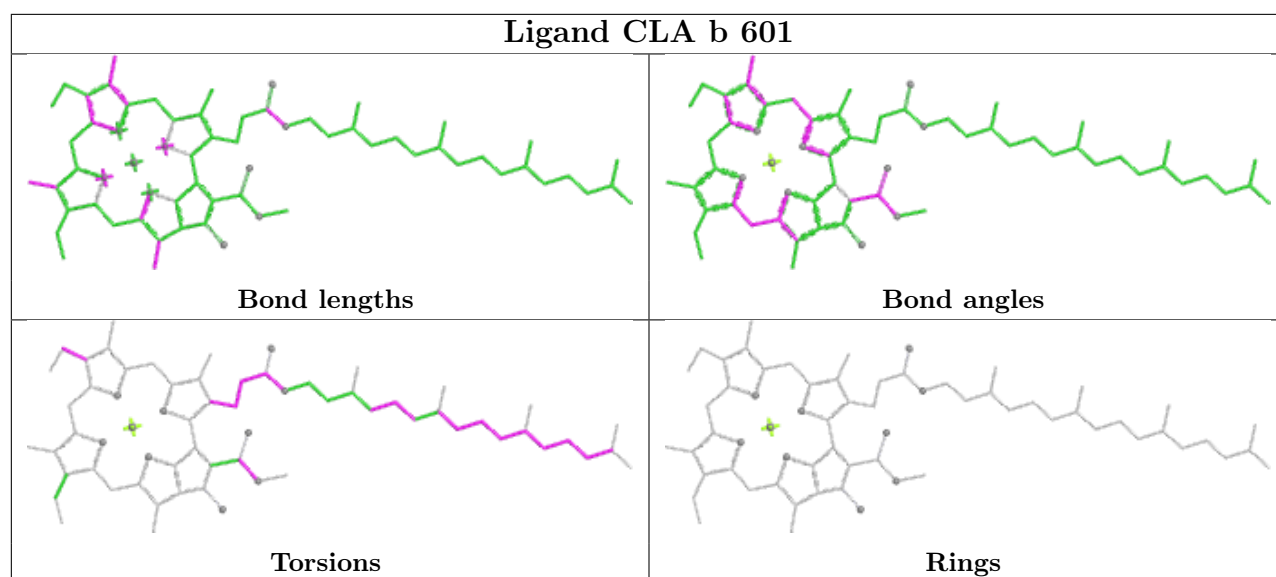
Ligand CLA c 507

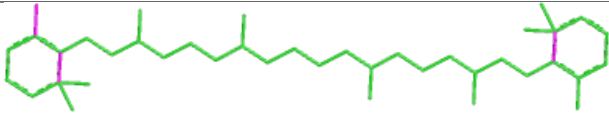
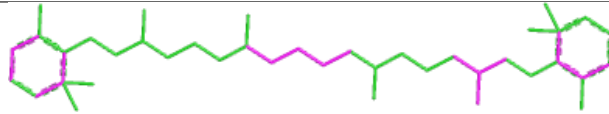
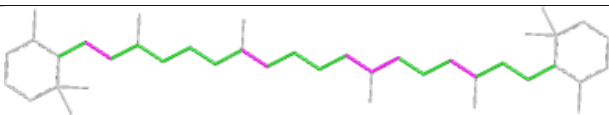
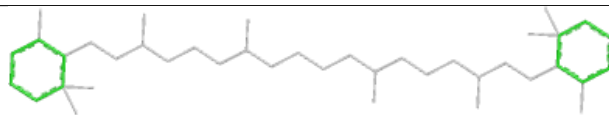


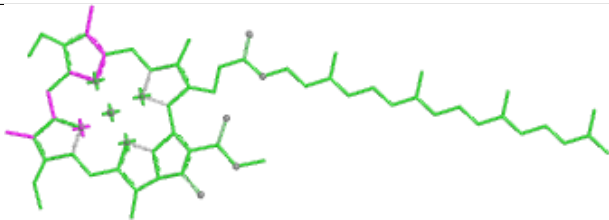
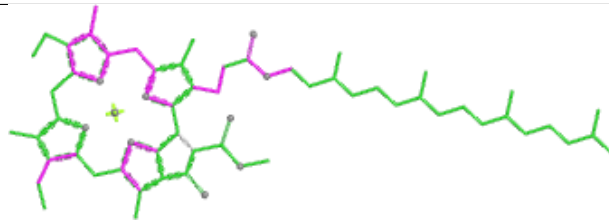
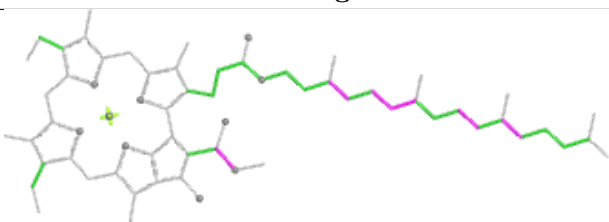
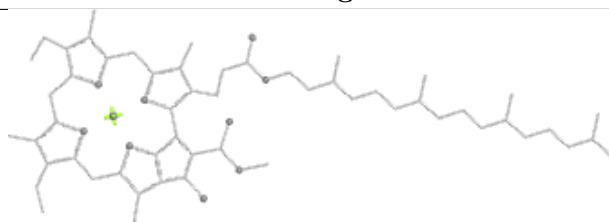
Ligand CLA d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

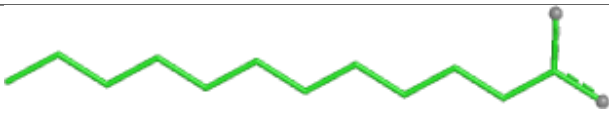
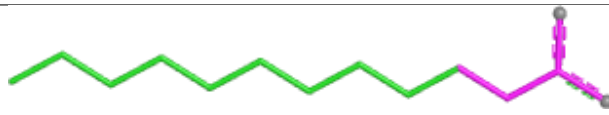
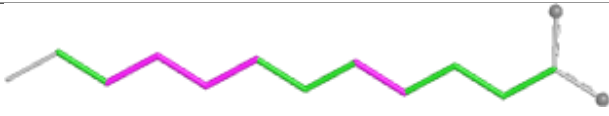
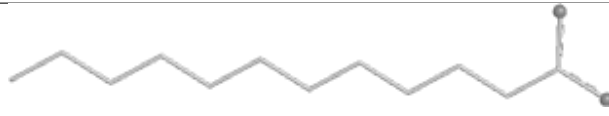
Ligand CLA d 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

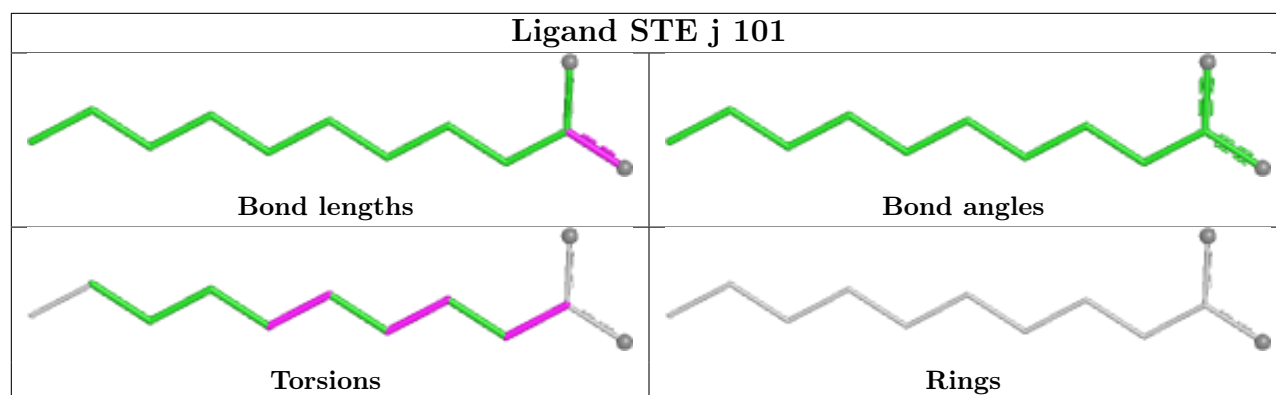
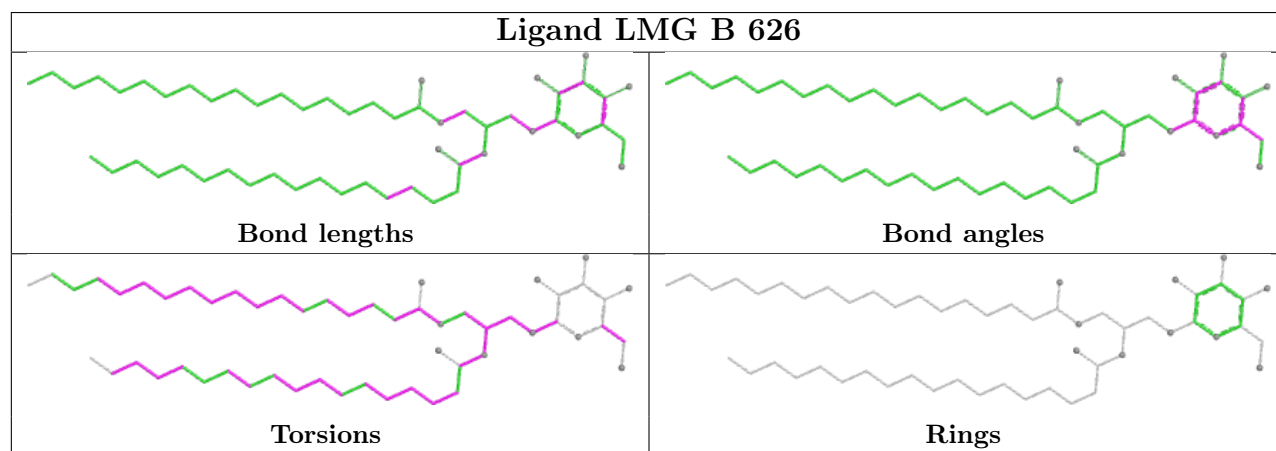
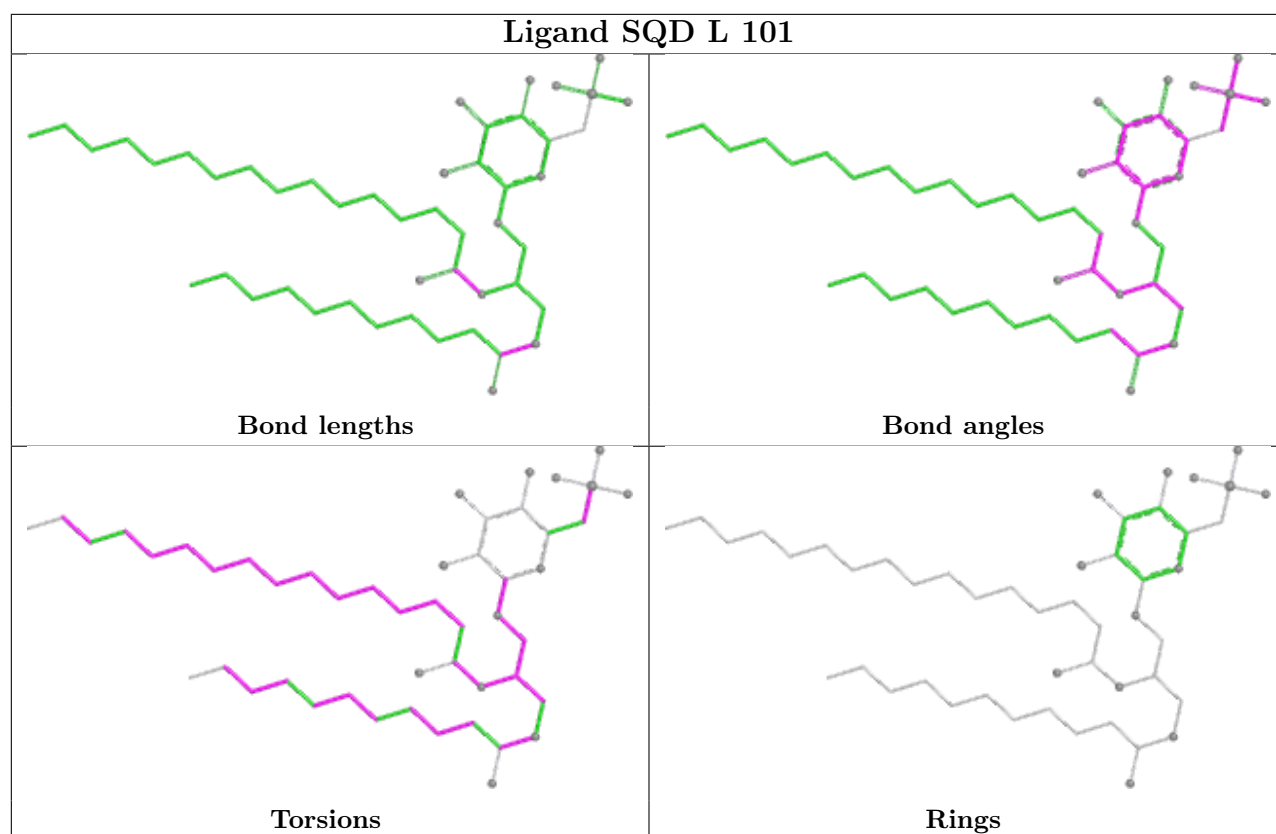
Ligand PL9 A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

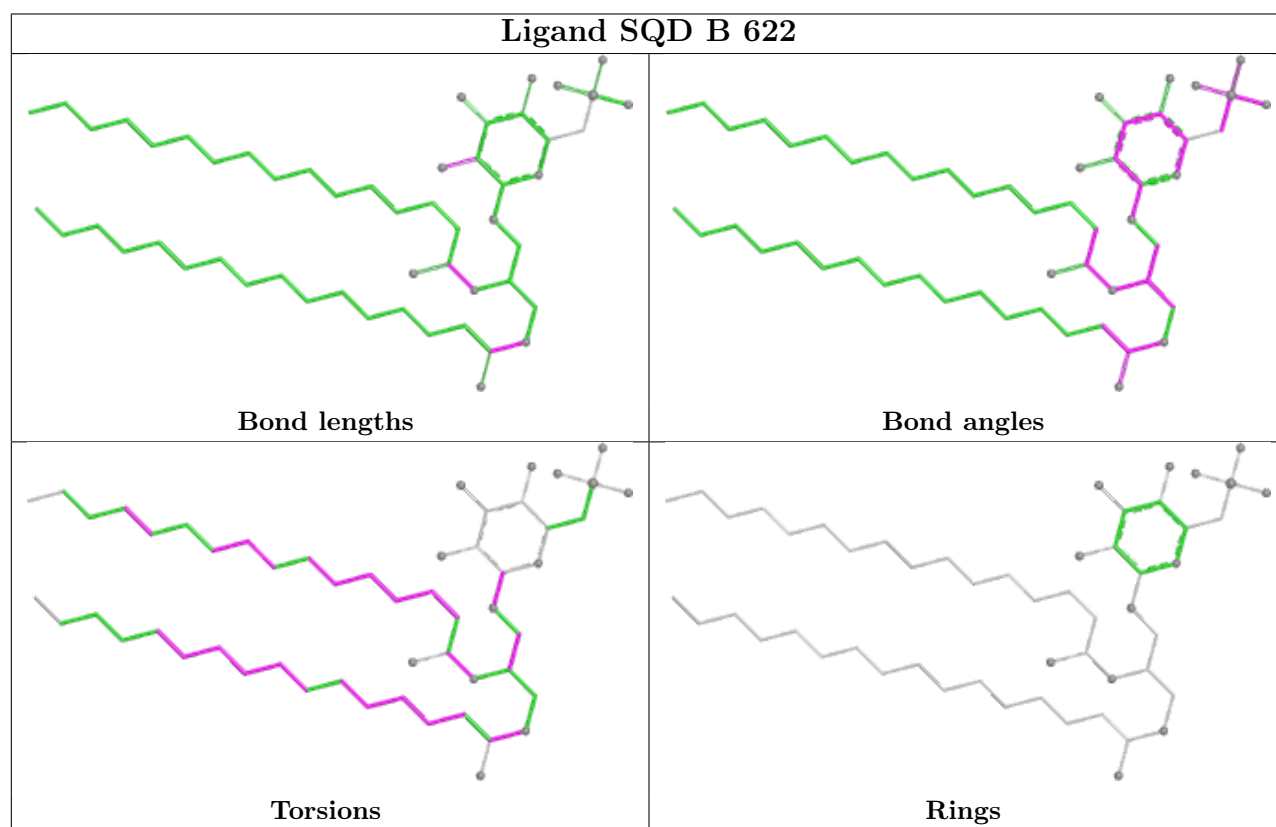
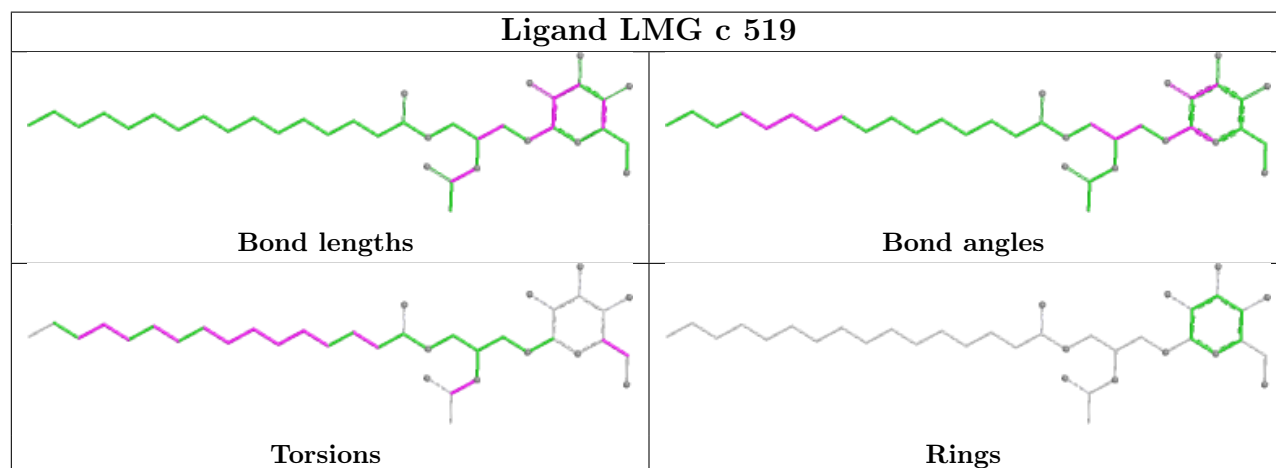
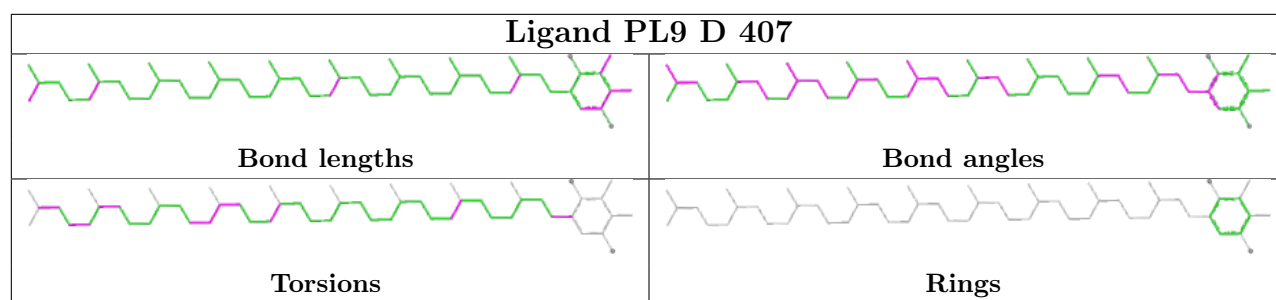


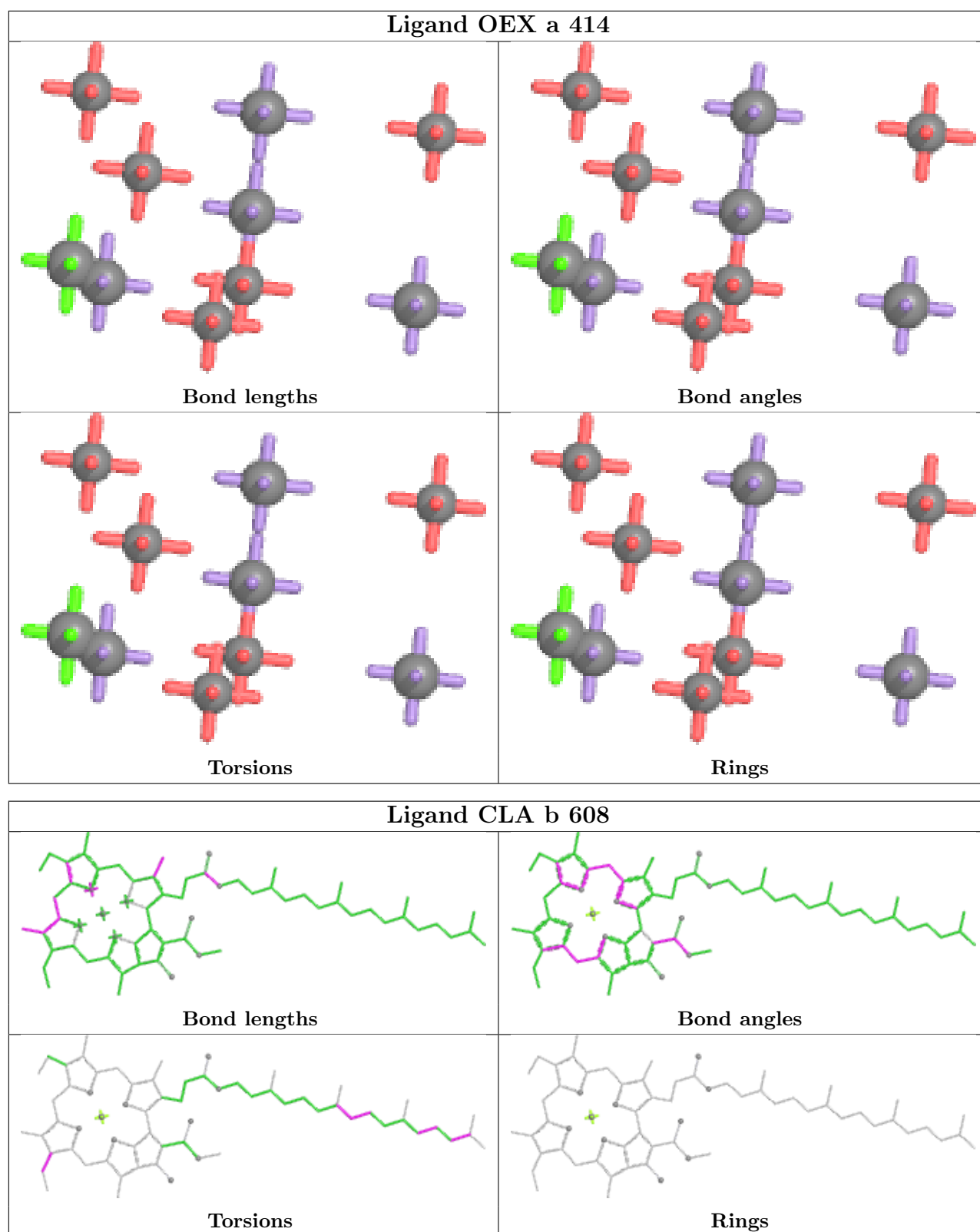
Ligand BCR B 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

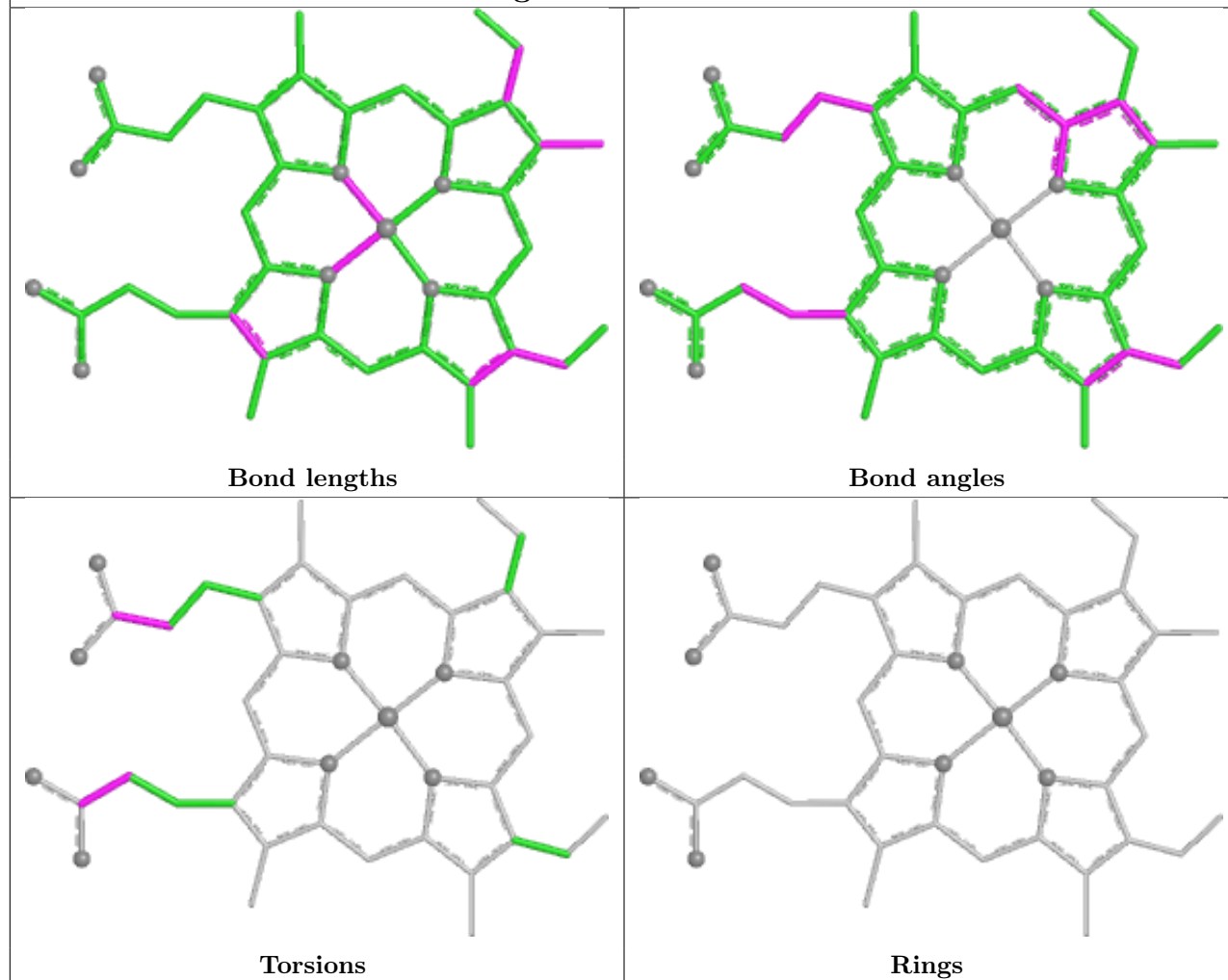
Ligand STE t 103	
	
Bond lengths	Bond angles
	
Torsions	Rings



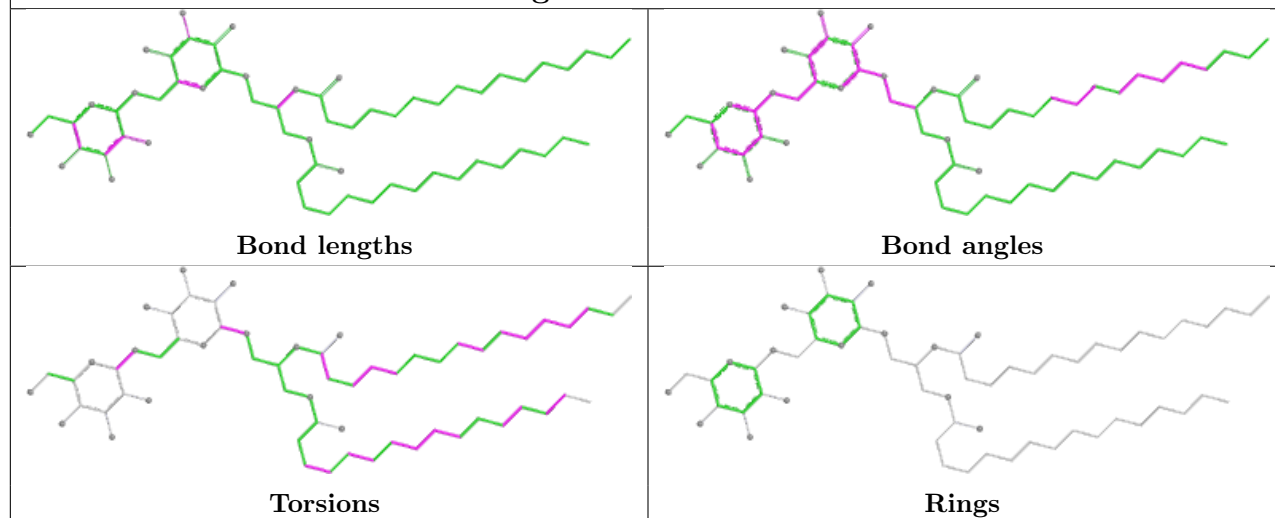


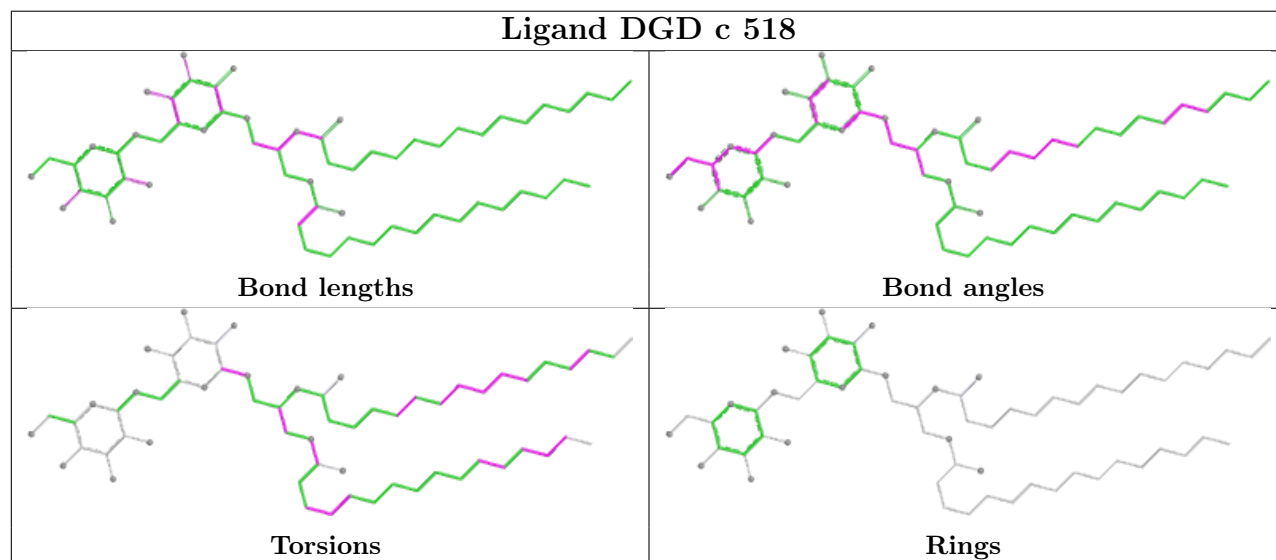
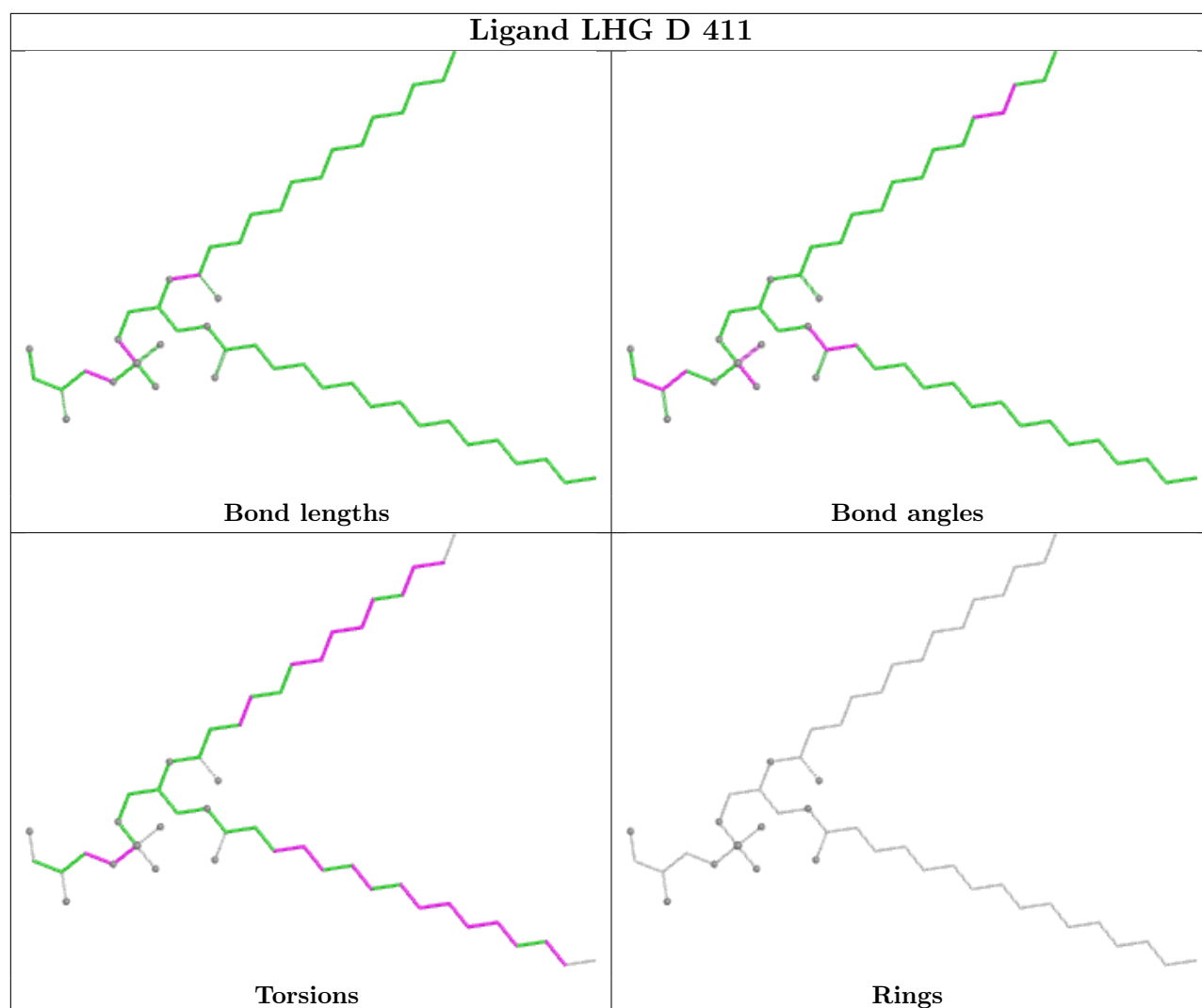


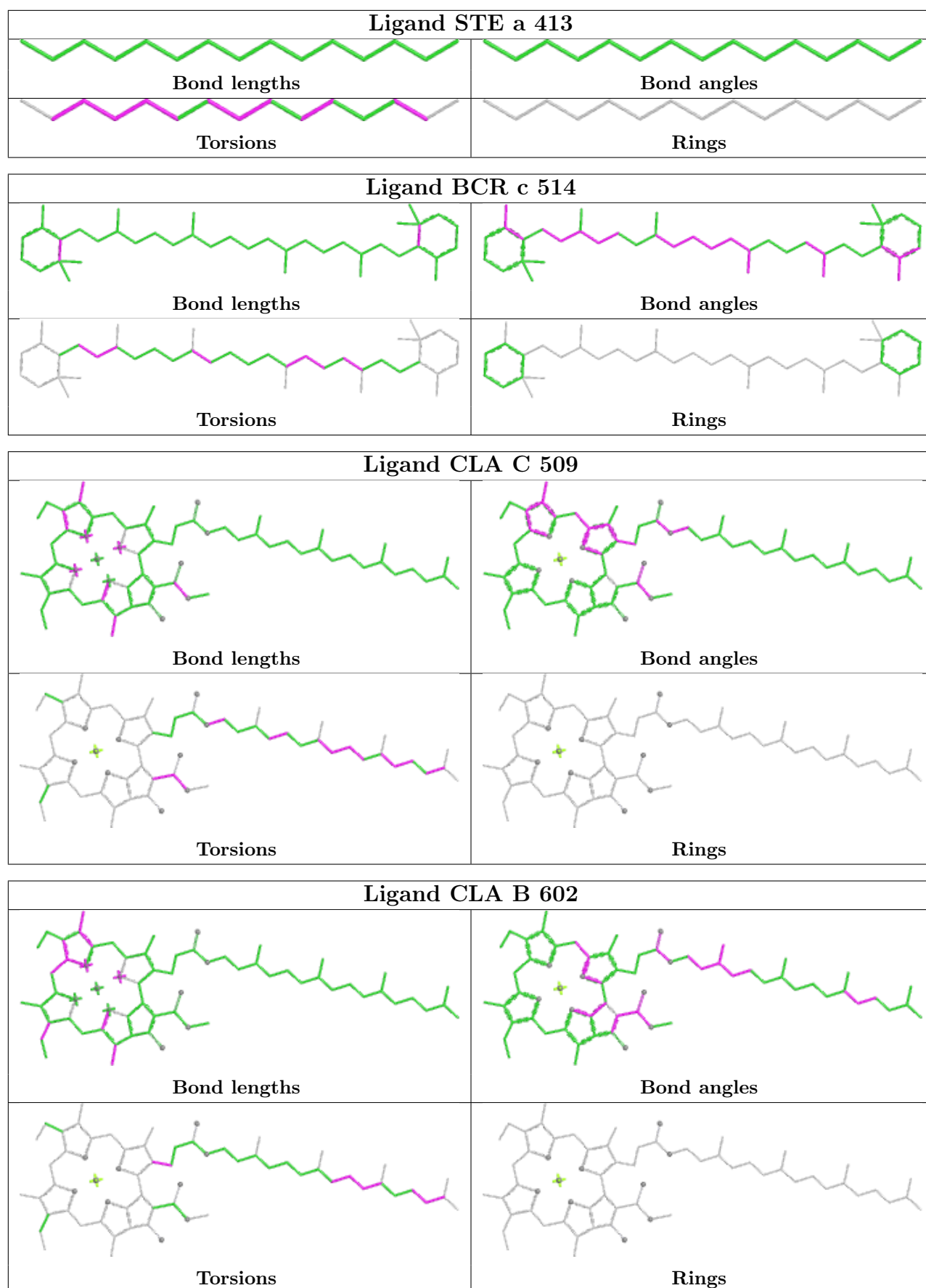
Ligand HEM f 101



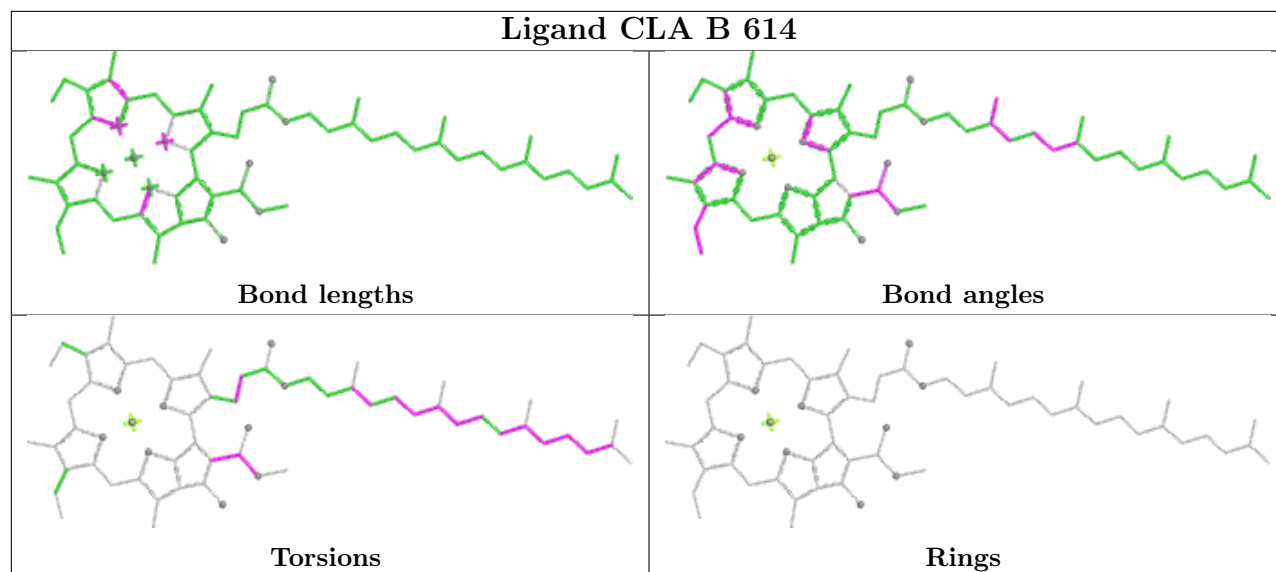
Ligand DGD c 517



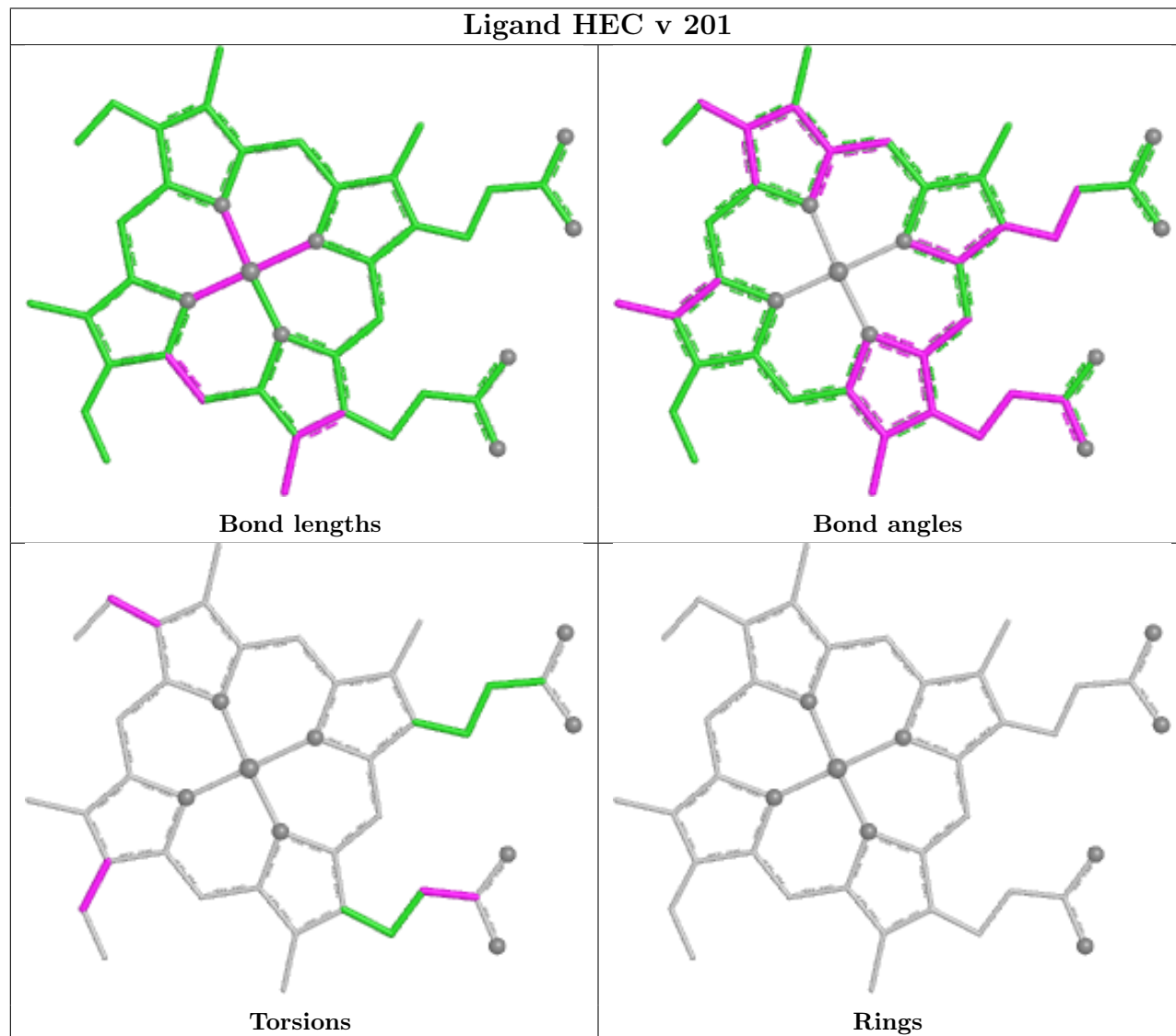


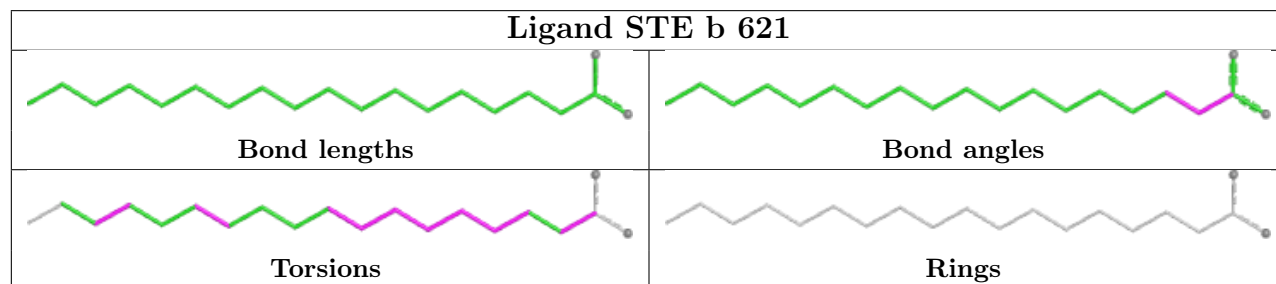
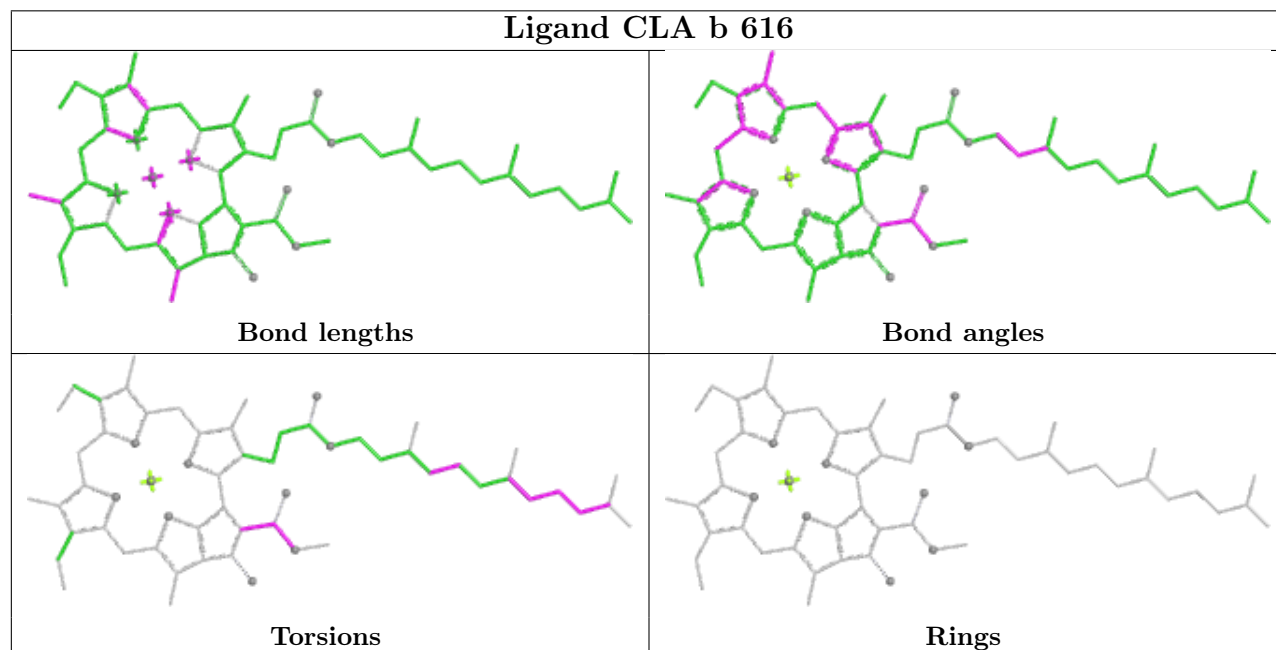
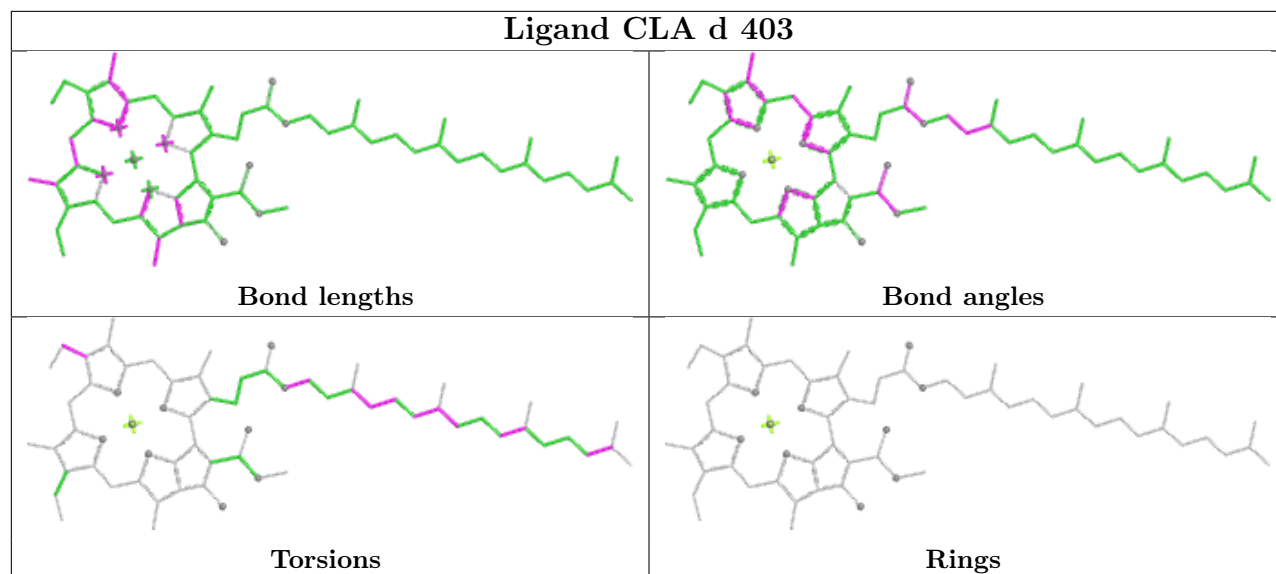


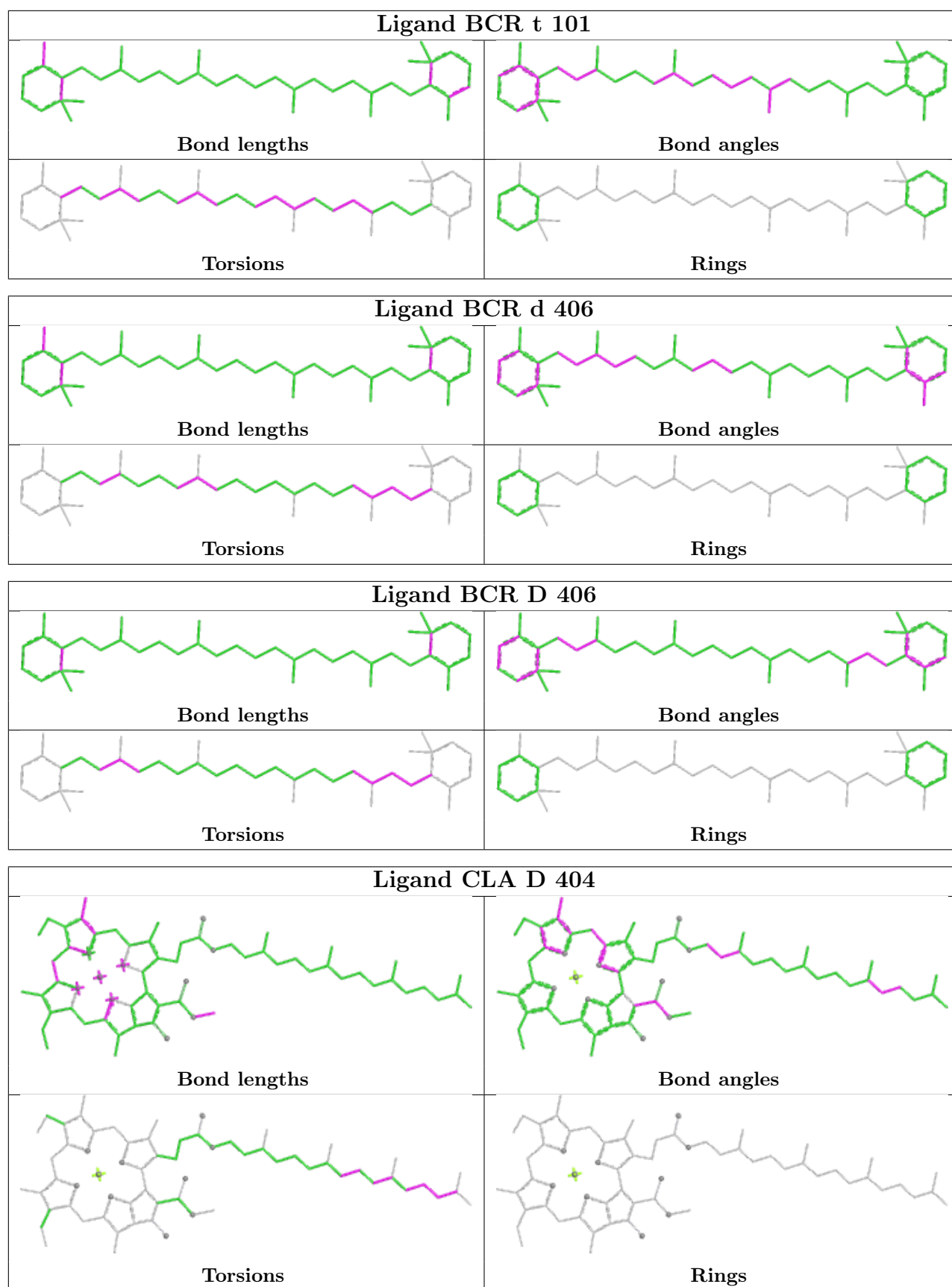
Ligand CLA B 614

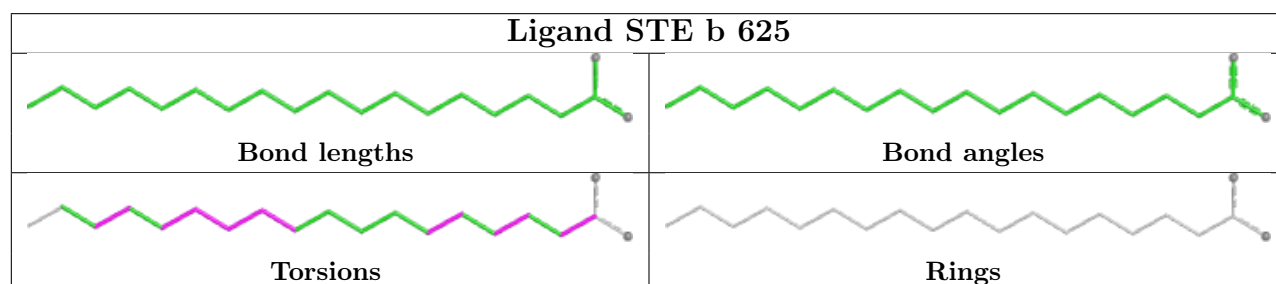
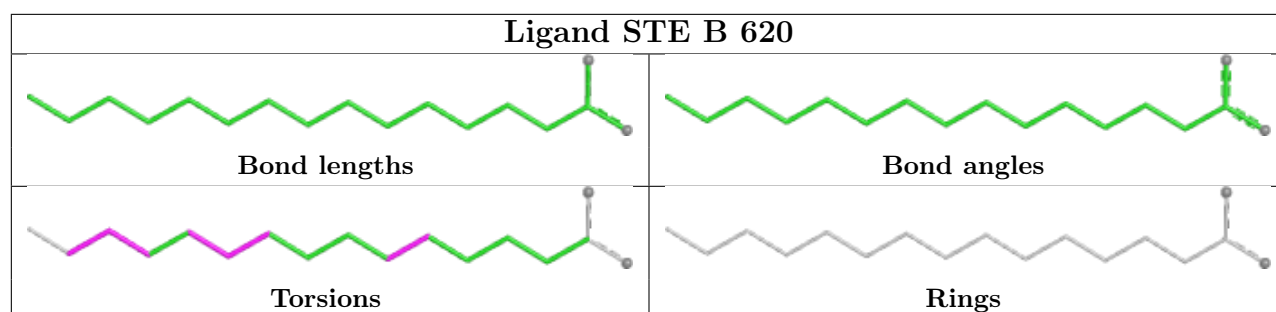
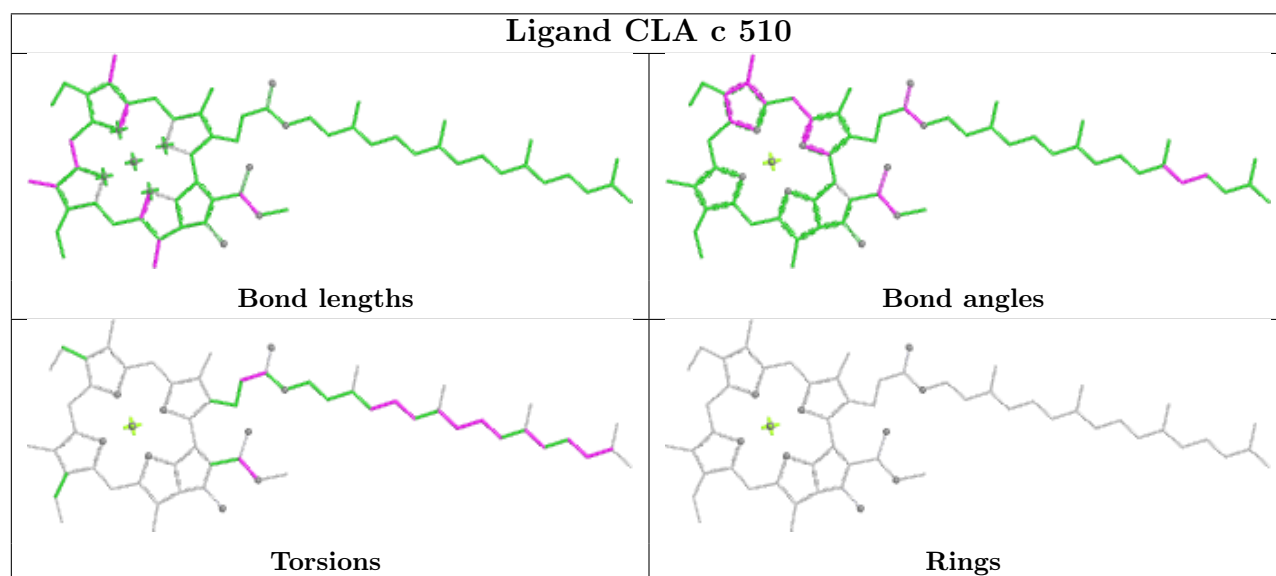
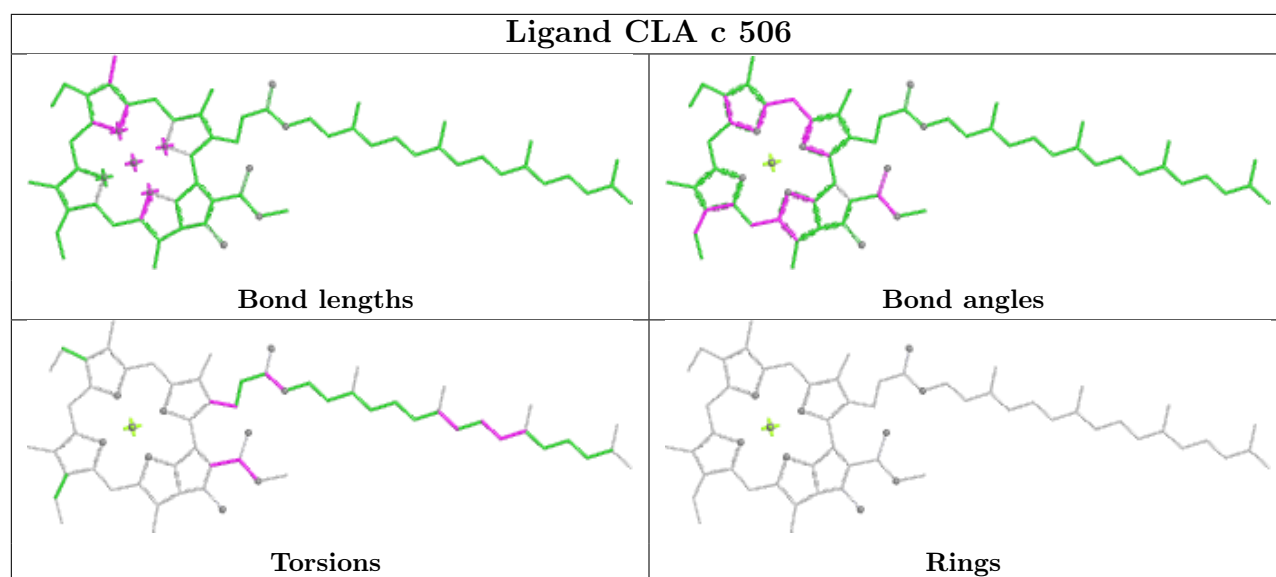


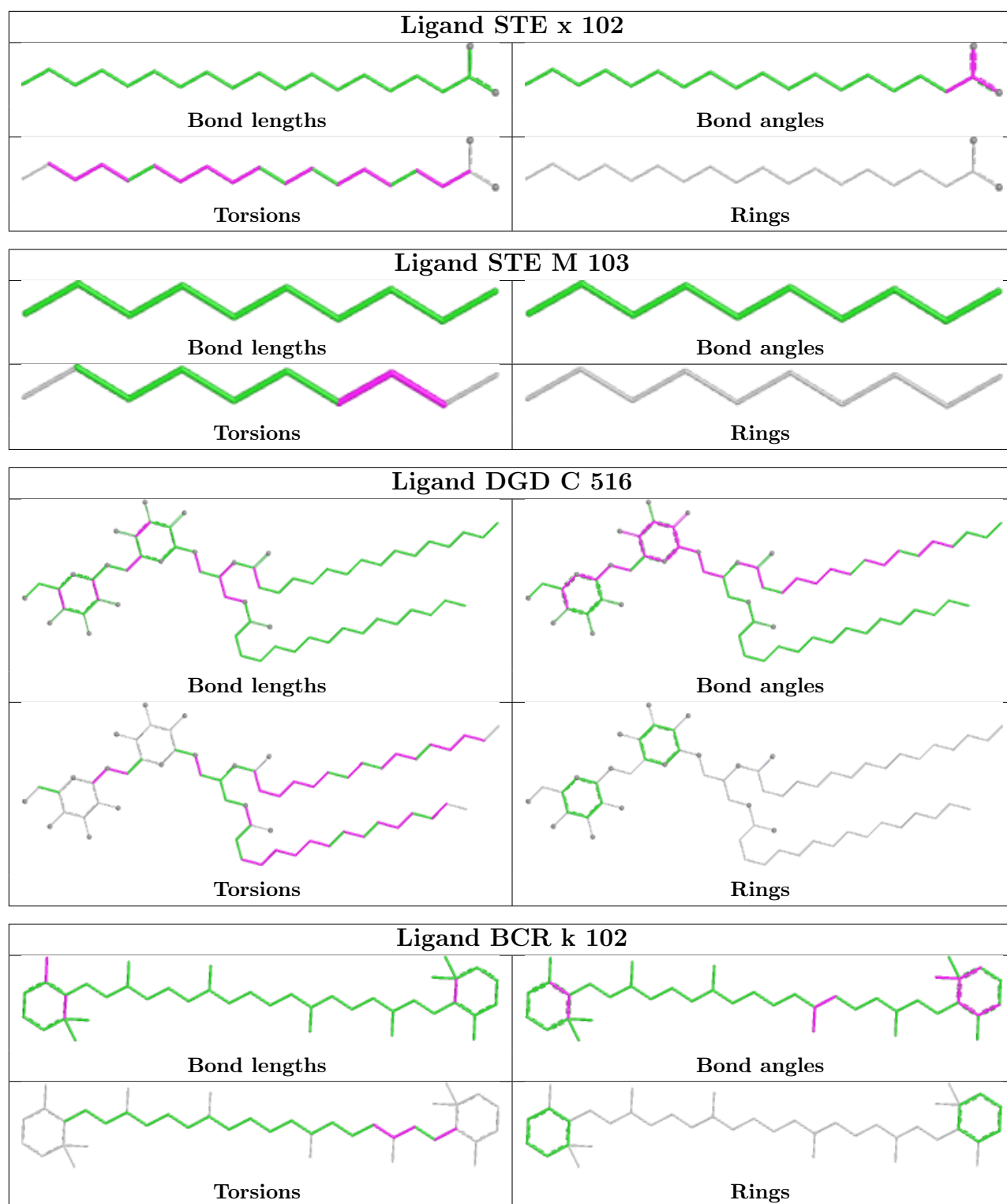
Ligand HEC v 201

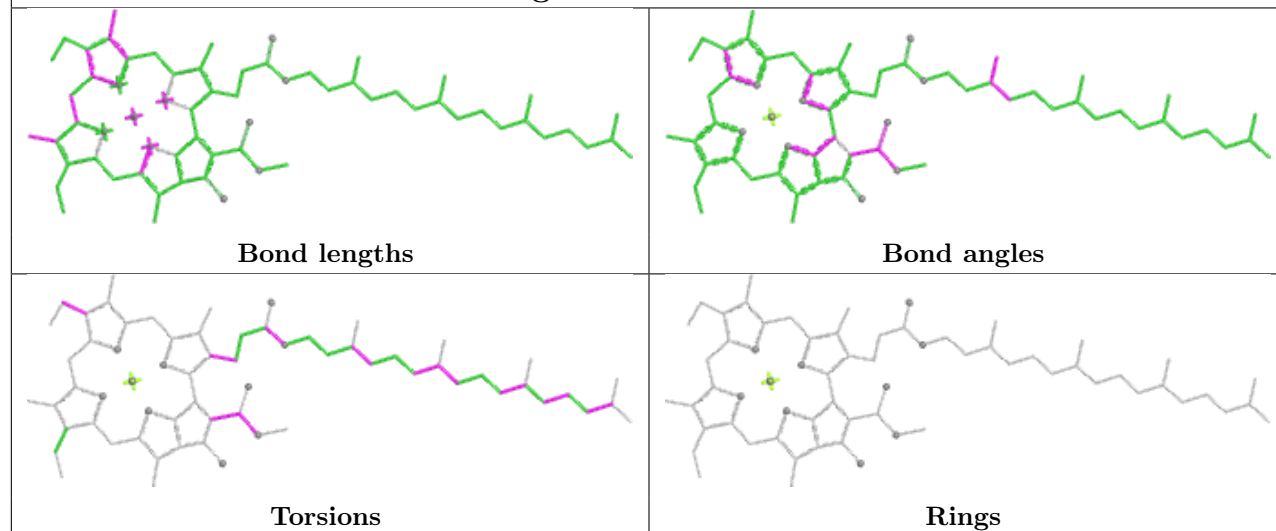
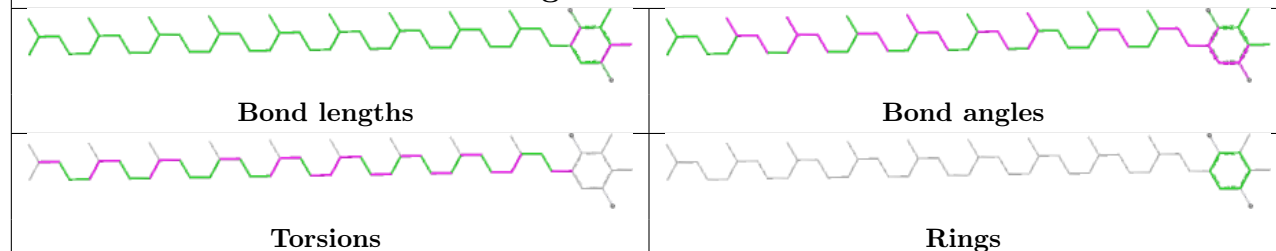
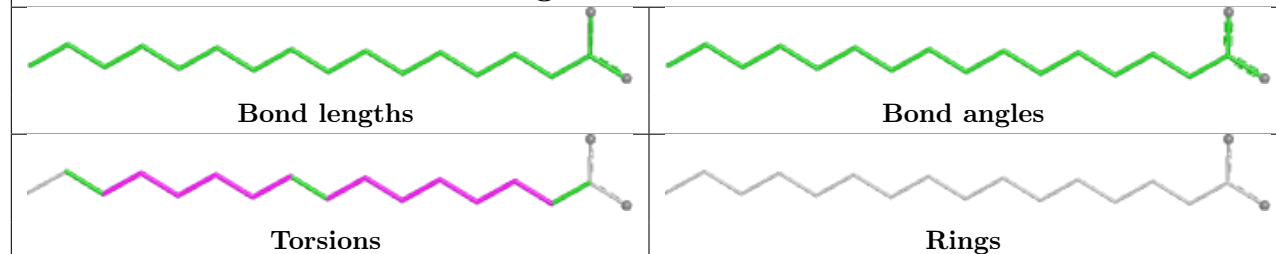


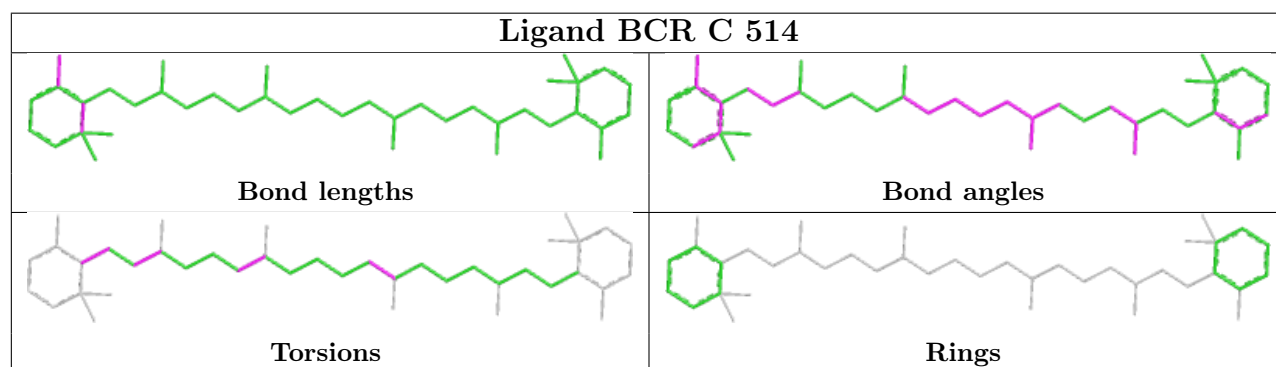
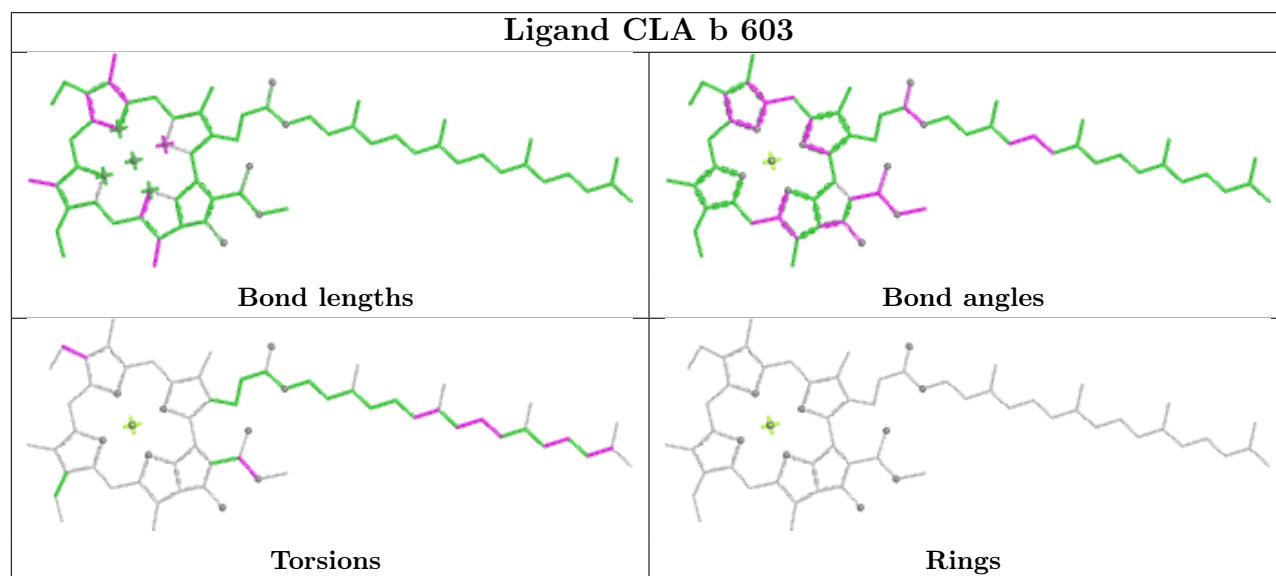
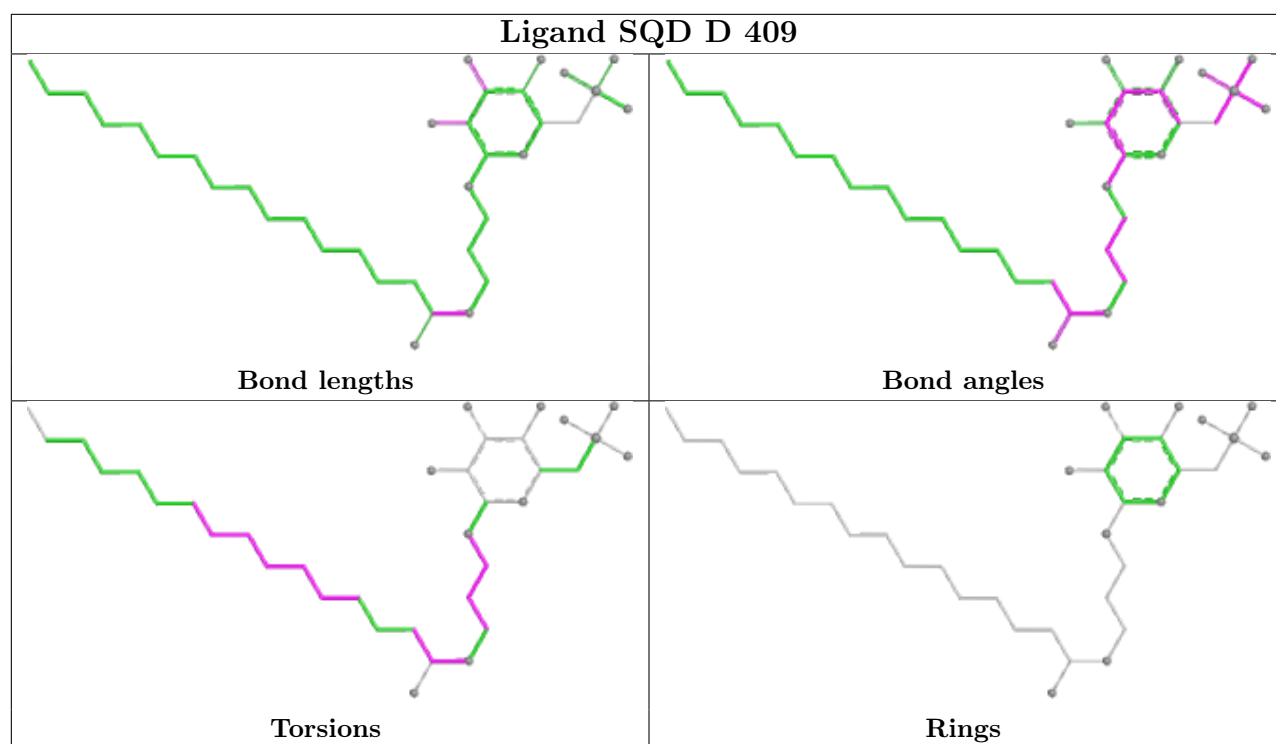


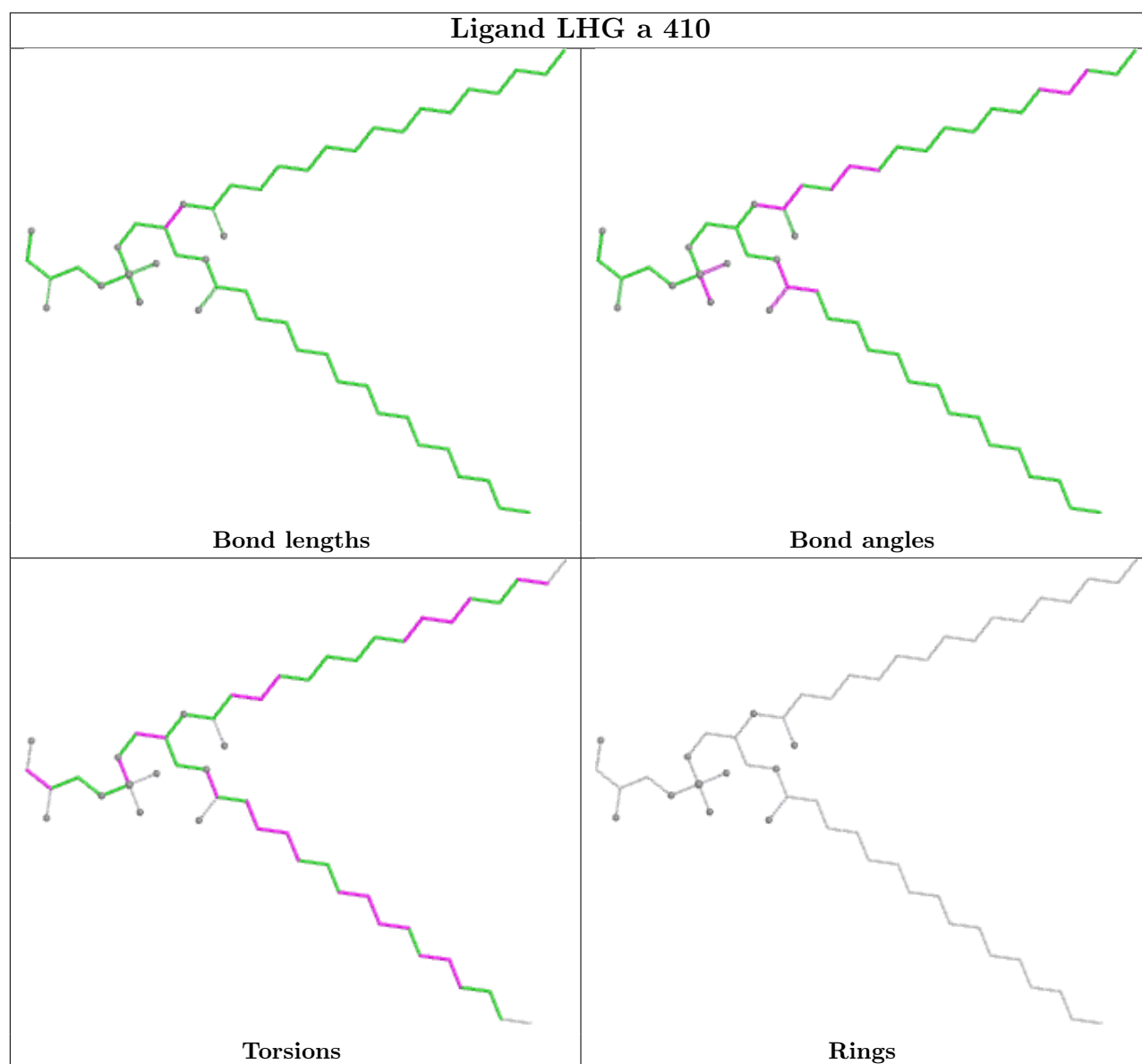


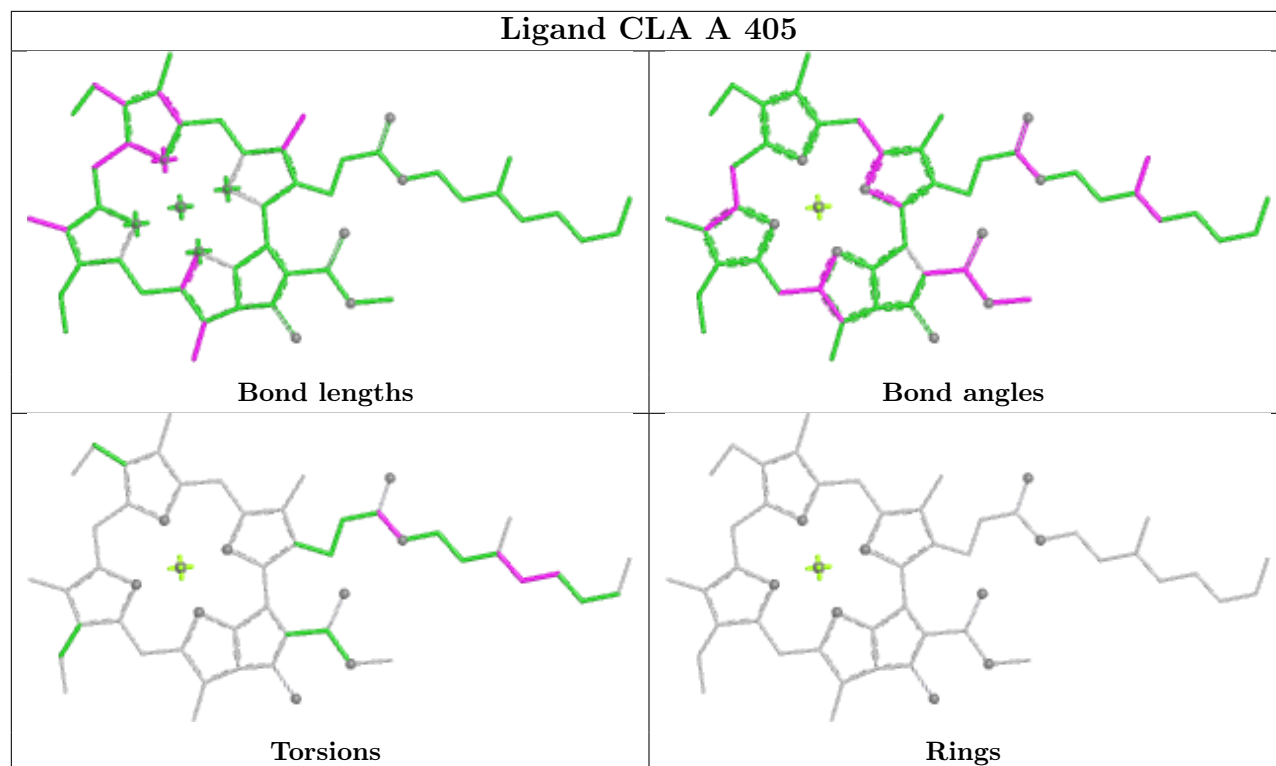


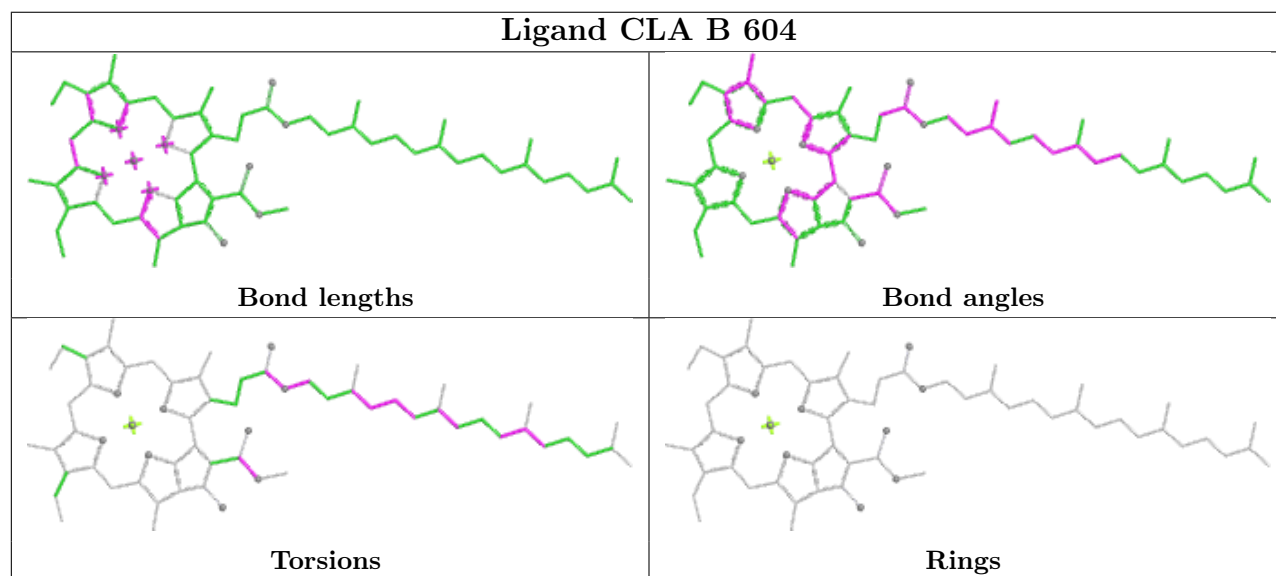
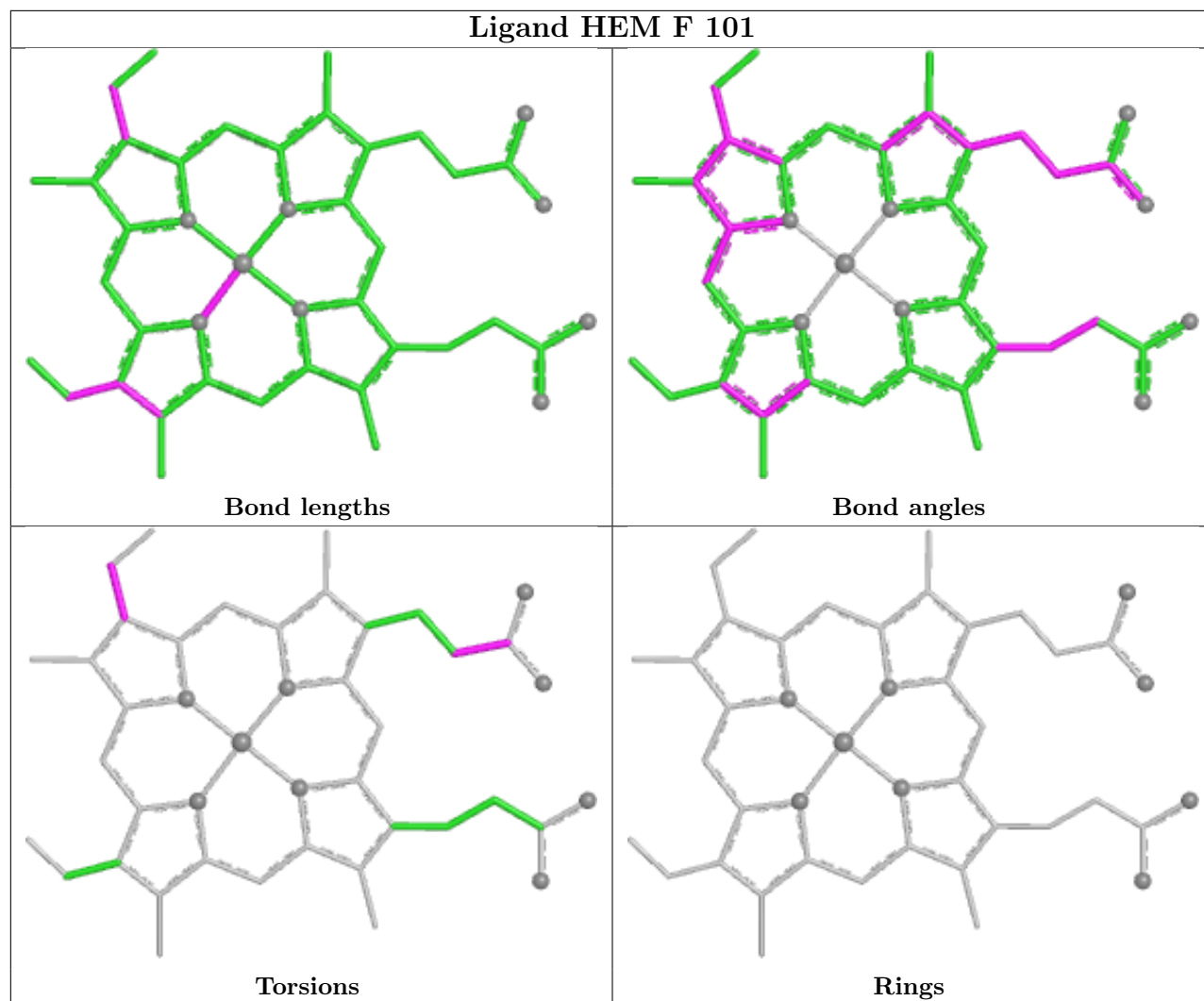


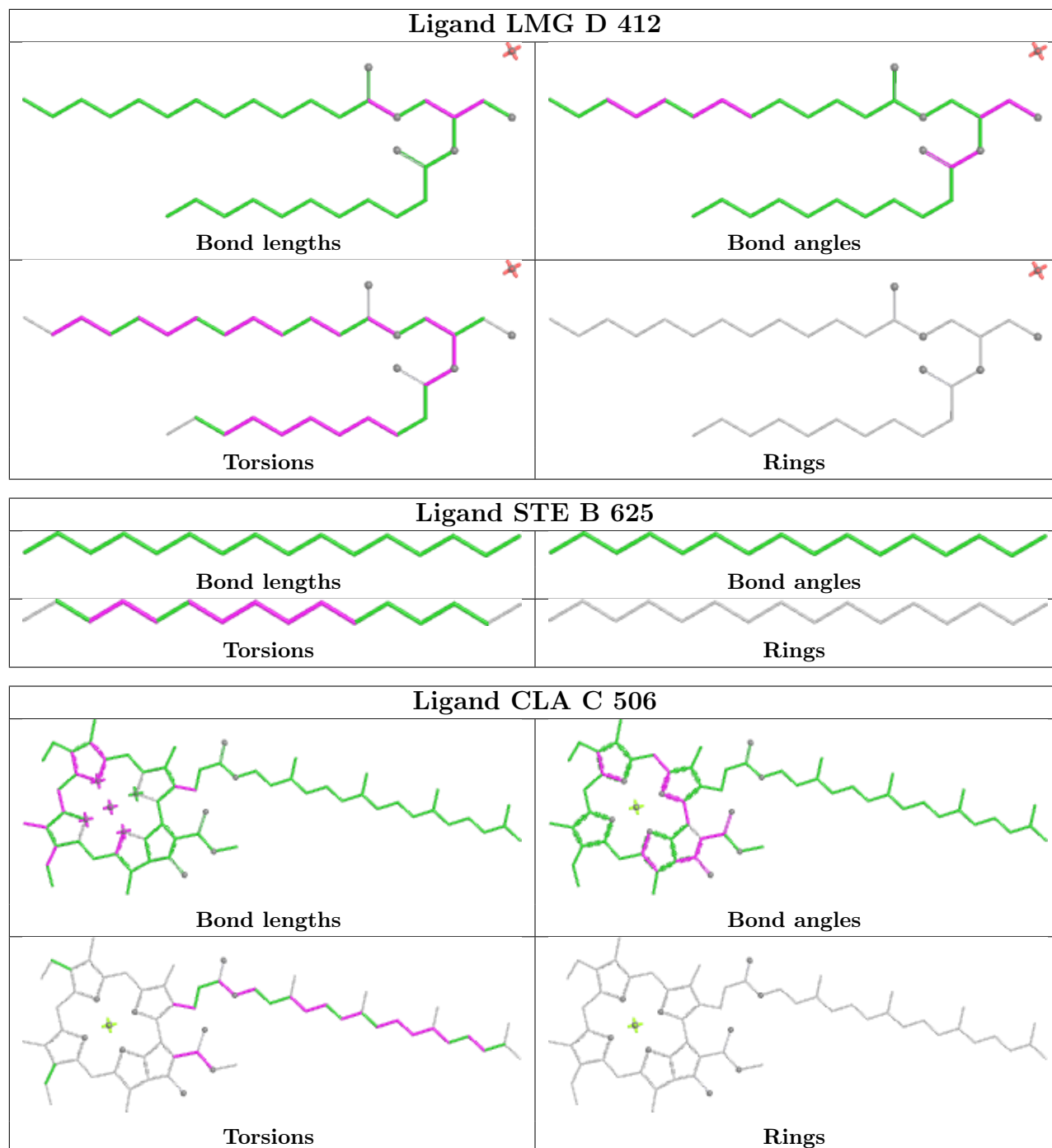
Ligand CLA B 601**Ligand PL9 a 409****Ligand STE B 624**



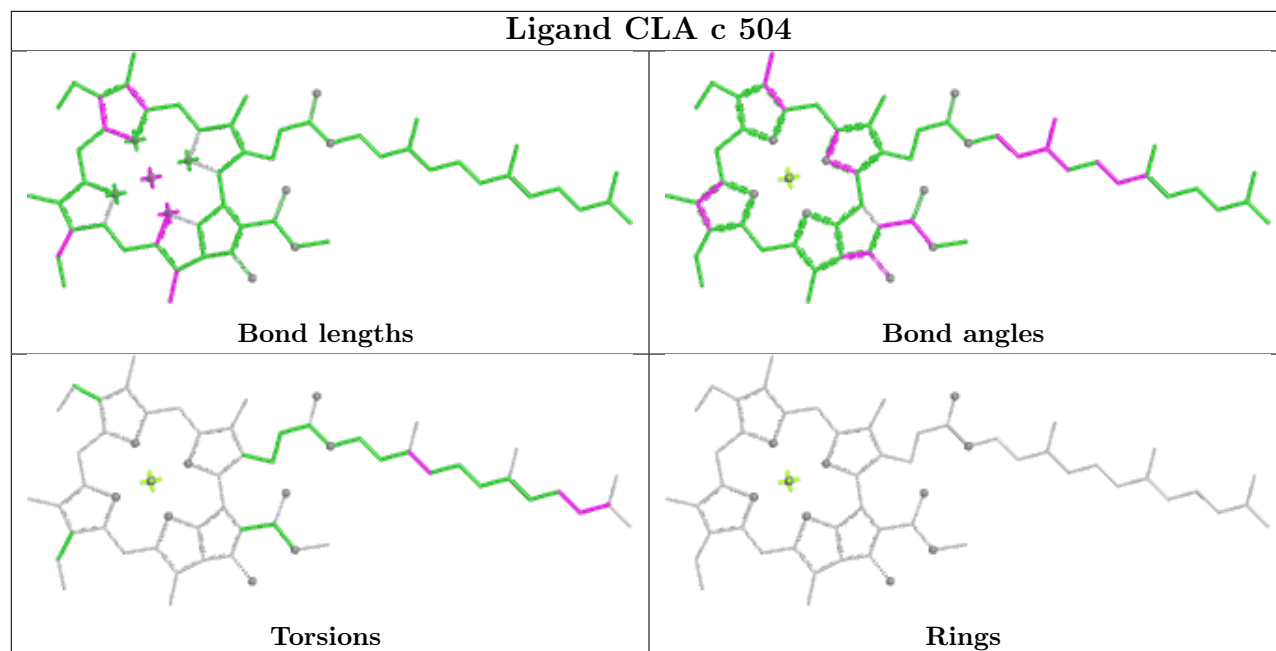




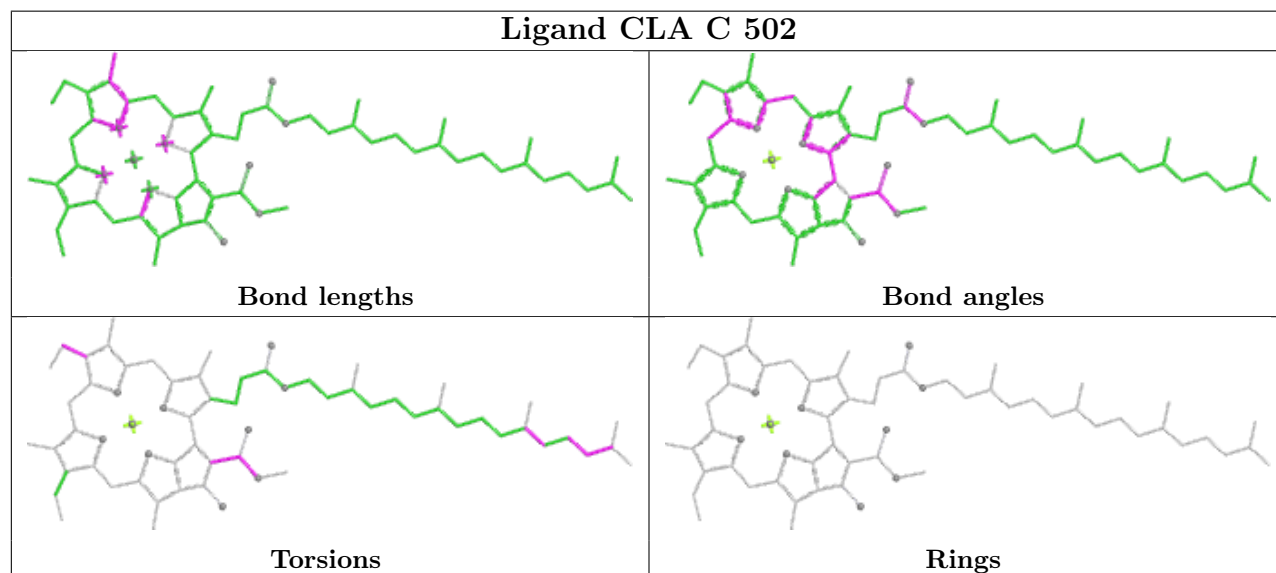


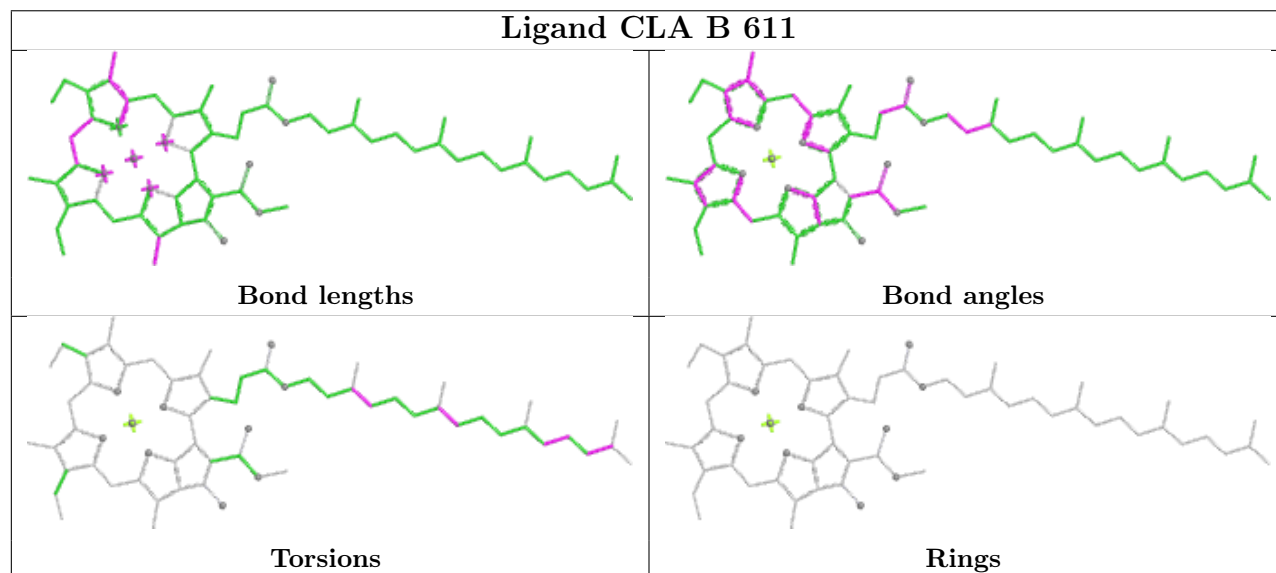
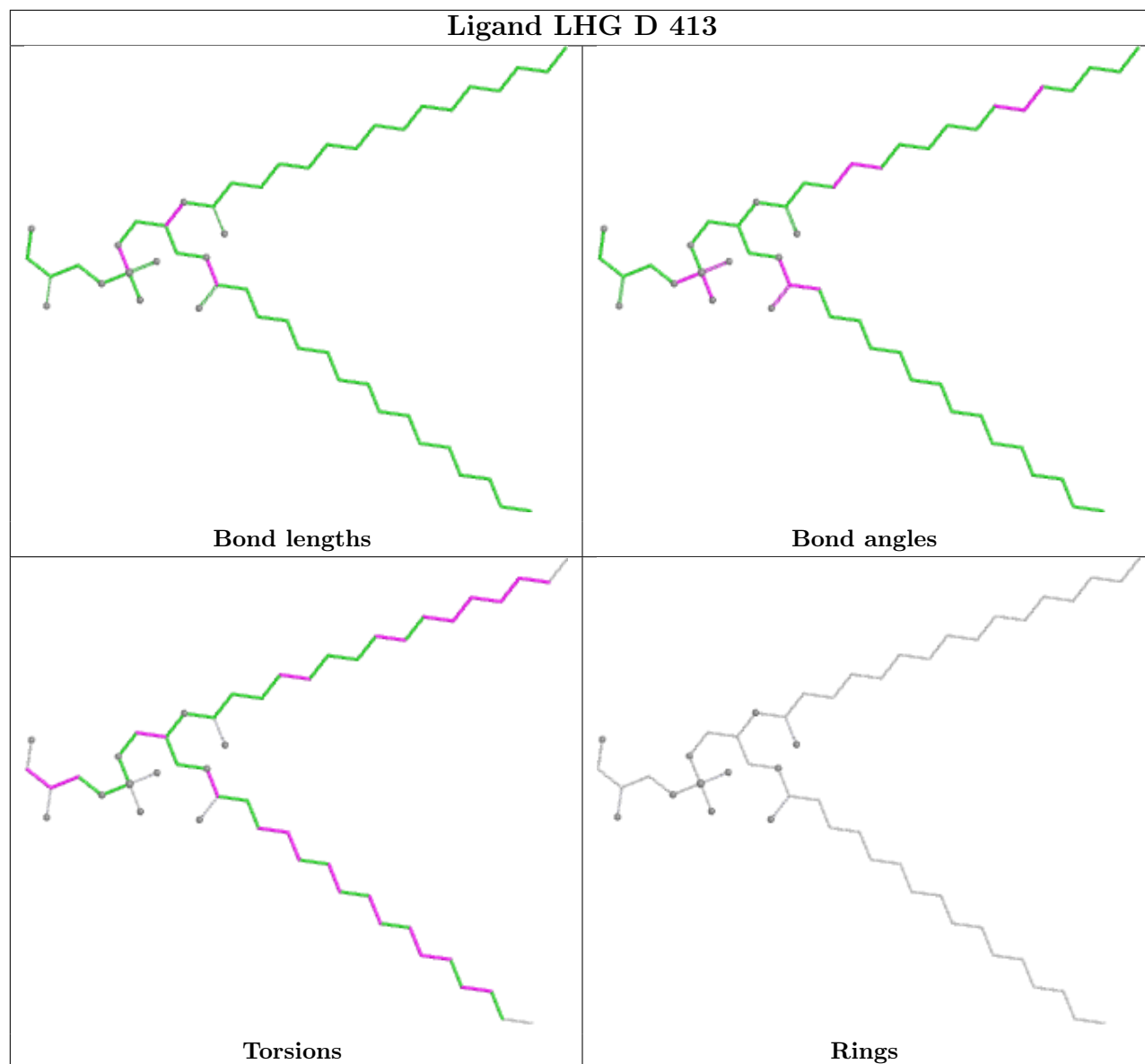


Ligand CLA c 504

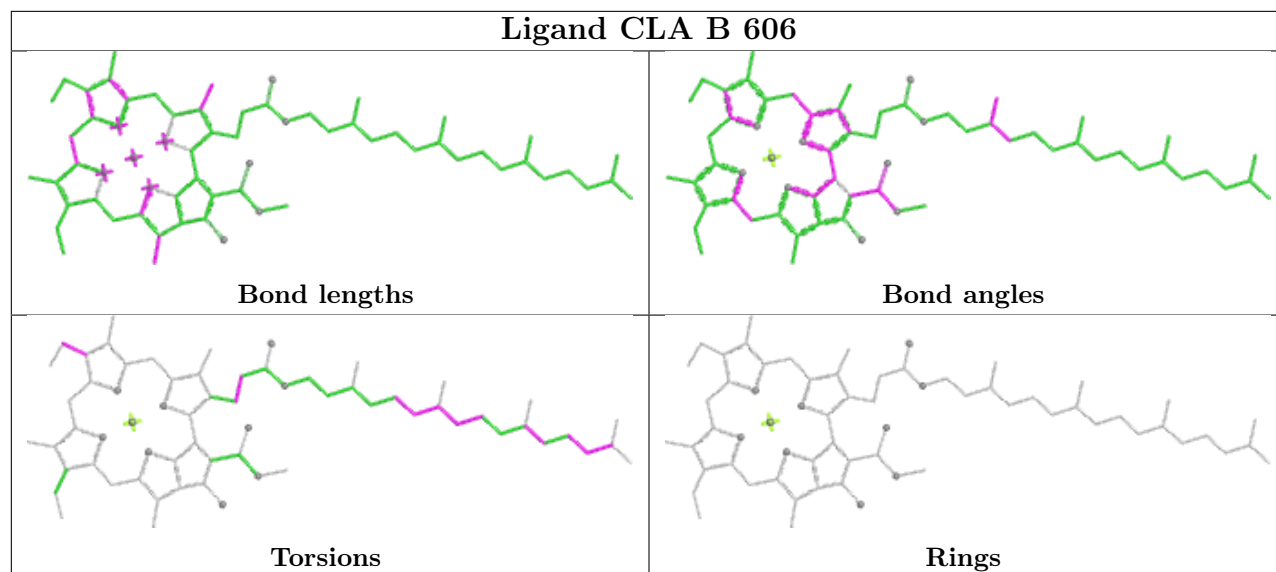


Ligand CLA C 502

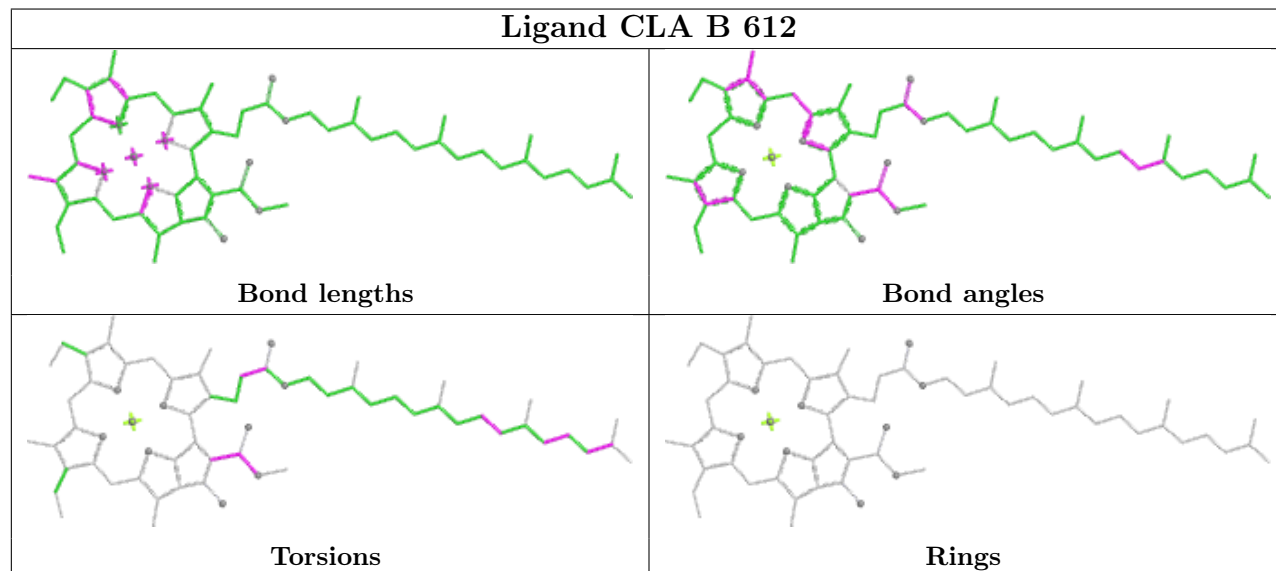




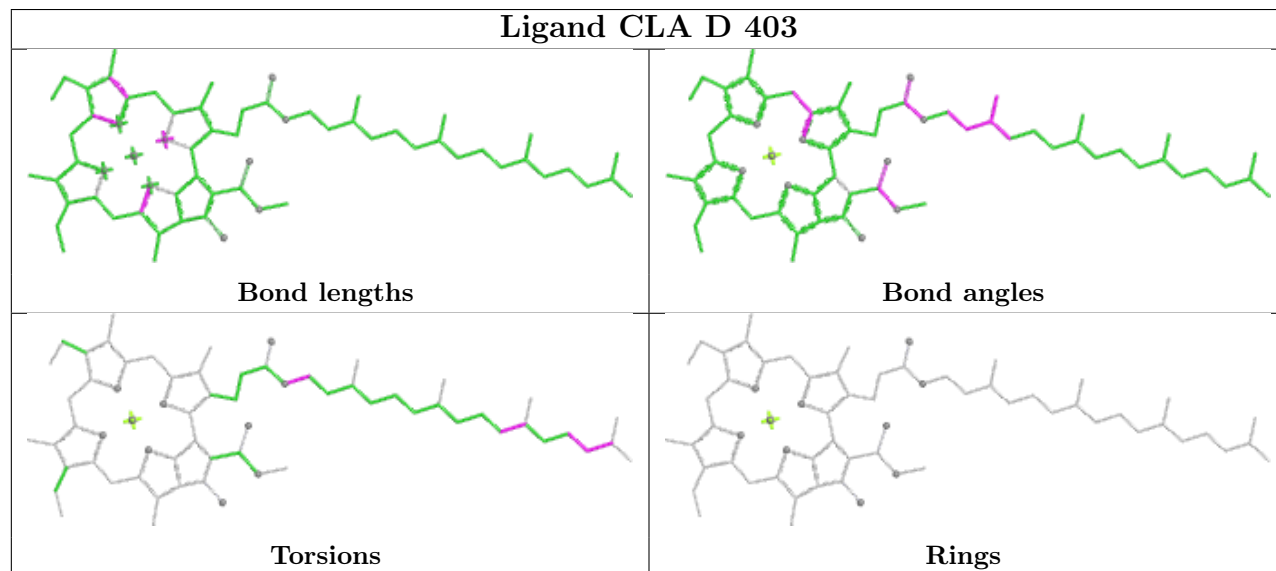
Ligand CLA B 606

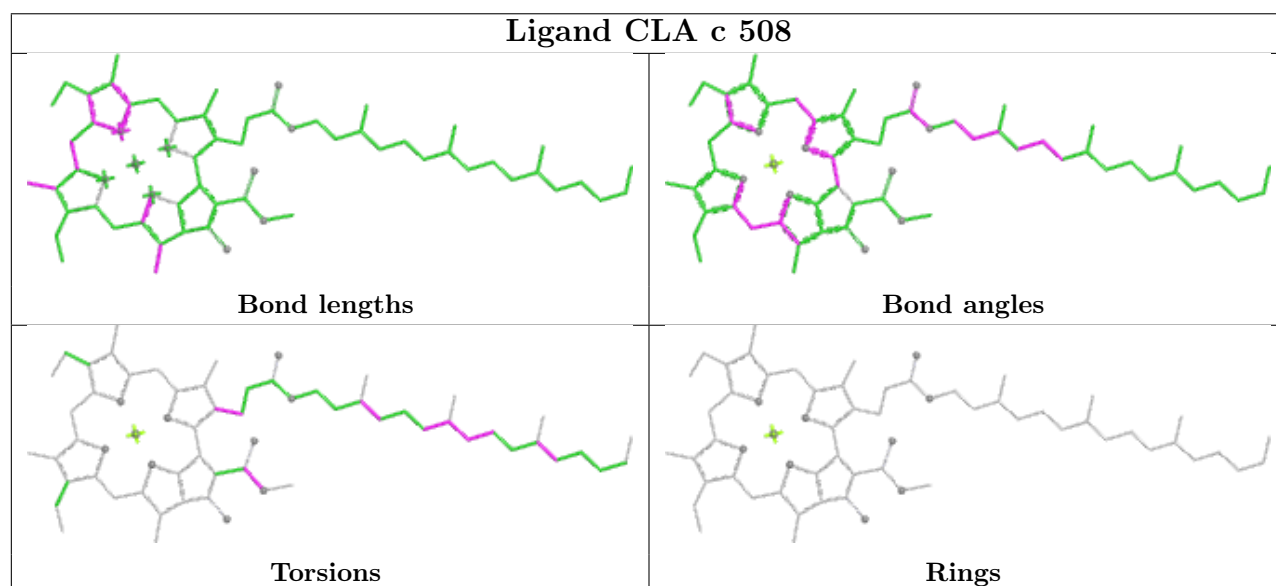
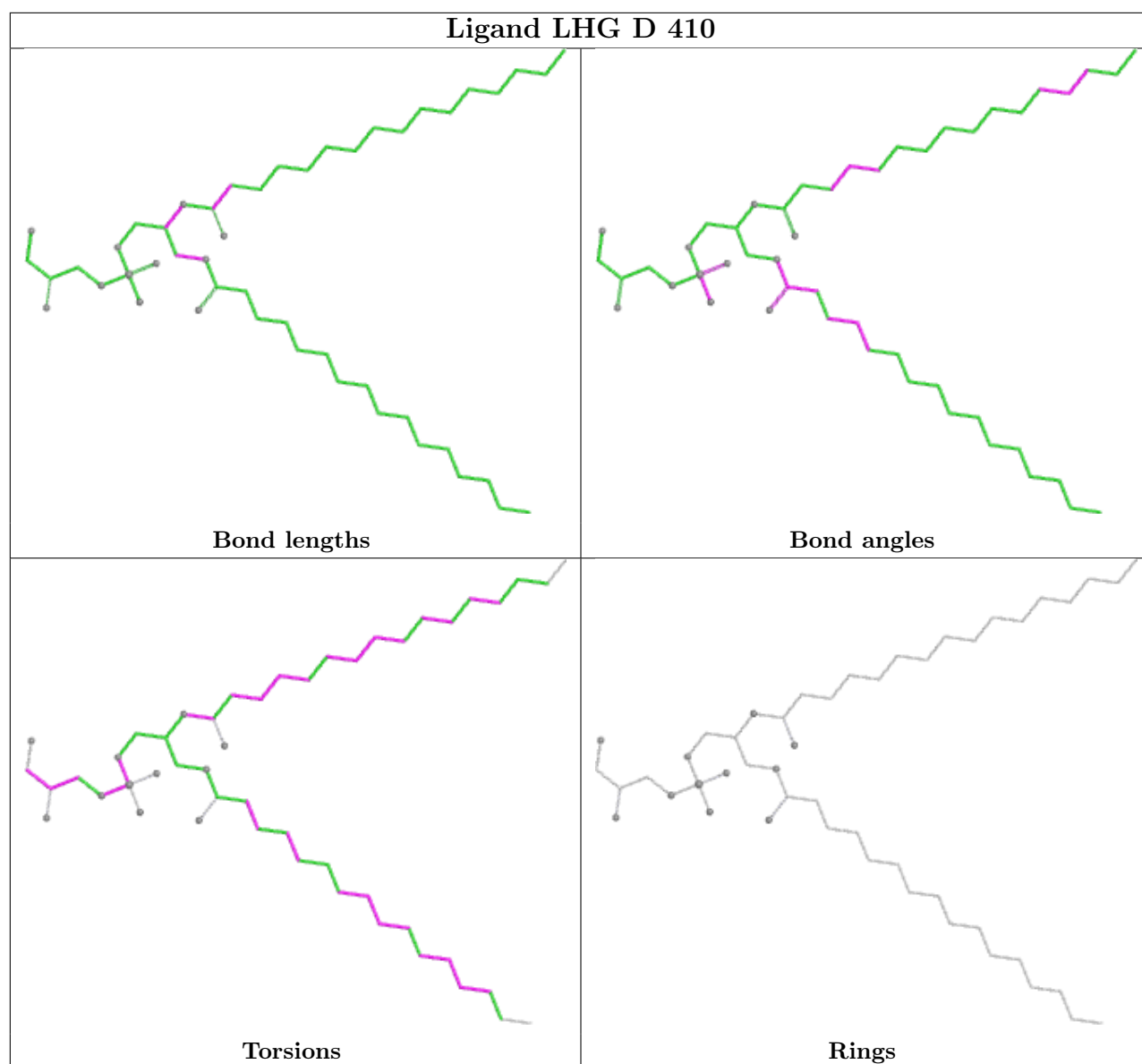


Ligand CLA B 612

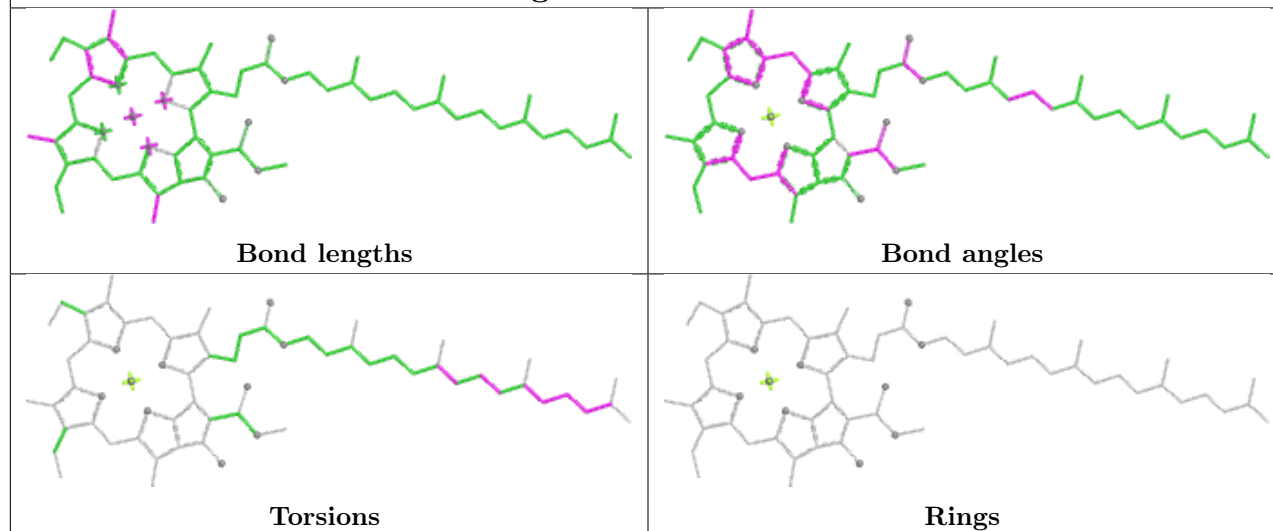


Ligand CLA D 403

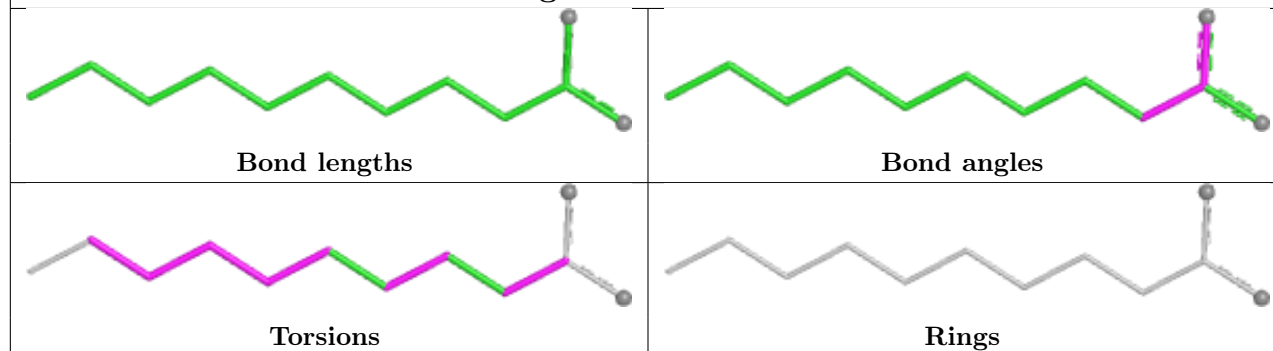




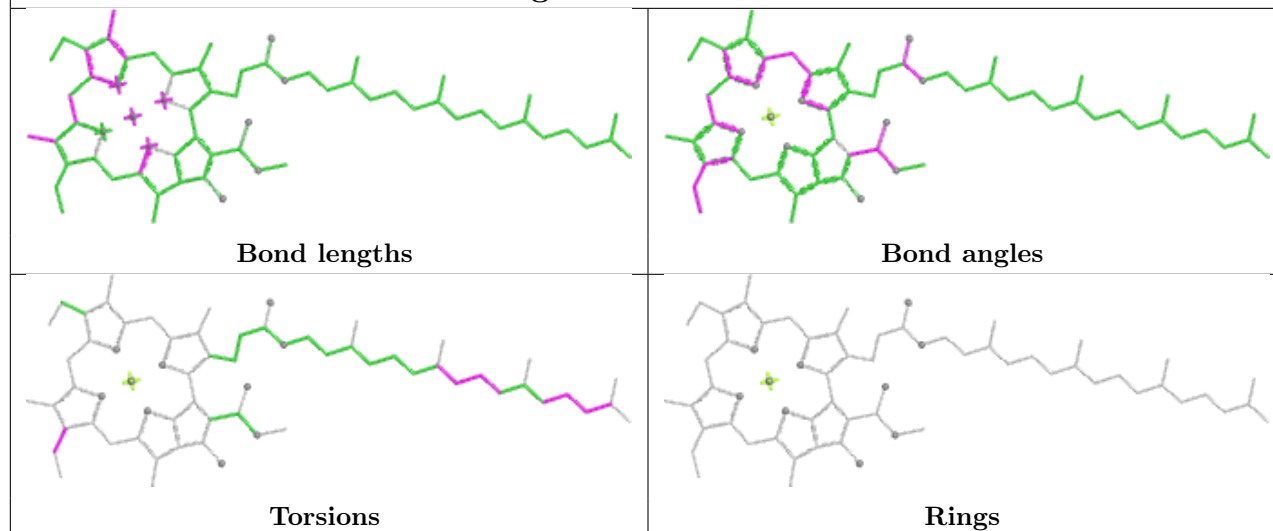
Ligand CLA C 508

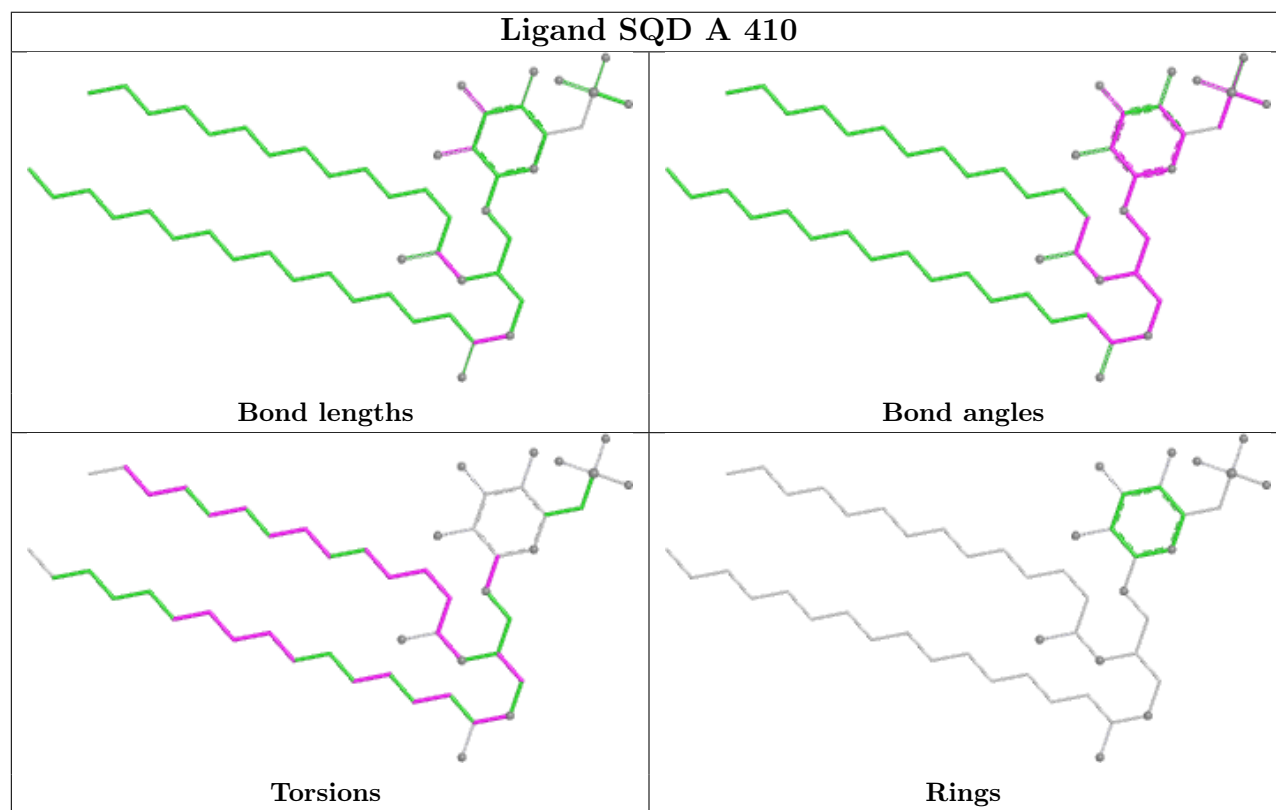
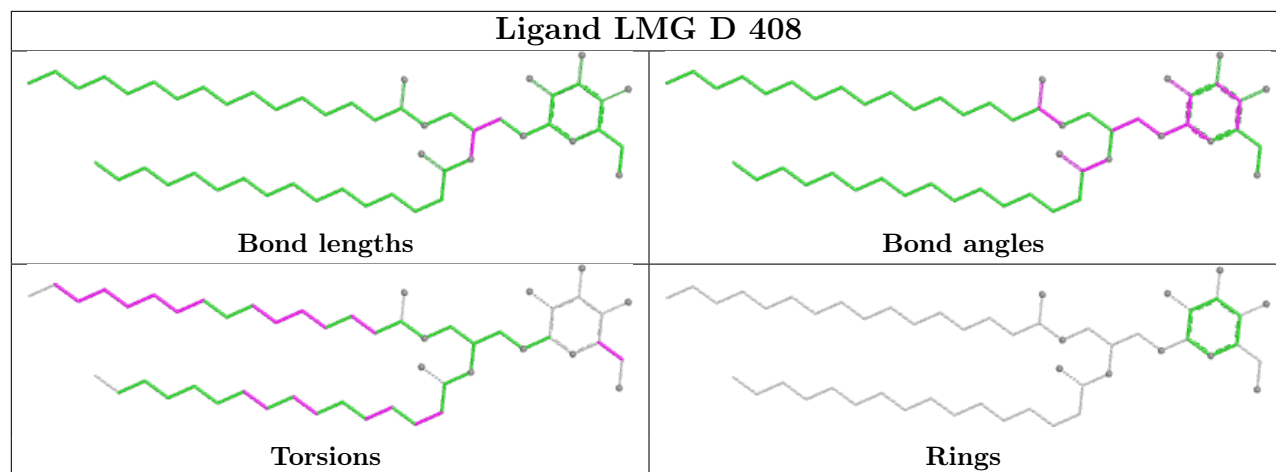


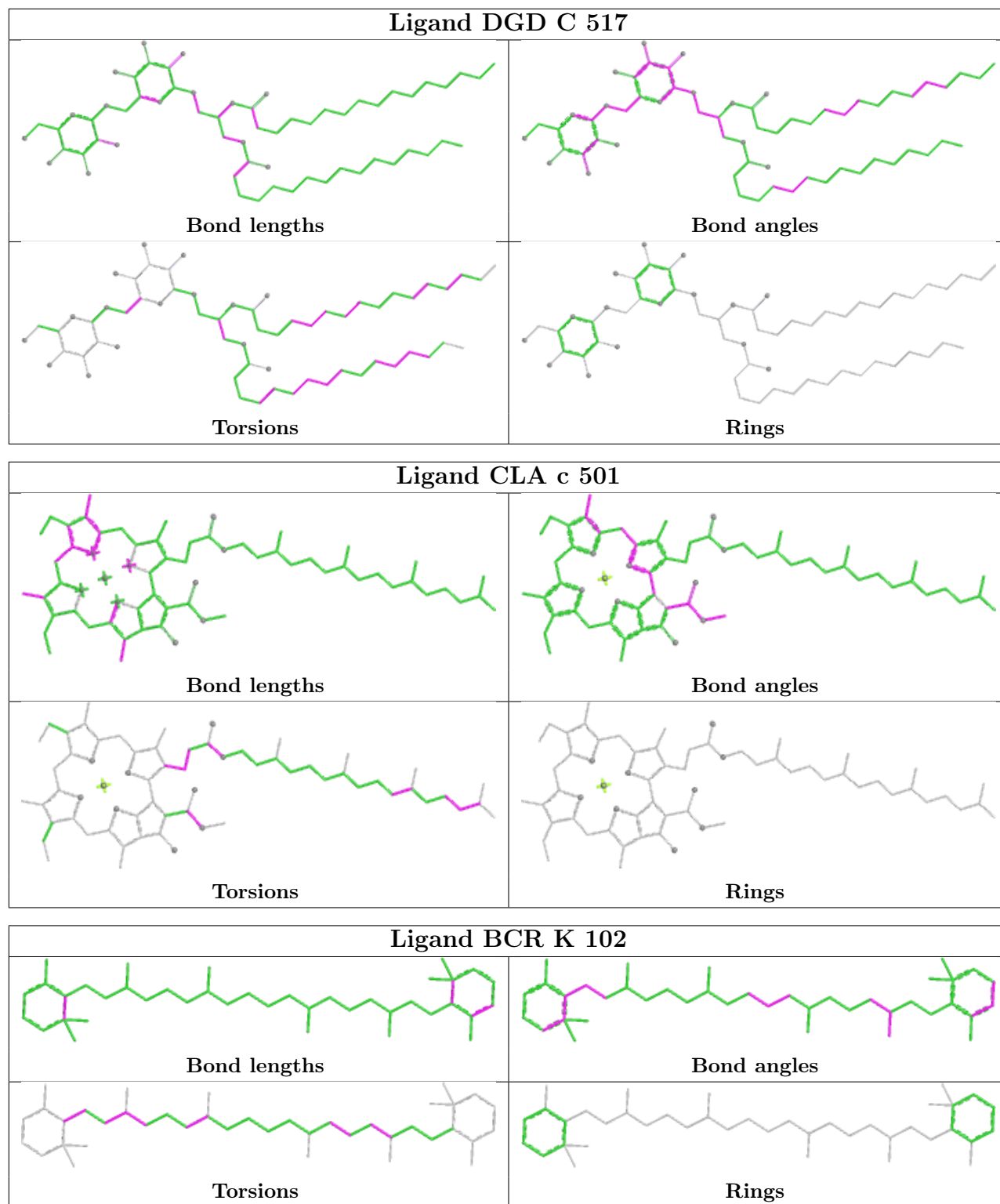
Ligand STE c 523

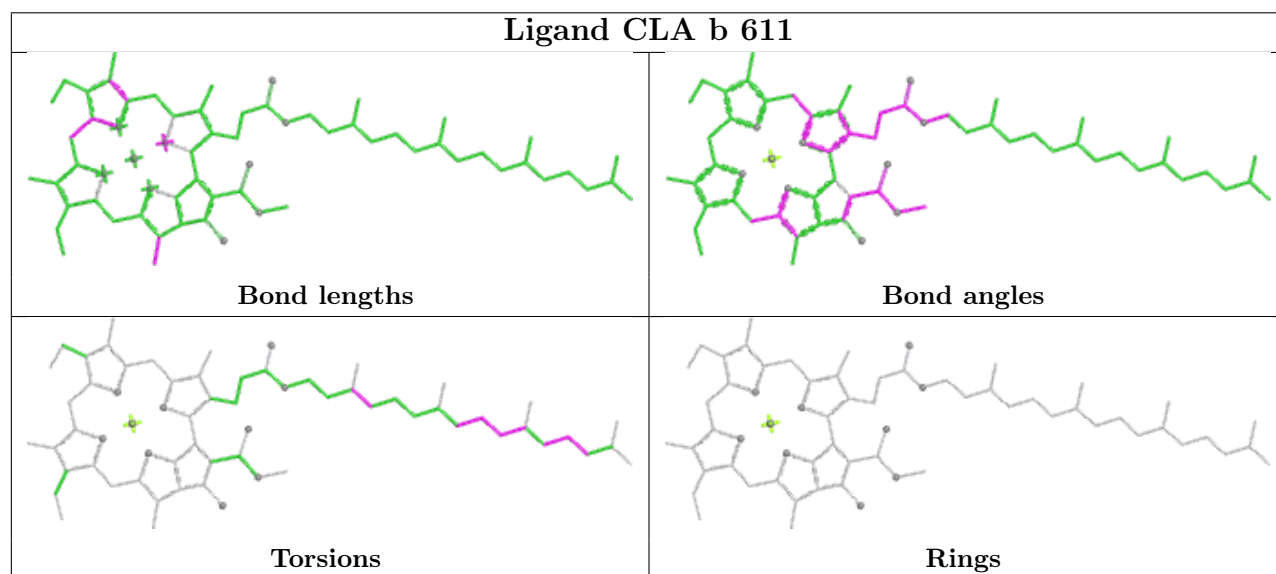
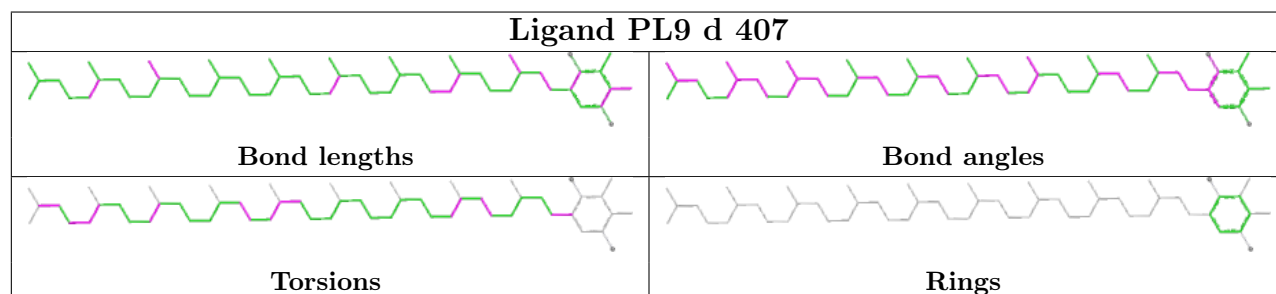
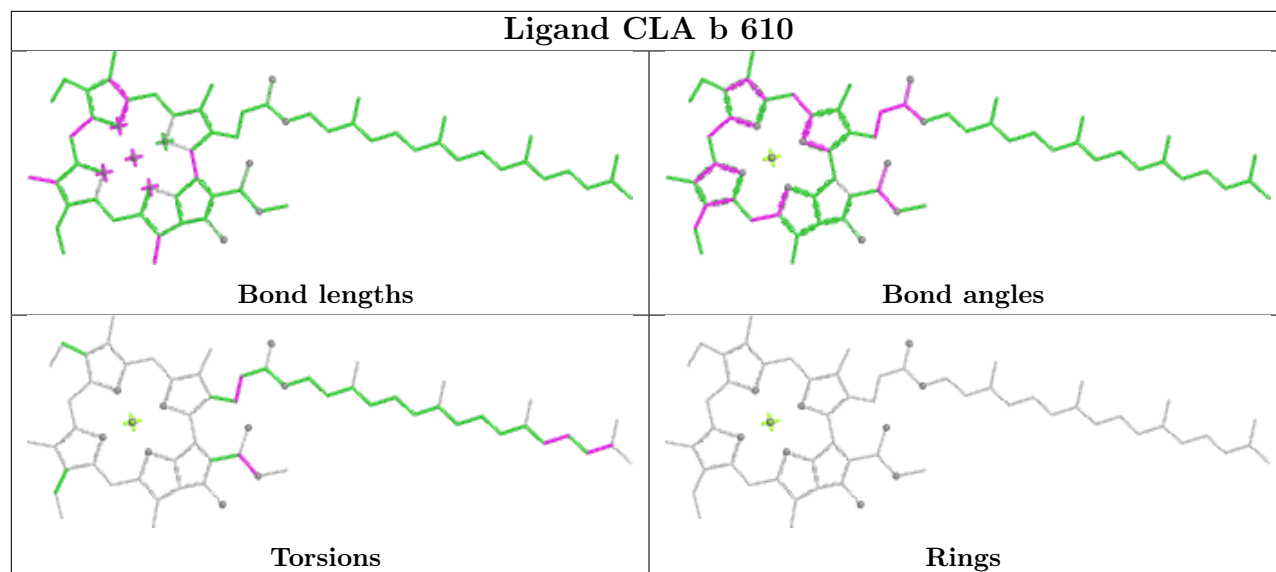


Ligand CLA C 513

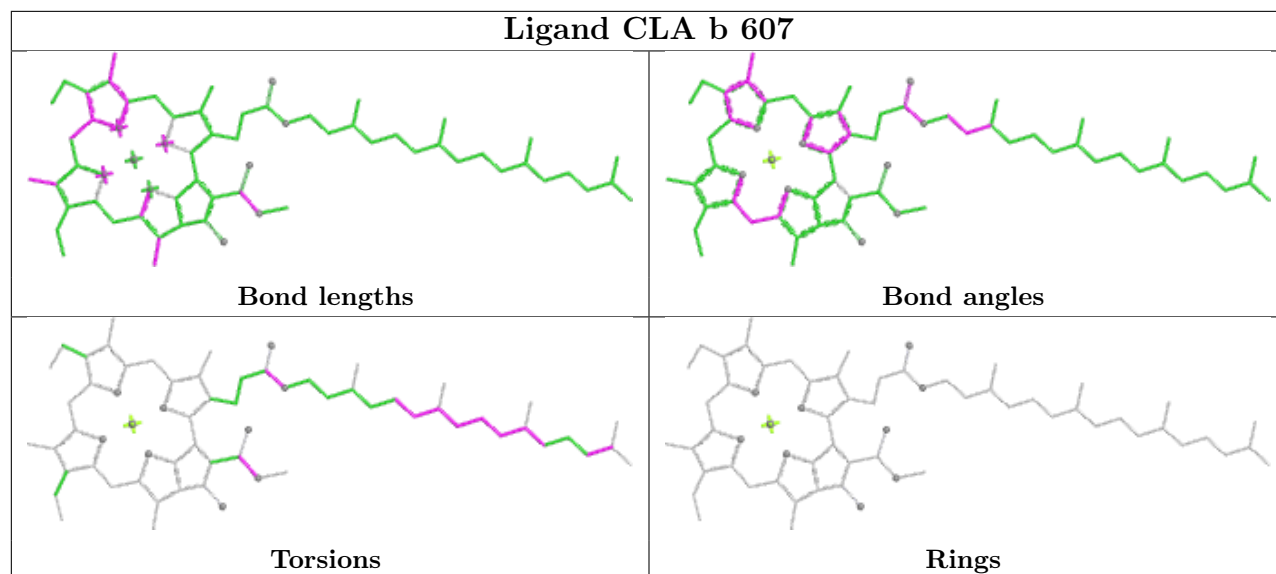




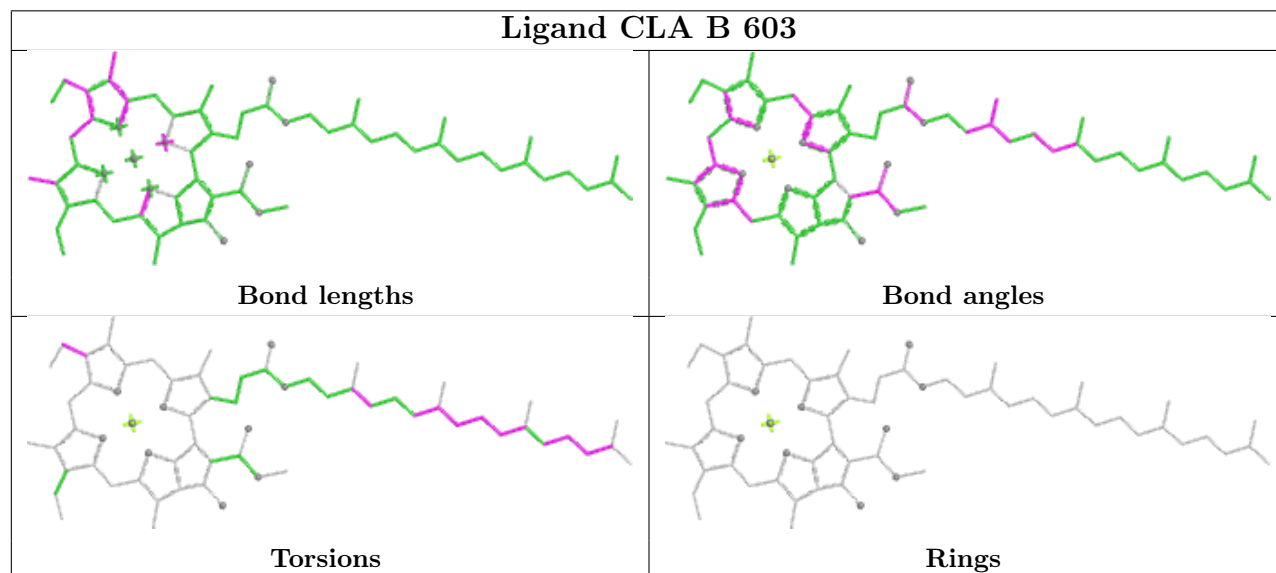




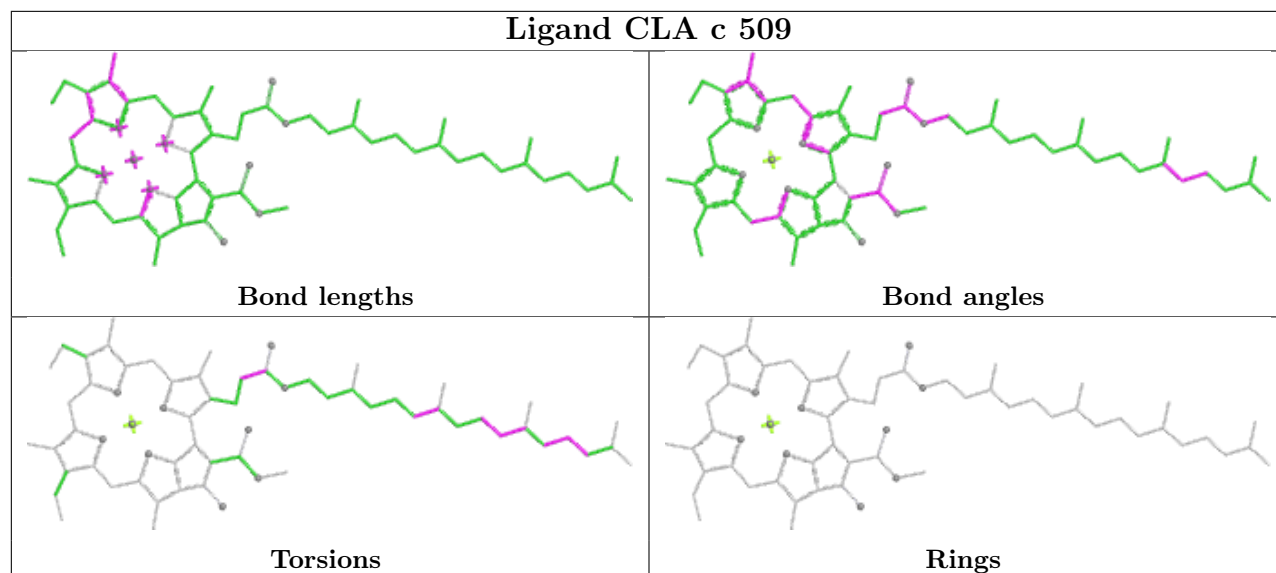
Ligand CLA b 607

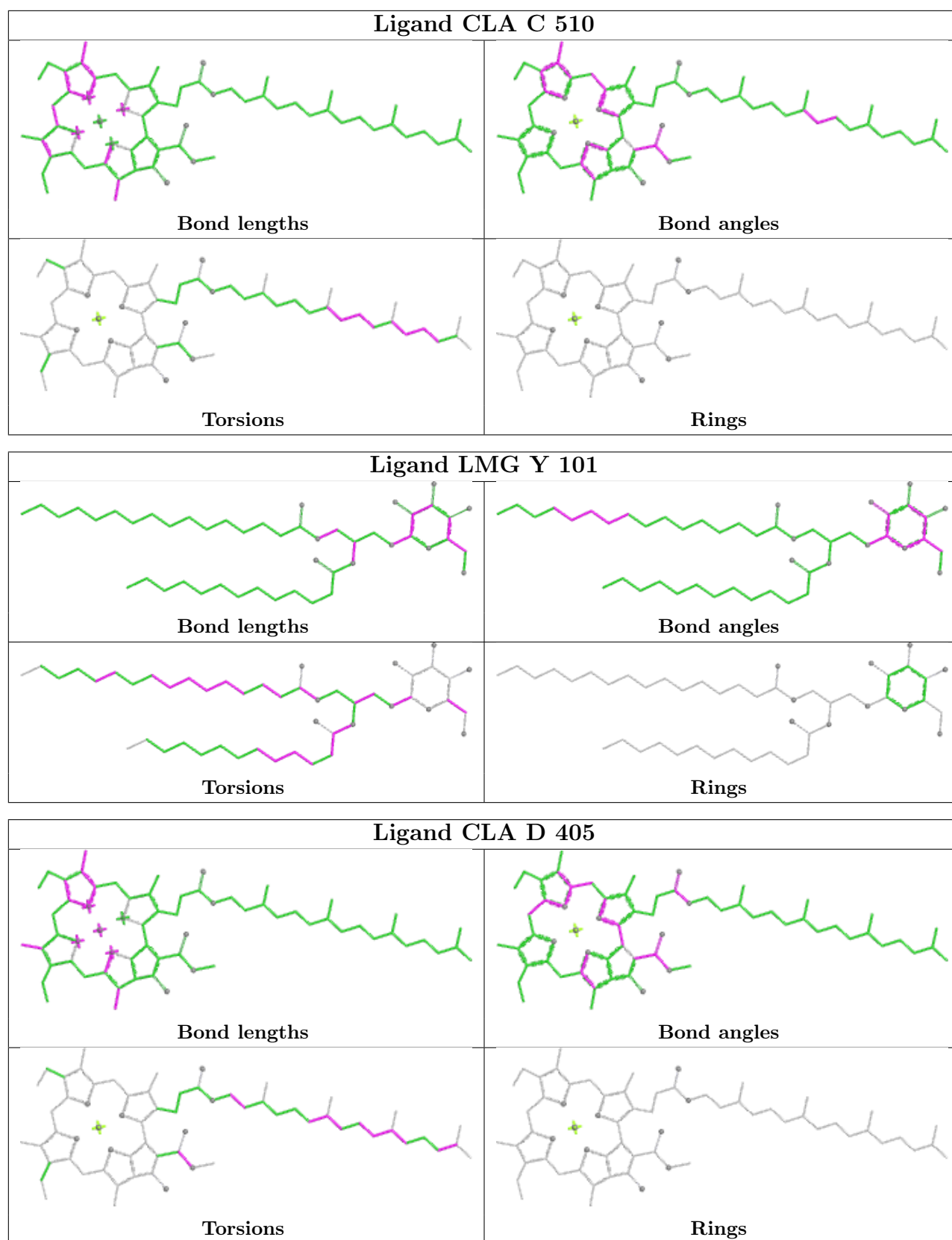


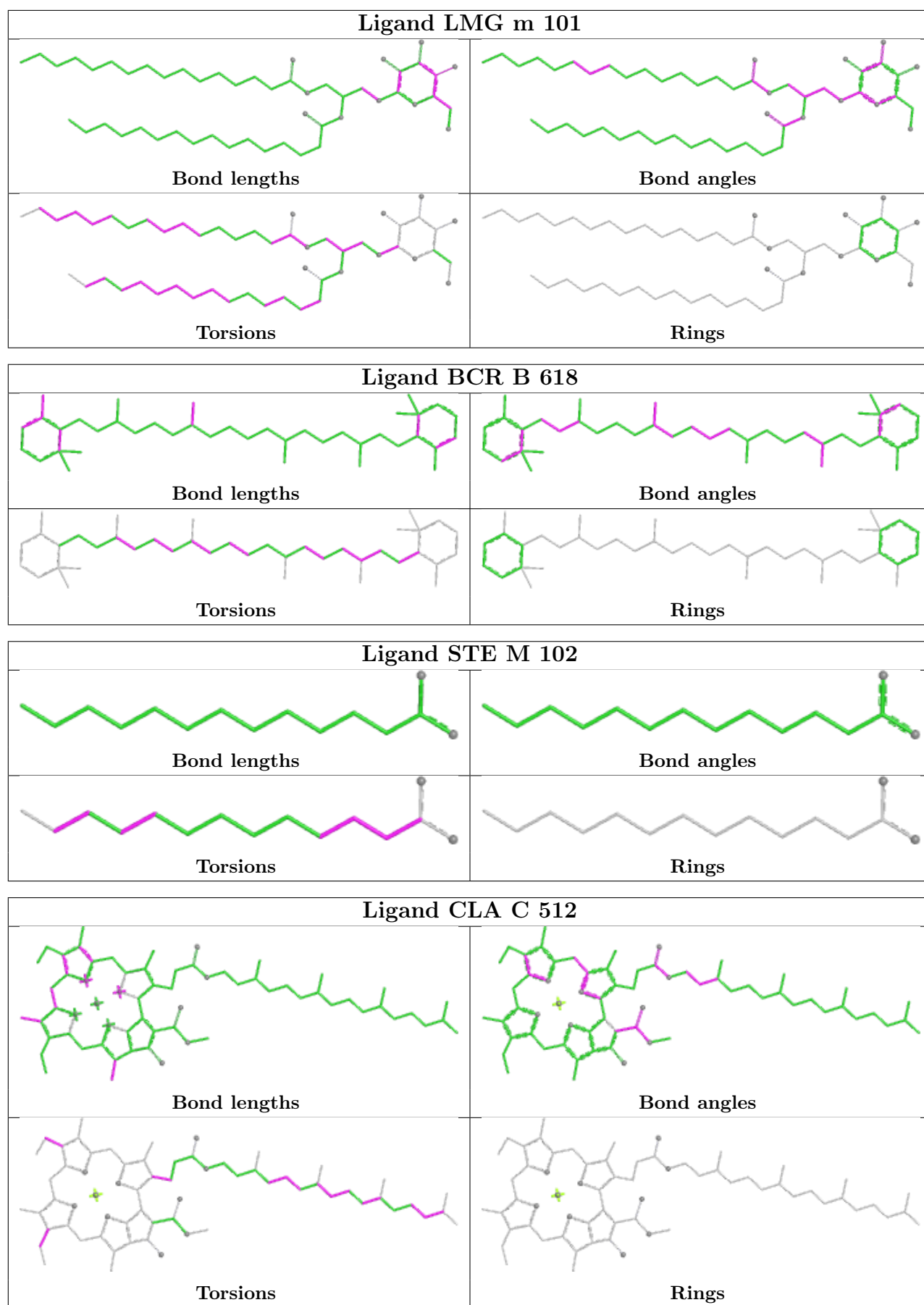
Ligand CLA B 603



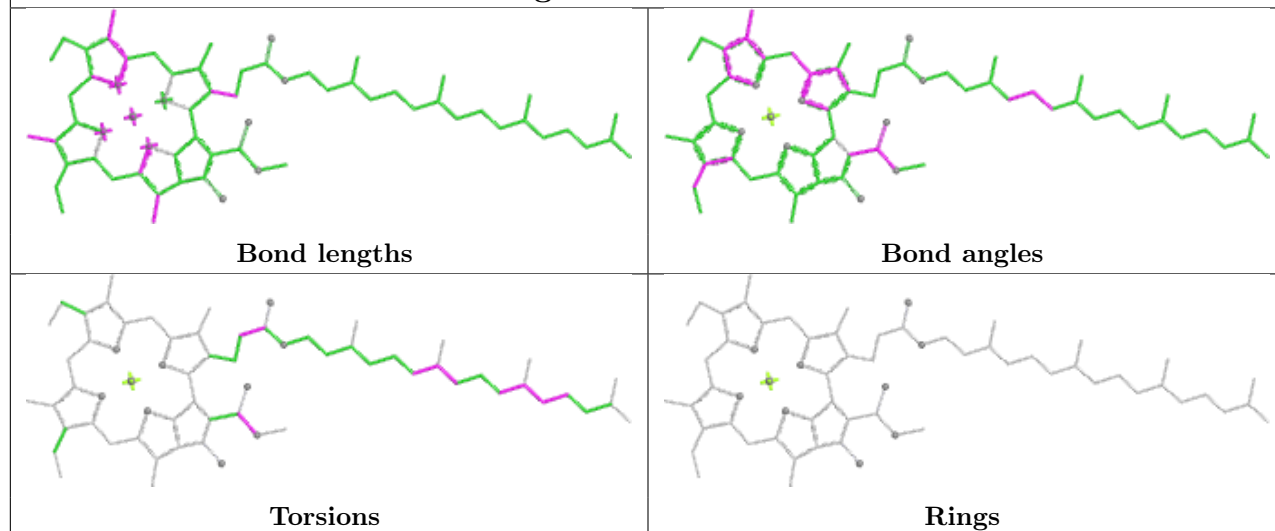
Ligand CLA c 509



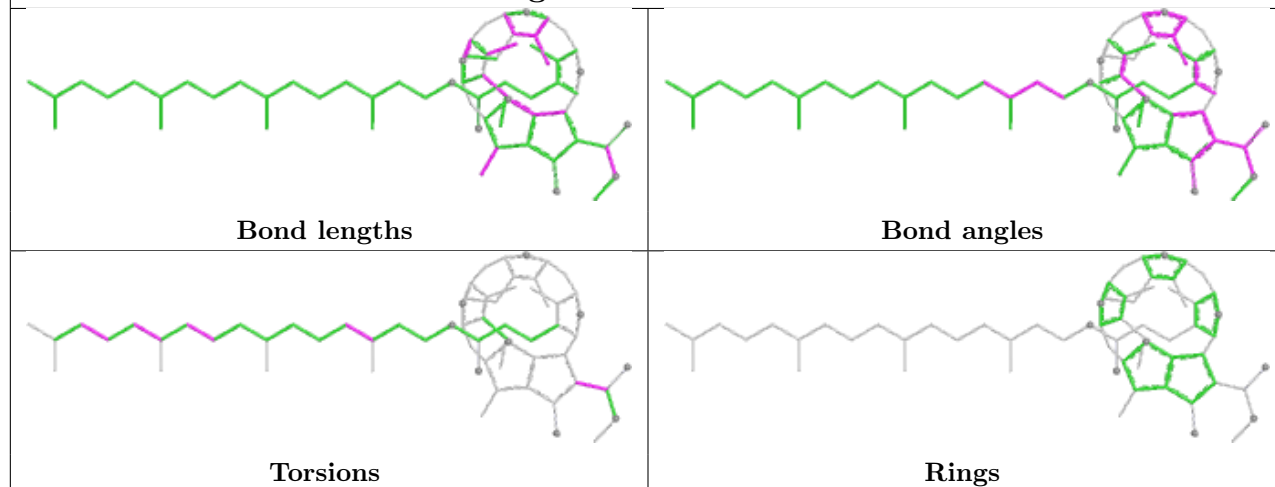




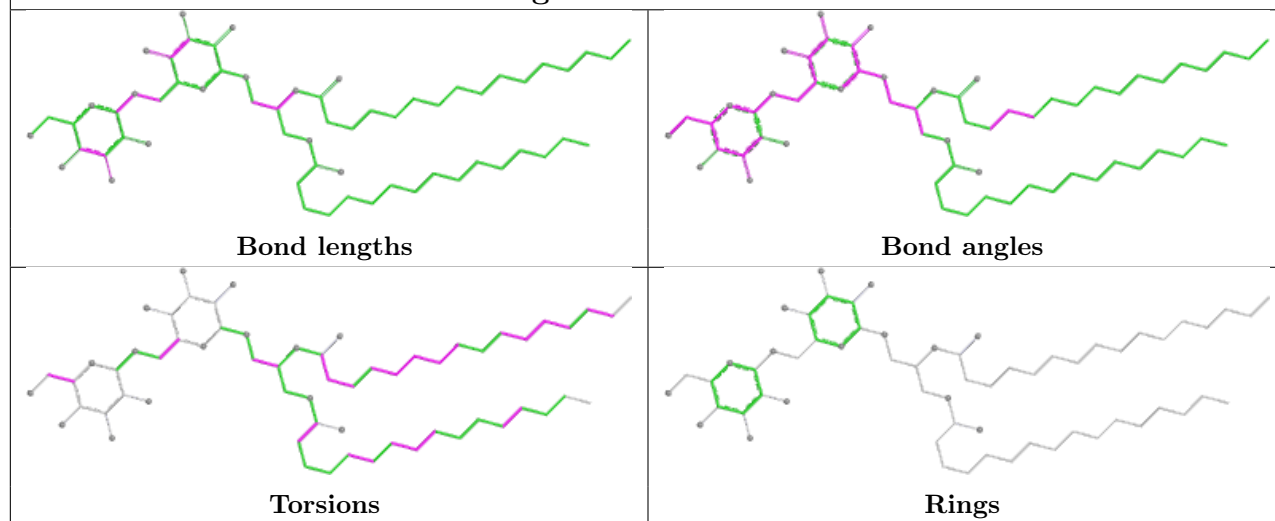
Ligand CLA b 613

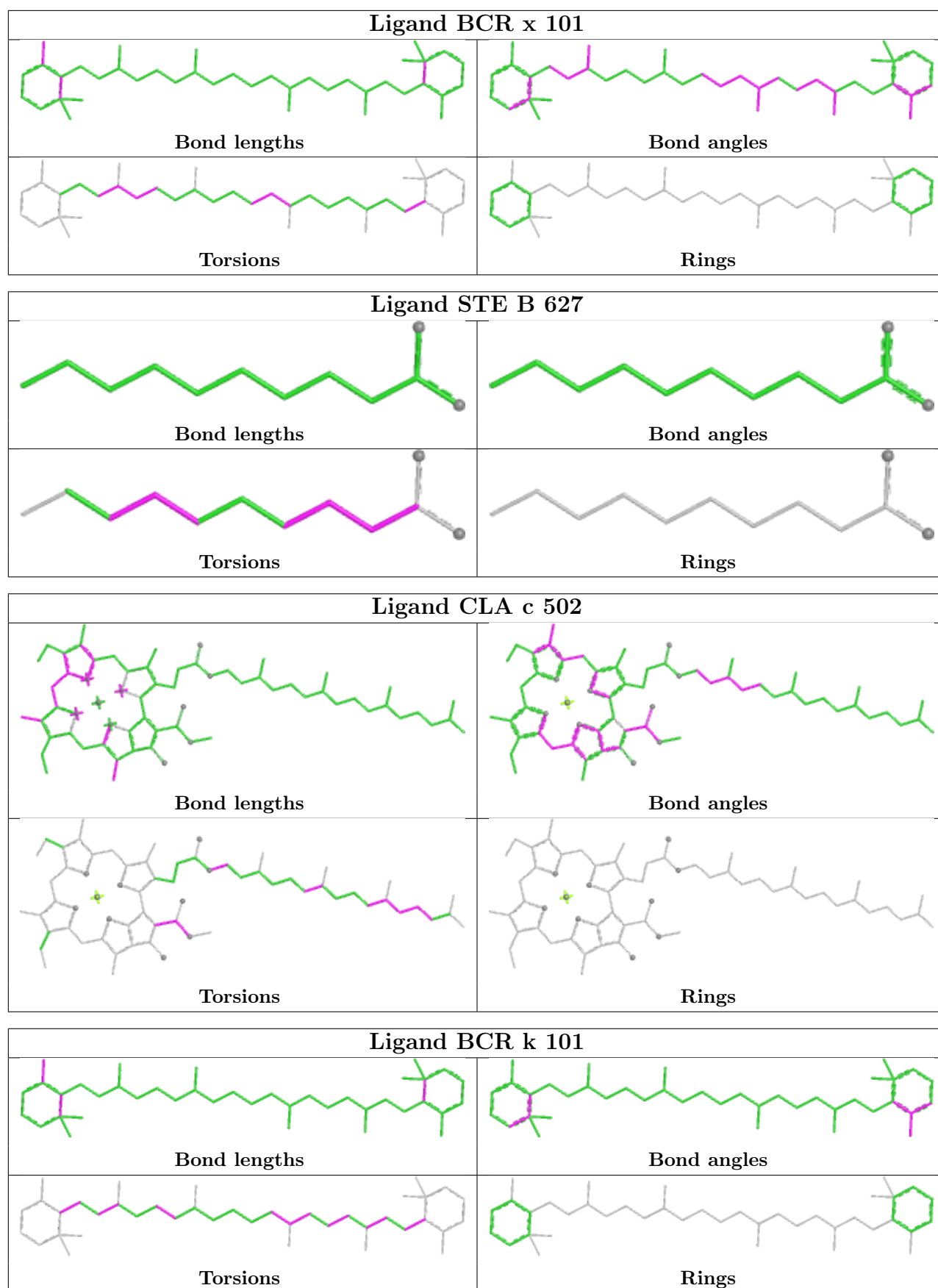


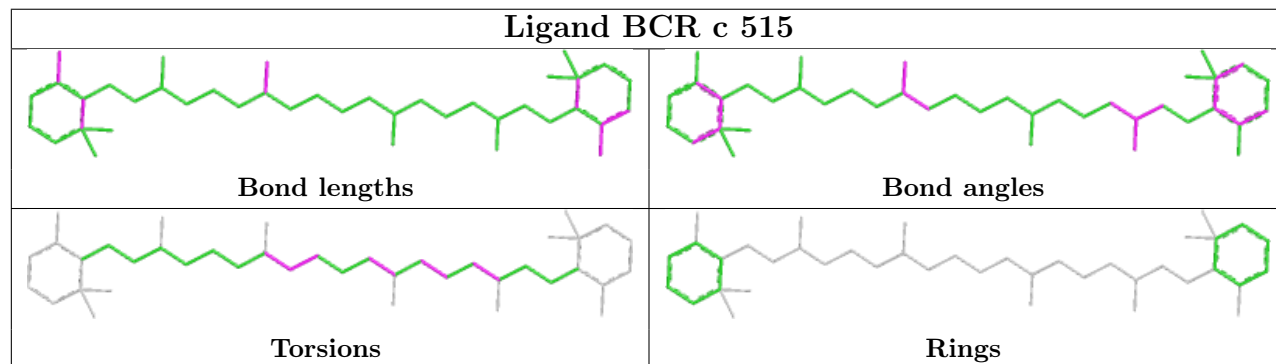
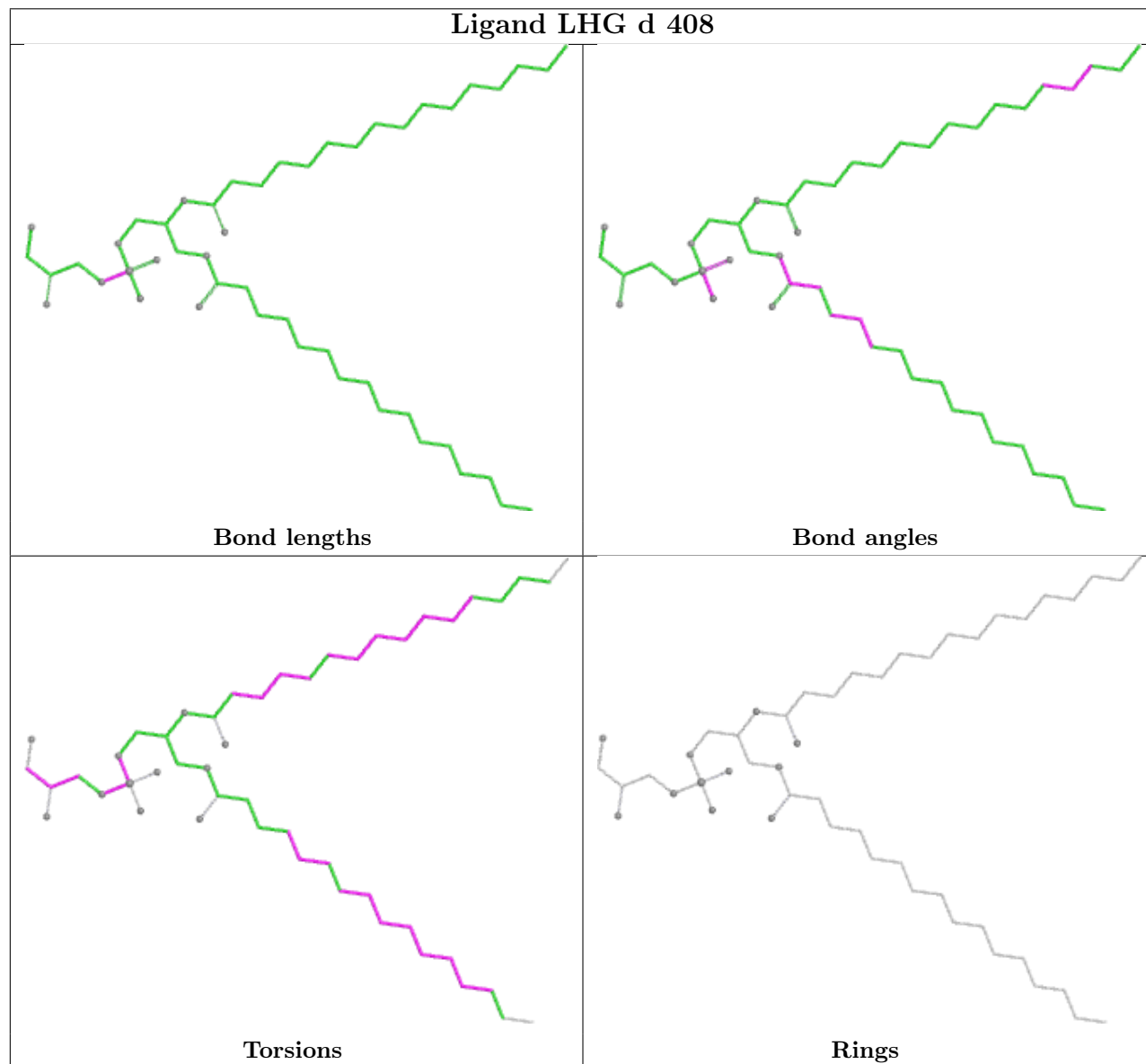
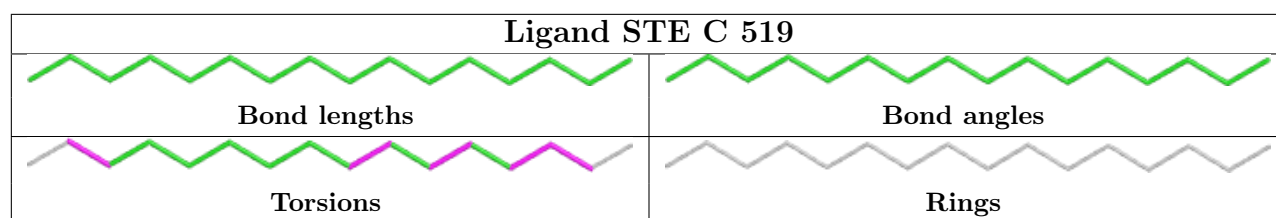
Ligand PHO A 404

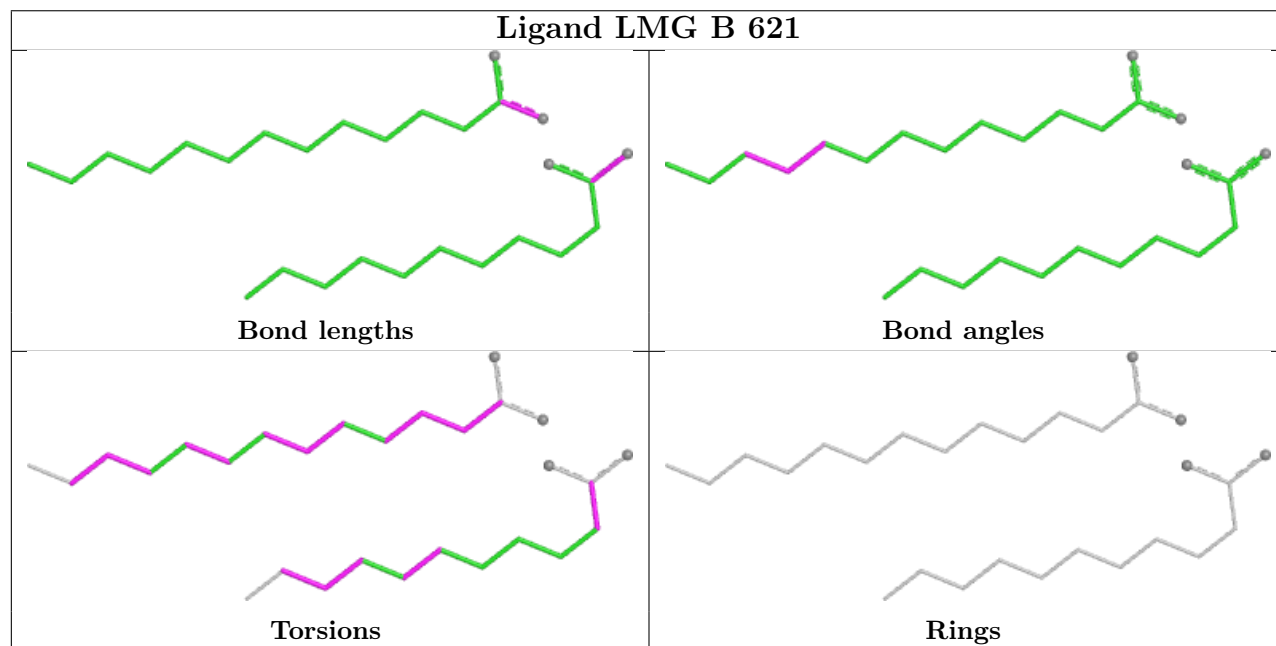
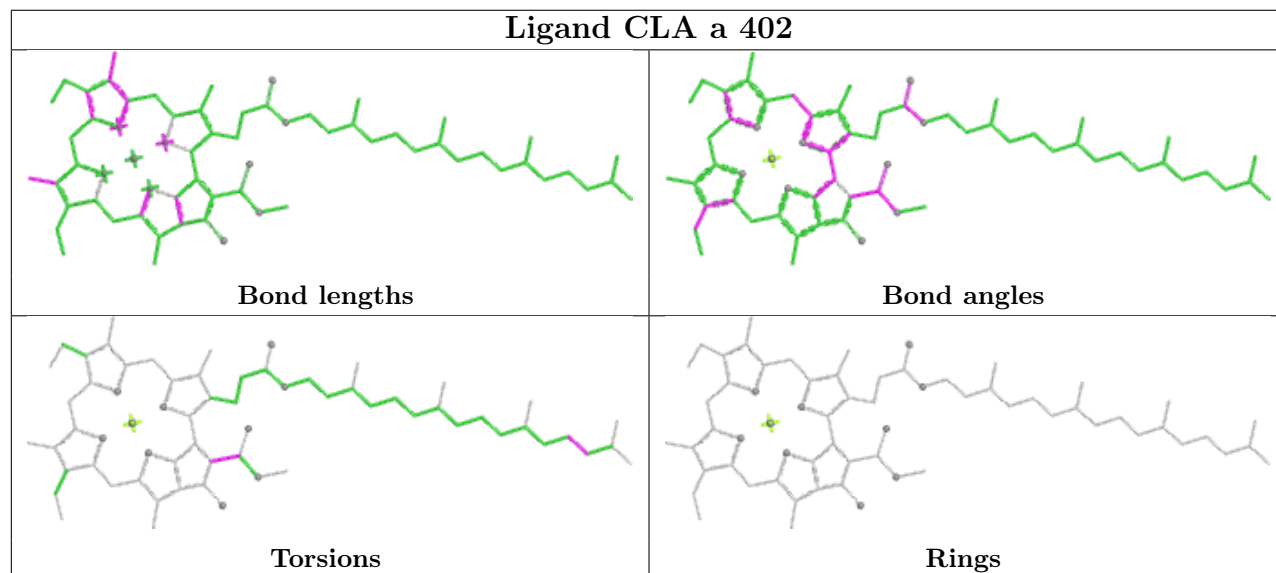
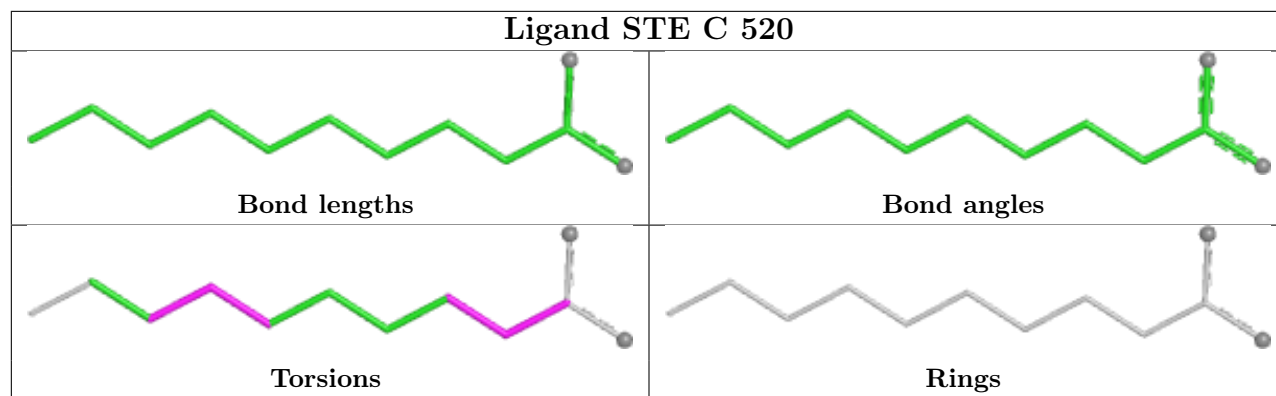


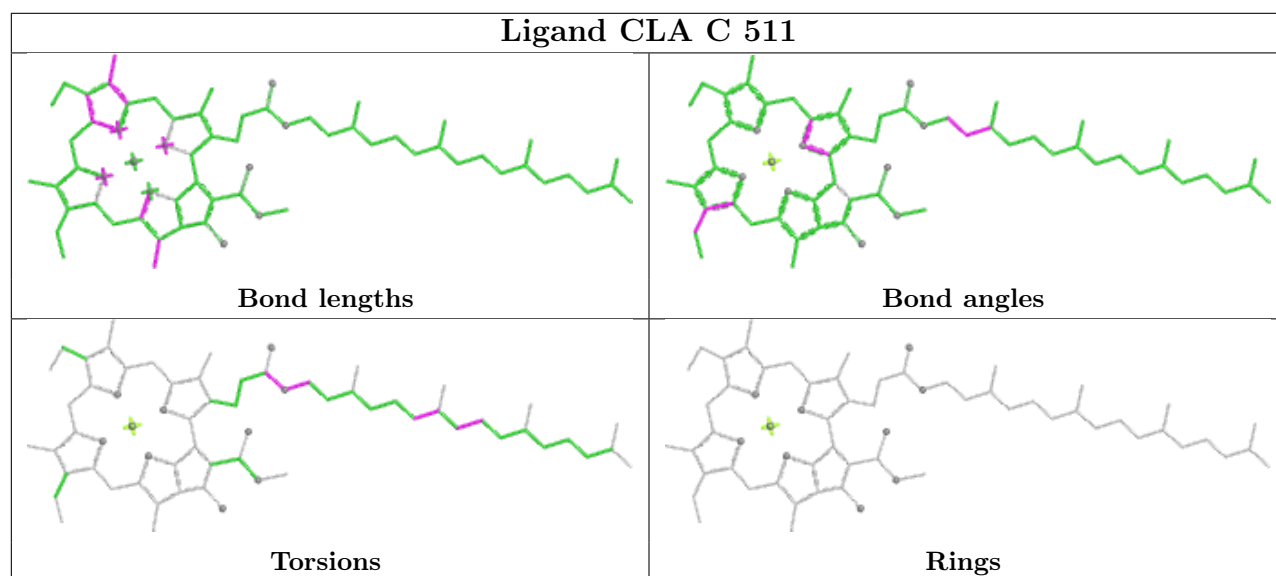
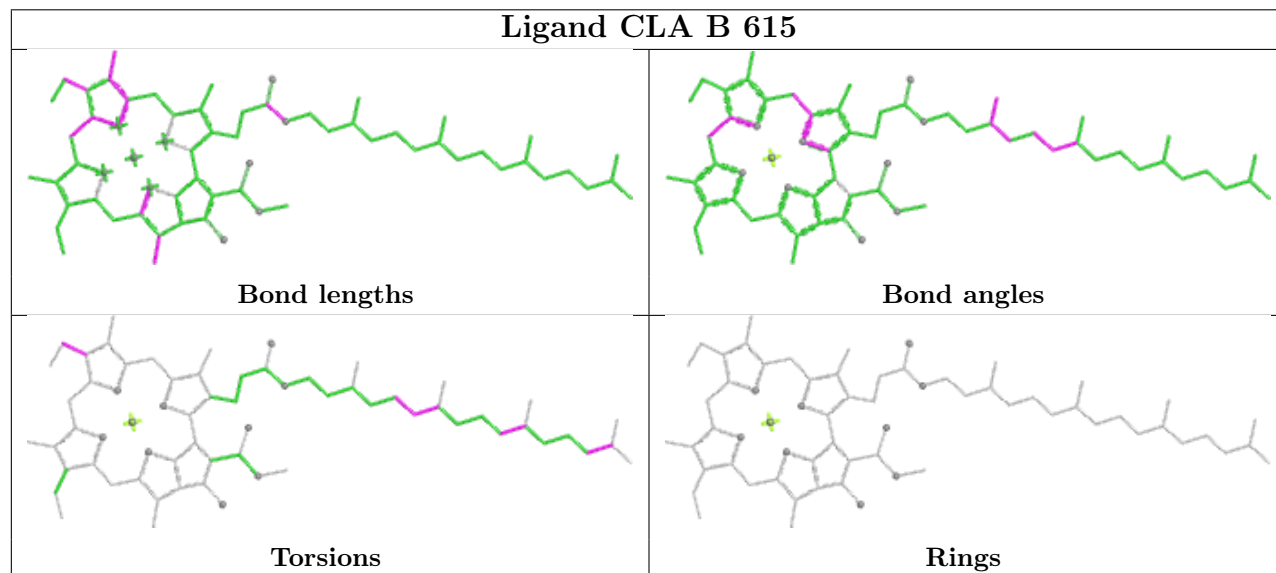
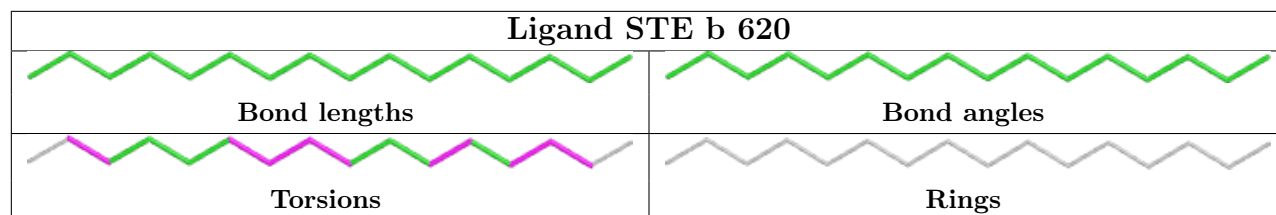
Ligand DGD c 516

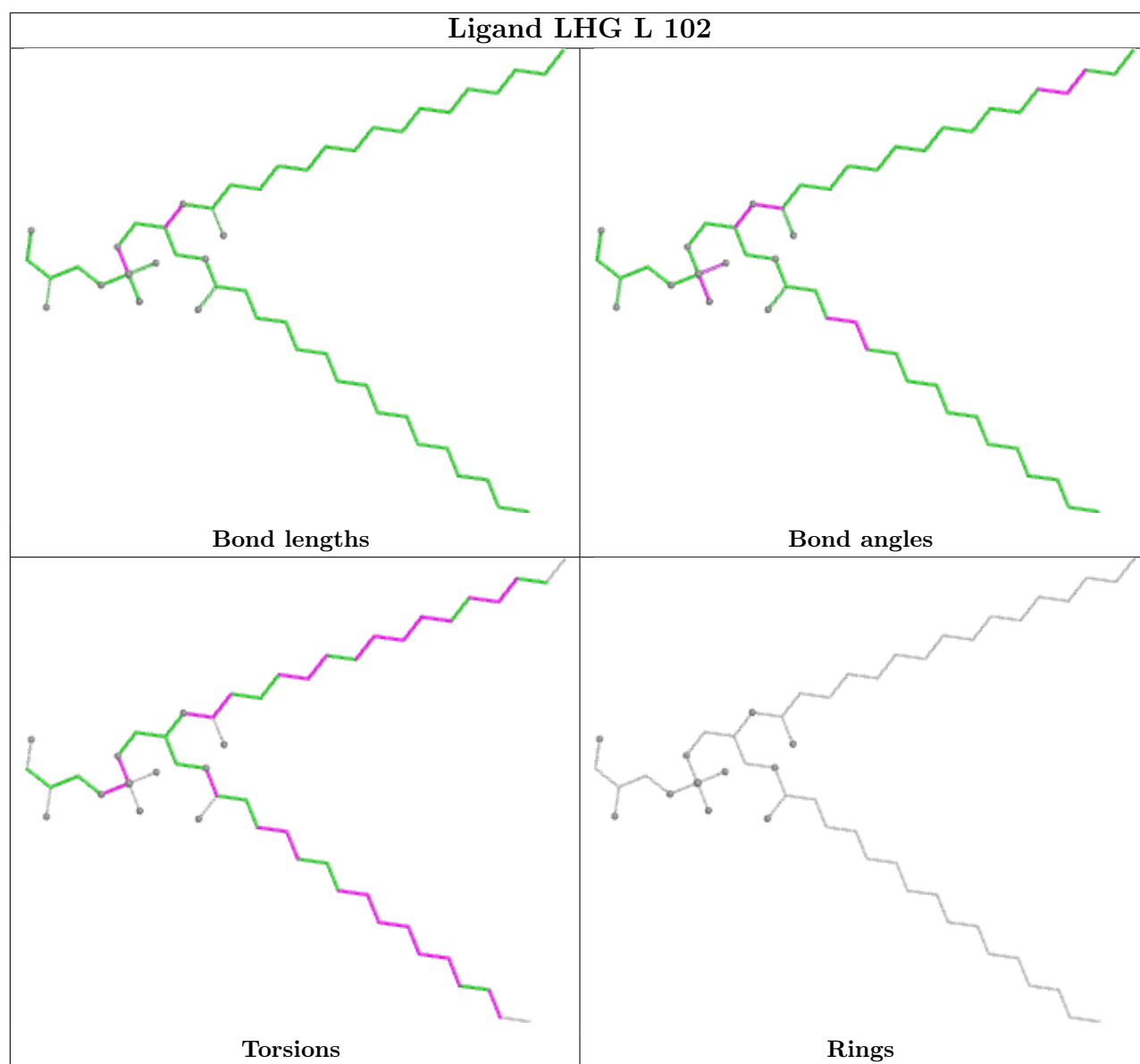


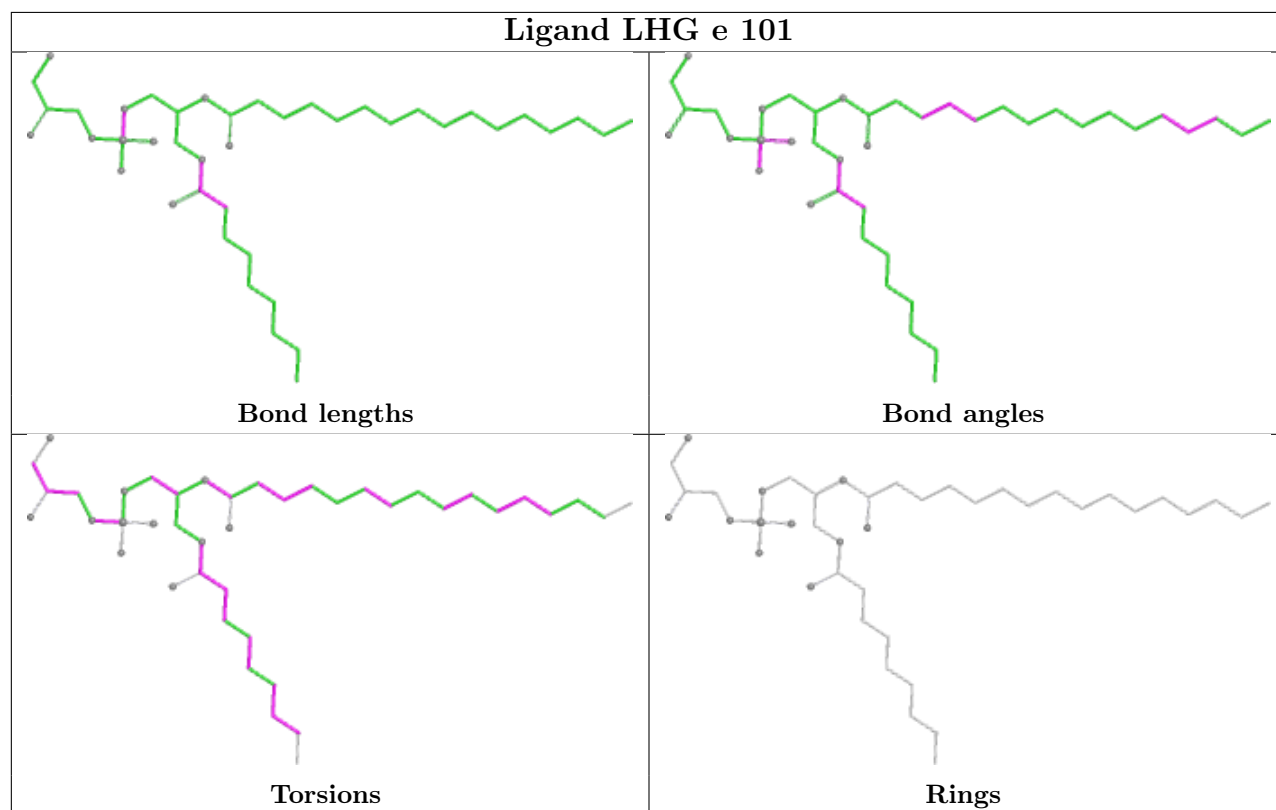
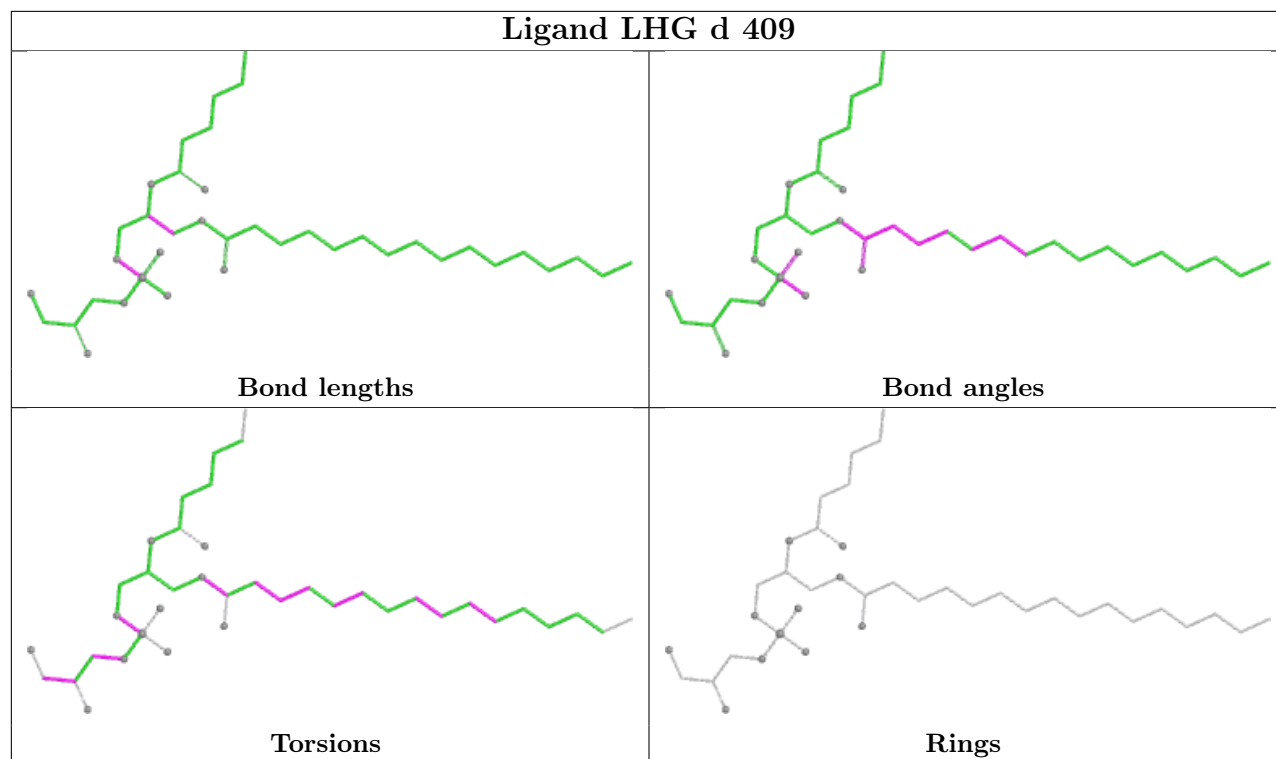


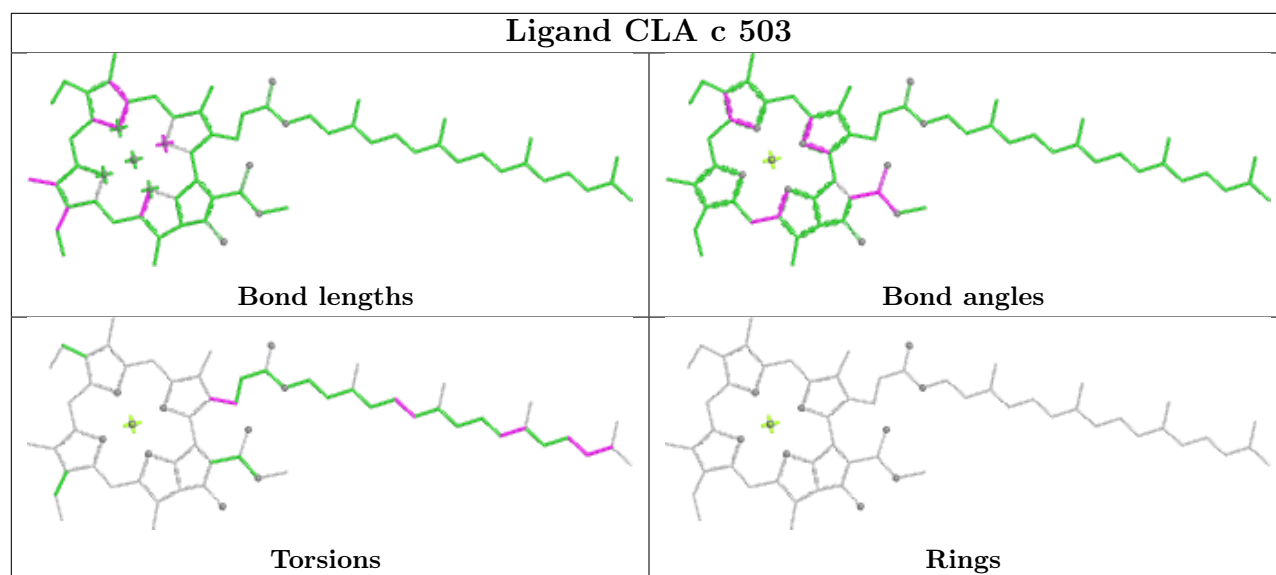
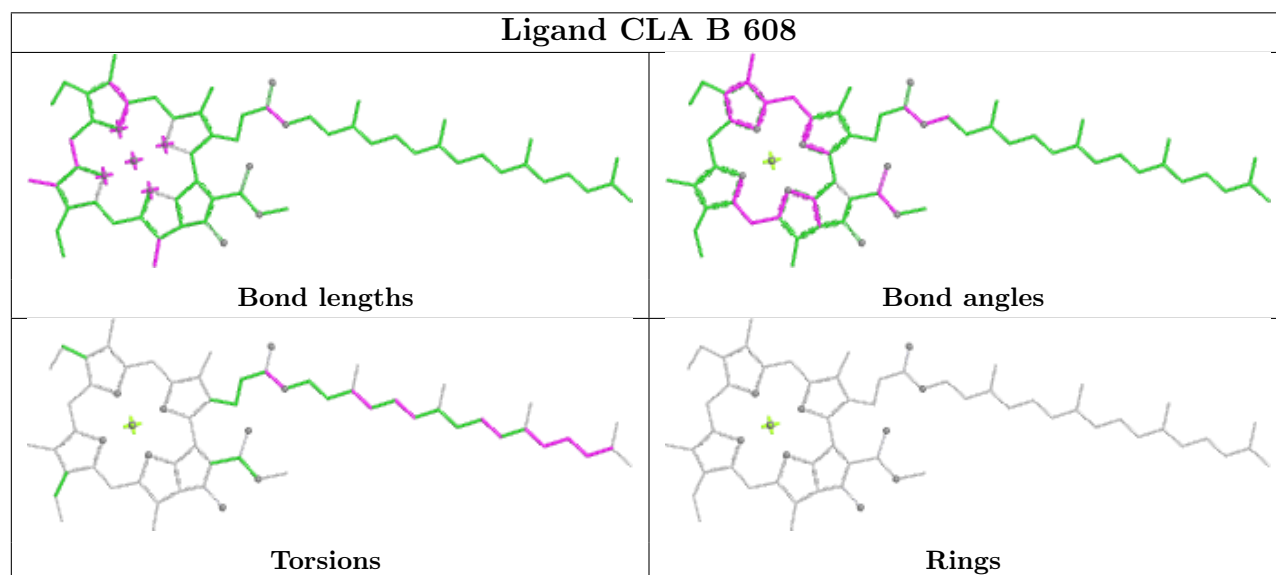
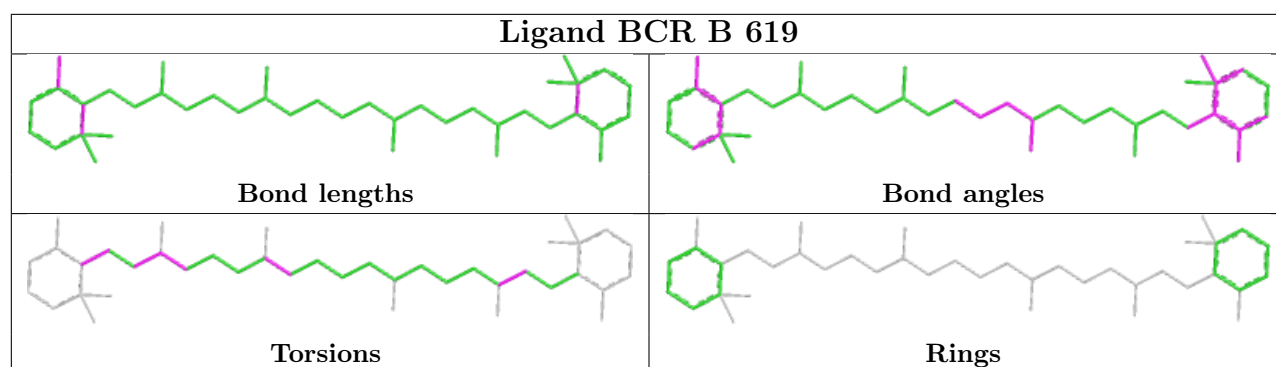


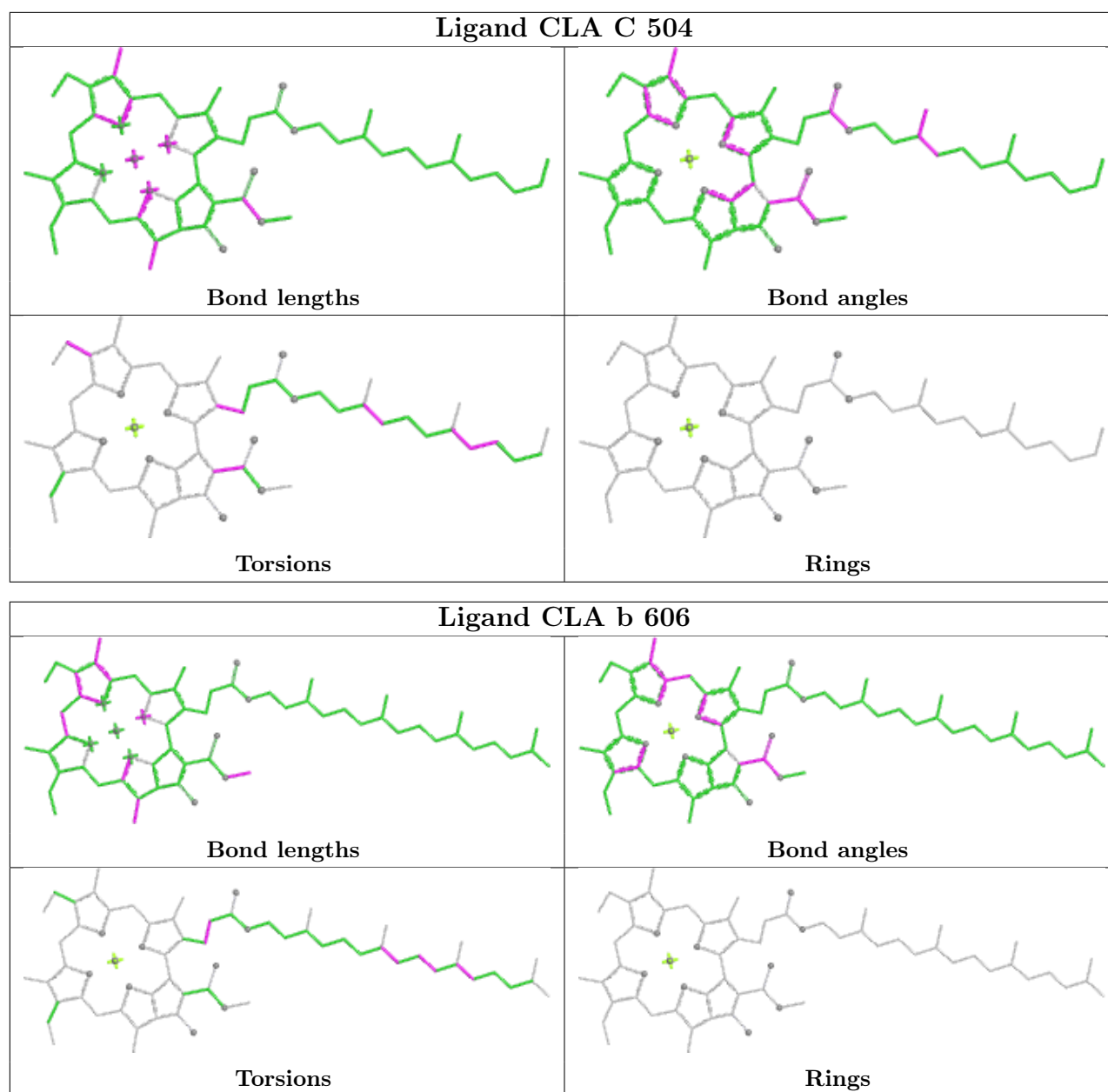












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	468:SER	C	469:MET	N	1.20

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%)	-0.55	1 (0%) 90 90	29, 38, 56, 86	0
1	a	334/344 (97%)	-0.44	4 (1%) 76 78	28, 40, 66, 86	0
2	B	505/510 (99%)	-0.40	0 100 100	22, 42, 70, 94	4 (0%)
2	b	505/510 (99%)	-0.29	4 (0%) 82 84	32, 46, 78, 112	0
3	C	442/461 (95%)	-0.36	0 100 100	22, 45, 63, 92	1 (0%)
3	c	451/461 (97%)	-0.25	1 (0%) 91 91	25, 50, 73, 105	2 (0%)
4	D	341/352 (96%)	-0.51	0 100 100	28, 39, 58, 89	0
4	d	341/352 (96%)	-0.37	0 100 100	28, 43, 69, 95	1 (0%)
5	E	82/84 (97%)	0.05	3 (3%) 45 47	35, 62, 78, 91	1 (1%)
5	e	82/84 (97%)	0.25	1 (1%) 76 78	46, 72, 89, 102	0
6	F	34/45 (75%)	-0.23	0 100 100	44, 53, 74, 88	0
6	f	34/45 (75%)	-0.10	0 100 100	51, 60, 89, 105	0
7	H	65/66 (98%)	-0.24	0 100 100	39, 51, 69, 75	0
7	h	63/66 (95%)	0.02	2 (3%) 50 52	48, 61, 72, 81	0
8	I	35/38 (92%)	-0.31	1 (2%) 53 55	40, 48, 75, 89	0
8	i	35/38 (92%)	-0.12	0 100 100	39, 51, 80, 92	0
9	J	36/40 (90%)	-0.13	0 100 100	43, 61, 87, 100	0
9	j	36/40 (90%)	0.06	0 100 100	48, 66, 99, 116	0
10	K	37/46 (80%)	-0.15	0 100 100	45, 62, 79, 86	0
10	k	37/46 (80%)	0.12	0 100 100	59, 67, 85, 91	0
11	L	37/37 (100%)	-0.59	0 100 100	31, 38, 71, 78	0
11	l	36/37 (97%)	-0.51	0 100 100	33, 41, 82, 92	0
12	M	32/36 (88%)	-0.37	1 (3%) 51 53	37, 44, 70, 82	0
12	m	31/36 (86%)	-0.45	0 100 100	36, 44, 62, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.20	2 (0%) 82 84	30, 52, 94, 132	1 (0%)
13	o	244/272 (89%)	-0.23	2 (0%) 82 84	30, 50, 90, 139	0
14	R	28/41 (68%)	0.65	1 (3%) 46 48	71, 81, 97, 101	0
14	r	28/41 (68%)	1.28	6 (21%) 2 2	88, 108, 129, 144	0
15	T	29/32 (90%)	-0.49	1 (3%) 48 50	32, 39, 68, 89	0
15	t	29/32 (90%)	-0.33	1 (3%) 48 50	36, 41, 85, 93	0
16	U	97/134 (72%)	-0.20	0 100 100	36, 54, 82, 102	0
16	u	97/134 (72%)	-0.27	0 100 100	39, 51, 66, 84	0
17	V	137/163 (84%)	-0.40	0 100 100	34, 50, 63, 81	0
17	v	137/163 (84%)	-0.17	0 100 100	40, 57, 81, 90	0
18	X	38/41 (92%)	-0.05	1 (2%) 57 59	50, 60, 83, 88	0
18	x	39/41 (95%)	0.07	1 (2%) 57 59	58, 67, 96, 110	0
19	Y	27/46 (58%)	0.84	2 (7%) 20 21	62, 84, 104, 114	0
19	y	30/46 (65%)	0.65	0 100 100	73, 89, 101, 113	0
20	Z	62/62 (100%)	0.55	2 (3%) 50 52	64, 80, 127, 137	0
20	z	62/62 (100%)	0.63	4 (6%) 25 26	71, 86, 124, 131	0
All	All	5293/5700 (92%)	-0.27	41 (0%) 82 84	22, 47, 85, 144	10 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	t	30	THR	4.9
13	o	58	ASN	4.6
20	z	33	TRP	4.2
7	h	64	ALA	3.6
18	x	40	SER	3.5
20	Z	62	VAL	3.4
14	r	20	VAL	3.3
5	E	3	GLY	3.2
19	Y	22	LEU	3.1
13	O	60	ARG	3.0
20	z	27	TYR	3.0
5	e	79	PHE	2.8
3	c	23	ALA	2.8
19	Y	20	ALA	2.8
2	b	495	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	79	PHE	2.7
14	r	29	LYS	2.6
2	b	84	THR	2.6
1	a	11	ALA	2.6
20	Z	30	PRO	2.5
14	r	9	LEU	2.5
7	h	21	VAL	2.4
13	O	221	SER	2.4
14	r	14	LEU	2.3
18	X	2	THR	2.3
8	I	36	ASP	2.3
20	z	30	PRO	2.3
1	a	248	ILE	2.3
1	A	11	ALA	2.3
5	E	84	LYS	2.3
2	b	133	LEU	2.2
1	a	250	ALA	2.2
15	T	30	THR	2.2
14	r	26	TYR	2.2
2	b	486	LEU	2.2
14	r	3	TRP	2.1
14	R	29	LYS	2.1
1	a	264	SER	2.1
12	M	33	GLN	2.1
20	z	62	VAL	2.0
13	o	57	LYS	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($\text{\AA}^2$)	Q<0.9
8	FME	I	1	10/11	0.92	0.11	46,58,68,81	0
15	FME	T	1	10/11	0.94	0.10	31,58,77,77	0
12	FME	m	1	10/11	0.95	0.08	44,53,72,80	0
15	FME	t	1	10/11	0.95	0.08	34,54,68,69	0
12	FME	M	1	10/11	0.96	0.07	45,56,70,76	0
8	FME	i	1	10/11	0.97	0.07	42,55,68,74	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	STE	d	412	20/20	0.75	0.18	40,68,83,90	0
32	STE	I	102	15/20	0.76	0.18	42,58,80,82	0
32	STE	B	625	16/20	0.78	0.16	40,64,82,85	0
32	STE	a	412	12/20	0.78	0.16	47,74,84,88	0
32	STE	H	103	18/20	0.78	0.16	52,77,88,89	0
32	STE	b	625	20/20	0.79	0.15	42,67,89,95	0
32	STE	b	624	15/20	0.79	0.17	50,66,87,92	0
32	STE	b	626	10/20	0.80	0.16	49,60,69,71	0
32	STE	c	523	12/20	0.80	0.13	55,74,88,90	0
28	LHG	A	411	49/49	0.80	0.14	45,84,111,116	0
32	STE	b	627	14/20	0.81	0.17	54,77,98,104	0
28	LHG	e	101	42/49	0.81	0.15	62,89,116,133	0
26	LMG	b	622	55/55	0.81	0.16	49,78,102,109	0
32	STE	L	103	12/20	0.82	0.17	48,66,88,88	0
32	STE	M	103	10/20	0.82	0.17	40,56,67,71	0
32	STE	B	624	18/20	0.82	0.14	52,72,90,94	0
26	LMG	c	521	48/55	0.83	0.14	34,77,102,106	0
27	SQD	A	412	39/54	0.83	0.14	45,66,96,103	0
32	STE	a	413	15/20	0.83	0.18	36,63,77,86	0
32	STE	c	520	20/20	0.83	0.12	42,64,85,89	0
32	STE	b	620	16/20	0.83	0.15	40,55,81,91	0
26	LMG	B	626	55/55	0.83	0.13	40,64,84,98	0
32	STE	x	102	20/20	0.83	0.14	50,66,80,86	0
32	STE	C	518	12/20	0.84	0.14	39,57,68,69	0
25	PL9	A	408	55/55	0.84	0.14	32,67,92,100	0
32	STE	B	627	12/20	0.85	0.12	42,68,79,82	0
22	CLA	b	601	65/65	0.85	0.12	48,73,101,104	0
32	STE	C	519	16/20	0.85	0.14	47,62,75,75	0
32	STE	R	101	12/20	0.85	0.14	60,82,101,105	0
32	STE	t	104	10/20	0.85	0.14	43,60,72,77	0
26	LMG	c	519	37/55	0.85	0.12	45,69,89,99	0
32	STE	b	623	16/20	0.86	0.14	53,73,83,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	LMG	D	412	33/55	0.86	0.13	32,62,92,94	0
32	STE	J	101	12/20	0.86	0.13	49,65,72,74	0
32	STE	j	101	12/20	0.86	0.11	50,64,71,72	0
27	SQD	t	102	36/54	0.86	0.13	31,66,91,95	0
29	DGD	A	413	66/66	0.86	0.11	47,64,83,89	0
32	STE	B	620	17/20	0.87	0.12	37,60,76,76	0
25	PL9	a	409	55/55	0.87	0.14	41,72,95,100	0
26	LMG	B	621	28/55	0.87	0.13	36,52,67,73	0
32	STE	l	102	18/20	0.87	0.12	38,52,75,78	0
32	STE	b	621	20/20	0.87	0.11	42,60,79,84	0
22	CLA	B	601	65/65	0.87	0.11	40,70,93,104	0
32	STE	B	623	12/20	0.88	0.12	38,60,72,73	0
27	SQD	L	101	49/54	0.88	0.11	40,66,100,105	0
26	LMG	A	409	48/55	0.88	0.10	34,63,79,96	0
26	LMG	Y	101	48/55	0.88	0.11	52,75,93,102	0
32	STE	d	411	17/20	0.89	0.12	48,63,70,78	0
32	STE	Z	102	8/20	0.89	0.14	43,65,79,79	0
27	SQD	f	102	41/54	0.89	0.12	62,87,107,118	0
26	LMG	M	101	51/55	0.90	0.10	36,54,76,86	0
27	SQD	B	622	54/54	0.90	0.10	38,65,89,98	0
26	LMG	c	522	49/55	0.90	0.10	28,62,92,100	0
26	LMG	d	410	44/55	0.90	0.11	41,61,89,106	0
32	STE	t	103	14/20	0.90	0.10	43,57,69,70	0
26	LMG	m	101	51/55	0.90	0.10	39,58,78,87	0
32	STE	C	520	12/20	0.90	0.12	36,47,59,66	0
31	BCR	K	101	40/40	0.91	0.10	40,57,75,78	0
31	BCR	c	514	40/40	0.91	0.11	45,67,82,87	0
31	BCR	d	406	40/40	0.91	0.10	35,61,97,109	0
31	BCR	x	101	40/40	0.91	0.09	37,58,76,80	0
32	STE	X	101	20/20	0.91	0.10	39,56,75,81	0
27	SQD	a	411	54/54	0.91	0.10	47,69,98,106	0
22	CLA	c	512	65/65	0.91	0.11	42,63,90,104	0
22	CLA	C	513	65/65	0.91	0.10	41,63,99,108	0
31	BCR	B	619	40/40	0.92	0.09	29,49,73,84	0
31	BCR	C	514	40/40	0.92	0.10	29,46,59,77	0
27	SQD	D	409	36/54	0.92	0.11	51,77,96,105	0
31	BCR	Z	101	40/40	0.92	0.10	42,64,78,82	0
32	STE	M	102	15/20	0.92	0.09	38,53,63,66	0
22	CLA	c	513	65/65	0.92	0.11	47,77,104,108	0
29	DGD	H	102	62/66	0.92	0.09	33,51,66,72	0
31	BCR	k	101	40/40	0.92	0.10	46,68,84,90	0
29	DGD	c	518	62/66	0.92	0.10	35,62,87,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	BCR	H	101	40/40	0.93	0.08	35,52,66,74	0
29	DGD	C	516	62/66	0.93	0.09	31,54,103,124	0
31	BCR	K	102	40/40	0.93	0.10	39,58,71,71	0
31	BCR	T	101	40/40	0.93	0.07	32,46,58,65	0
22	CLA	c	506	65/65	0.93	0.10	35,57,100,103	0
31	BCR	b	617	40/40	0.93	0.08	32,48,65,66	0
31	BCR	b	619	40/40	0.93	0.09	30,55,81,85	0
29	DGD	c	517	62/66	0.93	0.08	38,60,95,104	0
31	BCR	c	515	40/40	0.93	0.09	33,53,70,76	0
28	LHG	d	409	39/49	0.93	0.09	32,52,69,75	0
29	DGD	h	101	62/66	0.93	0.09	34,52,67,70	0
31	BCR	k	102	40/40	0.93	0.11	46,63,76,78	0
31	BCR	B	618	40/40	0.93	0.08	29,45,60,67	0
27	SQD	A	410	52/54	0.93	0.09	37,66,96,101	0
26	LMG	D	408	51/55	0.93	0.11	32,65,89,99	0
31	BCR	D	406	40/40	0.93	0.09	34,51,88,99	0
22	CLA	c	511	65/65	0.94	0.10	43,63,80,86	0
29	DGD	C	517	62/66	0.94	0.08	31,53,79,87	0
31	BCR	I	101	40/40	0.94	0.07	27,40,50,54	0
22	CLA	C	512	65/65	0.94	0.10	39,61,93,102	0
22	CLA	b	606	65/65	0.94	0.08	28,46,80,92	0
28	LHG	D	411	47/49	0.94	0.10	28,53,83,89	0
28	LHG	a	410	49/49	0.94	0.11	39,57,79,91	0
31	BCR	a	405	40/40	0.94	0.07	24,39,58,59	0
31	BCR	B	617	40/40	0.94	0.08	30,45,64,65	0
31	BCR	b	618	40/40	0.94	0.07	29,44,60,62	0
22	CLA	c	503	65/65	0.94	0.08	34,49,61,67	0
22	CLA	C	510	65/65	0.94	0.07	29,48,65,73	0
22	CLA	c	508	64/65	0.94	0.09	37,55,93,115	0
33	BCT	a	408	4/4	0.94	0.09	34,44,53,64	0
22	CLA	c	502	65/65	0.95	0.08	32,48,68,72	0
22	CLA	C	503	65/65	0.95	0.07	31,47,57,61	0
22	CLA	c	504	60/65	0.95	0.07	35,51,84,100	0
22	CLA	C	504	59/65	0.95	0.08	32,48,87,92	0
22	CLA	C	506	65/65	0.95	0.08	30,50,89,98	0
22	CLA	c	509	65/65	0.95	0.09	30,53,72,80	0
22	CLA	c	510	65/65	0.95	0.07	35,50,66,84	0
22	CLA	C	508	65/65	0.95	0.08	30,49,107,117	0
22	CLA	C	509	65/65	0.95	0.08	30,50,68,77	0
22	CLA	B	606	65/65	0.95	0.08	30,45,78,92	0
22	CLA	d	405	65/65	0.95	0.08	32,54,94,107	0
23	PHO	D	401	64/64	0.95	0.06	26,40,50,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	PHO	d	402	64/64	0.95	0.07	28,43,55,68	0
22	CLA	C	511	65/65	0.95	0.08	32,59,76,80	0
25	PL9	D	407	55/55	0.95	0.07	26,39,54,62	0
22	CLA	B	614	65/65	0.95	0.08	26,46,80,96	0
25	PL9	d	407	55/55	0.95	0.07	24,40,53,63	0
22	CLA	B	615	65/65	0.95	0.08	27,42,67,84	0
31	BCR	t	101	40/40	0.95	0.06	27,44,59,62	0
29	DGD	C	515	62/66	0.95	0.10	27,47,83,98	0
22	CLA	a	404	65/65	0.95	0.09	24,44,87,96	0
22	CLA	B	616	60/65	0.95	0.10	23,43,89,97	0
22	CLA	C	502	65/65	0.95	0.07	28,47,68,78	0
22	CLA	b	608	65/65	0.95	0.08	31,48,71,77	0
22	CLA	b	609	65/65	0.95	0.08	31,52,71,79	0
22	CLA	b	614	65/65	0.95	0.08	25,43,80,87	0
22	CLA	b	615	65/65	0.95	0.08	27,46,66,74	0
22	CLA	b	616	60/65	0.95	0.09	31,49,92,99	0
36	NA	V	202	1/1	0.95	0.12	60,60,60,60	0
22	CLA	d	404	65/65	0.96	0.07	22,37,52,55	0
28	LHG	D	413	49/49	0.96	0.08	32,47,74,88	0
28	LHG	L	102	49/49	0.96	0.07	30,45,63,73	0
22	CLA	b	602	65/65	0.96	0.08	33,47,65,71	0
28	LHG	d	408	49/49	0.96	0.08	29,47,61,72	0
23	PHO	A	404	64/64	0.96	0.06	17,35,45,49	0
22	CLA	b	604	65/65	0.96	0.08	26,44,80,95	0
28	LHG	l	101	49/49	0.96	0.07	34,49,63,70	0
23	PHO	a	403	64/64	0.96	0.06	23,36,44,47	0
22	CLA	b	605	65/65	0.96	0.07	25,38,56,62	0
22	CLA	B	610	65/65	0.96	0.07	24,38,49,60	0
22	CLA	b	607	65/65	0.96	0.07	24,41,81,86	0
22	CLA	C	505	65/65	0.96	0.08	26,47,73,76	0
29	DGD	c	516	62/66	0.96	0.08	30,47,80,87	0
22	CLA	B	611	65/65	0.96	0.07	20,36,53,58	0
22	CLA	b	610	65/65	0.96	0.07	28,43,58,68	0
22	CLA	b	611	65/65	0.96	0.07	24,41,57,66	0
22	CLA	b	612	65/65	0.96	0.07	27,41,52,54	0
22	CLA	b	613	65/65	0.96	0.08	23,41,82,97	0
22	CLA	C	507	65/65	0.96	0.07	26,46,66,68	0
22	CLA	B	612	65/65	0.96	0.07	23,36,50,60	0
22	CLA	B	613	65/65	0.96	0.08	22,40,73,81	0
22	CLA	c	501	65/65	0.96	0.07	32,49,65,71	0
22	CLA	B	602	65/65	0.96	0.07	26,43,63,67	0
22	CLA	B	604	65/65	0.96	0.08	25,40,87,96	0

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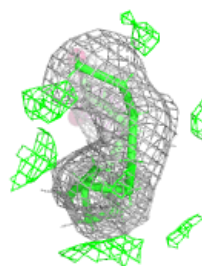
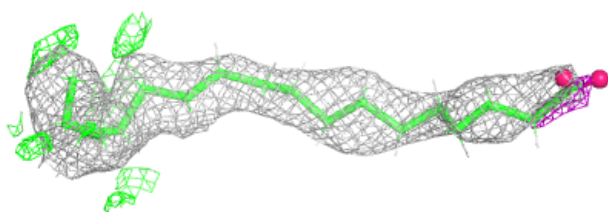
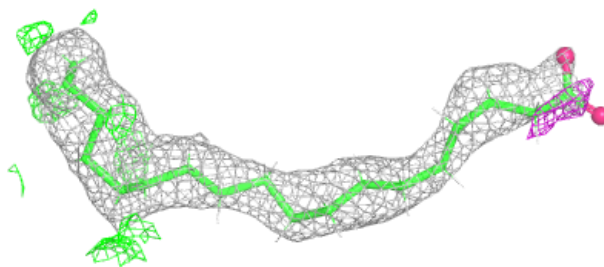
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	B	605	65/65	0.96	0.07	21,38,53,60	0
22	CLA	c	505	65/65	0.96	0.08	31,46,72,76	0
22	CLA	C	501	65/65	0.96	0.06	26,42,59,65	0
22	CLA	c	507	65/65	0.96	0.07	31,50,65,78	0
22	CLA	D	403	65/65	0.96	0.07	22,36,54,66	0
22	CLA	D	404	65/65	0.96	0.07	23,35,56,65	0
22	CLA	D	405	65/65	0.96	0.08	26,50,128,138	0
22	CLA	a	402	65/65	0.96	0.07	23,36,50,58	0
22	CLA	A	402	65/65	0.96	0.07	20,33,48,57	0
22	CLA	B	609	65/65	0.96	0.07	28,43,61,65	0
22	CLA	d	401	65/65	0.96	0.09	28,47,105,111	0
33	BCT	D	402	4/4	0.96	0.08	28,35,45,54	0
22	CLA	d	403	65/65	0.96	0.09	23,41,64,74	0
34	HEM	f	101	43/43	0.96	0.09	43,64,91,99	0
28	LHG	D	410	49/49	0.96	0.08	31,46,59,66	0
22	CLA	B	608	65/65	0.97	0.06	27,43,64,69	0
22	CLA	A	403	65/65	0.97	0.08	25,41,95,103	0
22	CLA	A	405	54/65	0.97	0.06	22,39,70,82	0
22	CLA	B	603	65/65	0.97	0.07	23,39,62,68	0
34	HEM	F	101	43/43	0.97	0.08	36,54,73,75	0
22	CLA	b	603	65/65	0.97	0.07	24,42,74,90	0
22	CLA	B	607	65/65	0.97	0.07	19,40,81,87	0
24	CL	A	407	1/1	0.98	0.03	37,37,37,37	0
24	CL	a	407	1/1	0.98	0.07	34,34,34,34	0
35	HEC	V	201	43/43	0.98	0.07	24,39,48,49	0
35	HEC	v	201	43/43	0.98	0.07	29,44,55,61	0
24	CL	A	406	1/1	0.98	0.04	36,36,36,36	0
24	CL	a	406	1/1	0.99	0.02	33,33,33,33	0
21	FE2	A	401	1/1	0.99	0.03	31,31,31,31	0
30	OEX	A	414	10/10	0.99	0.04	27,36,39,39	0
30	OEX	a	414	10/10	0.99	0.03	29,35,39,44	0
21	FE2	a	401	1/1	1.00	0.02	36,36,36,36	0

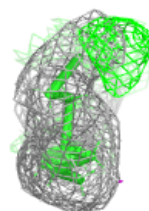
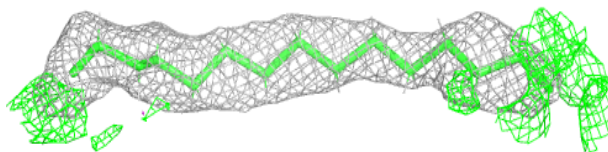
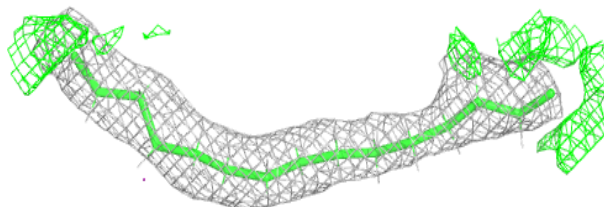
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

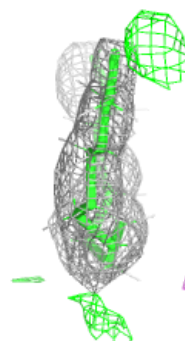
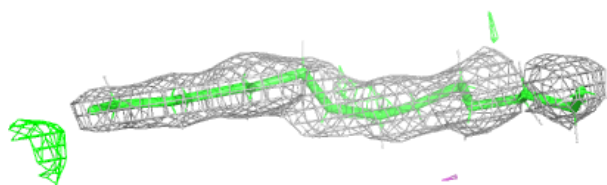
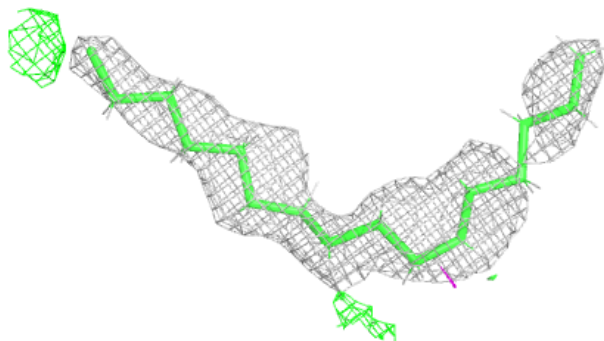
**Electron density around STE I 102:**

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

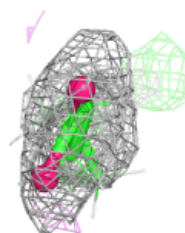
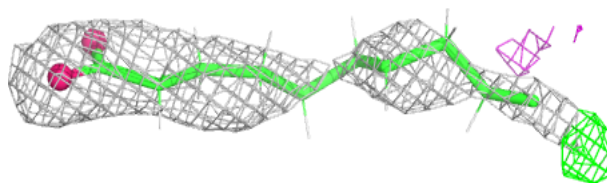
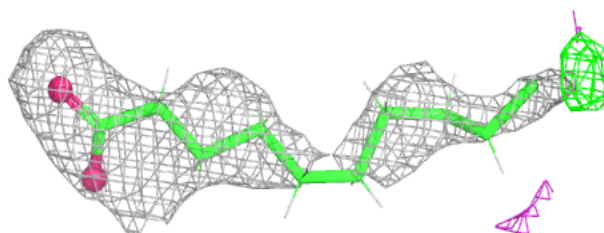


Electron density around STE B 625:

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

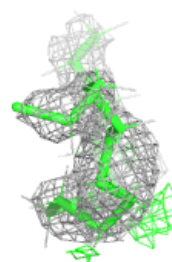
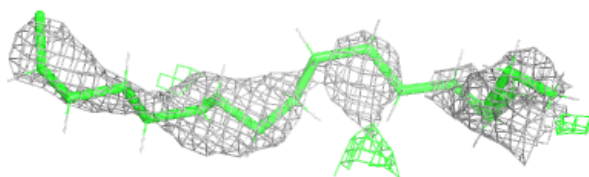
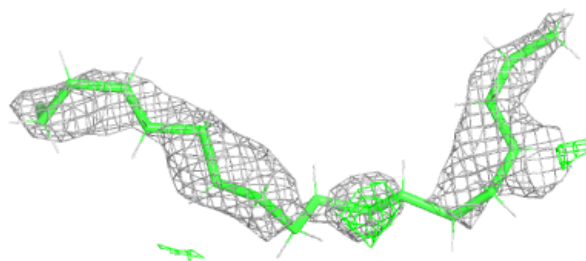
**Electron density around STE a 412:**

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

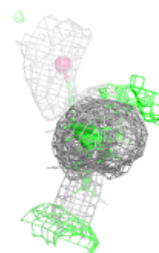
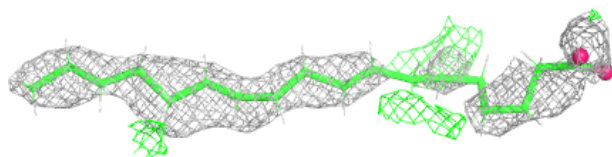
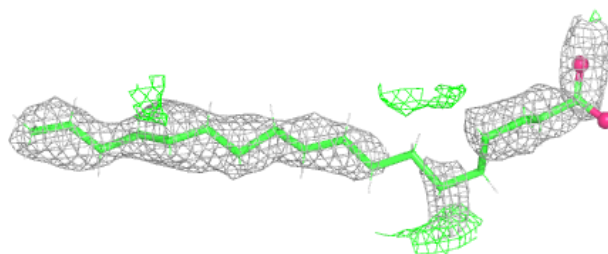


Electron density around STE H 103:

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

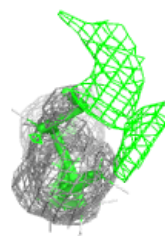
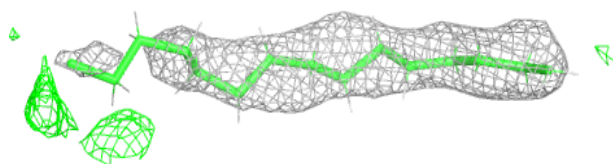
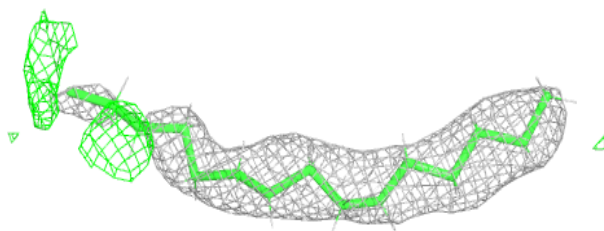
**Electron density around STE b 625:**

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

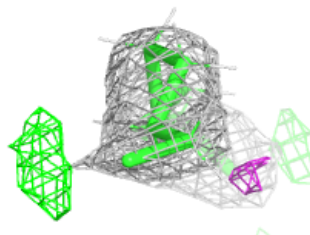
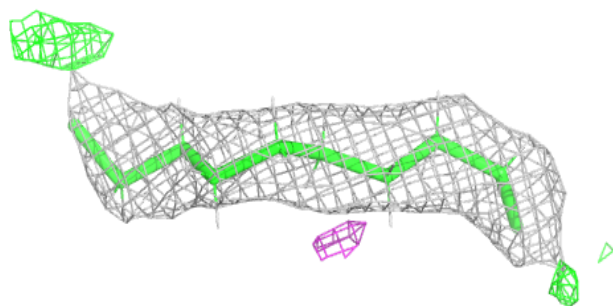
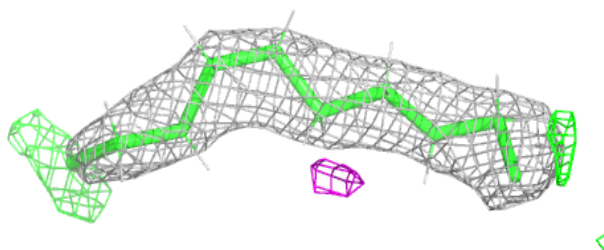


Electron density around STE b 624:

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

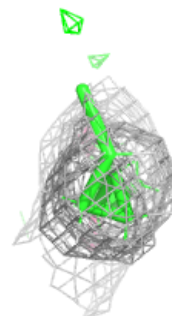
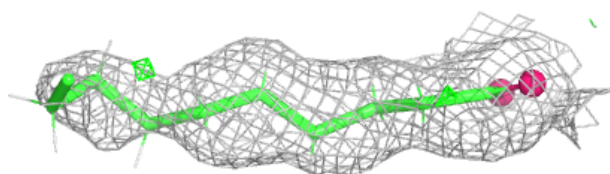
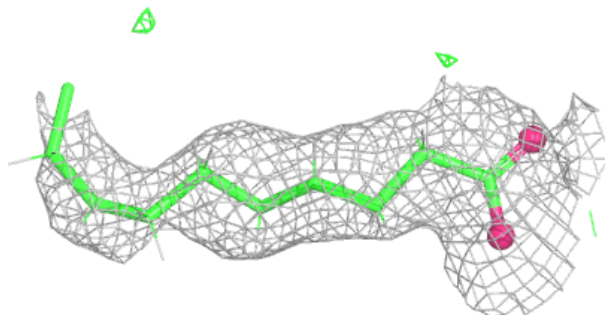
**Electron density around STE b 626:**

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



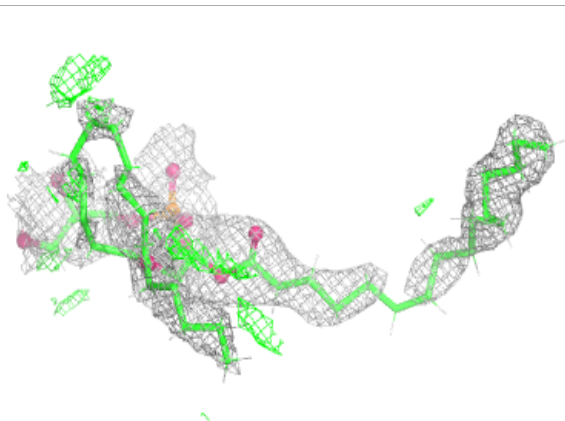
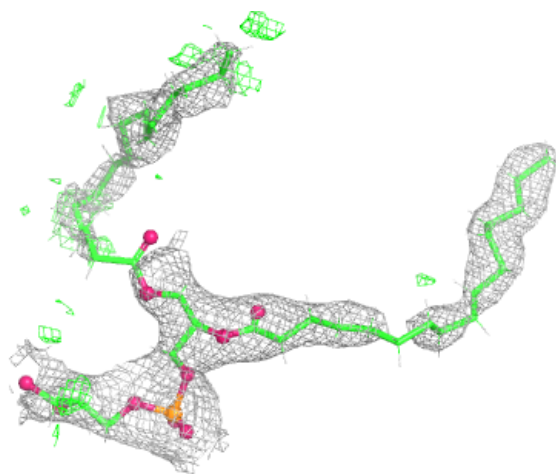
Electron density around STE c 523:

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



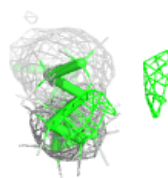
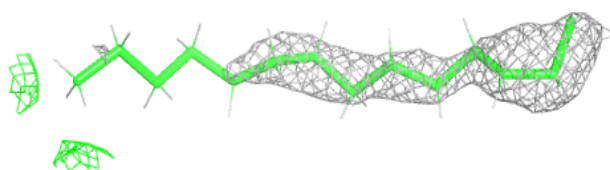
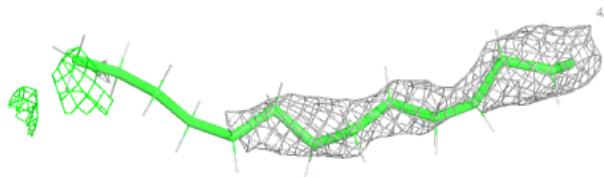
Electron density around LHG A 411:

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

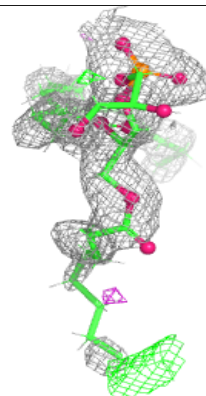
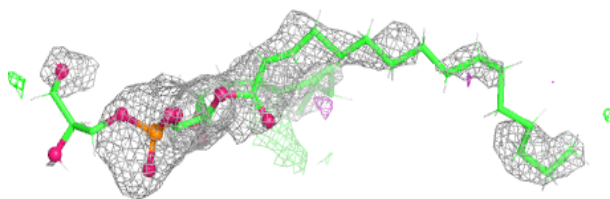
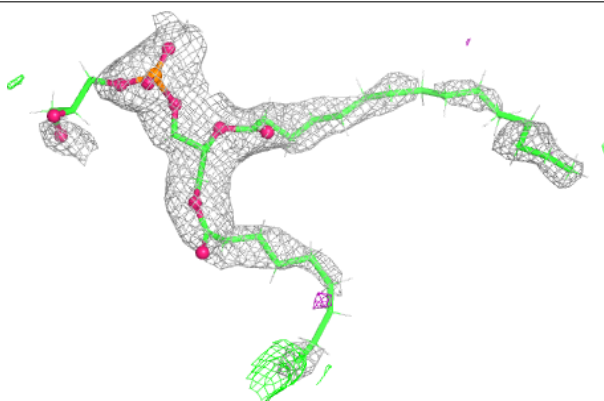


Electron density around STE b 627:

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

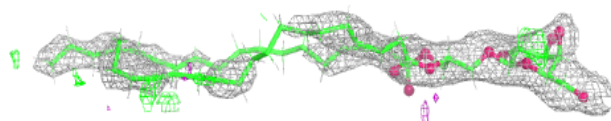
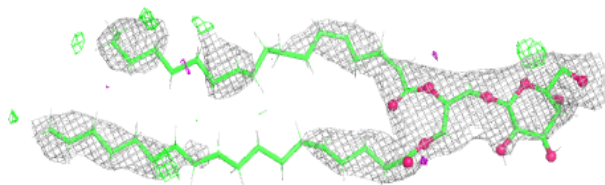
**Electron density around LHG e 101:**

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

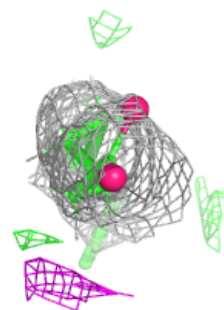
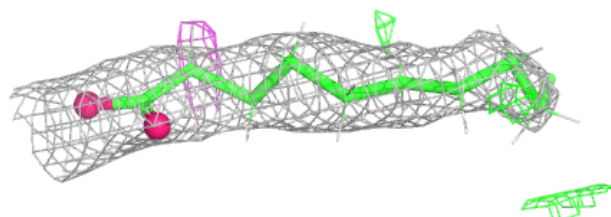
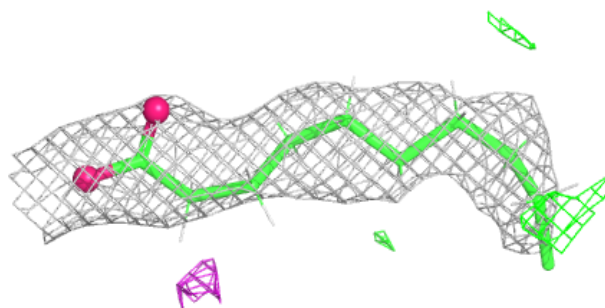


Electron density around LMG b 622:

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

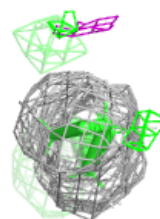
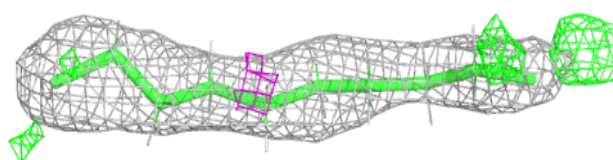
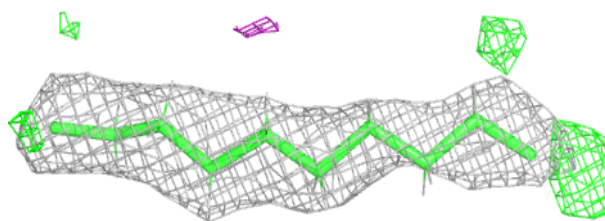
**Electron density around STE L 103:**

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

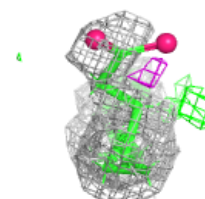
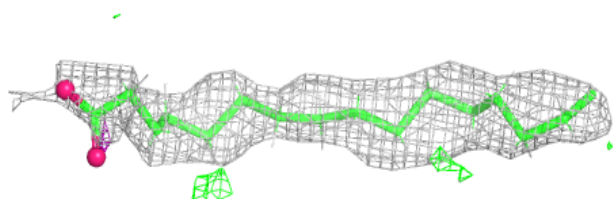
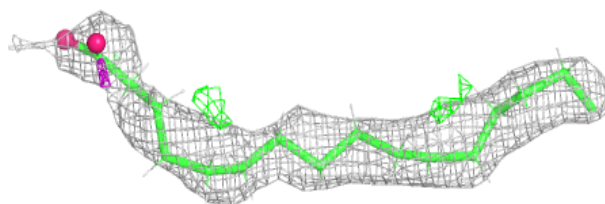


Electron density around STE M 103:

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

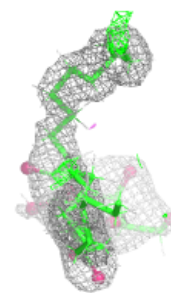
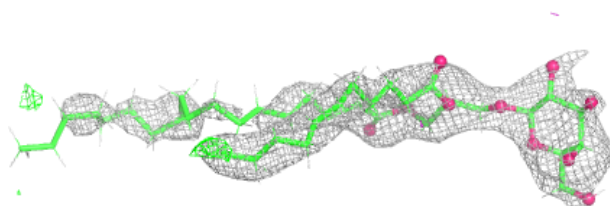
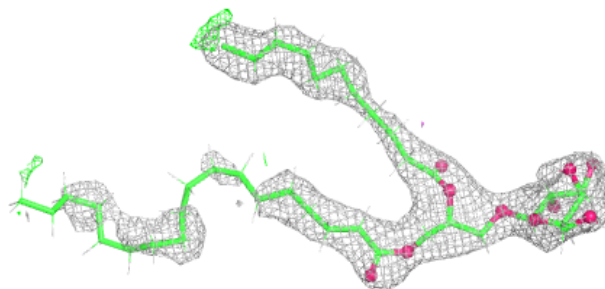
**Electron density around STE B 624:**

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



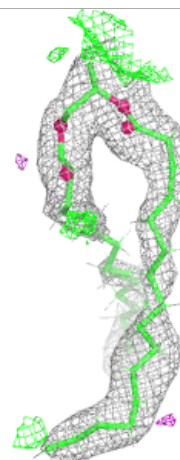
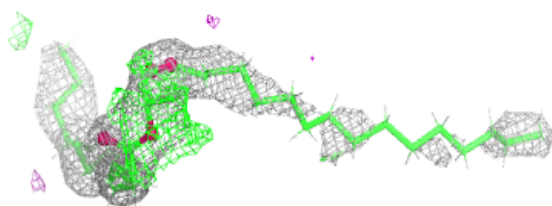
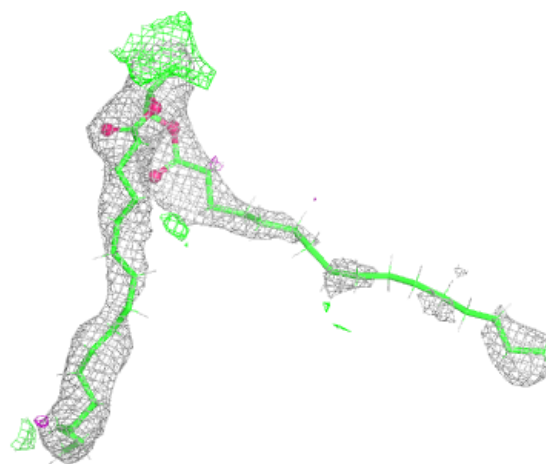
Electron density around LMG c 521:

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



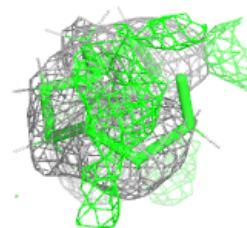
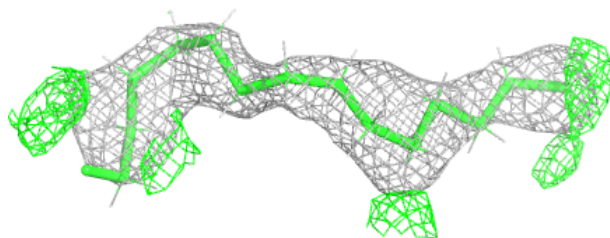
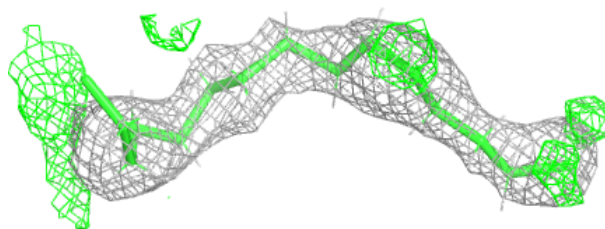
Electron density around SQD A 412:

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

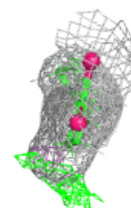
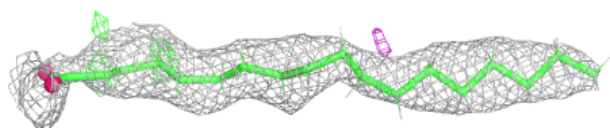
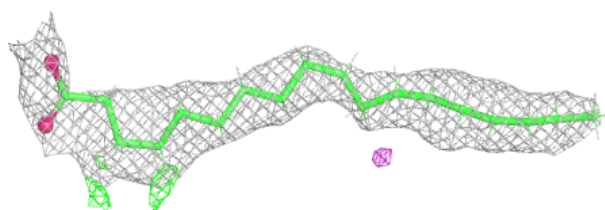


Electron density around STE a 413:

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

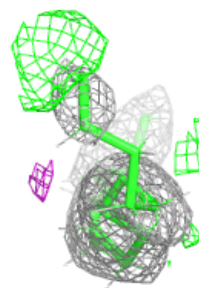
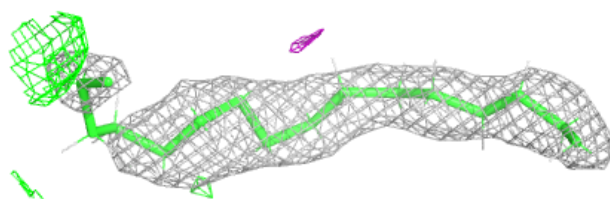
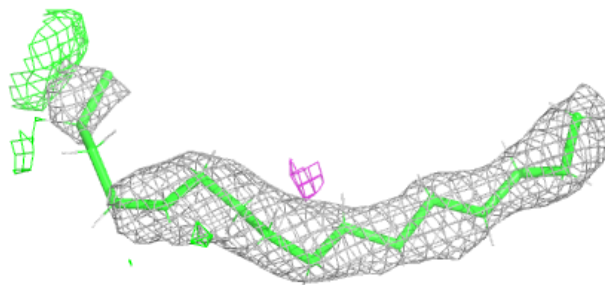
**Electron density around STE c 520:**

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

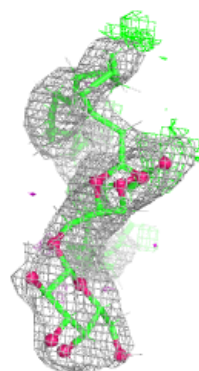
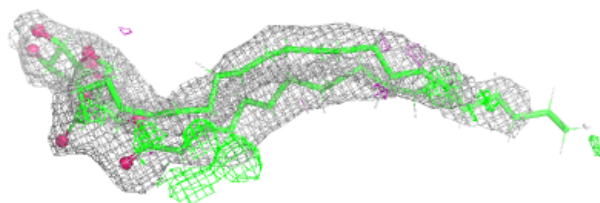
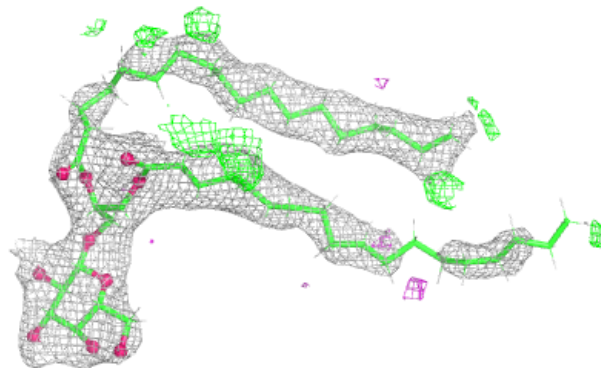


Electron density around STE b 620:

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

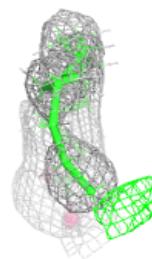
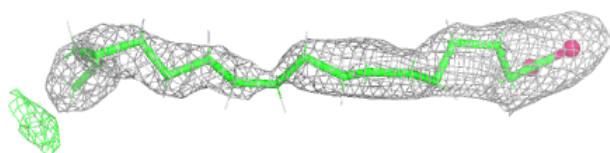
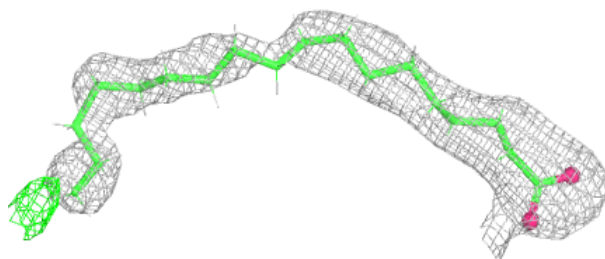
**Electron density around LMG B 626:**

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

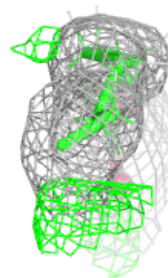
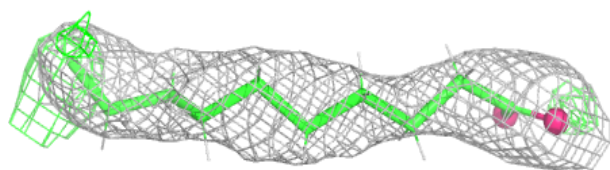
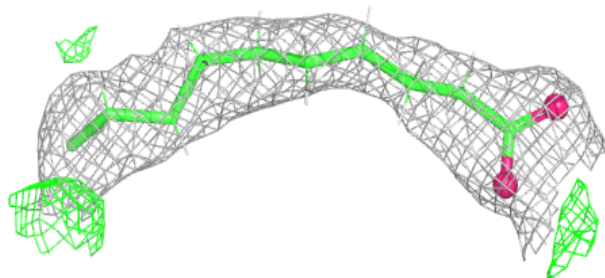


Electron density around STE x 102:

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

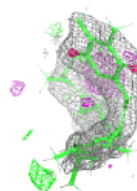
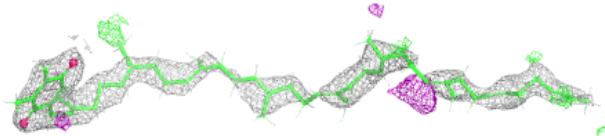
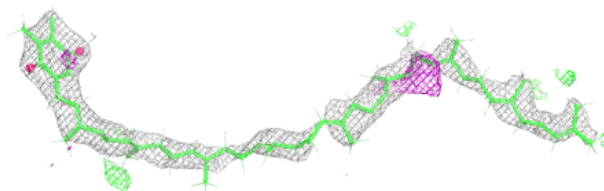
**Electron density around STE C 518:**

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

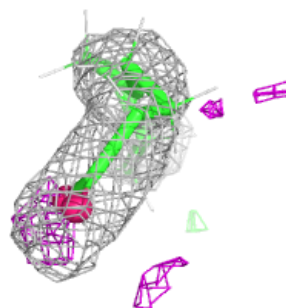
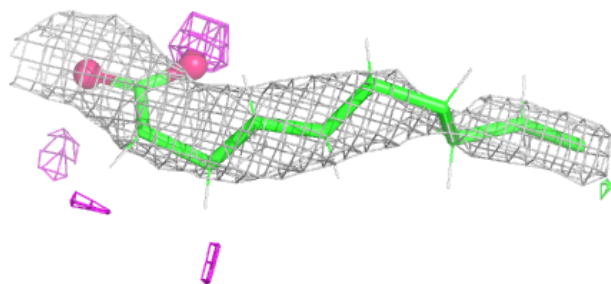
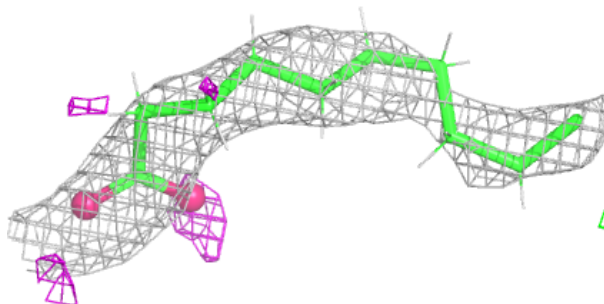


Electron density around PL9 A 408:

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

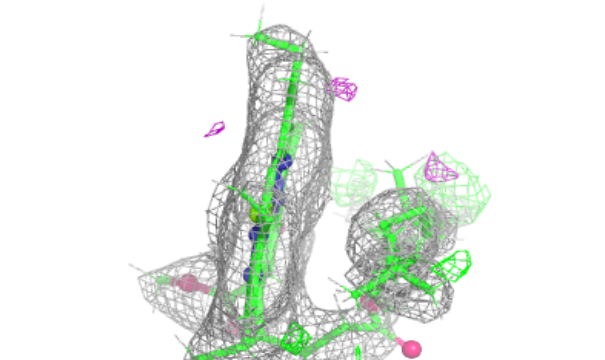
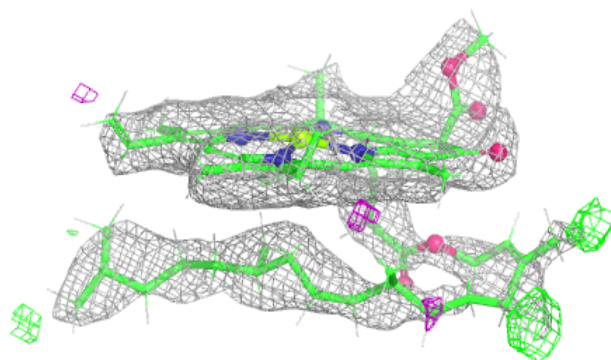
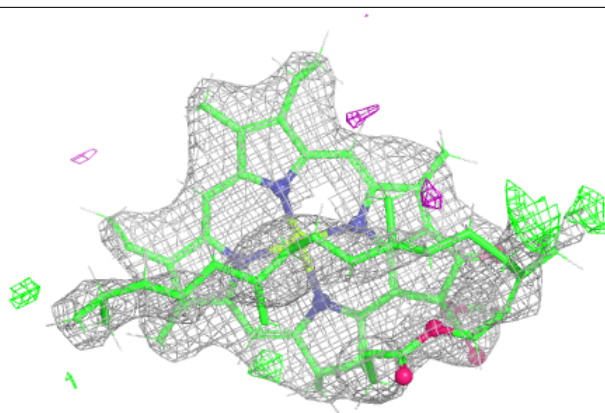
**Electron density around STE B 627:**

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

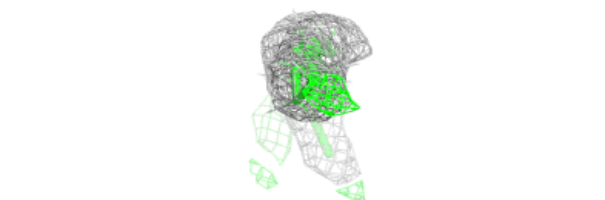
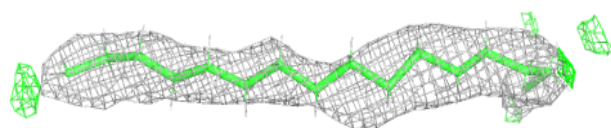
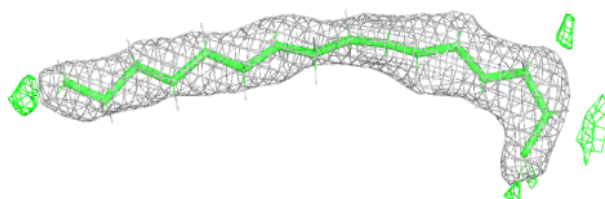


Electron density around CLA b 601:

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

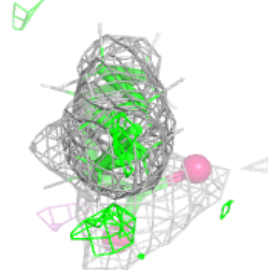
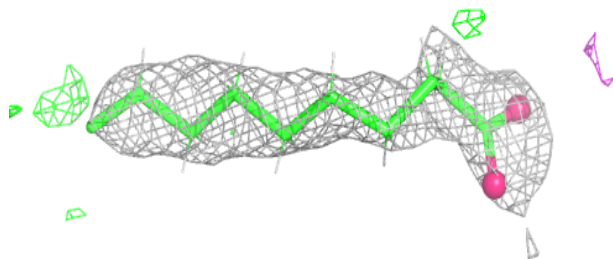
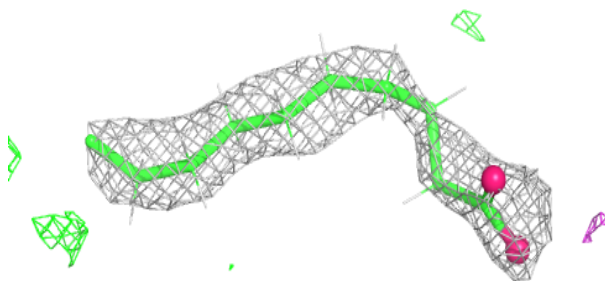
**Electron density around STE C 519:**

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

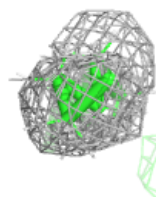
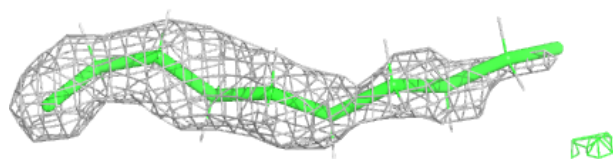
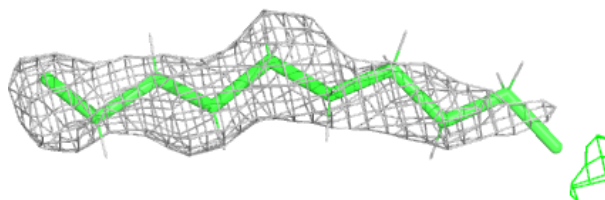


Electron density around STE R 101:

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

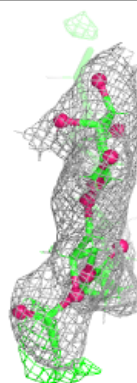
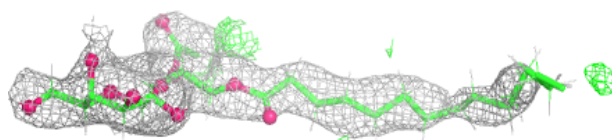
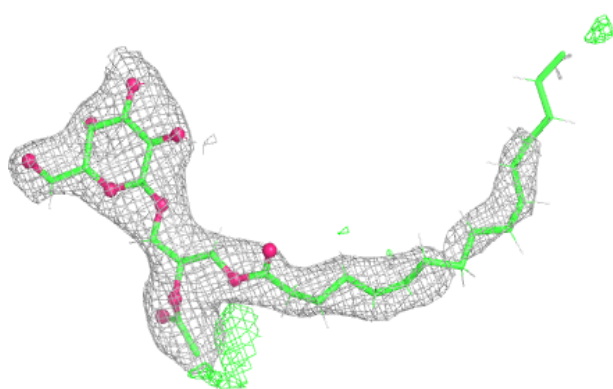
**Electron density around STE t 104:**

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

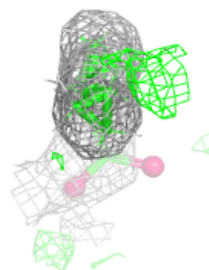
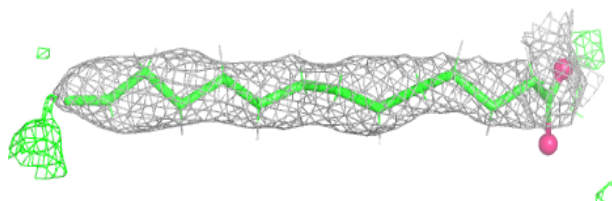
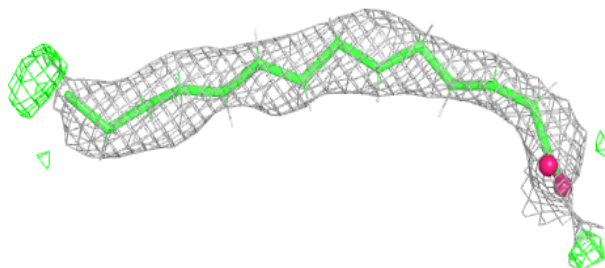


Electron density around LMG c 519:

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

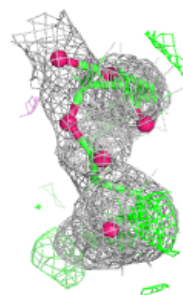
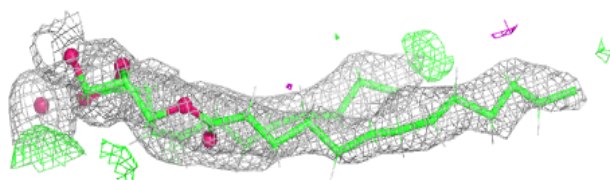
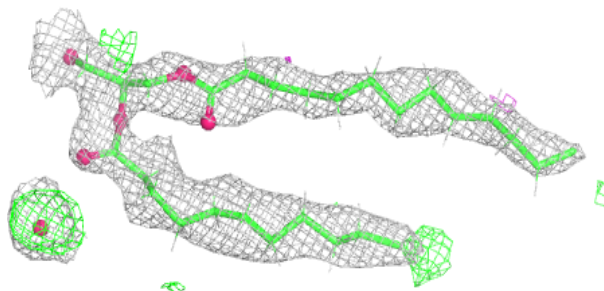
**Electron density around STE b 623:**

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

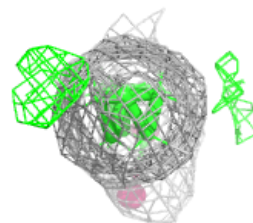
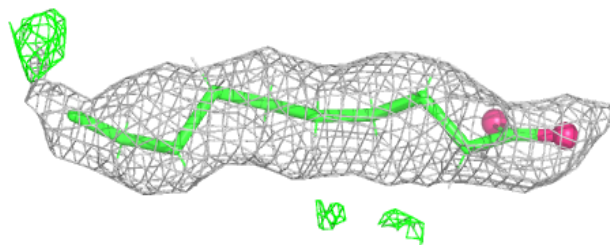
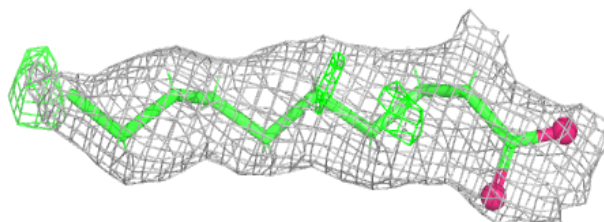


Electron density around LMG D 412:

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

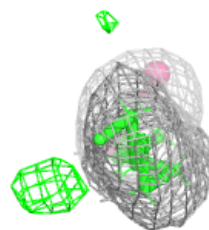
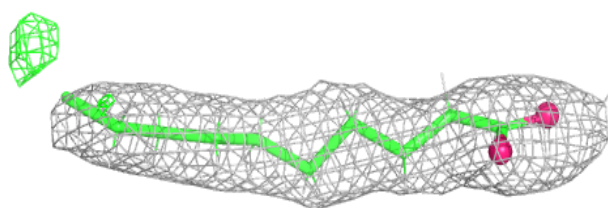
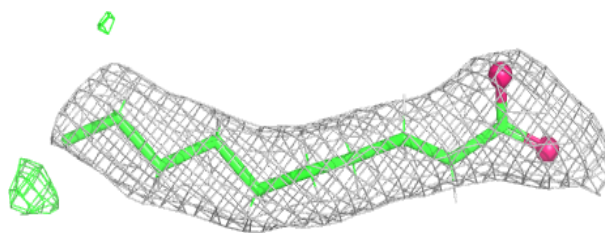
**Electron density around STE J 101:**

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



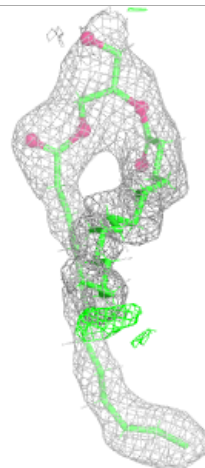
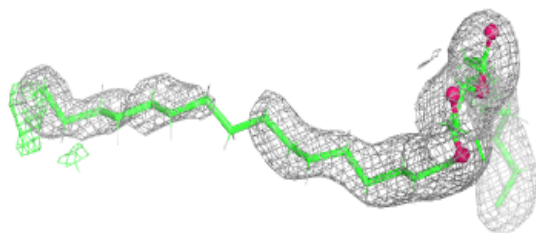
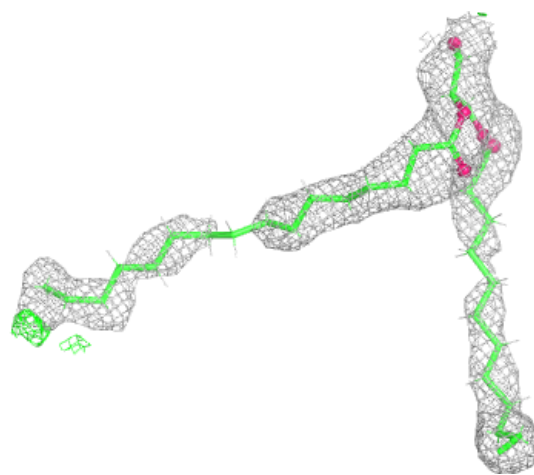
Electron density around STE j 101:

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



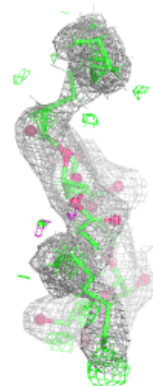
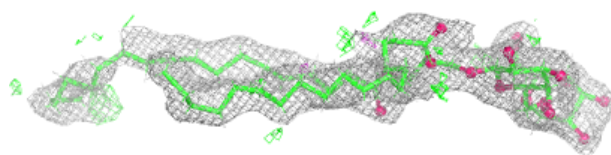
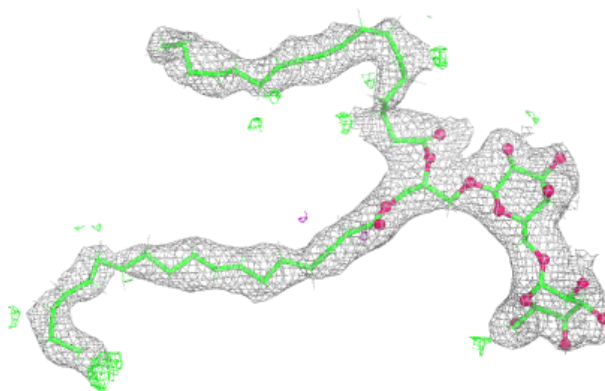
Electron density around SQD t 102:

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

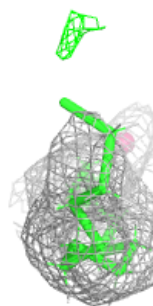
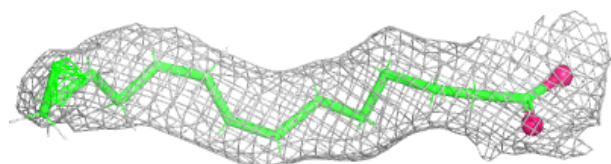
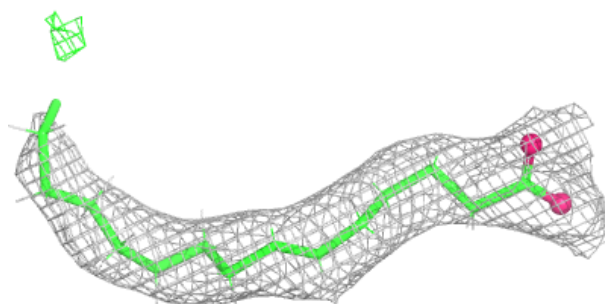


Electron density around DGD A 413:

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

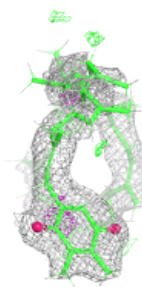
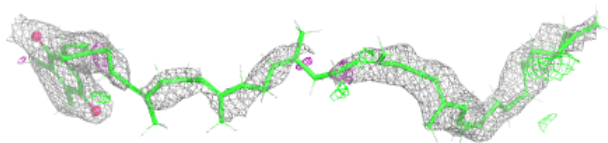
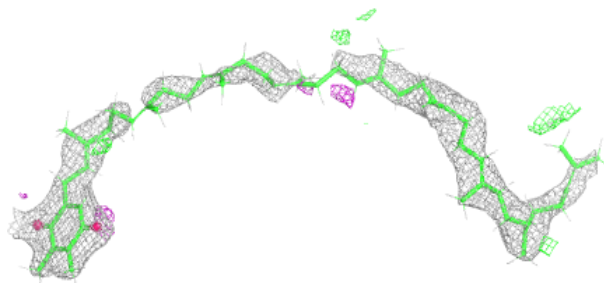
**Electron density around STE B 620:**

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

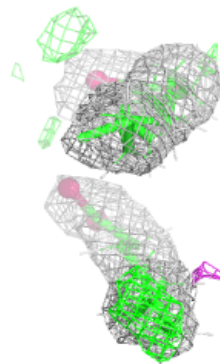
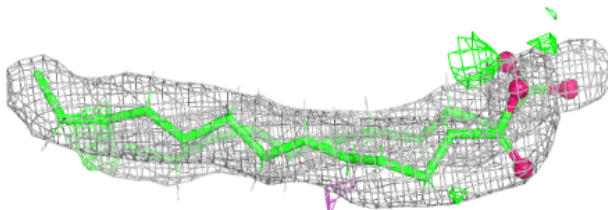
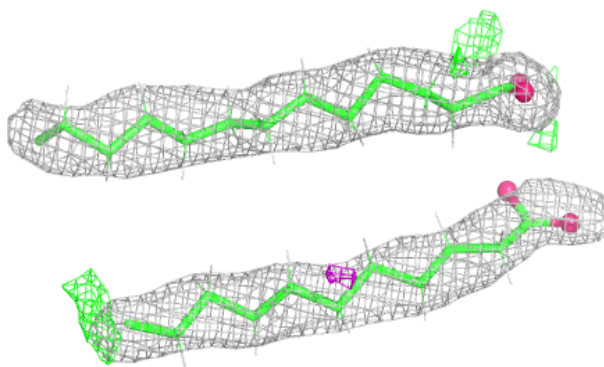


Electron density around PL9 a 409:

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

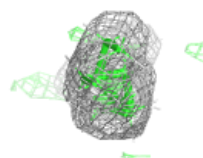
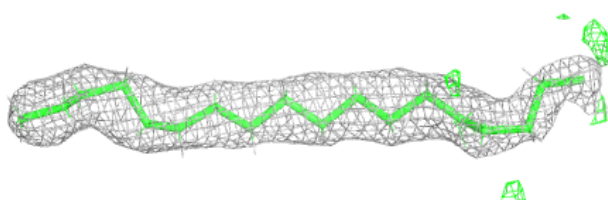
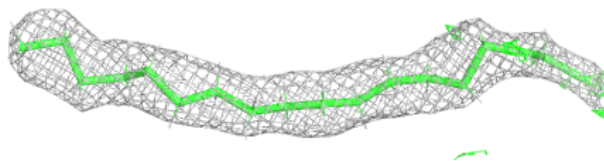
**Electron density around LMG B 621:**

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

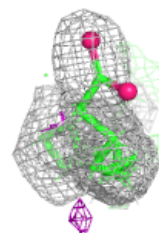
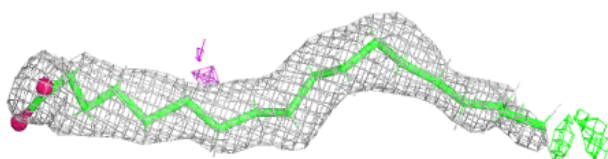
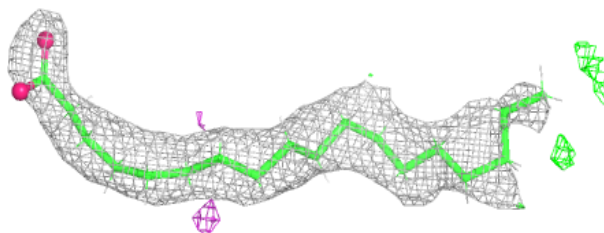


Electron density around STE l 102:

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

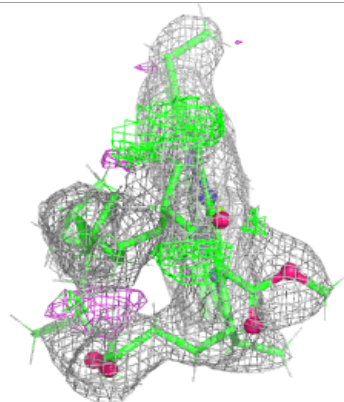
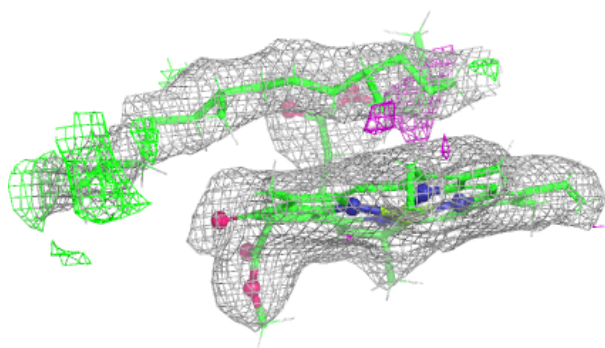
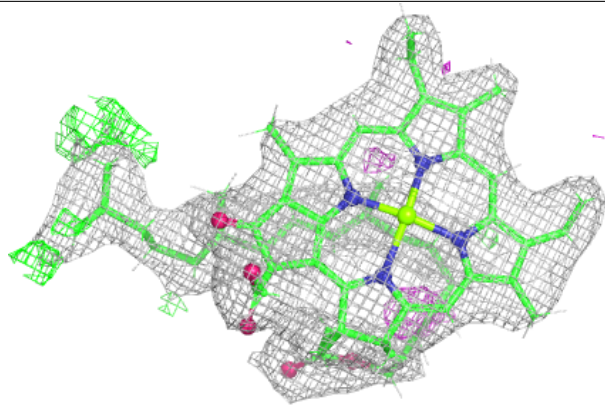
**Electron density around STE b 621:**

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

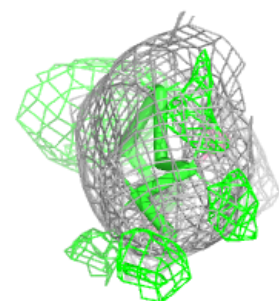
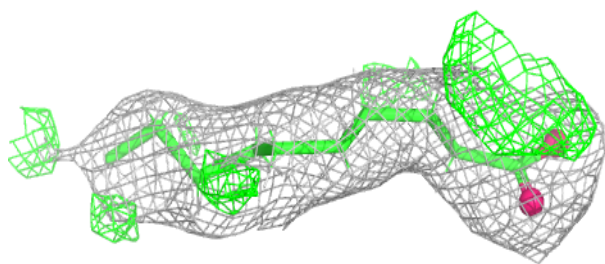
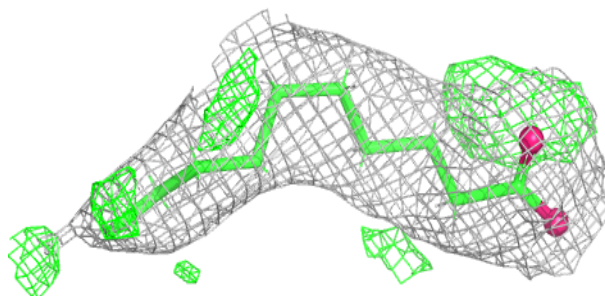


Electron density around CLA B 601:

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

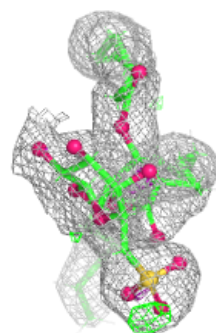
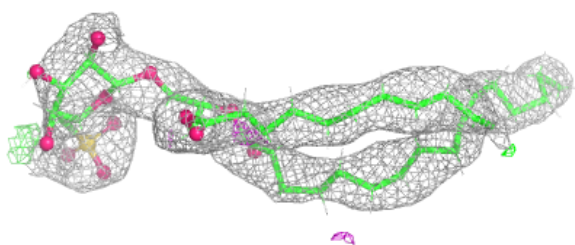
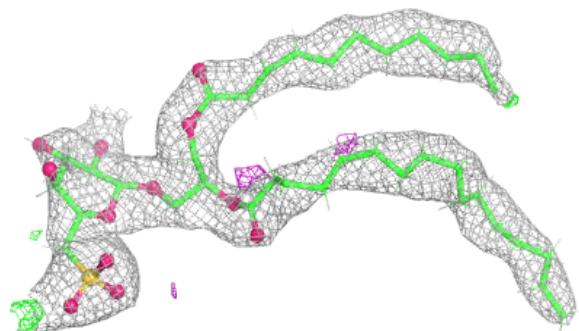
**Electron density around STE B 623:**

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

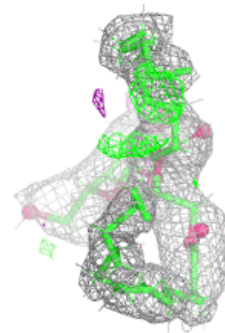
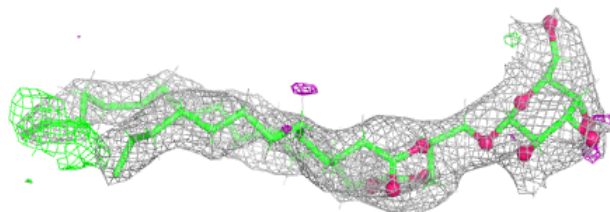
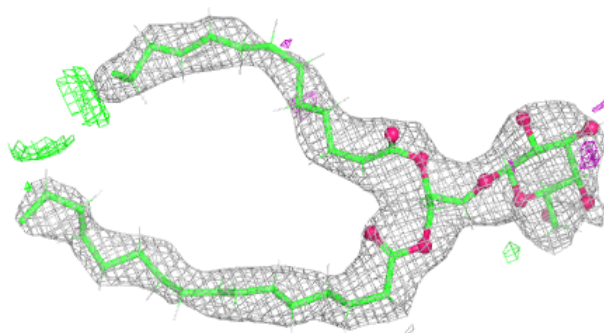


Electron density around SQD L 101:

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

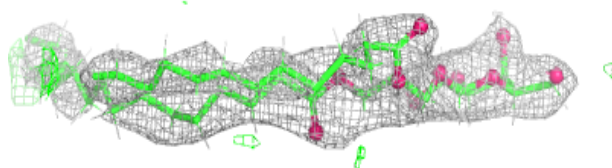
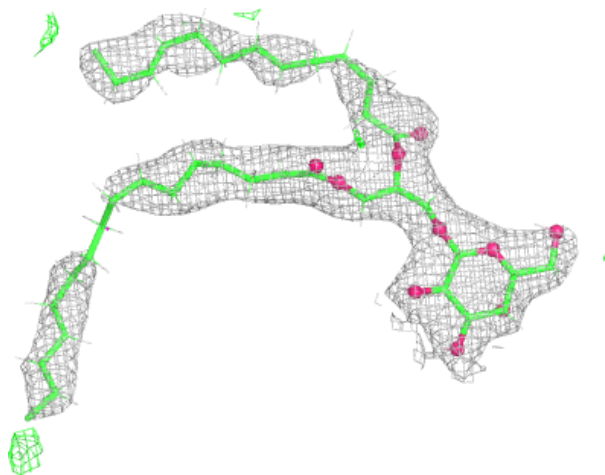
**Electron density around LMG A 409:**

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



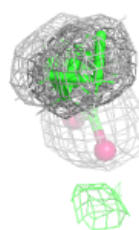
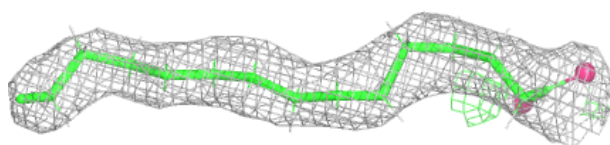
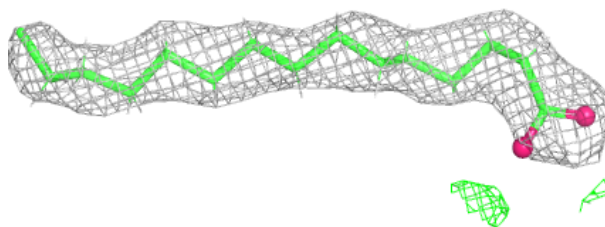
Electron density around LMG Y 101:

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

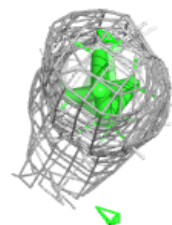
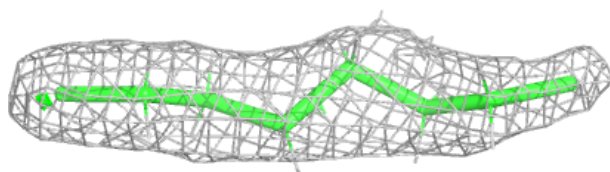
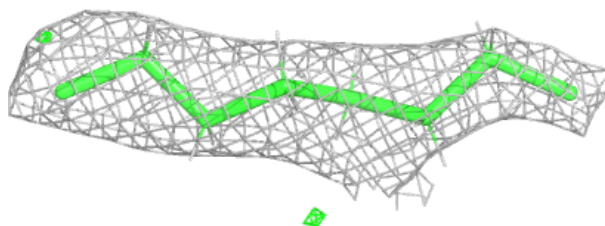


Electron density around STE d 411:

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

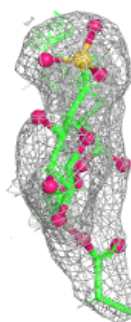
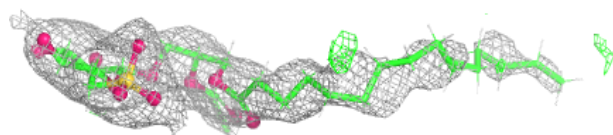
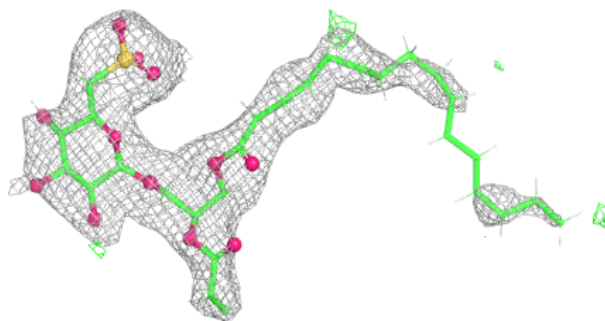
**Electron density around STE Z 102:**

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

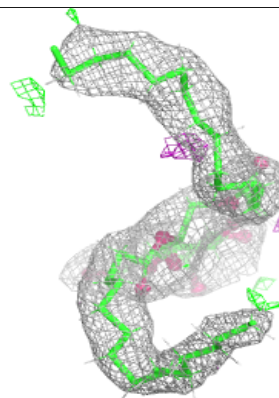
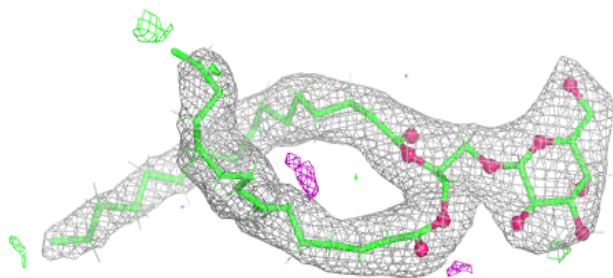
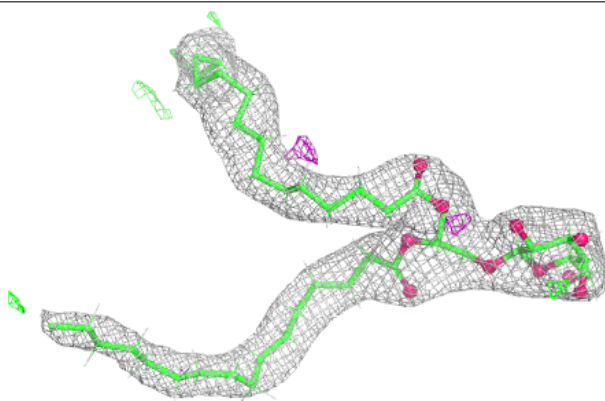


Electron density around SQD f 102:

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

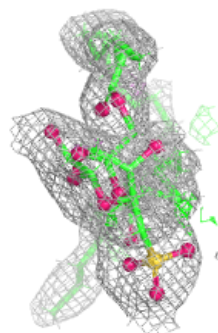
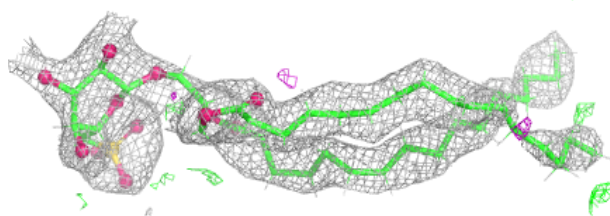
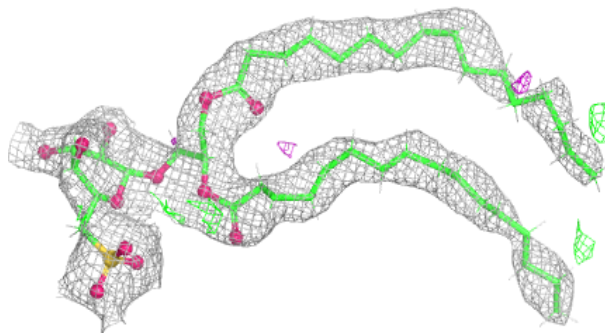
**Electron density around LMG M 101:**

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

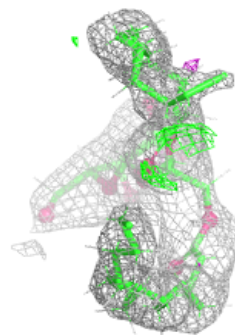
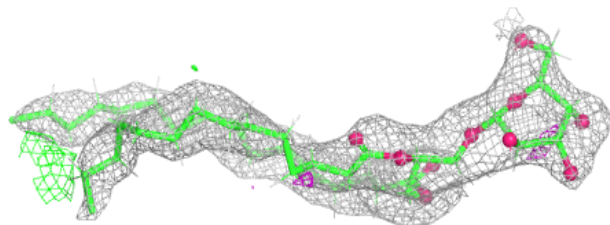
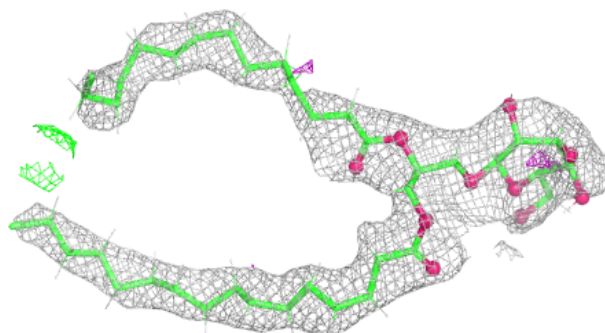


Electron density around SQD B 622:

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

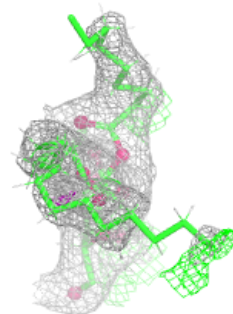
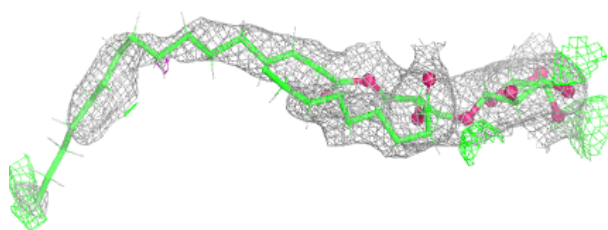
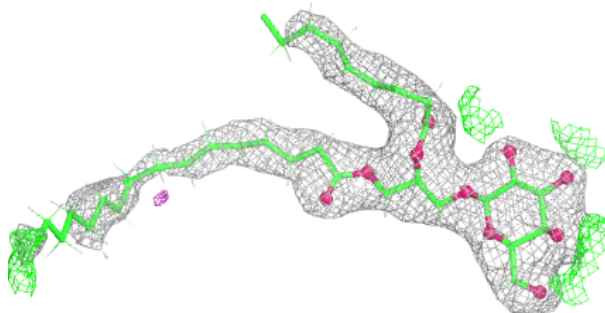
**Electron density around LMG c 522:**

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

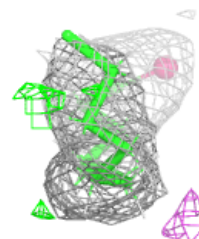
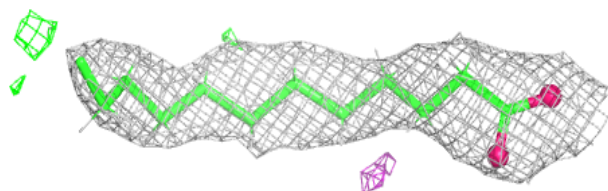
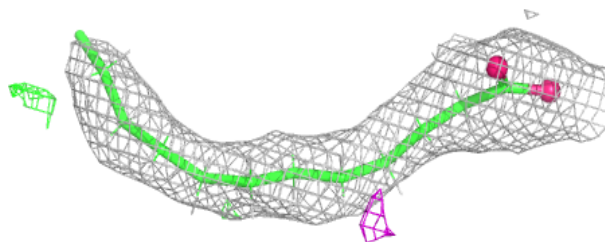


Electron density around LMG d 410:

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

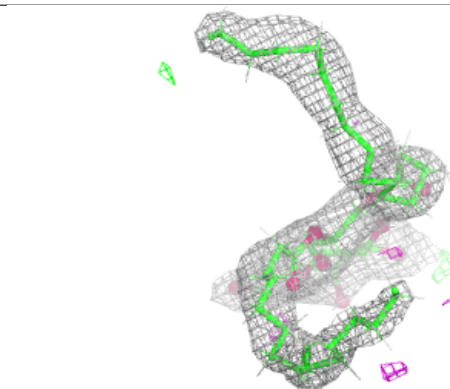
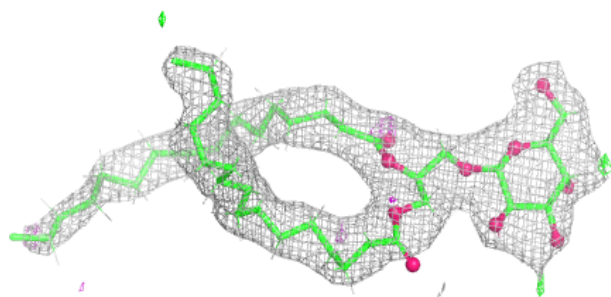
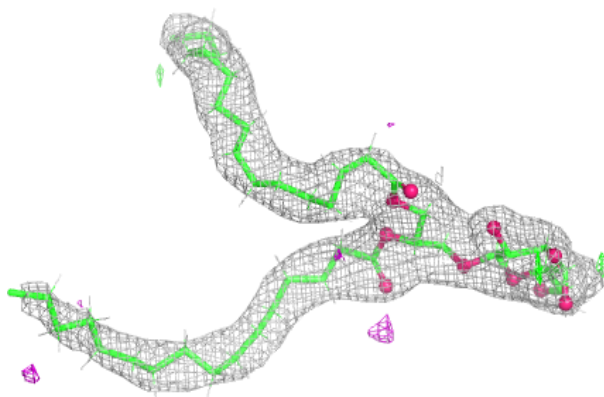
**Electron density around STE t 103:**

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

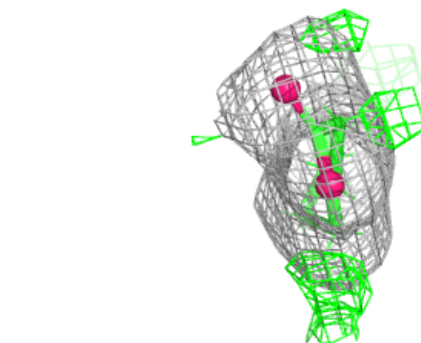
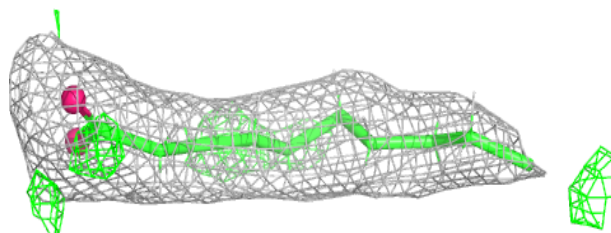
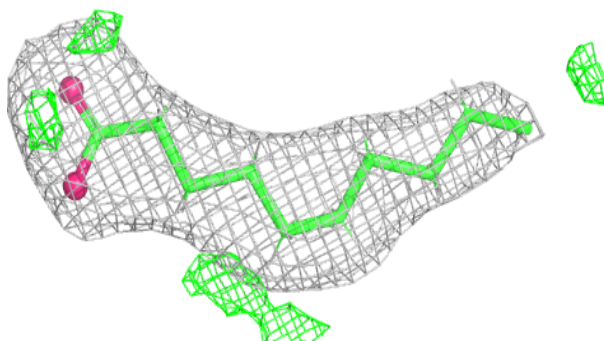


Electron density around LMG m 101:

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

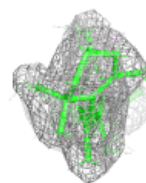
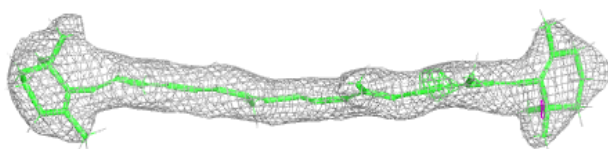
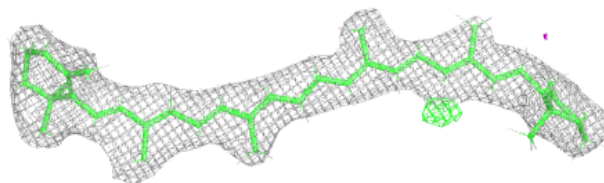
**Electron density around STE C 520:**

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

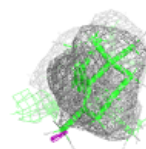
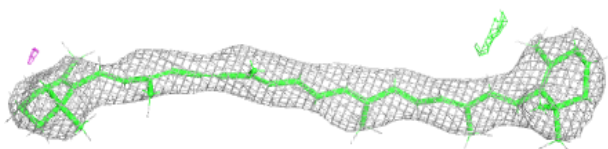
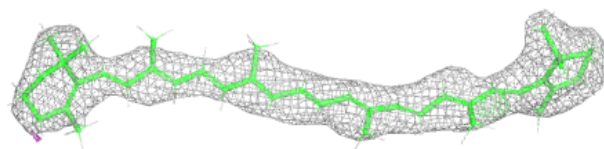


Electron density around BCR K 101:

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

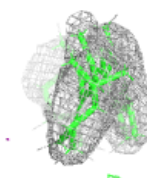
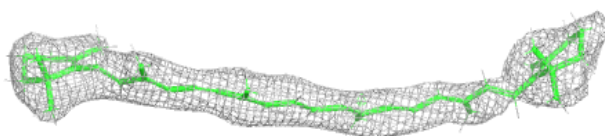
**Electron density around BCR c 514:**

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

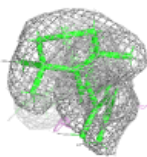
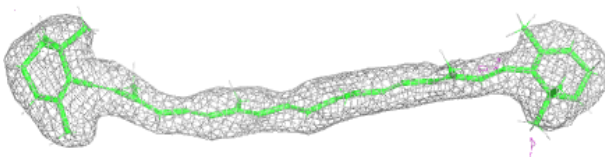
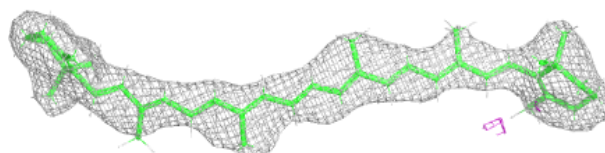


Electron density around BCR d 406:

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

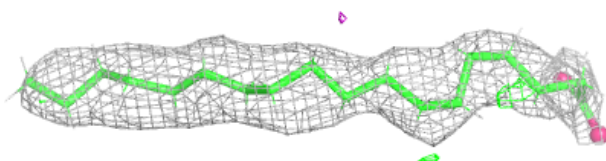
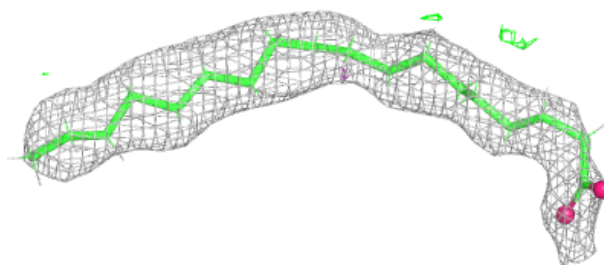
**Electron density around BCR x 101:**

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



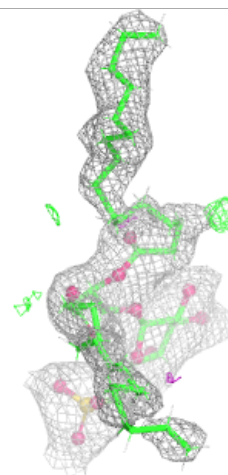
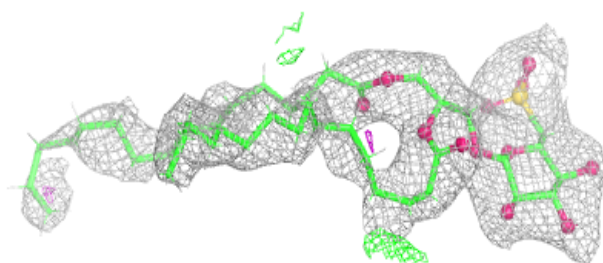
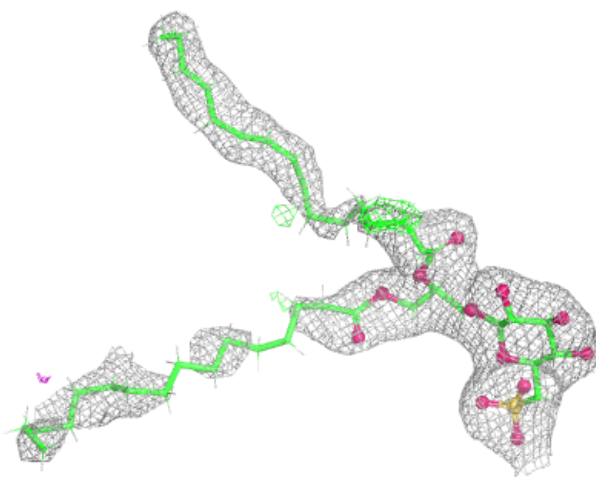
Electron density around STE X 101:

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



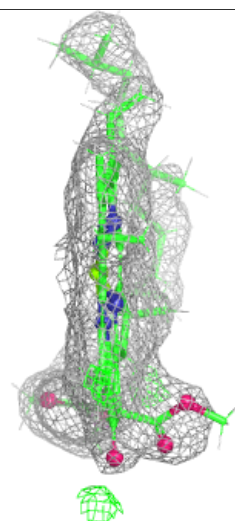
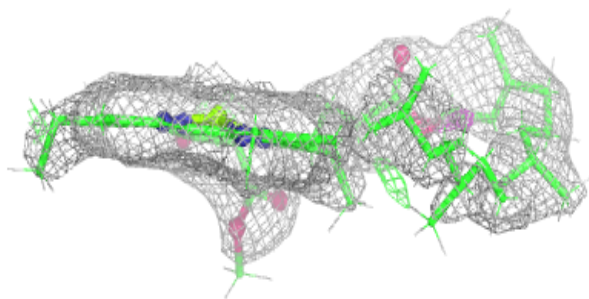
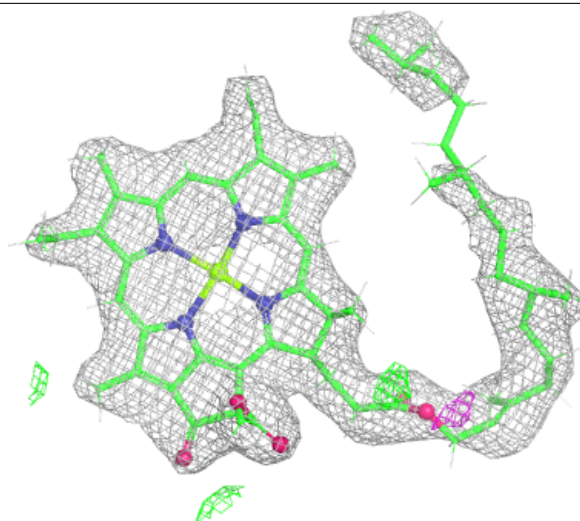
Electron density around SQD a 411:

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



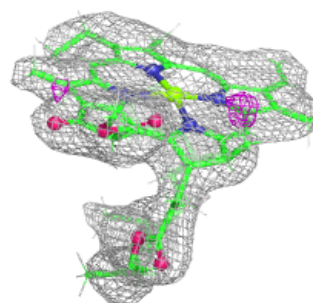
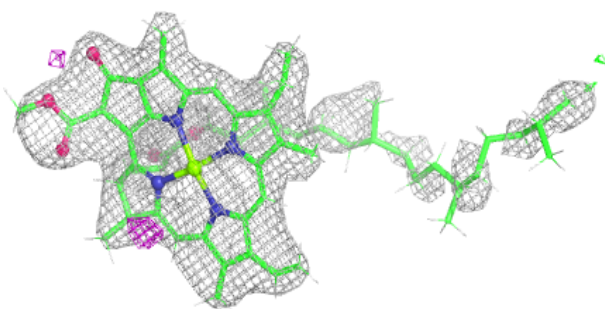
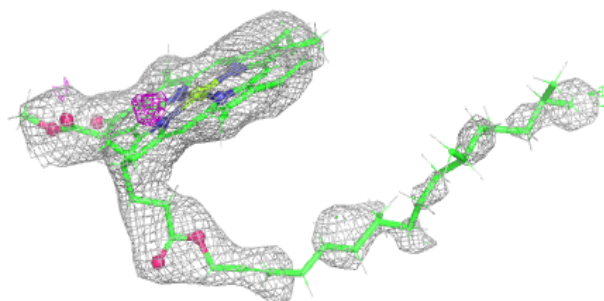
Electron density around CLA c 512:

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

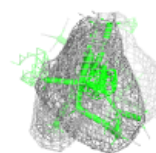
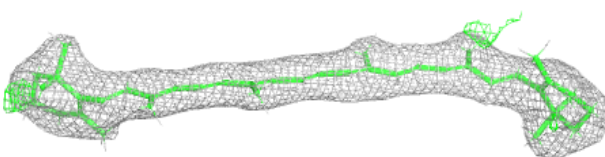
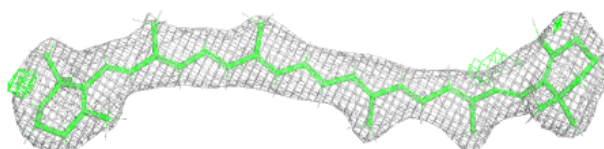


Electron density around CLA C 513:

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

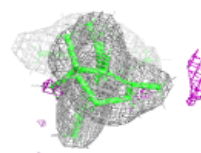
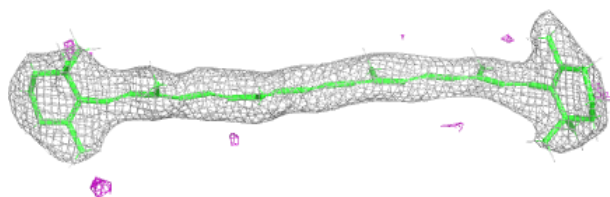
**Electron density around BCR B 619:**

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

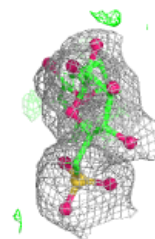
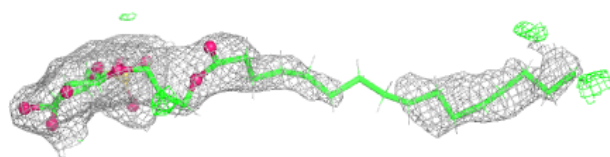
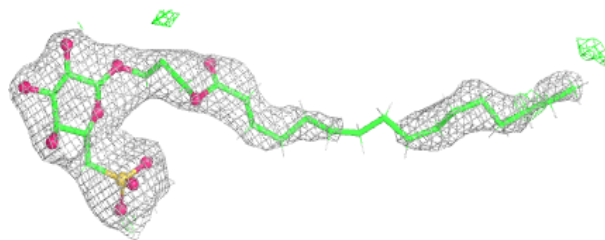


Electron density around BCR C 514:

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

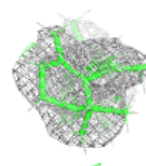
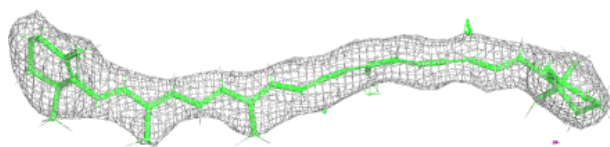
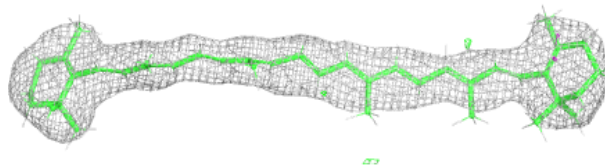
**Electron density around SQD D 409:**

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

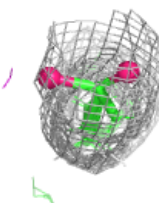
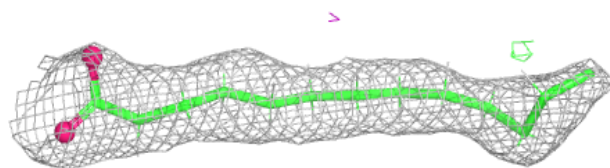
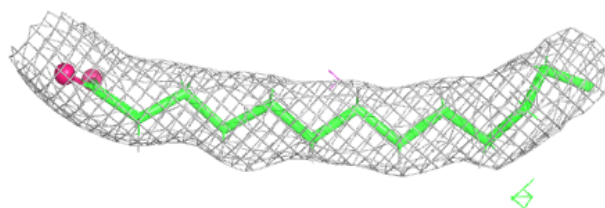


Electron density around BCR Z 101:

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

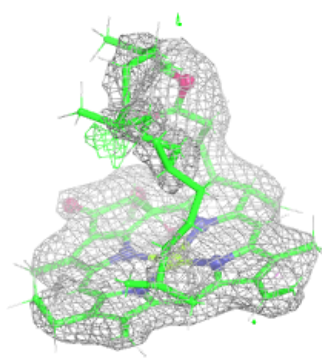
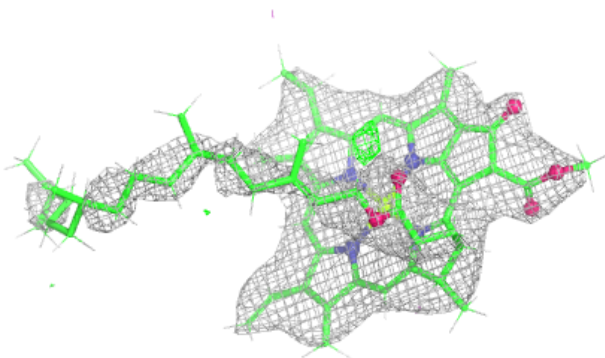
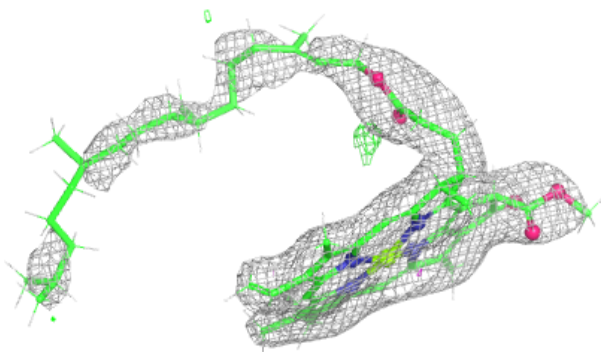
**Electron density around STE M 102:**

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

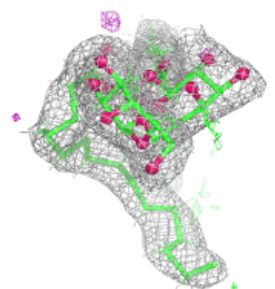
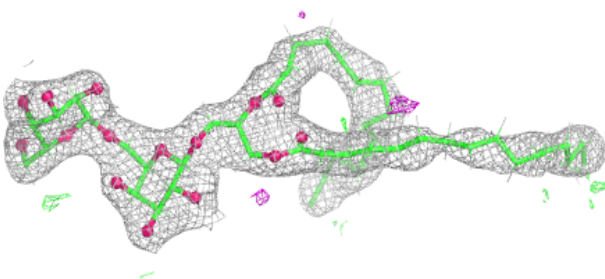
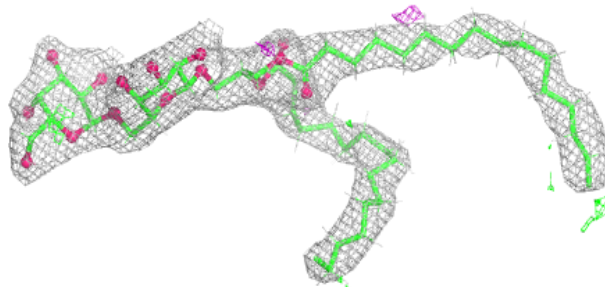


Electron density around CLA c 513:

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

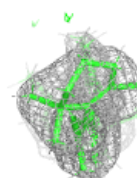
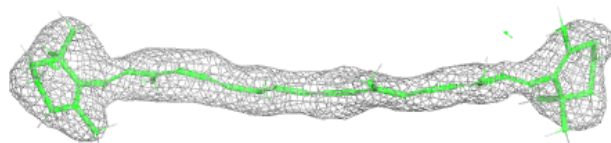
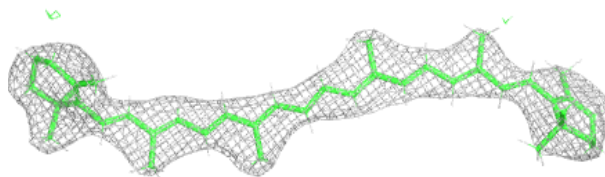
**Electron density around DGD H 102:**

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

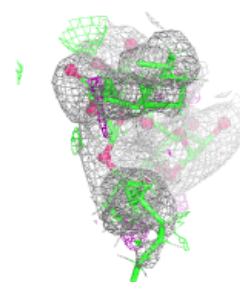
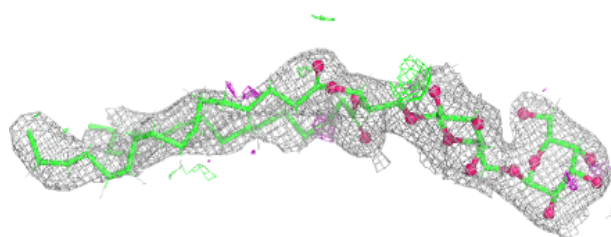
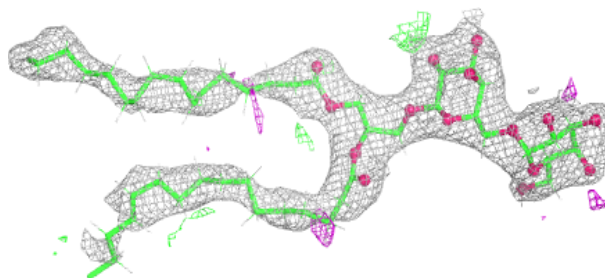


Electron density around BCR k 101:

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

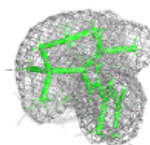
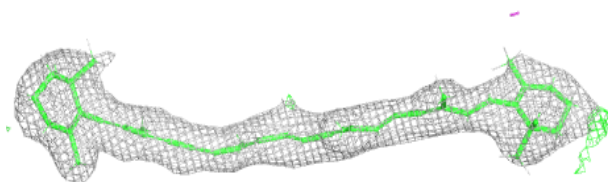
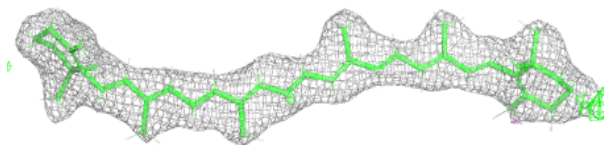
**Electron density around DGD c 518:**

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



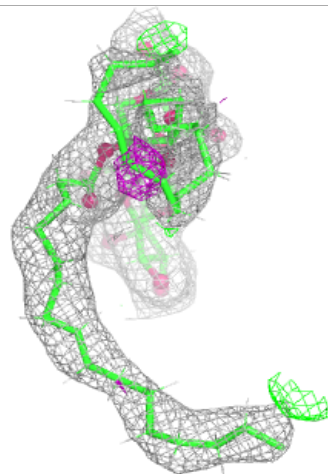
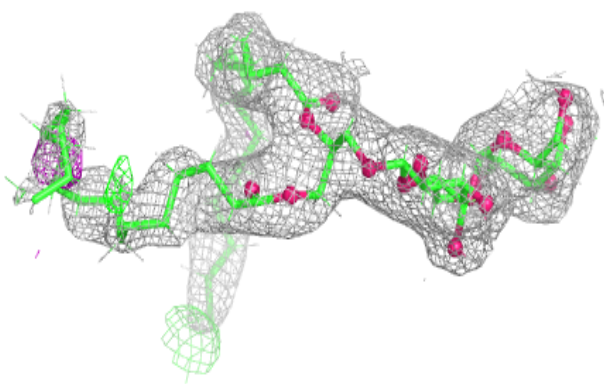
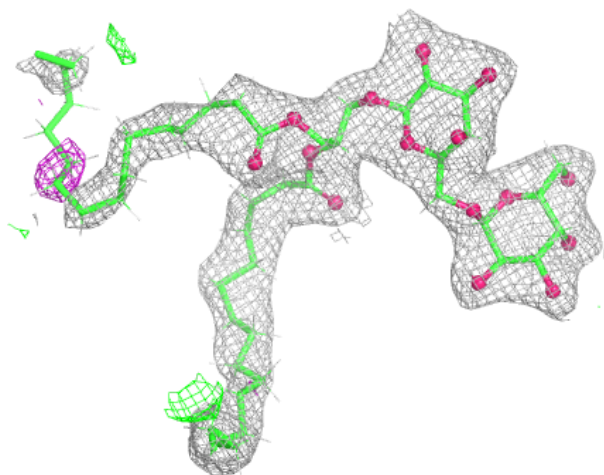
Electron density around BCR H 101:

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



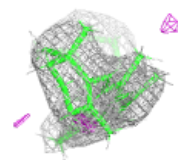
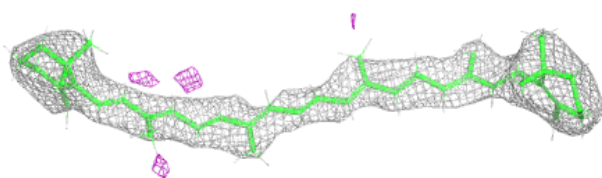
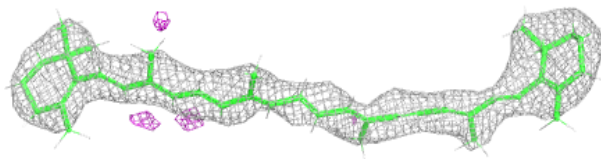
Electron density around DGD C 516:

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

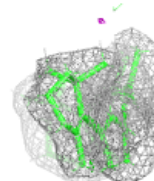
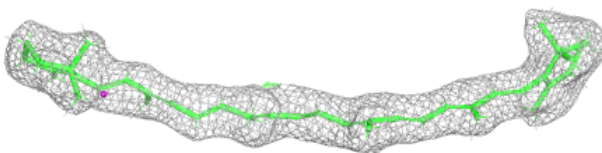
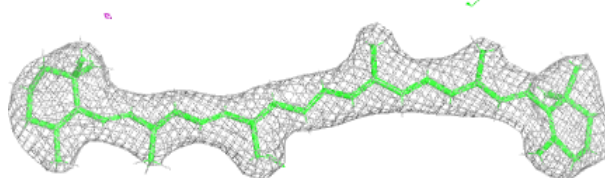


Electron density around BCR K 102:

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

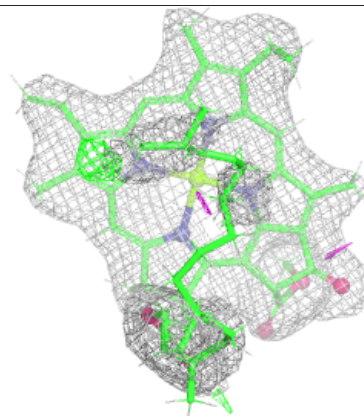
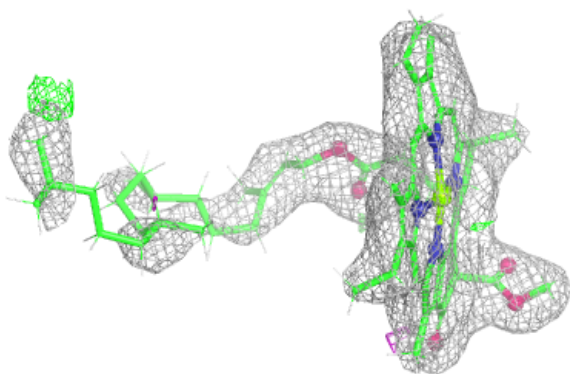
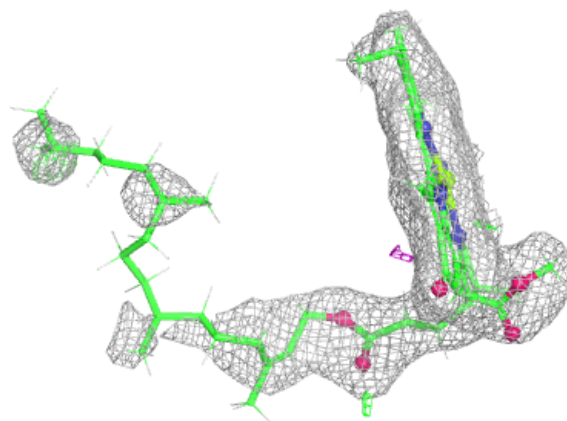
**Electron density around BCR T 101:**

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

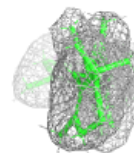
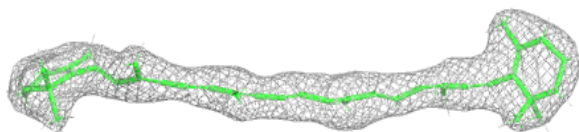


Electron density around CLA c 506:

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

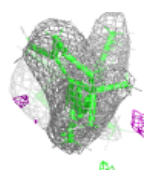
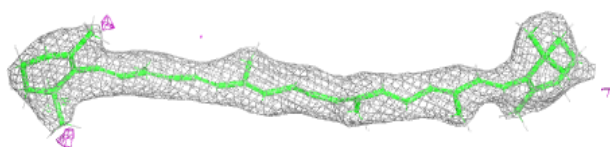
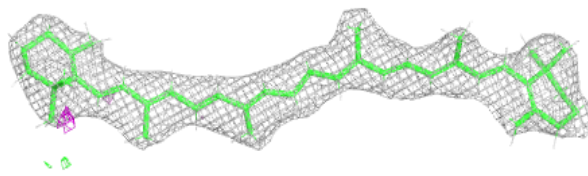
**Electron density around BCR b 617:**

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

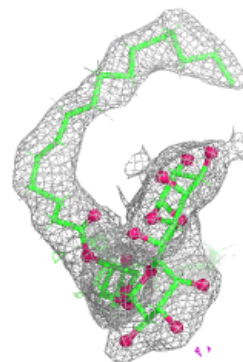
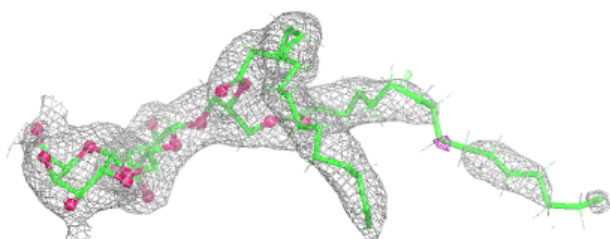
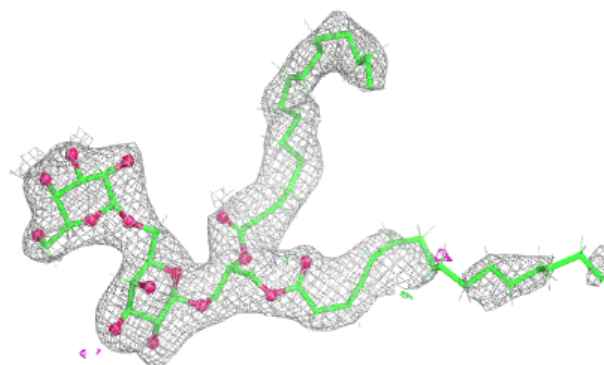


Electron density around BCR b 619:

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

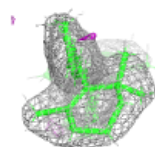
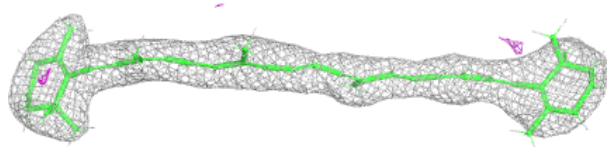
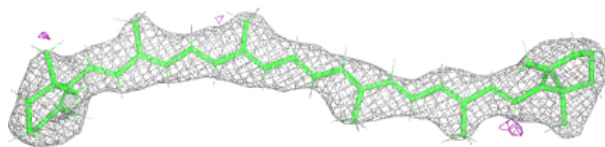
**Electron density around DGD c 517:**

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

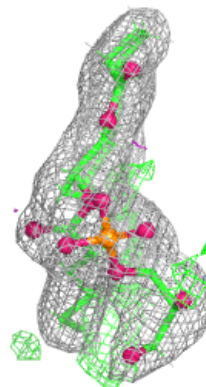
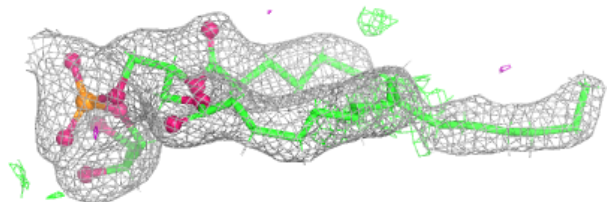
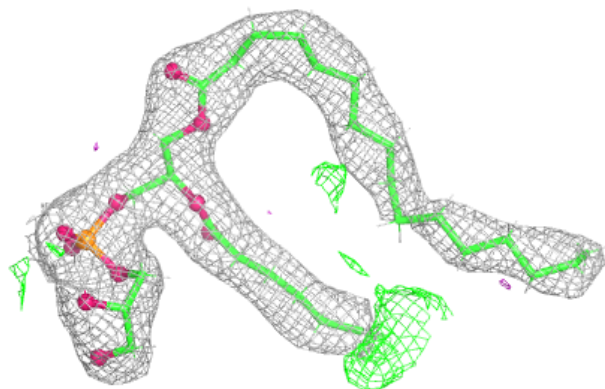


Electron density around BCR c 515:

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

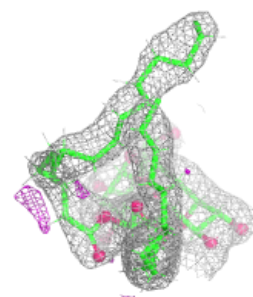
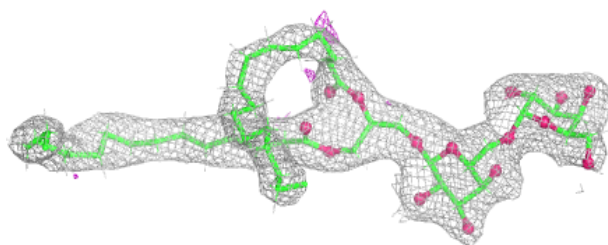
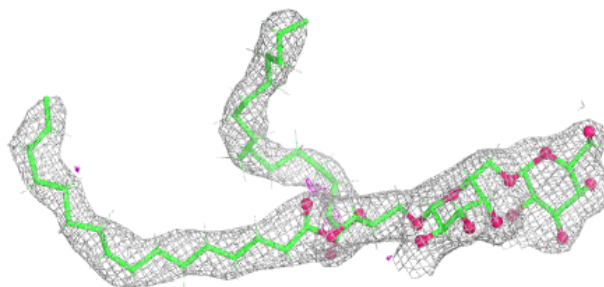
**Electron density around LHG d 409:**

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

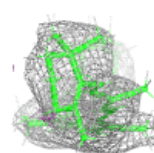
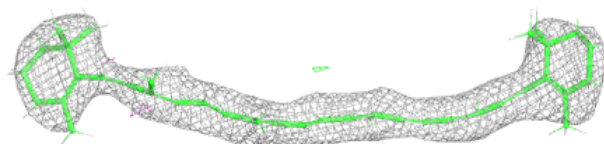


Electron density around DGD h 101:

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

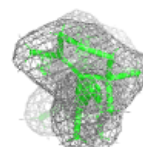
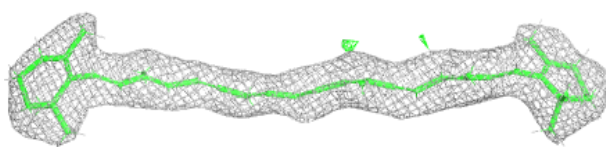
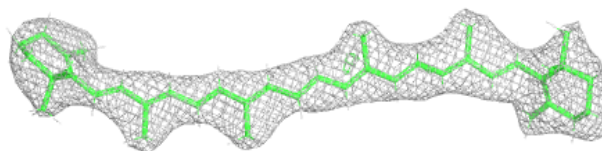
**Electron density around BCR k 102:**

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



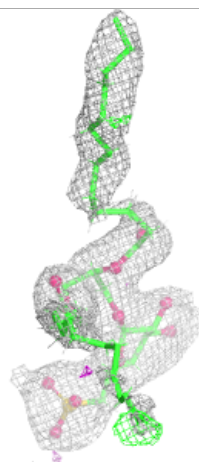
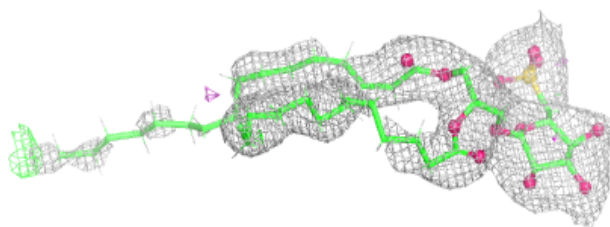
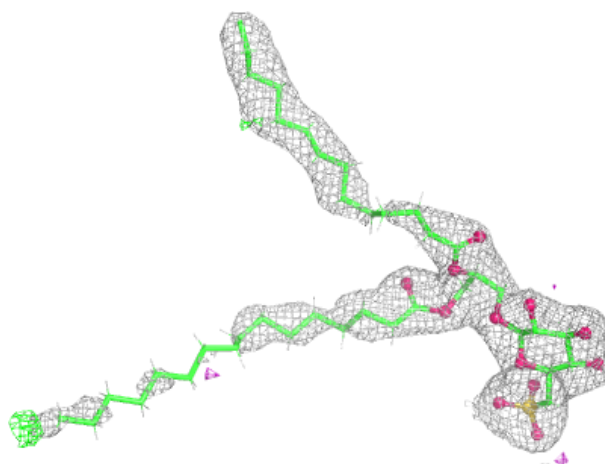
Electron density around BCR B 618:

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



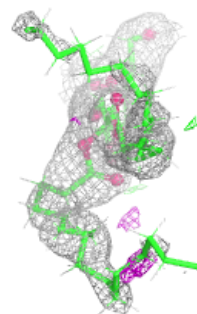
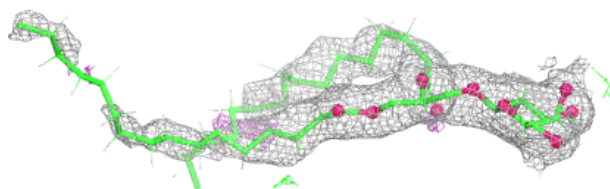
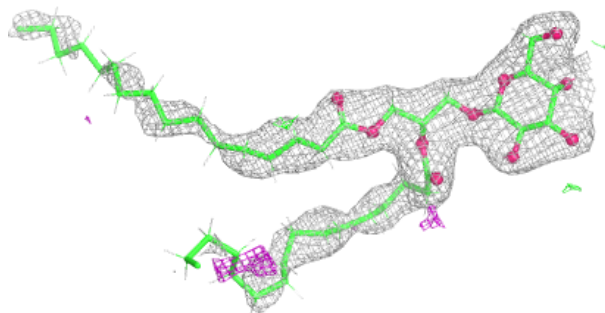
Electron density around SQD A 410:

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

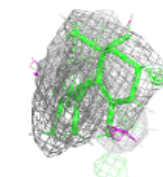
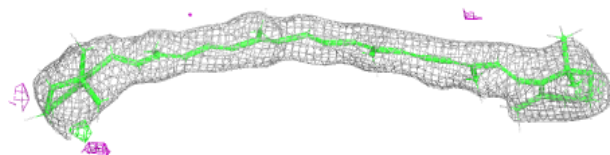
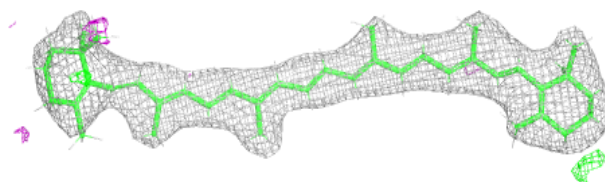


Electron density around LMG D 408:

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

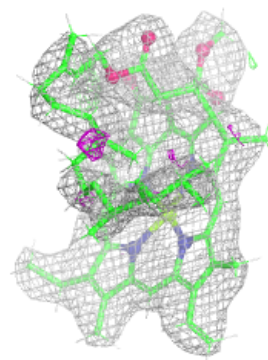
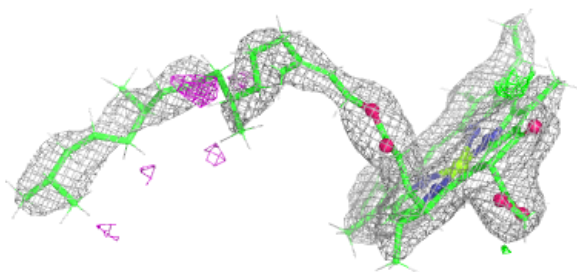
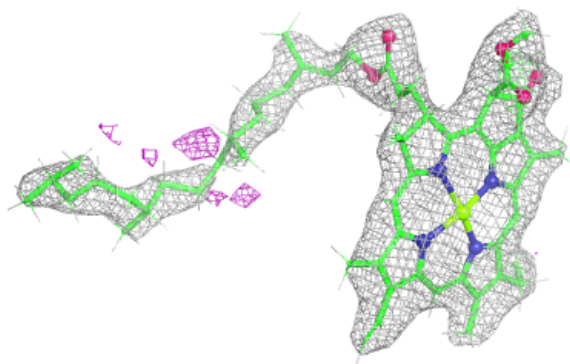
**Electron density around BCR D 406:**

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

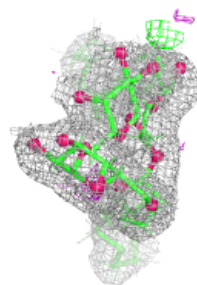
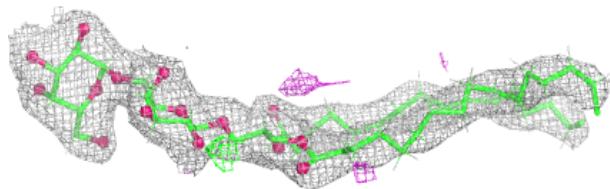
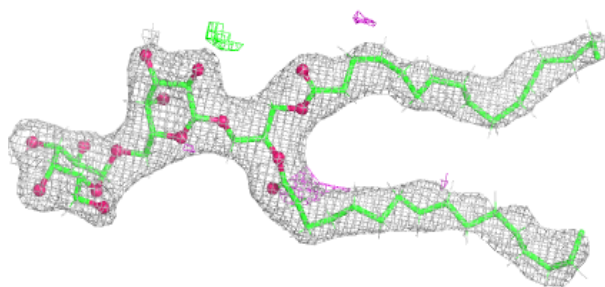


Electron density around CLA c 511:

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

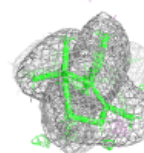
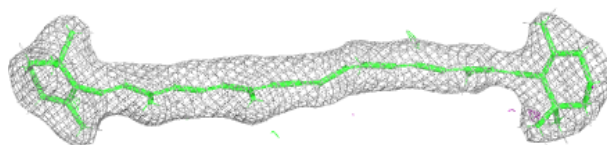
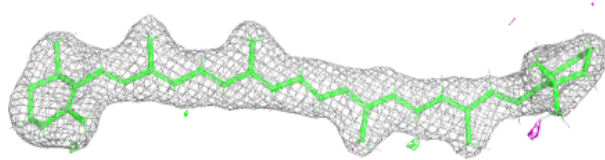
**Electron density around DGD C 517:**

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



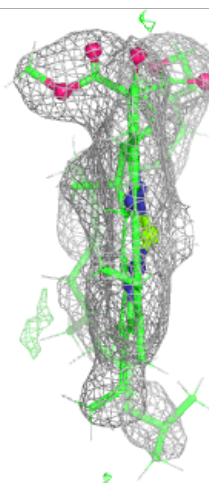
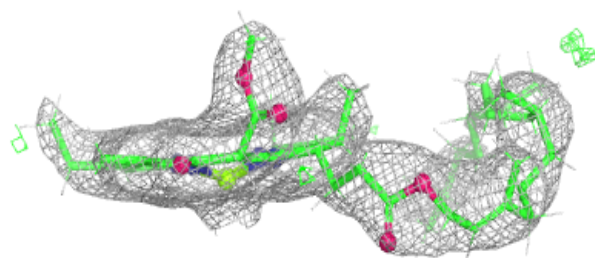
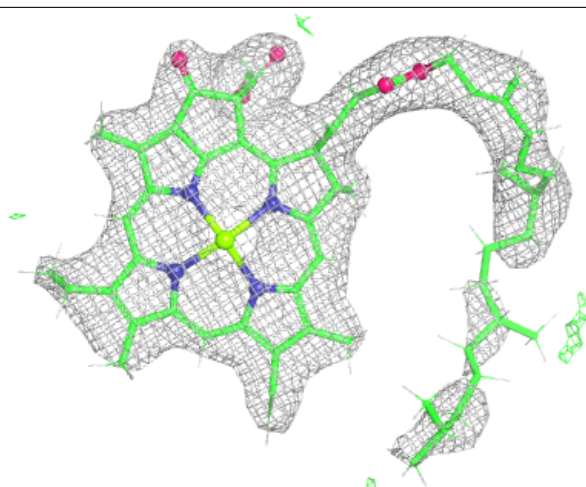
Electron density around BCR I 101:

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



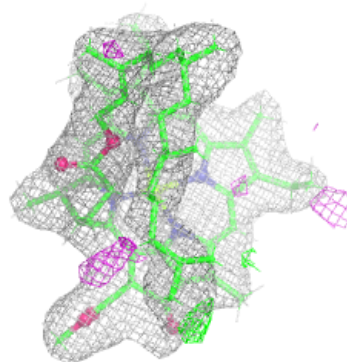
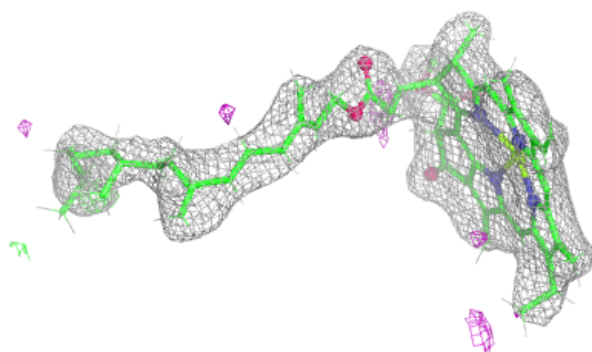
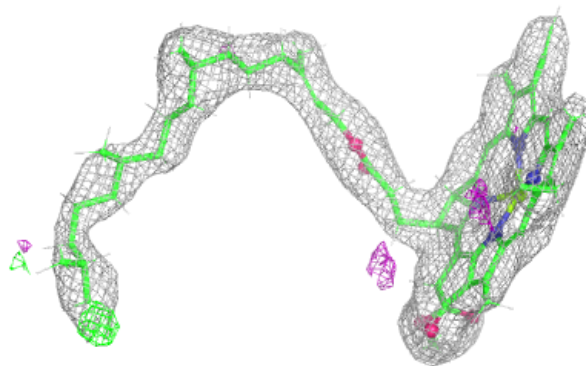
Electron density around CLA C 512:

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

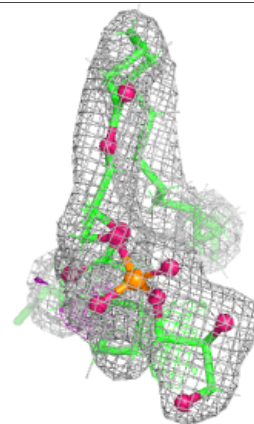
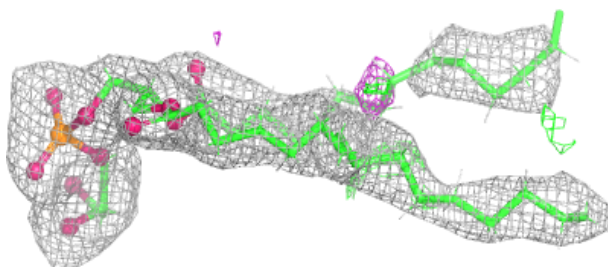
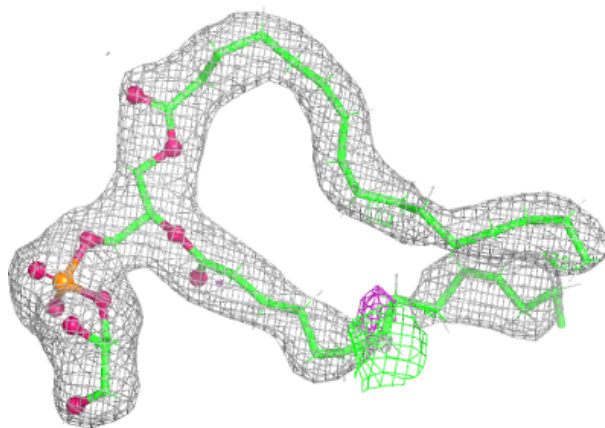


Electron density around CLA b 606:

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

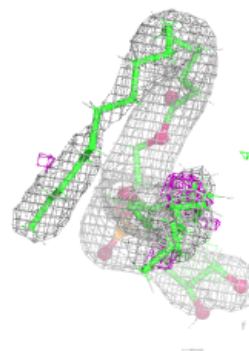
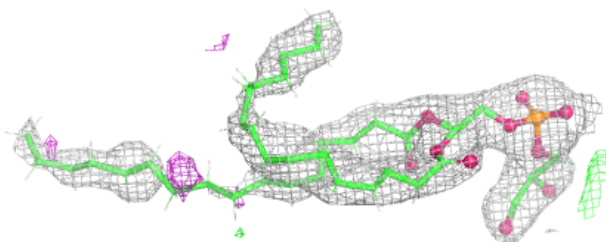
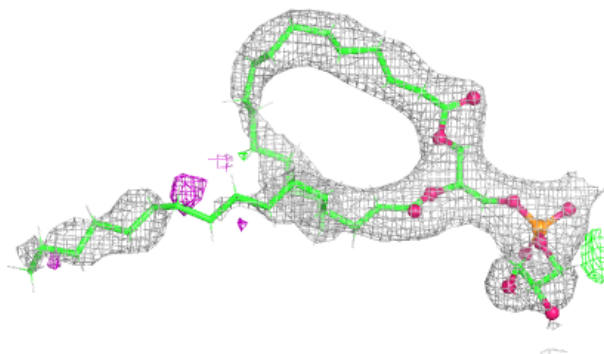
**Electron density around LHG D 411:**

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

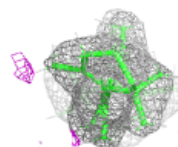
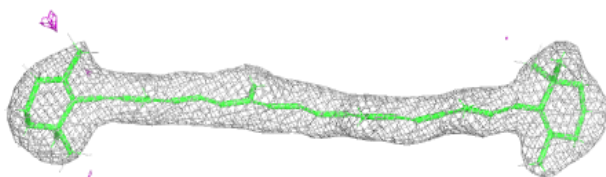
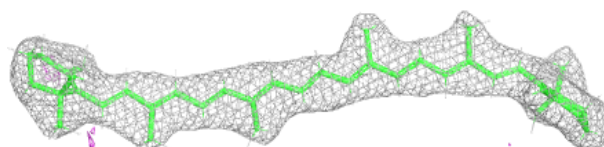


Electron density around LHG a 410:

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

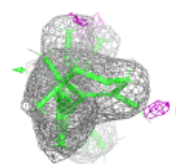
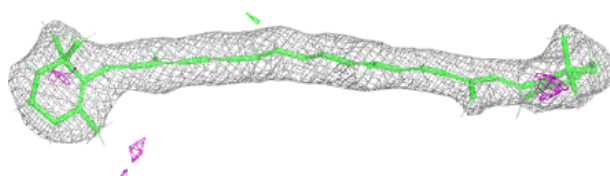
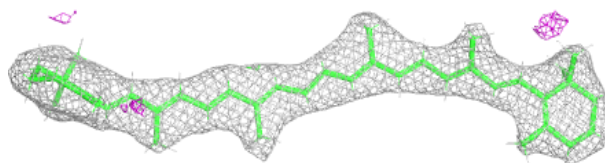
**Electron density around BCR a 405:**

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

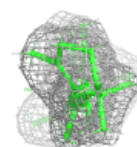
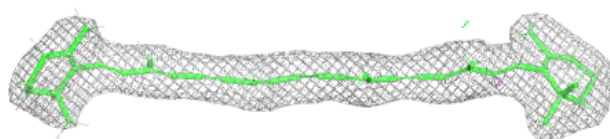
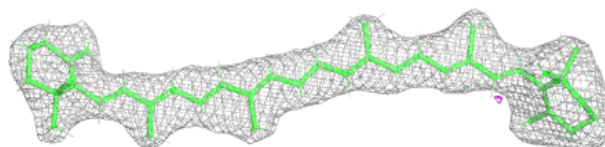


Electron density around BCR B 617:

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

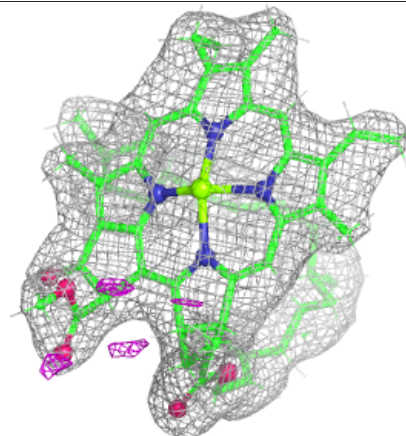
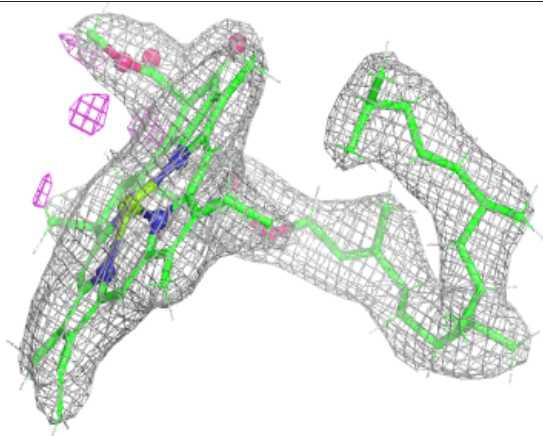
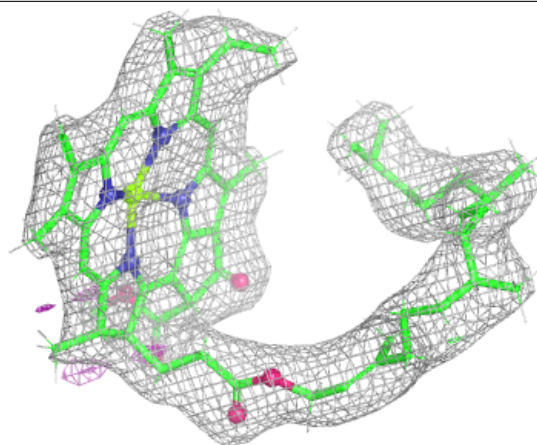
**Electron density around BCR b 618:**

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



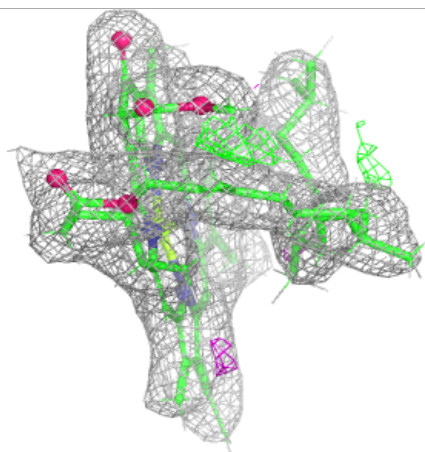
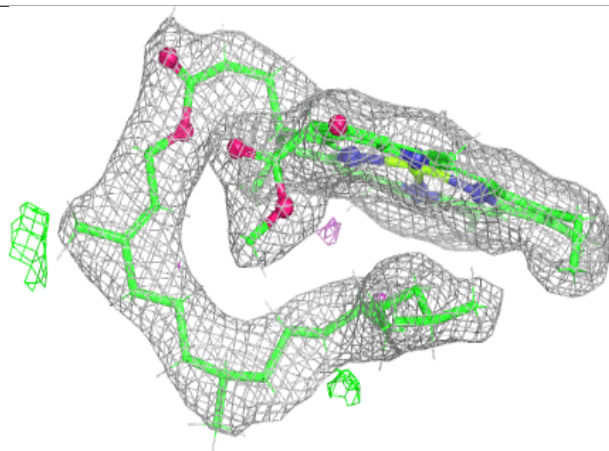
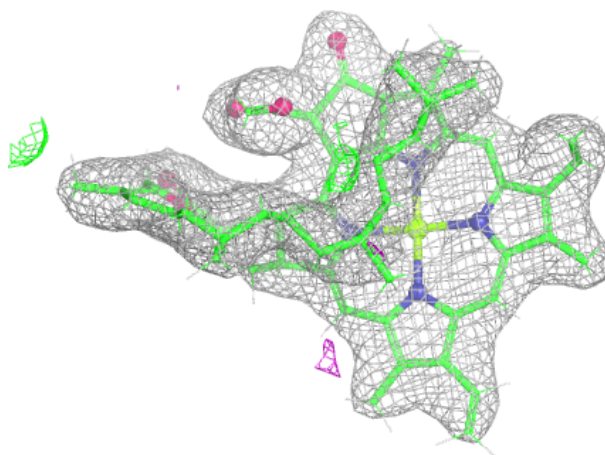
Electron density around CLA c 503:

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



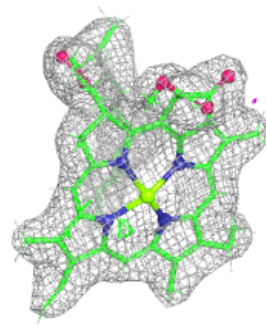
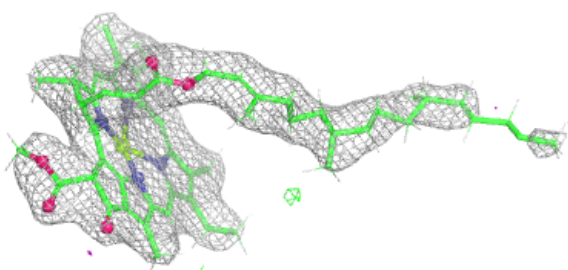
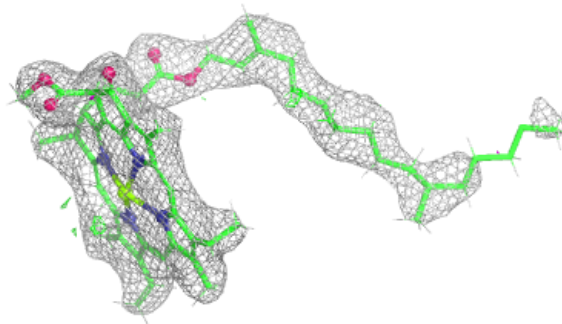
Electron density around CLA C 510:

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

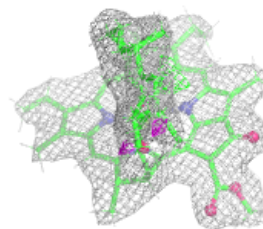
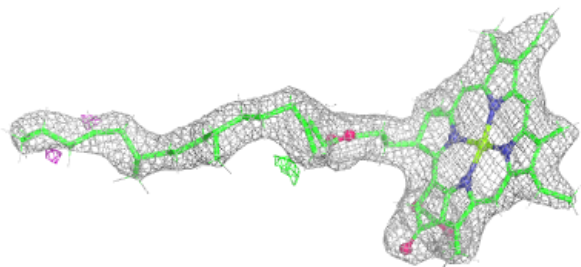
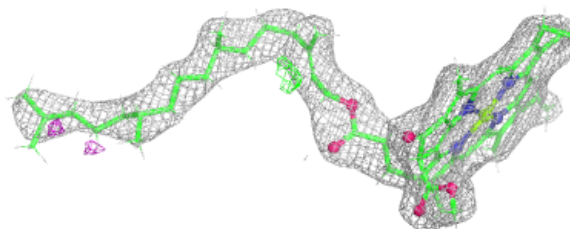


Electron density around CLA c 508:

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

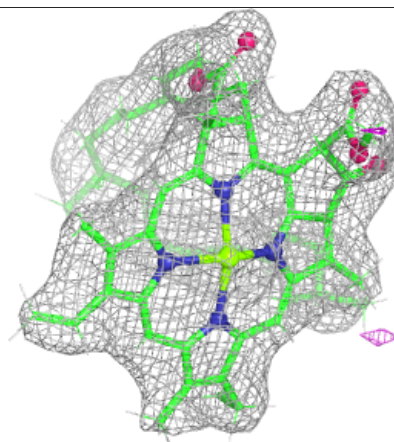
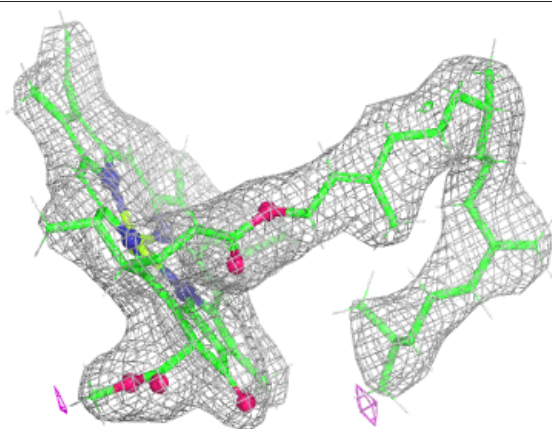
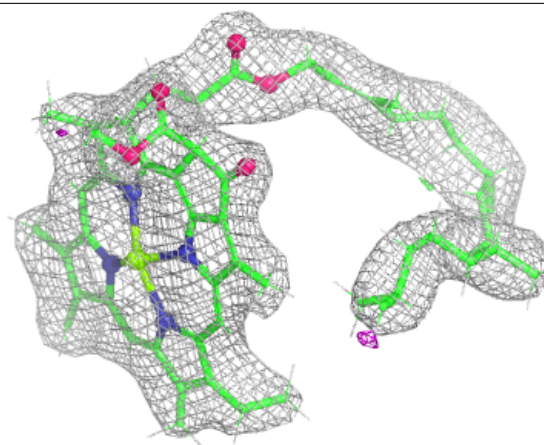
**Electron density around CLA c 502:**

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

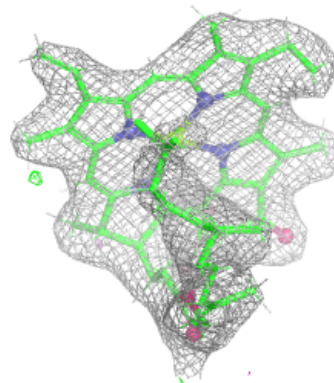
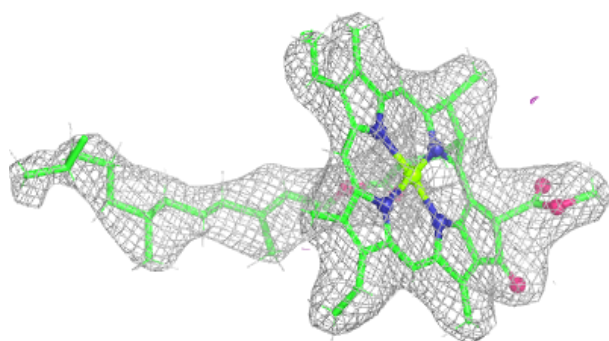
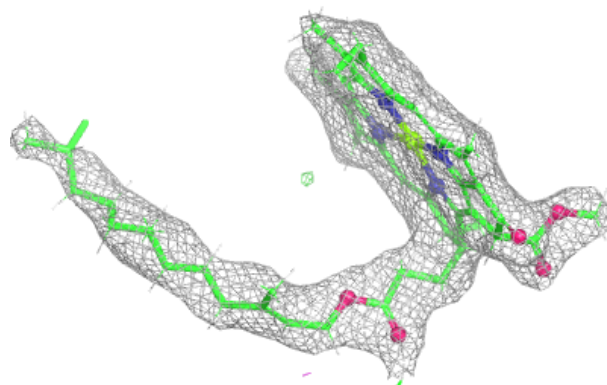


Electron density around CLA C 503:

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

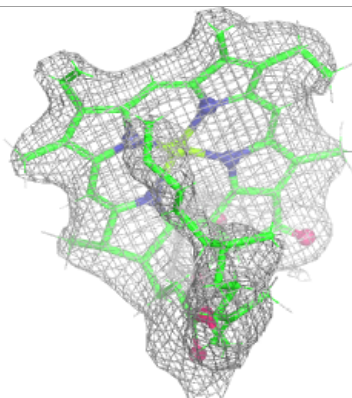
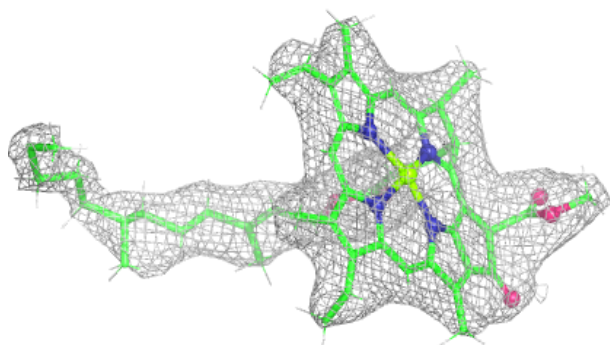
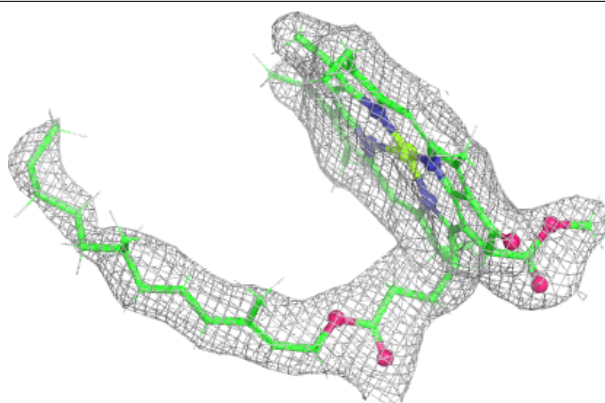
**Electron density around CLA c 504:**

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

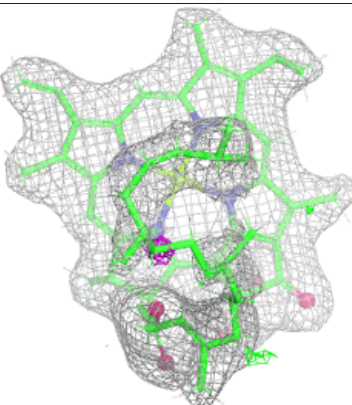
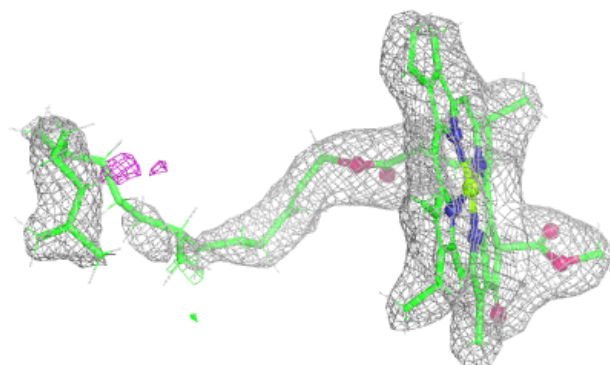
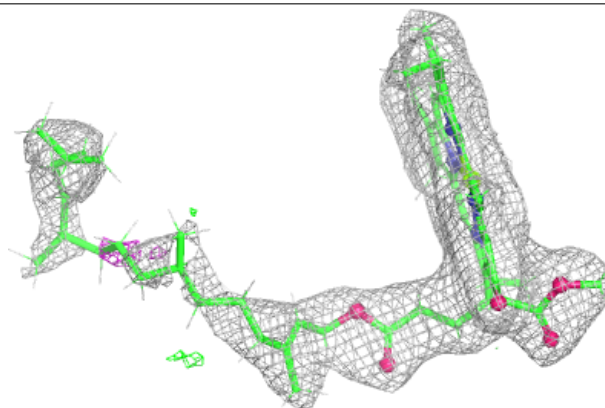


Electron density around CLA C 504:

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

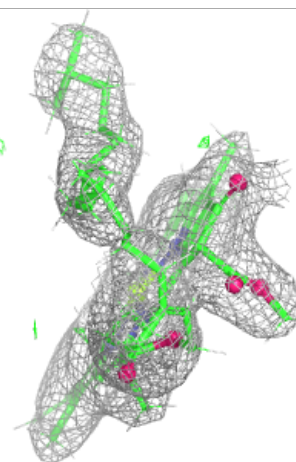
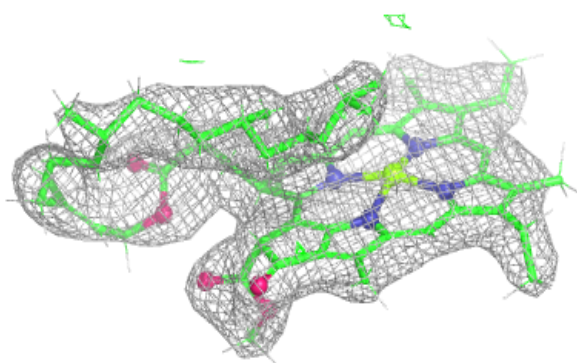
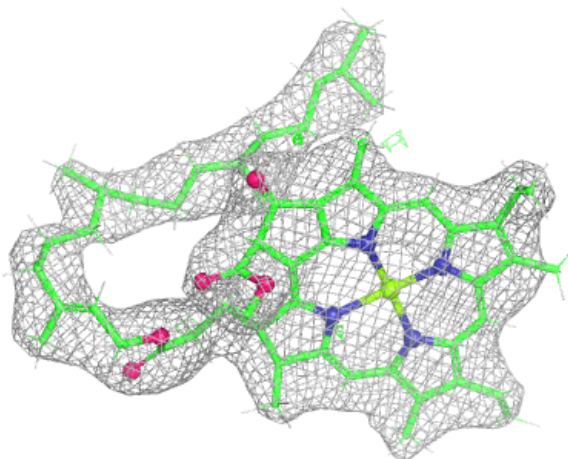
**Electron density around CLA C 506:**

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



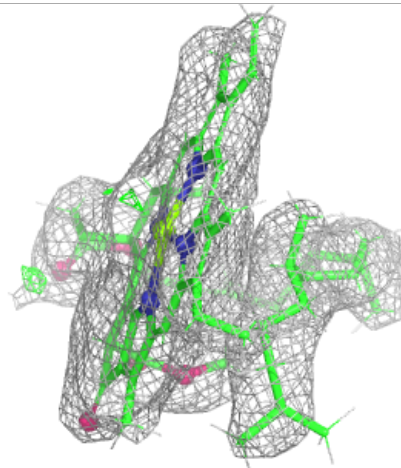
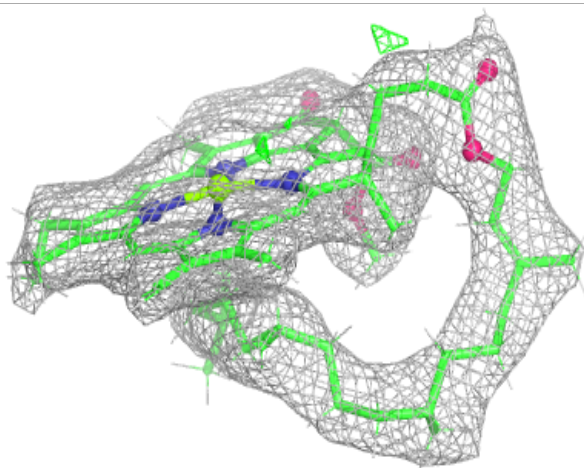
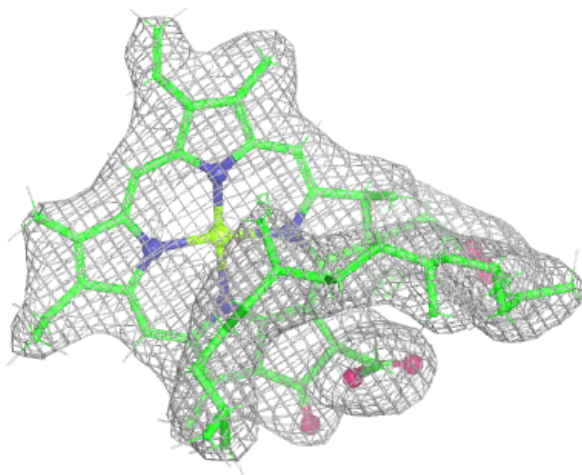
Electron density around CLA c 509:

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



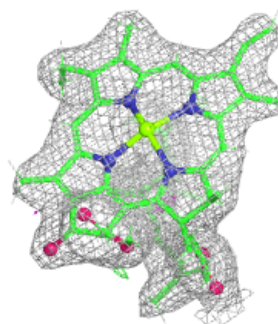
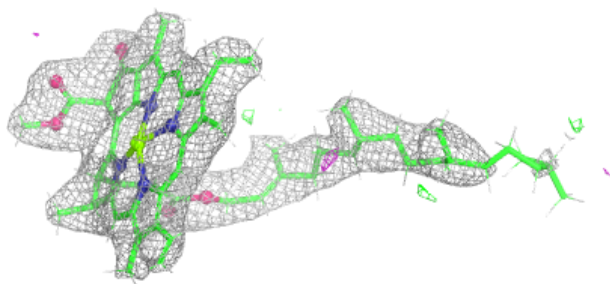
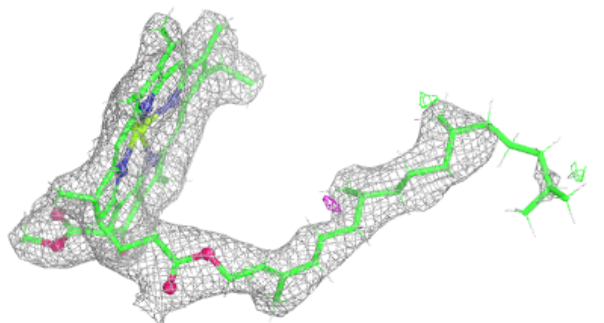
Electron density around CLA c 510:

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

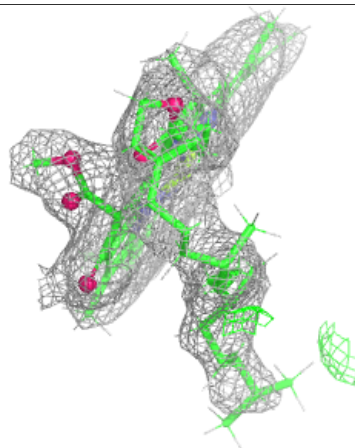
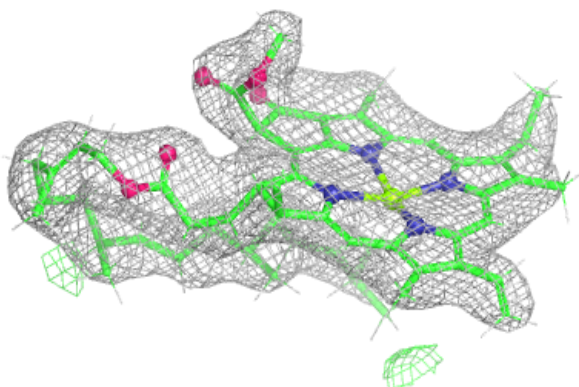
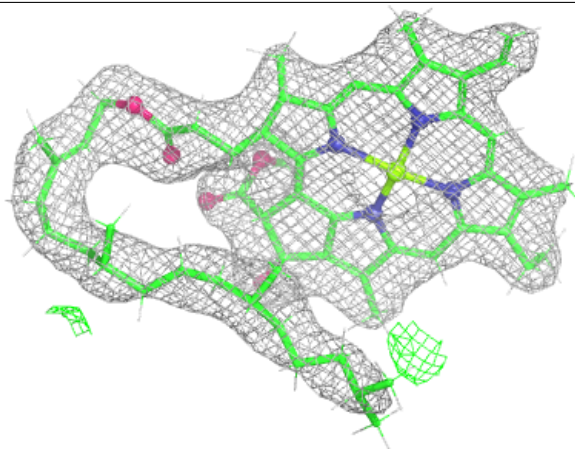


Electron density around CLA C 508:

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

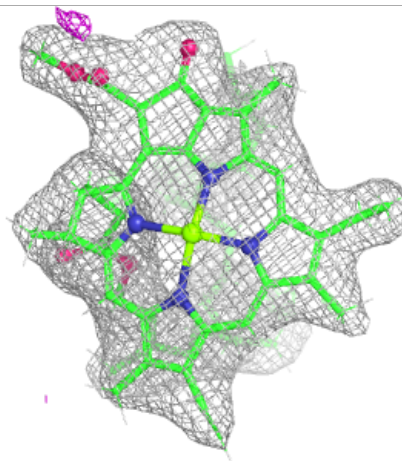
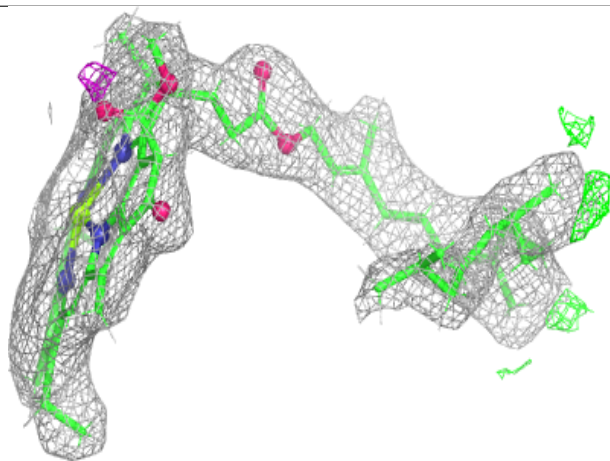
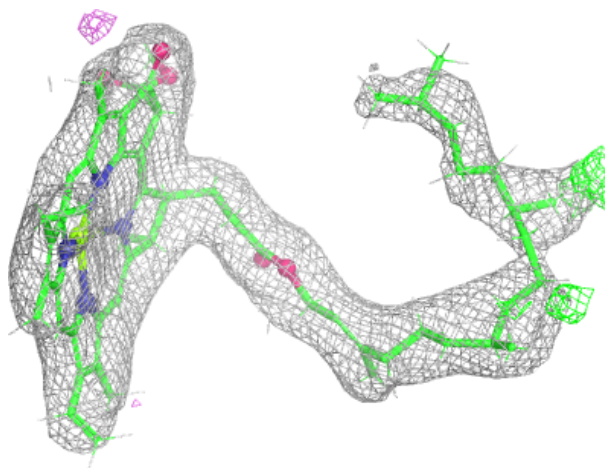
**Electron density around CLA C 509:**

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



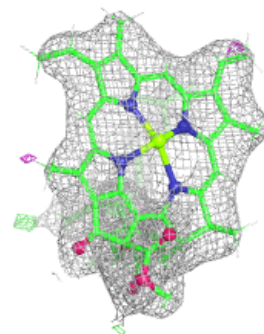
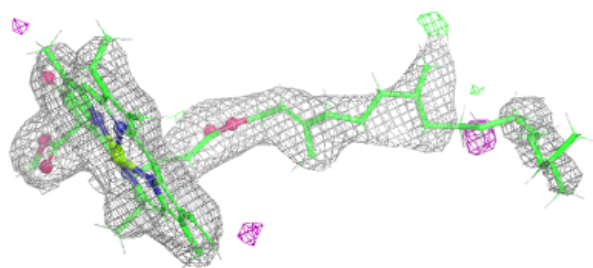
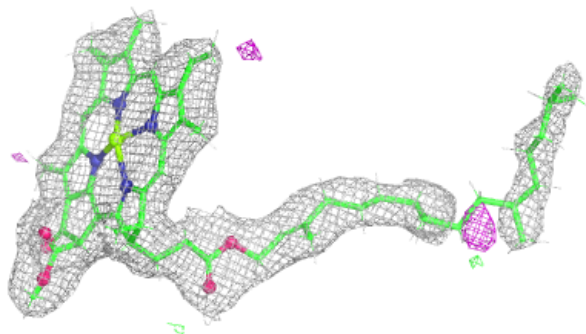
Electron density around CLA B 606:

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



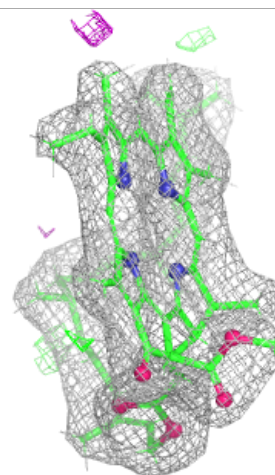
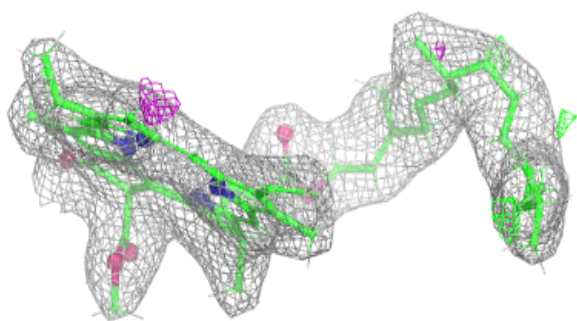
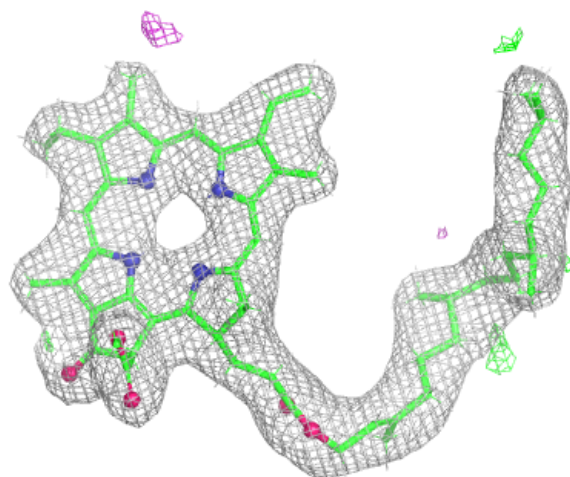
Electron density around CLA d 405:

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



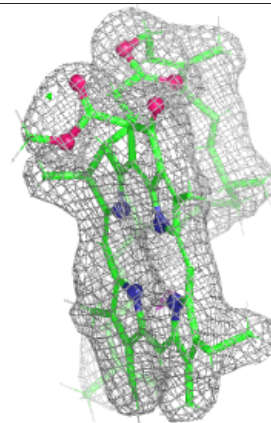
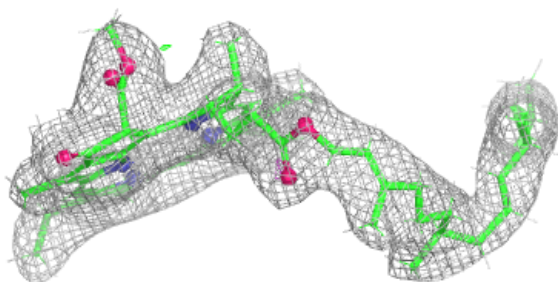
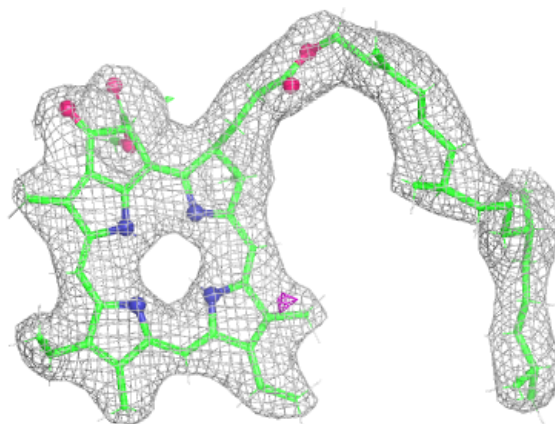
Electron density around PHO D 401:

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

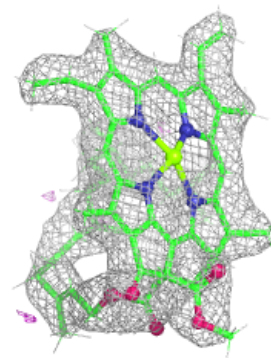
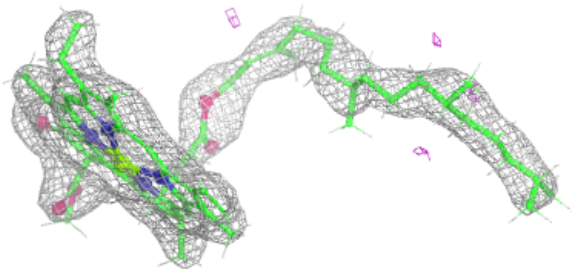
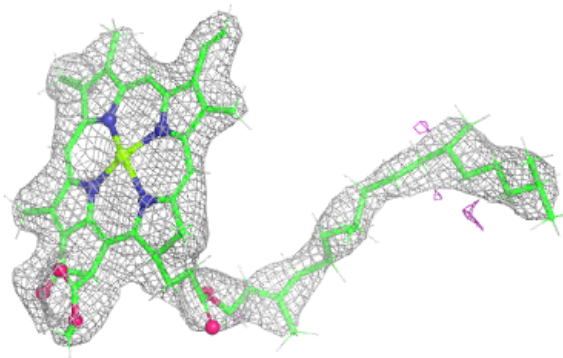


Electron density around PHO d 402:

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

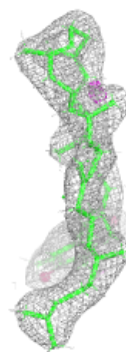
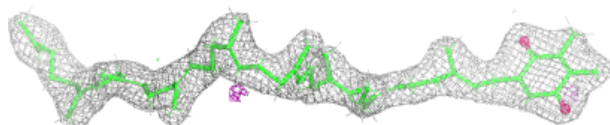
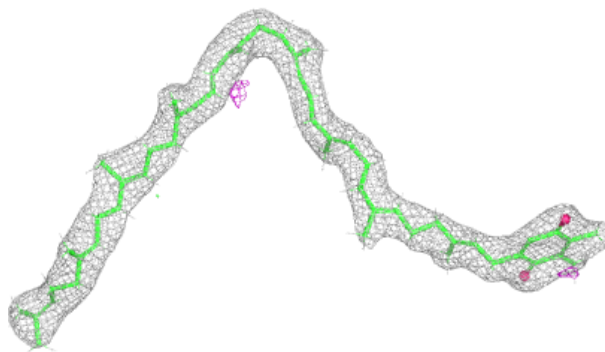
**Electron density around CLA C 511:**

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

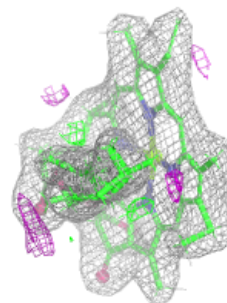
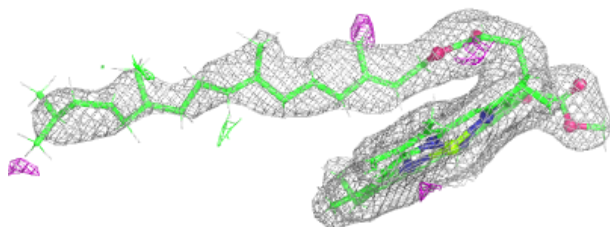
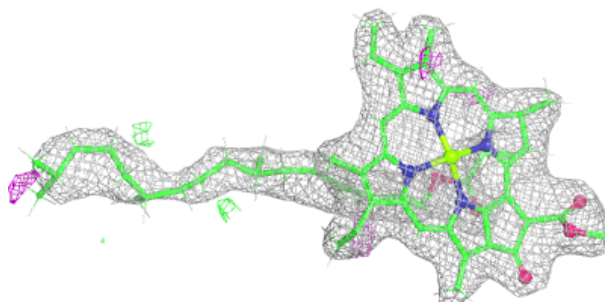


Electron density around PL9 D 407:

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

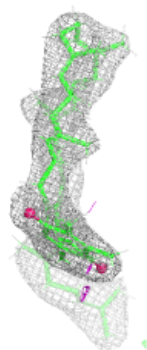
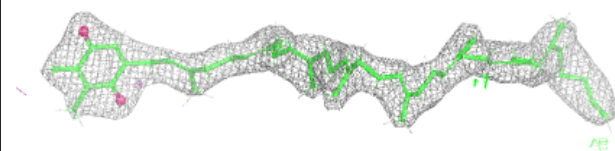
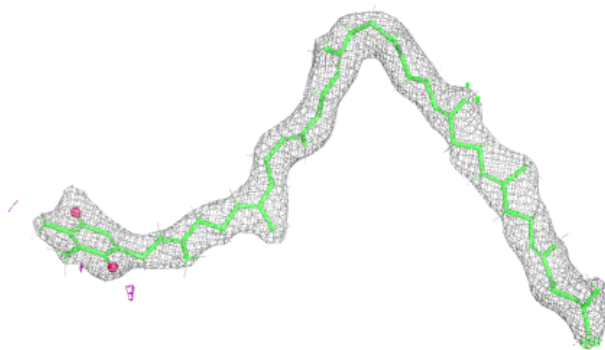
**Electron density around CLA B 614:**

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



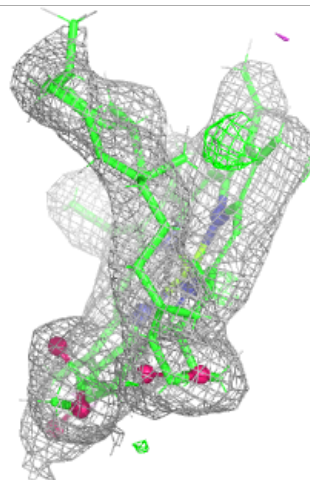
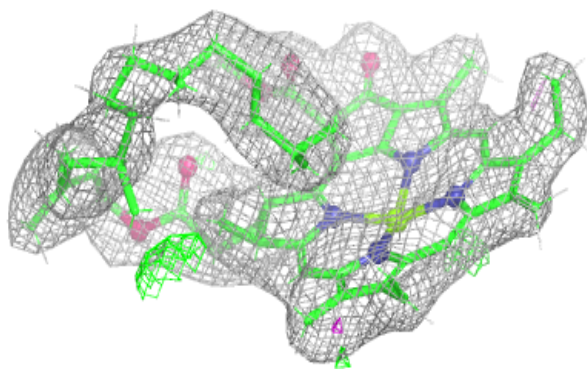
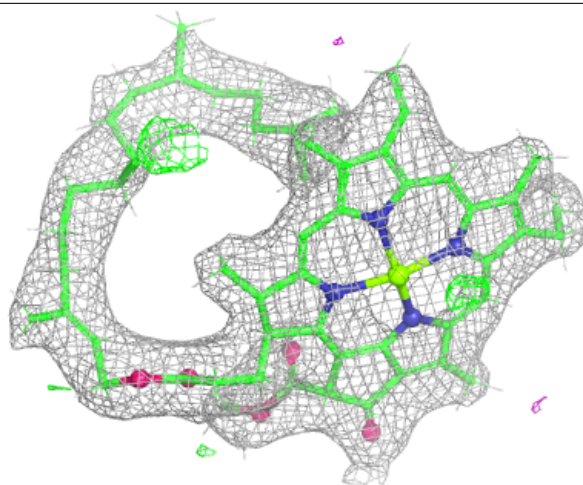
Electron density around PL9 d 407:

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



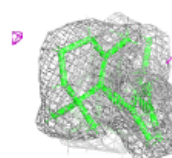
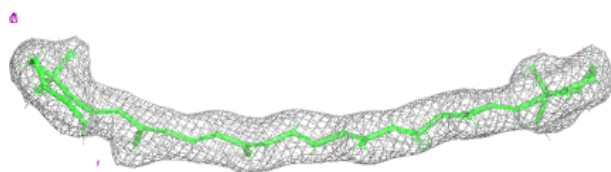
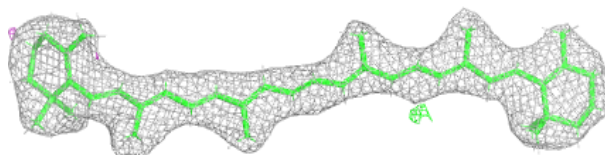
Electron density around CLA B 615:

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

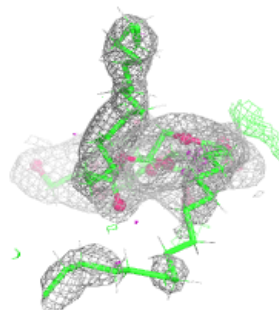
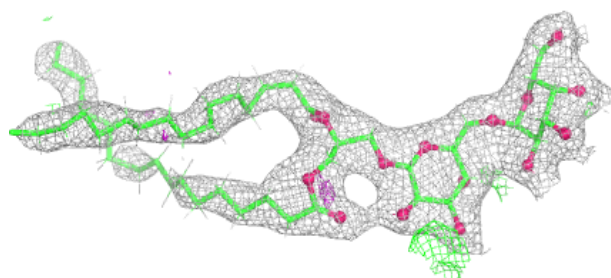
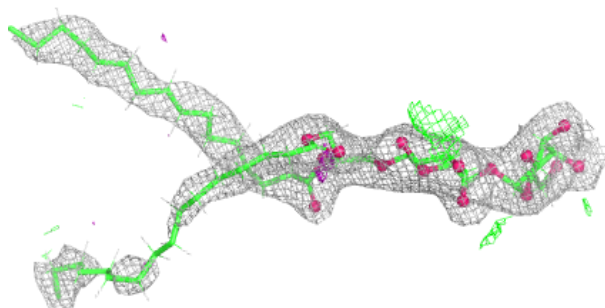


Electron density around BCR t 101:

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

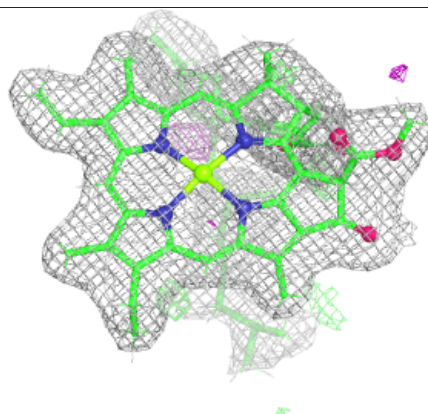
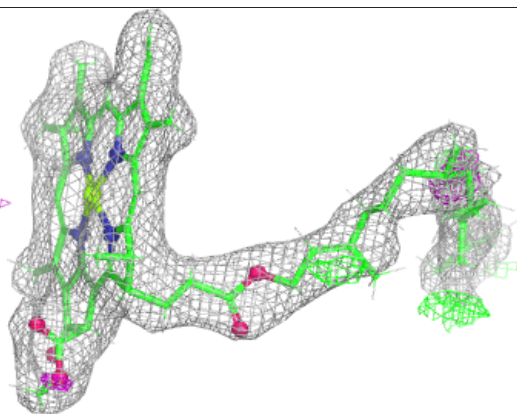
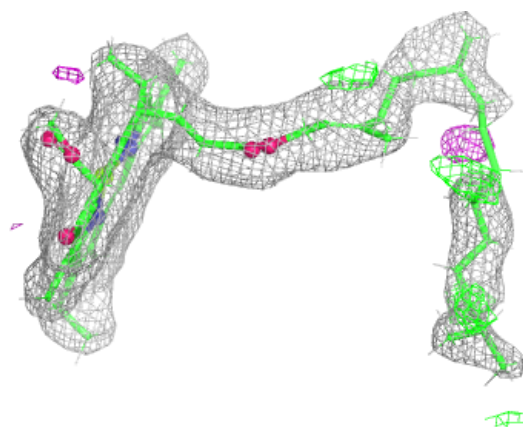
**Electron density around DGD C 515:**

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



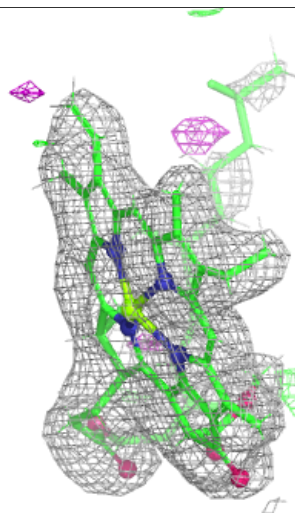
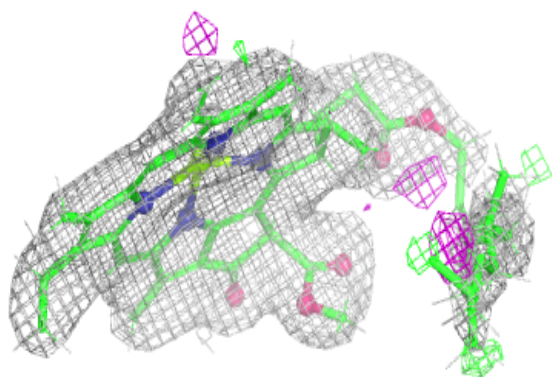
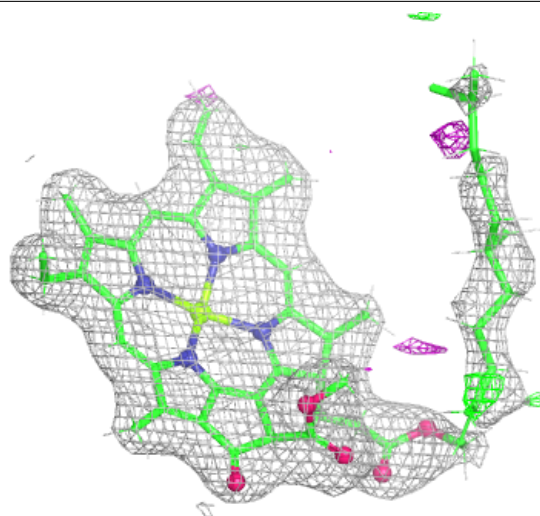
Electron density around CLA a 404:

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



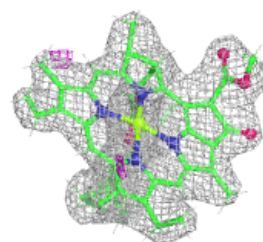
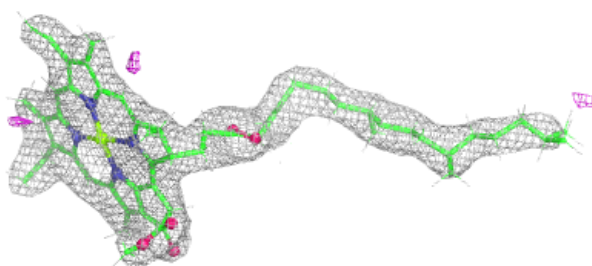
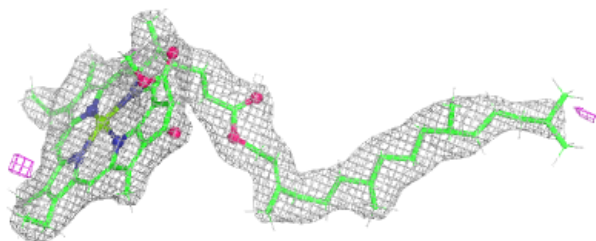
Electron density around CLA B 616:

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

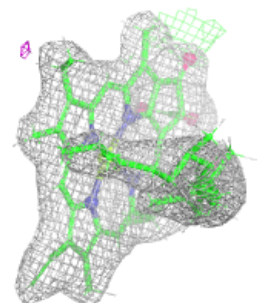
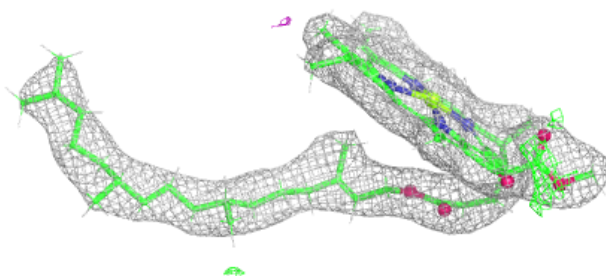
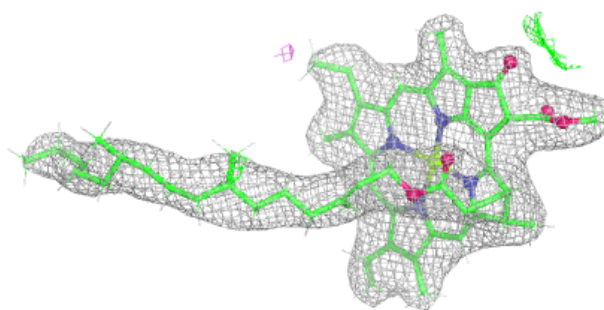


Electron density around CLA C 502:

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

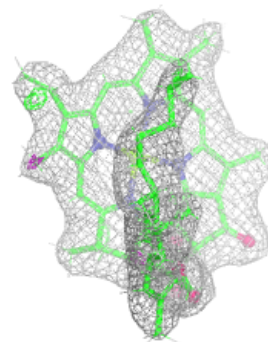
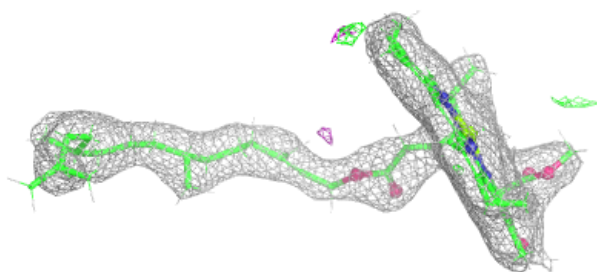
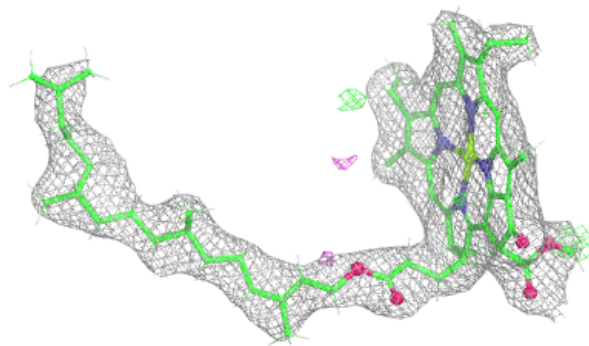
**Electron density around CLA b 608:**

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

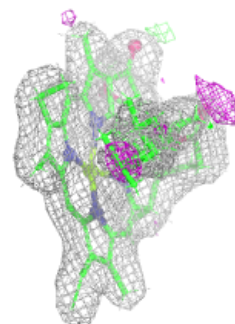
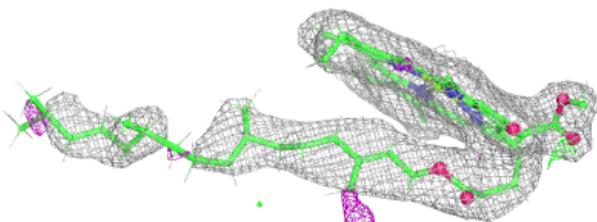
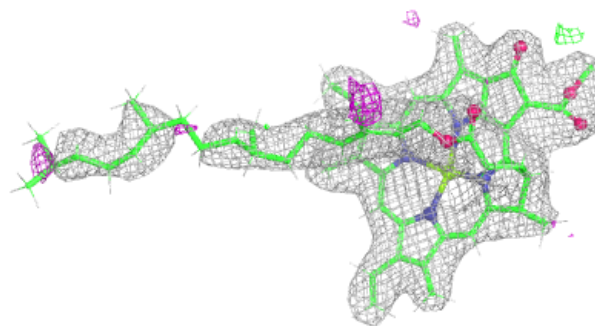


Electron density around CLA b 609:

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

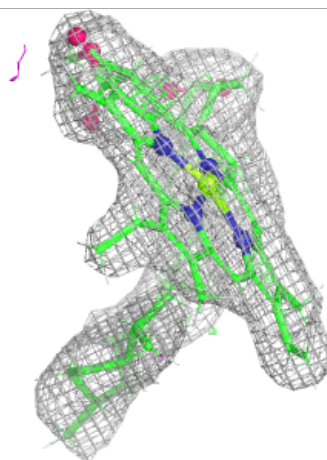
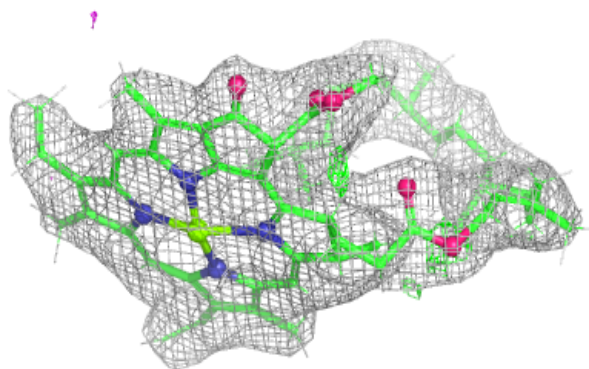
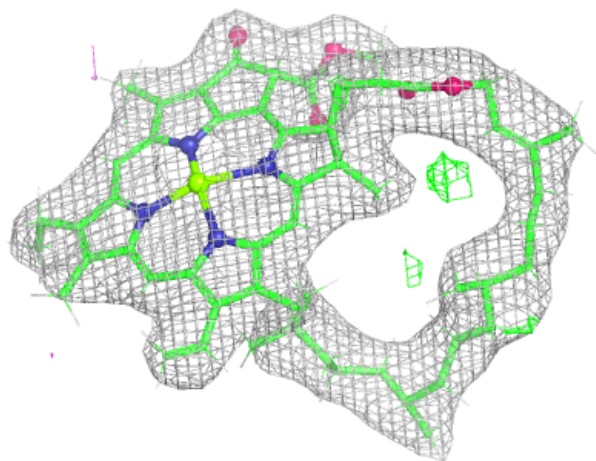
**Electron density around CLA b 614:**

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



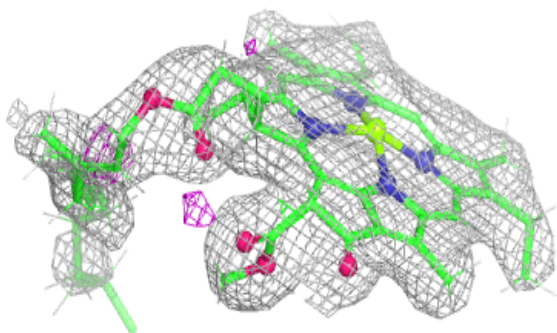
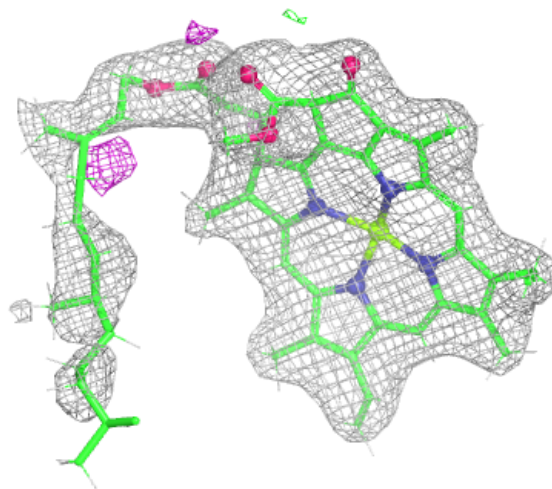
Electron density around CLA b 615:

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



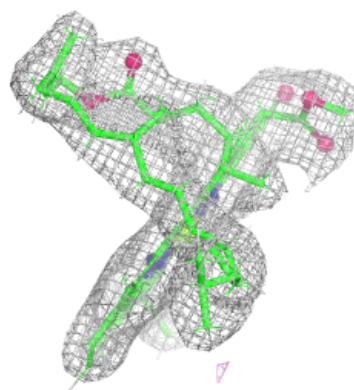
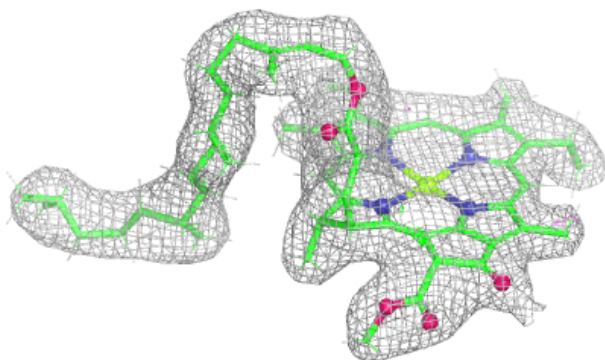
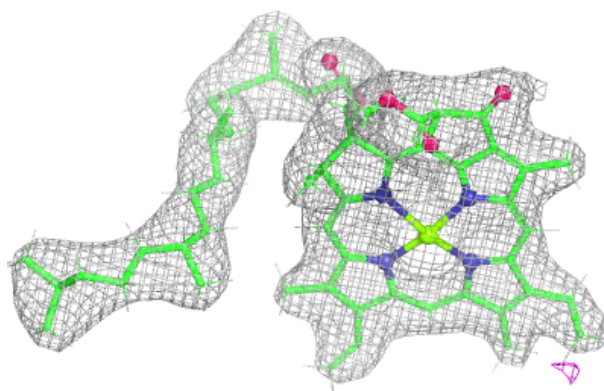
Electron density around CLA b 616:

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

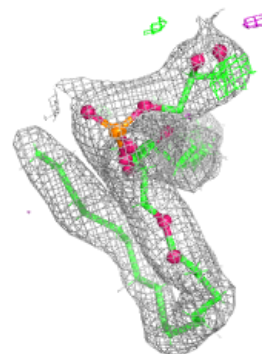
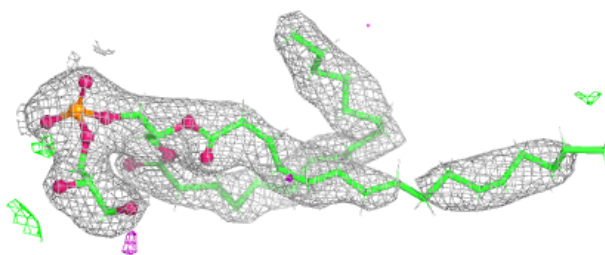
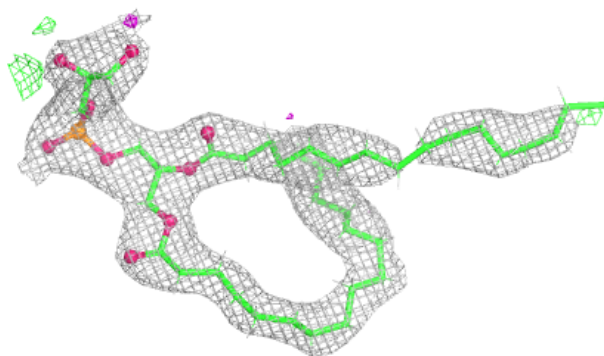


Electron density around CLA d 404:

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

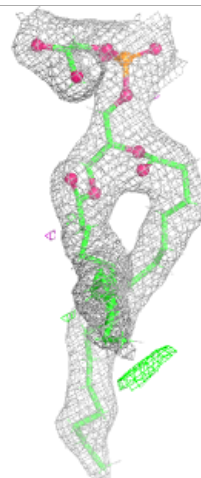
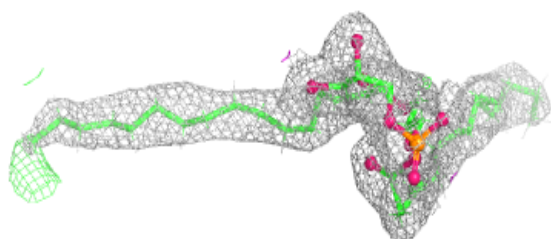
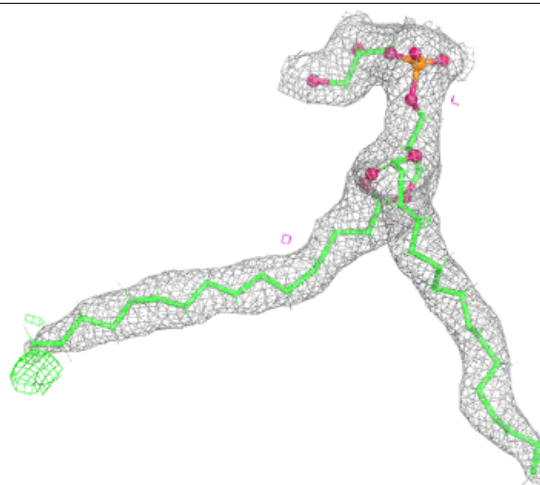
**Electron density around LHG D 413:**

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



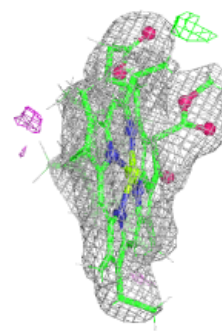
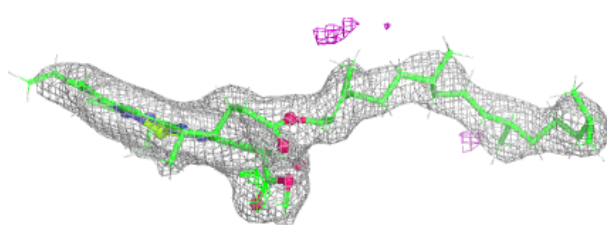
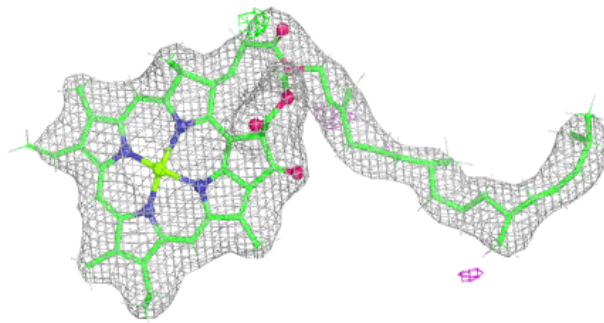
Electron density around LHG L 102:

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

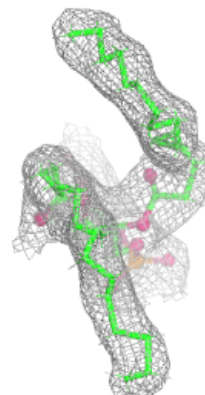
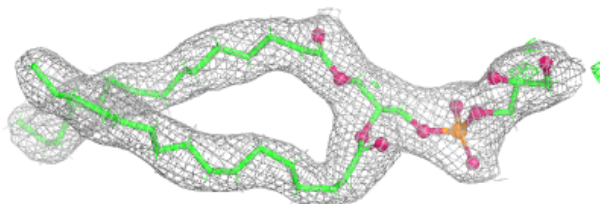
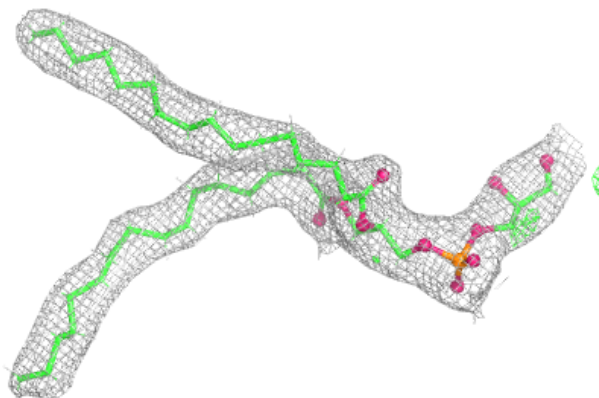


Electron density around CLA b 602:

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

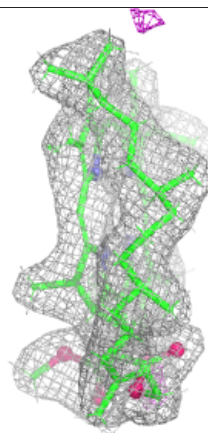
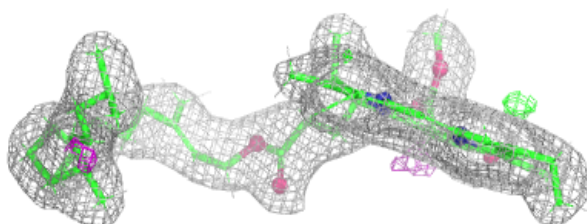
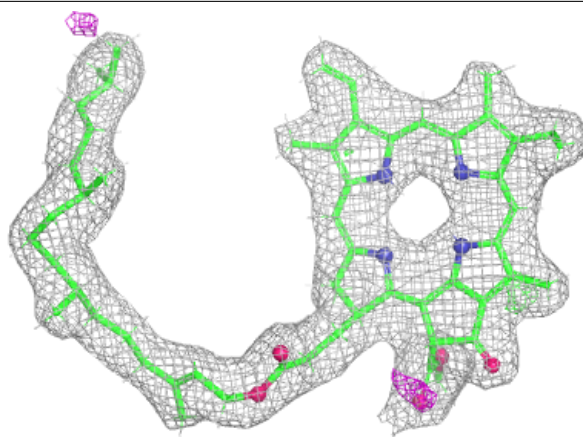
**Electron density around LHG d 408:**

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



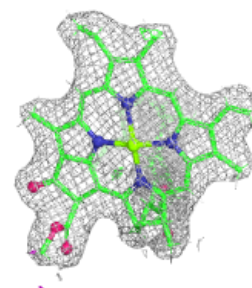
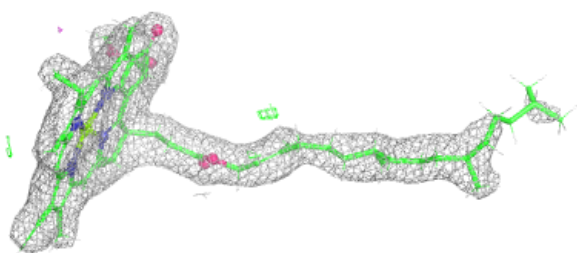
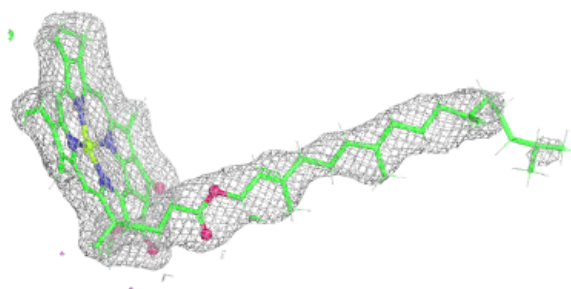
Electron density around PHO A 404:

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



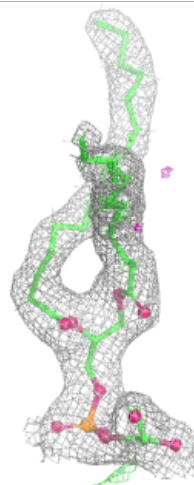
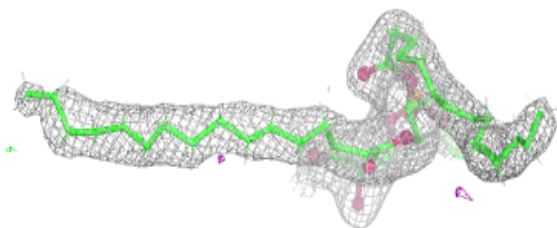
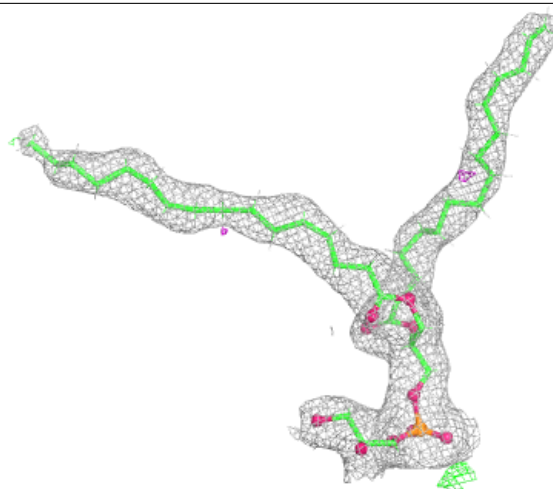
Electron density around CLA b 604:

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



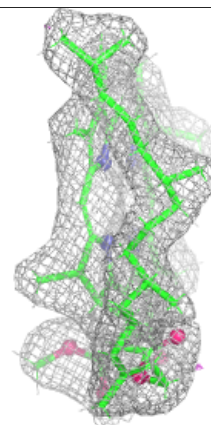
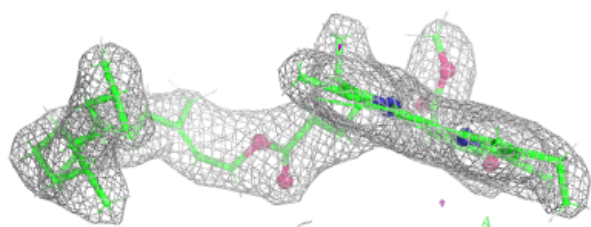
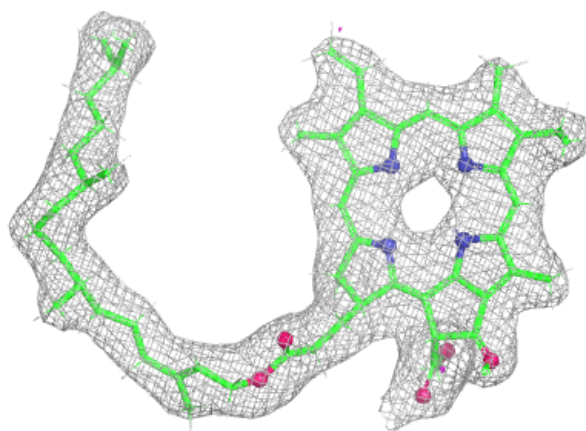
Electron density around LHG 1 101:

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

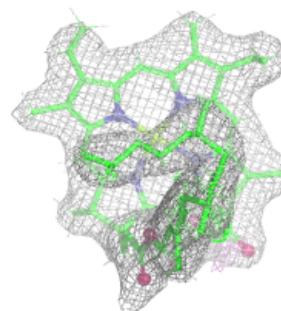
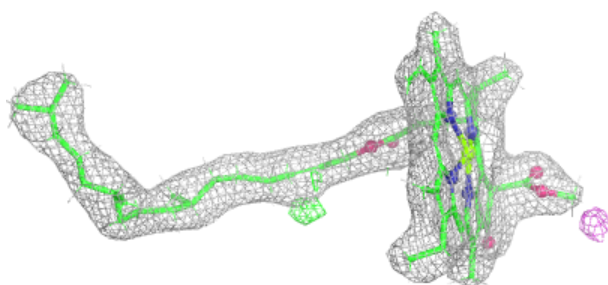
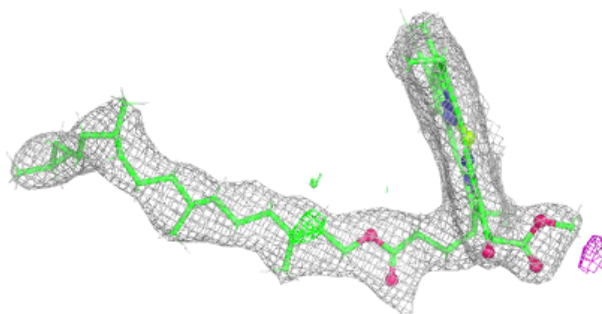


Electron density around PHO a 403:

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

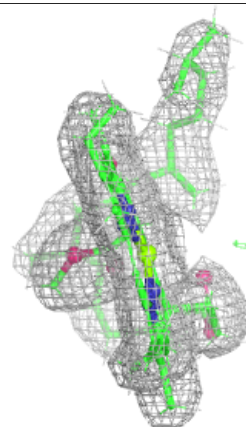
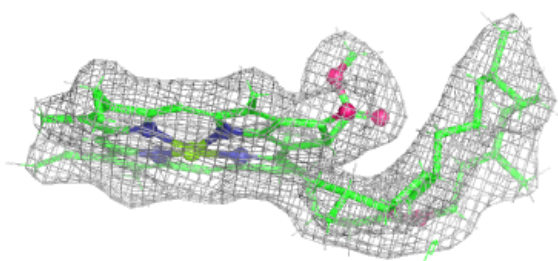
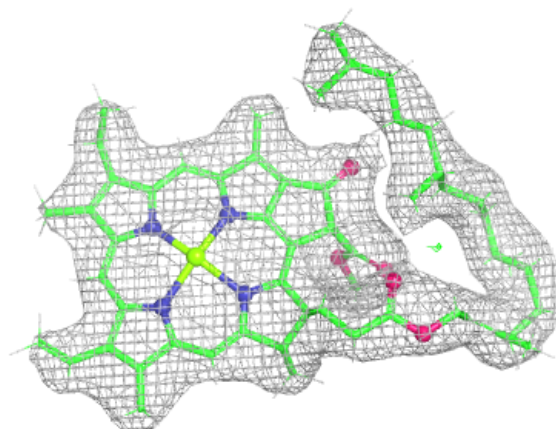
**Electron density around CLA b 605:**

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

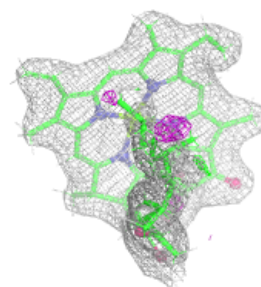
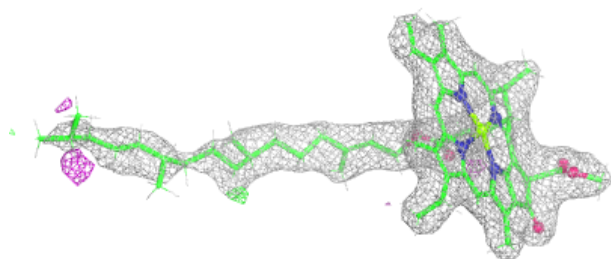
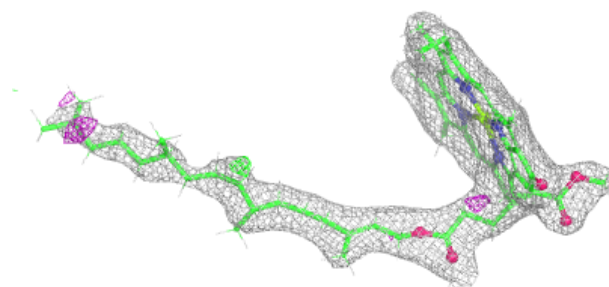


Electron density around CLA B 610:

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

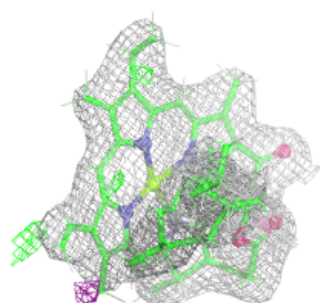
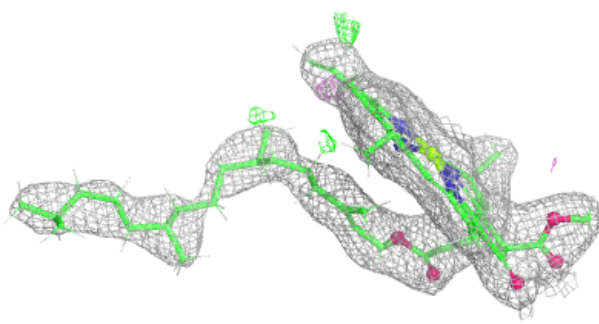
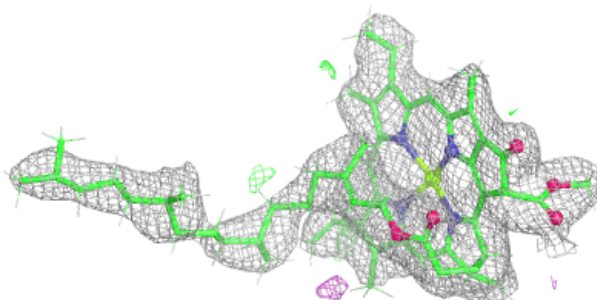
**Electron density around CLA b 607:**

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

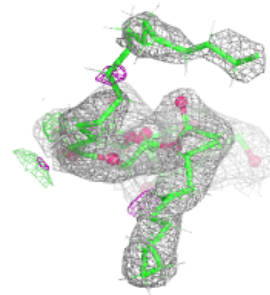
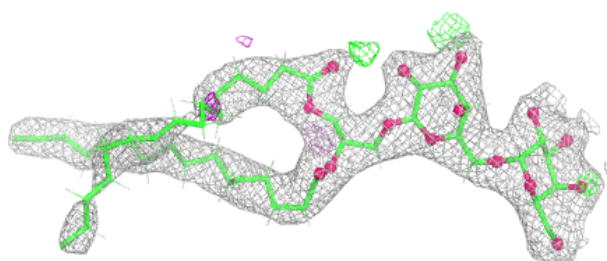
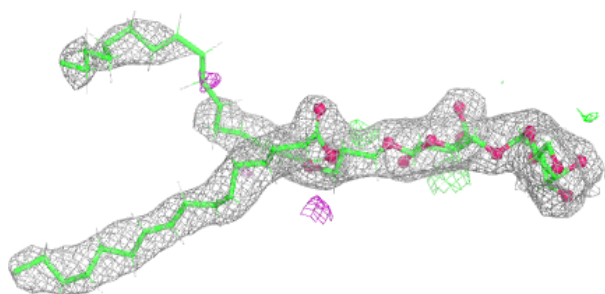


Electron density around CLA C 505:

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

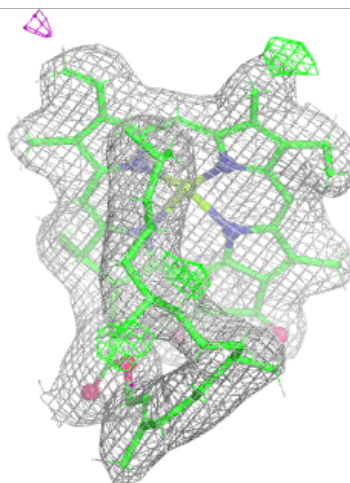
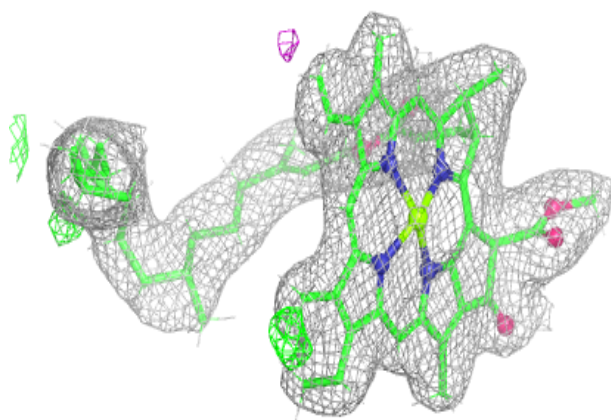
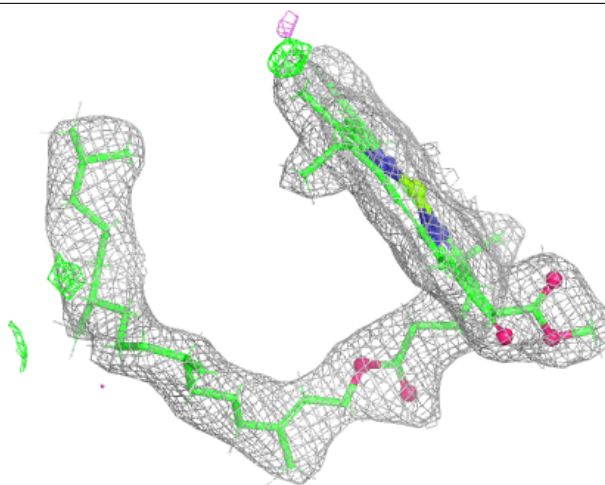
**Electron density around DGD c 516:**

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



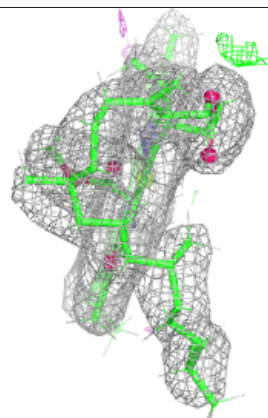
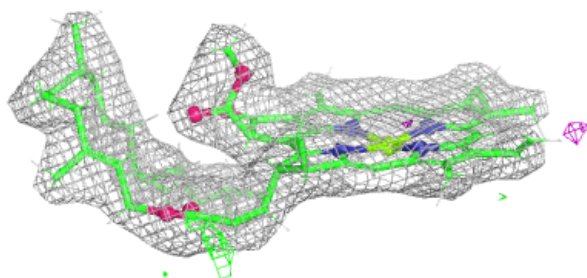
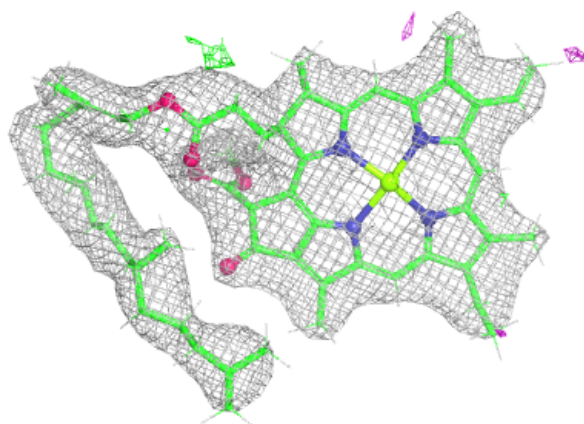
Electron density around CLA B 611:

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



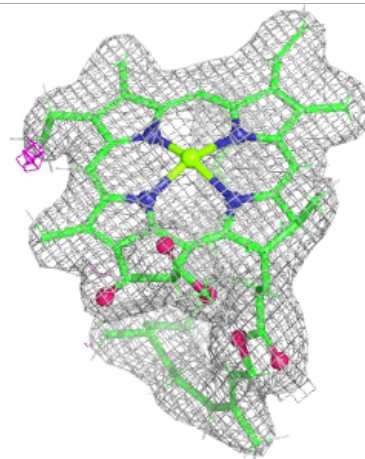
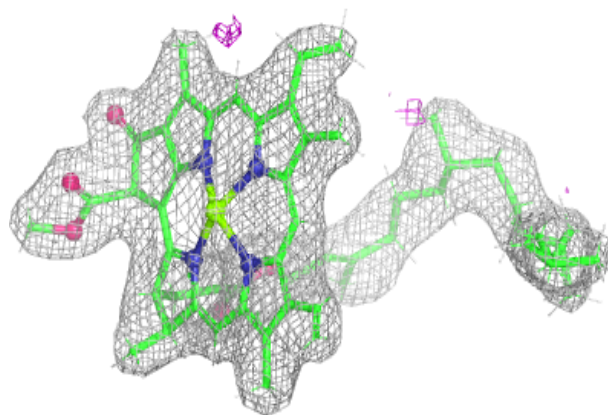
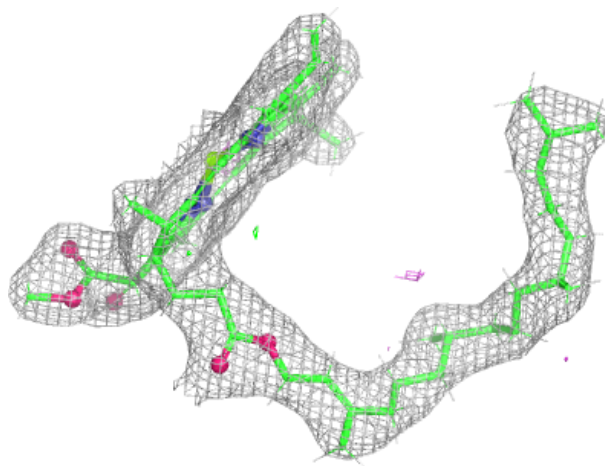
Electron density around CLA b 610:

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



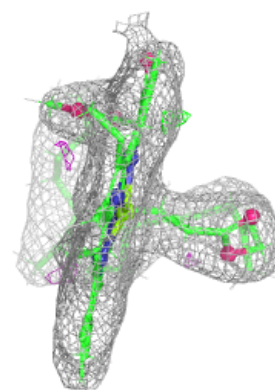
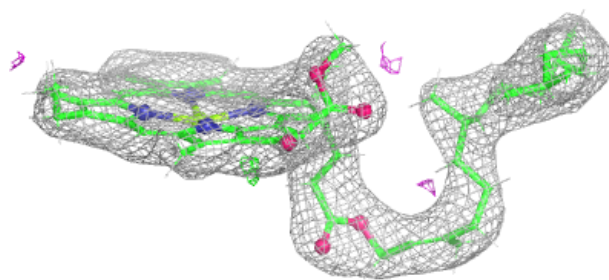
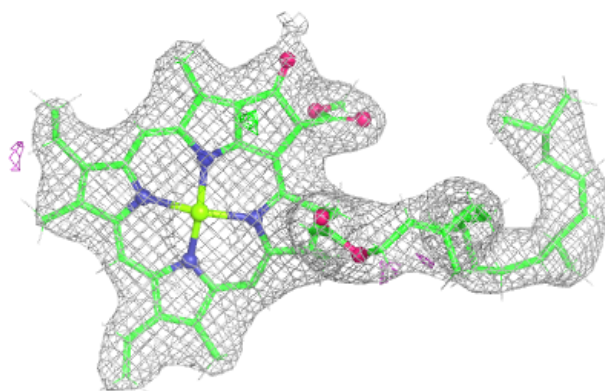
Electron density around CLA b 611:

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



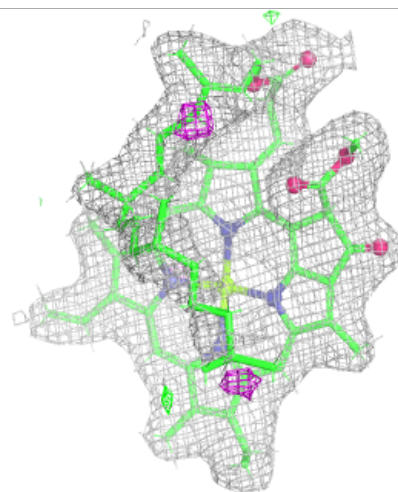
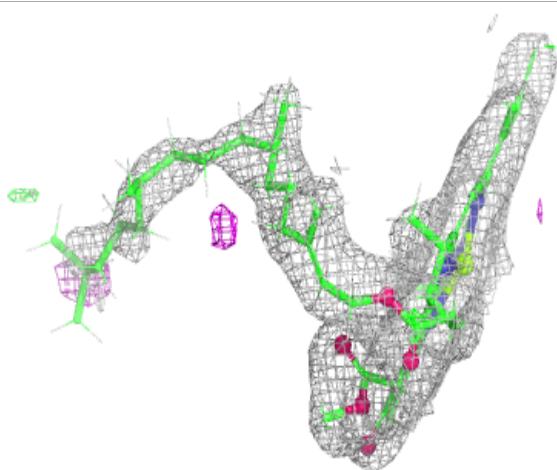
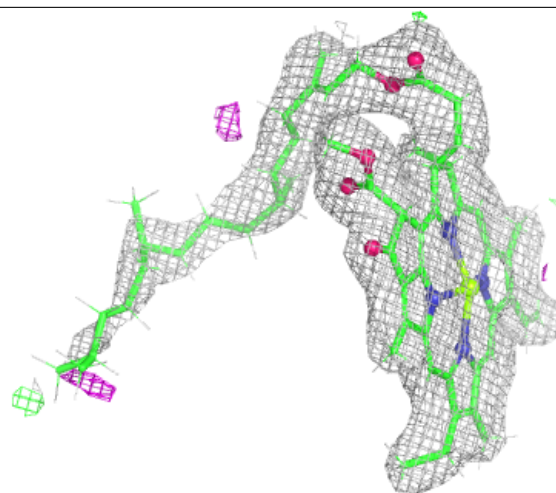
Electron density around CLA b 612:

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



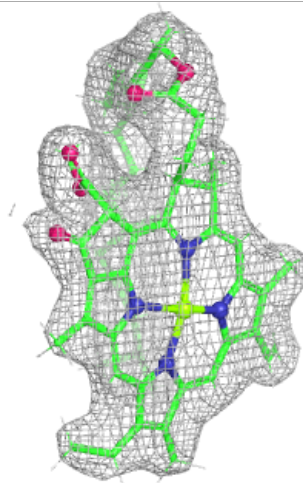
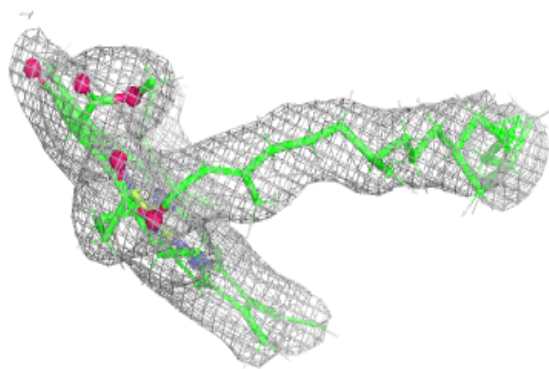
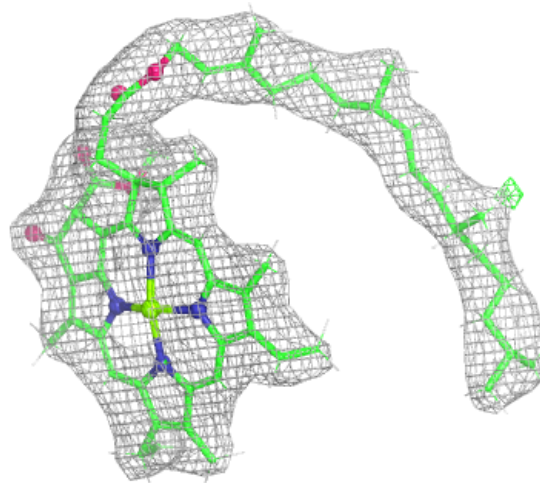
Electron density around CLA b 613:

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



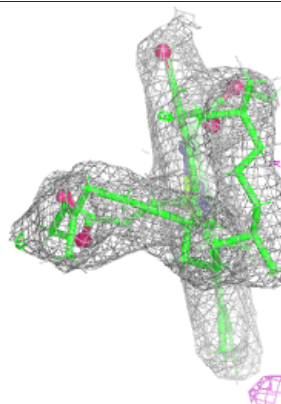
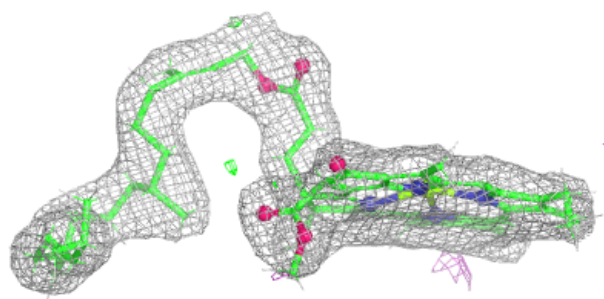
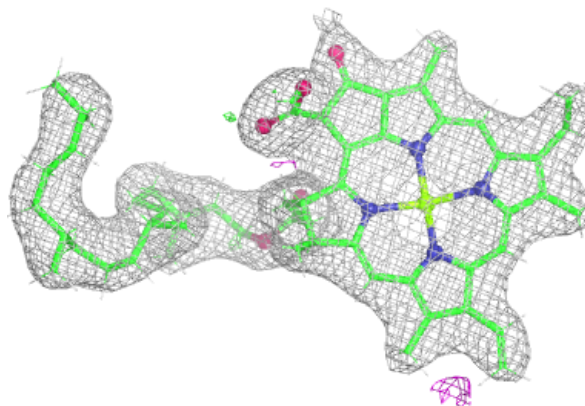
Electron density around CLA C 507:

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



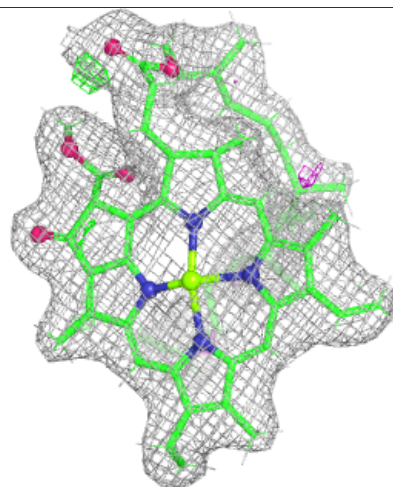
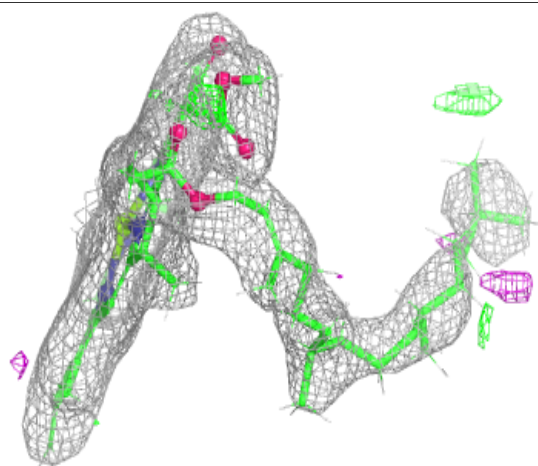
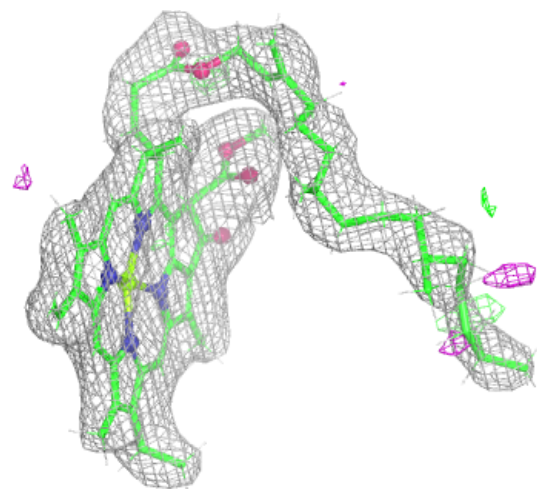
Electron density around CLA B 612:

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



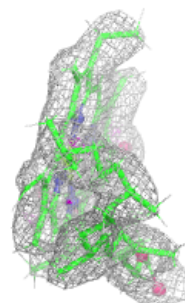
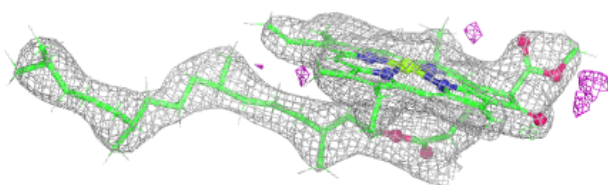
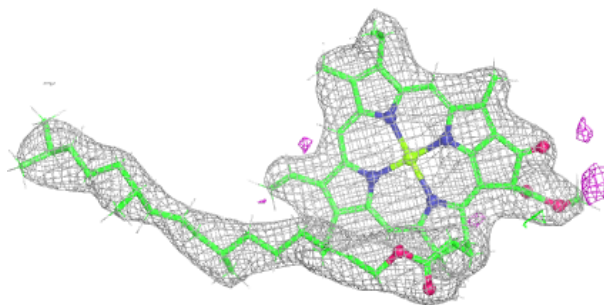
Electron density around CLA B 613:

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

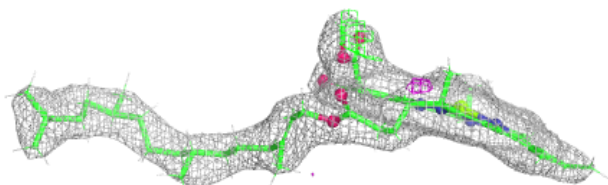
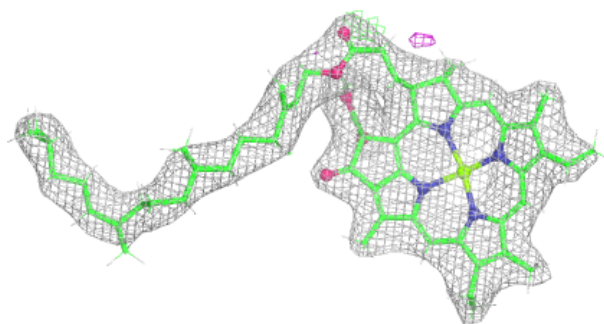


Electron density around CLA c 501:

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

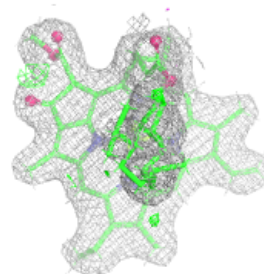
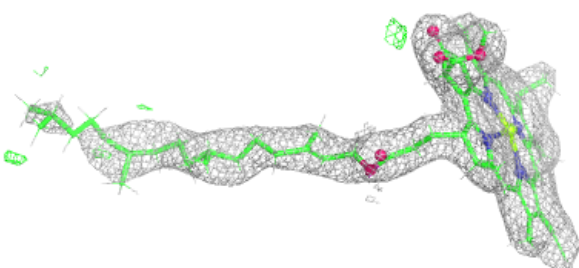
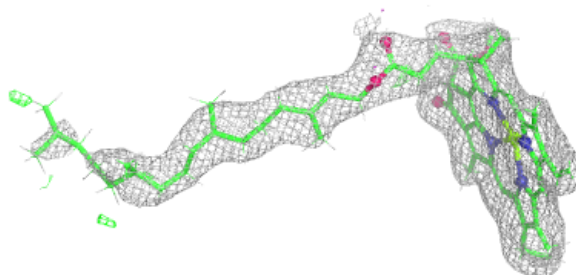
**Electron density around CLA B 602:**

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

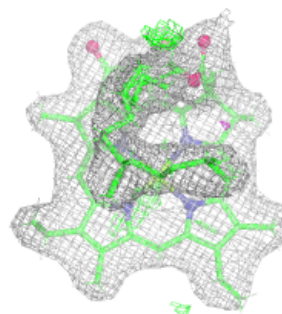
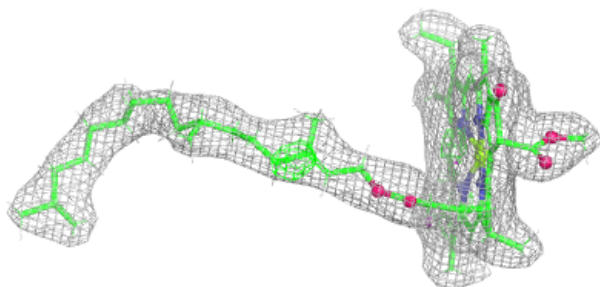
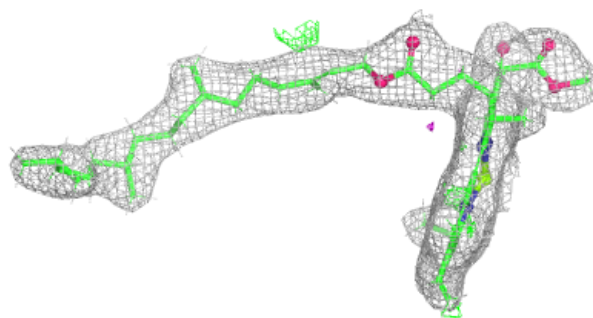


Electron density around CLA B 604:

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

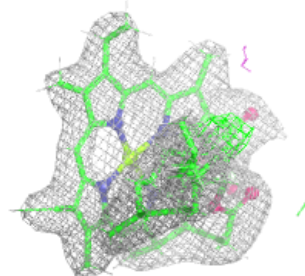
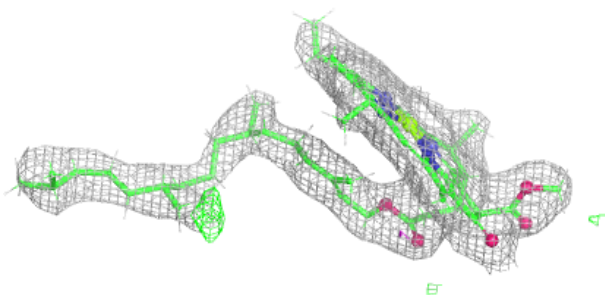
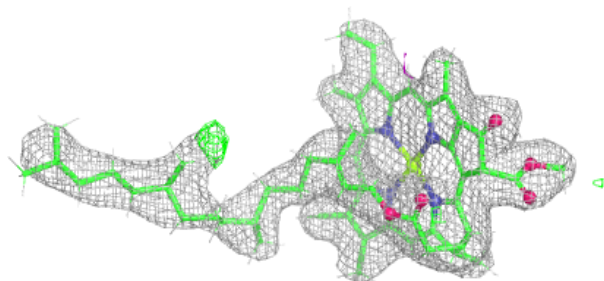
**Electron density around CLA B 605:**

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

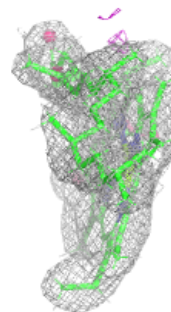
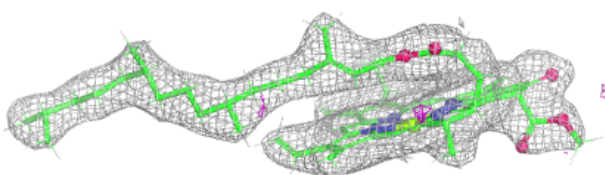
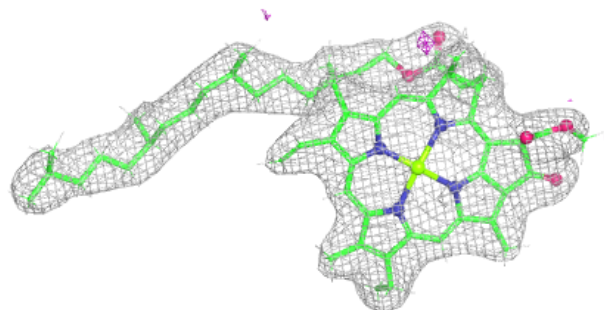


Electron density around CLA c 505:

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

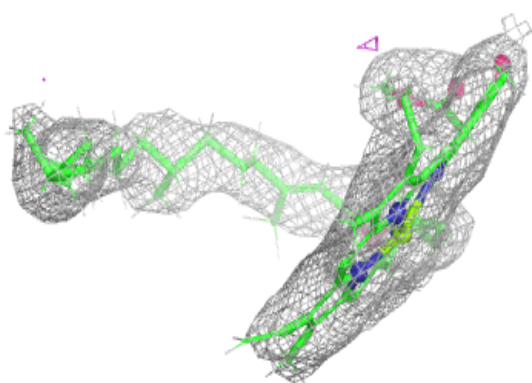
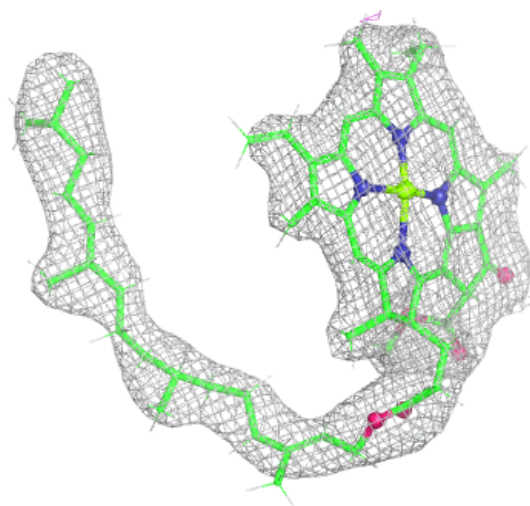
**Electron density around CLA C 501:**

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



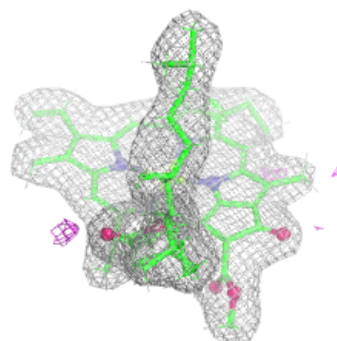
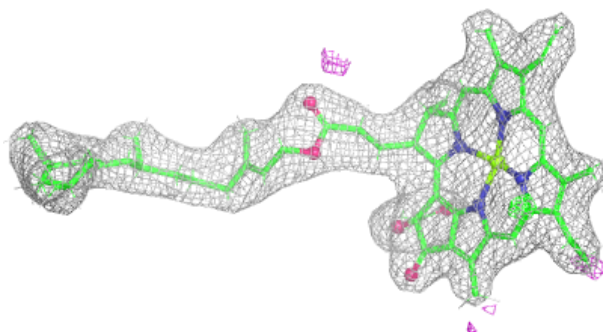
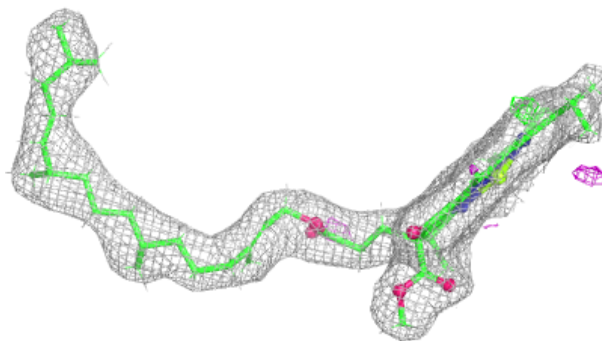
Electron density around CLA c 507:

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

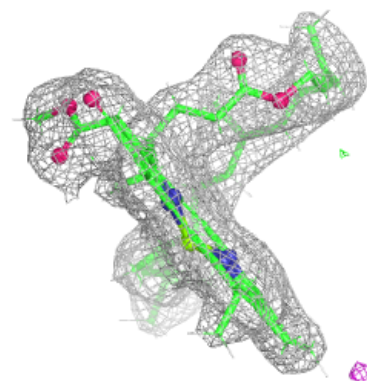
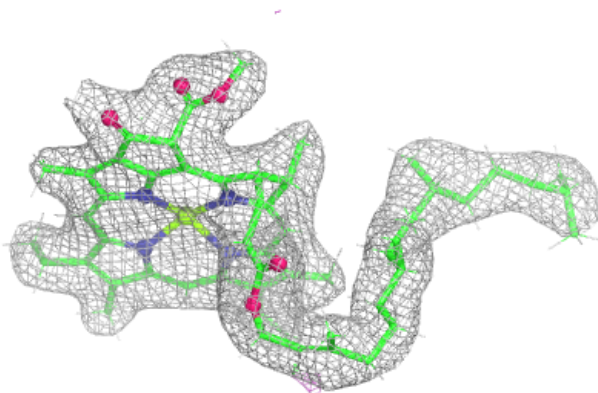
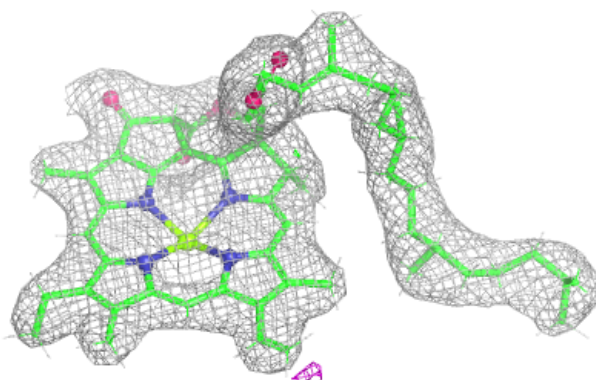


Electron density around CLA D 403:

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

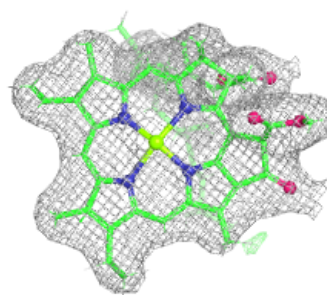
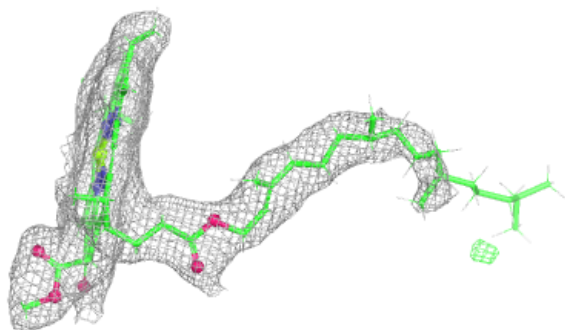
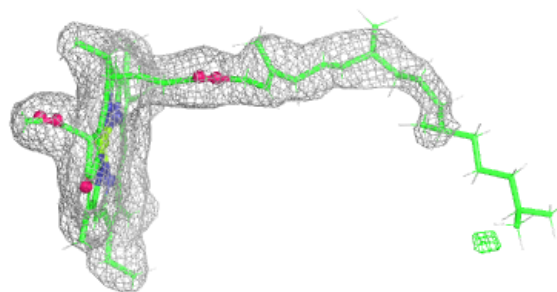
**Electron density around CLA D 404:**

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

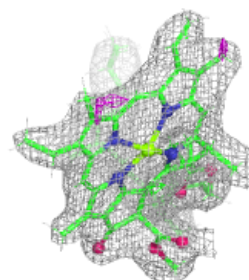
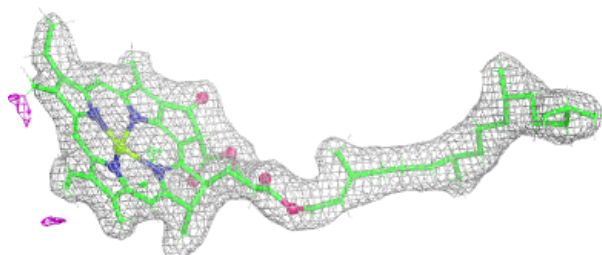
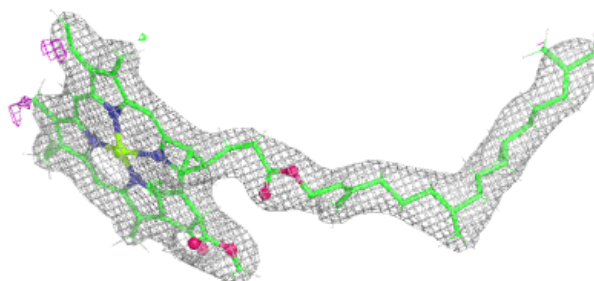


Electron density around CLA D 405:

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

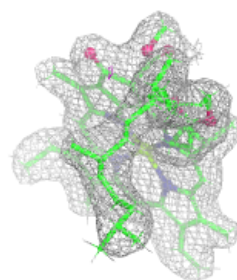
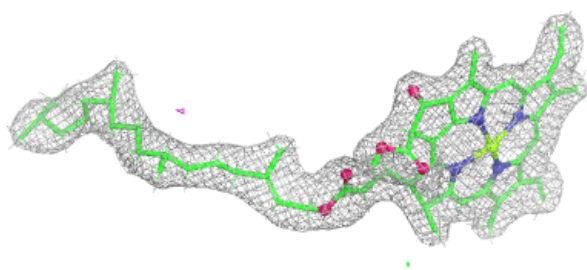
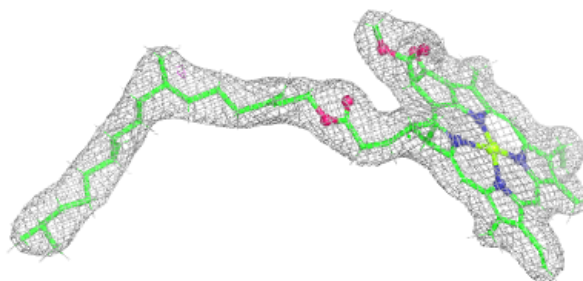
**Electron density around CLA a 402:**

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

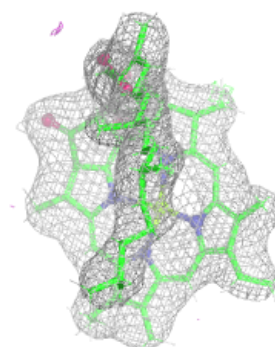
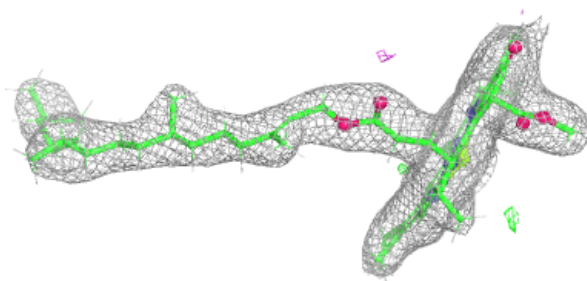
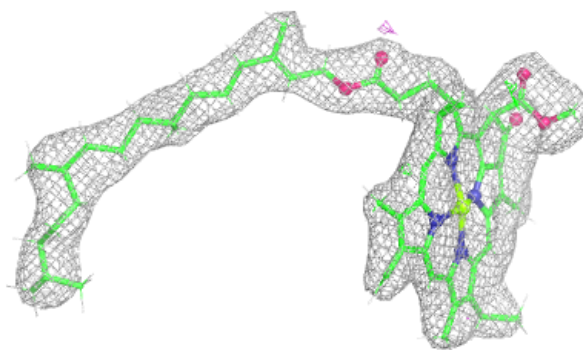


Electron density around CLA A 402:

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

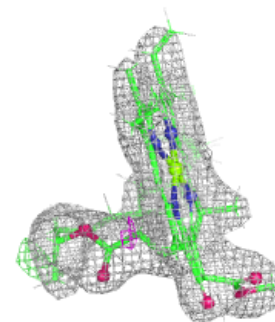
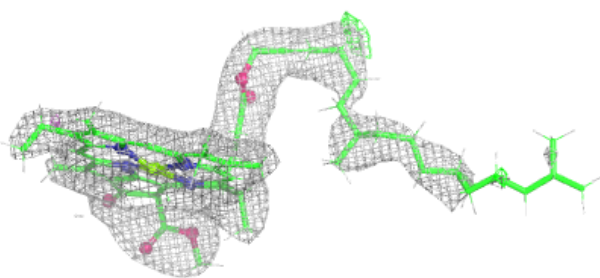
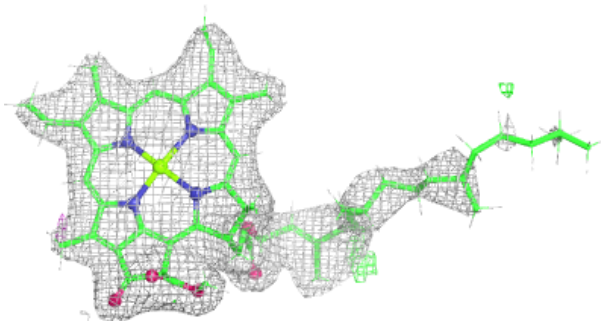
**Electron density around CLA B 609:**

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

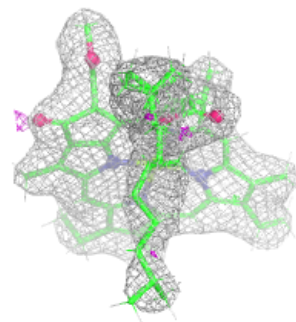
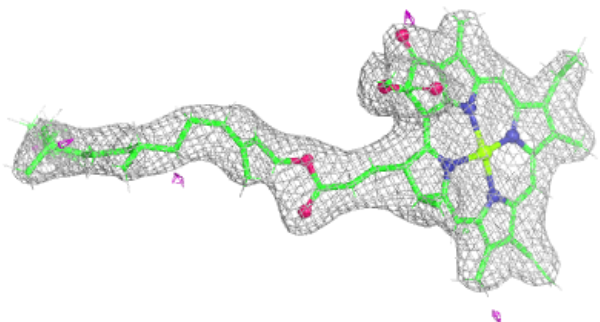
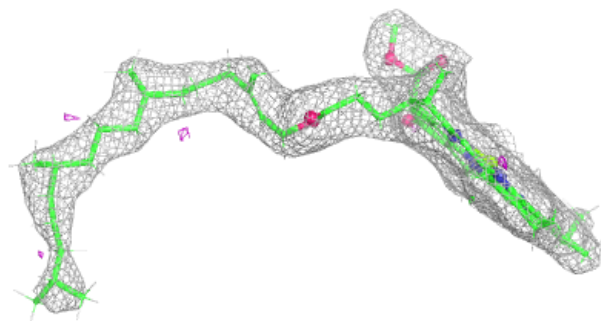


Electron density around CLA d 401:

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

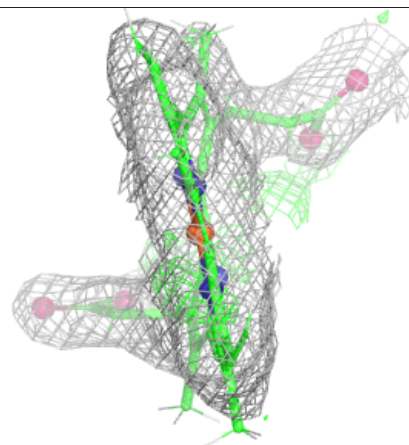
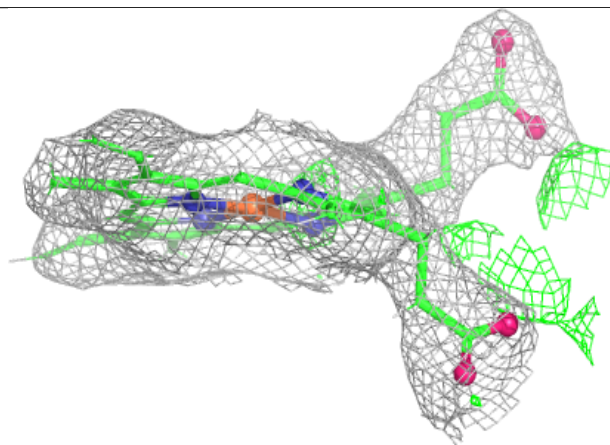
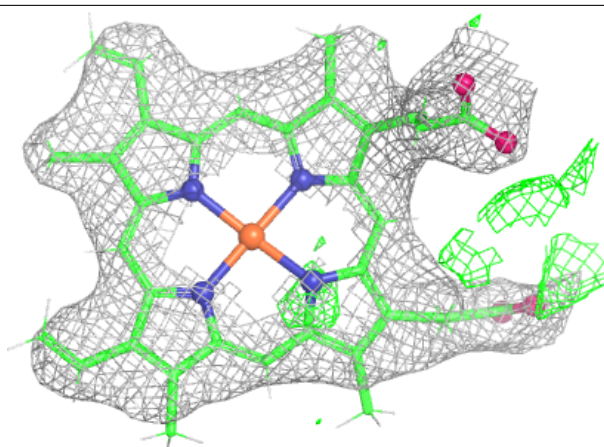
**Electron density around CLA d 403:**

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



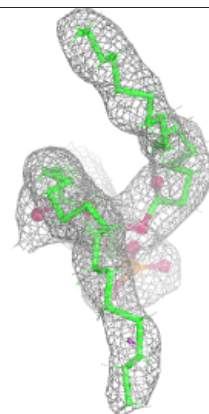
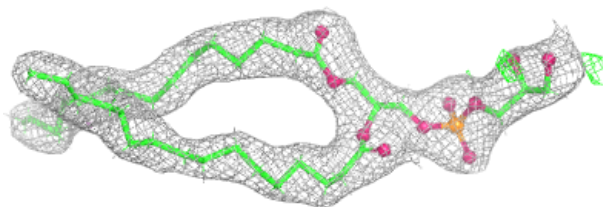
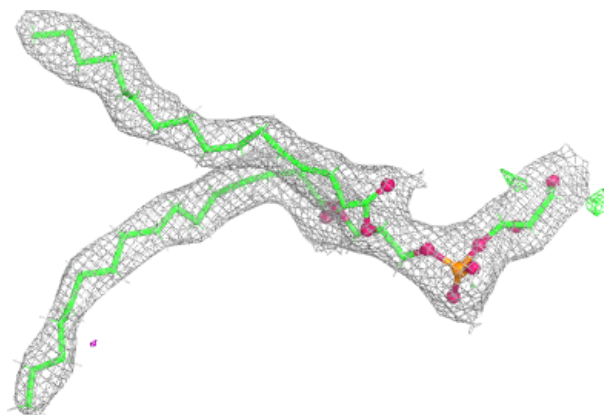
Electron density around HEM f 101:

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

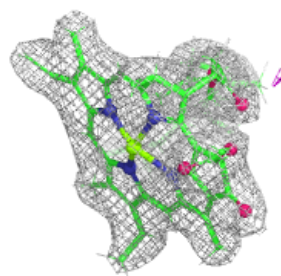
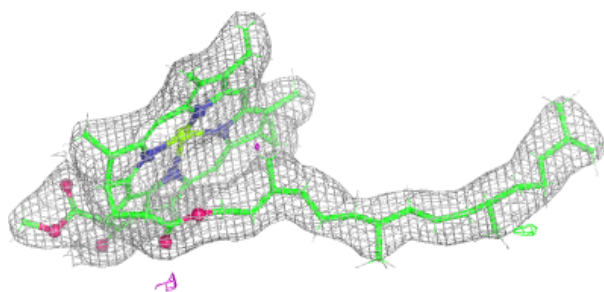
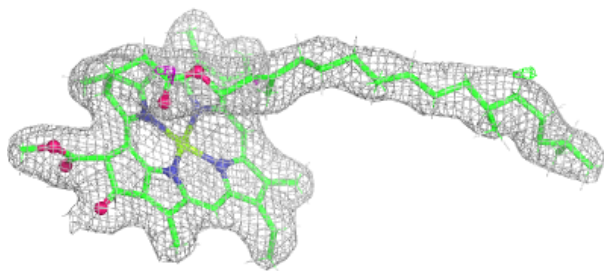


Electron density around LHG D 410:

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

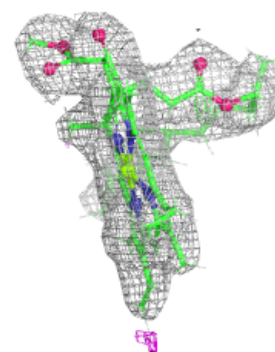
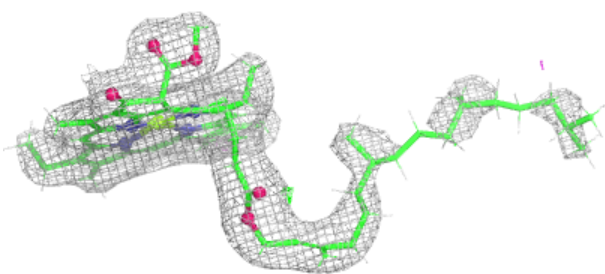
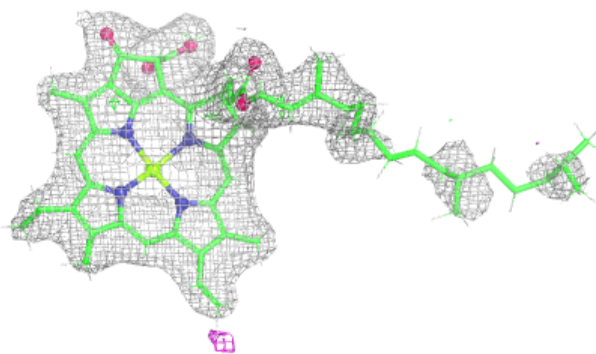
**Electron density around CLA B 608:**

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

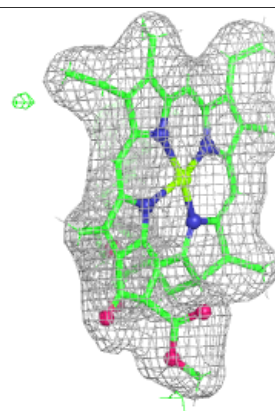
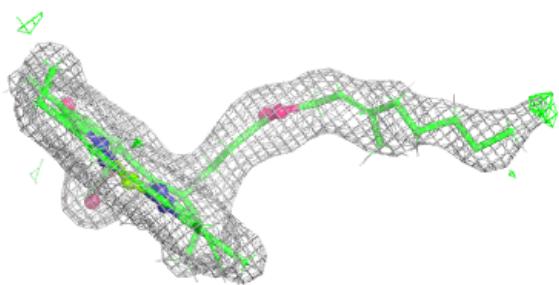
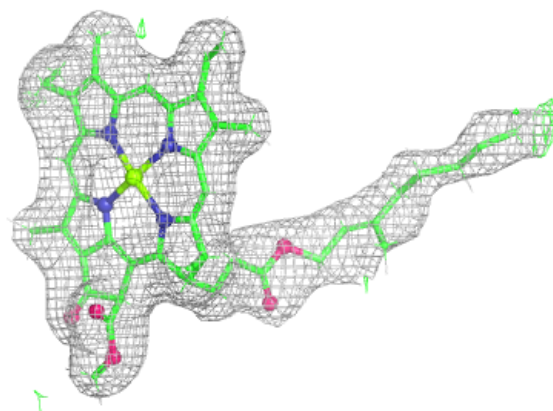


Electron density around CLA A 403:

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

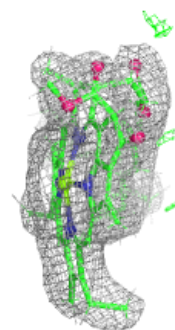
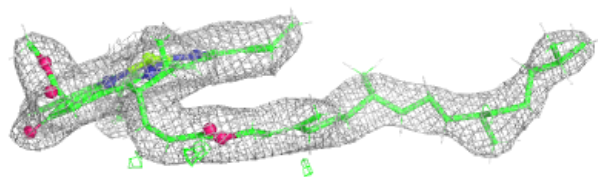
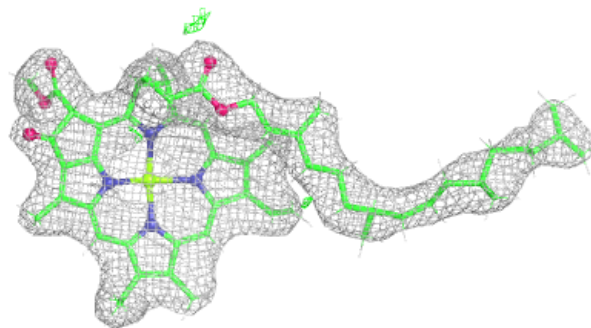
**Electron density around CLA A 405:**

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



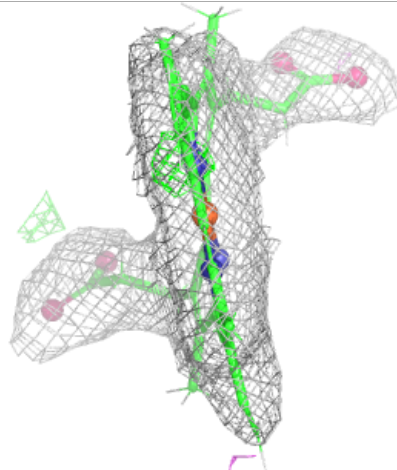
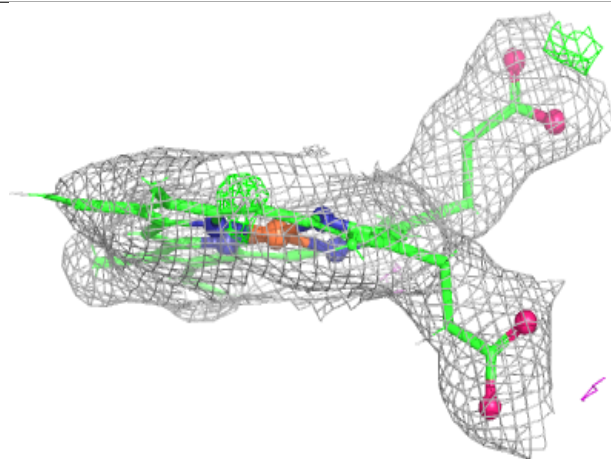
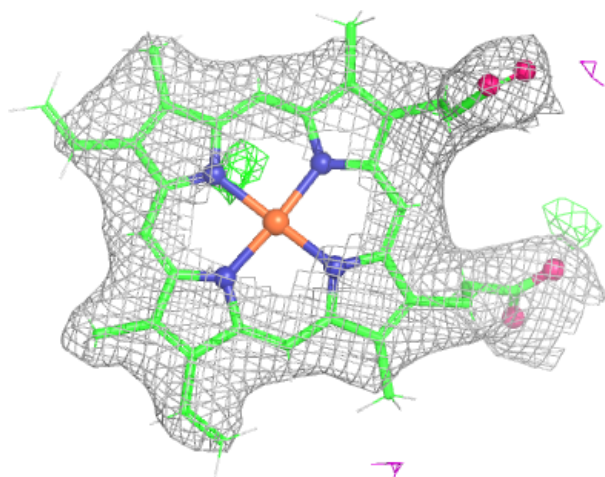
Electron density around CLA B 603:

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



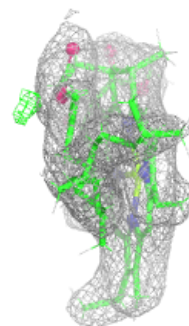
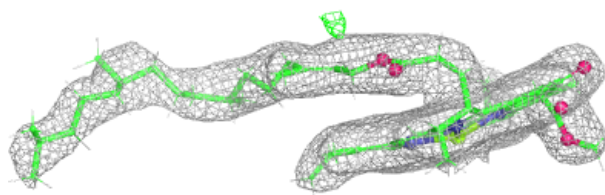
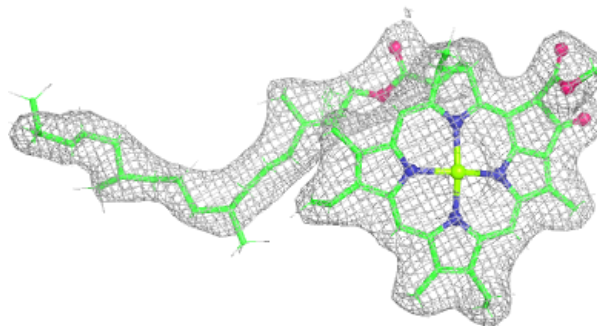
Electron density around HEM F 101:

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

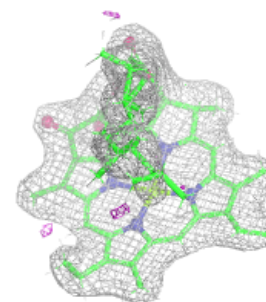
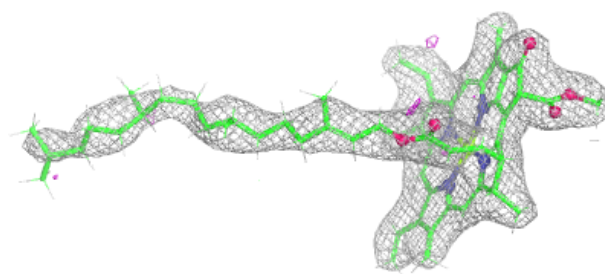
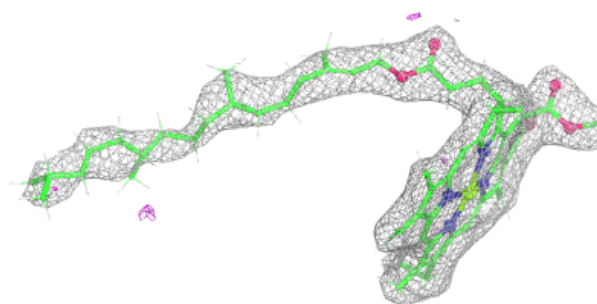


Electron density around CLA b 603:

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

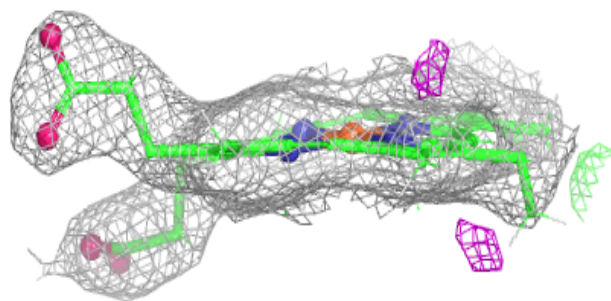
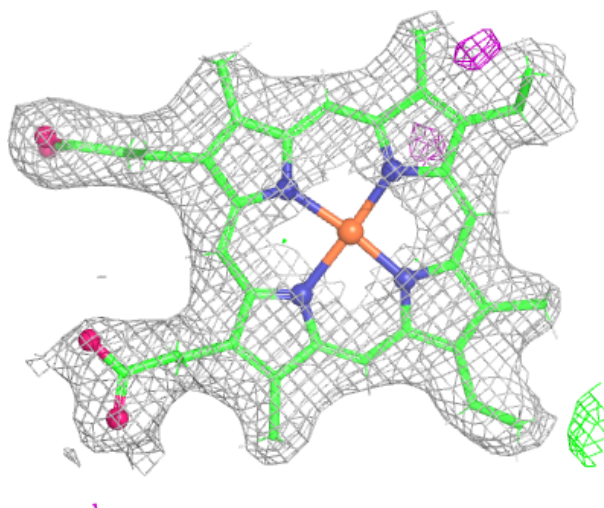
**Electron density around CLA B 607:**

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



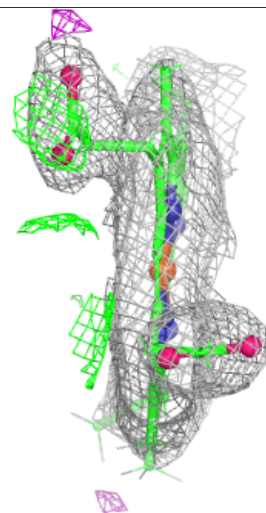
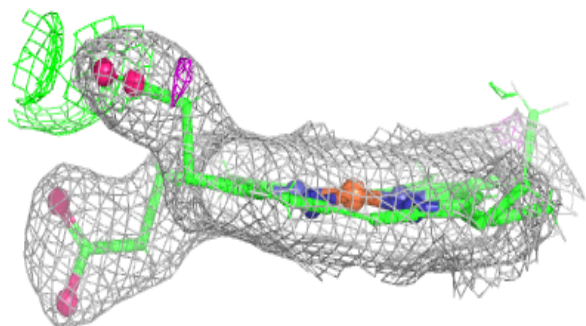
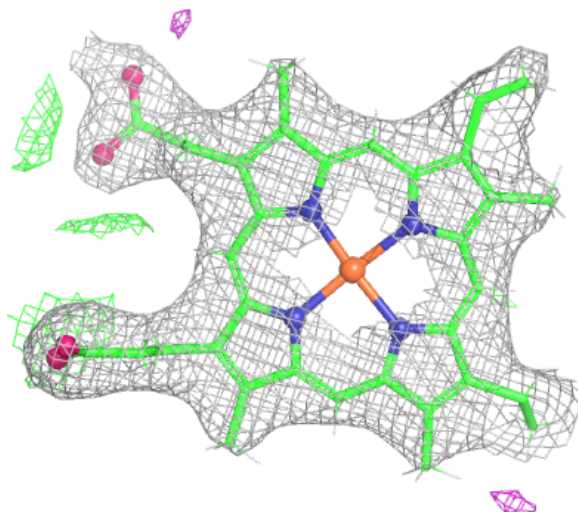
Electron density around HEC V 201:

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



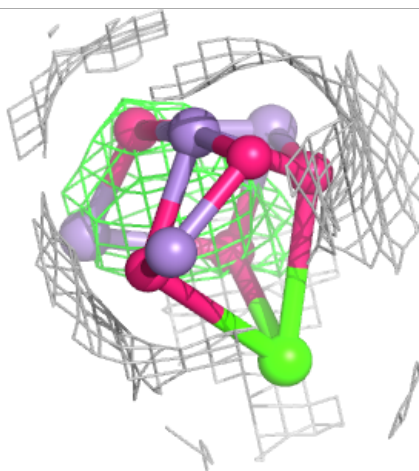
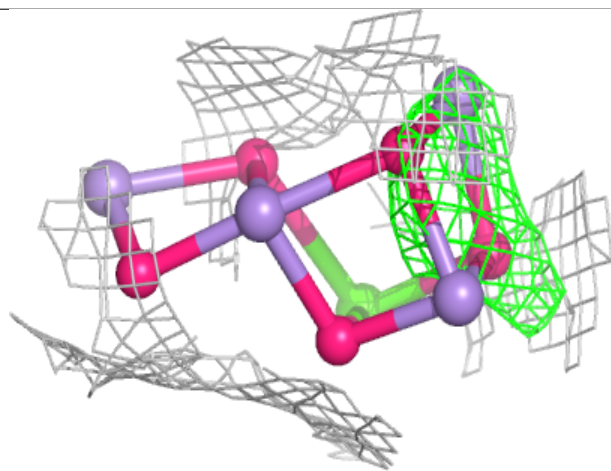
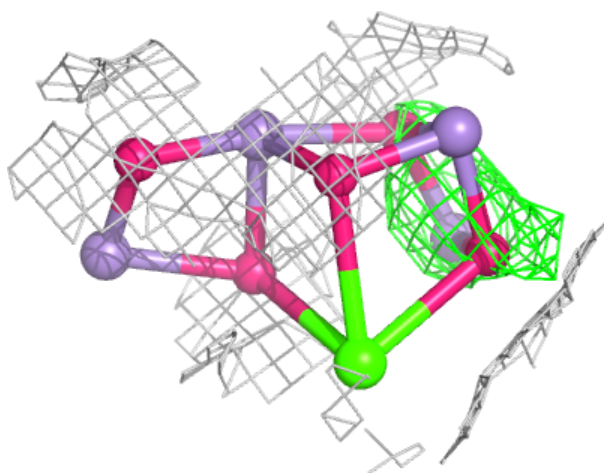
Electron density around HEC v 201:

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



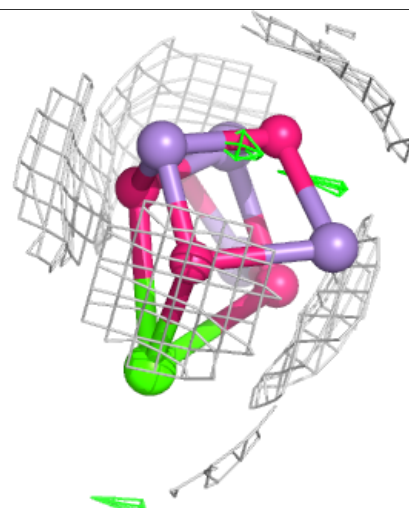
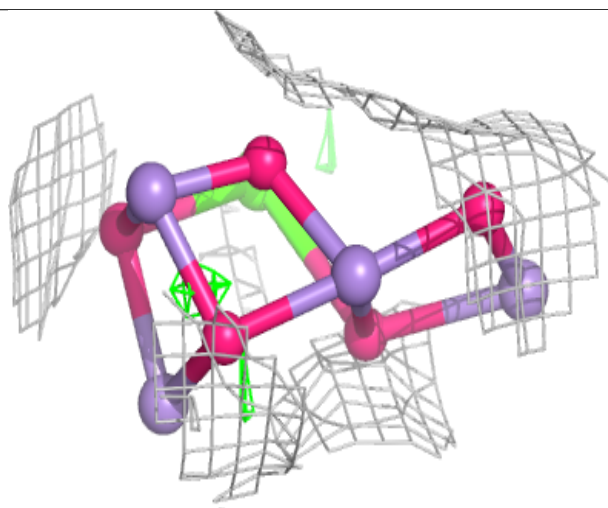
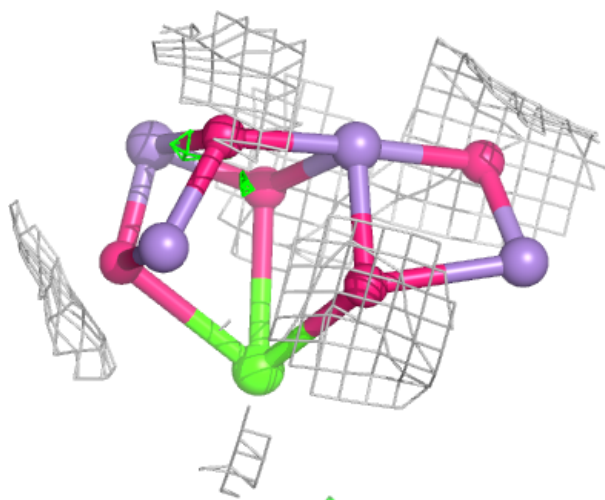
Electron density around OEX A 414:

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



Electron density around OEX a 414:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.