



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:51 AM EDT

PDB ID : 7RF2 / pdb_00007rf2
Title : RT XFEL structure of dark-stable state of Photosystem II (0F, S1 rich) at 2.08 Angstrom
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 : 2.08 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)

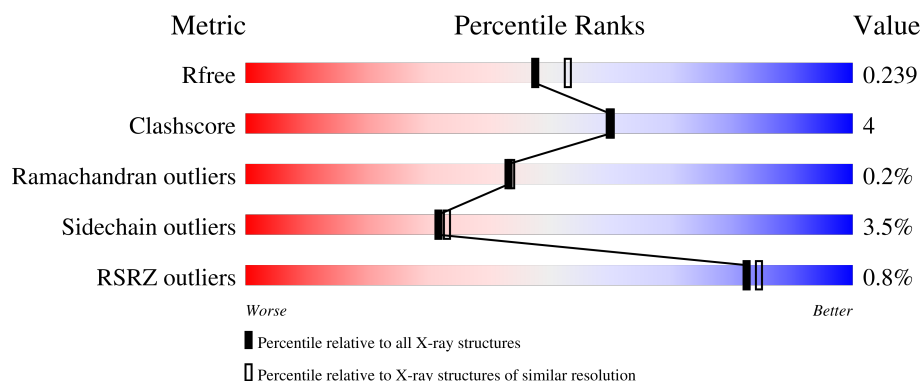
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

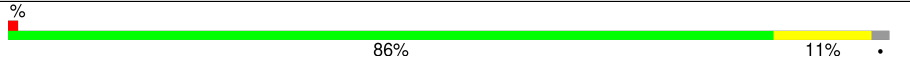
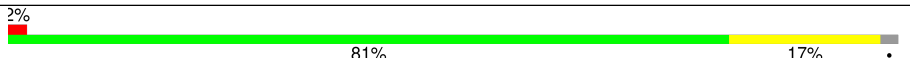
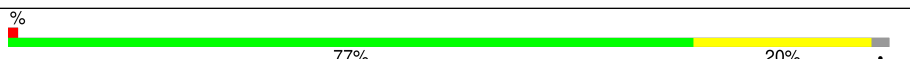
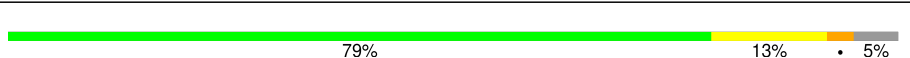
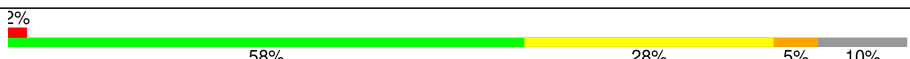
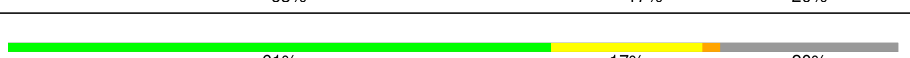
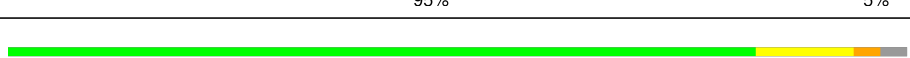
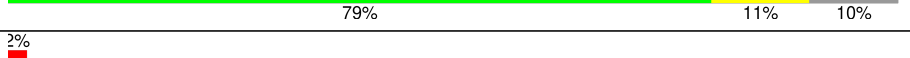
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Mol	Chain	Length	Quality of chain
1	A	344	 85% 11% .
1	a	344	 85% 11% .

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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 [i](#)

There are 36 unique types of molecules in this entry. The entry contains 103670 atoms, of which 51532 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
			5128	1714	2509	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			

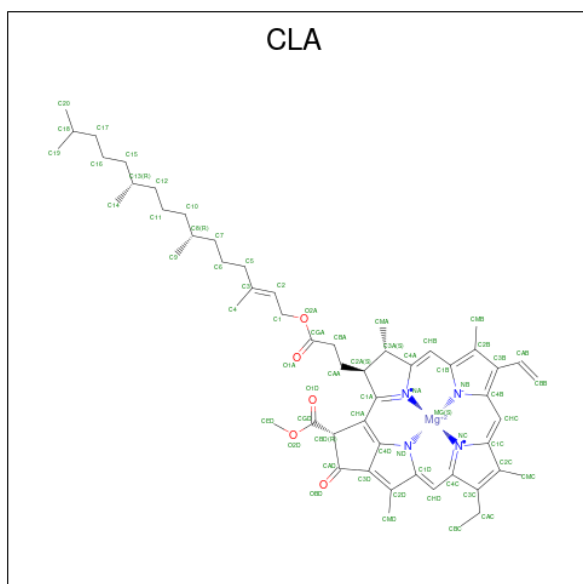
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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: $C_{55}H_{72}MgN_4O_5$).



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

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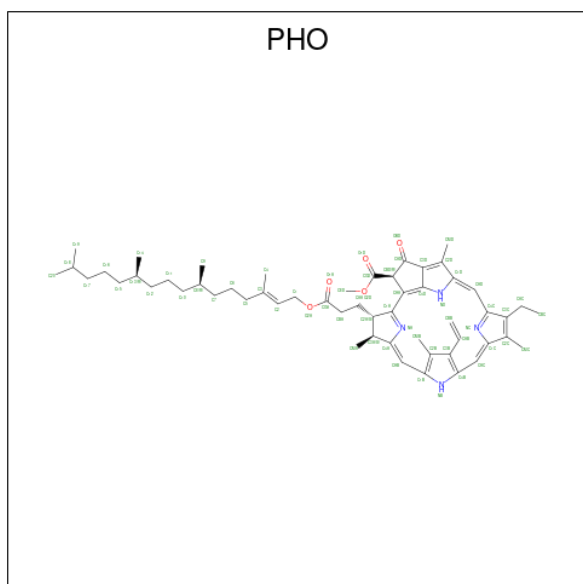
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
22	b	1	Total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

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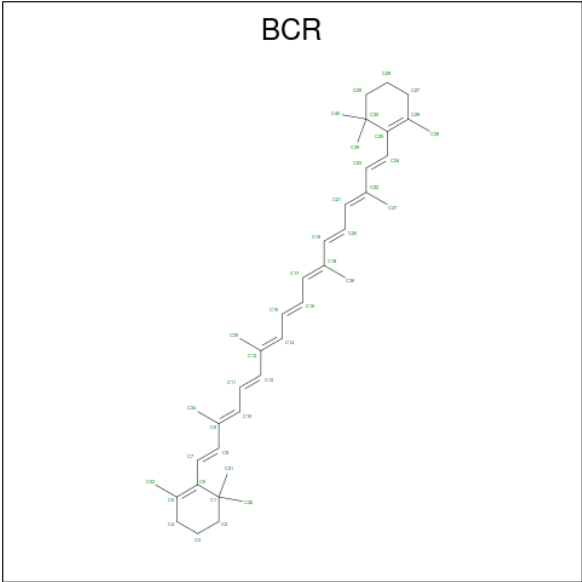
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4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

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



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

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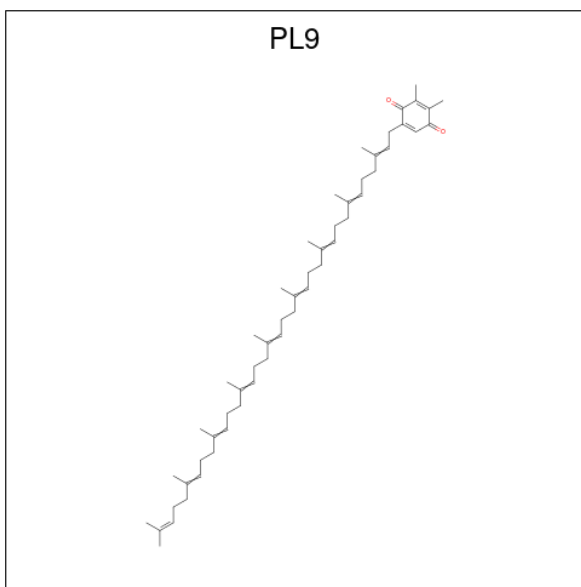
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	h	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40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

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

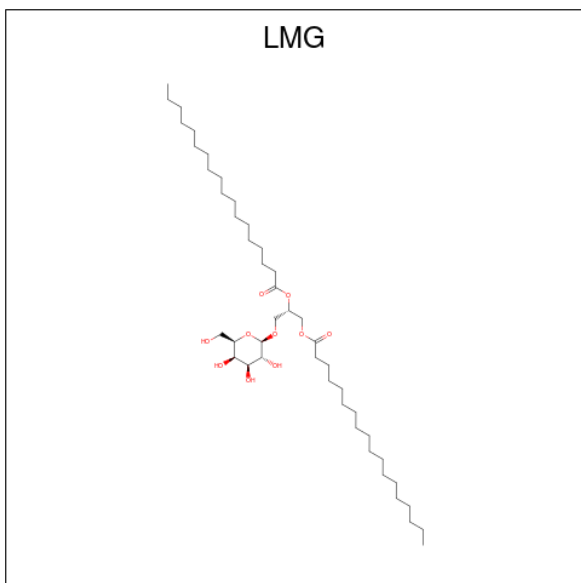
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- Molecule 26 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



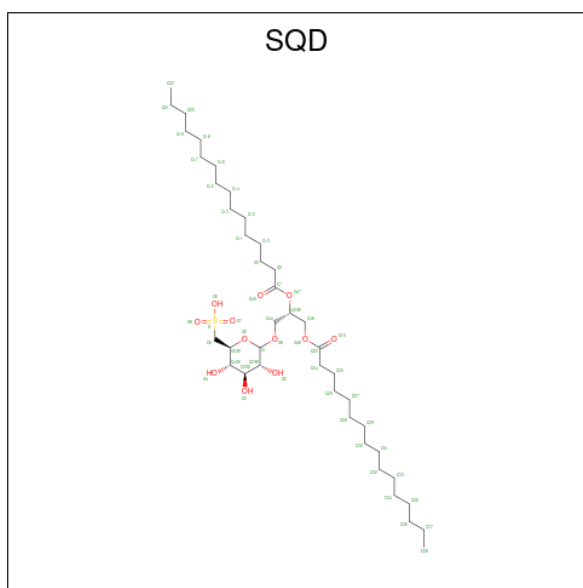
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



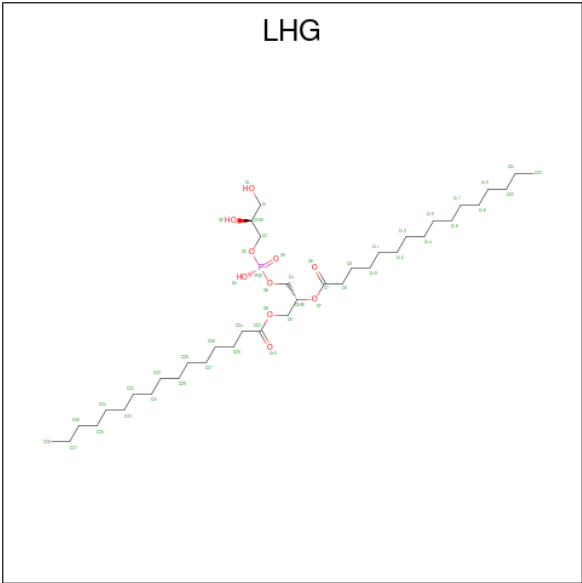
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			114	38	66	10		
27	D	1	Total	C	H	O	0	0
			123	41	72	10		
27	D	1	Total	C	H	O	0	0
			77	27	45	5		
27	M	1	Total	C	H	O	0	0
			123	41	72	10		
27	Y	1	Total	C	H	O	0	0
			114	38	66	10		
27	a	1	Total	C	H	O	0	0
			117	39	68	10		
27	b	1	Total	C	H	O	0	0
			141	45	86	10		
27	c	1	Total	C	H	O	0	0
			81	27	44	10		
27	c	1	Total	C	H	O	0	0
			117	38	69	10		
27	d	1	Total	C	H	O	0	0
			102	34	58	10		
27	h	1	Total	C	H	O	0	0
			57	21	34	2		
27	m	1	Total	C	H	O	0	0
			123	41	72	10		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	S	0	0
			122	39	70	12	1		
28	A	1	Total	C	H	O		0	0
			104	35	65	4			
28	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	F	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
28	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
28	a	1	Total	C	H	O		0	0
			92	31	56	5			
28	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
28	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



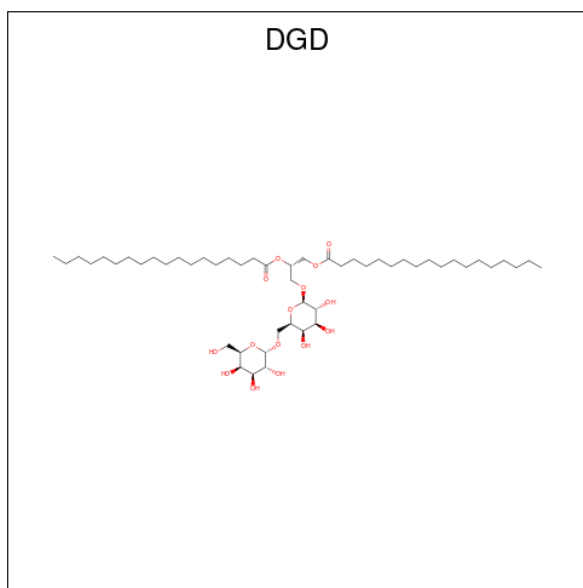
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
29	D	1	Total	C	H	O	P	0	0
			114	36	67	10	1		

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

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



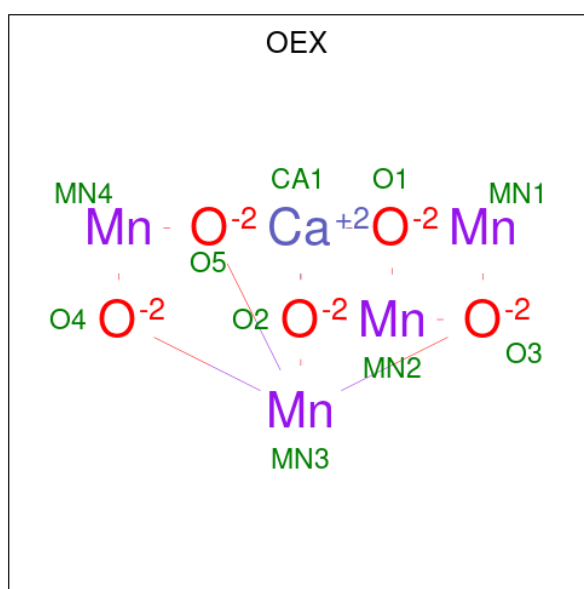
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			162	51	96	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		
30	C	1	Total	C	H	O	0	0
			144	47	82	15		

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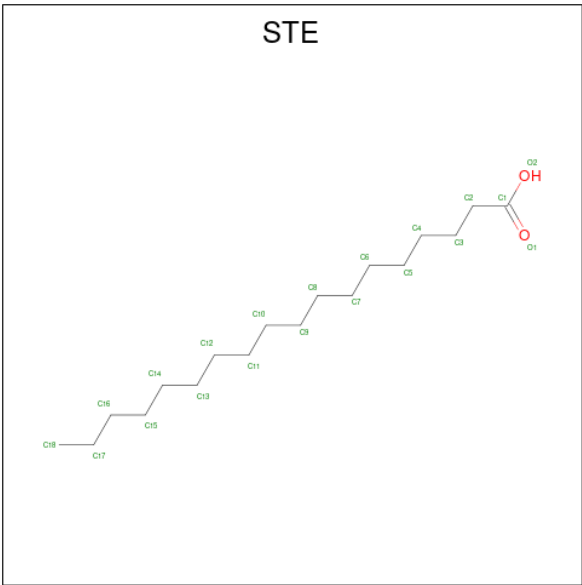
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	H	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			143	47	81	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	c	1	Total	C	H	O	0	0
			144	47	82	15		
30	h	1	Total	C	H	O	0	0
			144	47	82	15		
30	o	1	Total	C	H	O	0	0
			119	39	75	5		

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



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

- Molecule 32 is STEARIC ACID (CCD ID: STE) (formula: $\text{C}_{18}\text{H}_{36}\text{O}_2$).



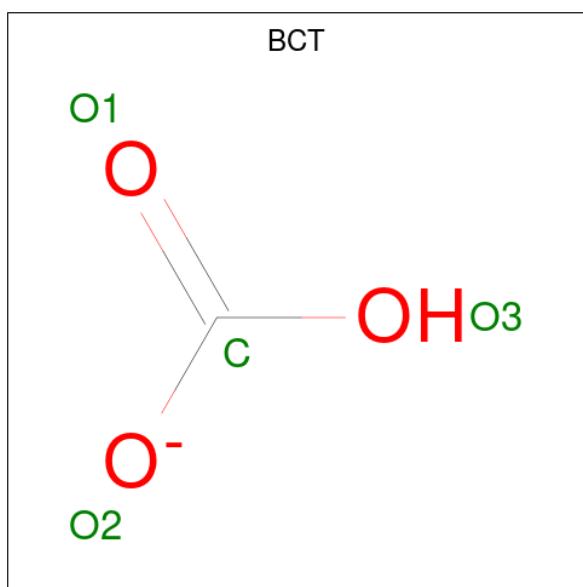
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	B	1	Total	C	H	O	0	0
			43	15	26	2		
32	B	1	Total	C	H	O	0	0
			34	12	20	2		
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	H	O	0	0
			46	16	28	2		
32	B	1	Total	C	H		0	0
			47	16	31			
32	B	1	Total	C	H	O	0	0
			28	10	16	2		
32	B	1	Total	C	O		0	0
			16	14	2			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	C	1	Total	C	H		0	0
			47	16	31			
32	C	1	Total	C	H	O	0	0
			28	10	16	2		
32	D	1	Total	C	H	O	0	0
			55	18	35	2		
32	D	1	Total	C	O		0	0
			15	13	2			
32	E	1	Total	C	H	O	0	0
			28	10	16	2		
32	H	1	Total	C	H		0	0
			53	18	35			

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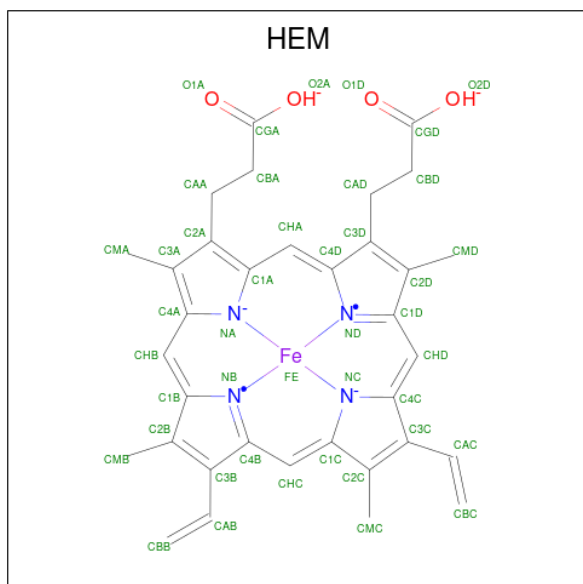
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	I	1	Total C H 41 15 26	0	0
32	J	1	Total C H O 28 10 16 2	0	0
32	M	1	Total C H O 37 13 22 2	0	0
32	M	1	Total C H 26 10 16	0	0
32	M	1	Total C H 53 18 35	0	0
32	T	1	Total C H 44 15 29	0	0
32	a	1	Total C H 26 10 16	0	0
32	a	1	Total C H O 28 10 16 2	0	0
32	b	1	Total C H 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 O 55 18 35 2	0	0
32	b	1	Total C H 26 10 16	0	0
32	c	1	Total C H O 55 18 35 2	0	0
32	c	1	Total C H O 28 10 16 2	0	0
32	d	1	Total C H O 43 15 26 2	0	0
32	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	m	1	Total C H O 28 10 16 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	d	1	Total	C	H	O	0	0
			5	1	1	3		

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



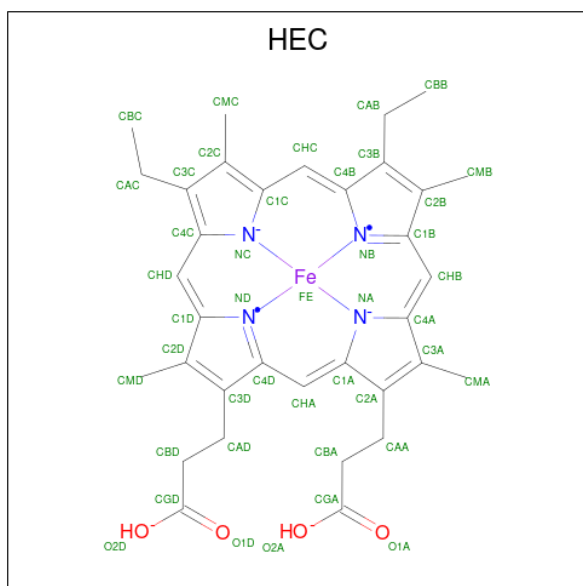
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
34	F	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	V	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		
35	v	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	144	Total	O	0	0
			144	144		
36	B	204	Total	O	0	0
			204	204		
36	C	182	Total	O	0	0
			182	182		
36	D	136	Total	O	0	0
			136	136		
36	E	30	Total	O	0	0
			30	30		
36	F	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	H	37	Total O 37 37	0	0
36	I	10	Total O 10 10	0	0
36	J	16	Total O 16 16	0	0
36	K	8	Total O 8 8	0	0
36	L	8	Total O 8 8	0	0
36	M	7	Total O 7 7	0	0
36	O	90	Total O 90 90	0	0
36	T	10	Total O 10 10	0	0
36	U	52	Total O 52 52	0	0
36	V	65	Total O 65 65	0	0
36	X	12	Total O 12 12	0	0
36	Y	6	Total O 6 6	0	0
36	Z	2	Total O 2 2	0	0
36	a	126	Total O 126 126	0	0
36	b	206	Total O 206 206	0	0
36	c	181	Total O 181 181	0	0
36	d	111	Total O 111 111	0	0
36	e	21	Total O 21 21	0	0
36	f	8	Total O 8 8	0	0
36	h	36	Total O 36 36	0	0
36	i	13	Total O 13 13	0	0

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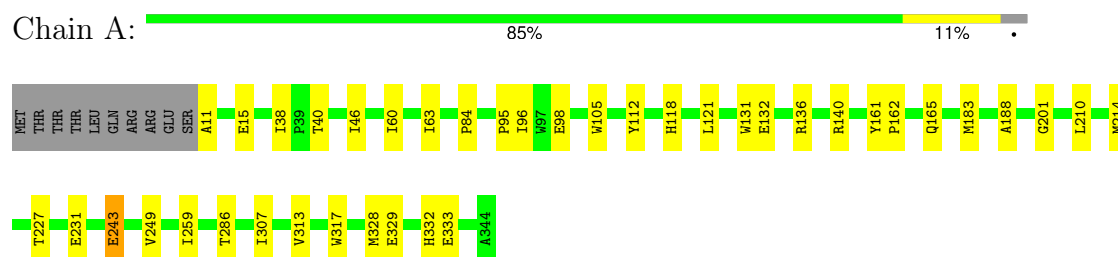
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	j	8	Total 8	O 8	0	0
36	k	6	Total 6	O 6	0	0
36	l	7	Total 7	O 7	0	0
36	m	6	Total 6	O 6	0	0
36	o	102	Total 102	O 102	0	0
36	r	3	Total 3	O 3	0	0
36	t	8	Total 8	O 8	0	0
36	u	58	Total 58	O 58	0	0
36	v	56	Total 56	O 56	0	0
36	x	8	Total 8	O 8	0	0
36	y	3	Total 3	O 3	0	0
36	z	9	Total 9	O 9	0	0

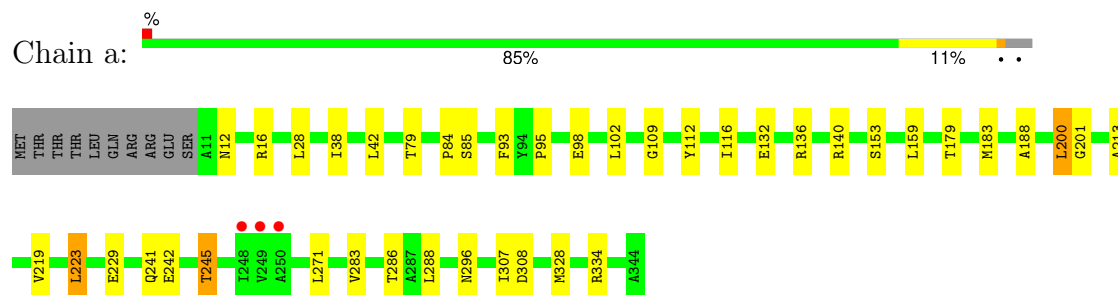
3 Residue-property plots

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.

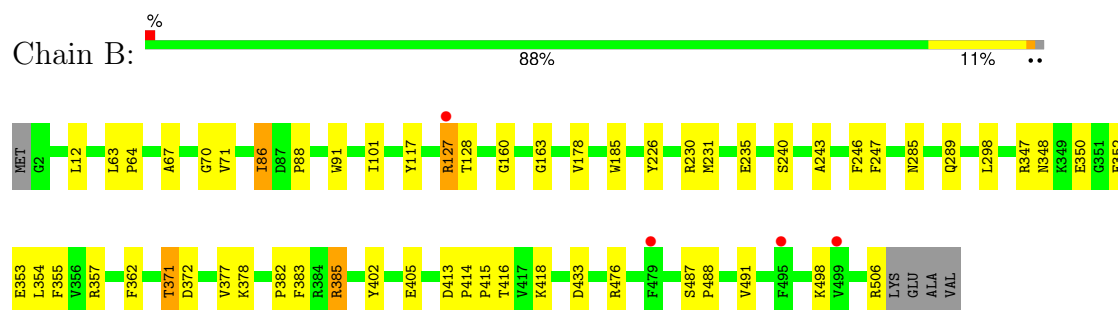
• Molecule 1: Photosystem II protein D1 1



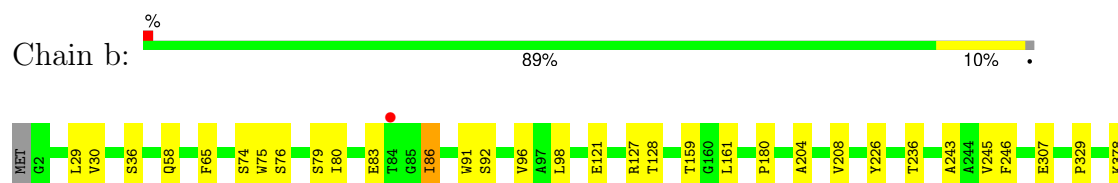
• Molecule 1: Photosystem II protein D1 1

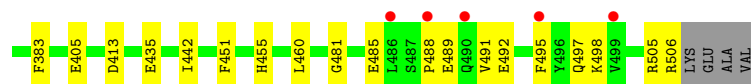


• Molecule 2: Photosystem II CP47 reaction center protein

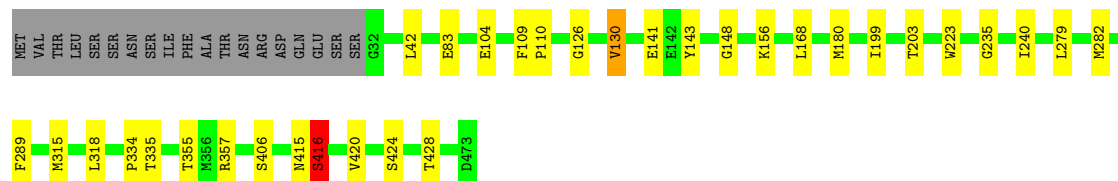
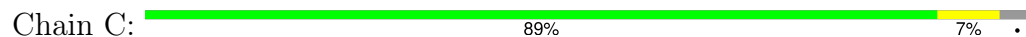


• Molecule 2: Photosystem II CP47 reaction center protein

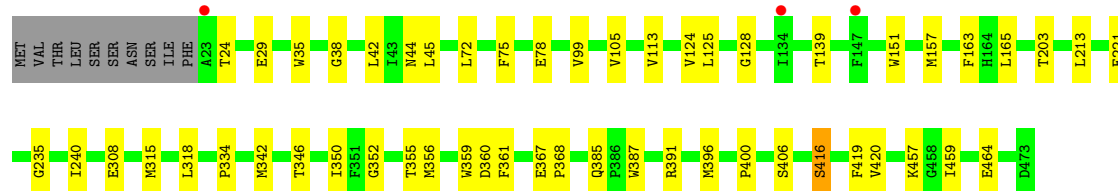
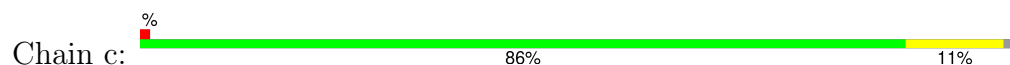




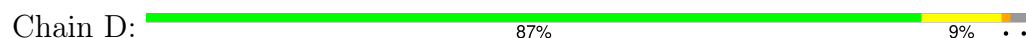
- Molecule 3: Photosystem II CP43 reaction center protein



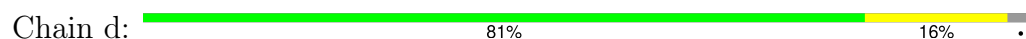
- Molecule 3: Photosystem II CP43 reaction center protein



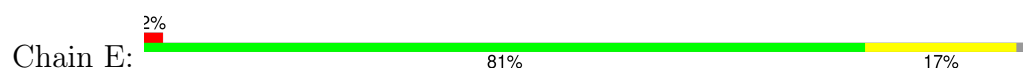
- Molecule 4: Photosystem II D2 protein



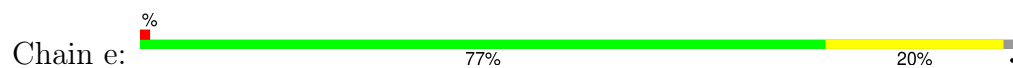
- Molecule 4: Photosystem II D2 protein



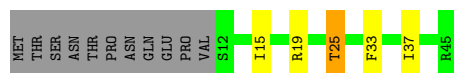
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha



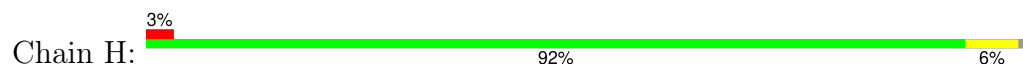
- Molecule 6: Cytochrome b559 subunit beta



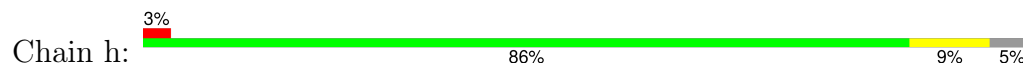
- Molecule 6: Cytochrome b559 subunit beta



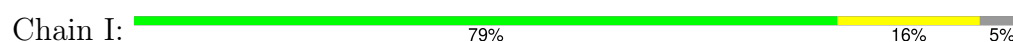
- Molecule 7: Photosystem II reaction center protein H



- Molecule 7: Photosystem II reaction center protein H

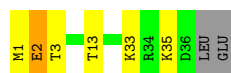


- Molecule 8: Photosystem II reaction center protein I



- Molecule 8: Photosystem II reaction center protein I

Chain i:  79% 13% • 5%



- Molecule 9: Photosystem II reaction center protein J

Chain J:  72% 18% 10%



- Molecule 9: Photosystem II reaction center protein J

Chain j:  2% 58% 28% 5% 10%



- Molecule 10: Photosystem II reaction center protein K

Chain K:  63% 17% 20%

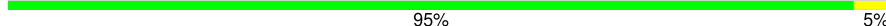


- Molecule 10: Photosystem II reaction center protein K

Chain k:  61% 17% • 20%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  95% 5%



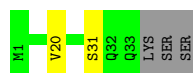
- Molecule 11: Photosystem II reaction center protein L

Chain l:  84% 11% • •



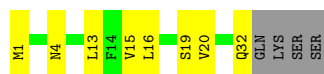
- Molecule 12: Photosystem II reaction center protein M

Chain M:  86% 6% 8%



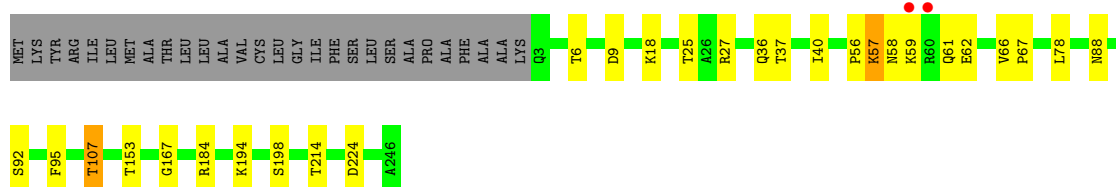
- Molecule 12: Photosystem II reaction center protein M

Chain m:  67% 22% 11%



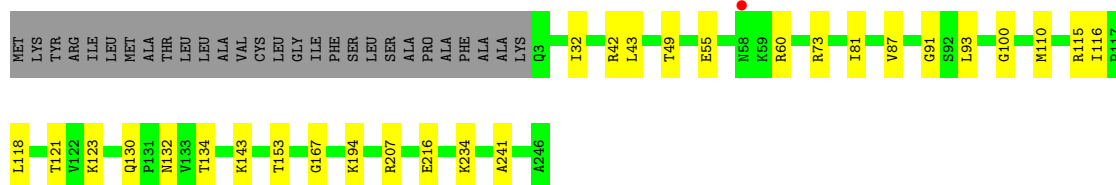
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  79% 10% 10%



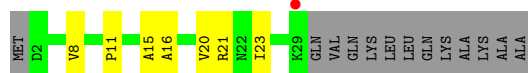
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  79% 11% 10%



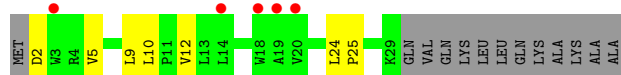
- Molecule 14: Photosystem II protein Y

Chain R:  2% 51% 17% 32%



- Molecule 14: Photosystem II protein Y

Chain r:  12% 51% 17% 32%

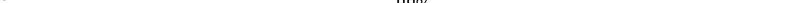


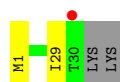
- Molecule 15: Photosystem II reaction center protein T

Chain T: 81% 9% • 6%

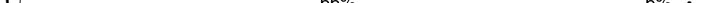


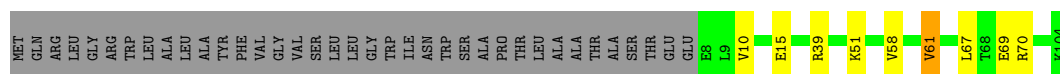
- Molecule 15: Photosystem II reaction center protein T

Chain t:  3% 88% 6% 6%

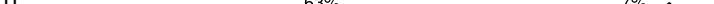


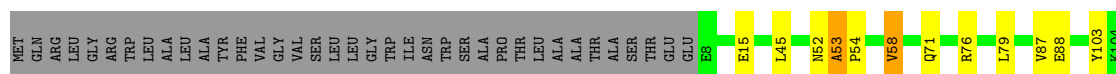
- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain U:  66% 6% 28%



- Molecule 16: Photosystem II 12 kDa extrinsic protein

Chain u:  63% 7% 28%

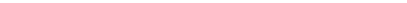


- Molecule 17: Cytochrome c-550

Chain V:  74% 9% • 16%

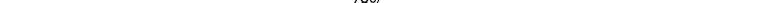


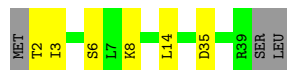
- Molecule 17: Cytochrome c-550

Chain v:  75% 7% • 16%

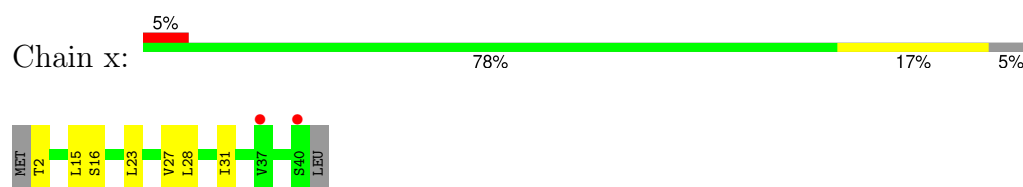


- Molecule 18: Photosystem II reaction center X protein

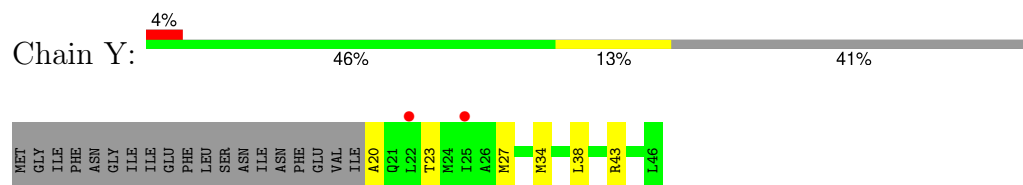
Chain X:  78% 15% 7%



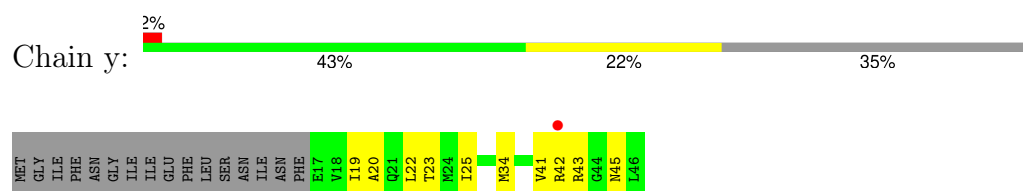
- Molecule 18: Photosystem II reaction center X protein



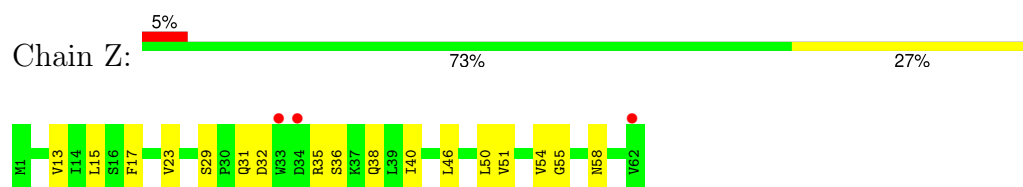
- Molecule 19: Photosystem II reaction center protein Ycf12



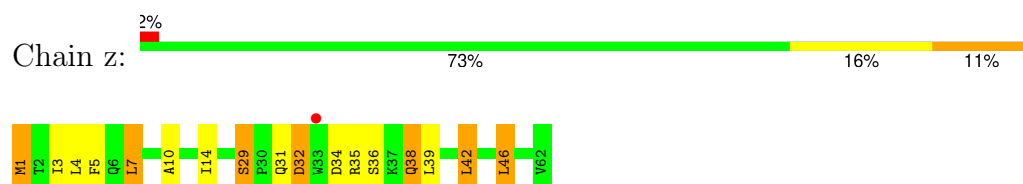
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.92Å 221.63Å 307.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.64 – 2.08 33.64 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.64-2.08) 85.0 (33.64-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.55 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.185 , 0.238 0.185 , 0.239	Depositor DCC
R_{free} test set	4226 reflections (0.67%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.4	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	103670	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	1/2707 (0.0%)	0.66	0/3692
1	a	0.58	1/2704 (0.0%)	0.65	0/3688
2	B	0.54	0/4161	0.60	0/5669
2	b	0.54	0/4118	0.60	0/5611
3	C	0.54	0/3547	0.61	0/4830
3	c	0.50	0/3619	0.58	0/4926
4	D	0.58	0/2812	0.64	0/3832
4	d	0.53	0/2821	0.62	0/3844
5	E	0.50	0/688	0.60	0/940
5	e	0.47	0/683	0.59	0/932
6	F	0.58	0/284	0.60	0/387
6	f	0.46	0/284	0.69	0/387
7	H	0.67	0/523	0.65	0/713
7	h	0.59	0/511	0.65	0/697
8	I	0.60	0/293	0.70	0/396
8	i	0.64	0/293	0.65	0/396
9	J	0.50	0/263	0.61	0/356
9	j	0.51	0/263	0.60	0/356
10	K	0.45	0/303	0.56	0/416
10	k	0.48	0/303	0.54	0/416
11	L	0.70	0/311	0.67	0/422
11	l	0.72	0/303	0.67	0/412
12	M	0.71	0/249	0.81	0/341
12	m	0.69	0/244	0.75	0/334
13	O	0.64	0/1904	0.71	0/2585
13	o	0.63	0/1905	0.68	0/2583
14	R	0.40	0/227	0.54	0/313
14	r	0.40	0/227	0.47	0/313
15	T	0.69	0/257	0.71	0/349
15	t	0.62	0/255	0.67	0/346
16	U	0.55	0/785	0.62	0/1064
16	u	0.75	1/785 (0.1%)	0.69	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.65	0/1085	0.69	0/1473
17	v	0.58	0/1085	0.63	0/1473
18	X	0.50	0/284	0.60	0/384
18	x	0.43	0/289	0.52	0/391
19	Y	0.48	0/197	0.57	0/264
19	y	0.44	0/219	0.56	0/294
20	Z	0.42	0/490	0.52	0/669
20	z	0.38	0/488	0.51	0/666
All	All	0.56	3/42769 (0.0%)	0.63	0/58224

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	V	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	u	103	TYR	CA-C	10.60	1.59	1.53
1	a	38	ILE	CA-CB	8.40	1.58	1.54
1	A	38	ILE	CA-CB	-7.59	1.50	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	2519	2519	24	0
1	a	2619	2509	2509	26	0
2	B	4005	3873	3867	36	0
2	b	3978	3836	3836	28	0
3	C	3426	3355	3343	18	0
3	c	3500	3426	3426	30	0
4	D	2717	2621	2621	23	0
4	d	2723	2627	2627	36	0
5	E	666	651	651	11	0
5	e	664	648	648	15	0
6	F	275	282	282	4	0
6	f	275	282	282	9	0
7	H	510	532	532	3	0
7	h	498	518	518	3	0
8	I	296	311	311	2	0
8	i	296	311	311	3	0
9	J	257	268	268	5	0
9	j	257	268	268	12	0
10	K	293	305	305	4	0
10	k	293	305	305	7	0
11	L	304	316	316	2	0
11	l	296	304	304	2	0
12	M	256	269	269	2	0
12	m	251	267	267	4	0
13	O	1870	1830	1830	17	0
13	o	1874	1846	1846	15	0
14	R	221	238	238	4	0
14	r	221	238	238	2	0
15	T	258	261	261	3	0
15	t	256	256	256	0	0
16	U	774	773	773	6	0
16	u	774	773	773	9	1
17	V	1064	1073	1073	10	1
17	v	1064	1073	1073	9	0
18	X	281	312	312	5	0
18	x	286	316	314	5	0
19	Y	196	217	217	3	0
19	y	218	241	241	4	0
20	Z	479	516	516	7	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	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	B	1035	1139	1139	13	0
22	C	839	922	922	10	0
22	D	195	216	216	3	0
22	a	195	216	216	2	0
22	b	1035	1139	1139	15	0
22	c	839	919	919	11	0
22	d	195	216	216	1	0
23	A	128	148	148	1	0
23	a	64	74	74	0	0
23	d	64	74	74	0	0
24	A	40	56	56	0	0
24	B	120	168	168	1	0
24	C	40	56	56	1	0
24	D	40	56	56	2	0
24	H	40	56	56	3	0
24	K	120	168	168	2	0
24	T	40	56	56	2	0
24	a	40	56	56	0	0
24	b	120	168	168	3	0
24	c	80	112	112	2	0
24	d	40	56	56	2	0
24	h	40	56	56	1	0
24	k	80	112	112	1	0
24	t	40	56	56	2	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	1	0
26	D	55	80	80	1	0
26	a	55	80	80	4	0
26	d	55	80	80	1	0
27	A	48	66	66	1	0
27	D	83	117	117	1	0
27	M	51	72	72	2	0
27	Y	48	66	66	0	0
27	a	49	68	68	0	0
27	b	55	86	86	0	0
27	c	85	113	112	0	0
27	d	44	58	58	0	0
27	h	23	34	34	0	0
27	m	51	72	72	1	0
28	A	91	135	135	2	0
28	B	54	78	78	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	F	36	46	45	0	0
28	a	90	134	133	0	0
28	b	49	65	65	1	0
28	f	41	48	48	2	0
29	A	49	74	74	3	0
29	D	145	215	215	4	0
29	L	49	74	74	1	0
29	a	49	74	74	1	0
29	d	88	125	125	1	0
29	e	42	57	57	2	0
29	l	49	74	74	1	0
30	A	66	96	96	5	0
30	C	186	246	245	1	0
30	H	62	82	80	0	0
30	c	186	245	241	2	0
30	h	62	82	80	0	0
30	o	44	75	75	3	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	B	105	137	161	4	0
32	C	40	63	63	0	0
32	D	35	35	57	1	0
32	E	12	16	16	0	0
32	H	18	35	35	1	0
32	I	15	26	26	2	0
32	J	12	16	16	0	0
32	M	43	73	73	1	0
32	T	15	29	29	0	0
32	a	22	32	32	0	0
32	b	82	141	141	1	0
32	c	32	51	51	2	0
32	d	37	61	61	1	0
32	j	12	16	16	0	0
32	m	12	16	16	0	0
33	D	4	1	1	0	0
33	d	4	1	1	0	0
34	F	43	30	30	1	0
34	f	43	30	30	6	0
35	V	43	32	30	2	0
35	v	43	32	30	2	0
36	A	144	0	0	5	0
36	B	204	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	C	182	0	0	0	0
36	D	136	0	0	1	0
36	E	30	0	0	2	0
36	F	7	0	0	0	0
36	H	37	0	0	0	0
36	I	10	0	0	0	0
36	J	16	0	0	2	0
36	K	8	0	0	0	0
36	L	8	0	0	0	0
36	M	7	0	0	0	0
36	O	90	0	0	3	0
36	T	10	0	0	1	0
36	U	52	0	0	2	0
36	V	65	0	0	1	0
36	X	12	0	0	1	0
36	Y	6	0	0	0	0
36	Z	2	0	0	0	0
36	a	126	0	0	2	0
36	b	206	0	0	6	0
36	c	181	0	0	5	0
36	d	111	0	0	0	0
36	e	21	0	0	1	0
36	f	8	0	0	0	0
36	h	36	0	0	0	0
36	i	13	0	0	0	0
36	j	8	0	0	2	0
36	k	6	0	0	1	0
36	l	7	0	0	2	0
36	m	6	0	0	0	0
36	o	102	0	0	5	0
36	r	3	0	0	0	0
36	t	8	0	0	0	0
36	u	58	0	0	5	0
36	v	56	0	0	2	0
36	x	8	0	0	0	0
36	y	3	0	0	0	0
36	z	9	0	0	1	0
All	All	52138	51532	51542	440	1

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 4.

All (440) 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)
16:u:53:ALA:O	36:u:201:HOH:O	1.77	1.02
16:u:15:GLU:OE1	36:u:202:HOH:O	1.89	0.90
2:B:235:GLU:HB3	36:B:701:HOH:O	1.71	0.89
3:c:44:ASN:O	36:c:601:HOH:O	1.99	0.81
16:u:88:GLU:OE1	36:u:203:HOH:O	1.98	0.80
2:b:29:LEU:HD23	28:b:620:SQD:H222	1.64	0.78
9:j:36:LEU:O	36:j:201:HOH:O	2.00	0.78
2:b:307:GLU:OE1	36:b:701:HOH:O	2.02	0.77
3:c:391[B]:ARG:NE	36:c:604:HOH:O	2.21	0.74
15:T:25:GLU:OE1	36:T:201:HOH:O	2.06	0.71
3:c:221:GLU:OE1	36:c:602:HOH:O	2.07	0.71
26:A:410:PL9:H361	6:F:25:THR:HG21	1.72	0.71
34:F:101:HEM:HBC2	34:F:101:HEM:HHD	1.74	0.70
5:e:17:VAL:N	36:e:201:HOH:O	2.23	0.70
9:J:36:LEU:O	36:J:201:HOH:O	2.10	0.69
20:z:34:ASP:O	20:z:38:GLN:NE2	2.25	0.69
13:O:58:ASN:HB3	36:b:701:HOH:O	1.93	0.68
13:o:60:ARG:NH2	36:o:402:HOH:O	2.25	0.68
13:O:57:LYS:NZ	36:b:701:HOH:O	2.26	0.68
17:V:109:GLU:OE1	36:V:301:HOH:O	2.11	0.68
3:c:360:ASP:OD1	36:c:603:HOH:O	2.12	0.68
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.27	0.67
26:a:409:PL9:H48	4:d:39:PRO:HG3	1.76	0.67
2:b:121:GLU:OE2	7:h:12:ARG:NH1	2.27	0.67
13:O:184:ARG:NE	36:O:302:HOH:O	2.28	0.67
2:b:127:ARG:NH2	7:h:18:TYR:O	2.27	0.67
16:U:70:ARG:NH2	17:V:85:GLU:OE1	2.28	0.66
13:O:224:ASP:OD2	36:O:301:HOH:O	2.14	0.65
16:u:53:ALA:HB1	16:u:54:PRO:HD2	1.77	0.65
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.79	0.65
22:b:615:CLA:HHC	22:b:615:CLA:HBB1	1.77	0.65
9:j:34:ALA:O	36:j:201:HOH:O	2.14	0.65
4:d:79:SER:HA	4:d:172:SER:HB3	1.80	0.64
6:f:24:HIS:O	6:f:28:VAL:HG13	1.98	0.63
12:m:4:ASN:ND2	27:m:101:LMG:O10	2.32	0.62
7:H:56:ASP:OD2	18:X:2:THR:OG1	2.16	0.62
13:o:194:LYS:NZ	36:o:403:HOH:O	2.25	0.62
13:O:107:THR:HG22	36:O:313:HOH:O	2.01	0.61
2:b:435:GLU:HB2	36:b:717:HOH:O	2.00	0.60
11:l:2:GLU:OE2	36:l:201:HOH:O	2.16	0.60
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.36	0.60
20:z:1:MET:SD	20:z:1:MET:N	2.73	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:ARG:NH1	36:B:705:HOH:O	2.31	0.60
5:E:7:GLU:OE2	36:E:201:HOH:O	2.16	0.60
13:O:88:ASN:OD1	13:O:92:SER:OG	2.19	0.60
16:U:58:VAL:O	16:U:61:VAL:HG22	2.01	0.60
2:B:371:THR:HG23	2:B:372:ASP:O	2.01	0.59
28:A:414:SQD:H383	22:b:606:CLA:H93	1.85	0.59
19:y:41:VAL:C	19:y:43:ARG:H	2.11	0.59
34:f:101:HEM:HHC	34:f:101:HEM:HBB2	1.83	0.59
2:B:86:ILE:HD12	2:B:88:PRO:HD3	1.85	0.59
17:v:104:MET:HA	17:v:107:LEU:HD22	1.86	0.58
1:A:11:ALA:N	36:A:506:HOH:O	2.36	0.58
5:e:30:LEU:HD11	34:f:101:HEM:HBB2	1.86	0.58
20:z:32:ASP:OD1	20:z:32:ASP:N	2.37	0.58
5:e:14:ILE:O	5:e:20:TRP:NE1	2.37	0.57
5:E:68:ASP:O	5:E:72:ALA:HB2	2.05	0.56
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.86	0.56
9:J:20:GLY:O	9:J:24:ILE:HG13	2.06	0.56
3:c:459:ILE:HG21	3:c:464:GLU:HG3	1.88	0.56
9:J:19:MET:O	9:J:23:VAL:HG23	2.05	0.56
1:a:84:PRO:HA	1:a:112:TYR:CG	2.41	0.56
2:b:498:LYS:HE3	4:d:20:ASP:HA	1.88	0.56
9:J:15:THR:HG22	9:J:19:MET:HE2	1.87	0.56
10:k:46:ARG:NH2	36:k:201:HOH:O	2.39	0.55
22:C:502:CLA:H61	22:C:512:CLA:H42	1.87	0.55
3:C:42:LEU:HD21	22:C:511:CLA:H2A	1.88	0.55
3:C:203:THR:O	3:C:235:GLY:HA3	2.06	0.55
4:D:246:MET:HE3	4:D:264:LYS:HE2	1.89	0.55
22:c:501:CLA:H192	22:c:507:CLA:HBB1	1.88	0.55
1:a:12:ASN:HA	36:a:574:HOH:O	2.06	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.54
17:v:57:GLU:OE2	36:v:301:HOH:O	2.18	0.54
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.23	0.54
32:M:104:STE:C1	36:l:204:HOH:O	2.56	0.54
4:d:126:MET:HE3	4:d:143:ALA:O	2.08	0.54
17:V:4:THR:O	17:V:7:VAL:HG12	2.08	0.53
20:Z:29:SER:HB3	20:Z:31:GLN:HE21	1.74	0.53
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.90	0.53
19:Y:20:ALA:N	19:Y:23:THR:HG1	2.06	0.53
13:O:56:PRO:O	13:O:58:ASN:N	2.37	0.52
16:U:10:VAL:HG21	16:U:15:GLU:OE2	2.10	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:VAL:HG13	4:D:244:TYR:CD1	2.45	0.52
16:U:70:ARG:NH1	36:U:205:HOH:O	2.42	0.52
3:c:151:TRP:HA	3:c:157:MET:HE3	1.92	0.52
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.45	0.51
17:V:41:HIS:HA	17:V:45:ILE:O	2.10	0.51
5:e:30:LEU:HD11	34:f:101:HEM:CBB	2.41	0.51
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.91	0.51
29:A:413:LHG:H281	36:A:624:HOH:O	2.10	0.51
26:D:406:PL9:H412	11:L:29:LEU:HD23	1.93	0.51
10:K:26:PRO:O	10:K:29:PRO:HD2	2.10	0.51
24:T:101:BCR:H321	24:T:101:BCR:HC8	1.93	0.51
2:B:67:ALA:HA	2:B:71:VAL:O	2.10	0.51
16:u:15:GLU:OE2	36:u:204:HOH:O	2.19	0.50
3:C:406:SER:HA	3:C:420:VAL:HG23	1.93	0.50
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.93	0.50
35:v:201:HEC:HMC1	35:v:201:HEC:HBC3	1.92	0.50
4:D:269:PHE:CD2	29:D:411:LHG:HC12	2.46	0.50
10:K:25:LEU:N	10:K:26:PRO:HD2	2.25	0.50
2:B:160:GLY:HA2	2:B:163:GLY:O	2.11	0.50
22:C:501:CLA:HHC	22:C:501:CLA:HBB1	1.94	0.50
28:f:102:SQD:H312	18:x:27:VAL:HG11	1.93	0.50
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.93	0.50
1:A:183:MET:HE2	22:D:402:CLA:HMC1	1.93	0.50
22:b:615:CLA:H2	22:b:616:CLA:HBB2	1.94	0.50
4:d:267:LEU:C	4:d:267:LEU:HD23	2.36	0.50
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.46	0.50
10:k:25:LEU:N	10:k:26:PRO:CD	2.75	0.50
1:A:201:GLY:HA3	1:A:286:THR:HB	1.93	0.50
27:M:101:LMG:HC71	27:M:101:LMG:O9	2.11	0.50
20:z:3:ILE:HG22	20:z:7:LEU:HD23	1.94	0.50
22:c:501:CLA:C3D	22:c:503:CLA:H2	2.42	0.49
6:f:19:ARG:NH2	34:f:101:HEM:O2D	2.42	0.49
3:c:406:SER:HA	3:c:420:VAL:HG23	1.95	0.49
13:O:27:ARG:O	13:O:27:ARG:HG2	2.12	0.49
15:T:15:ALA:HB2	24:T:101:BCR:H14C	1.93	0.49
22:B:607:CLA:C20	29:D:411:LHG:H142	2.42	0.49
1:a:140:ARG:HB2	4:d:220:ASN:HA	1.93	0.49
26:a:409:PL9:H372	6:f:22:ALA:HA	1.94	0.49
30:A:415:DGD:HD5	2:b:75:TRP:HB3	1.94	0.49
2:b:65:PHE:HE1	22:b:604:CLA:HED2	1.78	0.49
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:SER:OG	2:B:488:PRO:HD2	2.13	0.49
32:d:412:STE:H71	18:x:16:SER:HB3	1.94	0.49
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.49
5:E:53:ASP:O	17:V:1:ALA:N	2.46	0.48
1:A:307:ILE:HG22	1:A:313:VAL:HA	1.96	0.48
2:B:117:TYR:HA	11:L:1:MET:HE1	1.95	0.48
2:b:226:TYR:OH	36:b:702:HOH:O	2.20	0.48
1:a:102:LEU:H	30:o:301:DGD:HA21	1.78	0.48
22:b:601:CLA:HBA1	36:b:789:HOH:O	2.13	0.48
3:c:44:ASN:HB3	36:c:601:HOH:O	2.12	0.48
1:a:79:THR:HG22	4:d:315:TYR:HB2	1.94	0.48
1:a:308:ASP:OD1	1:a:308:ASP:C	2.56	0.48
3:C:279:LEU:HD23	3:C:282:MET:HE3	1.95	0.48
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.12	0.48
16:U:39:ARG:NH2	17:V:60:ALA:O	2.45	0.48
5:e:13:ILE:HG22	5:e:19:TYR:CD2	2.48	0.48
20:z:36:SER:HA	20:z:39:LEU:HD23	1.95	0.48
32:B:627:STE:H32	32:D:413:STE:O1	2.14	0.48
9:j:18:GLY:O	9:j:22:ILE:HD13	2.13	0.48
10:K:13:GLU:N	10:K:13:GLU:OE1	2.46	0.48
20:z:1:MET:HB2	20:z:4:LEU:HB3	1.94	0.48
30:A:415:DGD:C6B	32:I:101:STE:H51	2.44	0.48
10:k:10:LYS:HD2	10:k:10:LYS:N	2.29	0.48
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.49	0.48
22:C:506:CLA:H8	24:C:514:BCR:H12C	1.96	0.48
2:B:382:PRO:HG2	2:B:385:ARG:HD2	1.96	0.48
14:R:16:ALA:O	14:R:20:VAL:HG23	2.14	0.48
2:b:489:GLU:HA	2:b:495:PHE:HD2	1.78	0.48
24:t:101:BCR:HC8	24:t:101:BCR:H311	1.94	0.48
13:o:32:ILE:HG21	13:o:93:LEU:HD21	1.96	0.47
2:B:433:ASP:OD1	2:B:433:ASP:C	2.55	0.47
9:J:5:GLY:N	36:J:203:HOH:O	2.47	0.47
2:b:497:GLN:HE21	4:d:24:ARG:HH12	1.61	0.47
17:v:87:GLU:CD	17:v:96:ARG:HH12	2.22	0.47
3:C:126:GLY:O	3:C:130:VAL:HG13	2.15	0.47
3:C:318:LEU:C	3:C:318:LEU:HD23	2.39	0.47
20:Z:51:VAL:O	20:Z:54:VAL:O	2.31	0.47
2:B:378:LYS:HE3	36:B:763:HOH:O	2.14	0.47
6:F:15:ILE:HD13	14:R:23:ILE:HD11	1.96	0.47
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.78	0.47
2:b:442:ILE:HD12	4:d:299:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:246:MET:HE2	4:d:246:MET:HA	1.96	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.47
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	1.96	0.47
1:a:179:THR:O	1:a:183:MET:HG3	2.15	0.47
1:a:271:LEU:HD21	26:a:409:PL9:C3	2.44	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.96	0.47
2:B:91:TRP:HE1	32:B:620:STE:H32	1.80	0.47
2:b:79:SER:HB3	2:b:86:ILE:HG12	1.97	0.47
3:c:334:PRO:HA	13:o:153:THR:OG1	2.15	0.47
14:r:2:ASP:HB3	14:r:5:VAL:HG23	1.95	0.47
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.96	0.47
13:O:58:ASN:ND2	13:O:61:GLN:OE1	2.47	0.47
2:b:91:TRP:HE1	32:b:622:STE:H111	1.80	0.47
4:d:191:TRP:CZ2	4:d:197:HIS:HB2	2.49	0.47
8:i:33:LYS:O	8:i:35:LYS:NZ	2.46	0.47
5:E:23:HIS:HA	5:E:26:THR:OG1	2.15	0.47
22:B:606:CLA:H72	24:B:619:BCR:H311	1.97	0.46
17:v:41:HIS:HA	17:v:45:ILE:O	2.15	0.46
30:A:415:DGD:HB61	32:I:101:STE:H31	1.98	0.46
22:C:512:CLA:H72	22:C:512:CLA:H41	1.96	0.46
24:d:406:BCR:H402	9:j:21:VAL:HG21	1.97	0.46
1:a:245:THR:HG22	4:d:265:ARG:NH2	2.31	0.46
1:a:283:VAL:HA	1:a:286:THR:HG22	1.97	0.46
20:Z:55:GLY:HA2	20:Z:58:ASN:HB3	1.97	0.46
2:B:377:VAL:HG11	4:D:342:PRO:HG3	1.98	0.46
29:a:410:LHG:O4	4:d:141:TYR:OH	2.29	0.46
5:e:17:VAL:HG23	9:j:7:ARG:HD3	1.98	0.46
27:D:410:LMG:O10	27:D:410:LMG:H132	2.16	0.46
2:b:92:SER:O	2:b:96:VAL:HG23	2.16	0.46
17:v:41:HIS:CD2	35:v:201:HEC:NB	2.83	0.46
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.97	0.46
4:d:161:PRO:HG3	4:d:170:ALA:HB2	1.97	0.46
13:o:194:LYS:NZ	36:o:412:HOH:O	2.49	0.46
16:u:45:LEU:HD21	16:u:71:GLN:HB3	1.98	0.46
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.04	0.46
2:B:357:ARG:NE	36:B:709:HOH:O	2.35	0.46
22:C:510:CLA:HBC3	22:C:510:CLA:H192	1.98	0.46
26:a:409:PL9:H453	18:x:28:LEU:HD21	1.97	0.45
3:c:42:LEU:HD21	22:c:511:CLA:H2A	1.98	0.45
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.50	0.45
32:c:520:STE:C1	32:c:520:STE:H51	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:37:ILE:HG22	9:j:28:PHE:CE1	2.52	0.45
5:E:8:ARG:O	6:F:19:ARG:NH2	2.35	0.45
2:b:488:PRO:HA	2:b:491:VAL:HG22	1.98	0.45
22:B:601:CLA:H92	24:H:101:BCR:H21C	1.97	0.45
4:D:24:ARG:NH2	18:X:35:ASP:OD2	2.49	0.45
24:D:405:BCR:H23C	24:D:405:BCR:H392	1.97	0.45
22:b:601:CLA:CHA	22:b:601:CLA:HBA2	2.46	0.45
1:A:161:TYR:CZ	1:A:165:GLN:HG3	2.52	0.45
24:K:102:BCR:H321	24:K:102:BCR:HC8	1.98	0.45
2:B:230:ARG:HH12	32:B:627:STE:H22	1.81	0.45
2:B:348:ASN:HB3	2:B:354:LEU:HD11	1.98	0.45
22:C:508:CLA:H203	30:C:516:DGD:HAE1	1.98	0.45
29:D:411:LHG:H152	29:L:101:LHG:H281	1.99	0.45
5:E:71:GLU:HG3	36:E:222:HOH:O	2.17	0.45
1:a:213:ALA:HB2	4:d:275:PRO:HG2	1.99	0.45
3:c:213:LEU:HD21	24:c:515:BCR:C20	2.47	0.45
13:o:121:THR:OG1	13:o:123:LYS:HG3	2.17	0.45
2:B:413:ASP:OD2	2:B:416:THR:HB	2.17	0.45
22:C:501:CLA:H203	22:C:507:CLA:H13	1.99	0.45
24:H:101:BCR:H331	24:H:101:BCR:C8	2.47	0.45
3:c:350:ILE:HG21	3:c:359:TRP:HB2	1.98	0.45
13:o:81:ILE:HA	13:o:100:GLY:HA3	1.97	0.45
22:c:503:CLA:H203	22:c:510:CLA:HAB	1.99	0.45
22:d:404:CLA:H52	26:d:407:PL9:H151	1.99	0.45
14:r:24:LEU:N	14:r:25:PRO:HD2	2.31	0.45
17:V:63:THR:HG22	17:V:64:PRO:CD	2.47	0.45
4:d:194:ASN:HA	4:d:295:SER:OG	2.17	0.45
24:t:101:BCR:H23C	24:t:101:BCR:H382	1.98	0.45
22:D:404:CLA:H142	18:X:14:LEU:HG	2.00	0.44
6:f:19:ARG:O	6:f:23:VAL:HG13	2.17	0.44
23:A:405:PHO:HBC3	4:D:279:LEU:HD22	1.99	0.44
2:B:235:GLU:CB	36:B:701:HOH:O	2.46	0.44
3:C:415:ASN:O	3:C:416:SER:HB2	2.17	0.44
1:a:95:PRO:HG2	1:a:98:GLU:HG2	1.99	0.44
17:v:109:GLU:OE2	36:v:302:HOH:O	2.21	0.44
2:B:235:GLU:C	36:B:701:HOH:O	2.59	0.44
3:c:38:GLY:HA3	22:c:511:CLA:HMD2	1.98	0.44
3:c:342:MET:SD	3:c:356:MET:HE2	2.58	0.44
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.00	0.44
2:B:63:LEU:N	2:B:64:PRO:HD2	2.32	0.44
3:C:109:PHE:N	3:C:110:PRO:CD	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:481:GLY:HA2	4:d:139:ARG:HD2	1.99	0.44
5:e:20:TRP:HD1	9:j:8:ILE:HD12	1.83	0.44
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.52	0.44
29:A:413:LHG:P	36:A:501:HOH:O	2.75	0.44
28:B:621:SQD:H262	11:l:18:TYR:HE1	1.82	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.52	0.44
28:f:102:SQD:H382	18:x:23:LEU:HB3	2.00	0.44
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.36	0.44
5:E:26:THR:HA	14:R:15:ALA:HB1	2.00	0.44
2:b:36:SER:OG	24:b:618:BCR:H362	2.18	0.44
4:d:49:LEU:HD13	24:d:406:BCR:C15	2.48	0.44
10:k:15:TYR:CE2	20:z:5:PHE:HZ	2.36	0.44
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.99	0.44
13:o:42:ARG:O	13:o:241:ALA:HA	2.18	0.44
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.53	0.43
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.43
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.99	0.43
19:Y:34:MET:O	19:Y:38:LEU:HG	2.18	0.43
3:c:113:VAL:HG11	32:c:520:STE:H72	1.99	0.43
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.48	0.43
13:o:91:GLY:HA3	13:o:132:ASN:HA	1.99	0.43
20:z:31:GLN:NE2	36:z:101:HOH:O	2.51	0.43
4:D:59:TYR:O	5:E:65:LEU:HD12	2.18	0.43
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.89	0.43
1:a:201:GLY:HA3	1:a:286:THR:HB	1.99	0.43
22:a:405:CLA:H102	8:i:13:THR:HG23	2.01	0.43
4:d:68:LEU:HA	6:f:40:MET:SD	2.58	0.43
28:A:414:SQD:H383	22:b:606:CLA:C9	2.49	0.43
5:E:35:TRP:CD1	5:E:35:TRP:C	2.96	0.43
2:B:347:ARG:HA	2:B:352:GLU:O	2.19	0.43
3:C:143:TYR:CE2	22:C:513:CLA:HED3	2.53	0.43
13:O:36:GLN:HG3	13:O:37:THR:N	2.34	0.43
2:b:204:ALA:O	2:b:208:VAL:HG23	2.19	0.43
17:v:76:MET:HE1	17:v:115:ILE:HD12	1.99	0.43
20:z:29:SER:HB3	20:z:32:ASP:OD1	2.18	0.43
27:A:411:LMG:H331	3:C:223:TRP:CE2	2.53	0.43
1:a:16:ARG:HH11	1:a:16:ARG:HB3	1.83	0.43
4:d:37:LEU:HD21	29:e:101:LHG:H221	1.99	0.43
1:a:132:GLU:O	1:a:136:ARG:HG2	2.19	0.43
22:b:610:CLA:H152	22:b:612:CLA:O1A	2.18	0.43
22:c:509:CLA:H142	22:c:509:CLA:H111	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:178:ILE:O	4:d:182:LEU:HD13	2.18	0.43
5:e:20:TRP:CD1	9:j:8:ILE:HD12	2.53	0.43
22:B:614:CLA:H141	22:B:614:CLA:H161	1.83	0.43
32:B:624:STE:H31	27:M:101:LMG:HC5	2.00	0.43
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.83	0.43
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.43
9:j:10:LEU:O	9:j:13:VAL:HG22	2.19	0.43
2:B:353:GLU:HG2	2:B:355:PHE:CZ	2.54	0.43
12:M:31:SER:O	12:m:32:GLN:HB3	2.19	0.43
2:B:414:PRO:N	2:B:415:PRO:HD2	2.34	0.43
4:d:52:THR:O	4:d:66:SER:HA	2.18	0.43
3:C:424:SER:O	3:C:428:THR:HG23	2.19	0.43
6:F:33:PHE:O	6:F:37:ILE:HG13	2.19	0.43
14:R:8:VAL:O	14:R:11:PRO:HD2	2.18	0.43
22:c:510:CLA:H102	22:c:510:CLA:H61	1.83	0.43
4:d:84:SER:O	5:e:69:ARG:HB2	2.19	0.43
4:d:213:ILE:HD11	4:d:253:TRP:CH2	2.54	0.43
1:A:136:ARG:NH2	8:I:27:ASP:OD1	2.49	0.42
3:C:148:GLY:O	3:C:156:LYS:NZ	2.51	0.42
1:a:153:SER:HB3	22:a:402:CLA:H43	1.99	0.42
1:a:334:ARG:NH2	36:a:509:HOH:O	2.50	0.42
2:b:460:LEU:HG	4:d:280:TRP:HZ3	1.84	0.42
3:c:128:GLY:HA3	22:c:513:CLA:C3C	2.49	0.42
22:c:509:CLA:H92	22:c:509:CLA:H61	1.93	0.42
16:u:52:ASN:O	16:u:53:ALA:O	2.37	0.42
22:B:611:CLA:H72	22:B:611:CLA:H112	1.82	0.42
29:D:408:LHG:H321	15:T:21:ILE:HD11	2.01	0.42
35:V:201:HEC:HMC1	35:V:201:HEC:HBC3	2.01	0.42
1:a:112:TYR:O	1:a:116:ILE:HG12	2.20	0.42
22:b:614:CLA:H62	22:b:614:CLA:H41	1.73	0.42
4:d:85:MET:HE1	5:e:72:ALA:HB2	2.02	0.42
12:m:15:VAL:O	12:m:19:SER:OG	2.33	0.42
16:u:87:VAL:HG23	36:u:247:HOH:O	2.19	0.42
3:c:350:ILE:CG2	3:c:359:TRP:HB2	2.50	0.42
19:y:41:VAL:C	19:y:43:ARG:N	2.77	0.42
1:A:95:PRO:HD2	1:A:98:GLU:HG3	2.02	0.42
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.54	0.42
1:A:161:TYR:N	1:A:162:PRO:CD	2.83	0.42
29:A:413:LHG:O3	36:A:501:HOH:O	2.22	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
24:b:618:BCR:H15C	24:b:618:BCR:H351	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42
5:e:52:PRO:HG3	9:j:36:LEU:HD21	2.01	0.42
34:f:101:HEM:HBC2	34:f:101:HEM:HMC1	2.00	0.42
10:k:32:PHE:CE2	24:k:102:BCR:C21	3.02	0.42
2:B:498:LYS:HE3	4:D:20:ASP:HA	2.01	0.42
22:B:601:CLA:HBA1	22:B:601:CLA:HBD	2.00	0.42
3:C:168:LEU:HD21	22:C:509:CLA:H61	2.01	0.42
3:C:334:PRO:HA	13:O:153:THR:OG1	2.20	0.42
18:X:8:LYS:NZ	36:X:101:HOH:O	2.52	0.42
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.54	0.42
1:a:85:SER:HA	1:a:109:GLY:HA3	2.02	0.42
2:b:30:VAL:HG12	22:b:605:CLA:HHD	2.01	0.42
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.54	0.42
5:e:56:TYR:HA	5:e:60:GLN:HE21	1.84	0.42
30:o:301:DGD:C3G	36:o:410:HOH:O	2.67	0.42
29:d:408:LHG:O1	29:l:101:LHG:O4	2.34	0.42
19:y:20:ALA:O	19:y:23:THR:HG22	2.20	0.42
22:B:616:CLA:HAB	22:B:616:CLA:HHC	1.86	0.42
3:C:83:GLU:OE1	17:V:103:LYS:NZ	2.53	0.42
7:H:38:PHE:HB2	24:H:101:BCR:C10	2.50	0.42
3:c:385:GLN:HB2	3:c:387:TRP:CD1	2.54	0.42
2:B:127:ARG:HG3	2:B:128:THR:HG23	2.02	0.42
2:B:285:ASN:O	2:B:289:GLN:HG2	2.20	0.42
36:D:572:HOH:O	18:X:6:SER:HA	2.19	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.42
22:b:616:CLA:H93	22:b:616:CLA:H112	1.95	0.42
3:c:352:GLY:O	3:c:355:THR:HG22	2.20	0.42
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.44	0.42
18:x:27:VAL:O	18:x:31:ILE:HG13	2.20	0.42
2:B:185:TRP:HB3	22:B:601:CLA:HMA3	2.02	0.41
4:D:272:LEU:C	4:D:272:LEU:HD23	2.45	0.41
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.19	0.41
24:h:101:BCR:H24C	24:h:101:BCR:H371	1.94	0.41
1:A:210:LEU:HD23	1:A:214:MET:HG2	2.02	0.41
1:A:332:HIS:O	1:A:333:GLU:C	2.63	0.41
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.55	0.41
4:D:52:THR:O	4:D:66:SER:HA	2.20	0.41
13:o:110:MET:HE2	13:o:116:ILE:CG1	2.50	0.41
1:a:188:ALA:HB2	1:a:328:MET:HB2	2.03	0.41
34:f:101:HEM:HBC2	34:f:101:HEM:CMC	2.50	0.41
20:z:42:LEU:O	20:z:46:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:17:GLU:OE2	7:H:20:LYS:HE2	2.21	0.41
22:b:602:CLA:H112	22:b:602:CLA:H152	1.85	0.41
4:d:40:CYS:HB3	4:d:117:HIS:O	2.21	0.41
1:A:243:GLU:CD	1:A:243:GLU:H	2.28	0.41
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.02	0.41
2:B:247:PHE:HE1	22:B:602:CLA:H102	1.85	0.41
22:B:604:CLA:HBD	22:B:605:CLA:H43	2.02	0.41
5:E:9:PRO:O	5:E:13:ILE:HG13	2.21	0.41
1:a:219:VAL:O	1:a:223:LEU:HD13	2.20	0.41
22:b:604:CLA:H142	22:b:604:CLA:H111	1.92	0.41
3:c:318:LEU:C	3:c:318:LEU:HD23	2.46	0.41
4:d:90:LEU:HD12	4:d:90:LEU:HA	1.81	0.41
1:a:200:LEU:HD13	30:c:518:DGD:CCA	2.51	0.41
1:A:40:THR:O	1:A:118:HIS:HB3	2.21	0.41
1:A:84:PRO:HA	1:A:112:TYR:CG	2.56	0.41
1:a:296:ASN:HB2	3:c:400:PRO:O	2.21	0.41
22:b:602:CLA:H43	7:h:45:ILE:HG22	2.02	0.41
6:f:28:VAL:N	6:f:29:PRO:CD	2.84	0.41
13:o:32:ILE:HG13	13:o:93:LEU:HD11	2.03	0.41
22:A:406:CLA:H41	22:A:406:CLA:H61	1.80	0.41
30:A:415:DGD:HE4	2:b:76:SER:HB3	2.03	0.41
22:B:606:CLA:H142	22:B:606:CLA:H111	1.89	0.41
24:D:405:BCR:H20C	24:D:405:BCR:H361	1.91	0.41
1:a:102:LEU:HD12	30:o:301:DGD:HB22	2.02	0.41
3:c:367:GLU:N	3:c:368:PRO:CD	2.84	0.41
4:d:26:ARG:HD2	4:d:30:VAL:HG23	2.02	0.41
4:d:342:PRO:O	4:d:345:VAL:HG22	2.21	0.41
5:e:10:PHE:N	29:e:101:LHG:O4	2.53	0.41
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.51	0.41
3:C:355:THR:C	3:C:357:ARG:N	2.77	0.41
4:D:295:SER:O	4:D:295:SER:OG	2.31	0.41
16:U:69:GLU:HG2	36:U:234:HOH:O	2.20	0.41
17:V:57:GLU:CD	17:V:57:GLU:H	2.29	0.41
3:c:45:LEU:HA	3:c:139:THR:HG22	2.02	0.41
3:c:419:PHE:HA	30:c:517:DGD:O3E	2.21	0.41
22:c:506:CLA:H102	22:c:506:CLA:H13	1.98	0.41
10:K:40:GLN:HB3	10:K:45:PHE:CD1	2.56	0.40
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.86	0.40
22:b:615:CLA:H112	22:b:615:CLA:H152	1.90	0.40
3:c:35:TRP:CD1	10:k:45:PHE:HB3	2.56	0.40
3:c:75:PHE:HZ	3:c:105:VAL:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.09	0.40
4:d:190:ASN:HB2	4:d:296:TYR:CD1	2.57	0.40
2:B:414:PRO:O	2:B:418:LYS:HG3	2.21	0.40
24:K:102:BCR:H322	20:Z:17:PHE:CD2	2.56	0.40
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.03	0.40
9:j:9:PRO:HG2	9:j:12:ILE:HD12	2.02	0.40
19:y:22:LEU:HA	19:y:25:ILE:HG22	2.03	0.40
20:z:32:ASP:HB2	20:z:35:ARG:HB2	2.02	0.40
2:B:12:LEU:HB2	22:B:612:CLA:HMC2	2.03	0.40
20:Z:36:SER:O	20:Z:40:ILE:HG12	2.21	0.40
24:b:619:BCR:H24C	24:b:619:BCR:H371	1.96	0.40
24:c:514:BCR:H371	24:c:514:BCR:H24C	1.83	0.40
8:i:2:GLU:HG3	8:i:3:THR:N	2.37	0.40
17:v:28:GLU:OE1	17:v:28:GLU:HA	2.21	0.40
1:A:329:GLU:HG3	36:A:617:HOH:O	2.21	0.40
22:B:601:CLA:HAB	32:H:103:STE:H131	2.02	0.40
13:O:58:ASN:OD1	13:O:61:GLN:HB2	2.22	0.40
35:V:201:HEC:HBC3	35:V:201:HEC:CMC	2.52	0.40
3:c:163:PHE:CD2	22:c:512:CLA:HAB	2.57	0.40
4:d:241:GLU:H	4:d:241:GLU:CD	2.28	0.40
20:z:10:ALA:O	20:z:14:ILE:HD13	2.21	0.40
1:A:46:ILE:HD13	30:A:415:DGD:HA81	2.03	0.40
3:C:180:MET:HG2	3:C:199:ILE:O	2.21	0.40
4:D:201:VAL:HG11	22:D:403:CLA:C3D	2.51	0.40
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.56	0.40
2:b:159:THR:O	2:b:180:PRO:HB3	2.21	0.40
4:d:126:MET:HA	4:d:129:GLN:OE1	2.21	0.40
13:o:115:ARG:NH1	36:o:408:HOH:O	2.44	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:V:70:GLU:OE2	16:u:76:ARG:HE[3_457]	1.57	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/344 (96%)	326 (98%)	5 (2%)	1 (0%)	36	36
1	a	332/344 (96%)	325 (98%)	7 (2%)	0	100	100
2	B	508/510 (100%)	503 (99%)	5 (1%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	442/461 (96%)	434 (98%)	7 (2%)	1 (0%)	43	44
3	c	451/461 (98%)	438 (97%)	12 (3%)	1 (0%)	43	44
4	D	339/352 (96%)	331 (98%)	8 (2%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	32 (100%)	0	0	100	100
7	H	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
7	h	61/66 (92%)	58 (95%)	3 (5%)	0	100	100
8	I	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
8	i	34/38 (90%)	32 (94%)	2 (6%)	0	100	100
9	J	34/40 (85%)	31 (91%)	3 (9%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	35 (100%)	0	0	100	100
10	k	35/46 (76%)	34 (97%)	1 (3%)	0	100	100
11	L	35/37 (95%)	35 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (100%)	0	0	100	100
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	226 (93%)	14 (6%)	3 (1%)	10	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	28
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	25 (96%)	1 (4%)	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	92 (97%)	2 (2%)	1 (1%)	11	7
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	14
17	v	135/163 (83%)	132 (98%)	3 (2%)	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%)	24 (96%)	0	1 (4%)	2	0
19	y	28/46 (61%)	24 (86%)	3 (11%)	1 (4%)	2	1
20	Z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
20	z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
All	All	5231/5700 (92%)	5092 (97%)	128 (2%)	11 (0%)	43	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
13	O	59	LYS
13	O	62	GLU
17	V	64	PRO
3	c	416	SER
16	u	53	ALA
19	Y	43	ARG
19	y	42	ARG
13	O	57	LYS
13	o	73	ARG
1	A	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/280 (96%)	267 (99%)	3 (1%)	65	73
1	a	269/280 (96%)	259 (96%)	10 (4%)	30	31
2	B	408/407 (100%)	398 (98%)	10 (2%)	42	46
2	b	402/407 (99%)	386 (96%)	16 (4%)	28	28
3	C	346/362 (96%)	339 (98%)	7 (2%)	48	54
3	c	354/362 (98%)	341 (96%)	13 (4%)	30	31
4	D	276/283 (98%)	271 (98%)	5 (2%)	51	58
4	d	277/283 (98%)	269 (97%)	8 (3%)	37	40
5	E	72/73 (99%)	70 (97%)	2 (3%)	38	42
5	e	71/73 (97%)	68 (96%)	3 (4%)	26	26
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	32
6	f	28/39 (72%)	25 (89%)	3 (11%)	6	3
7	H	54/55 (98%)	54 (100%)	0	100	100
7	h	53/55 (96%)	50 (94%)	3 (6%)	18	16
8	I	32/34 (94%)	30 (94%)	2 (6%)	16	13
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	38
9	J	24/28 (86%)	24 (100%)	0	100	100
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	11
10	k	30/37 (81%)	27 (90%)	3 (10%)	7	4
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	3
12	M	28/32 (88%)	28 (100%)	0	100	100
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	34
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	29
14	R	22/33 (67%)	21 (96%)	1 (4%)	24	24
14	r	22/33 (67%)	19 (86%)	3 (14%)	3	2
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	30
15	t	25/28 (89%)	24 (96%)	1 (4%)	28	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	32
16	u	84/112 (75%)	83 (99%)	1 (1%)	63	70
17	V	117/138 (85%)	114 (97%)	3 (3%)	40	45
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	34
18	X	31/34 (91%)	30 (97%)	1 (3%)	34	36
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	12
19	Y	19/37 (51%)	19 (100%)	0	100	100
19	y	22/37 (60%)	19 (86%)	3 (14%)	3	2
20	Z	52/52 (100%)	46 (88%)	6 (12%)	5	3
20	z	51/52 (98%)	44 (86%)	7 (14%)	3	2
All	All	4321/4654 (93%)	4170 (96%)	151 (4%)	32	33

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	121	LEU
1	A	243	GLU
2	B	86	ILE
2	B	101	ILE
2	B	127	ARG
2	B	240	SER
2	B	350	GLU
2	B	362	PHE
2	B	371	THR
2	B	385	ARG
2	B	405	GLU
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	416	SER
4	D	43	LEU
4	D	136	VAL
4	D	154	VAL

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Mol	Chain	Res	Type
4	D	264	LYS
4	D	295	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
6	F	25	THR
8	I	4	LEU
8	I	6	ILE
10	K	17	ILE
10	K	27	VAL
13	O	18	LYS
13	O	25	THR
13	O	78	LEU
13	O	107	THR
13	O	194	LYS
13	O	198	SER
13	O	214	THR
14	R	21	ARG
15	T	25	GLU
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	19	ILE
17	V	24	LYS
17	V	57	GLU
18	X	3	ILE
20	Z	13	VAL
20	Z	15	LEU
20	Z	35	ARG
20	Z	38	GLN
20	Z	46	LEU
20	Z	50	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159	LEU
1	a	200	LEU
1	a	223	LEU
1	a	229	GLU
1	a	242	GLU
1	a	245	THR
1	a	288	LEU
1	a	307	ILE
2	b	74	SER

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Mol	Chain	Res	Type
2	b	80	ILE
2	b	83	GLU
2	b	86	ILE
2	b	98	LEU
2	b	128	THR
2	b	161	LEU
2	b	236	THR
2	b	245	VAL
2	b	378	LYS
2	b	405	GLU
2	b	413	ASP
2	b	485	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	ARG
3	c	24	THR
3	c	29	GLU
3	c	72	LEU
3	c	78	GLU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	315	MET
3	c	346	THR
3	c	396	MET
3	c	416	SER
4	d	90	LEU
4	d	230	SER
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	66	VAL
5	e	83	LEU
6	f	15	ILE
6	f	23	VAL
6	f	28	VAL

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Mol	Chain	Res	Type
7	h	3	ARG
7	h	7	LEU
7	h	39	LEU
8	i	2	GLU
9	j	7	ARG
9	j	13	VAL
10	k	10	LYS
10	k	30	VAL
10	k	35	LEU
11	l	2	GLU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	49	THR
13	o	55	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	143	LYS
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
14	r	12	VAL
15	t	29	ILE
16	u	58	VAL
17	v	19	ILE
17	v	30	LYS
17	v	45	ILE
17	v	107	LEU
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	34	MET
19	y	45	ASN
20	z	1	MET
20	z	7	LEU
20	z	29	SER
20	z	32	ASP
20	z	38	GLN

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Mol	Chain	Res	Type
20	z	42	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	338	ASN
2	B	274	GLN
2	B	374	ASN
3	C	201	ASN
3	C	311	GLN
3	C	327	ASN
3	C	385	GLN
3	C	415	ASN
11	L	8	GLN
13	O	88	ASN
14	R	22	ASN
16	U	37	GLN
18	X	38	GLN
20	Z	6	GLN
20	Z	31	GLN
20	Z	38	GLN
1	a	19	ASN
1	a	165	GLN
1	a	181	ASN
1	a	234	ASN
1	a	296	ASN
2	b	179	GLN
2	b	274	GLN
2	b	281	GLN
2	b	338	GLN
2	b	409	GLN
3	c	28	GLN
3	c	322	GLN
4	d	186	GLN
4	d	338	ASN
5	e	60	GLN
7	h	59	ASN
13	o	61	GLN
13	o	124	ASN
13	o	147	ASN

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Mol	Chain	Res	Type
13	o	231	HIS
20	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	i	1	8	8,9,10	1.30	1 (12%)	8,9,11	1.42	1 (12%)
12	FME	M	1	12	8,9,10	1.04	0	8,9,11	0.85	0
15	FME	t	1	15	8,9,10	1.22	1 (12%)	8,9,11	1.07	0
15	FME	T	1	15	8,9,10	1.14	1 (12%)	8,9,11	0.92	0
12	FME	m	1	12	8,9,10	1.16	1 (12%)	8,9,11	0.66	0
8	FME	I	1	8	8,9,10	0.98	0	8,9,11	1.15	1 (12%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	1	FME	CA-N	-3.07	1.42	1.46
12	m	1	FME	CA-N	-2.53	1.42	1.46
15	t	1	FME	CA-N	-2.34	1.43	1.46
15	T	1	FME	CN-N	2.13	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	CB-CA-N	3.03	116.04	110.52
8	I	1	FME	CB-CA-N	2.05	114.25	110.52

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 6 are monoatomic - leaving 181 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	CLA	B	610	36	69,73,73	1.39	9 (13%)	82,113,113	1.44	12 (14%)
22	CLA	C	511	3	69,73,73	1.24	7 (10%)	82,113,113	1.27	3 (3%)
22	CLA	c	509	3	69,73,73	1.17	7 (10%)	82,113,113	1.56	11 (13%)
24	BCR	a	406	-	41,41,41	1.24	4 (9%)	56,56,56	1.20	5 (8%)
22	CLA	b	616	2	64,68,73	1.13	6 (9%)	76,107,113	1.56	13 (17%)
27	LMG	A	411	-	48,48,55	1.05	1 (2%)	56,56,63	1.45	8 (14%)
22	CLA	B	613	2	69,73,73	1.64	13 (18%)	82,113,113	1.42	10 (12%)
30	DGD	c	517	-	63,63,67	1.15	8 (12%)	77,77,81	1.38	10 (12%)
22	CLA	A	403	36	69,73,73	1.23	7 (10%)	82,113,113	1.32	13 (15%)
32	STE	M	104	-	17,17,19	0.37	0	16,16,19	0.86	0
23	PHO	a	404	-	58,69,69	2.00	10 (17%)	55,99,99	1.54	9 (16%)
22	CLA	A	402	1	69,73,73	1.41	8 (11%)	82,113,113	1.31	5 (6%)
22	CLA	B	607	36	69,73,73	1.17	7 (10%)	82,113,113	1.45	10 (12%)
32	STE	d	412	-	19,19,19	0.73	0	19,19,19	0.77	1 (5%)
32	STE	C	518	-	11,11,19	0.68	0	11,11,19	1.11	1 (9%)
27	LMG	D	407	-	51,51,55	1.01	1 (1%)	59,59,63	1.33	8 (13%)
22	CLA	d	405	4	69,73,73	1.20	7 (10%)	82,113,113	1.18	10 (12%)
24	BCR	D	405	-	41,41,41	1.26	2 (4%)	56,56,56	1.20	7 (12%)
26	PL9	A	410	-	55,55,55	0.89	2 (3%)	68,69,69	1.48	13 (19%)
32	STE	b	624	-	15,15,19	0.85	1 (6%)	15,15,19	0.96	1 (6%)
24	BCR	d	406	-	41,41,41	1.30	2 (4%)	56,56,56	1.24	6 (10%)
22	CLA	B	615	2	69,73,73	1.46	9 (13%)	82,113,113	1.33	7 (8%)
26	PL9	a	409	1	55,55,55	1.31	3 (5%)	68,69,69	1.84	12 (17%)
32	STE	I	101	-	14,14,19	0.62	0	13,13,19	0.36	0
22	CLA	C	509	3	69,73,73	1.31	11 (15%)	82,113,113	1.29	7 (8%)
22	CLA	C	503	3	69,73,73	1.42	10 (14%)	82,113,113	1.43	8 (9%)
35	HEC	V	201	17	50,50,50	1.62	4 (8%)	68,82,82	1.39	8 (11%)
27	LMG	b	623	-	55,55,55	1.03	4 (7%)	63,63,63	1.76	11 (17%)
31	OEX	A	416	1,3,36	0,14,14	-	-	-	-	-
32	STE	T	102	-	14,14,19	0.43	0	13,13,19	0.83	0
32	STE	b	621	-	15,15,19	0.49	0	14,14,19	0.69	0
32	STE	c	522	-	11,11,19	0.86	0	11,11,19	1.17	1 (9%)
22	CLA	b	604	2	69,73,73	1.44	10 (14%)	82,113,113	1.50	8 (9%)
22	CLA	c	511	3	69,73,73	1.55	8 (11%)	82,113,113	1.34	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	d	411	-	16,16,19	0.67	0	16,16,19	1.03	1 (6%)
32	STE	c	520	-	19,19,19	0.71	1 (5%)	19,19,19	0.91	1 (5%)
29	LHG	D	411	-	48,48,48	0.88	3 (6%)	51,54,54	1.38	8 (15%)
30	DGD	H	102	-	63,63,67	1.31	8 (12%)	77,77,81	1.57	13 (16%)
32	STE	b	625	-	19,19,19	0.67	0	19,19,19	1.26	3 (15%)
22	CLA	B	614	2	69,73,73	1.32	7 (10%)	82,113,113	1.28	10 (12%)
22	CLA	c	502	3	69,73,73	1.16	7 (10%)	82,113,113	1.33	9 (10%)
30	DGD	o	301	-	43,43,67	1.15	2 (4%)	45,45,81	1.49	5 (11%)
24	BCR	b	618	-	41,41,41	1.23	2 (4%)	56,56,56	1.20	8 (14%)
22	CLA	c	507	36	69,73,73	1.23	7 (10%)	82,113,113	1.31	9 (10%)
22	CLA	B	605	2	69,73,73	1.23	10 (14%)	82,113,113	1.50	11 (13%)
22	CLA	c	512	3	69,73,73	1.32	10 (14%)	82,113,113	1.23	7 (8%)
32	STE	j	101	-	11,11,19	0.97	1 (9%)	11,11,19	1.44	2 (18%)
31	OEX	a	416	1,3,36	0,14,14	-	-	-	-	-
29	LHG	A	413	-	48,48,48	1.00	3 (6%)	51,54,54	1.20	2 (3%)
24	BCR	k	101	-	41,41,41	1.05	4 (9%)	56,56,56	1.08	3 (5%)
32	STE	m	102	-	11,11,19	0.67	0	11,11,19	1.73	2 (18%)
27	LMG	D	410	-	31,31,55	1.20	3 (9%)	33,33,63	1.14	1 (3%)
27	LMG	c	521	-	48,48,55	1.25	7 (14%)	56,56,63	1.20	4 (7%)
22	CLA	b	609	2	69,73,73	1.34	11 (15%)	82,113,113	1.24	8 (9%)
22	CLA	b	611	2	69,73,73	1.27	10 (14%)	82,113,113	1.60	9 (10%)
29	LHG	a	410	-	48,48,48	1.03	3 (6%)	51,54,54	1.45	6 (11%)
29	LHG	e	101	-	41,41,48	1.01	3 (7%)	44,47,54	1.24	4 (9%)
24	BCR	B	619	-	41,41,41	1.23	2 (4%)	56,56,56	1.43	8 (14%)
23	PHO	A	404	-	58,69,69	1.88	14 (24%)	55,99,99	1.46	9 (16%)
22	CLA	A	406	1	58,62,73	1.36	9 (15%)	68,99,113	1.51	9 (13%)
29	LHG	l	101	-	48,48,48	0.63	0	51,54,54	1.26	6 (11%)
22	CLA	d	404	36	69,73,73	1.44	7 (10%)	82,113,113	1.51	9 (10%)
32	STE	B	627	-	15,15,19	0.85	1 (6%)	15,15,19	1.27	2 (13%)
28	SQD	f	102	-	39,41,54	1.14	4 (10%)	49,52,65	1.86	11 (22%)
28	SQD	B	621	-	52,54,54	1.01	3 (5%)	62,65,65	1.77	12 (19%)
24	BCR	K	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.18	3 (5%)
30	DGD	c	516	-	63,63,67	1.38	7 (11%)	77,77,81	1.29	6 (7%)
32	STE	C	519	-	15,15,19	0.73	0	14,14,19	0.27	0
32	STE	B	626	-	11,11,19	0.75	0	11,11,19	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	a	402	1	69,73,73	1.37	9 (13%)	82,113,113	1.31	7 (8%)
22	CLA	B	609	2	69,73,73	1.27	7 (10%)	82,113,113	1.37	8 (9%)
22	CLA	B	601	36	69,73,73	1.52	10 (14%)	82,113,113	1.41	8 (9%)
22	CLA	c	510	3	69,73,73	1.25	7 (10%)	82,113,113	1.45	9 (10%)
24	BCR	B	618	-	41,41,41	1.12	3 (7%)	56,56,56	1.38	6 (10%)
22	CLA	b	602	2	69,73,73	1.33	9 (13%)	82,113,113	1.34	8 (9%)
22	CLA	b	607	36	69,73,73	1.39	12 (17%)	82,113,113	1.24	10 (12%)
24	BCR	K	101	-	41,41,41	1.15	3 (7%)	56,56,56	1.36	6 (10%)
22	CLA	C	512	3	69,73,73	1.50	8 (11%)	82,113,113	1.25	8 (9%)
24	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.44	9 (16%)
28	SQD	a	411	-	52,54,54	0.98	3 (5%)	62,65,65	2.16	14 (22%)
32	STE	E	101	-	11,11,19	1.04	1 (9%)	11,11,19	0.89	0
24	BCR	t	101	-	41,41,41	1.06	3 (7%)	56,56,56	1.56	12 (21%)
30	DGD	C	515	-	63,63,67	1.65	13 (20%)	77,77,81	1.45	12 (15%)
26	PL9	D	406	-	55,55,55	1.39	7 (12%)	68,69,69	1.68	17 (25%)
22	CLA	C	513	3	69,73,73	1.20	10 (14%)	82,113,113	1.37	8 (9%)
22	CLA	b	601	36	69,73,73	1.46	10 (14%)	82,113,113	1.38	7 (8%)
22	CLA	b	608	2	69,73,73	1.31	9 (13%)	82,113,113	1.40	10 (12%)
22	CLA	D	402	4	69,73,73	1.19	7 (10%)	82,113,113	1.39	11 (13%)
32	STE	a	415	-	11,11,19	0.75	0	11,11,19	1.20	1 (9%)
32	STE	B	623	-	11,11,19	0.93	1 (9%)	11,11,19	1.07	1 (9%)
22	CLA	d	403	4	69,73,73	1.13	7 (10%)	82,113,113	1.14	8 (9%)
24	BCR	k	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.20	4 (7%)
22	CLA	B	611	2	69,73,73	1.26	8 (11%)	82,113,113	1.38	12 (14%)
24	BCR	b	617	-	41,41,41	1.26	3 (7%)	56,56,56	1.36	7 (12%)
22	CLA	b	614	2	69,73,73	1.25	10 (14%)	82,113,113	1.15	7 (8%)
24	BCR	b	619	-	41,41,41	1.20	2 (4%)	56,56,56	1.34	9 (16%)
29	LHG	D	408	-	48,48,48	1.01	2 (4%)	51,54,54	1.27	7 (13%)
32	STE	B	622	-	13,13,19	0.57	0	13,13,19	1.32	3 (23%)
22	CLA	b	610	36	69,73,73	1.18	4 (5%)	82,113,113	1.40	12 (14%)
24	BCR	K	103	-	41,41,41	1.14	4 (9%)	56,56,56	1.30	9 (16%)
27	LMG	m	101	-	51,51,55	1.15	6 (11%)	59,59,63	1.49	11 (18%)
29	LHG	d	408	-	48,48,48	0.94	1 (2%)	51,54,54	1.15	2 (3%)
33	BCT	d	402	21	3,3,3	1.22	0	2,3,3	3.07	2 (100%)
28	SQD	A	414	-	38,38,54	1.08	3 (7%)	40,40,65	1.30	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	d	410	-	44,44,55	1.24	4 (9%)	52,52,63	1.42	6 (11%)
22	CLA	B	602	2	69,73,73	1.28	9 (13%)	82,113,113	1.35	9 (10%)
22	CLA	B	606	2	69,73,73	1.42	10 (14%)	82,113,113	1.45	9 (10%)
22	CLA	b	613	2	69,73,73	1.28	9 (13%)	82,113,113	1.43	12 (14%)
28	SQD	F	102	-	34,36,54	0.99	2 (5%)	42,45,65	1.86	10 (23%)
26	PL9	d	407	-	55,55,55	1.58	7 (12%)	68,69,69	1.79	14 (20%)
22	CLA	b	605	2	69,73,73	1.17	7 (10%)	82,113,113	1.49	13 (15%)
22	CLA	c	504	36	64,68,73	1.30	10 (15%)	76,107,113	1.34	10 (13%)
32	STE	D	413	-	14,14,19	0.88	1 (7%)	14,14,19	1.09	1 (7%)
22	CLA	b	606	2	69,73,73	1.48	8 (11%)	82,113,113	1.37	7 (8%)
24	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.26	7 (12%)
34	HEM	f	101	6,5	50,50,50	1.45	8 (16%)	67,82,82	1.29	7 (10%)
30	DGD	h	103	-	63,63,67	1.22	8 (12%)	77,77,81	1.38	11 (14%)
32	STE	b	622	-	19,19,19	0.73	0	19,19,19	0.95	0
22	CLA	c	505	3	69,73,73	1.10	8 (11%)	82,113,113	1.28	8 (9%)
23	PHO	A	405	-	58,69,69	1.96	8 (13%)	55,99,99	1.51	6 (10%)
24	BCR	c	515	-	41,41,41	1.30	4 (9%)	56,56,56	1.30	5 (8%)
29	LHG	L	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.18	3 (5%)
27	LMG	M	101	-	51,51,55	1.13	2 (3%)	59,59,63	1.44	7 (11%)
22	CLA	C	505	3	69,73,73	1.17	7 (10%)	82,113,113	1.44	10 (12%)
24	BCR	C	514	-	41,41,41	1.27	3 (7%)	56,56,56	1.28	7 (12%)
32	STE	C	520	-	11,11,19	0.55	0	11,11,19	1.52	1 (9%)
22	CLA	b	615	2	69,73,73	1.59	12 (17%)	82,113,113	1.42	7 (8%)
32	STE	a	413	-	9,9,19	0.65	0	8,8,19	0.38	0
24	BCR	B	617	-	41,41,41	1.18	3 (7%)	56,56,56	1.24	5 (8%)
23	PHO	d	401	-	58,69,69	2.07	9 (15%)	55,99,99	1.69	11 (20%)
27	LMG	h	102	-	21,21,55	0.96	1 (4%)	20,20,63	1.08	1 (5%)
22	CLA	C	508	3	69,73,73	1.39	7 (10%)	82,113,113	1.38	7 (8%)
32	STE	B	624	-	17,17,19	0.66	0	17,17,19	1.18	1 (5%)
32	STE	b	626	-	9,9,19	0.51	0	8,8,19	0.60	0
22	CLA	c	513	3	69,73,73	1.43	10 (14%)	82,113,113	1.19	11 (13%)
22	CLA	B	604	2	69,73,73	1.29	7 (10%)	82,113,113	1.57	12 (14%)
35	HEC	v	201	17	50,50,50	1.68	6 (12%)	68,82,82	1.61	15 (22%)
28	SQD	b	620	-	47,49,54	0.93	2 (4%)	57,60,65	2.34	14 (24%)
24	BCR	T	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.17	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	DGD	A	415	-	67,67,67	1.43	10 (14%)	81,81,81	1.50	13 (16%)
30	DGD	C	517	-	63,63,67	1.28	7 (11%)	77,77,81	1.40	10 (12%)
22	CLA	c	501	3	69,73,73	1.14	7 (10%)	82,113,113	1.47	8 (9%)
30	DGD	C	516	-	63,63,67	1.28	8 (12%)	77,77,81	1.43	9 (11%)
32	STE	H	103	-	17,17,19	0.41	0	16,16,19	0.84	0
22	CLA	D	404	4	69,73,73	1.48	11 (15%)	82,113,113	1.10	3 (3%)
22	CLA	C	504	36	63,67,73	1.18	8 (12%)	74,105,113	1.33	9 (12%)
22	CLA	C	502	3	69,73,73	1.22	8 (11%)	82,113,113	1.15	8 (9%)
29	LHG	D	409	-	46,46,48	0.98	3 (6%)	49,52,54	1.25	5 (10%)
32	STE	B	625	-	15,15,19	0.49	0	14,14,19	0.71	0
22	CLA	a	405	1	69,73,73	1.25	10 (14%)	82,113,113	1.26	5 (6%)
32	STE	J	101	-	11,11,19	0.70	0	11,11,19	1.58	2 (18%)
33	BCT	D	401	21	3,3,3	1.11	0	2,3,3	2.76	2 (100%)
32	STE	B	620	-	16,16,19	0.87	0	16,16,19	0.76	0
22	CLA	B	612	2	69,73,73	1.11	5 (7%)	82,113,113	1.39	10 (12%)
22	CLA	C	510	3	69,73,73	1.19	7 (10%)	82,113,113	1.20	7 (8%)
28	SQD	a	412	-	35,35,54	1.25	2 (5%)	37,37,65	1.67	6 (16%)
32	STE	M	102	-	14,14,19	1.03	1 (7%)	14,14,19	0.77	1 (7%)
28	SQD	A	412	-	50,52,54	1.08	5 (10%)	60,63,65	1.68	8 (13%)
22	CLA	B	603	2	69,73,73	1.34	9 (13%)	82,113,113	1.37	14 (17%)
34	HEM	F	101	6,5	50,50,50	1.37	7 (14%)	67,82,82	1.20	6 (8%)
24	BCR	c	514	-	41,41,41	1.19	2 (4%)	56,56,56	1.12	5 (8%)
27	LMG	Y	101	-	48,48,55	0.97	2 (4%)	56,56,63	1.47	10 (17%)
22	CLA	a	403	36	69,73,73	1.20	9 (13%)	82,113,113	1.36	9 (10%)
27	LMG	c	519	-	37,37,55	1.22	5 (13%)	45,45,63	1.38	6 (13%)
22	CLA	C	506	3	69,73,73	1.68	9 (13%)	82,113,113	1.19	6 (7%)
22	CLA	c	508	3	68,72,73	1.41	9 (13%)	80,111,113	1.35	12 (15%)
24	BCR	A	407	-	41,41,41	1.21	3 (7%)	56,56,56	1.41	8 (14%)
22	CLA	B	616	2	64,68,73	1.57	11 (17%)	76,107,113	1.54	9 (11%)
27	LMG	a	414	-	49,49,55	1.01	5 (10%)	57,57,63	1.33	6 (10%)
32	STE	D	412	-	19,19,19	0.76	1 (5%)	19,19,19	0.98	0
22	CLA	C	507	36	69,73,73	1.46	10 (14%)	82,113,113	1.58	9 (10%)
22	CLA	C	501	3	69,73,73	1.47	12 (17%)	82,113,113	1.39	9 (10%)
29	LHG	d	409	-	38,38,48	1.02	2 (5%)	41,44,54	1.07	4 (9%)
22	CLA	D	403	36	69,73,73	1.31	5 (7%)	82,113,113	1.31	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	STE	M	103	-	9,9,19	0.55	0	8,8,19	0.66	0
30	DGD	c	518	-	63,63,67	1.20	7 (11%)	77,77,81	1.47	12 (15%)
22	CLA	B	608	2	69,73,73	1.45	11 (15%)	82,113,113	1.28	9 (10%)
22	CLA	c	506	3	69,73,73	1.24	9 (13%)	82,113,113	1.16	6 (7%)
22	CLA	b	612	2	69,73,73	1.13	7 (10%)	82,113,113	1.26	9 (10%)
22	CLA	c	503	3	69,73,73	1.20	10 (14%)	82,113,113	1.39	9 (10%)
22	CLA	b	603	2	69,73,73	1.32	10 (14%)	82,113,113	1.46	13 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	610	36	-	4/39/115/115	-
22	CLA	C	511	3	-	8/39/115/115	-
22	CLA	c	509	3	-	15/39/115/115	-
24	BCR	a	406	-	-	0/29/63/63	0/2/2/2
22	CLA	b	616	2	-	13/33/109/115	-
27	LMG	A	411	-	-	16/43/63/70	0/1/1/1
22	CLA	B	613	2	-	14/39/115/115	-
30	DGD	c	517	-	-	20/51/91/95	0/2/2/2
22	CLA	A	403	36	-	14/39/115/115	-
32	STE	M	104	-	-	7/15/15/17	-
23	PHO	a	404	-	-	5/37/103/103	0/5/6/6
22	CLA	A	402	1	-	3/39/115/115	-
22	CLA	B	607	36	-	4/39/115/115	-
32	STE	d	412	-	-	11/17/17/17	-
32	STE	C	518	-	-	4/9/9/17	-
27	LMG	D	407	-	-	14/46/66/70	0/1/1/1
22	CLA	d	405	4	-	4/39/115/115	-
24	BCR	D	405	-	-	5/29/63/63	0/2/2/2
26	PL9	A	410	-	-	23/53/73/73	0/1/1/1
32	STE	b	624	-	-	5/13/13/17	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
22	CLA	B	615	2	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PL9	a	409	1	-	19/53/73/73	0/1/1/1
32	STE	I	101	-	-	5/12/12/17	-
22	CLA	C	509	3	-	14/39/115/115	-
22	CLA	C	503	3	-	4/39/115/115	-
35	HEC	V	201	17	1/1/7/7	6/14/54/54	-
27	LMG	b	623	-	-	25/50/70/70	0/1/1/1
32	STE	T	102	-	-	7/12/12/17	-
32	STE	c	522	-	-	4/9/9/17	-
32	STE	b	621	-	-	8/13/13/17	-
22	CLA	b	604	2	-	9/39/115/115	-
22	CLA	c	511	3	-	9/39/115/115	-
32	STE	d	411	-	-	8/14/14/17	-
32	STE	c	520	-	-	13/17/17/17	-
29	LHG	D	411	-	-	19/53/53/53	-
30	DGD	H	102	-	-	19/51/91/95	0/2/2/2
32	STE	b	625	-	-	10/17/17/17	-
22	CLA	B	614	2	-	8/39/115/115	-
22	CLA	c	502	3	-	6/39/115/115	-
30	DGD	o	301	-	-	20/45/45/95	-
24	BCR	b	618	-	-	5/29/63/63	0/2/2/2
22	CLA	c	507	36	-	12/39/115/115	-
22	CLA	B	605	2	-	7/39/115/115	-
22	CLA	c	512	3	-	18/39/115/115	-
32	STE	j	101	-	-	3/9/9/17	-
29	LHG	A	413	-	-	27/53/53/53	-
24	BCR	k	101	-	-	12/29/63/63	0/2/2/2
32	STE	m	102	-	-	1/9/9/17	-
27	LMG	D	410	-	-	13/33/33/70	-
27	LMG	c	521	-	-	25/43/63/70	0/1/1/1
22	CLA	b	609	2	-	8/39/115/115	-
22	CLA	b	611	2	-	7/39/115/115	-
29	LHG	a	410	-	-	17/53/53/53	-
29	LHG	e	101	-	-	21/46/46/53	-
24	BCR	B	619	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	A	404	-	-	3/37/103/103	0/5/6/6
22	CLA	A	406	1	-	3/26/102/115	-
29	LHG	l	101	-	-	21/53/53/53	-
22	CLA	d	404	36	-	5/39/115/115	-
32	STE	B	627	-	-	8/13/13/17	-
28	SQD	f	102	-	-	17/36/56/69	0/1/1/1
28	SQD	B	621	-	-	19/49/69/69	0/1/1/1
24	BCR	K	102	-	-	5/29/63/63	0/2/2/2
30	DGD	c	516	-	-	27/51/91/95	0/2/2/2
32	STE	C	519	-	-	5/13/13/17	-
32	STE	B	626	-	-	3/9/9/17	-
22	CLA	a	402	1	-	4/39/115/115	-
22	CLA	B	609	2	-	3/39/115/115	-
22	CLA	B	601	36	-	21/39/115/115	-
22	CLA	c	510	3	-	6/39/115/115	-
24	BCR	B	618	-	-	10/29/63/63	0/2/2/2
22	CLA	b	602	2	-	9/39/115/115	-
22	CLA	b	607	36	-	13/39/115/115	-
24	BCR	K	101	-	-	8/29/63/63	0/2/2/2
22	CLA	C	512	3	-	14/39/115/115	-
24	BCR	h	101	-	-	3/29/63/63	0/2/2/2
28	SQD	a	411	-	-	23/49/69/69	0/1/1/1
32	STE	E	101	-	-	3/9/9/17	-
24	BCR	t	101	-	-	2/29/63/63	0/2/2/2
30	DGD	C	515	-	-	19/51/91/95	0/2/2/2
26	PL9	D	406	-	-	10/53/73/73	0/1/1/1
22	CLA	C	513	3	-	15/39/115/115	-
22	CLA	b	601	36	-	18/39/115/115	-
22	CLA	b	608	2	-	6/39/115/115	-
22	CLA	D	402	4	-	6/39/115/115	-
32	STE	a	415	-	-	4/9/9/17	-
32	STE	B	623	-	-	5/9/9/17	-
22	CLA	d	403	4	-	12/39/115/115	-
24	BCR	k	102	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	611	2	-	6/39/115/115	-
24	BCR	b	617	-	-	5/29/63/63	0/2/2/2
22	CLA	b	614	2	-	15/39/115/115	-
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
29	LHG	D	408	-	-	23/53/53/53	-
32	STE	B	622	-	-	2/11/11/17	-
22	CLA	b	610	36	-	3/39/115/115	-
24	BCR	K	103	-	-	4/29/63/63	0/2/2/2
27	LMG	m	101	-	-	16/46/66/70	0/1/1/1
29	LHG	d	408	-	-	20/53/53/53	-
28	SQD	A	414	-	-	17/39/39/69	-
27	LMG	d	410	-	-	12/39/59/70	0/1/1/1
22	CLA	B	602	2	-	6/39/115/115	-
22	CLA	B	606	2	-	15/39/115/115	-
22	CLA	b	613	2	-	7/39/115/115	-
28	SQD	F	102	-	-	12/28/48/69	0/1/1/1
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
22	CLA	b	605	2	-	7/39/115/115	-
22	CLA	c	504	36	-	7/33/109/115	-
32	STE	D	413	-	-	7/12/12/17	-
22	CLA	b	606	2	-	5/39/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
34	HEM	f	101	6,5	-	5/14/54/54	-
30	DGD	h	103	-	-	19/51/91/95	0/2/2/2
32	STE	b	622	-	-	12/17/17/17	-
22	CLA	c	505	3	-	8/39/115/115	-
23	PHO	A	405	-	-	1/37/103/103	0/5/6/6
24	BCR	c	515	-	-	2/29/63/63	0/2/2/2
29	LHG	L	101	-	-	17/53/53/53	-
27	LMG	M	101	-	-	25/46/66/70	0/1/1/1
22	CLA	C	505	3	-	12/39/115/115	-
24	BCR	C	514	-	-	7/29/63/63	0/2/2/2
32	STE	C	520	-	-	5/9/9/17	-
22	CLA	b	615	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	STE	a	413	-	-	5/7/7/17	-
24	BCR	B	617	-	-	6/29/63/63	0/2/2/2
23	PHO	d	401	-	-	5/37/103/103	0/5/6/6
27	LMG	h	102	-	-	11/17/17/70	-
22	CLA	C	508	3	-	6/39/115/115	-
32	STE	B	624	-	-	14/15/15/17	-
35	HEC	v	201	17	1/1/7/7	6/14/54/54	-
22	CLA	c	513	3	-	11/39/115/115	-
22	CLA	B	604	2	-	11/39/115/115	-
32	STE	b	626	-	-	4/7/7/17	-
28	SQD	b	620	-	-	24/44/64/69	0/1/1/1
24	BCR	T	101	-	-	14/29/63/63	0/2/2/2
30	DGD	A	415	-	-	33/55/95/95	0/2/2/2
30	DGD	C	517	-	-	14/51/91/95	0/2/2/2
22	CLA	c	501	3	-	2/39/115/115	-
30	DGD	C	516	-	-	20/51/91/95	0/2/2/2
32	STE	H	103	-	-	9/15/15/17	-
22	CLA	D	404	4	-	12/39/115/115	-
22	CLA	C	504	36	-	4/32/108/115	-
22	CLA	C	502	3	-	8/39/115/115	-
29	LHG	D	409	-	-	21/51/51/53	-
32	STE	B	625	-	-	7/13/13/17	-
22	CLA	a	405	1	-	5/39/115/115	-
32	STE	J	101	-	-	5/9/9/17	-
32	STE	B	620	-	-	8/14/14/17	-
22	CLA	B	612	2	-	11/39/115/115	-
22	CLA	C	510	3	-	9/39/115/115	-
28	SQD	a	412	-	-	16/37/37/69	-
32	STE	M	102	-	-	5/12/12/17	-
28	SQD	A	412	-	-	15/47/67/69	0/1/1/1
22	CLA	B	603	2	-	10/39/115/115	-
34	HEM	F	101	6,5	-	3/14/54/54	-
24	BCR	c	514	-	-	7/29/63/63	0/2/2/2
27	LMG	Y	101	-	-	23/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	a	403	36	-	13/39/115/115	-
27	LMG	c	519	-	-	11/31/51/70	0/1/1/1
22	CLA	C	506	3	-	9/39/115/115	-
22	CLA	c	508	3	-	6/38/114/115	-
24	BCR	A	407	-	-	7/29/63/63	0/2/2/2
22	CLA	B	616	2	-	8/33/109/115	-
27	LMG	a	414	-	-	23/44/64/70	0/1/1/1
32	STE	D	412	-	-	7/17/17/17	-
22	CLA	C	507	36	-	5/39/115/115	-
22	CLA	C	501	3	-	3/39/115/115	-
29	LHG	d	409	-	-	13/43/43/53	-
22	CLA	D	403	36	-	6/39/115/115	-
32	STE	M	103	-	-	4/7/7/17	-
30	DGD	c	518	-	-	16/51/91/95	0/2/2/2
22	CLA	B	608	2	-	3/39/115/115	-
22	CLA	c	506	3	-	13/39/115/115	-
22	CLA	b	612	2	-	5/39/115/115	-
22	CLA	c	503	3	-	10/39/115/115	-
22	CLA	b	603	2	-	8/39/115/115	-

All (923) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	401	PHO	C1B-C2B	9.07	1.49	1.39
23	d	401	PHO	C3B-C4B	9.04	1.50	1.41
23	a	404	PHO	C1B-C2B	8.87	1.49	1.39
23	A	405	PHO	C1B-C2B	8.36	1.48	1.39
23	A	405	PHO	C3B-C4B	7.87	1.49	1.41
22	b	615	CLA	MG-NA	7.85	2.24	2.06
22	c	511	CLA	MG-NA	7.71	2.24	2.06
35	v	201	HEC	C3D-C2D	7.50	1.52	1.36
22	b	606	CLA	MG-NA	7.48	2.24	2.06
22	C	506	CLA	MG-ND	-7.48	1.91	2.05
22	B	613	CLA	MG-ND	-7.43	1.91	2.05
22	C	512	CLA	MG-NB	7.41	2.20	2.05
23	a	404	PHO	C3B-C4B	7.40	1.49	1.41
22	B	616	CLA	MG-NA	7.19	2.23	2.06
22	D	404	CLA	MG-NB	-6.59	1.92	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	503	CLA	MG-NA	6.54	2.21	2.06
22	b	604	CLA	MG-NA	6.51	2.21	2.06
23	A	404	PHO	C1B-C2B	6.47	1.46	1.39
22	C	507	CLA	MG-NA	6.35	2.21	2.06
23	A	404	PHO	C3B-C4B	6.32	1.47	1.41
22	B	603	CLA	MG-ND	6.31	2.18	2.05
35	V	201	HEC	C3D-C2D	6.08	1.49	1.36
22	b	601	CLA	MG-NA	6.01	2.20	2.06
22	C	508	CLA	MG-NA	5.98	2.20	2.06
22	d	404	CLA	MG-NA	5.84	2.20	2.06
22	B	608	CLA	MG-NA	5.82	2.20	2.06
35	V	201	HEC	FE-ND	5.77	2.12	1.94
22	C	506	CLA	MG-NA	5.73	2.19	2.06
22	B	601	CLA	MG-NA	5.58	2.19	2.06
22	D	403	CLA	MG-NA	5.57	2.19	2.06
22	c	513	CLA	MG-NC	-5.53	1.93	2.06
22	b	608	CLA	MG-NA	5.40	2.19	2.06
26	a	409	PL9	C3-C4	5.34	1.58	1.49
22	c	508	CLA	MG-NA	5.25	2.18	2.06
22	B	604	CLA	MG-NA	5.16	2.18	2.06
26	a	409	PL9	O1-C4	5.09	1.34	1.23
22	B	606	CLA	MG-NB	-5.06	1.95	2.05
30	C	515	DGD	C6E-C5E	5.04	1.68	1.51
26	d	407	PL9	C6-C1	-5.02	1.40	1.48
22	b	607	CLA	MG-NB	-4.97	1.95	2.05
22	B	610	CLA	MG-ND	-4.95	1.96	2.05
22	b	602	CLA	MG-NA	4.94	2.18	2.06
26	D	406	PL9	C7-C3	-4.84	1.44	1.51
22	B	606	CLA	MG-NA	4.80	2.17	2.06
22	a	402	CLA	MG-NA	4.78	2.17	2.06
24	b	618	BCR	C30-C25	-4.76	1.47	1.53
30	H	102	DGD	C4E-C5E	4.74	1.63	1.53
22	B	601	CLA	MG-NB	-4.72	1.96	2.05
34	f	101	HEM	FE-NA	4.69	2.10	1.95
22	c	510	CLA	MG-NA	4.66	2.17	2.06
27	A	411	LMG	O1-C7	-4.65	1.35	1.43
30	C	515	DGD	O5D-C1E	4.64	1.47	1.40
22	B	615	CLA	MG-NA	4.61	2.17	2.06
29	D	408	LHG	O7-C5	-4.59	1.35	1.46
24	c	515	BCR	C1-C6	-4.57	1.47	1.53
30	C	517	DGD	O2G-C2G	-4.56	1.35	1.46
22	B	614	CLA	MG-NA	4.53	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	514	BCR	C1-C6	-4.53	1.48	1.53
30	c	516	DGD	O2G-C2G	-4.51	1.36	1.46
30	o	301	DGD	O1G-C1A	4.49	1.46	1.33
22	b	613	CLA	MG-ND	-4.47	1.96	2.05
22	A	402	CLA	MG-ND	-4.45	1.97	2.05
28	a	412	SQD	O47-C7	4.44	1.46	1.34
22	B	608	CLA	MG-NC	-4.39	1.95	2.06
22	b	604	CLA	MG-ND	-4.38	1.97	2.05
22	C	501	CLA	MG-ND	-4.36	1.97	2.05
23	a	404	PHO	C1D-C2D	4.36	1.44	1.39
22	c	513	CLA	MG-NA	4.33	2.16	2.06
22	B	614	CLA	MG-ND	-4.30	1.97	2.05
22	A	402	CLA	MG-NB	4.30	2.14	2.05
30	c	516	DGD	C3G-C2G	4.29	1.64	1.50
22	B	615	CLA	MG-NB	4.27	2.14	2.05
24	d	406	BCR	C30-C25	-4.23	1.48	1.53
27	D	407	LMG	C4-C5	4.22	1.62	1.53
22	C	501	CLA	C1D-ND	4.21	1.43	1.37
23	A	405	PHO	C4D-ND	-4.19	1.32	1.38
24	T	101	BCR	C1-C6	-4.19	1.48	1.53
22	b	610	CLA	C1D-ND	4.19	1.43	1.37
22	b	607	CLA	MG-ND	-4.14	1.97	2.05
22	B	610	CLA	C1D-ND	4.13	1.43	1.37
22	b	603	CLA	MG-NB	-4.13	1.97	2.05
26	d	407	PL9	C31-C29	-4.12	1.42	1.51
22	C	502	CLA	MG-NA	4.10	2.16	2.06
22	b	609	CLA	MG-NA	4.08	2.16	2.06
24	d	406	BCR	C1-C6	-4.08	1.48	1.53
22	B	602	CLA	C1D-ND	4.05	1.43	1.37
22	C	512	CLA	MG-ND	-4.04	1.97	2.05
28	a	411	SQD	O48-C23	4.04	1.45	1.33
22	b	615	CLA	MG-NB	4.03	2.13	2.05
30	A	415	DGD	C3E-C2E	4.02	1.62	1.52
27	d	410	LMG	C4-C5	4.00	1.61	1.53
22	b	603	CLA	MG-NA	3.98	2.15	2.06
24	D	405	BCR	C1-C6	-3.97	1.48	1.53
27	m	101	LMG	O7-C8	-3.94	1.37	1.46
22	B	613	CLA	C4B-NB	3.94	1.43	1.37
24	B	619	BCR	C1-C6	-3.93	1.48	1.53
30	c	516	DGD	O3E-C3E	-3.93	1.33	1.43
22	b	604	CLA	C4B-NB	3.92	1.43	1.37
22	B	609	CLA	MG-ND	3.91	2.13	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	102	BCR	C30-C25	-3.90	1.48	1.53
27	c	521	LMG	O1-C1	3.87	1.46	1.40
30	C	515	DGD	C4E-C3E	3.87	1.62	1.52
22	c	504	CLA	MG-ND	-3.84	1.98	2.05
22	D	402	CLA	C1D-ND	3.84	1.42	1.37
22	C	507	CLA	MG-NB	-3.84	1.98	2.05
24	D	405	BCR	C30-C25	-3.84	1.48	1.53
24	c	514	BCR	C1-C6	-3.80	1.48	1.53
22	B	609	CLA	MG-NA	3.79	2.15	2.06
22	b	602	CLA	C1D-ND	3.79	1.42	1.37
22	b	609	CLA	C1D-ND	3.78	1.42	1.37
24	b	619	BCR	C30-C25	-3.78	1.48	1.53
22	b	611	CLA	MG-ND	3.77	2.13	2.05
35	v	201	HEC	FE-ND	3.76	2.06	1.94
22	C	501	CLA	MG-NA	3.76	2.15	2.06
22	c	509	CLA	C1D-ND	3.75	1.42	1.37
22	B	616	CLA	C1D-ND	3.75	1.42	1.37
24	b	617	BCR	C30-C25	-3.75	1.49	1.53
24	b	619	BCR	C1-C6	-3.74	1.49	1.53
22	c	512	CLA	MG-NB	3.74	2.13	2.05
24	A	407	BCR	C1-C6	-3.74	1.49	1.53
22	c	511	CLA	MG-ND	3.72	2.13	2.05
22	D	404	CLA	C1D-ND	3.70	1.42	1.37
22	c	508	CLA	MG-NB	3.69	2.13	2.05
22	B	607	CLA	MG-NA	3.68	2.15	2.06
30	A	415	DGD	O3G-C3G	-3.66	1.37	1.43
24	B	617	BCR	C30-C25	-3.63	1.49	1.53
22	b	603	CLA	CMD-C2D	-3.62	1.43	1.50
29	d	408	LHG	O8-C6	-3.62	1.37	1.45
22	B	610	CLA	MG-NC	-3.62	1.97	2.06
30	o	301	DGD	O2G-C2G	-3.61	1.38	1.46
22	b	615	CLA	CMD-C2D	-3.61	1.43	1.50
27	M	101	LMG	O7-C8	-3.61	1.38	1.46
24	T	101	BCR	C30-C25	-3.59	1.49	1.53
24	B	618	BCR	C30-C25	-3.57	1.49	1.53
22	C	509	CLA	MG-NB	-3.57	1.98	2.05
22	b	611	CLA	MG-NA	3.54	2.14	2.06
30	c	517	DGD	C3E-C2E	3.54	1.61	1.52
22	b	615	CLA	C4B-NB	3.53	1.42	1.37
22	c	505	CLA	MG-NA	3.52	2.14	2.06
22	B	616	CLA	MG-NB	-3.51	1.98	2.05
23	A	404	PHO	CBD-CGD	-3.51	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	613	CLA	MG-NC	3.51	2.14	2.06
24	c	514	BCR	C30-C25	-3.50	1.49	1.53
29	A	413	LHG	C24-C23	3.50	1.60	1.50
27	d	410	LMG	O7-C8	-3.49	1.38	1.46
22	B	605	CLA	C1B-C2B	3.49	1.51	1.43
26	D	406	PL9	C52-C5	-3.49	1.43	1.50
22	c	504	CLA	C4B-NB	3.49	1.42	1.37
22	D	403	CLA	C1D-ND	3.48	1.42	1.37
22	C	511	CLA	C1B-C2B	3.48	1.51	1.43
26	d	407	PL9	C3-C4	-3.47	1.44	1.49
27	D	410	LMG	C7-C8	3.47	1.59	1.51
22	c	501	CLA	C1D-ND	3.46	1.42	1.37
22	A	406	CLA	C1D-ND	3.46	1.42	1.37
22	C	513	CLA	C1D-ND	3.46	1.42	1.37
30	A	415	DGD	O5D-C6D	-3.44	1.37	1.43
22	B	601	CLA	C4B-NB	3.44	1.42	1.37
22	B	601	CLA	C1D-ND	3.42	1.42	1.37
22	a	405	CLA	MG-NB	-3.42	1.99	2.05
22	b	609	CLA	MG-NB	-3.42	1.99	2.05
26	d	407	PL9	C25-C24	-3.41	1.42	1.50
30	C	515	DGD	O2G-C2G	-3.41	1.38	1.46
28	a	412	SQD	O48-C23	3.41	1.43	1.33
24	a	406	BCR	C1-C6	-3.41	1.49	1.53
24	h	101	BCR	C30-C25	-3.41	1.49	1.53
24	H	101	BCR	C30-C25	-3.40	1.49	1.53
22	b	614	CLA	MG-ND	-3.39	1.99	2.05
24	b	617	BCR	C1-C6	-3.39	1.49	1.53
22	C	506	CLA	C1B-NB	-3.39	1.33	1.37
27	D	410	LMG	C9-C8	3.39	1.61	1.50
22	A	402	CLA	C1B-C2B	3.38	1.51	1.43
22	B	602	CLA	C4B-NB	3.38	1.42	1.37
22	C	501	CLA	C4B-NB	3.38	1.42	1.37
28	f	102	SQD	O48-C23	3.38	1.43	1.33
28	B	621	SQD	O47-C7	3.38	1.43	1.34
22	b	612	CLA	MG-ND	-3.38	1.99	2.05
30	c	518	DGD	O3G-C3G	-3.37	1.37	1.43
22	B	605	CLA	C1D-ND	3.36	1.42	1.37
22	c	512	CLA	MG-NA	3.36	2.14	2.06
22	C	510	CLA	MG-NC	3.36	2.14	2.06
24	k	102	BCR	C30-C25	-3.35	1.49	1.53
22	b	613	CLA	MG-NA	3.35	2.14	2.06
23	d	401	PHO	C4D-ND	-3.35	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	PHO	CMD-C2D	-3.35	1.44	1.51
28	B	621	SQD	O48-C23	3.34	1.43	1.33
22	c	512	CLA	C1D-ND	3.34	1.42	1.37
22	C	508	CLA	C1B-C2B	3.33	1.51	1.43
28	A	414	SQD	O47-C45	-3.33	1.41	1.47
22	B	611	CLA	MG-NA	3.32	2.14	2.06
23	a	404	PHO	CBD-CGD	-3.32	1.48	1.52
30	H	102	DGD	C1G-C2G	3.32	1.61	1.50
22	c	506	CLA	CMD-C2D	-3.32	1.44	1.50
22	b	601	CLA	C1B-C2B	3.32	1.50	1.43
35	V	201	HEC	FE-NB	3.31	2.05	1.94
22	C	506	CLA	C4B-NB	3.31	1.42	1.37
22	A	406	CLA	C4B-NB	3.31	1.42	1.37
22	c	507	CLA	MG-NB	-3.31	1.99	2.05
30	H	102	DGD	C4D-C5D	3.30	1.60	1.53
22	B	613	CLA	C1D-ND	3.30	1.42	1.37
29	a	410	LHG	C24-C23	3.30	1.60	1.50
24	K	101	BCR	C30-C25	-3.29	1.49	1.53
30	c	517	DGD	C4D-C3D	3.29	1.60	1.52
22	B	610	CLA	CMB-C2B	-3.28	1.44	1.50
22	C	502	CLA	C1B-C2B	3.28	1.50	1.43
30	c	516	DGD	C4D-C3D	3.26	1.60	1.52
22	d	403	CLA	C1B-C2B	3.25	1.50	1.43
22	c	508	CLA	C1D-ND	3.25	1.42	1.37
22	C	506	CLA	MG-NB	3.25	2.12	2.05
24	B	617	BCR	C1-C6	-3.25	1.49	1.53
22	b	614	CLA	C1D-ND	3.24	1.42	1.37
30	A	415	DGD	C1E-C2E	3.24	1.62	1.52
22	B	615	CLA	CMD-C2D	-3.24	1.44	1.50
22	B	611	CLA	C1B-NB	-3.24	1.33	1.37
22	b	601	CLA	C1D-ND	3.23	1.42	1.37
22	B	611	CLA	CMB-C2B	-3.23	1.44	1.50
28	A	414	SQD	O48-C23	3.22	1.42	1.33
24	a	406	BCR	C30-C25	-3.22	1.49	1.53
35	v	201	HEC	FE-NA	3.22	2.05	1.95
30	A	415	DGD	O1G-C1G	-3.22	1.38	1.45
30	h	103	DGD	O1G-C1G	-3.22	1.38	1.45
28	f	102	SQD	O47-C7	3.21	1.43	1.34
30	A	415	DGD	C4D-C3D	3.21	1.60	1.52
30	c	518	DGD	O2E-C2E	-3.20	1.35	1.43
22	C	507	CLA	MG-ND	3.19	2.12	2.05
22	d	404	CLA	MG-NB	3.19	2.12	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	511	CLA	MG-NA	3.19	2.13	2.06
30	h	103	DGD	O3D-C3D	-3.18	1.35	1.43
30	c	518	DGD	O3D-C3D	-3.18	1.35	1.43
23	A	404	PHO	C1D-C2D	3.18	1.43	1.39
22	b	602	CLA	CMD-C2D	-3.18	1.44	1.50
28	A	412	SQD	O48-C23	3.18	1.42	1.33
22	b	616	CLA	C1D-ND	3.18	1.42	1.37
28	A	414	SQD	O47-C7	3.17	1.43	1.34
22	a	405	CLA	CMC-C2C	-3.17	1.44	1.50
28	F	102	SQD	O48-C23	3.17	1.42	1.33
22	b	606	CLA	C1B-C2B	3.17	1.50	1.43
22	c	503	CLA	MG-NA	3.16	2.13	2.06
22	b	606	CLA	C1D-ND	3.16	1.42	1.37
23	d	401	PHO	CMC-C2C	-3.16	1.45	1.50
22	d	405	CLA	C1B-C2B	3.15	1.50	1.43
27	a	414	LMG	C4-C5	3.15	1.59	1.53
30	C	516	DGD	C1E-C2E	3.15	1.61	1.52
22	C	509	CLA	MG-NC	-3.15	1.98	2.06
22	C	505	CLA	C4B-NB	3.14	1.42	1.37
30	A	415	DGD	C4E-C5E	3.14	1.59	1.53
22	d	404	CLA	C1D-ND	3.14	1.42	1.37
23	A	404	PHO	CMC-C2C	-3.13	1.45	1.50
22	b	607	CLA	CMD-C2D	-3.13	1.44	1.50
22	A	406	CLA	MG-NB	-3.13	1.99	2.05
23	A	405	PHO	CMB-C2B	-3.12	1.45	1.51
28	b	620	SQD	O47-C7	3.12	1.43	1.34
22	c	507	CLA	C1D-ND	3.12	1.42	1.37
22	c	502	CLA	MG-NA	3.12	2.13	2.06
24	K	101	BCR	C1-C6	-3.11	1.49	1.53
22	A	403	CLA	C1D-ND	3.11	1.41	1.37
29	D	409	LHG	P-O6	3.11	1.71	1.59
22	B	606	CLA	C1D-ND	3.10	1.41	1.37
22	C	511	CLA	C1D-ND	3.10	1.41	1.37
29	A	413	LHG	P-O6	3.09	1.71	1.59
24	c	515	BCR	C30-C25	-3.08	1.49	1.53
22	b	608	CLA	C1D-ND	3.08	1.41	1.37
22	B	611	CLA	C1B-C2B	3.08	1.50	1.43
22	c	513	CLA	MG-ND	-3.07	1.99	2.05
22	a	402	CLA	C1B-C2B	3.07	1.50	1.43
22	C	505	CLA	MG-NA	3.07	2.13	2.06
27	Y	101	LMG	O7-C8	-3.07	1.39	1.46
23	A	404	PHO	CAC-C3C	-3.07	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	506	CLA	CHC-C1C	3.06	1.44	1.38
22	c	511	CLA	C1B-C2B	3.06	1.50	1.43
22	C	509	CLA	MG-NA	3.06	2.13	2.06
27	M	101	LMG	C4-C3	3.06	1.60	1.52
22	b	605	CLA	MG-NA	3.05	2.13	2.06
28	b	620	SQD	O48-C23	3.04	1.42	1.33
22	c	510	CLA	CMB-C2B	-3.04	1.44	1.50
30	H	102	DGD	C3E-C2E	3.04	1.60	1.52
22	C	505	CLA	CHC-C1C	3.04	1.44	1.38
22	a	402	CLA	C4B-NB	3.04	1.41	1.37
22	B	612	CLA	CMC-C2C	-3.03	1.44	1.50
23	a	404	PHO	C4D-ND	-3.02	1.34	1.38
22	a	405	CLA	CHC-C4B	-3.02	1.32	1.39
22	B	601	CLA	C1B-C2B	3.01	1.50	1.43
22	b	607	CLA	CMB-C2B	-3.01	1.44	1.50
22	c	506	CLA	C4B-NB	3.01	1.41	1.37
22	d	404	CLA	C1B-C2B	3.00	1.50	1.43
22	c	508	CLA	CHC-C1C	3.00	1.44	1.38
22	A	402	CLA	C1B-NB	-2.99	1.33	1.37
22	B	602	CLA	MG-NB	2.99	2.11	2.05
22	B	603	CLA	CMD-C2D	-2.98	1.44	1.50
22	C	508	CLA	C3B-C4B	2.98	1.51	1.42
27	c	521	LMG	C3-C2	2.98	1.60	1.52
30	C	517	DGD	O3G-C1D	2.97	1.45	1.40
22	B	615	CLA	MG-NC	2.97	2.13	2.06
29	d	409	LHG	P-O6	2.97	1.71	1.59
22	c	507	CLA	MG-NA	2.97	2.13	2.06
22	d	405	CLA	C1D-ND	2.97	1.41	1.37
22	B	616	CLA	C1B-C2B	2.96	1.50	1.43
22	a	402	CLA	C1B-NB	-2.96	1.34	1.37
22	D	404	CLA	CMD-C2D	-2.96	1.44	1.50
22	b	606	CLA	MG-NB	2.96	2.11	2.05
24	K	102	BCR	C1-C6	-2.96	1.50	1.53
22	a	402	CLA	CHC-C1C	2.96	1.44	1.38
30	C	515	DGD	O1G-C1G	-2.95	1.38	1.45
22	b	613	CLA	CMB-C2B	-2.95	1.44	1.50
22	C	503	CLA	C1B-C2B	2.95	1.50	1.43
34	F	101	HEM	FE-NA	2.94	2.04	1.95
22	C	506	CLA	C1D-ND	2.94	1.41	1.37
22	A	403	CLA	C3B-C4B	2.94	1.51	1.42
22	C	512	CLA	C1D-ND	2.93	1.41	1.37
22	B	614	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	MG-NB	2.92	2.11	2.05
30	C	515	DGD	O3E-C3E	-2.92	1.35	1.43
27	c	519	LMG	O1-C1	2.92	1.45	1.40
24	T	101	BCR	C38-C26	-2.91	1.46	1.50
22	B	615	CLA	C1B-C2B	2.91	1.50	1.43
22	C	501	CLA	C1B-NB	-2.91	1.34	1.37
22	B	606	CLA	C4B-NB	2.90	1.41	1.37
24	b	617	BCR	C33-C5	-2.90	1.46	1.50
22	B	604	CLA	C1D-ND	2.90	1.41	1.37
23	A	404	PHO	C3B-C2B	-2.90	1.36	1.40
23	A	405	PHO	CMD-C2D	-2.90	1.45	1.51
27	h	102	LMG	O7-C10	2.90	1.40	1.30
22	c	509	CLA	C1B-C2B	2.90	1.49	1.43
28	A	412	SQD	O2-C2	-2.89	1.35	1.43
35	v	201	HEC	CMA-C3A	2.89	1.56	1.50
30	A	415	DGD	O2G-C2G	-2.89	1.39	1.46
22	b	609	CLA	C4B-NB	2.88	1.41	1.37
30	C	516	DGD	O3G-C3G	-2.88	1.38	1.43
22	B	606	CLA	MG-NC	2.88	2.13	2.06
24	A	407	BCR	C30-C25	-2.88	1.50	1.53
22	b	601	CLA	MG-NC	-2.88	1.99	2.06
30	C	516	DGD	C4E-C3E	2.87	1.59	1.52
22	c	511	CLA	CHC-C1C	2.87	1.44	1.38
27	m	101	LMG	O1-C7	-2.87	1.38	1.43
22	C	505	CLA	C1B-C2B	2.87	1.49	1.43
22	b	614	CLA	C4B-NB	2.87	1.41	1.37
30	C	516	DGD	C6E-C5E	2.87	1.61	1.51
22	c	512	CLA	C1B-C2B	2.86	1.49	1.43
22	B	608	CLA	C1B-C2B	2.86	1.49	1.43
24	C	514	BCR	C30-C25	-2.86	1.50	1.53
30	h	103	DGD	C4E-C5E	2.85	1.59	1.53
22	a	405	CLA	CMD-C2D	-2.85	1.44	1.50
22	b	601	CLA	C4B-NB	2.84	1.41	1.37
22	c	513	CLA	CHC-C1C	2.84	1.44	1.38
22	B	607	CLA	MG-ND	-2.84	2.00	2.05
22	a	402	CLA	C1D-ND	2.84	1.41	1.37
22	B	613	CLA	MG-NB	2.82	2.11	2.05
22	c	502	CLA	C1D-ND	2.81	1.41	1.37
29	a	410	LHG	O7-C5	-2.81	1.40	1.46
22	C	512	CLA	C4B-NB	2.81	1.41	1.37
27	c	521	LMG	C1-C2	2.81	1.60	1.52
22	b	608	CLA	CHC-C1C	2.80	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C1B-C2B	2.80	1.49	1.43
22	C	504	CLA	C1B-NB	-2.79	1.34	1.37
24	B	619	BCR	C30-C25	-2.79	1.50	1.53
22	a	402	CLA	MG-NB	2.78	2.11	2.05
22	c	506	CLA	C1D-ND	2.78	1.41	1.37
23	d	401	PHO	CMD-C2D	-2.77	1.46	1.51
22	a	405	CLA	C1B-C2B	2.77	1.49	1.43
22	c	504	CLA	C1B-NB	-2.77	1.34	1.37
22	b	609	CLA	CMB-C2B	-2.77	1.45	1.50
22	C	510	CLA	C1D-ND	2.77	1.41	1.37
22	C	511	CLA	C4B-NB	2.77	1.41	1.37
29	D	411	LHG	P-O4	-2.76	1.42	1.55
22	B	602	CLA	C1B-C2B	2.76	1.49	1.43
22	C	509	CLA	C1D-ND	2.75	1.41	1.37
22	A	403	CLA	CMD-C2D	-2.75	1.45	1.50
22	b	611	CLA	C1B-C2B	2.75	1.49	1.43
22	B	609	CLA	MG-NB	-2.75	2.00	2.05
26	D	406	PL9	C27-C28	-2.75	1.42	1.50
30	c	518	DGD	O4D-C4D	-2.74	1.36	1.43
29	L	101	LHG	O8-C23	2.74	1.41	1.33
22	C	513	CLA	C1B-C2B	2.74	1.49	1.43
27	c	519	LMG	O7-C10	2.73	1.41	1.35
22	d	404	CLA	MG-NC	-2.73	1.99	2.06
27	d	410	LMG	O6-C5	-2.72	1.37	1.44
22	C	507	CLA	C1B-C2B	2.72	1.49	1.43
22	b	605	CLA	MG-ND	2.72	2.11	2.05
23	A	404	PHO	C4D-ND	-2.72	1.34	1.38
22	D	404	CLA	CMB-C2B	-2.72	1.45	1.50
29	e	101	LHG	P-O6	2.71	1.70	1.59
22	D	404	CLA	C1B-C2B	2.71	1.49	1.43
22	B	610	CLA	MG-NA	2.71	2.12	2.06
22	b	603	CLA	CMC-C2C	-2.71	1.45	1.50
22	C	513	CLA	MG-NA	2.71	2.12	2.06
30	C	515	DGD	O6D-C5D	-2.71	1.37	1.44
22	d	403	CLA	CMD-C2D	-2.71	1.45	1.50
22	c	511	CLA	C4B-NB	2.70	1.41	1.37
28	A	412	SQD	O47-C7	2.70	1.41	1.34
22	a	403	CLA	CMD-C2D	-2.70	1.45	1.50
22	b	610	CLA	MG-NB	-2.70	2.00	2.05
22	d	403	CLA	C1B-NB	-2.70	1.34	1.37
22	B	608	CLA	MG-ND	-2.70	2.00	2.05
22	D	403	CLA	CHC-C1C	2.70	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	MG-NC	-2.70	1.99	2.06
24	A	407	BCR	C33-C5	-2.69	1.46	1.50
22	d	405	CLA	C4B-NB	2.69	1.41	1.37
22	a	403	CLA	CMB-C2B	-2.69	1.45	1.50
22	c	501	CLA	C4B-NB	2.69	1.41	1.37
22	c	507	CLA	C1B-C2B	2.69	1.49	1.43
23	A	404	PHO	CMB-C2B	-2.68	1.46	1.51
22	c	512	CLA	CMD-C2D	-2.68	1.45	1.50
22	b	604	CLA	C1B-C2B	2.68	1.49	1.43
27	b	623	LMG	C4-C5	2.68	1.58	1.53
22	B	611	CLA	MG-NC	-2.67	1.99	2.06
27	c	521	LMG	C7-C8	2.67	1.59	1.50
22	b	613	CLA	C1D-ND	2.67	1.41	1.37
22	C	511	CLA	CMB-C2B	-2.67	1.45	1.50
22	A	406	CLA	CMD-C2D	-2.66	1.45	1.50
24	k	101	BCR	C1-C6	-2.66	1.50	1.53
27	a	414	LMG	C1-C2	2.66	1.60	1.52
22	C	507	CLA	C1D-ND	2.66	1.41	1.37
26	D	406	PL9	C31-C29	-2.66	1.45	1.51
24	K	103	BCR	C1-C6	-2.66	1.50	1.53
22	B	614	CLA	CMC-C2C	-2.66	1.45	1.50
24	a	406	BCR	C38-C26	-2.66	1.46	1.50
22	C	509	CLA	C1B-C2B	2.65	1.49	1.43
22	B	613	CLA	CHC-C1C	2.65	1.43	1.38
22	a	403	CLA	C1D-ND	2.65	1.41	1.37
22	C	511	CLA	C3B-C4B	2.65	1.50	1.42
22	c	503	CLA	C1D-ND	2.64	1.41	1.37
27	c	519	LMG	O2-C2	-2.64	1.36	1.43
27	m	101	LMG	C4-C5	2.63	1.58	1.53
22	D	402	CLA	C4B-NB	2.63	1.41	1.37
22	c	508	CLA	MG-NC	-2.62	2.00	2.06
22	A	403	CLA	C1B-C2B	2.62	1.49	1.43
22	C	501	CLA	C3B-C4B	2.62	1.50	1.42
22	C	503	CLA	C4B-NB	2.62	1.41	1.37
22	b	611	CLA	C1D-ND	2.62	1.41	1.37
22	B	602	CLA	MG-ND	-2.62	2.00	2.05
22	c	501	CLA	CMD-C2D	-2.61	1.45	1.50
22	c	506	CLA	C1B-C2B	2.61	1.49	1.43
30	C	517	DGD	C6E-C5E	2.61	1.60	1.51
22	b	601	CLA	MG-ND	2.61	2.11	2.05
22	b	616	CLA	C3B-C4B	2.61	1.50	1.42
22	c	512	CLA	C4B-NB	2.60	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	c	519	LMG	C7-C8	2.60	1.58	1.50
22	b	605	CLA	C1B-C2B	2.60	1.49	1.43
22	B	604	CLA	C3B-C4B	2.60	1.50	1.42
22	C	501	CLA	C1B-C2B	2.59	1.49	1.43
29	A	413	LHG	O8-C23	2.59	1.40	1.33
22	C	511	CLA	CMC-C2C	-2.59	1.45	1.50
24	T	101	BCR	C27-C26	-2.58	1.46	1.51
22	b	606	CLA	CMB-C2B	-2.58	1.45	1.50
22	A	403	CLA	C4B-NB	2.58	1.41	1.37
22	C	502	CLA	C1D-ND	2.58	1.41	1.37
24	k	102	BCR	C1-C6	-2.58	1.50	1.53
22	a	403	CLA	C4B-NB	2.58	1.41	1.37
22	b	602	CLA	C1B-C2B	2.58	1.49	1.43
30	H	102	DGD	O2D-C2D	-2.58	1.36	1.43
22	D	404	CLA	CHC-C4B	-2.58	1.33	1.39
22	a	403	CLA	MG-NC	2.57	2.12	2.06
30	C	517	DGD	O1G-C1G	-2.57	1.39	1.45
24	K	103	BCR	C30-C25	-2.57	1.50	1.53
22	b	613	CLA	C4B-NB	2.56	1.41	1.37
22	b	607	CLA	C1B-C2B	2.56	1.49	1.43
22	c	508	CLA	C1B-C2B	2.56	1.49	1.43
22	d	403	CLA	CMB-C2B	-2.56	1.45	1.50
22	B	616	CLA	CMC-C2C	-2.56	1.45	1.50
22	A	406	CLA	CHC-C4B	-2.56	1.33	1.39
22	a	402	CLA	CMB-C2B	-2.56	1.45	1.50
24	k	101	BCR	C30-C25	-2.56	1.50	1.53
30	C	517	DGD	C3D-C2D	2.55	1.59	1.52
22	c	507	CLA	CMD-C2D	-2.55	1.45	1.50
22	d	403	CLA	CHC-C4B	-2.55	1.33	1.39
22	C	509	CLA	CMB-C2B	-2.54	1.45	1.50
22	C	513	CLA	CMC-C2C	-2.54	1.45	1.50
27	b	623	LMG	C4-C3	2.54	1.58	1.52
22	b	604	CLA	C1D-ND	2.54	1.41	1.37
22	B	613	CLA	C1B-C2B	2.54	1.49	1.43
22	b	613	CLA	CMD-C2D	-2.54	1.45	1.50
26	D	406	PL9	C26-C24	-2.54	1.46	1.51
22	a	403	CLA	C1B-C2B	2.54	1.49	1.43
22	C	504	CLA	O2D-CGD	2.54	1.39	1.33
23	a	404	PHO	CMD-C2D	-2.53	1.46	1.51
22	B	615	CLA	CMB-C2B	-2.53	1.45	1.50
22	C	501	CLA	CMD-C2D	-2.53	1.45	1.50
22	C	506	CLA	CMC-C2C	-2.53	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	101	HEM	C3B-C2B	-2.53	1.32	1.37
30	C	515	DGD	C4D-C3D	2.53	1.58	1.52
22	c	511	CLA	C3B-C4B	2.52	1.50	1.42
22	c	509	CLA	CHC-C1C	2.52	1.43	1.38
22	C	512	CLA	C1B-C2B	2.52	1.49	1.43
22	a	405	CLA	C1D-ND	2.52	1.41	1.37
22	b	611	CLA	C1B-NB	-2.52	1.34	1.37
22	b	601	CLA	CHC-C1C	2.52	1.43	1.38
22	C	504	CLA	C4B-NB	2.52	1.41	1.37
22	d	405	CLA	MG-NB	-2.52	2.00	2.05
22	B	608	CLA	C1B-NB	-2.51	1.34	1.37
22	C	502	CLA	C4B-NB	2.51	1.41	1.37
22	c	513	CLA	C3B-C4B	2.51	1.50	1.42
22	c	506	CLA	C3B-C4B	2.51	1.50	1.42
22	B	612	CLA	C3B-C4B	2.51	1.50	1.42
22	c	510	CLA	C1D-ND	2.51	1.41	1.37
22	C	507	CLA	C1B-NB	-2.51	1.34	1.37
22	C	513	CLA	C3B-C4B	2.50	1.50	1.42
22	B	605	CLA	C1B-NB	-2.50	1.34	1.37
22	b	607	CLA	C1D-ND	2.50	1.41	1.37
30	C	516	DGD	C4D-C5D	2.50	1.58	1.53
30	H	102	DGD	C1E-C2E	2.50	1.59	1.52
24	C	514	BCR	C33-C5	-2.50	1.47	1.50
22	B	613	CLA	O2D-CED	-2.49	1.39	1.45
22	c	502	CLA	CMD-C2D	-2.49	1.45	1.50
34	f	101	HEM	CAC-C3C	2.48	1.54	1.47
26	d	407	PL9	C53-C6	-2.48	1.45	1.50
22	b	610	CLA	C1B-C2B	2.48	1.49	1.43
30	c	517	DGD	O1G-C1G	-2.48	1.39	1.45
24	c	515	BCR	C33-C5	-2.48	1.47	1.50
22	c	503	CLA	CMB-C2B	-2.48	1.45	1.50
22	d	405	CLA	C3B-C4B	2.47	1.49	1.42
22	D	402	CLA	MG-ND	-2.47	2.00	2.05
22	b	612	CLA	C3B-C4B	2.47	1.49	1.42
28	A	412	SQD	O47-C45	-2.47	1.40	1.46
24	B	617	BCR	C33-C5	-2.46	1.47	1.50
22	c	513	CLA	C4B-NB	2.46	1.41	1.37
22	C	504	CLA	C3B-C4B	2.46	1.49	1.42
22	b	614	CLA	CHC-C1C	2.46	1.43	1.38
30	c	517	DGD	O2E-C2E	-2.46	1.36	1.43
22	A	402	CLA	MG-NA	2.46	2.12	2.06
23	A	404	PHO	C4D-CHA	2.46	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	MG-ND	-2.46	2.00	2.05
24	b	618	BCR	C1-C6	-2.46	1.50	1.53
30	h	103	DGD	C4D-C3D	2.46	1.58	1.52
22	c	509	CLA	MG-NB	-2.46	2.00	2.05
22	b	615	CLA	CMC-C2C	-2.46	1.45	1.50
22	b	611	CLA	CHC-C1C	2.46	1.43	1.38
22	B	601	CLA	CMB-C2B	-2.46	1.45	1.50
22	C	508	CLA	C4B-NB	2.46	1.41	1.37
22	B	607	CLA	CMD-C2D	-2.46	1.45	1.50
22	c	508	CLA	C3B-C4B	2.45	1.49	1.42
22	c	502	CLA	C1B-C2B	2.45	1.48	1.43
22	d	403	CLA	C3B-C4B	2.45	1.49	1.42
22	b	614	CLA	CMC-C2C	-2.45	1.45	1.50
22	B	613	CLA	C3B-C4B	2.45	1.49	1.42
22	B	615	CLA	C1D-ND	2.45	1.41	1.37
22	C	502	CLA	C3B-C4B	2.45	1.49	1.42
24	t	101	BCR	C30-C25	-2.44	1.50	1.53
22	b	605	CLA	C4B-NB	2.44	1.41	1.37
22	a	405	CLA	C4B-NB	2.44	1.41	1.37
22	C	504	CLA	MG-NB	2.44	2.10	2.05
27	b	623	LMG	C3-C2	2.44	1.58	1.52
35	v	201	HEC	FE-NC	2.44	2.03	1.95
22	C	502	CLA	CHC-C1C	2.44	1.43	1.38
22	B	605	CLA	C3B-C4B	2.44	1.49	1.42
30	C	515	DGD	C1G-C2G	2.44	1.58	1.50
22	b	603	CLA	C1B-C2B	2.44	1.48	1.43
22	c	513	CLA	C1B-C2B	2.44	1.48	1.43
22	b	615	CLA	C3B-C4B	2.43	1.49	1.42
22	B	615	CLA	O2D-CGD	2.43	1.39	1.33
22	B	612	CLA	C1C-NC	-2.43	1.34	1.37
22	B	613	CLA	CMD-C2D	-2.43	1.45	1.50
22	b	614	CLA	O2D-CGD	2.43	1.39	1.33
22	C	513	CLA	CMB-C2B	-2.43	1.45	1.50
27	m	101	LMG	C1-C2	2.43	1.59	1.52
34	f	101	HEM	CMA-C3A	2.42	1.55	1.50
30	C	515	DGD	O1G-C1A	2.42	1.40	1.33
22	c	503	CLA	C4B-NB	2.42	1.41	1.37
23	d	401	PHO	CAC-C3C	-2.42	1.47	1.51
22	D	402	CLA	CMB-C2B	-2.42	1.45	1.50
22	B	603	CLA	C3B-C4B	2.42	1.49	1.42
22	C	503	CLA	CHC-C4B	-2.42	1.34	1.39
27	c	521	LMG	O6-C1	2.42	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	605	CLA	C3B-C4B	2.42	1.49	1.42
22	b	608	CLA	C3B-C4B	2.42	1.49	1.42
22	b	601	CLA	O2A-CGA	2.42	1.40	1.33
22	B	614	CLA	C4B-NB	2.42	1.41	1.37
22	B	603	CLA	MG-NA	2.42	2.12	2.06
22	d	404	CLA	CMB-C2B	-2.41	1.45	1.50
22	D	404	CLA	CMC-C2C	-2.41	1.45	1.50
27	a	414	LMG	O1-C7	-2.41	1.39	1.43
22	d	405	CLA	CHC-C4B	-2.41	1.34	1.39
22	A	402	CLA	C1D-ND	2.41	1.41	1.37
22	b	612	CLA	C4B-NB	2.40	1.41	1.37
22	B	608	CLA	C1D-ND	2.40	1.41	1.37
26	d	407	PL9	C30-C29	-2.40	1.44	1.50
22	b	605	CLA	CMD-C2D	-2.40	1.45	1.50
22	c	502	CLA	CHC-C1C	2.40	1.43	1.38
22	c	503	CLA	MG-NC	2.40	2.12	2.06
22	C	512	CLA	C3B-C4B	2.39	1.49	1.42
22	a	402	CLA	C3B-C4B	2.39	1.49	1.42
22	c	503	CLA	C1B-C2B	2.39	1.48	1.43
30	c	518	DGD	C2A-C1A	-2.39	1.43	1.50
22	B	612	CLA	C1B-NB	-2.38	1.34	1.37
22	C	504	CLA	C1B-C2B	2.38	1.48	1.43
22	b	615	CLA	MG-ND	-2.38	2.01	2.05
22	C	501	CLA	CMC-C2C	-2.38	1.45	1.50
22	C	510	CLA	CMD-C2D	-2.38	1.45	1.50
22	B	608	CLA	C3C-C2C	2.38	1.41	1.36
29	e	101	LHG	C3-C2	2.38	1.59	1.51
22	c	501	CLA	CMC-C2C	-2.37	1.45	1.50
27	m	101	LMG	C9-C8	2.37	1.58	1.50
22	D	402	CLA	C1B-C2B	2.37	1.48	1.43
22	C	508	CLA	C1D-ND	2.37	1.41	1.37
22	B	605	CLA	O2D-CED	-2.37	1.40	1.45
22	c	504	CLA	C1B-C2B	2.37	1.48	1.43
22	b	614	CLA	CMB-C2B	-2.36	1.45	1.50
29	D	411	LHG	C24-C23	2.36	1.57	1.50
22	B	603	CLA	CMB-C2B	-2.36	1.45	1.50
34	f	101	HEM	CAB-C3B	2.36	1.53	1.47
23	a	404	PHO	C4D-CHA	2.36	1.43	1.39
22	b	604	CLA	C3B-C4B	2.36	1.49	1.42
22	B	606	CLA	CMB-C2B	-2.36	1.45	1.50
34	F	101	HEM	CAB-C3B	2.36	1.53	1.47
29	L	101	LHG	O7-C5	-2.35	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	513	CLA	CMD-C2D	-2.35	1.45	1.50
22	b	616	CLA	CMB-C2B	-2.35	1.46	1.50
22	A	406	CLA	CMA-C3A	-2.35	1.48	1.53
22	b	606	CLA	CHC-C4B	-2.35	1.34	1.39
22	B	614	CLA	CHC-C1C	2.35	1.43	1.38
22	C	506	CLA	CHC-C1C	2.35	1.43	1.38
22	b	612	CLA	C1B-NB	-2.34	1.34	1.37
22	C	512	CLA	CMD-C2D	-2.34	1.46	1.50
22	B	611	CLA	C1D-ND	2.34	1.40	1.37
27	Y	101	LMG	O8-C9	-2.34	1.39	1.45
22	c	505	CLA	C4B-NB	2.34	1.40	1.37
34	F	101	HEM	C2A-C3A	-2.34	1.32	1.38
22	B	605	CLA	CMD-C2D	-2.34	1.46	1.50
22	B	609	CLA	C1D-ND	2.34	1.40	1.37
22	a	403	CLA	CHC-C1C	2.33	1.43	1.38
22	b	612	CLA	CMB-C2B	-2.33	1.46	1.50
22	C	509	CLA	C1B-NB	-2.33	1.34	1.37
22	c	501	CLA	C1B-C2B	2.32	1.48	1.43
22	B	605	CLA	CMC-C2C	-2.32	1.46	1.50
22	B	608	CLA	CMD-C2D	-2.32	1.46	1.50
28	B	621	SQD	O2-C2	-2.32	1.37	1.43
22	B	606	CLA	CHC-C1C	2.32	1.43	1.38
22	c	503	CLA	CMD-C2D	-2.32	1.46	1.50
22	B	616	CLA	MG-ND	2.32	2.10	2.05
22	C	508	CLA	C1D-C2D	2.31	1.49	1.45
22	C	507	CLA	C3B-C4B	2.31	1.49	1.42
22	b	613	CLA	CAA-C2A	-2.31	1.49	1.54
22	B	616	CLA	CMD-C2D	-2.31	1.46	1.50
27	m	101	LMG	C4-C3	2.31	1.58	1.52
22	B	602	CLA	CMB-C2B	-2.31	1.46	1.50
22	b	603	CLA	C1D-ND	2.31	1.40	1.37
24	k	101	BCR	C33-C5	-2.31	1.47	1.50
22	B	601	CLA	C3B-C4B	2.30	1.49	1.42
22	c	505	CLA	CHC-C1C	2.30	1.43	1.38
28	A	412	SQD	O3-C3	-2.30	1.37	1.43
34	F	101	HEM	CAC-C3C	2.30	1.53	1.47
28	f	102	SQD	O2-C2	-2.30	1.37	1.43
22	D	402	CLA	CHC-C1C	2.30	1.43	1.38
29	D	411	LHG	O7-C5	-2.30	1.41	1.46
22	B	608	CLA	CHC-C4B	-2.30	1.34	1.39
22	b	609	CLA	C3B-C4B	2.30	1.49	1.42
22	B	611	CLA	C4B-NB	2.29	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	408	LHG	O8-C6	-2.29	1.40	1.45
30	c	517	DGD	O6E-C5E	2.29	1.50	1.44
22	b	604	CLA	CMC-C2C	-2.29	1.46	1.50
22	c	508	CLA	CMC-C2C	-2.29	1.46	1.50
22	b	603	CLA	C1B-NB	-2.29	1.34	1.37
22	c	508	CLA	CMD-C2D	-2.29	1.46	1.50
22	B	615	CLA	C1B-NB	-2.28	1.34	1.37
29	D	409	LHG	O3-C3	-2.28	1.36	1.44
22	b	611	CLA	MG-NB	2.28	2.10	2.05
22	c	513	CLA	CMC-C2C	-2.28	1.46	1.50
22	b	603	CLA	CMB-C2B	-2.27	1.46	1.50
22	C	503	CLA	C1D-ND	2.27	1.40	1.37
26	A	410	PL9	C31-C29	-2.27	1.46	1.51
22	b	602	CLA	MG-NC	-2.27	2.00	2.06
22	B	607	CLA	C1B-NB	-2.27	1.34	1.37
22	b	606	CLA	C3B-C4B	2.27	1.49	1.42
22	B	601	CLA	CMC-C2C	-2.27	1.46	1.50
34	F	101	HEM	FE-ND	2.27	2.01	1.94
22	a	405	CLA	C3B-C4B	2.27	1.49	1.42
22	b	602	CLA	CHC-C4B	-2.27	1.34	1.39
22	C	504	CLA	CMD-C2D	-2.26	1.46	1.50
22	B	605	CLA	MG-ND	2.26	2.10	2.05
23	A	405	PHO	CAC-C3C	-2.26	1.47	1.51
22	b	601	CLA	C1D-C2D	2.26	1.49	1.45
22	b	609	CLA	O2D-CGD	2.26	1.38	1.33
22	c	512	CLA	C1B-NB	-2.26	1.34	1.37
22	C	510	CLA	C1B-C2B	2.26	1.48	1.43
22	c	511	CLA	C3D-C4D	2.26	1.49	1.44
22	C	509	CLA	C3B-C4B	2.26	1.49	1.42
22	B	606	CLA	CMC-C2C	-2.26	1.46	1.50
23	d	401	PHO	CMB-C2B	-2.26	1.47	1.51
23	A	404	PHO	CHA-CBD	-2.25	1.49	1.51
22	c	506	CLA	CMC-C2C	-2.25	1.46	1.50
22	B	610	CLA	C3B-C4B	2.25	1.49	1.42
30	c	517	DGD	O3D-C3D	-2.25	1.37	1.43
22	b	605	CLA	CHC-C4B	-2.25	1.34	1.39
22	c	506	CLA	MG-ND	-2.25	2.01	2.05
22	b	612	CLA	C1D-ND	2.25	1.40	1.37
30	H	102	DGD	C4E-C3E	2.25	1.58	1.52
22	B	613	CLA	MG-NA	2.25	2.11	2.06
23	d	401	PHO	C4D-CHA	2.25	1.42	1.39
30	C	515	DGD	O3G-C1D	-2.24	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	608	CLA	C4B-NB	2.24	1.40	1.37
22	c	507	CLA	C4B-NB	2.24	1.40	1.37
22	b	608	CLA	C1B-C2B	2.24	1.48	1.43
22	b	614	CLA	C1A-CHA	-2.24	1.33	1.43
27	a	414	LMG	O7-C8	-2.24	1.41	1.46
22	C	503	CLA	CMB-C2B	-2.24	1.46	1.50
22	b	616	CLA	CMC-C2C	-2.24	1.46	1.50
22	B	603	CLA	O2D-CED	-2.24	1.40	1.45
22	b	610	CLA	CMD-C2D	-2.24	1.46	1.50
22	C	501	CLA	C1D-C2D	2.23	1.49	1.45
22	c	511	CLA	C1D-ND	2.23	1.40	1.37
22	c	501	CLA	C1B-NB	-2.23	1.34	1.37
22	B	613	CLA	CMC-C2C	-2.23	1.46	1.50
24	t	101	BCR	C5-C6	2.23	1.38	1.34
30	c	518	DGD	O6D-C5D	-2.23	1.38	1.44
22	A	403	CLA	MG-ND	2.23	2.10	2.05
22	c	505	CLA	C3B-C4B	2.23	1.49	1.42
30	C	516	DGD	O3D-C3D	-2.23	1.37	1.43
32	B	623	STE	C2-C1	2.23	1.55	1.50
32	D	413	STE	O1-C1	2.22	1.29	1.22
22	C	510	CLA	O2D-CED	-2.22	1.40	1.45
22	D	403	CLA	CMD-C2D	-2.22	1.46	1.50
22	C	503	CLA	C3B-C4B	2.22	1.49	1.42
22	d	404	CLA	C1B-NB	-2.22	1.34	1.37
26	D	406	PL9	C53-C6	-2.22	1.46	1.50
22	c	505	CLA	CMC-C2C	-2.22	1.46	1.50
22	c	503	CLA	C3D-C4D	2.22	1.49	1.44
24	a	406	BCR	C33-C5	-2.21	1.47	1.50
22	b	603	CLA	C4B-NB	2.21	1.40	1.37
27	b	623	LMG	O6-C1	2.21	1.47	1.41
32	D	412	STE	C2-C1	2.21	1.55	1.50
22	c	509	CLA	C1B-NB	-2.21	1.35	1.37
22	C	501	CLA	CHC-C1C	2.21	1.42	1.38
22	A	402	CLA	C3B-C4B	2.21	1.49	1.42
22	b	611	CLA	CMD-C2D	-2.20	1.46	1.50
32	B	627	STE	C2-C1	2.20	1.55	1.50
27	c	521	LMG	C4-C3	2.20	1.58	1.52
22	c	504	CLA	C3B-C4B	2.20	1.49	1.42
22	c	506	CLA	C1B-NB	-2.20	1.35	1.37
23	a	404	PHO	C3D-CAD	-2.20	1.43	1.47
22	C	504	CLA	CHC-C1C	2.20	1.42	1.38
30	h	103	DGD	O5D-C6D	2.20	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	606	CLA	CAB-C3B	-2.20	1.41	1.47
24	B	618	BCR	C33-C5	-2.19	1.47	1.50
22	b	609	CLA	C3D-C4D	2.19	1.49	1.44
35	V	201	HEC	C2A-C3A	-2.19	1.32	1.36
32	E	101	STE	C2-C1	2.19	1.55	1.50
22	a	405	CLA	MG-ND	-2.19	2.01	2.05
22	C	503	CLA	CMC-C2C	-2.19	1.46	1.50
22	b	602	CLA	CMB-C2B	-2.19	1.46	1.50
22	b	612	CLA	C1B-C2B	2.19	1.48	1.43
23	A	405	PHO	C1D-C2D	2.19	1.42	1.39
28	a	411	SQD	O3-C3	-2.18	1.37	1.43
22	c	504	CLA	CMD-C2D	-2.18	1.46	1.50
22	D	403	CLA	C4B-NB	2.18	1.40	1.37
22	B	610	CLA	C3D-C4D	2.18	1.49	1.44
22	b	607	CLA	C4B-NB	2.18	1.40	1.37
29	a	410	LHG	P-O4	-2.17	1.45	1.55
22	C	503	CLA	C1D-C2D	2.17	1.49	1.45
22	b	615	CLA	CMB-C2B	-2.17	1.46	1.50
30	c	516	DGD	C4D-C5D	2.17	1.57	1.53
28	f	102	SQD	O3-C3	-2.17	1.37	1.43
22	B	613	CLA	C1B-NB	-2.17	1.35	1.37
22	D	402	CLA	C3B-C4B	2.17	1.49	1.42
22	b	607	CLA	C1B-NB	-2.17	1.35	1.37
22	B	603	CLA	MG-NB	-2.16	2.01	2.05
22	C	505	CLA	MG-NB	-2.16	2.01	2.05
23	A	405	PHO	CMC-C2C	-2.16	1.47	1.50
22	D	404	CLA	C3B-C4B	2.16	1.49	1.42
29	e	101	LHG	P-O3	2.16	1.67	1.59
26	A	410	PL9	C53-C6	-2.16	1.46	1.50
30	C	516	DGD	C4D-C3D	2.16	1.57	1.52
22	B	602	CLA	C3B-C4B	2.16	1.49	1.42
22	C	513	CLA	CMD-C2D	-2.16	1.46	1.50
22	C	505	CLA	C3B-C4B	2.16	1.49	1.42
30	C	515	DGD	C3E-C2E	2.16	1.57	1.52
22	c	504	CLA	MG-NC	2.16	2.11	2.06
34	f	101	HEM	CMB-C2B	2.16	1.55	1.50
22	b	614	CLA	C3B-C4B	2.15	1.49	1.42
22	c	504	CLA	MG-NB	-2.15	2.01	2.05
22	C	509	CLA	C4B-NB	2.15	1.40	1.37
22	C	509	CLA	CMC-C2C	-2.15	1.46	1.50
22	b	615	CLA	CHC-C1C	2.15	1.42	1.38
28	a	411	SQD	O47-C7	2.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	503	CLA	CMC-C2C	-2.15	1.46	1.50
22	c	510	CLA	C5-C3	-2.15	1.46	1.51
22	b	607	CLA	C3B-C4B	2.15	1.49	1.42
22	c	504	CLA	CMB-C2B	-2.15	1.46	1.50
30	h	103	DGD	O3E-C3E	-2.15	1.37	1.43
22	C	513	CLA	C4B-NB	2.14	1.40	1.37
30	A	415	DGD	C4D-C5D	2.14	1.57	1.53
22	b	601	CLA	C3B-C4B	2.14	1.49	1.42
22	c	501	CLA	MG-ND	-2.14	2.01	2.05
22	b	608	CLA	MG-NB	2.14	2.10	2.05
22	B	604	CLA	C1B-C2B	2.14	1.48	1.43
22	C	509	CLA	O2D-CGD	2.14	1.38	1.33
27	c	519	LMG	C4-C3	2.14	1.57	1.52
24	K	101	BCR	C33-C5	-2.14	1.47	1.50
22	d	403	CLA	C4B-NB	2.14	1.40	1.37
23	d	401	PHO	C1D-ND	2.14	1.42	1.38
22	B	616	CLA	CAC-C3C	-2.14	1.45	1.51
22	C	512	CLA	CHC-C1C	2.13	1.42	1.38
34	f	101	HEM	FE-NB	2.13	2.01	1.94
22	b	606	CLA	CMD-C2D	-2.13	1.46	1.50
22	c	510	CLA	C3B-C4B	2.13	1.49	1.42
23	a	404	PHO	CMB-C2B	-2.13	1.47	1.51
22	A	402	CLA	C5-C3	-2.13	1.46	1.51
27	a	414	LMG	O8-C9	-2.13	1.40	1.45
30	C	517	DGD	C4E-C3E	2.13	1.57	1.52
26	a	409	PL9	C53-C6	-2.13	1.46	1.50
22	b	604	CLA	C3D-C4D	2.13	1.49	1.44
22	B	604	CLA	O2A-CGA	2.13	1.39	1.33
22	C	510	CLA	MG-NA	2.13	2.11	2.06
22	b	615	CLA	CAC-C3C	-2.13	1.45	1.51
22	c	502	CLA	CMC-C2C	-2.13	1.46	1.50
30	C	516	DGD	O2G-C2G	-2.13	1.41	1.46
22	a	405	CLA	CMB-C2B	-2.12	1.46	1.50
27	d	410	LMG	O1-C7	-2.12	1.40	1.43
22	B	607	CLA	C3B-C4B	2.12	1.48	1.42
22	c	505	CLA	C1B-C2B	2.12	1.48	1.43
22	b	607	CLA	MG-NA	2.12	2.11	2.06
22	b	607	CLA	O2D-CED	-2.12	1.40	1.45
22	B	607	CLA	C1B-C2B	2.12	1.48	1.43
34	F	101	HEM	C3C-C2C	-2.12	1.32	1.37
22	B	611	CLA	CMD-C2D	-2.11	1.46	1.50
22	c	507	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	609	CLA	C3B-C4B	2.11	1.48	1.42
22	c	504	CLA	CMC-C2C	-2.11	1.46	1.50
22	b	607	CLA	C1A-CHA	-2.11	1.34	1.43
23	a	404	PHO	O2D-CGD	2.11	1.38	1.33
22	B	616	CLA	CMB-C2B	-2.11	1.46	1.50
22	C	513	CLA	CHC-C4B	-2.11	1.34	1.39
22	b	611	CLA	CMB-C2B	-2.11	1.46	1.50
32	j	101	STE	C2-C1	2.11	1.55	1.50
27	c	521	LMG	O7-C8	-2.10	1.41	1.46
22	b	615	CLA	C1D-ND	2.10	1.40	1.37
22	B	602	CLA	MG-NA	2.10	2.11	2.06
22	B	609	CLA	CMD-C2D	-2.10	1.46	1.50
22	B	603	CLA	C1B-NB	-2.10	1.35	1.37
30	h	103	DGD	O2E-C2E	-2.10	1.37	1.43
22	d	405	CLA	CMC-C2C	-2.10	1.46	1.50
32	M	102	STE	O1-C1	2.10	1.28	1.22
22	c	513	CLA	C1D-ND	2.09	1.40	1.37
34	F	101	HEM	C3B-C2B	-2.09	1.32	1.37
30	H	102	DGD	O6D-C5D	-2.09	1.39	1.44
22	c	512	CLA	MG-NC	2.09	2.11	2.06
22	c	510	CLA	C1B-NB	-2.09	1.35	1.37
24	K	103	BCR	C38-C26	-2.09	1.47	1.50
22	A	403	CLA	CAA-C2A	-2.09	1.50	1.54
22	b	604	CLA	C1D-C2D	2.08	1.49	1.45
22	B	605	CLA	CAA-C2A	-2.08	1.50	1.54
30	h	103	DGD	C1E-C2E	2.08	1.58	1.52
24	K	103	BCR	C27-C26	-2.08	1.47	1.51
22	B	610	CLA	CMC-C2C	-2.08	1.46	1.50
22	C	510	CLA	O2A-CGA	2.08	1.39	1.33
29	D	409	LHG	P-O4	-2.08	1.45	1.55
22	b	613	CLA	CMC-C2C	-2.08	1.46	1.50
26	D	406	PL9	C6-C1	-2.08	1.45	1.48
22	a	403	CLA	C3B-C4B	2.08	1.48	1.42
22	c	502	CLA	O2D-CGD	2.08	1.38	1.33
30	A	415	DGD	C3G-C2G	2.08	1.57	1.50
28	F	102	SQD	O4-C4	-2.08	1.37	1.43
30	c	517	DGD	O6D-C5D	-2.08	1.39	1.44
30	c	517	DGD	C6E-C5E	2.07	1.58	1.51
23	A	404	PHO	C3D-CAD	-2.07	1.43	1.47
22	C	505	CLA	CMC-C2C	-2.07	1.46	1.50
22	D	404	CLA	MG-ND	-2.07	2.01	2.05
22	c	505	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	517	DGD	O3D-C3D	-2.07	1.37	1.43
22	B	605	CLA	C5-C3	-2.07	1.47	1.51
24	c	515	BCR	C36-C18	-2.07	1.46	1.50
22	b	616	CLA	MG-ND	-2.06	2.01	2.05
22	c	512	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	612	CLA	MG-NA	2.06	2.11	2.06
22	B	601	CLA	MG-ND	-2.06	2.01	2.05
22	B	604	CLA	CMD-C2D	-2.06	1.46	1.50
22	C	501	CLA	CMB-C2B	-2.06	1.46	1.50
22	C	507	CLA	MG-NC	-2.06	2.01	2.06
22	B	610	CLA	C1B-C2B	2.06	1.48	1.43
22	C	507	CLA	C4D-CHA	2.06	1.45	1.38
30	c	518	DGD	O2G-C2G	-2.06	1.41	1.46
30	c	516	DGD	O3D-C3D	-2.05	1.37	1.43
22	b	614	CLA	C1B-NB	-2.05	1.35	1.37
32	c	520	STE	C2-C1	2.05	1.55	1.50
22	B	607	CLA	C1D-ND	2.05	1.40	1.37
22	b	611	CLA	O2D-CED	-2.05	1.40	1.45
22	b	608	CLA	C3D-C4D	2.05	1.48	1.44
22	b	609	CLA	C1A-CHA	-2.05	1.34	1.43
22	C	503	CLA	CHC-C1C	2.05	1.42	1.38
22	b	608	CLA	CMC-C2C	-2.05	1.46	1.50
22	C	502	CLA	CMD-C2D	-2.05	1.46	1.50
22	b	609	CLA	MG-NC	2.04	2.11	2.06
22	b	616	CLA	CAC-C3C	-2.04	1.45	1.51
22	C	507	CLA	CMC-C2C	-2.04	1.46	1.50
22	B	608	CLA	CMB-C2B	-2.04	1.46	1.50
26	d	407	PL9	C11-C9	-2.04	1.47	1.51
22	C	513	CLA	CHC-C1C	2.04	1.42	1.38
22	B	608	CLA	C1D-C2D	2.04	1.49	1.45
22	B	614	CLA	C1B-NB	-2.04	1.35	1.37
22	c	509	CLA	O2D-CED	-2.04	1.40	1.45
29	d	409	LHG	C9-C8	2.03	1.59	1.52
32	b	624	STE	C2-C1	2.03	1.55	1.50
22	B	602	CLA	CMD-C2D	-2.03	1.46	1.50
22	b	615	CLA	C1B-C2B	2.03	1.47	1.43
30	C	515	DGD	C2A-C1A	-2.03	1.44	1.50
22	c	509	CLA	MG-ND	2.03	2.09	2.05
22	B	606	CLA	C1B-C2B	2.03	1.47	1.43
22	A	406	CLA	C1B-C2B	2.03	1.47	1.43
22	C	506	CLA	C3D-C4D	2.03	1.48	1.44
35	v	201	HEC	CAB-C3B	2.03	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	406	CLA	CMB-C2B	-2.03	1.46	1.50
22	C	508	CLA	CMC-C2C	-2.03	1.46	1.50
27	D	410	LMG	C30-C29	2.02	1.59	1.52
22	D	404	CLA	C1B-NB	-2.02	1.35	1.37
24	B	618	BCR	C1-C6	-2.02	1.51	1.53
22	c	512	CLA	C3B-C4B	2.02	1.48	1.42
22	b	613	CLA	MG-NB	2.02	2.09	2.05
22	a	403	CLA	MG-NA	2.02	2.11	2.06
22	b	609	CLA	CHC-C1C	2.02	1.42	1.38
22	c	510	CLA	CHC-C1C	2.02	1.42	1.38
22	B	616	CLA	C1B-NB	-2.01	1.35	1.37
22	D	404	CLA	O2D-CED	-2.01	1.40	1.45
22	C	502	CLA	MG-NB	-2.01	2.01	2.05
24	t	101	BCR	C27-C26	-2.01	1.47	1.51
30	c	516	DGD	C6D-C5D	2.01	1.57	1.51
22	B	616	CLA	C3B-C4B	2.01	1.48	1.42
22	b	602	CLA	CAC-C3C	-2.01	1.45	1.51
22	b	604	CLA	CHC-C1C	2.01	1.42	1.38
24	k	101	BCR	C36-C18	-2.01	1.46	1.50
23	A	404	PHO	O2D-CGD	2.01	1.38	1.33
22	b	603	CLA	C3B-C4B	2.01	1.48	1.42
34	f	101	HEM	CMC-C2C	2.01	1.54	1.50
22	c	503	CLA	CHC-C1C	2.01	1.42	1.38
22	B	603	CLA	C1B-C2B	2.01	1.47	1.43
22	b	602	CLA	C3B-C4B	2.01	1.48	1.42
22	B	601	CLA	C1D-C2D	2.01	1.49	1.45

All (1223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	620	SQD	O6-C1-C2	10.28	123.88	108.27
28	a	411	SQD	O6-C1-C2	9.94	123.37	108.27
22	c	509	CLA	C4A-NA-C1A	8.90	110.74	106.68
22	C	507	CLA	C4A-NA-C1A	8.48	110.55	106.68
22	b	611	CLA	C4A-NA-C1A	8.26	110.45	106.68
22	d	404	CLA	C4A-NA-C1A	8.17	110.41	106.68
22	B	604	CLA	C4A-NA-C1A	8.04	110.35	106.68
22	B	616	CLA	C4A-NA-C1A	8.03	110.34	106.68
22	C	511	CLA	C4A-NA-C1A	7.90	110.28	106.68
22	b	604	CLA	C4A-NA-C1A	7.61	110.15	106.68
26	a	409	PL9	C7-C3-C4	7.56	123.14	116.91
22	c	511	CLA	C4A-NA-C1A	7.53	110.12	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	D	403	CLA	C4A-NA-C1A	7.33	110.02	106.68
28	A	412	SQD	O6-C1-C2	7.07	119.01	108.27
22	c	501	CLA	C4A-NA-C1A	6.94	109.84	106.68
22	B	601	CLA	C4A-NA-C1A	6.86	109.81	106.68
22	C	508	CLA	C4A-NA-C1A	6.76	109.76	106.68
22	B	605	CLA	C4A-NA-C1A	6.70	109.73	106.68
22	B	609	CLA	C4A-NA-C1A	6.65	109.71	106.68
22	c	503	CLA	C4A-NA-C1A	6.64	109.71	106.68
22	C	513	CLA	C4A-NA-C1A	6.59	109.68	106.68
22	a	403	CLA	C4A-NA-C1A	6.55	109.67	106.68
26	a	409	PL9	C7-C3-C2	-6.52	115.70	123.39
22	B	606	CLA	C4A-NA-C1A	6.42	109.61	106.68
22	C	501	CLA	C4A-NA-C1A	6.40	109.60	106.68
22	C	503	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	b	601	CLA	C4A-NA-C1A	6.30	109.55	106.68
22	c	510	CLA	C4A-NA-C1A	6.23	109.52	106.68
22	B	607	CLA	C4A-NA-C1A	6.20	109.51	106.68
28	b	620	SQD	O7-S-C6	6.20	116.01	106.76
27	b	623	LMG	O1-C1-C2	-6.17	98.90	108.27
22	c	502	CLA	C4A-NA-C1A	6.17	109.49	106.68
28	f	102	SQD	O9-S-C6	6.17	115.96	106.76
26	d	407	PL9	C7-C3-C4	6.14	121.97	116.91
22	b	606	CLA	C4A-NA-C1A	6.06	109.44	106.68
23	a	404	PHO	C4D-CHA-CBD	-5.95	105.60	108.45
28	B	621	SQD	O6-C1-C2	5.94	117.30	108.27
22	C	505	CLA	C4A-NA-C1A	5.88	109.36	106.68
28	a	412	SQD	O47-C7-C8	5.87	124.19	111.48
22	b	615	CLA	C4A-NA-C1A	5.85	109.35	106.68
22	A	402	CLA	C4A-NA-C1A	5.74	109.30	106.68
22	B	615	CLA	C4A-NA-C1A	5.67	109.27	106.68
28	a	411	SQD	O9-S-C6	5.66	115.21	106.76
22	c	507	CLA	C4A-NA-C1A	5.64	109.25	106.68
23	A	404	PHO	C4D-CHA-CBD	-5.61	105.76	108.45
22	B	610	CLA	C4A-NA-C1A	5.60	109.23	106.68
22	B	612	CLA	C4A-NA-C1A	5.60	109.23	106.68
22	D	402	CLA	C4A-NA-C1A	5.51	109.19	106.68
22	b	602	CLA	C4A-NA-C1A	5.41	109.14	106.68
28	F	102	SQD	O6-C1-C2	5.40	116.47	108.27
22	b	616	CLA	C4A-NA-C1A	5.38	109.13	106.68
22	a	402	CLA	C4A-NA-C1A	5.34	109.12	106.68
22	B	613	CLA	C4A-NA-C1A	5.28	109.09	106.68
22	b	605	CLA	C4A-NA-C1A	5.28	109.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	406	CLA	C4A-NA-C1A	5.27	109.08	106.68
22	b	613	CLA	C4A-NA-C1A	5.18	109.04	106.68
30	H	102	DGD	O3G-C3G-C2G	-5.18	98.21	110.82
22	a	405	CLA	C4A-NA-C1A	5.15	109.03	106.68
22	C	509	CLA	C4A-NA-C1A	5.13	109.02	106.68
22	b	615	CLA	C3B-C4B-NB	-5.05	106.02	110.53
26	D	406	PL9	C7-C3-C4	5.05	121.07	116.91
22	c	501	CLA	O2D-CGD-O1D	-5.02	114.08	123.85
30	o	301	DGD	O3G-C3G-C2G	-5.01	98.89	111.77
22	c	512	CLA	C4A-NA-C1A	4.95	108.94	106.68
22	B	602	CLA	C4A-NA-C1A	4.94	108.93	106.68
22	b	603	CLA	C4A-NA-C1A	4.89	108.91	106.68
26	d	407	PL9	C40-C39-C41	4.88	123.69	115.23
28	f	102	SQD	O6-C1-C2	4.83	115.61	108.27
35	V	201	HEC	C1D-ND-C4D	4.81	110.90	105.21
23	d	401	PHO	C4D-CHA-CBD	-4.74	106.18	108.45
28	F	102	SQD	O9-S-C6	4.68	113.75	106.76
34	f	101	HEM	CBD-CAD-C3D	-4.66	99.64	112.53
35	v	201	HEC	C1D-ND-C4D	4.66	110.73	105.21
23	d	401	PHO	O1D-CGD-CBD	4.63	131.74	124.72
23	A	405	PHO	C4D-CHA-CBD	-4.62	106.24	108.45
24	b	617	BCR	C2-C1-C6	4.59	117.10	110.44
27	b	623	LMG	C1-O6-C5	-4.54	104.86	113.72
22	b	616	CLA	O2D-CGD-O1D	-4.53	115.03	123.85
28	b	620	SQD	C1-C2-C3	-4.49	100.56	110.01
22	B	610	CLA	O2D-CGD-O1D	-4.48	115.12	123.85
22	b	611	CLA	O2D-CGD-O1D	-4.44	115.20	123.85
22	c	508	CLA	C4A-NA-C1A	4.44	108.70	106.68
22	B	613	CLA	C1-C2-C3	-4.43	118.93	126.20
23	a	404	PHO	CMB-C2B-C3B	4.43	133.54	124.68
29	A	413	LHG	O4-P-O5	4.42	133.01	112.44
28	F	102	SQD	C44-O6-C1	4.41	121.21	113.68
29	L	101	LHG	O4-P-O5	4.38	132.82	112.44
23	A	405	PHO	C2B-C1B-NB	-4.34	106.29	109.43
30	C	516	DGD	O3G-C3G-C2G	-4.34	100.27	110.82
28	a	411	SQD	C1-O5-C5	-4.32	105.28	113.72
28	B	621	SQD	O47-C7-C8	4.30	120.79	111.48
28	A	414	SQD	C45-O47-C7	4.29	123.97	117.78
28	a	411	SQD	O47-C7-O49	-4.28	113.69	123.70
29	e	101	LHG	O4-P-O5	4.28	132.37	112.44
29	D	409	LHG	O4-P-O5	4.27	132.31	112.44
28	f	102	SQD	O9-S-O7	-4.27	99.94	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	620	SQD	O48-C23-C24	4.27	124.85	111.83
22	b	616	CLA	O1D-CGD-CBD	4.16	132.72	124.52
29	a	410	LHG	O8-C23-C24	4.15	124.50	111.83
30	c	518	DGD	O3G-C3G-C2G	-4.13	100.77	110.82
22	D	404	CLA	C4A-NA-C1A	4.13	108.56	106.68
29	d	408	LHG	O4-P-O5	4.12	131.63	112.44
22	B	614	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
30	C	515	DGD	O6D-C1D-O3G	-4.10	100.36	110.04
28	B	621	SQD	C1-O5-C5	-4.10	105.72	113.72
28	b	620	SQD	O9-S-O7	-4.09	100.53	113.82
26	d	407	PL9	C7-C3-C2	-4.07	118.59	123.39
22	b	605	CLA	C1-C2-C3	-4.07	119.53	126.20
29	D	408	LHG	O4-P-O5	4.06	131.33	112.44
22	b	613	CLA	CMB-C2B-C1B	-4.05	119.25	125.42
32	m	102	STE	O2-C1-C2	4.04	126.78	114.00
28	A	412	SQD	C1-C2-C3	-4.04	101.51	110.01
28	a	412	SQD	C46-C45-C44	-4.02	102.51	111.80
24	B	619	BCR	C2-C1-C6	4.01	116.27	110.44
28	A	412	SQD	O47-C7-O49	-4.01	114.33	123.70
22	B	603	CLA	C3B-C4B-NB	-4.00	106.96	110.53
22	c	505	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
22	A	406	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
22	B	601	CLA	CAA-CBA-CGA	-3.99	101.88	113.21
22	b	605	CLA	O2D-CGD-O1D	-3.99	116.09	123.85
30	C	517	DGD	O3G-C3G-C2G	-3.98	101.13	110.82
29	a	410	LHG	O4-P-O5	3.97	130.91	112.44
28	B	621	SQD	O5-C5-C4	3.97	116.85	109.70
27	d	410	LMG	O1-C1-C2	-3.96	102.26	108.27
22	B	605	CLA	O2D-CGD-O1D	-3.95	116.16	123.85
22	B	606	CLA	C3B-C4B-NB	-3.95	107.01	110.53
29	l	101	LHG	O4-P-O5	3.95	130.81	112.44
24	T	101	BCR	C7-C8-C9	-3.94	120.41	126.23
22	b	602	CLA	O2D-CGD-CBD	3.93	118.10	111.23
22	A	403	CLA	O2D-CGD-O1D	-3.93	116.20	123.85
22	b	606	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
22	b	608	CLA	C4A-NA-C1A	3.90	108.46	106.68
22	b	603	CLA	O2D-CGD-O1D	-3.90	116.27	123.85
22	c	509	CLA	O2A-CGA-O1A	-3.89	113.89	123.63
29	D	411	LHG	O4-P-O5	3.89	130.53	112.44
24	B	617	BCR	C2-C1-C6	3.88	116.08	110.44
30	C	516	DGD	O6E-C1E-O5D	-3.87	100.90	110.04
22	c	504	CLA	CMB-C2B-C1B	-3.86	119.53	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	601	CLA	CHB-C4A-NA	3.86	129.97	124.40
22	B	612	CLA	CMB-C2B-C1B	-3.86	119.54	125.42
22	c	501	CLA	O2D-CGD-CBD	3.86	117.98	111.23
22	b	608	CLA	C3B-C4B-NB	-3.85	107.09	110.53
23	A	405	PHO	C1-C2-C3	-3.84	119.90	126.20
28	a	411	SQD	C1-C2-C3	-3.84	101.93	110.01
22	B	601	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
22	D	403	CLA	C3B-C4B-NB	-3.80	107.14	110.53
22	C	510	CLA	C4A-NA-C1A	3.80	108.41	106.68
22	c	504	CLA	C4A-NA-C1A	3.80	108.41	106.68
29	a	410	LHG	O8-C23-O10	-3.79	114.14	123.63
22	A	406	CLA	C4-C3-C5	3.79	121.81	115.23
26	D	406	PL9	C22-C23-C24	-3.79	118.95	127.62
22	C	502	CLA	C4A-NA-C1A	3.79	108.41	106.68
28	B	621	SQD	O7-S-C6	3.78	112.40	106.76
22	B	613	CLA	C3B-C4B-NB	-3.78	107.16	110.53
23	A	404	PHO	CMB-C2B-C3B	3.78	132.23	124.68
29	d	409	LHG	O4-P-O5	3.76	129.92	112.44
22	C	505	CLA	CMB-C2B-C1B	-3.75	119.72	125.42
22	c	502	CLA	C1-C2-C3	-3.74	120.08	126.20
22	c	505	CLA	C4A-NA-C1A	3.73	108.38	106.68
27	d	410	LMG	O2-C2-C1	-3.73	101.19	110.08
22	b	606	CLA	O2D-CGD-CBD	3.72	117.74	111.23
23	A	405	PHO	CMB-C2B-C3B	3.72	132.12	124.68
35	v	201	HEC	CHB-C1B-NB	3.72	128.43	124.42
22	c	510	CLA	C6-C5-C3	-3.72	104.41	113.47
32	C	520	STE	C3-C2-C1	-3.70	104.85	114.51
30	c	516	DGD	O3G-C3G-C2G	-3.70	101.83	110.82
35	v	201	HEC	CHA-C4D-ND	3.70	128.40	124.42
26	A	410	PL9	C7-C3-C4	3.69	119.95	116.91
27	m	101	LMG	O1-C1-C2	-3.69	102.67	108.27
30	C	515	DGD	O3G-C3G-C2G	-3.69	101.85	110.82
22	B	611	CLA	O2D-CGD-O1D	-3.68	116.68	123.85
22	b	616	CLA	CHB-C4A-NA	3.68	129.71	124.40
22	D	402	CLA	C1D-ND-C4D	-3.68	103.73	106.31
22	B	602	CLA	CHB-C4A-NA	3.68	129.71	124.40
28	A	414	SQD	O47-C7-C8	3.67	119.43	111.48
24	A	407	BCR	C27-C26-C25	3.67	127.66	122.70
22	B	614	CLA	C3B-C4B-NB	-3.67	107.26	110.53
22	D	403	CLA	CHB-C4A-NA	3.66	129.69	124.40
22	c	509	CLA	CHB-C4A-NA	3.66	129.69	124.40
22	d	404	CLA	CHB-C4A-NA	3.64	129.66	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	506	CLA	O2D-CGD-O1D	-3.63	116.77	123.85
22	B	602	CLA	O2D-CGD-CBD	3.63	117.57	111.23
28	A	412	SQD	C1-O5-C5	-3.62	106.66	113.72
22	B	608	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
33	d	402	BCT	O2-C-O1	3.61	128.91	119.68
22	C	506	CLA	C3B-C4B-NB	-3.61	107.31	110.53
24	K	101	BCR	C2-C1-C6	3.60	115.67	110.44
26	D	406	PL9	C42-C43-C44	-3.60	119.39	127.62
28	b	620	SQD	O2-C2-C1	3.59	118.64	110.08
22	b	608	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
22	B	612	CLA	C11-C12-C13	-3.59	104.04	115.97
22	C	512	CLA	CHB-C4A-NA	3.59	129.57	124.40
23	d	401	PHO	CMB-C2B-C3B	3.58	131.84	124.68
22	B	605	CLA	O1D-CGD-CBD	3.57	131.57	124.52
22	c	513	CLA	C3B-C4B-NB	-3.57	107.34	110.53
23	d	401	PHO	O2D-CGD-O1D	-3.57	116.90	123.85
22	B	608	CLA	C4A-NA-C1A	3.57	108.31	106.68
26	D	406	PL9	C40-C39-C41	3.56	121.41	115.23
22	B	606	CLA	O2A-CGA-O1A	-3.56	114.73	123.63
24	h	101	BCR	C38-C26-C25	-3.55	120.61	124.48
22	B	610	CLA	O2A-CGA-O1A	-3.55	114.75	123.63
22	B	601	CLA	O2D-CGD-CBD	3.55	117.43	111.23
24	b	619	BCR	C29-C30-C25	3.54	115.58	110.44
22	a	402	CLA	C3B-C4B-NB	-3.53	107.38	110.53
30	A	415	DGD	O3G-C3G-C2G	-3.53	102.23	110.82
30	c	516	DGD	C3D-C4D-C5D	-3.53	103.84	110.23
22	B	604	CLA	C1-C2-C3	-3.53	120.42	126.20
22	c	503	CLA	C3B-C4B-NB	-3.51	107.39	110.53
28	f	102	SQD	O5-C5-C4	3.51	116.03	109.70
22	b	601	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
27	m	101	LMG	O3-C3-C2	-3.50	102.12	110.38
24	c	515	BCR	C27-C26-C25	3.50	127.44	122.70
22	A	402	CLA	CHB-C4A-NA	3.49	129.44	124.40
28	a	411	SQD	O2-C2-C1	3.47	118.35	110.08
27	Y	101	LMG	O1-C7-C8	-3.47	102.38	110.82
28	F	102	SQD	O8-S-C6	3.47	112.67	105.97
27	M	101	LMG	C1-O6-C5	-3.45	106.99	113.72
28	B	621	SQD	C3-C4-C5	3.44	116.47	110.23
32	b	625	STE	C3-C2-C1	-3.44	105.53	114.51
24	h	101	BCR	C27-C26-C25	3.43	127.33	122.70
29	D	411	LHG	O8-C23-C24	3.42	122.28	111.83
22	B	616	CLA	O1D-CGD-CBD	3.42	131.26	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	403	CLA	C4A-NA-C1A	3.42	108.24	106.68
22	B	611	CLA	O2D-CGD-CBD	3.39	117.16	111.23
22	c	510	CLA	CMB-C2B-C1B	-3.39	120.26	125.42
24	K	101	BCR	C15-C16-C17	-3.39	116.58	123.52
22	C	512	CLA	O2D-CGD-CBD	3.39	117.16	111.23
22	b	610	CLA	C1-C2-C3	-3.39	120.65	126.20
26	a	409	PL9	C3-C4-C5	-3.38	114.35	118.57
27	b	623	LMG	C8-O7-C10	3.38	125.89	117.80
22	B	602	CLA	CMB-C2B-C1B	-3.38	120.27	125.42
24	T	101	BCR	C27-C26-C25	3.38	127.27	122.70
22	C	504	CLA	O2A-CGA-O1A	-3.38	115.18	123.63
26	d	407	PL9	C22-C23-C24	-3.37	119.90	127.62
35	v	201	HEC	CAB-C3B-C4B	3.37	129.17	124.79
26	D	406	PL9	C7-C3-C2	-3.37	119.42	123.39
22	C	507	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
22	C	513	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
22	b	612	CLA	C11-C12-C13	-3.36	104.79	115.97
27	c	521	LMG	O7-C10-O9	-3.36	115.85	123.70
24	b	618	BCR	C36-C18-C17	-3.36	117.38	122.82
22	C	504	CLA	C4A-NA-C1A	3.35	108.21	106.68
24	t	101	BCR	C36-C18-C19	3.35	123.20	118.09
22	C	506	CLA	C4A-NA-C1A	3.34	108.20	106.68
32	B	624	STE	C3-C2-C1	-3.33	105.83	114.51
30	H	102	DGD	O6E-C5E-C4E	3.33	115.69	109.70
30	c	517	DGD	C3G-O3G-C1D	3.32	120.92	113.80
22	A	406	CLA	CMB-C2B-C1B	-3.31	120.37	125.42
29	D	411	LHG	O8-C23-O10	-3.31	115.36	123.63
30	C	516	DGD	O2D-C2D-C1D	-3.31	102.20	110.08
22	b	607	CLA	C4-C3-C5	3.30	120.96	115.23
22	C	501	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
22	b	604	CLA	C3B-C4B-NB	-3.29	107.59	110.53
22	B	608	CLA	O2D-CGD-CBD	3.29	116.99	111.23
22	b	611	CLA	O2D-CGD-CBD	3.29	116.99	111.23
28	A	412	SQD	O47-C7-C8	3.29	118.59	111.48
22	b	604	CLA	CMB-C2B-C1B	-3.29	120.42	125.42
22	B	614	CLA	C4-C3-C5	3.27	120.91	115.23
22	b	603	CLA	C3B-C4B-NB	-3.27	107.61	110.53
22	d	404	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
22	C	506	CLA	O1D-CGD-CBD	3.26	130.96	124.52
22	B	613	CLA	C4-C3-C5	3.26	120.89	115.23
30	c	518	DGD	C1D-C2D-C3D	-3.26	103.15	110.01
30	A	415	DGD	O5E-C6E-C5E	-3.26	100.23	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	623	LMG	C3-C4-C5	-3.26	104.32	110.23
22	C	504	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
23	d	401	PHO	C1-C2-C3	-3.25	120.87	126.20
22	B	615	CLA	CHC-C4B-NB	3.25	128.92	124.05
27	c	519	LMG	O3-C3-C2	-3.24	102.73	110.38
22	B	612	CLA	CMB-C2B-C3B	3.24	134.17	126.55
30	C	517	DGD	O3E-C3E-C2E	-3.23	102.75	110.38
27	b	623	LMG	O8-C28-O10	-3.23	115.54	123.63
30	c	518	DGD	C3D-C4D-C5D	-3.23	104.38	110.23
22	C	508	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
22	c	508	CLA	CHD-C1D-ND	-3.22	120.27	124.80
22	b	616	CLA	CMB-C2B-C3B	3.22	134.13	126.55
22	C	513	CLA	C4-C3-C5	3.22	120.81	115.23
26	a	409	PL9	C35-C34-C36	3.22	120.81	115.23
22	c	510	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
23	d	401	PHO	C2B-C1B-NB	-3.21	107.11	109.43
26	A	410	PL9	C36-C34-C33	-3.21	113.96	121.17
24	B	618	BCR	C2-C1-C6	3.21	115.10	110.44
22	C	503	CLA	C7-C6-C5	-3.21	104.71	113.26
28	f	102	SQD	O7-S-C6	3.21	111.54	106.76
30	c	517	DGD	O3G-C3G-C2G	-3.21	103.02	110.82
22	C	501	CLA	C3B-C4B-NB	-3.20	107.67	110.53
28	a	412	SQD	O48-C23-O10	-3.20	115.63	123.63
22	b	602	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
33	D	401	BCT	O2-C-O1	3.19	127.84	119.68
22	B	615	CLA	C3B-C4B-NB	-3.19	107.68	110.53
28	a	412	SQD	O48-C23-C24	3.18	121.55	111.83
22	c	508	CLA	CHB-C4A-NA	3.18	129.00	124.40
22	b	610	CLA	CHB-C4A-NA	3.17	128.98	124.40
24	B	618	BCR	C29-C30-C25	3.17	115.04	110.44
30	A	415	DGD	O6E-C5E-C4E	3.17	115.41	109.70
27	b	623	LMG	C4-C3-C2	-3.17	105.27	110.83
22	B	608	CLA	CMB-C2B-C1B	-3.17	120.60	125.42
22	c	502	CLA	C3B-C4B-NB	-3.16	107.71	110.53
24	t	101	BCR	C7-C8-C9	-3.15	121.57	126.23
24	B	618	BCR	C37-C22-C21	-3.15	117.71	122.82
32	j	101	STE	O2-C1-C2	3.15	123.94	114.00
24	K	103	BCR	C37-C22-C21	-3.15	117.72	122.82
26	A	410	PL9	C22-C23-C24	-3.13	120.46	127.62
27	Y	101	LMG	O1-C1-C2	-3.13	103.52	108.27
22	b	610	CLA	O2D-CGD-O1D	-3.13	117.76	123.85
22	b	601	CLA	O2D-CGD-CBD	3.13	116.70	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	510	CLA	C3B-C4B-NB	-3.12	107.74	110.53
22	b	603	CLA	O2D-CGD-CBD	3.12	116.68	111.23
22	B	610	CLA	CHB-C4A-NA	3.12	128.90	124.40
28	a	411	SQD	O9-S-O7	-3.12	103.69	113.82
26	d	407	PL9	C36-C34-C33	-3.11	114.18	121.17
28	a	411	SQD	O8-S-O9	-3.11	103.61	111.40
22	B	613	CLA	CMB-C2B-C1B	-3.11	120.69	125.42
22	c	506	CLA	C3B-C4B-NB	-3.11	107.76	110.53
22	B	615	CLA	CHB-C4A-NA	3.10	128.87	124.40
22	b	615	CLA	CHB-C1B-NB	3.09	128.68	124.05
22	b	603	CLA	CHC-C4B-NB	3.08	128.67	124.05
22	c	511	CLA	C3B-C4B-NB	-3.08	107.78	110.53
22	b	614	CLA	O2A-CGA-O1A	-3.08	115.92	123.63
22	B	603	CLA	C2D-C1D-ND	-3.07	107.09	110.13
22	c	513	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
22	B	612	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
24	h	101	BCR	C37-C22-C21	-3.06	117.86	122.82
27	a	414	LMG	O8-C28-O10	-3.05	115.99	123.63
26	d	407	PL9	C7-C8-C9	-3.05	121.57	126.83
34	F	101	HEM	CBD-CAD-C3D	-3.05	104.11	112.53
22	a	403	CLA	CHB-C4A-NA	3.05	128.79	124.40
35	V	201	HEC	CBD-CAD-C3D	-3.03	104.16	112.53
22	C	508	CLA	CHD-C1D-ND	-3.03	120.54	124.80
26	a	409	PL9	C22-C23-C24	-3.03	120.69	127.62
22	c	508	CLA	C3B-C4B-NB	-3.02	107.83	110.53
22	b	613	CLA	C1-C2-C3	-3.02	121.24	126.20
23	d	401	PHO	C3B-C4B-NB	-3.02	105.49	107.46
22	C	509	CLA	CHB-C4A-NA	3.02	128.76	124.40
27	b	623	LMG	O2-C2-C1	-3.02	102.88	110.08
22	c	512	CLA	C1-C2-C3	-3.02	121.25	126.20
22	d	404	CLA	O2D-CGD-CBD	3.02	116.50	111.23
30	H	102	DGD	O2D-C2D-C1D	-3.02	102.89	110.08
22	B	607	CLA	O2A-CGA-O1A	-3.01	116.09	123.63
32	J	101	STE	C3-C2-C1	-3.01	106.64	114.51
22	b	616	CLA	CMB-C2B-C1B	-3.01	120.83	125.42
26	d	407	PL9	C30-C29-C31	-3.01	110.00	115.23
22	b	609	CLA	C4A-NA-C1A	3.01	108.05	106.68
22	B	606	CLA	CHC-C4B-NB	3.00	128.55	124.05
22	D	404	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
22	B	606	CLA	CGD-CBD-CAD	-3.00	101.14	110.85
24	D	405	BCR	C7-C8-C9	-3.00	121.80	126.23
22	b	608	CLA	CMB-C2B-C1B	-2.99	120.86	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	415	DGD	C4E-C3E-C2E	-2.99	105.57	110.83
30	c	518	DGD	C3G-C2G-C1G	-2.99	104.81	111.78
30	C	515	DGD	O5D-C6D-C5D	-2.99	102.67	109.42
22	C	509	CLA	CMB-C2B-C1B	-2.99	120.86	125.42
22	C	503	CLA	C4D-CHA-C1A	2.99	124.81	121.24
22	C	512	CLA	C4A-NA-C1A	2.99	108.04	106.68
24	d	406	BCR	C38-C26-C25	-2.98	121.23	124.48
22	B	615	CLA	O2D-CGD-CBD	2.98	116.44	111.23
28	b	620	SQD	C45-O47-C7	2.98	124.92	117.80
22	c	505	CLA	C3B-C4B-NB	-2.98	107.87	110.53
28	a	412	SQD	O49-C7-C8	-2.97	112.15	123.78
28	b	620	SQD	C3-C4-C5	2.97	115.62	110.23
24	H	101	BCR	C2-C1-C6	2.97	114.76	110.44
22	b	615	CLA	CMB-C2B-C1B	-2.97	120.89	125.42
27	D	407	LMG	O6-C1-O1	-2.97	103.02	110.04
22	B	604	CLA	C3B-C4B-NB	-2.97	107.88	110.53
24	B	617	BCR	C37-C22-C23	2.97	122.62	118.09
22	b	610	CLA	CAC-C3C-C4C	2.96	128.65	124.79
24	B	619	BCR	C29-C30-C25	2.96	114.74	110.44
22	b	613	CLA	CAC-C3C-C4C	2.96	128.64	124.79
22	b	606	CLA	CHB-C4A-NA	2.96	128.67	124.40
30	h	103	DGD	O3G-C3G-C2G	-2.96	103.62	110.82
22	b	612	CLA	CHB-C4A-NA	2.96	128.67	124.40
26	d	407	PL9	C35-C34-C36	2.96	120.36	115.23
32	B	627	STE	O2-C1-C2	2.95	123.33	114.00
22	B	611	CLA	CHD-C4C-NC	2.95	128.81	124.23
22	C	505	CLA	C1-C2-C3	-2.95	121.36	126.20
22	b	607	CLA	C4A-NA-C1A	2.95	108.03	106.68
24	d	406	BCR	C24-C23-C22	-2.95	121.87	126.23
22	b	604	CLA	C1-C2-C3	-2.95	121.37	126.20
22	B	604	CLA	C11-C10-C8	-2.94	106.19	115.97
22	B	616	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
26	A	410	PL9	C20-C19-C21	2.93	120.32	115.23
22	a	405	CLA	O2D-CGD-CBD	2.93	116.35	111.23
30	A	415	DGD	O5D-C1E-C2E	2.93	112.72	108.27
22	b	612	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
27	A	411	LMG	C1-O6-C5	-2.93	108.00	113.72
23	a	404	PHO	C1-C2-C3	-2.93	121.40	126.20
24	t	101	BCR	C15-C16-C17	-2.92	117.54	123.52
22	B	613	CLA	CHB-C4A-NA	2.92	128.61	124.40
35	v	201	HEC	CBD-CAD-C3D	-2.92	104.46	112.53
26	D	406	PL9	C35-C34-C36	2.92	120.29	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	k	102	BCR	C2-C1-C6	2.91	114.67	110.44
22	b	610	CLA	CAA-CBA-CGA	-2.91	104.94	113.21
30	h	103	DGD	C3D-C4D-C5D	-2.91	104.95	110.23
30	C	517	DGD	O6D-C1D-O3G	-2.91	103.16	110.04
22	C	512	CLA	C3B-C4B-NB	-2.91	107.93	110.53
22	b	605	CLA	C4-C3-C5	2.91	120.28	115.23
27	a	414	LMG	C1-O6-C5	-2.90	108.05	113.72
22	C	504	CLA	C3B-C4B-NB	-2.90	107.94	110.53
22	b	611	CLA	C1D-ND-C4D	2.90	108.35	106.31
28	a	411	SQD	O48-C23-C24	2.90	120.68	111.83
26	A	410	PL9	O1-C4-C3	-2.89	117.69	120.73
22	B	611	CLA	C7-C6-C5	-2.89	105.57	113.26
29	e	101	LHG	O8-C23-C24	2.89	120.63	111.83
27	b	623	LMG	O6-C5-C6	2.89	113.59	106.44
22	b	611	CLA	C2D-C1D-ND	-2.88	107.27	110.13
24	H	101	BCR	C38-C26-C25	-2.88	121.34	124.48
24	c	515	BCR	C7-C8-C9	-2.88	121.97	126.23
30	A	415	DGD	C1D-C2D-C3D	-2.88	103.95	110.01
24	K	101	BCR	C7-C8-C9	-2.88	121.98	126.23
26	D	406	PL9	C50-C49-C48	-2.88	114.03	122.66
24	B	619	BCR	C38-C26-C25	-2.87	121.35	124.48
30	C	517	DGD	O6D-C5D-C6D	-2.87	101.00	106.69
22	D	402	CLA	CHB-C4A-NA	2.87	128.55	124.40
24	c	514	BCR	C24-C23-C22	-2.87	121.98	126.23
27	m	101	LMG	O7-C10-O9	-2.87	116.99	123.70
30	o	301	DGD	CAB-C9B-C8B	-2.87	99.86	114.37
30	H	102	DGD	O6E-C5E-C6E	-2.87	99.33	106.44
22	B	605	CLA	C16-C15-C13	-2.87	106.44	115.97
22	A	402	CLA	CAA-CBA-CGA	-2.87	105.07	113.21
22	b	601	CLA	CHD-C1D-ND	-2.86	120.77	124.80
22	B	610	CLA	O2D-CGD-CBD	2.86	116.23	111.23
24	H	101	BCR	C29-C30-C25	2.86	114.59	110.44
24	d	406	BCR	C27-C26-C25	2.86	126.57	122.70
29	D	408	LHG	O8-C23-C24	2.86	120.55	111.83
28	F	102	SQD	O9-S-O7	-2.86	104.53	113.82
22	c	501	CLA	CED-O2D-CGD	-2.85	109.45	115.92
22	B	603	CLA	CMB-C2B-C1B	-2.85	121.08	125.42
22	C	507	CLA	O2D-CGD-CBD	2.85	116.21	111.23
26	D	406	PL9	C37-C38-C39	-2.85	121.11	127.62
24	t	101	BCR	C1-C6-C5	-2.85	118.75	122.64
22	b	609	CLA	C3B-C4B-NB	-2.84	107.99	110.53
30	A	415	DGD	O2D-C2D-C1D	-2.84	103.31	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C36-C18-C17	-2.84	118.22	122.82
22	C	505	CLA	CMB-C2B-C3B	2.84	133.22	126.55
22	B	603	CLA	CHD-C1D-C2D	2.83	131.38	125.49
24	D	405	BCR	C24-C23-C22	-2.83	122.04	126.23
22	a	403	CLA	O2A-CGA-O1A	-2.83	116.56	123.63
22	C	501	CLA	O2A-CGA-O1A	-2.82	116.56	123.63
24	A	407	BCR	C15-C16-C17	-2.82	117.75	123.52
22	C	509	CLA	C1-C2-C3	-2.82	121.58	126.20
35	v	201	HEC	CHC-C4B-NB	-2.81	120.89	124.37
30	o	301	DGD	C8B-C7B-C6B	-2.81	100.17	114.37
27	b	623	LMG	O7-C10-O9	-2.81	117.14	123.70
22	b	602	CLA	CHB-C4A-NA	2.81	128.45	124.40
22	A	403	CLA	O2D-CGD-CBD	2.80	116.13	111.23
27	A	411	LMG	C1-C2-C3	-2.80	104.11	110.01
27	D	407	LMG	O8-C28-O10	-2.80	116.62	123.63
22	a	405	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
22	b	607	CLA	C6-C7-C8	-2.80	106.67	115.97
32	j	101	STE	O2-C1-O1	-2.79	116.15	123.33
28	f	102	SQD	C1-C2-C3	-2.79	104.13	110.01
22	d	404	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	d	407	PL9	C41-C39-C38	-2.79	114.90	121.17
22	c	504	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
22	c	512	CLA	CHB-C4A-NA	2.79	128.42	124.40
22	c	503	CLA	C7-C6-C5	-2.78	105.84	113.26
22	c	503	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
22	b	610	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
27	A	411	LMG	O6-C1-O1	-2.78	103.47	110.04
24	K	103	BCR	C27-C26-C25	2.78	126.46	122.70
34	f	101	HEM	CHD-C4C-NC	2.78	127.48	124.45
22	C	505	CLA	C3B-C4B-NB	-2.78	108.05	110.53
22	c	512	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
24	t	101	BCR	C2-C1-C6	2.77	114.47	110.44
22	b	614	CLA	C3B-C4B-NB	-2.77	108.06	110.53
22	b	614	CLA	CHB-C4A-NA	2.77	128.39	124.40
22	b	604	CLA	CMB-C2B-C3B	2.77	133.06	126.55
26	A	410	PL9	C7-C3-C2	-2.76	120.13	123.39
24	k	102	BCR	C40-C30-C25	2.76	114.58	110.24
22	C	503	CLA	CHD-C1D-ND	-2.76	120.92	124.80
28	a	412	SQD	O47-C45-C44	2.76	118.12	108.30
24	b	619	BCR	C38-C26-C25	-2.76	121.47	124.48
22	C	507	CLA	CHD-C1D-ND	-2.76	120.92	124.80
22	B	607	CLA	C3B-C4B-NB	-2.76	108.07	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	504	CLA	CMB-C2B-C3B	2.75	133.02	126.55
27	h	102	LMG	O7-C10-O9	-2.75	116.26	123.33
22	B	613	CLA	CHA-C1A-NA	-2.75	120.17	126.39
22	C	501	CLA	O2D-CGD-CBD	2.75	116.03	111.23
22	A	402	CLA	C6-C5-C3	2.75	120.16	113.47
24	B	618	BCR	C38-C26-C25	-2.74	121.49	124.48
22	c	512	CLA	C3B-C4B-NB	-2.74	108.08	110.53
28	F	102	SQD	O48-C23-O10	-2.74	116.77	123.63
22	a	405	CLA	CHB-C4A-NA	2.74	128.35	124.40
22	C	504	CLA	O2D-CGD-CBD	2.74	116.02	111.23
22	a	402	CLA	CHB-C4A-NA	2.73	128.35	124.40
30	C	516	DGD	O5D-C6D-C5D	-2.73	103.26	109.42
27	c	519	LMG	O2-C2-C3	-2.73	103.93	110.38
22	B	610	CLA	C1-C2-C3	-2.73	121.72	126.20
22	D	402	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
22	a	402	CLA	CMB-C2B-C1B	-2.73	121.26	125.42
26	d	407	PL9	C20-C19-C21	2.73	119.96	115.23
28	B	621	SQD	O48-C23-C24	2.73	120.15	111.83
22	b	611	CLA	CHB-C4A-NA	2.72	128.33	124.40
22	b	604	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
24	K	102	BCR	C27-C26-C25	2.72	126.38	122.70
22	b	615	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
22	B	603	CLA	C1D-ND-C4D	2.72	108.22	106.31
27	Y	101	LMG	C1-O6-C5	-2.72	108.42	113.72
32	J	101	STE	O2-C1-C2	2.72	122.58	114.00
22	c	505	CLA	C6-C7-C8	-2.71	106.95	115.97
28	F	102	SQD	C1-O5-C5	-2.71	108.43	113.72
23	a	404	PHO	C2B-C1B-NB	-2.71	107.47	109.43
35	v	201	HEC	CMD-C2D-C1D	2.71	129.27	125.03
22	b	602	CLA	CHC-C1C-NC	2.71	128.39	124.31
35	V	201	HEC	CMD-C2D-C1D	2.71	129.26	125.03
22	B	604	CLA	CHB-C4A-NA	2.70	128.30	124.40
22	C	505	CLA	CHB-C1B-NB	2.70	128.10	124.05
27	A	411	LMG	C9-C8-C7	-2.70	105.49	111.78
24	D	405	BCR	C2-C1-C6	2.70	114.36	110.44
23	A	405	PHO	O2D-CGD-O1D	-2.70	118.60	123.85
24	k	102	BCR	C27-C26-C25	2.70	126.35	122.70
22	a	403	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	K	101	BCR	C27-C26-C25	2.69	126.34	122.70
27	Y	101	LMG	O2-C2-C1	-2.69	103.67	110.08
24	C	514	BCR	C15-C16-C17	-2.69	118.02	123.52
27	d	410	LMG	O6-C1-O1	-2.69	103.69	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	406	CLA	O2D-CGD-CBD	2.69	115.93	111.23
27	m	101	LMG	O6-C1-O1	-2.69	103.70	110.04
22	c	507	CLA	C3B-C4B-NB	-2.69	108.13	110.53
22	B	607	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
22	b	612	CLA	CAC-C3C-C4C	2.68	128.28	124.79
22	C	510	CLA	C3B-C4B-NB	-2.68	108.14	110.53
27	m	101	LMG	C1-O6-C5	-2.68	108.49	113.72
24	b	617	BCR	C27-C26-C25	2.68	126.32	122.70
22	c	504	CLA	O2D-CGD-CBD	2.67	115.89	111.23
22	B	606	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
30	C	516	DGD	O6D-C1D-O3G	-2.67	103.75	110.04
22	B	605	CLA	C7-C6-C5	-2.67	106.16	113.26
22	b	605	CLA	C3B-C4B-NB	-2.66	108.15	110.53
30	H	102	DGD	O5D-C1E-C2E	2.66	112.32	108.27
22	C	512	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
28	b	620	SQD	O47-C7-C8	2.66	117.23	111.48
22	d	403	CLA	C2D-C1D-ND	-2.66	107.50	110.13
22	A	403	CLA	C1-C2-C3	-2.66	121.84	126.20
24	b	617	BCR	C15-C16-C17	-2.66	118.08	123.52
28	b	620	SQD	O9-S-C6	2.66	110.72	106.76
22	B	602	CLA	C3B-C4B-NB	-2.65	108.16	110.53
22	b	601	CLA	C3B-C4B-NB	-2.65	108.16	110.53
30	H	102	DGD	C6D-C5D-C4D	2.65	117.63	112.07
24	b	617	BCR	C38-C26-C25	-2.65	121.59	124.48
22	b	613	CLA	C7-C6-C5	-2.65	106.20	113.26
22	c	504	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
24	h	101	BCR	C36-C18-C17	-2.65	118.52	122.82
22	b	603	CLA	C4D-CHA-C1A	2.65	124.41	121.24
22	B	603	CLA	O2A-CGA-O1A	-2.65	117.00	123.63
27	D	410	LMG	O8-C28-O10	-2.64	117.01	123.63
24	a	406	BCR	C8-C7-C6	-2.64	119.94	127.00
24	c	515	BCR	C15-C16-C17	-2.64	118.11	123.52
22	C	507	CLA	C4-C3-C5	2.64	119.81	115.23
24	k	101	BCR	C27-C26-C25	2.64	126.27	122.70
30	C	516	DGD	O5D-C1E-C2E	2.64	112.28	108.27
22	C	505	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
22	b	608	CLA	CMB-C2B-C3B	2.64	132.75	126.55
22	B	614	CLA	O2A-CGA-O1A	-2.64	117.03	123.63
22	A	406	CLA	CHB-C4A-NA	2.64	128.21	124.40
24	t	101	BCR	C37-C22-C23	2.64	122.11	118.09
22	B	603	CLA	C4A-NA-C1A	2.63	107.88	106.68
24	D	405	BCR	C27-C26-C25	2.63	126.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	b	620	SQD	O5-C1-C2	-2.63	104.96	110.37
22	C	513	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
29	l	101	LHG	O8-C23-C24	2.63	119.86	111.83
27	M	101	LMG	O2-C2-C1	-2.63	103.81	110.08
24	B	618	BCR	C15-C16-C17	-2.63	118.14	123.52
22	b	613	CLA	CHB-C4A-NA	2.62	128.19	124.40
22	b	614	CLA	C1-C2-C3	-2.62	121.90	126.20
22	a	402	CLA	C7-C6-C5	-2.62	106.28	113.26
24	a	406	BCR	C27-C26-C25	2.61	126.24	122.70
22	C	504	CLA	C4-C3-C5	2.61	119.77	115.23
28	b	620	SQD	O48-C23-O10	-2.61	117.10	123.63
30	h	103	DGD	C4E-C3E-C2E	-2.61	106.25	110.83
22	B	614	CLA	C4A-NA-C1A	2.61	107.87	106.68
22	B	613	CLA	CMB-C2B-C3B	2.61	132.68	126.55
28	B	621	SQD	O3-C3-C2	-2.61	104.23	110.38
30	c	518	DGD	O3D-C3D-C4D	-2.61	104.23	110.38
22	C	507	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
22	a	403	CLA	O2D-CGD-CBD	2.60	115.77	111.23
30	C	515	DGD	C3D-C4D-C5D	-2.60	105.52	110.23
27	M	101	LMG	O6-C1-O1	-2.60	103.91	110.04
22	C	512	CLA	C1-C2-C3	-2.59	121.95	126.20
30	h	103	DGD	C1D-C2D-C3D	-2.59	104.55	110.01
22	b	614	CLA	CHD-C1D-ND	-2.59	121.15	124.80
22	B	602	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
22	c	509	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
22	B	611	CLA	C14-C13-C15	-2.59	102.04	111.27
28	a	411	SQD	O7-S-C6	2.59	110.62	106.76
22	D	402	CLA	C1-C2-C3	-2.59	121.95	126.20
34	F	101	HEM	O2D-CGD-CBD	2.59	122.17	114.00
22	b	610	CLA	C4A-NA-C1A	2.58	107.86	106.68
22	B	604	CLA	CGD-CBD-CAD	-2.58	102.49	110.85
22	b	613	CLA	CMB-C2B-C3B	2.58	132.62	126.55
22	c	508	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
22	c	508	CLA	O2A-CGA-O1A	-2.58	117.18	123.63
22	c	506	CLA	CHB-C4A-NA	2.58	128.12	124.40
24	h	101	BCR	C2-C1-C6	2.57	114.18	110.44
22	c	502	CLA	CHB-C1B-NB	2.57	127.91	124.05
30	H	102	DGD	O6D-C1D-O3G	-2.57	103.96	110.04
32	b	625	STE	O2-C1-C2	2.57	122.12	114.00
30	c	517	DGD	C3D-C4D-C5D	-2.57	105.58	110.23
24	C	514	BCR	C27-C26-C25	2.57	126.17	122.70
24	b	618	BCR	C27-C26-C25	2.57	126.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	B	621	SQD	O8-S-C6	2.57	110.93	105.97
22	C	513	CLA	CHD-C1D-ND	-2.57	121.19	124.80
22	B	604	CLA	C6-C5-C3	-2.56	107.22	113.47
32	b	625	STE	O1-C1-C2	-2.56	114.97	123.09
22	b	603	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
22	B	612	CLA	C1-C2-C3	-2.56	122.00	126.20
22	c	501	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
22	C	508	CLA	CHB-C4A-NA	2.55	128.08	124.40
35	V	201	HEC	CAD-CBD-CGD	-2.55	106.90	113.67
32	m	102	STE	O1-C1-C2	-2.55	115.00	123.09
30	A	415	DGD	O3G-C1D-C2D	-2.55	104.40	108.27
22	c	503	CLA	C4-C3-C5	2.55	119.65	115.23
24	b	619	BCR	C2-C1-C6	2.55	114.14	110.44
24	K	101	BCR	C11-C10-C9	-2.55	123.70	127.28
22	c	508	CLA	C7-C6-C5	-2.55	106.48	113.26
23	A	405	PHO	O2D-CGD-CBD	2.55	113.74	110.95
24	B	619	BCR	C15-C16-C17	-2.55	118.31	123.52
22	b	608	CLA	CHB-C1B-NB	2.54	127.87	124.05
32	d	411	STE	O2-C1-C2	2.54	122.03	114.00
22	B	611	CLA	CHD-C1D-ND	-2.54	121.23	124.80
22	C	509	CLA	CMB-C2B-C3B	2.54	132.52	126.55
26	d	407	PL9	C37-C38-C39	-2.54	121.82	127.62
30	A	415	DGD	C3G-C2G-C1G	-2.54	105.87	111.78
32	B	627	STE	O1-C1-C2	-2.53	115.06	123.09
22	C	510	CLA	C11-C10-C8	-2.53	107.55	115.97
22	A	406	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
29	A	413	LHG	O8-C23-C24	2.53	119.54	111.83
22	b	609	CLA	CHA-C1A-NA	-2.53	120.67	126.39
30	h	103	DGD	O6E-C5E-C4E	2.53	114.25	109.70
22	b	603	CLA	CHD-C1D-ND	-2.53	121.25	124.80
22	b	607	CLA	CHA-C1A-NA	-2.52	120.68	126.39
24	K	103	BCR	C15-C16-C17	-2.52	118.36	123.52
34	F	101	HEM	CHC-C1C-NC	2.52	127.20	124.45
27	a	414	LMG	O6-C1-O1	-2.52	104.09	110.04
26	D	406	PL9	C7-C8-C9	-2.52	122.49	126.83
28	a	411	SQD	O47-C7-C8	2.52	116.93	111.48
22	c	507	CLA	O2A-CGA-O1A	-2.52	117.34	123.63
24	H	101	BCR	C27-C26-C25	2.51	126.10	122.70
24	t	101	BCR	C27-C26-C25	2.51	126.10	122.70
22	c	507	CLA	CHD-C1D-ND	-2.51	121.26	124.80
22	C	504	CLA	CHB-C4A-NA	2.51	128.03	124.40
22	b	608	CLA	O2A-CGA-O1A	-2.51	117.34	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	505	CLA	O2D-CGD-CBD	2.51	115.62	111.23
30	c	518	DGD	C3E-C4E-C5E	-2.51	105.69	110.23
35	v	201	HEC	C3C-C4C-NC	-2.51	107.37	110.15
22	C	502	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
22	d	404	CLA	CHD-C1D-ND	-2.50	121.28	124.80
22	d	403	CLA	C4-C3-C5	2.50	119.56	115.23
30	c	518	DGD	O6D-C1D-O3G	-2.49	104.15	110.04
28	F	102	SQD	C1-C2-C3	-2.49	104.76	110.01
30	C	517	DGD	O2D-C2D-C1D	-2.49	104.13	110.08
22	B	611	CLA	C1-C2-C3	-2.49	122.11	126.20
24	K	103	BCR	C7-C8-C9	-2.49	122.55	126.23
28	a	411	SQD	O5-C5-C4	2.49	114.19	109.70
22	B	611	CLA	C4A-NA-C1A	2.49	107.82	106.68
22	B	607	CLA	CHB-C1B-NB	2.49	127.79	124.05
26	a	409	PL9	O2-C1-C2	-2.49	116.17	121.83
22	c	501	CLA	C3B-C4B-NB	-2.49	108.31	110.53
30	o	301	DGD	C6B-C5B-C4B	-2.49	101.78	114.37
22	B	603	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
34	f	101	HEM	O2D-CGD-CBD	2.49	121.86	114.00
22	b	609	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
22	A	403	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	c	501	CLA	CHB-C4A-NA	2.49	127.99	124.40
22	A	406	CLA	CMB-C2B-C3B	2.49	132.40	126.55
22	c	507	CLA	C4-C3-C5	2.48	119.54	115.23
26	a	409	PL9	O2-C1-C6	2.48	124.43	120.48
22	B	614	CLA	CHC-C4B-NB	2.48	127.78	124.05
22	b	609	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
27	c	519	LMG	C1-O6-C5	-2.48	108.88	113.72
27	m	101	LMG	O1-C7-C8	-2.48	104.79	110.82
35	v	201	HEC	CMC-C2C-C1C	-2.48	121.64	125.42
24	C	514	BCR	C36-C18-C17	-2.48	118.80	122.82
30	c	517	DGD	C8B-C7B-C6B	-2.48	101.85	114.37
22	D	402	CLA	CED-O2D-CGD	2.48	121.53	115.92
32	B	622	STE	C3-C2-C1	-2.48	108.05	114.51
22	B	604	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
29	D	408	LHG	O8-C23-O10	-2.48	117.44	123.63
22	B	608	CLA	CMB-C2B-C3B	2.48	132.37	126.55
30	C	515	DGD	O1G-C1A-C2A	-2.48	104.29	111.83
30	c	518	DGD	O6E-C5E-C4E	2.47	114.16	109.70
27	c	519	LMG	O8-C28-O10	-2.47	117.44	123.63
23	a	404	PHO	CBC-CAC-C3C	-2.47	109.34	112.87
24	C	514	BCR	C2-C1-C6	2.47	114.02	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	406	CLA	C1-C2-C3	-2.47	122.16	126.20
22	d	405	CLA	O2A-CGA-O1A	-2.47	117.46	123.63
24	b	619	BCR	C37-C22-C21	-2.46	118.82	122.82
22	c	502	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
22	B	603	CLA	CMB-C2B-C3B	2.46	132.34	126.55
26	D	406	PL9	C36-C34-C33	-2.46	115.64	121.17
27	a	414	LMG	C9-C8-C7	-2.46	106.05	111.78
22	C	506	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
22	B	613	CLA	CAC-C3C-C4C	2.46	127.99	124.79
27	Y	101	LMG	O6-C5-C6	2.46	112.53	106.44
32	B	622	STE	O2-C1-C2	2.46	121.76	114.00
30	c	517	DGD	O2G-C1B-O1B	-2.45	117.97	123.70
22	d	405	CLA	CMB-C2B-C3B	2.45	132.31	126.55
30	H	102	DGD	C1D-C2D-C3D	-2.45	104.86	110.01
26	A	410	PL9	C40-C39-C38	-2.45	117.34	123.63
34	f	101	HEM	C3B-C2B-C1B	2.45	108.25	106.41
28	a	411	SQD	O5-C1-C2	-2.45	105.34	110.37
26	D	406	PL9	O2-C1-C2	-2.44	116.27	121.83
28	F	102	SQD	O48-C23-C24	2.44	119.29	111.83
22	C	511	CLA	CHB-C4A-NA	2.44	127.93	124.40
22	b	615	CLA	CHB-C4A-NA	2.44	127.93	124.40
22	C	512	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
30	C	515	DGD	C4E-C3E-C2E	-2.44	106.55	110.83
24	c	514	BCR	C38-C26-C25	-2.44	121.83	124.48
22	B	614	CLA	O1D-CGD-CBD	2.43	129.32	124.52
22	B	602	CLA	C1-C2-C3	-2.43	122.21	126.20
22	b	607	CLA	CAC-C3C-C4C	2.43	127.95	124.79
22	a	403	CLA	C3B-C4B-NB	-2.43	108.36	110.53
22	b	614	CLA	C4A-NA-C1A	2.43	107.79	106.68
29	l	101	LHG	C27-C26-C25	-2.43	102.09	114.37
24	H	101	BCR	C37-C22-C23	2.43	121.80	118.09
22	B	602	CLA	CMB-C2B-C3B	2.43	132.26	126.55
22	B	606	CLA	O2D-CGD-CBD	2.43	115.47	111.23
22	D	402	CLA	C4-C3-C5	2.43	119.44	115.23
22	b	612	CLA	C1-C2-C3	-2.43	122.22	126.20
34	f	101	HEM	CHB-C1B-NB	2.42	127.36	124.37
22	d	405	CLA	CHB-C4A-NA	2.42	127.89	124.40
29	D	411	LHG	O4-P-O6	-2.42	96.59	107.57
30	C	517	DGD	CAB-C9B-C8B	-2.42	102.13	114.37
22	b	607	CLA	CHB-C1B-NB	2.42	127.68	124.05
22	d	405	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
29	D	411	LHG	C18-C17-C16	-2.42	102.14	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	CHB-C4A-NA	2.42	127.89	124.40
32	b	624	STE	O2-C1-C2	2.42	121.64	114.00
33	d	402	BCT	O3-C-O1	-2.42	113.50	119.68
22	c	508	CLA	CMB-C2B-C3B	2.41	132.23	126.55
29	a	410	LHG	C11-C10-C9	-2.41	102.18	114.37
27	c	521	LMG	C6-C5-C4	-2.41	107.10	113.02
22	B	615	CLA	C2D-C1D-ND	-2.41	107.74	110.13
30	H	102	DGD	C1E-O6E-C5E	2.41	118.42	113.72
24	k	101	BCR	C38-C26-C25	-2.41	121.86	124.48
22	B	608	CLA	C11-C12-C13	-2.41	107.96	115.97
30	C	516	DGD	C1D-C2D-C3D	-2.41	104.95	110.01
23	a	404	PHO	OBD-CAD-CBD	-2.40	122.30	125.82
22	b	605	CLA	C16-C15-C13	-2.40	107.98	115.97
22	c	513	CLA	CMB-C2B-C1B	-2.40	121.76	125.42
27	D	407	LMG	C31-C30-C29	-2.40	104.30	113.13
22	C	505	CLA	CAA-CBA-CGA	-2.40	106.39	113.21
30	c	516	DGD	O6D-C1D-O3G	-2.40	104.37	110.04
34	f	101	HEM	CAB-C3B-C2B	-2.40	120.63	128.43
22	C	502	CLA	CHA-C1A-NA	-2.40	120.96	126.39
30	C	515	DGD	C5B-C4B-C3B	-2.40	102.24	114.37
22	C	507	CLA	C1-C2-C3	-2.40	122.27	126.20
24	A	407	BCR	C37-C22-C21	-2.39	118.94	122.82
26	a	409	PL9	C12-C13-C14	-2.39	122.14	127.62
24	c	515	BCR	C38-C26-C25	-2.39	121.87	124.48
22	B	604	CLA	C1-O2A-CGA	-2.39	110.86	116.65
27	m	101	LMG	O8-C28-O10	-2.39	117.64	123.63
22	B	610	CLA	C3B-C4B-NB	-2.39	108.39	110.53
22	B	608	CLA	CHA-C1A-NA	-2.39	120.98	126.39
22	b	605	CLA	CHD-C1D-ND	-2.39	121.44	124.80
30	c	517	DGD	O4D-C4D-C3D	2.39	116.00	110.38
29	D	409	LHG	C6-C5-C4	2.39	117.35	111.78
22	B	607	CLA	CED-O2D-CGD	2.39	121.33	115.92
22	c	503	CLA	C5-C3-C2	-2.39	115.81	121.17
22	B	605	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	C	501	CLA	CHD-C1D-C2D	2.38	130.44	125.49
24	b	619	BCR	C16-C15-C14	-2.38	118.65	123.52
22	B	609	CLA	CHC-C4B-NB	2.38	127.61	124.05
22	C	501	CLA	C2D-C1D-ND	-2.38	107.78	110.13
22	D	402	CLA	C3B-C4B-NB	-2.37	108.41	110.53
22	A	403	CLA	C2D-C1D-ND	-2.37	107.78	110.13
30	A	415	DGD	C8B-C7B-C6B	-2.37	102.38	114.37
22	b	603	CLA	CMA-C3A-C4A	2.37	118.15	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	F	102	SQD	O5-C5-C4	2.37	113.97	109.70
35	V	201	HEC	C1B-C2B-C3B	2.37	109.47	106.98
22	C	504	CLA	CHD-C1D-ND	-2.37	121.47	124.80
32	a	415	STE	C3-C2-C1	-2.37	108.33	114.51
29	D	408	LHG	C18-C17-C16	-2.37	102.41	114.37
22	b	612	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
26	A	410	PL9	C27-C28-C29	-2.36	122.21	127.62
22	c	507	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
22	c	510	CLA	CHB-C4A-NA	2.36	127.81	124.40
32	d	412	STE	C3-C2-C1	-2.36	108.35	114.51
22	C	510	CLA	CMB-C2B-C3B	2.36	132.10	126.55
22	B	612	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
23	a	404	PHO	O2A-CGA-O1A	-2.36	117.72	123.63
30	A	415	DGD	CDB-CCB-CBB	-2.36	102.45	114.37
28	a	411	SQD	O10-C23-C24	-2.36	114.56	123.78
22	B	610	CLA	O1A-CGA-CBA	2.36	133.00	123.78
22	C	505	CLA	O2D-CGD-O1D	-2.36	119.26	123.85
24	b	618	BCR	C15-C16-C17	-2.35	118.71	123.52
27	m	101	LMG	C38-C37-C36	-2.35	102.49	114.37
29	D	409	LHG	O8-C23-C24	2.35	119.00	111.83
32	c	522	STE	C3-C2-C1	-2.35	108.38	114.51
27	A	411	LMG	C40-C39-C38	-2.35	102.51	114.37
22	c	503	CLA	O1D-CGD-CBD	2.35	129.15	124.52
24	K	102	BCR	C38-C26-C25	-2.35	121.92	124.48
22	B	603	CLA	CHD-C1D-ND	-2.35	121.50	124.80
22	B	611	CLA	CHB-C4A-NA	2.34	127.78	124.40
22	b	616	CLA	C4-C3-C5	2.34	119.30	115.23
30	H	102	DGD	O5E-C6E-C5E	-2.34	103.35	111.33
22	c	512	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
22	A	403	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
22	b	605	CLA	CHB-C4A-NA	2.34	127.77	124.40
22	a	405	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
28	A	412	SQD	O7-S-C6	2.34	110.25	106.76
26	a	409	PL9	C27-C28-C29	-2.34	122.28	127.62
22	c	512	CLA	O1D-CGD-CBD	2.34	129.13	124.52
22	B	605	CLA	CAC-C3C-C4C	2.34	127.83	124.79
22	C	502	CLA	O1D-CGD-CBD	2.34	129.12	124.52
28	f	102	SQD	O5-C1-O6	2.34	115.56	110.04
22	c	510	CLA	CMB-C2B-C3B	2.33	132.04	126.55
22	C	505	CLA	C11-C10-C8	-2.33	108.21	115.97
28	b	620	SQD	O47-C45-C46	2.33	116.69	108.34
23	A	404	PHO	O2D-CGD-CBD	2.33	113.50	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	BCR	C38-C26-C25	-2.33	121.95	124.48
22	b	611	CLA	C3B-C4B-NB	-2.32	108.45	110.53
22	B	616	CLA	CAA-CBA-CGA	-2.32	106.61	113.21
22	A	403	CLA	CHD-C1D-C2D	2.32	130.32	125.49
22	D	404	CLA	CAC-C3C-C4C	2.32	127.81	124.79
22	B	605	CLA	C11-C10-C8	-2.32	108.25	115.97
32	D	413	STE	C3-C2-C1	-2.32	108.46	114.51
34	F	101	HEM	CHB-C1B-NB	2.32	127.23	124.37
22	B	616	CLA	C2C-C1C-NC	2.32	112.42	109.98
24	A	407	BCR	C37-C22-C23	2.32	121.63	118.09
24	b	617	BCR	C8-C7-C6	-2.32	120.81	127.00
22	d	405	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
22	b	613	CLA	CHB-C1B-NB	2.32	127.52	124.05
22	B	613	CLA	C2A-C1A-CHA	2.31	127.88	123.87
22	c	510	CLA	CHB-C1B-NB	2.31	127.52	124.05
22	B	606	CLA	CHB-C4A-NA	2.31	127.74	124.40
22	c	511	CLA	O2D-CGD-CBD	2.31	115.27	111.23
22	B	609	CLA	C2C-C1C-NC	2.31	112.41	109.98
22	d	403	CLA	CBA-CAA-C2A	-2.31	106.92	113.79
27	Y	101	LMG	C40-C39-C38	-2.31	102.70	114.37
24	b	618	BCR	C38-C26-C25	-2.31	121.97	124.48
22	c	508	CLA	CHD-C1D-C2D	2.30	130.28	125.49
22	C	502	CLA	C3B-C4B-NB	-2.30	108.47	110.53
22	C	513	CLA	O2D-CGD-CBD	2.30	115.26	111.23
30	C	517	DGD	CBB-CAB-C9B	-2.30	102.72	114.37
22	c	505	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
28	f	102	SQD	O5-C1-C2	-2.30	105.65	110.37
24	b	619	BCR	C36-C18-C17	-2.30	119.10	122.82
22	d	403	CLA	C4A-NA-C1A	2.29	107.73	106.68
22	b	608	CLA	CHA-C1A-NA	-2.29	121.20	126.39
22	b	611	CLA	CHD-C1D-C2D	2.29	130.25	125.49
22	c	511	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
22	b	613	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
22	B	608	CLA	CHD-C1D-ND	-2.29	121.58	124.80
22	c	507	CLA	CHD-C4C-NC	2.29	127.78	124.23
24	K	103	BCR	C16-C15-C14	-2.28	118.85	123.52
29	l	101	LHG	O8-C23-O10	-2.28	117.92	123.63
30	c	516	DGD	C3E-C4E-C5E	-2.28	106.10	110.23
24	K	103	BCR	C36-C18-C19	2.28	121.57	118.09
22	B	604	CLA	CMB-C2B-C3B	2.28	131.91	126.55
22	b	606	CLA	C4-C3-C5	2.28	119.19	115.23
26	d	407	PL9	O1-C4-C3	-2.28	118.33	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	604	CLA	CHA-C1A-NA	-2.28	121.23	126.39
26	A	410	PL9	C7-C8-C9	-2.28	122.91	126.83
22	c	505	CLA	CHB-C4A-NA	2.28	127.69	124.40
34	F	101	HEM	C1D-C2D-C3D	2.28	109.37	106.98
26	A	410	PL9	O2-C1-C2	-2.28	116.66	121.83
27	A	411	LMG	C38-C37-C36	-2.28	102.87	114.37
22	b	604	CLA	CHB-C1B-NB	2.27	127.46	124.05
22	c	503	CLA	CHC-C4B-NB	2.27	127.46	124.05
22	b	613	CLA	CHA-C1A-NA	-2.27	121.24	126.39
26	D	406	PL9	C27-C28-C29	-2.27	122.42	127.62
22	c	508	CLA	CHD-C4C-NC	2.27	127.75	124.23
35	V	201	HEC	CHB-C4A-NA	2.26	126.92	124.45
23	A	404	PHO	C5-C3-C2	2.26	126.24	121.17
22	C	504	CLA	CHC-C1C-NC	2.26	127.72	124.31
27	M	101	LMG	C40-C39-C38	-2.26	102.94	114.37
30	o	301	DGD	CDB-CCB-CBB	-2.26	102.95	114.37
22	c	509	CLA	C1-O2A-CGA	-2.26	111.18	116.65
22	d	403	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
22	b	616	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
30	c	516	DGD	CBB-CAB-C9B	-2.26	102.96	114.37
26	d	407	PL9	C27-C28-C29	-2.25	122.47	127.62
28	B	621	SQD	C4-C3-C2	2.25	114.78	110.83
27	c	519	LMG	O8-C28-C29	2.25	118.70	111.83
30	C	515	DGD	O2G-C1B-C2B	-2.25	106.61	111.48
22	B	607	CLA	C3A-C2A-C1A	2.25	104.71	101.34
34	F	101	HEM	CBA-CAA-C2A	-2.25	106.31	112.53
22	C	509	CLA	CHA-C4D-ND	2.25	137.19	132.55
30	c	518	DGD	O6E-C1E-O5D	-2.25	104.73	110.04
22	b	601	CLA	CHD-C1D-C2D	2.25	130.16	125.49
24	d	406	BCR	C2-C1-C6	2.24	113.70	110.44
22	c	505	CLA	C11-C10-C8	-2.24	108.51	115.97
22	B	616	CLA	C2A-C3A-C4A	2.24	105.49	101.87
22	B	609	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
22	b	606	CLA	C6-C5-C3	2.24	118.92	113.47
22	b	605	CLA	O1D-CGD-CBD	2.24	128.93	124.52
24	K	103	BCR	C40-C30-C25	2.24	113.75	110.24
33	D	401	BCT	O3-C-O1	-2.24	113.95	119.68
32	c	520	STE	O2-C1-C2	2.24	121.07	114.00
24	B	618	BCR	C40-C30-C25	2.24	113.75	110.24
30	H	102	DGD	C7B-C6B-C5B	-2.24	103.07	114.37
22	c	513	CLA	CMB-C2B-C3B	2.24	131.81	126.55
23	d	401	PHO	C16-C15-C13	-2.23	108.54	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	H	102	DGD	C1D-O6D-C5D	-2.23	109.36	113.72
26	A	410	PL9	C35-C34-C36	2.23	119.11	115.23
22	b	607	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
30	A	415	DGD	O5D-C6D-C5D	-2.23	104.39	109.42
22	D	402	CLA	C2D-C1D-ND	2.23	112.33	110.13
22	c	509	CLA	CHD-C1D-ND	-2.23	121.67	124.80
22	c	507	CLA	CHC-C4B-NB	2.23	127.39	124.05
22	c	504	CLA	C4-C3-C5	2.22	119.09	115.23
30	C	515	DGD	C3B-C2B-C1B	-2.22	105.55	113.69
24	k	101	BCR	C1-C6-C5	-2.22	119.60	122.64
35	v	201	HEC	C2A-C1A-NA	-2.22	108.18	110.32
27	b	623	LMG	C40-C39-C38	-2.22	103.14	114.37
24	c	514	BCR	C2-C1-C6	2.22	113.67	110.44
22	c	509	CLA	O2A-CGA-CBA	2.22	118.61	111.83
22	B	609	CLA	CMC-C2C-C1C	2.22	128.50	125.03
22	d	405	CLA	C4A-NA-C1A	2.22	107.69	106.68
22	b	612	CLA	CMB-C2B-C3B	2.22	131.77	126.55
22	b	609	CLA	CHB-C1B-NB	2.22	127.37	124.05
30	C	517	DGD	C8B-C7B-C6B	-2.22	103.17	114.37
30	C	515	DGD	C1E-C2E-C3E	-2.21	105.35	110.01
22	b	612	CLA	CHD-C1D-ND	-2.21	121.69	124.80
23	d	401	PHO	C3D-C4D-ND	2.21	110.54	107.71
35	v	201	HEC	O1D-CGD-CBD	-2.21	116.08	123.09
22	b	603	CLA	CHB-C1B-NB	2.21	127.37	124.05
22	C	506	CLA	CHA-C1A-NA	-2.21	121.38	126.39
22	B	610	CLA	CHD-C1D-ND	-2.21	121.69	124.80
22	d	405	CLA	C1-C2-C3	-2.21	122.58	126.20
28	f	102	SQD	O47-C7-O49	-2.21	118.54	123.70
27	c	521	LMG	O8-C28-O10	-2.21	118.10	123.63
22	D	402	CLA	C6-C5-C3	2.21	118.85	113.47
26	A	410	PL9	C40-C39-C41	2.21	119.06	115.23
30	C	515	DGD	C2G-O2G-C1B	2.20	123.07	117.80
24	t	101	BCR	C3-C4-C5	-2.20	110.12	114.06
27	d	410	LMG	O7-C10-O9	-2.20	118.56	123.70
22	b	613	CLA	C16-C15-C13	-2.20	108.65	115.97
26	a	409	PL9	C37-C38-C39	-2.20	122.59	127.62
27	D	407	LMG	O3-C3-C2	-2.19	105.20	110.38
22	B	606	CLA	CHB-C1B-NB	2.19	127.34	124.05
22	b	605	CLA	CHD-C1D-C2D	2.19	130.05	125.49
30	h	103	DGD	C1D-O6D-C5D	-2.19	109.44	113.72
26	d	407	PL9	C8-C7-C3	2.19	117.69	112.03
22	b	609	CLA	CHD-C1D-ND	-2.19	121.72	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	513	CLA	CHD-C1D-ND	-2.19	121.72	124.80
22	B	607	CLA	C2C-C1C-NC	2.19	112.28	109.98
22	b	616	CLA	C2B-C1B-NB	2.19	112.59	110.33
26	a	409	PL9	C7-C8-C9	-2.19	123.06	126.83
22	c	509	CLA	CHC-C1C-NC	2.19	127.61	124.31
22	B	607	CLA	CHD-C1D-ND	-2.19	121.72	124.80
29	D	408	LHG	O7-C7-C8	-2.19	106.75	111.48
29	d	409	LHG	O8-C6-C5	-2.19	102.09	108.40
29	d	409	LHG	C26-C25-C24	2.19	121.16	113.13
22	C	510	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
22	b	602	CLA	CHA-C4D-ND	2.19	137.06	132.55
22	c	509	CLA	CMB-C2B-C3B	2.19	131.69	126.55
28	A	412	SQD	O48-C23-C24	2.19	118.50	111.83
22	B	611	CLA	C3D-C4D-ND	2.18	113.54	109.99
22	C	503	CLA	O2A-C1-C2	-2.18	99.70	108.11
22	c	513	CLA	CHD-C4C-C3C	-2.18	121.59	124.77
28	B	621	SQD	O47-C45-C46	2.18	116.18	108.34
30	c	518	DGD	C4E-C3E-C2E	-2.18	107.00	110.83
22	B	612	CLA	C3B-C4B-NB	-2.18	108.58	110.53
22	B	605	CLA	CHB-C4A-NA	2.18	127.55	124.40
35	v	201	HEC	CAD-CBD-CGD	-2.18	107.88	113.67
27	Y	101	LMG	O7-C10-O9	-2.18	118.61	123.70
22	b	603	CLA	CHD-C1D-C2D	2.18	130.02	125.49
22	C	509	CLA	CHD-C1D-ND	-2.18	121.73	124.80
22	B	603	CLA	CHD-C4C-NC	2.18	127.61	124.23
29	D	409	LHG	O8-C23-O10	-2.18	118.17	123.63
24	A	407	BCR	C4-C5-C6	2.18	125.65	122.70
22	b	608	CLA	O2D-CGD-CBD	2.18	115.04	111.23
26	D	406	PL9	O2-C1-C6	2.18	123.94	120.48
22	B	608	CLA	CHD-C4C-NC	2.18	127.61	124.23
22	d	405	CLA	O1D-CGD-CBD	2.17	128.81	124.52
22	C	510	CLA	CHA-C1A-NA	-2.17	121.47	126.39
22	B	605	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
22	c	508	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
22	A	403	CLA	C3B-C4B-NB	-2.17	108.59	110.53
28	B	621	SQD	O2-C2-C1	2.17	115.25	110.08
28	f	102	SQD	C45-O47-C7	2.17	122.99	117.80
22	d	403	CLA	O1D-CGD-CBD	2.17	128.80	124.52
28	f	102	SQD	O47-C7-C8	2.17	118.90	110.93
27	Y	101	LMG	O8-C28-O10	-2.17	118.21	123.63
22	b	611	CLA	CED-O2D-CGD	-2.16	111.01	115.92
22	B	601	CLA	C2A-C1A-CHA	2.16	127.62	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	CHC-C1C-NC	2.16	127.57	124.31
30	c	517	DGD	CDB-CCB-CBB	-2.16	103.45	114.37
22	a	402	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
22	b	602	CLA	CMB-C2B-C1B	-2.16	122.14	125.42
27	b	623	LMG	C1-C2-C3	-2.16	105.47	110.01
26	D	406	PL9	C12-C13-C14	-2.16	122.69	127.62
24	b	619	BCR	C8-C7-C6	-2.15	121.24	127.00
22	B	614	CLA	CHA-C1A-NA	-2.15	121.52	126.39
24	C	514	BCR	C15-C14-C13	-2.15	124.26	127.28
22	B	616	CLA	CHB-C4A-NA	2.15	127.51	124.40
22	a	403	CLA	CED-O2D-CGD	-2.15	111.03	115.92
27	m	101	LMG	C20-C19-C18	-2.15	103.50	114.37
24	A	407	BCR	C1-C6-C5	-2.15	119.70	122.64
27	a	414	LMG	C4-C3-C2	-2.15	107.06	110.83
22	c	507	CLA	CHB-C4A-NA	2.15	127.50	124.40
22	D	403	CLA	O2D-CGD-CBD	2.15	114.98	111.23
22	C	501	CLA	CHD-C1D-ND	-2.15	121.78	124.80
22	c	513	CLA	CHD-C4C-NC	2.15	127.56	124.23
29	e	101	LHG	C20-C19-C18	-2.14	103.53	114.37
22	c	502	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
22	c	506	CLA	CMB-C2B-C1B	-2.14	122.15	125.42
27	d	410	LMG	C3-C4-C5	-2.14	106.34	110.23
22	b	616	CLA	CHD-C1D-ND	-2.14	121.79	124.80
24	b	617	BCR	C3-C4-C5	-2.14	110.23	114.06
22	d	403	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
24	d	406	BCR	C16-C15-C14	-2.14	119.14	123.52
30	c	517	DGD	O2D-C2D-C1D	-2.14	104.97	110.08
22	C	508	CLA	O2D-CGD-CBD	2.14	114.97	111.23
29	a	410	LHG	C25-C24-C23	2.14	121.53	113.69
27	a	414	LMG	O5-C6-C5	-2.14	104.05	111.33
24	B	617	BCR	C3-C4-C5	-2.14	110.24	114.06
24	b	619	BCR	C15-C16-C17	-2.14	119.14	123.52
24	K	101	BCR	C33-C5-C6	-2.14	122.15	124.48
29	e	101	LHG	C11-C10-C9	-2.14	103.56	114.37
26	a	409	PL9	C45-C44-C46	-2.14	111.52	115.23
24	c	514	BCR	C27-C26-C25	2.14	125.59	122.70
23	A	404	PHO	C1-O2A-CGA	2.14	121.82	116.65
22	c	509	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
22	b	614	CLA	C4-C3-C5	2.14	118.94	115.23
23	d	401	PHO	C4B-NB-C1B	2.14	111.93	108.82
24	a	406	BCR	C37-C22-C23	2.13	121.35	118.09
35	V	201	HEC	CMC-C2C-C1C	-2.13	122.17	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	h	103	DGD	C7B-C6B-C5B	-2.13	103.58	114.37
35	v	201	HEC	C1B-C2B-C3B	2.13	109.22	106.98
22	B	612	CLA	CED-O2D-CGD	-2.13	111.08	115.92
22	C	507	CLA	CHB-C4A-NA	2.13	127.48	124.40
24	A	407	BCR	C36-C18-C19	2.13	121.35	118.09
22	c	502	CLA	CHD-C1D-ND	-2.13	121.80	124.80
24	b	618	BCR	C2-C1-C6	2.13	113.54	110.44
22	b	610	CLA	C16-C17-C18	-2.13	106.42	115.94
22	C	503	CLA	CHA-C1A-NA	-2.13	121.56	126.39
24	b	617	BCR	C29-C30-C25	2.13	113.53	110.44
24	C	514	BCR	C7-C8-C9	-2.13	123.08	126.23
22	B	603	CLA	CHB-C1B-NB	2.13	127.24	124.05
27	m	101	LMG	C22-C21-C20	-2.13	103.61	114.37
22	B	614	CLA	CHB-C1B-NB	2.13	127.24	124.05
23	d	401	PHO	CAA-CBA-CGA	-2.13	107.17	113.21
29	d	409	LHG	C27-C26-C25	-2.13	103.61	114.37
24	c	515	BCR	C2-C1-C6	2.13	113.53	110.44
24	h	101	BCR	C11-C10-C9	-2.13	124.29	127.28
22	c	503	CLA	CHB-C4A-NA	2.13	127.47	124.40
22	d	403	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
22	b	610	CLA	C2C-C1C-NC	2.13	112.22	109.98
22	B	601	CLA	CHA-C4D-ND	2.13	136.93	132.55
22	b	615	CLA	CMB-C2B-C3B	2.13	131.55	126.55
22	b	603	CLA	O1A-CGA-CBA	2.12	132.09	123.78
22	C	513	CLA	CHD-C4C-NC	2.12	127.52	124.23
22	b	616	CLA	C3B-C4B-NB	-2.12	108.64	110.53
24	h	101	BCR	C16-C17-C18	-2.12	124.30	127.28
30	c	518	DGD	CDB-CCB-CBB	-2.12	103.64	114.37
22	b	605	CLA	CHB-C1B-NB	2.12	127.23	124.05
30	H	102	DGD	CAB-C9B-C8B	-2.12	103.65	114.37
24	B	619	BCR	C28-C27-C26	-2.12	110.28	114.06
22	c	501	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
29	D	409	LHG	O8-C6-C5	-2.12	102.29	108.40
22	b	612	CLA	C3D-C4D-ND	2.12	113.43	109.99
22	A	403	CLA	C7-C6-C5	-2.12	107.62	113.26
22	C	512	CLA	C6-C5-C3	-2.12	108.31	113.47
22	B	609	CLA	CHB-C4A-NA	2.11	127.45	124.40
22	C	503	CLA	C3B-C4B-NB	-2.11	108.64	110.53
29	d	408	LHG	O8-C6-C5	-2.11	102.31	108.40
22	B	601	CLA	C4-C3-C5	2.11	118.89	115.23
27	c	521	LMG	O3-C3-C2	-2.11	105.40	110.38
30	h	103	DGD	O5E-C6E-C5E	-2.11	104.14	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	102	BCR	C8-C7-C6	-2.11	121.36	127.00
24	B	619	BCR	C37-C22-C23	2.11	121.31	118.09
22	a	403	CLA	C2D-C1D-ND	-2.11	108.04	110.13
22	b	607	CLA	C3B-C4B-NB	-2.11	108.65	110.53
22	b	605	CLA	O2D-CGD-CBD	2.11	114.91	111.23
22	B	615	CLA	C1-O2A-CGA	2.11	121.75	116.65
27	D	407	LMG	O2-C2-C1	-2.10	105.06	110.08
22	a	402	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
30	C	517	DGD	O3D-C3D-C4D	-2.10	105.42	110.38
22	C	510	CLA	C7-C6-C5	-2.10	107.66	113.26
29	L	101	LHG	C12-C11-C10	-2.10	103.75	114.37
24	C	514	BCR	C29-C30-C25	2.10	113.49	110.44
22	B	611	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
22	c	513	CLA	CHB-C4A-NA	2.10	127.43	124.40
22	b	616	CLA	CGD-CBD-CAD	-2.10	104.05	110.85
24	a	406	BCR	C2-C1-C6	2.10	113.48	110.44
22	c	502	CLA	CMB-C2B-C3B	2.10	131.48	126.55
27	c	519	LMG	C40-C39-C38	-2.10	103.78	114.37
22	c	510	CLA	O2D-CGD-CBD	2.09	114.89	111.23
32	C	518	STE	O2-C1-C2	2.09	120.61	114.00
22	d	404	CLA	C2A-C1A-CHA	2.09	127.50	123.87
27	M	101	LMG	C38-C37-C36	-2.09	103.80	114.37
29	l	101	LHG	O10-C23-C24	-2.09	115.60	123.78
22	b	602	CLA	CMB-C2B-C3B	2.09	131.47	126.55
29	D	411	LHG	O3-P-O5	-2.09	100.65	108.94
29	D	411	LHG	C11-C10-C9	-2.09	103.81	114.37
22	B	607	CLA	C2A-C1A-CHA	2.09	127.49	123.87
27	D	407	LMG	C9-C8-C7	-2.09	106.92	111.78
27	D	407	LMG	C3-C4-C5	-2.09	106.45	110.23
22	C	507	CLA	C4D-CHA-C1A	2.09	123.73	121.24
27	M	101	LMG	C17-C16-C15	-2.09	103.82	114.37
24	t	101	BCR	C40-C30-C29	-2.09	100.94	108.95
27	Y	101	LMG	O6-C1-O1	-2.09	105.11	110.04
34	f	101	HEM	O1D-CGD-CBD	-2.08	116.48	123.09
24	k	102	BCR	C16-C15-C14	-2.08	119.25	123.52
22	b	604	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
22	B	610	CLA	O1D-CGD-CBD	2.08	128.63	124.52
24	t	101	BCR	C19-C18-C17	-2.08	115.73	119.01
26	D	406	PL9	C30-C29-C31	-2.08	111.61	115.23
29	D	411	LHG	C20-C19-C18	-2.08	103.84	114.37
24	B	617	BCR	C27-C26-C25	2.08	125.52	122.70
22	d	405	CLA	CHD-C1D-ND	-2.08	121.87	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	101	BCR	C1-C6-C5	-2.08	119.79	122.64
30	c	517	DGD	C4E-C3E-C2E	-2.08	107.18	110.83
22	c	508	CLA	C11-C10-C8	-2.08	109.05	115.97
22	c	504	CLA	C1C-C2C-C3C	-2.08	104.79	106.98
22	D	402	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
22	C	513	CLA	C3A-C2A-C1A	2.08	104.45	101.34
30	C	516	DGD	O1G-C1A-O1A	-2.08	118.43	123.63
27	m	101	LMG	C6-C5-C4	-2.08	107.92	113.02
29	a	410	LHG	C20-C19-C18	-2.08	103.86	114.37
26	D	406	PL9	C8-C7-C3	2.08	117.40	112.03
30	A	415	DGD	O1G-C1A-O1A	-2.08	118.44	123.63
22	c	511	CLA	CHB-C4A-NA	2.07	127.39	124.40
22	C	502	CLA	C1-C2-C3	-2.07	122.80	126.20
24	t	101	BCR	C30-C25-C26	-2.07	119.81	122.64
22	C	501	CLA	OBD-CAD-C3D	2.07	133.25	128.42
22	c	513	CLA	O1D-CGD-CBD	2.07	128.60	124.52
30	C	517	DGD	C3D-C4D-C5D	-2.07	106.48	110.23
22	c	506	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
28	A	414	SQD	O47-C45-C46	2.07	110.96	106.21
22	C	502	CLA	CAA-C2A-C3A	-2.07	107.42	113.00
22	D	403	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
32	B	622	STE	O1-C1-C2	-2.07	116.54	123.09
22	b	606	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
27	M	101	LMG	O8-C28-O10	-2.06	118.47	123.63
30	c	517	DGD	C6D-O5D-C1E	2.06	118.22	113.80
22	C	508	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
24	a	406	BCR	C40-C30-C25	2.06	113.48	110.24
22	B	612	CLA	CHB-C4A-NA	2.06	127.37	124.40
22	d	404	CLA	C1D-ND-C4D	2.06	107.76	106.31
23	A	404	PHO	C3B-C4B-NB	-2.06	106.12	107.46
24	B	617	BCR	C15-C16-C17	-2.06	119.31	123.52
22	B	601	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
22	A	403	CLA	CHD-C1D-ND	-2.06	121.91	124.80
22	a	403	CLA	C4D-CHA-C1A	2.06	123.70	121.24
22	B	605	CLA	CHD-C1D-C2D	2.06	129.76	125.49
28	b	620	SQD	O5-C5-C4	2.06	113.40	109.70
22	C	503	CLA	C1-O2A-CGA	2.05	121.62	116.65
22	c	506	CLA	CMB-C2B-C3B	2.05	131.38	126.55
30	c	518	DGD	C6B-C5B-C4B	-2.05	104.00	114.37
22	A	403	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
22	B	610	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
23	A	404	PHO	C3D-C4D-ND	2.05	110.33	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	BCR	C15-C16-C17	-2.05	119.33	123.52
22	c	509	CLA	O1D-CGD-CBD	2.05	128.55	124.52
22	B	616	CLA	CHA-C1A-NA	-2.05	121.76	126.39
27	Y	101	LMG	C3-C4-C5	-2.04	106.53	110.23
30	c	516	DGD	C4A-C3A-C2A	-2.04	105.62	113.13
24	c	514	BCR	C7-C8-C9	-2.04	123.21	126.23
22	B	609	CLA	CHD-C4C-NC	2.04	127.40	124.23
26	D	406	PL9	C20-C19-C21	2.04	118.77	115.23
22	c	513	CLA	C4A-NA-C1A	2.04	107.61	106.68
22	B	614	CLA	CHA-C4D-ND	2.04	136.76	132.55
26	A	410	PL9	C41-C39-C38	-2.04	116.58	121.17
29	l	101	LHG	C20-C19-C18	-2.04	104.05	114.37
22	B	604	CLA	C11-C12-C13	-2.04	109.18	115.97
30	C	516	DGD	C8B-C7B-C6B	-2.04	104.05	114.37
29	D	408	LHG	C20-C19-C18	-2.04	104.06	114.37
24	h	101	BCR	C20-C21-C22	-2.04	124.42	127.28
29	D	408	LHG	C27-C26-C25	-2.04	104.06	114.37
24	d	406	BCR	C1-C6-C5	-2.04	119.85	122.64
22	B	603	CLA	CHB-C4A-NA	2.04	127.34	124.40
22	b	609	CLA	C1-C2-C3	-2.04	122.86	126.20
28	A	412	SQD	O9-S-O7	-2.04	107.20	113.82
22	b	607	CLA	O1D-CGD-CBD	2.04	128.53	124.52
24	b	618	BCR	C30-C25-C26	-2.04	119.85	122.64
32	M	102	STE	O2-C1-O1	-2.04	118.10	123.33
22	d	405	CLA	C4-C3-C5	2.03	118.76	115.23
23	a	404	PHO	C3D-C4D-ND	2.03	110.31	107.71
22	B	611	CLA	OBD-CAD-C3D	2.03	133.17	128.42
24	t	101	BCR	C38-C26-C27	-2.03	109.26	113.60
23	A	404	PHO	CBC-CAC-C3C	2.03	115.78	112.87
24	K	103	BCR	C3-C4-C5	-2.03	110.44	114.06
24	B	619	BCR	C1-C6-C5	-2.03	119.86	122.64
22	B	610	CLA	CHC-C1C-NC	2.03	127.37	124.31
24	b	619	BCR	C11-C10-C9	-2.03	124.43	127.28
22	c	502	CLA	CMB-C2B-C1B	-2.03	122.33	125.42
27	A	411	LMG	O8-C28-O10	-2.03	118.56	123.63
22	b	603	CLA	C4-C3-C5	2.03	118.74	115.23
22	d	404	CLA	CHD-C1D-C2D	2.03	129.70	125.49
22	B	602	CLA	CGD-CBD-CAD	-2.02	104.29	110.85
30	h	103	DGD	O6E-C5E-C6E	-2.02	101.42	106.44
24	K	103	BCR	C11-C10-C9	-2.02	124.44	127.28
22	C	502	CLA	C4D-CHA-C1A	2.02	123.66	121.24
32	B	623	STE	O2-C1-C2	2.02	120.39	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	PHO	OBD-CAD-C3D	2.02	131.04	127.89
22	b	613	CLA	CAA-CBA-CGA	2.02	118.94	113.21
24	h	101	BCR	C15-C16-C17	-2.02	119.39	123.52
22	c	504	CLA	CHB-C4A-NA	2.02	127.31	124.40
22	b	610	CLA	CHD-C1D-ND	-2.02	121.96	124.80
29	L	101	LHG	C27-C26-C25	-2.02	104.17	114.37
27	D	407	LMG	C38-C37-C36	-2.02	104.18	114.37
22	B	609	CLA	CHD-C1D-ND	-2.02	121.97	124.80
23	A	404	PHO	O2A-CGA-O1A	-2.02	118.59	123.63
24	b	618	BCR	C15-C14-C13	-2.01	124.45	127.28
30	h	103	DGD	O3E-C3E-C2E	-2.01	105.63	110.38
22	B	616	CLA	CHA-C4D-ND	2.01	136.70	132.55
22	C	508	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
22	B	603	CLA	O1A-CGA-CBA	2.01	131.65	123.78
22	b	610	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
30	h	103	DGD	O2D-C2D-C1D	-2.01	105.28	110.08
24	D	405	BCR	C8-C7-C6	-2.01	121.63	127.00
22	c	513	CLA	C1D-ND-C4D	-2.01	104.90	106.31
22	b	610	CLA	C11-C12-C13	-2.01	109.29	115.97
22	C	511	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
24	b	618	BCR	C8-C7-C6	-2.01	121.64	127.00
24	H	101	BCR	C16-C15-C14	-2.01	119.41	123.52
27	d	410	LMG	C1-O6-C5	-2.01	109.80	113.72
30	C	515	DGD	CDB-CCB-CBB	-2.01	104.23	114.37
22	c	506	CLA	CHA-C1A-NA	-2.01	121.85	126.39
22	b	616	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
22	b	607	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
22	A	402	CLA	C1-C2-C3	-2.00	122.92	126.20
35	v	201	HEC	C3D-C4D-ND	-2.00	108.42	110.35
27	A	411	LMG	O7-C10-O9	-2.00	119.03	123.70
35	V	201	HEC	CHC-C1C-NC	2.00	127.49	123.86
22	c	504	CLA	CMC-C2C-C1C	2.00	128.16	125.03
35	v	201	HEC	C1D-C2D-C3D	-2.00	104.88	106.98
22	A	403	CLA	CHB-C1B-NB	2.00	127.05	124.05
24	A	407	BCR	C8-C7-C6	-2.00	121.65	127.00

All (2) chirality outliers are listed below:

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

All (1793) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C2B-C3B-CAB-CBB
22	A	403	CLA	C4B-C3B-CAB-CBB
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	614	CLA	CAD-CBD-CGD-O1D
22	B	614	CLA	CAD-CBD-CGD-O2D
22	C	507	CLA	CHA-CBD-CGD-O1D
22	C	507	CLA	CHA-CBD-CGD-O2D
22	C	509	CLA	C11-C10-C8-C9
22	C	512	CLA	C2B-C3B-CAB-CBB
22	C	512	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C11-C10-C8-C9
22	C	513	CLA	C6-C7-C8-C9
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	C2-C3-C5-C6
22	b	616	CLA	C4-C3-C5-C6
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
24	B	617	BCR	C35-C13-C14-C15
24	B	618	BCR	C20-C21-C22-C37
24	C	514	BCR	C16-C17-C18-C19
24	C	514	BCR	C36-C18-C19-C20
24	D	405	BCR	C35-C13-C14-C15
24	D	405	BCR	C23-C24-C25-C26
24	H	101	BCR	C11-C12-C13-C14
24	H	101	BCR	C11-C12-C13-C35
24	K	101	BCR	C10-C11-C12-C13
24	K	101	BCR	C16-C17-C18-C19
24	K	101	BCR	C16-C17-C18-C36
24	K	102	BCR	C5-C6-C7-C8
24	K	102	BCR	C21-C22-C23-C24
24	K	102	BCR	C37-C22-C23-C24
24	T	101	BCR	C1-C6-C7-C8
24	T	101	BCR	C7-C8-C9-C10
24	T	101	BCR	C12-C13-C14-C15
24	T	101	BCR	C16-C17-C18-C36
24	b	617	BCR	C20-C21-C22-C37
24	b	617	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	b	619	BCR	C35-C13-C14-C15
24	b	619	BCR	C20-C21-C22-C37
24	c	514	BCR	C11-C12-C13-C14
24	c	514	BCR	C18-C19-C20-C21
24	d	406	BCR	C7-C8-C9-C34
24	d	406	BCR	C37-C22-C23-C24
24	d	406	BCR	C22-C23-C24-C25
24	k	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C7-C8-C9-C34
24	k	101	BCR	C17-C18-C19-C20
26	A	410	PL9	C22-C23-C24-C25
26	A	410	PL9	C32-C33-C34-C36
26	A	410	PL9	C37-C38-C39-C40
26	A	410	PL9	C37-C38-C39-C41
26	D	406	PL9	C32-C33-C34-C35
26	D	406	PL9	C32-C33-C34-C36
26	D	406	PL9	C47-C48-C49-C51
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C42-C43-C44-C45
26	a	409	PL9	C47-C48-C49-C51
26	d	407	PL9	C32-C33-C34-C36
26	d	407	PL9	C42-C43-C44-C46
27	A	411	LMG	O9-C10-O7-C8
27	A	411	LMG	C11-C10-O7-C8
27	a	414	LMG	O6-C1-O1-C7
27	a	414	LMG	O10-C28-O8-C9
28	A	414	SQD	C44-C45-C46-O48
28	A	414	SQD	C46-C45-O47-C7
28	B	621	SQD	C2-C1-O6-C44
28	B	621	SQD	O5-C1-O6-C44
28	B	621	SQD	O6-C44-C45-O47
28	B	621	SQD	O49-C7-O47-C45
28	B	621	SQD	C8-C7-O47-C45
28	F	102	SQD	C45-C44-O6-C1
28	F	102	SQD	C2-C1-O6-C44
28	a	412	SQD	C8-C7-O47-C45
28	a	412	SQD	O10-C23-O48-C46
28	b	620	SQD	C46-C45-O47-C7
28	b	620	SQD	C8-C7-O47-C45
28	b	620	SQD	O10-C23-O48-C46
28	b	620	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
28	f	102	SQD	O5-C1-O6-C44
28	f	102	SQD	O49-C7-O47-C45
29	D	408	LHG	O1-C1-C2-C3
29	D	408	LHG	O2-C2-C3-O3
29	D	408	LHG	C3-O3-P-O4
29	D	408	LHG	C3-O3-P-O6
29	D	408	LHG	C4-O6-P-O4
29	D	409	LHG	C1-C2-C3-O3
29	D	409	LHG	O2-C2-C3-O3
29	D	409	LHG	C3-O3-P-O4
29	D	409	LHG	C3-O3-P-O5
29	D	409	LHG	C3-O3-P-O6
29	D	411	LHG	O1-C1-C2-C3
29	L	101	LHG	C3-O3-P-O4
29	L	101	LHG	C4-O6-P-O4
29	a	410	LHG	C3-O3-P-O4
29	a	410	LHG	C3-O3-P-O5
29	a	410	LHG	C3-O3-P-O6
29	d	408	LHG	C3-O3-P-O4
29	d	408	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O4
29	d	408	LHG	C4-O6-P-O5
29	e	101	LHG	C3-O3-P-O5
29	e	101	LHG	C3-O3-P-O6
29	l	101	LHG	C4-O6-P-O3
29	l	101	LHG	C4-O6-P-O4
29	l	101	LHG	C4-O6-P-O5
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
30	o	301	DGD	C2B-C1B-O2G-C2G
30	o	301	DGD	O1B-C1B-O2G-C2G
22	c	509	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	CBD-CGD-O2D-CED
22	c	509	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
23	d	401	PHO	CBD-CGD-O2D-CED
27	M	101	LMG	O10-C28-O8-C9
29	e	101	LHG	O10-C23-O8-C6
26	a	409	PL9	C47-C48-C49-C50
26	d	407	PL9	C47-C48-C49-C51
27	a	414	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
28	F	102	SQD	C24-C23-O48-C46
28	a	412	SQD	C24-C23-O48-C46
28	F	102	SQD	O10-C23-O48-C46
27	c	521	LMG	O10-C28-O8-C9
27	c	521	LMG	O9-C10-O7-C8
28	b	620	SQD	O49-C7-O47-C45
22	A	403	CLA	C3-C5-C6-C7
22	b	601	CLA	C3-C5-C6-C7
22	b	602	CLA	C3-C5-C6-C7
22	c	513	CLA	C3-C5-C6-C7
35	V	201	HEC	C2C-C3C-CAC-CBC
27	M	101	LMG	C29-C28-O8-C9
28	f	102	SQD	C24-C23-O48-C46
29	e	101	LHG	C24-C23-O8-C6
22	c	513	CLA	CBD-CGD-O2D-CED
28	f	102	SQD	C8-C7-O47-C45
22	A	406	CLA	C4-C3-C5-C6
22	C	507	CLA	C4-C3-C5-C6
22	A	406	CLA	C2-C3-C5-C6
22	C	507	CLA	C2-C3-C5-C6
26	A	410	PL9	C23-C24-C26-C27
26	a	409	PL9	C33-C34-C36-C37
28	f	102	SQD	O10-C23-O48-C46
22	B	608	CLA	C3-C5-C6-C7
22	C	513	CLA	C3-C5-C6-C7
22	b	614	CLA	C3-C5-C6-C7
27	c	521	LMG	C29-C28-O8-C9
26	a	409	PL9	C7-C8-C9-C10
26	A	410	PL9	C22-C23-C24-C26
26	a	409	PL9	C42-C43-C44-C46
30	h	103	DGD	O6E-C5E-C6E-O5E
27	b	623	LMG	O10-C28-O8-C9
30	o	301	DGD	O1A-C1A-O1G-C1G
28	a	412	SQD	O49-C7-O47-C45
22	c	511	CLA	O1D-CGD-O2D-CED
22	B	616	CLA	C3-C5-C6-C7
22	C	501	CLA	CBD-CGD-O2D-CED
27	Y	101	LMG	C29-C28-O8-C9
30	c	518	DGD	O1A-C1A-O1G-C1G
27	M	101	LMG	O6-C5-C6-O5
27	Y	101	LMG	C11-C10-O7-C8
23	d	401	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	V	201	HEC	C4C-C3C-CAC-CBC
30	C	515	DGD	O6E-C5E-C6E-O5E
22	C	513	CLA	CBA-CGA-O2A-C1
22	B	614	CLA	C4-C3-C5-C6
22	C	513	CLA	C4-C3-C5-C6
22	b	614	CLA	C4-C3-C5-C6
22	c	507	CLA	C4-C3-C5-C6
26	a	409	PL9	C35-C34-C36-C37
26	d	407	PL9	C40-C39-C41-C42
22	B	614	CLA	C2-C3-C5-C6
22	c	507	CLA	C2-C3-C5-C6
26	A	410	PL9	C18-C19-C21-C22
26	d	407	PL9	C38-C39-C41-C42
26	A	410	PL9	C9-C11-C12-C13
26	A	410	PL9	C14-C16-C17-C18
26	A	410	PL9	C19-C21-C22-C23
26	A	410	PL9	C24-C26-C27-C28
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C34-C36-C37-C38
30	h	103	DGD	C4E-C5E-C6E-O5E
22	C	511	CLA	CBD-CGD-O2D-CED
22	c	503	CLA	CBD-CGD-O2D-CED
34	f	101	HEM	C2A-CAA-CBA-CGA
27	b	623	LMG	O6-C1-O1-C7
28	b	620	SQD	O5-C1-O6-C44
30	H	102	DGD	O6E-C5E-C6E-O5E
27	M	101	LMG	C4-C5-C6-O5
30	o	301	DGD	C2A-C1A-O1G-C1G
22	C	513	CLA	CBD-CGD-O2D-CED
26	A	410	PL9	C12-C13-C14-C15
22	C	513	CLA	O1A-CGA-O2A-C1
30	A	415	DGD	O6E-C5E-C6E-O5E
26	D	406	PL9	C47-C48-C49-C50
29	l	101	LHG	C7-C8-C9-C10
30	A	415	DGD	C4E-C5E-C6E-O5E
27	b	623	LMG	O9-C10-O7-C8
22	c	506	CLA	CBA-CGA-O2A-C1
28	B	621	SQD	C24-C23-O48-C46
30	c	518	DGD	C2A-C1A-O1G-C1G
32	B	625	STE	C11-C12-C13-C14
22	C	513	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C2-C3-C5-C6
26	d	407	PL9	C47-C48-C49-C50
22	A	403	CLA	C14-C13-C15-C16
22	B	601	CLA	C11-C12-C13-C14
22	B	613	CLA	C11-C12-C13-C14
22	C	503	CLA	C11-C10-C8-C9
22	C	506	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C10-C8-C9
22	b	604	CLA	C6-C7-C8-C9
22	b	605	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	509	CLA	C6-C7-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	c	511	CLA	C14-C13-C15-C16
22	c	512	CLA	C6-C7-C8-C9
22	c	513	CLA	C6-C7-C8-C9
22	d	404	CLA	C14-C13-C15-C16
28	A	414	SQD	C44-C45-O47-C7
27	b	623	LMG	C2-C1-O1-C7
32	d	412	STE	C1-C2-C3-C4
24	B	618	BCR	C7-C8-C9-C34
24	B	619	BCR	C11-C12-C13-C35
24	C	514	BCR	C7-C8-C9-C34
24	K	101	BCR	C11-C12-C13-C35
24	b	618	BCR	C11-C12-C13-C35
24	b	619	BCR	C7-C8-C9-C34
24	b	619	BCR	C11-C12-C13-C35
24	c	514	BCR	C11-C12-C13-C35
24	k	101	BCR	C36-C18-C19-C20
24	k	101	BCR	C37-C22-C23-C24
24	d	406	BCR	C21-C22-C23-C24
22	c	512	CLA	C2A-CAA-CBA-CGA
35	v	201	HEC	C4C-C3C-CAC-CBC
27	D	407	LMG	C10-C11-C12-C13
30	A	415	DGD	O2G-C2G-C3G-O3G
27	m	101	LMG	C29-C28-O8-C9
22	c	513	CLA	O1D-CGD-O2D-CED
22	c	502	CLA	CBD-CGD-O2D-CED
22	C	505	CLA	C5-C6-C7-C8
22	b	605	CLA	C10-C11-C12-C13
28	b	620	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	c	507	CLA	C5-C6-C7-C8
22	C	508	CLA	C12-C13-C15-C16
22	C	510	CLA	C12-C13-C15-C16
22	D	404	CLA	C11-C10-C8-C7
22	b	614	CLA	C11-C12-C13-C15
22	c	506	CLA	C12-C13-C15-C16
30	A	415	DGD	C2A-C1A-O1G-C1G
27	Y	101	LMG	O6-C5-C6-O5
22	D	403	CLA	C13-C15-C16-C17
26	A	410	PL9	C34-C36-C37-C38
26	A	410	PL9	C44-C46-C47-C48
27	a	414	LMG	C15-C16-C17-C18
22	b	602	CLA	C15-C16-C17-C18
22	c	509	CLA	C10-C11-C12-C13
29	A	413	LHG	C24-C25-C26-C27
27	c	521	LMG	O6-C5-C6-O5
27	A	411	LMG	C28-C29-C30-C31
27	D	410	LMG	C10-C11-C12-C13
28	A	412	SQD	C7-C8-C9-C10
28	B	621	SQD	C23-C24-C25-C26
30	o	301	DGD	C1B-C2B-C3B-C4B
32	C	518	STE	C1-C2-C3-C4
22	c	506	CLA	O1A-CGA-O2A-C1
22	B	614	CLA	C13-C15-C16-C17
22	C	512	CLA	C10-C11-C12-C13
22	b	604	CLA	C10-C11-C12-C13
22	b	608	CLA	C13-C15-C16-C17
22	b	616	CLA	C8-C10-C11-C12
24	K	103	BCR	C18-C19-C20-C21
22	B	603	CLA	C8-C10-C11-C12
22	C	509	CLA	C13-C15-C16-C17
22	C	513	CLA	C5-C6-C7-C8
22	c	511	CLA	C15-C16-C17-C18
22	d	404	CLA	C15-C16-C17-C18
28	f	102	SQD	C23-C24-C25-C26
29	e	101	LHG	C23-C24-C25-C26
22	b	613	CLA	CBD-CGD-O2D-CED
30	C	516	DGD	O6E-C1E-O5D-C6D
32	C	520	STE	C4-C5-C6-C7
30	C	515	DGD	C4E-C5E-C6E-O5E
22	B	602	CLA	C13-C15-C16-C17
22	B	607	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	B	614	CLA	C8-C10-C11-C12
22	C	506	CLA	C13-C15-C16-C17
22	C	512	CLA	C13-C15-C16-C17
22	a	405	CLA	C10-C11-C12-C13
22	b	607	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
22	b	611	CLA	C13-C15-C16-C17
22	b	615	CLA	C8-C10-C11-C12
22	c	505	CLA	C15-C16-C17-C18
22	c	506	CLA	C13-C15-C16-C17
29	A	413	LHG	O2-C2-C3-O3
22	B	616	CLA	C5-C6-C7-C8
22	C	511	CLA	C8-C10-C11-C12
22	c	503	CLA	C8-C10-C11-C12
22	c	505	CLA	C13-C15-C16-C17
22	c	509	CLA	C5-C6-C7-C8
27	D	410	LMG	O9-C10-O7-C8
27	m	101	LMG	O9-C10-O7-C8
22	B	607	CLA	C13-C15-C16-C17
22	C	513	CLA	C15-C16-C17-C18
22	a	405	CLA	C15-C16-C17-C18
22	b	614	CLA	C5-C6-C7-C8
22	c	512	CLA	C13-C15-C16-C17
27	d	410	LMG	C28-C29-C30-C31
29	a	410	LHG	C23-C24-C25-C26
22	A	403	CLA	C13-C15-C16-C17
22	B	613	CLA	C8-C10-C11-C12
22	B	615	CLA	C5-C6-C7-C8
22	C	504	CLA	C8-C10-C11-C12
22	C	506	CLA	C8-C10-C11-C12
22	b	603	CLA	C5-C6-C7-C8
22	B	604	CLA	CBA-CGA-O2A-C1
22	B	614	CLA	C15-C16-C17-C18
30	A	415	DGD	O6D-C5D-C6D-O5D
22	C	505	CLA	C10-C11-C12-C13
22	c	503	CLA	C5-C6-C7-C8
32	B	623	STE	C1-C2-C3-C4
27	Y	101	LMG	O9-C10-O7-C8
29	A	413	LHG	C1-C2-C3-O3
22	b	606	CLA	C2A-CAA-CBA-CGA
28	F	102	SQD	O6-C44-C45-C46
22	A	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	C	502	CLA	C13-C15-C16-C17
22	C	510	CLA	C13-C15-C16-C17
22	D	404	CLA	C13-C15-C16-C17
22	a	403	CLA	C8-C10-C11-C12
22	b	616	CLA	C10-C11-C12-C13
22	c	511	CLA	C13-C15-C16-C17
22	a	405	CLA	C5-C6-C7-C8
22	b	605	CLA	C5-C6-C7-C8
22	B	606	CLA	C10-C11-C12-C13
22	B	606	CLA	C15-C16-C17-C18
22	C	503	CLA	C5-C6-C7-C8
22	C	512	CLA	C8-C10-C11-C12
22	D	402	CLA	C15-C16-C17-C18
22	B	601	CLA	CBA-CGA-O2A-C1
22	c	503	CLA	O1D-CGD-O2D-CED
22	c	507	CLA	C14-C13-C15-C16
28	f	102	SQD	C2-C1-O6-C44
30	C	516	DGD	C2E-C1E-O5D-C6D
30	c	517	DGD	C2E-C1E-O5D-C6D
22	b	606	CLA	C10-C11-C12-C13
27	c	521	LMG	C10-C11-C12-C13
30	C	515	DGD	C1B-C2B-C3B-C4B
27	b	623	LMG	C29-C28-O8-C9
22	B	616	CLA	C11-C12-C13-C15
22	b	611	CLA	C16-C17-C18-C20
24	A	407	BCR	C35-C13-C14-C15
24	B	617	BCR	C11-C10-C9-C34
24	K	103	BCR	C11-C10-C9-C34
24	K	103	BCR	C20-C21-C22-C37
24	T	101	BCR	C35-C13-C14-C15
24	T	101	BCR	C20-C21-C22-C37
24	b	617	BCR	C35-C13-C14-C15
24	b	618	BCR	C35-C13-C14-C15
24	b	618	BCR	C16-C17-C18-C36
24	d	406	BCR	C20-C21-C22-C37
24	k	101	BCR	C35-C13-C14-C15
32	b	625	STE	C1-C2-C3-C4
24	B	618	BCR	C37-C22-C23-C24
24	K	103	BCR	C7-C8-C9-C34
24	T	101	BCR	C7-C8-C9-C34
24	T	101	BCR	C11-C12-C13-C35
24	h	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	A	407	BCR	C11-C12-C13-C14
24	T	101	BCR	C17-C18-C19-C20
22	B	606	CLA	C2A-CAA-CBA-CGA
22	b	601	CLA	C2A-CAA-CBA-CGA
22	B	609	CLA	C13-C15-C16-C17
22	C	509	CLA	C5-C6-C7-C8
22	b	601	CLA	C10-C11-C12-C13
22	b	606	CLA	C15-C16-C17-C18
22	b	612	CLA	C13-C15-C16-C17
29	a	410	LHG	O1-C1-C2-C3
29	d	409	LHG	O1-C1-C2-C3
27	b	623	LMG	C9-C8-O7-C10
26	A	410	PL9	C47-C48-C49-C51
22	B	603	CLA	C16-C17-C18-C20
22	B	609	CLA	C16-C17-C18-C20
22	B	612	CLA	C16-C17-C18-C20
22	C	502	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C20
22	b	615	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C20
22	c	509	CLA	C16-C17-C18-C20
22	C	501	CLA	O1D-CGD-O2D-CED
24	B	617	BCR	C11-C10-C9-C8
24	B	617	BCR	C12-C13-C14-C15
24	B	618	BCR	C11-C10-C9-C8
24	B	619	BCR	C12-C13-C14-C15
24	C	514	BCR	C12-C13-C14-C15
24	T	101	BCR	C16-C17-C18-C19
24	b	617	BCR	C20-C21-C22-C23
24	h	101	BCR	C11-C10-C9-C8
24	k	101	BCR	C12-C13-C14-C15
30	c	516	DGD	CAA-CBA-CCA-CDA
32	B	624	STE	C11-C12-C13-C14
28	F	102	SQD	O5-C1-O6-C44
30	c	517	DGD	O6E-C1E-O5D-C6D
27	D	410	LMG	C11-C10-O7-C8
27	c	521	LMG	C11-C10-O7-C8
26	A	410	PL9	C33-C34-C36-C37
27	M	101	LMG	C28-C29-C30-C31
22	B	616	CLA	C11-C12-C13-C14
22	C	506	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	b	615	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C20
27	Y	101	LMG	C13-C14-C15-C16
28	A	412	SQD	C34-C35-C36-C37
28	A	414	SQD	C13-C14-C15-C16
30	C	516	DGD	C5A-C6A-C7A-C8A
30	h	103	DGD	C3A-C4A-C5A-C6A
24	K	101	BCR	C14-C15-C16-C17
27	M	101	LMG	C33-C34-C35-C36
27	M	101	LMG	C36-C37-C38-C39
28	B	621	SQD	C11-C12-C13-C14
28	a	411	SQD	C9-C10-C11-C12
28	a	412	SQD	C15-C16-C17-C18
28	a	412	SQD	C24-C25-C26-C27
28	f	102	SQD	C28-C29-C30-C31
28	f	102	SQD	C33-C34-C35-C36
29	A	413	LHG	C10-C11-C12-C13
30	A	415	DGD	CEB-CFB-CGB-CHB
30	C	515	DGD	C3B-C4B-C5B-C6B
30	o	301	DGD	C2A-C3A-C4A-C5A
32	B	626	STE	C5-C6-C7-C8
32	B	627	STE	C5-C6-C7-C8
32	T	102	STE	C9-C10-C11-C12
32	b	624	STE	C3-C4-C5-C6
32	c	520	STE	C9-C10-C11-C12
30	c	517	DGD	C1A-C2A-C3A-C4A
22	C	513	CLA	C8-C10-C11-C12
22	b	607	CLA	C8-C10-C11-C12
27	c	519	LMG	C33-C34-C35-C36
29	d	409	LHG	C34-C35-C36-C37
30	c	517	DGD	CBB-CCB-CDB-CEB
30	h	103	DGD	C6A-C7A-C8A-C9A
32	B	620	STE	C10-C11-C12-C13
32	M	104	STE	C9-C10-C11-C12
22	c	512	CLA	CBA-CGA-O2A-C1
27	h	102	LMG	C36-C37-C38-C39
29	D	411	LHG	C16-C17-C18-C19
29	d	408	LHG	C28-C29-C30-C31
29	l	101	LHG	C17-C18-C19-C20
30	c	518	DGD	CCB-CDB-CEB-CFB
32	b	622	STE	C14-C15-C16-C17
27	c	519	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C17-C18-C19-C20
27	a	414	LMG	C29-C30-C31-C32
27	a	414	LMG	C31-C32-C33-C34
30	A	415	DGD	CCB-CDB-CEB-CFB
30	o	301	DGD	C6A-C7A-C8A-C9A
30	o	301	DGD	C2B-C3B-C4B-C5B
22	C	513	CLA	O1D-CGD-O2D-CED
22	b	613	CLA	O1D-CGD-O2D-CED
22	B	606	CLA	C4B-C3B-CAB-CBB
22	b	601	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C4B-C3B-CAB-CBB
29	L	101	LHG	C14-C15-C16-C17
29	L	101	LHG	C30-C31-C32-C33
30	C	515	DGD	C5B-C6B-C7B-C8B
30	C	516	DGD	C4A-C5A-C6A-C7A
30	C	516	DGD	C6A-C7A-C8A-C9A
30	c	518	DGD	C4A-C5A-C6A-C7A
30	h	103	DGD	C6B-C7B-C8B-C9B
22	B	609	CLA	C16-C17-C18-C19
22	C	506	CLA	C16-C17-C18-C19
22	b	611	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C19
22	C	511	CLA	O1D-CGD-O2D-CED
29	A	413	LHG	C28-C29-C30-C31
30	C	517	DGD	CBA-CCA-CDA-CEA
30	c	518	DGD	C5B-C6B-C7B-C8B
30	o	301	DGD	C9A-CAA-CBA-CCA
32	T	102	STE	C7-C8-C9-C10
22	C	507	CLA	C5-C6-C7-C8
22	b	616	CLA	C5-C6-C7-C8
28	A	412	SQD	C16-C17-C18-C19
32	D	413	STE	C11-C10-C9-C8
32	b	621	STE	C9-C10-C11-C12
32	d	412	STE	C6-C7-C8-C9
22	b	602	CLA	C11-C12-C13-C15
22	c	504	CLA	C11-C10-C8-C7
32	b	621	STE	C6-C7-C8-C9
32	c	520	STE	C7-C8-C9-C10
32	J	101	STE	C1-C2-C3-C4
32	j	101	STE	C1-C2-C3-C4
22	c	510	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	h	102	LMG	C37-C38-C39-C40
28	B	621	SQD	C33-C34-C35-C36
28	a	411	SQD	C12-C13-C14-C15
28	b	620	SQD	C16-C17-C18-C19
29	A	413	LHG	C30-C31-C32-C33
29	a	410	LHG	C28-C29-C30-C31
29	e	101	LHG	C16-C17-C18-C19
30	C	515	DGD	C6A-C7A-C8A-C9A
30	C	517	DGD	C4A-C5A-C6A-C7A
30	c	516	DGD	C4A-C5A-C6A-C7A
30	c	516	DGD	C3B-C4B-C5B-C6B
32	d	412	STE	C3-C4-C5-C6
22	B	604	CLA	O1A-CGA-O2A-C1
22	b	604	CLA	C3-C5-C6-C7
22	b	601	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
26	A	410	PL9	C40-C39-C41-C42
26	A	410	PL9	C45-C44-C46-C47
27	D	407	LMG	C17-C18-C19-C20
27	c	521	LMG	C30-C31-C32-C33
28	a	411	SQD	C34-C35-C36-C37
29	D	409	LHG	C29-C30-C31-C32
30	o	301	DGD	CCA-CDA-CEA-CFA
32	b	624	STE	C11-C10-C9-C8
29	D	408	LHG	C30-C31-C32-C33
29	D	409	LHG	C32-C33-C34-C35
22	b	604	CLA	C15-C16-C17-C18
22	c	502	CLA	O1D-CGD-O2D-CED
24	c	514	BCR	C13-C14-C15-C16
22	B	615	CLA	C16-C17-C18-C20
22	a	402	CLA	C16-C17-C18-C19
22	d	403	CLA	C16-C17-C18-C20
28	f	102	SQD	C25-C26-C27-C28
27	b	623	LMG	C32-C33-C34-C35
29	d	408	LHG	C26-C27-C28-C29
32	M	102	STE	C6-C7-C8-C9
32	a	415	STE	C4-C5-C6-C7
29	D	408	LHG	C1-C2-C3-O3
28	a	411	SQD	C24-C23-O48-C46
27	h	102	LMG	C33-C34-C35-C36
28	B	621	SQD	C17-C18-C19-C20
29	A	413	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
30	h	103	DGD	C2B-C3B-C4B-C5B
27	M	101	LMG	C10-C11-C12-C13
32	c	520	STE	C1-C2-C3-C4
27	A	411	LMG	C33-C34-C35-C36
27	a	414	LMG	C11-C12-C13-C14
27	a	414	LMG	C17-C18-C19-C20
27	b	623	LMG	C15-C16-C17-C18
29	D	409	LHG	C25-C26-C27-C28
29	a	410	LHG	C15-C16-C17-C18
29	d	408	LHG	C29-C30-C31-C32
30	A	415	DGD	CAA-CBA-CCA-CDA
30	c	518	DGD	CBA-CCA-CDA-CEA
30	c	518	DGD	CCA-CDA-CEA-CFA
32	D	412	STE	C9-C10-C11-C12
29	L	101	LHG	C12-C13-C14-C15
30	C	516	DGD	C8B-C9B-CAB-CBB
30	o	301	DGD	C4A-C5A-C6A-C7A
32	M	102	STE	C11-C10-C9-C8
27	b	623	LMG	C18-C19-C20-C21
27	c	519	LMG	C38-C39-C40-C41
29	D	408	LHG	C29-C30-C31-C32
30	C	517	DGD	C8A-C9A-CAA-CBA
32	H	103	STE	C6-C7-C8-C9
22	b	603	CLA	C8-C10-C11-C12
27	D	407	LMG	C15-C16-C17-C18
29	A	413	LHG	C12-C13-C14-C15
30	o	301	DGD	CDB-CEB-CFB-CGB
32	b	625	STE	C12-C13-C14-C15
32	d	411	STE	C11-C12-C13-C14
26	d	407	PL9	C42-C43-C44-C45
22	B	603	CLA	C16-C17-C18-C19
27	Y	101	LMG	O10-C28-O8-C9
24	D	405	BCR	C23-C24-C25-C30
24	K	102	BCR	C1-C6-C7-C8
24	T	101	BCR	C5-C6-C7-C8
24	k	101	BCR	C1-C6-C7-C8
27	c	521	LMG	C39-C40-C41-C42
28	a	411	SQD	C24-C25-C26-C27
29	l	101	LHG	C31-C32-C33-C34
32	M	102	STE	C9-C10-C11-C12
27	b	623	LMG	C11-C10-O7-C8
27	Y	101	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
27	c	519	LMG	C39-C40-C41-C42
28	b	620	SQD	C12-C13-C14-C15
27	D	407	LMG	C35-C36-C37-C38
28	A	412	SQD	C10-C11-C12-C13
28	A	414	SQD	C18-C19-C20-C21
29	D	409	LHG	C13-C14-C15-C16
30	c	517	DGD	C8B-C9B-CAB-CBB
30	c	517	DGD	C4E-C5E-C6E-O5E
29	A	413	LHG	C23-C24-C25-C26
22	B	604	CLA	C10-C11-C12-C13
27	A	411	LMG	C12-C13-C14-C15
27	b	623	LMG	C40-C41-C42-C43
30	C	515	DGD	C4B-C5B-C6B-C7B
22	B	601	CLA	O1A-CGA-O2A-C1
22	c	512	CLA	O1A-CGA-O2A-C1
27	a	414	LMG	C32-C33-C34-C35
32	C	519	STE	C4-C5-C6-C7
32	d	412	STE	C11-C12-C13-C14
27	h	102	LMG	C34-C35-C36-C37
27	m	101	LMG	C33-C34-C35-C36
30	c	516	DGD	C4B-C5B-C6B-C7B
24	B	618	BCR	C18-C19-C20-C21
24	K	102	BCR	C10-C11-C12-C13
26	d	407	PL9	C33-C34-C36-C37
22	B	615	CLA	C16-C17-C18-C19
22	C	502	CLA	C16-C17-C18-C19
22	c	503	CLA	C16-C17-C18-C19
27	a	414	LMG	C12-C13-C14-C15
27	b	623	LMG	C19-C20-C21-C22
32	B	625	STE	C5-C6-C7-C8
32	B	627	STE	C4-C5-C6-C7
32	M	104	STE	C14-C15-C16-C17
32	b	621	STE	C5-C6-C7-C8
32	B	627	STE	C1-C2-C3-C4
22	a	405	CLA	CBA-CGA-O2A-C1
28	A	414	SQD	C24-C23-O48-C46
22	B	606	CLA	C11-C10-C8-C9
32	b	622	STE	C6-C7-C8-C9
22	B	605	CLA	C15-C16-C17-C18
27	D	407	LMG	C30-C31-C32-C33
30	h	103	DGD	C5B-C6B-C7B-C8B
32	B	622	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
32	H	103	STE	C4-C5-C6-C7
32	d	411	STE	C5-C6-C7-C8
24	c	514	BCR	C22-C23-C24-C25
30	A	415	DGD	C4D-C5D-C6D-O5D
24	k	101	BCR	C14-C15-C16-C17
29	d	409	LHG	C24-C25-C26-C27
30	C	516	DGD	C7A-C8A-C9A-CAA
30	C	517	DGD	C6B-C7B-C8B-C9B
27	a	414	LMG	C2-C1-O1-C7
22	B	601	CLA	C8-C10-C11-C12
22	B	603	CLA	C10-C11-C12-C13
22	b	615	CLA	C15-C16-C17-C18
27	M	101	LMG	C16-C17-C18-C19
28	a	412	SQD	C14-C15-C16-C17
30	A	415	DGD	C2B-C3B-C4B-C5B
30	A	415	DGD	C5B-C6B-C7B-C8B
32	T	102	STE	C10-C11-C12-C13
26	A	410	PL9	C47-C48-C49-C50
27	m	101	LMG	C37-C38-C39-C40
29	d	408	LHG	C13-C14-C15-C16
32	D	413	STE	C4-C5-C6-C7
27	D	407	LMG	C37-C38-C39-C40
27	M	101	LMG	C32-C33-C34-C35
29	L	101	LHG	C32-C33-C34-C35
32	C	518	STE	C4-C5-C6-C7
32	H	103	STE	C2-C3-C4-C5
32	c	520	STE	C6-C7-C8-C9
22	B	606	CLA	C16-C17-C18-C20
29	D	408	LHG	C8-C7-O7-C5
27	Y	101	LMG	C17-C18-C19-C20
22	C	509	CLA	C10-C11-C12-C13
28	A	414	SQD	C24-C25-C26-C27
29	a	410	LHG	C16-C17-C18-C19
30	c	517	DGD	CAA-CBA-CCA-CDA
30	o	301	DGD	C3B-C4B-C5B-C6B
22	c	510	CLA	C10-C11-C12-C13
24	c	515	BCR	C7-C8-C9-C34
27	D	410	LMG	C36-C37-C38-C39
28	a	412	SQD	C11-C12-C13-C14
27	c	521	LMG	C38-C39-C40-C41
32	I	101	STE	C7-C8-C9-C10
22	D	403	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	d	409	LHG	C27-C28-C29-C30
30	C	517	DGD	C5A-C6A-C7A-C8A
32	M	102	STE	C7-C8-C9-C10
32	M	104	STE	C10-C11-C12-C13
27	d	410	LMG	C36-C37-C38-C39
30	c	518	DGD	C9B-CAB-CBB-CCB
32	d	411	STE	C3-C4-C5-C6
30	H	102	DGD	CCB-CDB-CEB-CFB
30	H	102	DGD	C4E-C5E-C6E-O5E
30	A	415	DGD	C4B-C5B-C6B-C7B
22	A	406	CLA	C3-C5-C6-C7
22	B	613	CLA	C5-C6-C7-C8
27	b	623	LMG	C38-C39-C40-C41
27	c	521	LMG	C11-C12-C13-C14
32	D	412	STE	C5-C6-C7-C8
30	c	517	DGD	C7A-C8A-C9A-CAA
27	c	519	LMG	O6-C5-C6-O5
30	c	516	DGD	O6E-C5E-C6E-O5E
28	a	411	SQD	C15-C16-C17-C18
29	D	409	LHG	C9-C10-C11-C12
29	D	411	LHG	C18-C19-C20-C21
30	c	516	DGD	CCB-CDB-CEB-CFB
32	c	520	STE	C3-C4-C5-C6
28	f	102	SQD	C27-C28-C29-C30
27	D	410	LMG	C28-C29-C30-C31
30	H	102	DGD	C1A-C2A-C3A-C4A
22	B	601	CLA	C5-C6-C7-C8
22	b	605	CLA	C15-C16-C17-C18
28	a	411	SQD	O6-C44-C45-O47
27	D	407	LMG	C12-C13-C14-C15
27	D	410	LMG	C34-C35-C36-C37
27	d	410	LMG	C38-C39-C40-C41
28	b	620	SQD	C24-C25-C26-C27
30	C	516	DGD	CCB-CDB-CEB-CFB
30	c	518	DGD	C9A-CAA-CBA-CCA
28	a	411	SQD	C18-C19-C20-C21
29	L	101	LHG	C26-C27-C28-C29
30	A	415	DGD	C7A-C8A-C9A-CAA
29	e	101	LHG	C11-C10-C9-C8
29	e	101	LHG	C27-C28-C29-C30
27	h	102	LMG	C32-C33-C34-C35
30	o	301	DGD	CAB-CBB-CCB-CDB

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Mol	Chain	Res	Type	Atoms
27	A	411	LMG	C35-C36-C37-C38
30	c	516	DGD	C6B-C7B-C8B-C9B
30	c	517	DGD	C7B-C8B-C9B-CAB
30	c	517	DGD	CCB-CDB-CEB-CFB
28	b	620	SQD	C13-C14-C15-C16
22	B	605	CLA	C3-C5-C6-C7
35	v	201	HEC	C2C-C3C-CAC-CBC
30	c	516	DGD	C1B-C2B-C3B-C4B
29	e	101	LHG	C1-C2-C3-O3
27	M	101	LMG	C20-C21-C22-C23
28	f	102	SQD	C32-C33-C34-C35
30	H	102	DGD	C4B-C5B-C6B-C7B
32	H	103	STE	C11-C10-C9-C8
28	b	620	SQD	C10-C11-C12-C13
29	l	101	LHG	C27-C28-C29-C30
29	D	408	LHG	C7-C8-C9-C10
29	a	410	LHG	C14-C15-C16-C17
27	c	519	LMG	C36-C37-C38-C39
29	D	408	LHG	C34-C35-C36-C37
30	C	516	DGD	C3A-C4A-C5A-C6A
30	H	102	DGD	CAB-CBB-CCB-CDB
22	c	503	CLA	C10-C11-C12-C13
29	D	408	LHG	O1-C1-C2-O2
29	a	410	LHG	O1-C1-C2-O2
27	c	521	LMG	C31-C32-C33-C34
27	Y	101	LMG	C36-C37-C38-C39
28	A	414	SQD	C15-C16-C17-C18
22	C	503	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	c	508	CLA	C1A-C2A-CAA-CBA
22	c	511	CLA	C1A-C2A-CAA-CBA
32	B	624	STE	C11-C10-C9-C8
32	D	412	STE	C4-C5-C6-C7
32	b	625	STE	C4-C5-C6-C7
28	F	102	SQD	C25-C26-C27-C28
28	F	102	SQD	C32-C33-C34-C35
29	e	101	LHG	C14-C15-C16-C17
30	A	415	DGD	C4A-C5A-C6A-C7A
30	H	102	DGD	C7B-C8B-C9B-CAB
27	a	414	LMG	O9-C10-O7-C8
29	e	101	LHG	O9-C7-O7-C5
27	c	521	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
28	B	621	SQD	C9-C10-C11-C12
30	C	517	DGD	C4B-C5B-C6B-C7B
22	B	602	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	C6-C7-C8-C10
22	B	613	CLA	C12-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C10
22	C	504	CLA	C11-C10-C8-C7
22	C	513	CLA	C6-C7-C8-C10
22	a	403	CLA	C11-C10-C8-C7
22	b	616	CLA	C11-C10-C8-C7
22	c	505	CLA	C6-C7-C8-C10
22	c	505	CLA	C11-C10-C8-C7
22	c	506	CLA	C11-C10-C8-C7
22	c	511	CLA	C12-C13-C15-C16
22	c	513	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C10-C8-C7
22	a	403	CLA	C15-C16-C17-C18
28	b	620	SQD	C14-C15-C16-C17
32	c	520	STE	C11-C12-C13-C14
22	B	613	CLA	CBD-CGD-O2D-CED
32	B	626	STE	C1-C2-C3-C4
29	D	409	LHG	C11-C12-C13-C14
22	C	505	CLA	C2-C3-C5-C6
32	E	101	STE	C6-C7-C8-C9
27	a	414	LMG	C11-C10-O7-C8
22	b	610	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C11-C12-C13-C14
22	B	604	CLA	C11-C12-C13-C14
22	B	613	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C14
22	C	505	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	C	510	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C10-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	b	615	CLA	C14-C13-C15-C16
27	D	407	LMG	C20-C21-C22-C23
28	b	620	SQD	C26-C27-C28-C29
29	a	410	LHG	C18-C19-C20-C21
29	d	408	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	C	520	STE	C5-C6-C7-C8
32	j	101	STE	C3-C4-C5-C6
22	c	509	CLA	C16-C17-C18-C19
22	d	403	CLA	C2C-C3C-CAC-CBC
35	v	201	HEC	C2B-C3B-CAB-CBB
27	b	623	LMG	O6-C5-C6-O5
27	D	407	LMG	C19-C20-C21-C22
27	M	101	LMG	C7-C8-C9-O8
28	B	621	SQD	O6-C44-C45-C46
28	a	411	SQD	O6-C44-C45-C46
22	b	616	CLA	CBD-CGD-O2D-CED
32	I	101	STE	C10-C11-C12-C13
28	B	621	SQD	C35-C36-C37-C38
27	D	410	LMG	C29-C28-O8-C9
27	D	407	LMG	O6-C5-C6-O5
27	d	410	LMG	O6-C5-C6-O5
22	B	606	CLA	C16-C17-C18-C19
22	b	616	CLA	C11-C12-C13-C15
22	c	511	CLA	C16-C17-C18-C19
30	A	415	DGD	C6A-C7A-C8A-C9A
22	B	605	CLA	C10-C11-C12-C13
27	m	101	LMG	C16-C17-C18-C19
28	a	411	SQD	C16-C17-C18-C19
27	Y	101	LMG	C4-C5-C6-O5
24	A	407	BCR	C11-C10-C9-C34
22	c	509	CLA	C8-C10-C11-C12
27	M	101	LMG	C35-C36-C37-C38
29	D	411	LHG	C29-C30-C31-C32
29	d	409	LHG	C30-C31-C32-C33
27	h	102	LMG	C10-C11-C12-C13
22	a	405	CLA	O1A-CGA-O2A-C1
29	d	408	LHG	C34-C35-C36-C37
22	C	505	CLA	C4-C3-C5-C6
22	C	505	CLA	CBD-CGD-O2D-CED
30	c	517	DGD	C2A-C3A-C4A-C5A
24	H	101	BCR	C36-C18-C19-C20
28	a	412	SQD	C17-C18-C19-C20
30	C	515	DGD	CCB-CDB-CEB-CFB
32	B	625	STE	C4-C5-C6-C7
32	b	622	STE	C5-C6-C7-C8
27	D	410	LMG	C14-C15-C16-C17
28	A	414	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	a	410	LHG	C11-C10-C9-C8
29	l	101	LHG	C26-C27-C28-C29
32	b	625	STE	C3-C4-C5-C6
24	D	405	BCR	C21-C22-C23-C24
22	c	503	CLA	C15-C16-C17-C18
30	c	516	DGD	CAB-CBB-CCB-CDB
32	c	522	STE	C2-C3-C4-C5
29	D	411	LHG	C32-C33-C34-C35
32	T	102	STE	C11-C10-C9-C8
30	C	517	DGD	C9A-CAA-CBA-CCA
29	l	101	LHG	C32-C33-C34-C35
28	B	621	SQD	C45-C46-O48-C23
27	D	407	LMG	C38-C39-C40-C41
24	B	619	BCR	C10-C11-C12-C13
24	C	514	BCR	C10-C11-C12-C13
28	A	412	SQD	C26-C27-C28-C29
28	b	620	SQD	C18-C19-C20-C21
29	d	409	LHG	C26-C27-C28-C29
30	A	415	DGD	CDB-CEB-CFB-CGB
27	d	410	LMG	C30-C31-C32-C33
32	H	103	STE	C14-C15-C16-C17
30	h	103	DGD	C3B-C4B-C5B-C6B
28	B	621	SQD	C16-C17-C18-C19
29	L	101	LHG	C13-C14-C15-C16
26	d	407	PL9	C43-C44-C46-C47
28	a	412	SQD	C31-C32-C33-C34
29	D	411	LHG	C9-C10-C11-C12
29	D	411	LHG	C11-C12-C13-C14
30	o	301	DGD	C5B-C6B-C7B-C8B
32	b	621	STE	C11-C10-C9-C8
22	c	511	CLA	C16-C17-C18-C20
23	a	404	PHO	CBD-CGD-O2D-CED
27	A	411	LMG	C31-C32-C33-C34
27	d	410	LMG	C14-C15-C16-C17
27	h	102	LMG	C31-C32-C33-C34
29	D	411	LHG	C28-C29-C30-C31
29	l	101	LHG	C14-C15-C16-C17
29	e	101	LHG	C28-C29-C30-C31
27	M	101	LMG	C34-C35-C36-C37
29	D	409	LHG	C24-C25-C26-C27
28	b	620	SQD	O6-C44-C45-O47
28	B	621	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	C11-C12-C13-C14
30	c	516	DGD	C7A-C8A-C9A-CAA
30	C	515	DGD	CDA-CEA-CFA-CGA
30	C	516	DGD	CDA-CEA-CFA-CGA
30	h	103	DGD	CDB-CEB-CFB-CGB
32	B	624	STE	C13-C14-C15-C16
32	M	104	STE	C12-C13-C14-C15
32	b	621	STE	C12-C13-C14-C15
30	h	103	DGD	O2G-C1B-C2B-C3B
27	a	414	LMG	C33-C34-C35-C36
27	h	102	LMG	C35-C36-C37-C38
28	A	412	SQD	C24-C25-C26-C27
22	C	509	CLA	C3-C5-C6-C7
22	C	512	CLA	C3-C5-C6-C7
27	d	410	LMG	C40-C41-C42-C43
22	b	616	CLA	C2-C1-O2A-CGA
27	Y	101	LMG	C37-C38-C39-C40
30	C	516	DGD	CDB-CEB-CFB-CGB
32	c	522	STE	C5-C6-C7-C8
27	a	414	LMG	C20-C21-C22-C23
28	A	412	SQD	C17-C18-C19-C20
22	c	506	CLA	CBD-CGD-O2D-CED
32	J	101	STE	C7-C8-C9-C10
29	D	411	LHG	C27-C28-C29-C30
30	H	102	DGD	C6B-C7B-C8B-C9B
32	d	412	STE	C5-C6-C7-C8
22	D	404	CLA	C3-C5-C6-C7
32	D	412	STE	C6-C7-C8-C9
29	d	409	LHG	C35-C36-C37-C38
32	b	624	STE	C1-C2-C3-C4
35	V	201	HEC	C2B-C3B-CAB-CBB
26	D	406	PL9	C30-C29-C31-C32
26	a	409	PL9	C15-C14-C16-C17
32	M	104	STE	C4-C5-C6-C7
32	T	102	STE	C4-C5-C6-C7
27	Y	101	LMG	C33-C34-C35-C36
29	l	101	LHG	C34-C35-C36-C37
30	c	516	DGD	C5B-C6B-C7B-C8B
29	d	408	LHG	C19-C20-C21-C22
27	Y	101	LMG	C35-C36-C37-C38
29	D	409	LHG	C16-C17-C18-C19
30	c	517	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
30	h	103	DGD	CAB-CBB-CCB-CDB
30	o	301	DGD	C7A-C8A-C9A-CAA
27	M	101	LMG	O9-C10-O7-C8
29	D	411	LHG	O1-C1-C2-O2
22	B	601	CLA	C11-C10-C8-C9
22	B	602	CLA	C11-C12-C13-C14
22	B	604	CLA	C14-C13-C15-C16
22	B	616	CLA	C6-C7-C8-C9
22	C	504	CLA	C11-C10-C8-C9
22	C	510	CLA	C6-C7-C8-C9
22	D	403	CLA	C11-C12-C13-C14
22	b	602	CLA	C14-C13-C15-C16
22	b	609	CLA	C14-C13-C15-C16
22	c	504	CLA	C11-C10-C8-C9
22	c	505	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C10-C8-C9
22	c	513	CLA	C11-C10-C8-C9
32	B	625	STE	C6-C7-C8-C9
22	a	403	CLA	C4B-C3B-CAB-CBB
22	c	507	CLA	C4B-C3B-CAB-CBB
29	A	413	LHG	C11-C12-C13-C14
30	o	301	DGD	CBA-CCA-CDA-CEA
32	a	413	STE	C1-C2-C3-C4
22	B	611	CLA	C8-C10-C11-C12
32	b	626	STE	C4-C5-C6-C7
30	h	103	DGD	C4A-C5A-C6A-C7A
32	B	620	STE	C3-C4-C5-C6
32	E	101	STE	C4-C5-C6-C7
22	b	609	CLA	C15-C16-C17-C18
30	C	517	DGD	C3B-C4B-C5B-C6B
27	M	101	LMG	C18-C19-C20-C21
27	c	519	LMG	C34-C35-C36-C37
29	D	408	LHG	C17-C18-C19-C20
30	H	102	DGD	CCA-CDA-CEA-CFA
32	I	101	STE	C12-C13-C14-C15
22	A	403	CLA	C11-C10-C8-C7
22	A	403	CLA	C11-C12-C13-C15
22	B	601	CLA	C11-C10-C8-C7
22	B	605	CLA	C11-C10-C8-C7
22	B	608	CLA	C6-C7-C8-C10
22	B	615	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C12-C13-C15-C16
22	C	509	CLA	C11-C10-C8-C7
22	C	510	CLA	C6-C7-C8-C10
22	C	510	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	D	403	CLA	C11-C12-C13-C15
22	b	602	CLA	C12-C13-C15-C16
22	b	605	CLA	C11-C10-C8-C7
22	b	607	CLA	C11-C12-C13-C15
22	b	608	CLA	C11-C10-C8-C7
22	b	609	CLA	C12-C13-C15-C16
22	b	614	CLA	C12-C13-C15-C16
22	b	615	CLA	C12-C13-C15-C16
22	c	507	CLA	C11-C10-C8-C7
22	c	513	CLA	C11-C12-C13-C15
23	a	404	PHO	C6-C7-C8-C10
22	b	603	CLA	C13-C15-C16-C17
29	L	101	LHG	O10-C23-O8-C6
29	D	409	LHG	C17-C18-C19-C20
30	c	518	DGD	CDA-CEA-CFA-CGA
22	B	601	CLA	C16-C17-C18-C19
28	B	621	SQD	O10-C23-O48-C46
28	a	411	SQD	C17-C18-C19-C20
29	D	409	LHG	C34-C35-C36-C37
22	B	601	CLA	C3A-C2A-CAA-CBA
26	d	407	PL9	C45-C44-C46-C47
30	C	516	DGD	CCA-CDA-CEA-CFA
29	D	411	LHG	C25-C26-C27-C28
30	A	415	DGD	O6E-C1E-O5D-C6D
32	m	102	STE	C3-C4-C5-C6
30	h	103	DGD	O1A-C1A-O1G-C1G
22	B	612	CLA	C10-C11-C12-C13
24	k	101	BCR	C19-C20-C21-C22
24	A	407	BCR	C7-C8-C9-C34
32	B	620	STE	C9-C10-C11-C12
32	b	625	STE	C15-C16-C17-C18
27	a	414	LMG	C18-C19-C20-C21
29	l	101	LHG	C13-C14-C15-C16
30	h	103	DGD	C2A-C3A-C4A-C5A
32	c	520	STE	C4-C5-C6-C7
27	A	411	LMG	C16-C17-C18-C19
27	D	407	LMG	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
29	A	413	LHG	C27-C28-C29-C30
30	H	102	DGD	C3A-C4A-C5A-C6A
32	T	102	STE	C11-C12-C13-C14
27	c	521	LMG	C28-C29-C30-C31
30	c	517	DGD	CDB-CEB-CFB-CGB
27	c	521	LMG	C40-C41-C42-C43
29	L	101	LHG	C18-C19-C20-C21
27	a	414	LMG	O1-C7-C8-C9
27	c	521	LMG	C7-C8-C9-O8
28	a	412	SQD	C44-C45-C46-O48
29	e	101	LHG	C4-C5-C6-O8
30	A	415	DGD	C1G-C2G-C3G-O3G
30	c	516	DGD	O6D-C5D-C6D-O5D
32	D	413	STE	C6-C7-C8-C9
22	B	601	CLA	C16-C17-C18-C20
22	b	616	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C14
22	B	606	CLA	C5-C6-C7-C8
29	A	413	LHG	C13-C14-C15-C16
27	Y	101	LMG	C31-C32-C33-C34
27	h	102	LMG	C11-C12-C13-C14
28	a	412	SQD	C30-C31-C32-C33
32	d	412	STE	C9-C10-C11-C12
28	A	412	SQD	C11-C10-C9-C8
32	B	627	STE	C6-C7-C8-C9
32	d	411	STE	C2-C3-C4-C5
30	c	517	DGD	O6E-C5E-C6E-O5E
32	B	624	STE	C4-C5-C6-C7
30	H	102	DGD	O2G-C1B-C2B-C3B
28	A	414	SQD	O47-C45-C46-O48
30	A	415	DGD	C5A-C6A-C7A-C8A
30	h	103	DGD	CCA-CDA-CEA-CFA
22	b	601	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C23-C24-C25-C30
24	B	618	BCR	C23-C24-C25-C30
24	c	514	BCR	C1-C6-C7-C8
29	L	101	LHG	C31-C32-C33-C34
29	D	411	LHG	C26-C27-C28-C29
27	c	521	LMG	C34-C35-C36-C37
28	F	102	SQD	C28-C29-C30-C31
32	b	622	STE	C12-C13-C14-C15
22	B	607	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
27	M	101	LMG	C12-C13-C14-C15
28	a	411	SQD	C29-C30-C31-C32
32	M	104	STE	C13-C14-C15-C16
29	D	409	LHG	C30-C31-C32-C33
22	A	402	CLA	C2C-C3C-CAC-CBC
29	e	101	LHG	O7-C5-C6-O8
26	A	410	PL9	C4-C3-C7-C8
29	l	101	LHG	C11-C12-C13-C14
30	C	515	DGD	O6D-C5D-C6D-O5D
32	D	412	STE	C10-C11-C12-C13
32	E	101	STE	C5-C6-C7-C8
32	J	101	STE	C2-C3-C4-C5
26	D	406	PL9	C15-C14-C16-C17
27	c	521	LMG	C32-C33-C34-C35
28	a	411	SQD	C30-C31-C32-C33
28	b	620	SQD	C29-C30-C31-C32
29	d	408	LHG	C25-C26-C27-C28
32	B	625	STE	C11-C10-C9-C8
29	A	413	LHG	C19-C20-C21-C22
27	D	407	LMG	C39-C40-C41-C42
27	Y	101	LMG	C15-C16-C17-C18
28	a	412	SQD	C29-C30-C31-C32
29	D	409	LHG	C27-C28-C29-C30
22	b	601	CLA	C16-C17-C18-C19
27	m	101	LMG	C39-C40-C41-C42
30	c	516	DGD	C9B-CAB-CBB-CCB
32	C	518	STE	C2-C3-C4-C5
32	a	413	STE	C2-C3-C4-C5
22	B	608	CLA	C6-C7-C8-C9
22	C	505	CLA	C11-C10-C8-C9
22	b	607	CLA	C11-C12-C13-C14
29	D	411	LHG	C33-C34-C35-C36
29	d	408	LHG	C10-C11-C12-C13
27	d	410	LMG	C15-C16-C17-C18
22	B	613	CLA	O1D-CGD-O2D-CED
30	H	102	DGD	C3B-C4B-C5B-C6B
30	c	518	DGD	C8B-C9B-CAB-CBB
24	D	405	BCR	C22-C23-C24-C25
22	B	612	CLA	C16-C17-C18-C19
27	A	411	LMG	C14-C15-C16-C17
29	D	408	LHG	C35-C36-C37-C38
28	A	412	SQD	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
32	b	621	STE	C3-C4-C5-C6
22	c	513	CLA	C8-C10-C11-C12
29	d	409	LHG	O1-C1-C2-O2
22	c	509	CLA	CAA-CBA-CGA-O2A
23	d	401	PHO	C2C-C3C-CAC-CBC
27	b	623	LMG	C29-C30-C31-C32
22	B	607	CLA	CBD-CGD-O2D-CED
29	A	413	LHG	C18-C19-C20-C21
30	H	102	DGD	CBA-CCA-CDA-CEA
26	a	409	PL9	C32-C33-C34-C36
30	o	301	DGD	CAA-CBA-CCA-CDA
32	B	624	STE	C12-C13-C14-C15
32	B	626	STE	C2-C3-C4-C5
24	c	515	BCR	C35-C13-C14-C15
24	t	101	BCR	C11-C10-C9-C34
22	B	611	CLA	C13-C15-C16-C17
22	D	403	CLA	C15-C16-C17-C18
29	A	413	LHG	O6-C4-C5-C6
22	B	610	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C19
28	A	414	SQD	C19-C20-C21-C22
24	T	101	BCR	C36-C18-C19-C20
29	l	101	LHG	C15-C16-C17-C18
32	D	412	STE	C11-C12-C13-C14
22	C	509	CLA	C12-C13-C15-C16
22	C	512	CLA	C12-C13-C15-C16
22	a	403	CLA	C12-C13-C15-C16
22	b	603	CLA	C11-C12-C13-C15
22	b	607	CLA	C6-C7-C8-C10
22	b	615	CLA	C11-C12-C13-C15
22	c	505	CLA	C12-C13-C15-C16
22	c	510	CLA	C12-C13-C15-C16
22	d	403	CLA	C6-C7-C8-C10
22	d	404	CLA	C12-C13-C15-C16
30	c	518	DGD	C3B-C4B-C5B-C6B
32	B	624	STE	C6-C7-C8-C9
32	B	624	STE	C7-C8-C9-C10
22	b	613	CLA	C13-C15-C16-C17
27	Y	101	LMG	C29-C30-C31-C32
30	C	517	DGD	C8B-C9B-CAB-CBB
30	c	517	DGD	C5B-C6B-C7B-C8B
30	C	516	DGD	C2G-C3G-O3G-C1D

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	C2G-C3G-O3G-C1D
30	c	517	DGD	C5D-C6D-O5D-C1E
32	B	623	STE	C4-C5-C6-C7
22	B	610	CLA	C16-C17-C18-C20
27	m	101	LMG	C11-C10-O7-C8
22	b	616	CLA	O1D-CGD-O2D-CED
30	c	518	DGD	C3A-C4A-C5A-C6A
27	D	410	LMG	C37-C38-C39-C40
28	b	620	SQD	C15-C16-C17-C18
32	I	101	STE	C4-C5-C6-C7
28	b	620	SQD	C19-C20-C21-C22
27	a	414	LMG	C35-C36-C37-C38
22	D	404	CLA	C8-C10-C11-C12
22	b	602	CLA	C8-C10-C11-C12
27	a	414	LMG	C9-C8-O7-C10
32	b	626	STE	C7-C8-C9-C10
27	c	521	LMG	C33-C34-C35-C36
29	A	413	LHG	C16-C17-C18-C19
32	B	624	STE	C9-C10-C11-C12
32	B	624	STE	C2-C3-C4-C5
22	C	508	CLA	C16-C17-C18-C19
27	A	411	LMG	C38-C39-C40-C41
22	B	606	CLA	C8-C10-C11-C12
27	c	521	LMG	C15-C16-C17-C18
29	A	413	LHG	O6-C4-C5-O7
29	D	409	LHG	O6-C4-C5-O7
32	D	412	STE	C2-C3-C4-C5
32	b	624	STE	C9-C10-C11-C12
34	f	101	HEM	C4B-C3B-CAB-CBB
22	B	611	CLA	C16-C17-C18-C20
22	b	602	CLA	C16-C17-C18-C19
27	A	411	LMG	C15-C16-C17-C18
30	c	516	DGD	C4D-C5D-C6D-O5D
29	D	408	LHG	C12-C13-C14-C15
22	b	615	CLA	C5-C6-C7-C8
32	d	412	STE	C13-C14-C15-C16
27	a	414	LMG	O1-C7-C8-O7
28	a	411	SQD	O47-C45-C46-O48
30	c	516	DGD	O1G-C1G-C2G-O2G
22	B	605	CLA	C6-C7-C8-C9
22	B	606	CLA	C11-C12-C13-C14
22	a	403	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	614	CLA	C6-C7-C8-C9
22	b	614	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C15
30	A	415	DGD	CBB-CCB-CDB-CEB
28	A	414	SQD	C35-C36-C37-C38
28	A	412	SQD	C11-C12-C13-C14
29	L	101	LHG	C33-C34-C35-C36
32	D	413	STE	C7-C8-C9-C10
30	A	415	DGD	C2A-C3A-C4A-C5A
27	d	410	LMG	C32-C33-C34-C35
30	A	415	DGD	CEA-CFA-CGA-CHA
22	c	506	CLA	O1D-CGD-O2D-CED
24	T	101	BCR	C13-C14-C15-C16
23	a	404	PHO	O1D-CGD-O2D-CED
22	C	508	CLA	C16-C17-C18-C20
30	H	102	DGD	C8B-C9B-CAB-CBB
30	C	517	DGD	CDA-CEA-CFA-CGA
28	A	414	SQD	C32-C33-C34-C35
30	c	517	DGD	CCA-CDA-CEA-CFA
22	b	612	CLA	C10-C11-C12-C13
29	e	101	LHG	O2-C2-C3-O3
29	D	411	LHG	C19-C20-C21-C22
29	d	408	LHG	C12-C13-C14-C15
30	C	515	DGD	C9B-CAB-CBB-CCB
32	M	103	STE	C3-C4-C5-C6
22	A	403	CLA	C16-C17-C18-C20
22	B	602	CLA	C16-C17-C18-C20
30	C	517	DGD	CAB-CBB-CCB-CDB
32	b	624	STE	C7-C8-C9-C10
22	C	506	CLA	C3-C5-C6-C7
32	a	413	STE	C7-C8-C9-C10
32	B	620	STE	C4-C5-C6-C7
32	a	415	STE	C6-C7-C8-C9
22	c	508	CLA	C16-C17-C18-C19
30	H	102	DGD	CDB-CEB-CFB-CGB
29	d	408	LHG	O1-C1-C2-O2
22	B	601	CLA	C4B-C3B-CAB-CBB
29	D	411	LHG	C24-C23-O8-C6
29	A	413	LHG	C31-C32-C33-C34
22	B	601	CLA	C4-C3-C5-C6
27	m	101	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
24	k	101	BCR	C7-C8-C9-C10
27	A	411	LMG	C13-C14-C15-C16
29	D	411	LHG	C24-C25-C26-C27
28	a	411	SQD	C32-C33-C34-C35
29	D	409	LHG	O6-C4-C5-C6
29	l	101	LHG	O6-C4-C5-C6
27	c	519	LMG	C32-C33-C34-C35
32	b	626	STE	C2-C3-C4-C5
28	a	411	SQD	C5-C6-S-O9
32	C	520	STE	C6-C7-C8-C9
32	a	415	STE	C5-C6-C7-C8
22	A	403	CLA	C6-C7-C8-C10
22	B	601	CLA	C11-C12-C13-C15
22	B	603	CLA	C12-C13-C15-C16
22	B	612	CLA	C11-C10-C8-C7
22	B	613	CLA	C6-C7-C8-C10
22	C	505	CLA	C6-C7-C8-C10
22	D	402	CLA	C11-C12-C13-C15
22	a	403	CLA	C11-C12-C13-C15
22	b	601	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C10-C8-C7
22	b	614	CLA	C11-C10-C8-C7
22	c	506	CLA	C6-C7-C8-C10
22	c	509	CLA	C6-C7-C8-C10
29	D	408	LHG	C14-C15-C16-C17
30	C	516	DGD	C5B-C6B-C7B-C8B
32	H	103	STE	C9-C10-C11-C12
22	b	603	CLA	CBD-CGD-O2D-CED
32	a	413	STE	C6-C7-C8-C9
30	C	517	DGD	O6D-C5D-C6D-O5D
22	b	609	CLA	C4-C3-C5-C6
32	c	520	STE	C15-C16-C17-C18
32	M	104	STE	C2-C3-C4-C5
22	A	403	CLA	C11-C10-C8-C9
22	B	605	CLA	C11-C10-C8-C9
22	C	509	CLA	C14-C13-C15-C16
22	C	513	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C12-C13-C14
22	c	505	CLA	C14-C13-C15-C16
22	c	510	CLA	C14-C13-C15-C16
30	C	516	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
29	e	101	LHG	C12-C13-C14-C15
24	K	101	BCR	C15-C16-C17-C18
22	C	509	CLA	C16-C17-C18-C19
29	d	409	LHG	C33-C34-C35-C36
32	B	624	STE	C10-C11-C12-C13
29	L	101	LHG	C11-C12-C13-C14
29	l	101	LHG	C33-C34-C35-C36
27	M	101	LMG	O7-C8-C9-O8
27	b	623	LMG	O1-C7-C8-O7
27	c	521	LMG	O7-C8-C9-O8
28	B	621	SQD	C13-C14-C15-C16
22	d	405	CLA	C5-C6-C7-C8
30	A	415	DGD	CAB-CBB-CCB-CDB
27	b	623	LMG	O1-C7-C8-C9
26	d	407	PL9	C15-C14-C16-C17
30	C	516	DGD	CBB-CCB-CDB-CEB
22	c	504	CLA	C8-C10-C11-C12
28	b	620	SQD	C27-C28-C29-C30
28	F	102	SQD	C30-C31-C32-C33
22	B	601	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
35	v	201	HEC	C4B-C3B-CAB-CBB
28	A	412	SQD	O10-C23-O48-C46
29	D	408	LHG	C31-C32-C33-C34
22	a	403	CLA	C13-C15-C16-C17
27	b	623	LMG	C35-C36-C37-C38
22	b	602	CLA	C16-C17-C18-C20
29	l	101	LHG	C24-C25-C26-C27
22	D	404	CLA	C10-C11-C12-C13
29	A	413	LHG	C9-C10-C11-C12
32	b	621	STE	C15-C16-C17-C18
30	C	516	DGD	C9A-CAA-CBA-CCA
30	c	516	DGD	C5A-C6A-C7A-C8A
30	H	102	DGD	CBB-CCB-CDB-CEB
32	B	623	STE	C6-C7-C8-C9
22	B	601	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O1D
22	C	509	CLA	CHA-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O1D
23	d	401	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	B	618	BCR	C15-C16-C17-C18
24	C	514	BCR	C15-C16-C17-C18
29	A	413	LHG	C3-O3-P-O5
29	D	408	LHG	C4-O6-P-O3
29	L	101	LHG	C4-O6-P-O3
29	e	101	LHG	C4-O6-P-O3
29	e	101	LHG	C4-O6-P-O4
29	e	101	LHG	C4-O6-P-O5
24	t	101	BCR	C14-C15-C16-C17
27	D	407	LMG	C31-C32-C33-C34
22	B	601	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C1-C6-C7-C8
30	A	415	DGD	CBA-CCA-CDA-CEA
32	d	412	STE	C12-C13-C14-C15
29	a	410	LHG	C7-C8-C9-C10
29	d	409	LHG	C2-C3-O3-P
27	d	410	LMG	O9-C10-O7-C8
27	Y	101	LMG	C14-C15-C16-C17
22	B	602	CLA	C16-C17-C18-C19
29	d	409	LHG	C23-C24-C25-C26
29	A	413	LHG	C29-C30-C31-C32
22	c	512	CLA	C8-C10-C11-C12
27	m	101	LMG	C32-C33-C34-C35
26	a	409	PL9	C4-C3-C7-C8
27	D	410	LMG	C9-C8-O7-C10
26	A	410	PL9	C20-C19-C21-C22
29	L	101	LHG	C16-C17-C18-C19
22	c	509	CLA	C13-C15-C16-C17
22	c	510	CLA	C5-C6-C7-C8
26	a	409	PL9	C13-C14-C16-C17
32	H	103	STE	C10-C11-C12-C13
28	f	102	SQD	C30-C31-C32-C33
32	b	621	STE	C10-C11-C12-C13
32	d	411	STE	C10-C11-C12-C13
29	d	408	LHG	O6-C4-C5-C6
22	B	603	CLA	C14-C13-C15-C16
22	B	604	CLA	C6-C7-C8-C9
22	B	604	CLA	C11-C10-C8-C9
22	D	402	CLA	C11-C10-C8-C9
22	D	404	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	607	CLA	C6-C7-C8-C9
22	c	507	CLA	C11-C10-C8-C9
23	A	404	PHO	C14-C13-C15-C16
22	B	606	CLA	C12-C13-C15-C16
22	B	611	CLA	C11-C10-C8-C7
22	C	505	CLA	C11-C10-C8-C7
22	b	608	CLA	C11-C12-C13-C15
32	M	102	STE	C1-C2-C3-C4
22	a	402	CLA	C2C-C3C-CAC-CBC
22	A	403	CLA	C16-C17-C18-C19
22	B	611	CLA	C16-C17-C18-C19
30	C	515	DGD	C4D-C5D-C6D-O5D
30	c	517	DGD	C5A-C6A-C7A-C8A
32	I	101	STE	C2-C3-C4-C5
30	A	415	DGD	C2E-C1E-O5D-C6D
22	c	504	CLA	C4-C3-C5-C6
22	d	405	CLA	C8-C10-C11-C12
29	a	410	LHG	C29-C30-C31-C32
28	a	412	SQD	O47-C45-C46-O48
30	C	515	DGD	O1G-C1G-C2G-O2G
27	b	623	LMG	C12-C13-C14-C15
28	A	414	SQD	C11-C10-C9-C8
27	M	101	LMG	C11-C12-C13-C14
32	C	519	STE	C9-C10-C11-C12
27	c	519	LMG	C35-C36-C37-C38
29	A	413	LHG	C33-C34-C35-C36
32	b	622	STE	C13-C14-C15-C16
22	b	614	CLA	C10-C11-C12-C13
27	Y	101	LMG	C32-C33-C34-C35
22	b	607	CLA	C4-C3-C5-C6
26	d	407	PL9	C44-C46-C47-C48
32	d	412	STE	C10-C11-C12-C13
28	F	102	SQD	C27-C28-C29-C30
30	C	515	DGD	O1G-C1A-C2A-C3A
30	c	516	DGD	O1G-C1A-C2A-C3A
22	b	614	CLA	C8-C10-C11-C12
26	a	409	PL9	C12-C13-C14-C16
27	m	101	LMG	O10-C28-O8-C9
32	C	518	STE	C7-C8-C9-C10
22	b	606	CLA	C3-C5-C6-C7
22	d	404	CLA	C4C-C3C-CAC-CBC
30	H	102	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
32	M	103	STE	C1-C2-C3-C4
30	c	516	DGD	C5D-C6D-O5D-C1E
32	b	625	STE	C9-C10-C11-C12
22	c	501	CLA	C2A-CAA-CBA-CGA
22	C	509	CLA	O1D-CGD-O2D-CED
24	C	514	BCR	C13-C14-C15-C16
22	D	404	CLA	C16-C17-C18-C19
30	c	518	DGD	CBB-CCB-CDB-CEB
29	A	413	LHG	C11-C10-C9-C8
22	c	512	CLA	C4-C3-C5-C6
32	B	620	STE	C11-C12-C13-C14
27	m	101	LMG	C36-C37-C38-C39
32	B	625	STE	C7-C8-C9-C10
32	B	625	STE	C3-C4-C5-C6
22	A	403	CLA	C6-C7-C8-C9
22	B	612	CLA	C11-C10-C8-C9
22	b	608	CLA	C11-C12-C13-C14
22	b	613	CLA	C6-C7-C8-C9
22	c	506	CLA	C6-C7-C8-C9
23	a	404	PHO	C6-C7-C8-C9
29	D	408	LHG	C33-C34-C35-C36
32	T	102	STE	C12-C13-C14-C15
28	A	414	SQD	C27-C28-C29-C30
32	a	413	STE	C4-C5-C6-C7
22	C	511	CLA	C16-C17-C18-C19
27	M	101	LMG	C22-C23-C24-C25
22	C	510	CLA	C4-C3-C5-C6
22	b	609	CLA	C2-C3-C5-C6
30	h	103	DGD	C7A-C8A-C9A-CAA
22	C	509	CLA	C16-C17-C18-C20
22	b	609	CLA	C16-C17-C18-C20
32	c	522	STE	C6-C7-C8-C9
22	B	604	CLA	C11-C10-C8-C7
22	C	513	CLA	C11-C10-C8-C7
22	d	403	CLA	C11-C12-C13-C15
22	d	403	CLA	C3-C5-C6-C7
27	D	410	LMG	C16-C17-C18-C19
27	m	101	LMG	C17-C18-C19-C20
30	C	517	DGD	O1A-C1A-O1G-C1G
29	d	409	LHG	C32-C33-C34-C35
32	B	620	STE	C7-C8-C9-C10
22	d	404	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	c	516	DGD	CDB-CEB-CFB-CGB
27	c	519	LMG	C30-C31-C32-C33
29	D	408	LHG	C18-C19-C20-C21
22	C	509	CLA	CBD-CGD-O2D-CED
29	d	408	LHG	C30-C31-C32-C33
22	c	508	CLA	C4-C3-C5-C6
28	A	412	SQD	C9-C10-C11-C12
26	A	410	PL9	C12-C13-C14-C16
30	c	516	DGD	C8B-C9B-CAB-CBB
24	B	618	BCR	C35-C13-C14-C15
29	A	413	LHG	C2-C3-O3-P
22	b	613	CLA	C10-C11-C12-C13
22	B	601	CLA	C2-C3-C5-C6
22	b	611	CLA	C2-C3-C5-C6
22	c	512	CLA	C2-C3-C5-C6
22	B	613	CLA	C10-C11-C12-C13
32	b	622	STE	C10-C11-C12-C13
27	Y	101	LMG	O1-C7-C8-C9
30	c	516	DGD	O1G-C1G-C2G-C3G
27	m	101	LMG	C18-C19-C20-C21
22	B	611	CLA	C11-C12-C13-C14
22	B	614	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
22	C	512	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	604	CLA	C14-C13-C15-C16
22	b	612	CLA	C14-C13-C15-C16
22	c	508	CLA	C14-C13-C15-C16
29	d	408	LHG	C9-C10-C11-C12
27	b	623	LMG	C17-C18-C19-C20
29	L	101	LHG	C17-C18-C19-C20
32	C	519	STE	C6-C7-C8-C9
32	b	622	STE	C3-C4-C5-C6
32	B	623	STE	O1-C1-C2-C3
32	B	627	STE	O1-C1-C2-C3
22	D	402	CLA	C10-C11-C12-C13
22	B	612	CLA	CBD-CGD-O2D-CED
27	b	623	LMG	C30-C31-C32-C33
29	A	413	LHG	O1-C1-C2-O2
34	f	101	HEM	CAA-CBA-CGA-O1A
35	V	201	HEC	CAD-CBD-CGD-O1D
24	H	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
24	k	101	BCR	C11-C10-C9-C8
27	c	521	LMG	C42-C43-C44-C45
28	a	412	SQD	C16-C17-C18-C19
30	C	517	DGD	C6A-C7A-C8A-C9A
29	l	101	LHG	O6-C4-C5-O7
22	a	403	CLA	C2B-C3B-CAB-CBB
22	d	403	CLA	C2B-C3B-CAB-CBB
24	A	407	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C30
24	K	101	BCR	C23-C24-C25-C30
24	b	618	BCR	C23-C24-C25-C30
24	c	514	BCR	C5-C6-C7-C8
24	d	406	BCR	C23-C24-C25-C30
32	B	623	STE	O2-C1-C2-C3
32	B	627	STE	O2-C1-C2-C3
34	F	101	HEM	CAD-CBD-CGD-O1D
34	F	101	HEM	CAD-CBD-CGD-O2D
29	D	409	LHG	C2-C3-O3-P
22	C	511	CLA	C16-C17-C18-C20
22	B	603	CLA	C13-C15-C16-C17
32	d	411	STE	O1-C1-C2-C3
22	A	402	CLA	C4C-C3C-CAC-CBC
26	D	406	PL9	C40-C39-C41-C42
32	B	624	STE	C5-C6-C7-C8
22	b	607	CLA	C2-C3-C5-C6
32	d	411	STE	C12-C13-C14-C15
30	C	516	DGD	C2B-C3B-C4B-C5B
30	c	516	DGD	C7B-C8B-C9B-CAB
32	b	622	STE	O2-C1-C2-C3
35	V	201	HEC	CAD-CBD-CGD-O2D
30	H	102	DGD	CDA-CEA-CFA-CGA
32	b	622	STE	C15-C16-C17-C18
22	A	403	CLA	C12-C13-C15-C16
22	B	601	CLA	C12-C13-C15-C16
22	B	605	CLA	C12-C13-C15-C16
22	C	502	CLA	C12-C13-C15-C16
22	b	606	CLA	C11-C12-C13-C15
22	b	607	CLA	C11-C10-C8-C7
22	c	507	CLA	C11-C12-C13-C15
22	c	512	CLA	C6-C7-C8-C10
27	c	519	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
32	b	622	STE	C11-C12-C13-C14
22	B	603	CLA	C2A-CAA-CBA-CGA
22	B	604	CLA	C13-C15-C16-C17
29	D	408	LHG	O7-C5-C6-O8
28	a	411	SQD	C11-C10-C9-C8
27	D	410	LMG	C31-C32-C33-C34
32	B	627	STE	C2-C3-C4-C5
32	b	625	STE	O2-C1-C2-C3
24	b	617	BCR	C36-C18-C19-C20
22	b	605	CLA	C4-C3-C5-C6
22	C	510	CLA	C2-C3-C5-C6
26	D	406	PL9	C28-C29-C31-C32
32	D	413	STE	C10-C11-C12-C13
22	b	612	CLA	C16-C17-C18-C20
22	c	502	CLA	C2C-C3C-CAC-CBC
32	d	412	STE	C4-C5-C6-C7
32	b	625	STE	O1-C1-C2-C3
22	C	508	CLA	C11-C10-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	506	CLA	C14-C13-C15-C16
22	c	512	CLA	C14-C13-C15-C16
22	b	608	CLA	C5-C6-C7-C8
30	c	516	DGD	O1B-C1B-O2G-C2G
27	h	102	LMG	C38-C39-C40-C41
28	A	414	SQD	C16-C17-C18-C19
28	f	102	SQD	C31-C32-C33-C34
32	M	103	STE	C5-C6-C7-C8
27	h	102	LMG	C40-C41-C42-C43
32	B	622	STE	C3-C4-C5-C6
22	a	402	CLA	C4C-C3C-CAC-CBC
22	c	508	CLA	C2-C3-C5-C6
26	a	409	PL9	C28-C29-C31-C32
22	B	612	CLA	O1A-CGA-O2A-C1
30	c	516	DGD	CBB-CCB-CDB-CEB
30	c	516	DGD	CBA-CCA-CDA-CEA
27	c	521	LMG	O1-C7-C8-C9
29	D	408	LHG	C4-C5-C6-O8
29	D	411	LHG	C4-C5-C6-O8
30	C	515	DGD	C1G-C2G-C3G-O3G
32	b	622	STE	O1-C1-C2-C3
28	f	102	SQD	C29-C30-C31-C32
27	D	410	LMG	O10-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
32	d	411	STE	O2-C1-C2-C3
22	d	405	CLA	O1D-CGD-O2D-CED
29	d	408	LHG	O6-C4-C5-O7
30	A	415	DGD	C3B-C4B-C5B-C6B
32	c	520	STE	O2-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O2D
22	c	509	CLA	CAA-CBA-CGA-O1A
30	A	415	DGD	C9A-CAA-CBA-CCA
22	D	404	CLA	C16-C17-C18-C20
22	b	610	CLA	C13-C15-C16-C17
26	a	409	PL9	C32-C33-C34-C35
22	b	603	CLA	C4B-C3B-CAB-CBB
22	c	503	CLA	C4B-C3B-CAB-CBB
22	d	403	CLA	C4B-C3B-CAB-CBB
34	f	101	HEM	CAA-CBA-CGA-O2A
28	f	102	SQD	C24-C25-C26-C27
29	D	409	LHG	C11-C10-C9-C8
23	A	404	PHO	CHA-CBD-CGD-O2D
23	d	401	PHO	CHA-CBD-CGD-O1D
24	A	407	BCR	C20-C21-C22-C37
32	c	520	STE	O1-C1-C2-C3
27	b	623	LMG	C28-C29-C30-C31
22	b	604	CLA	C13-C15-C16-C17
22	B	612	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
28	a	412	SQD	C18-C19-C20-C21
32	b	622	STE	C11-C10-C9-C8
26	A	410	PL9	C25-C24-C26-C27
27	A	411	LMG	O1-C7-C8-O7
29	A	413	LHG	O7-C5-C6-O8
32	B	624	STE	C1-C2-C3-C4
32	B	620	STE	O2-C1-C2-C3
30	A	415	DGD	C8B-C9B-CAB-CBB
32	c	520	STE	C11-C10-C9-C8
22	B	603	CLA	C5-C6-C7-C8
22	b	601	CLA	C15-C16-C17-C18
30	C	515	DGD	CBA-CCA-CDA-CEA
32	j	101	STE	C2-C3-C4-C5
32	B	620	STE	O1-C1-C2-C3
32	H	103	STE	C13-C14-C15-C16
22	c	510	CLA	C3-C5-C6-C7
22	C	504	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	601	CLA	C11-C12-C13-C14
27	M	101	LMG	C8-C7-O1-C1
27	m	101	LMG	C8-C7-O1-C1
28	a	411	SQD	C5-C6-S-O8
32	J	101	STE	O2-C1-C2-C3
22	B	613	CLA	C2-C1-O2A-CGA
29	l	101	LHG	O10-C23-O8-C6
26	D	406	PL9	C16-C17-C18-C19
35	V	201	HEC	C4B-C3B-CAB-CBB
22	D	404	CLA	C3A-C2A-CAA-CBA
22	c	504	CLA	C2-C3-C5-C6
23	A	404	PHO	C10-C11-C12-C13
27	d	410	LMG	C34-C35-C36-C37
22	b	613	CLA	C16-C17-C18-C19
23	a	404	PHO	O2A-C1-C2-C3
22	a	403	CLA	O1D-CGD-O2D-CED
24	B	618	BCR	C10-C11-C12-C13
24	T	101	BCR	C14-C15-C16-C17
29	a	410	LHG	C10-C11-C12-C13
32	B	624	STE	O1-C1-C2-C3
35	v	201	HEC	CAD-CBD-CGD-O1D
27	Y	101	LMG	C34-C35-C36-C37
27	c	521	LMG	C13-C14-C15-C16
27	M	101	LMG	O1-C7-C8-C9
30	h	103	DGD	C1G-C2G-C3G-O3G
30	C	516	DGD	C8A-C9A-CAA-CBA
34	F	101	HEM	C4C-C3C-CAC-CBC
30	h	103	DGD	CBA-CCA-CDA-CEA
27	M	101	LMG	C13-C14-C15-C16
32	B	627	STE	C7-C8-C9-C10
22	b	603	CLA	C4-C3-C5-C6
26	D	406	PL9	C45-C44-C46-C47
32	J	101	STE	O1-C1-C2-C3
24	d	406	BCR	C19-C20-C21-C22
30	A	415	DGD	C6B-C7B-C8B-C9B
32	B	624	STE	O2-C1-C2-C3
28	a	411	SQD	C25-C26-C27-C28
32	c	520	STE	C10-C11-C12-C13
27	Y	101	LMG	O1-C7-C8-O7
28	b	620	SQD	O47-C45-C46-O48
22	B	613	CLA	C6-C7-C8-C9
22	B	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
22	C	505	CLA	C6-C7-C8-C9
22	C	508	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C12-C13-C14
22	d	403	CLA	C6-C7-C8-C9
23	A	405	PHO	C6-C7-C8-C9
32	a	415	STE	C7-C8-C9-C10
29	l	101	LHG	O7-C7-C8-C9
24	K	101	BCR	C21-C22-C23-C24
22	B	612	CLA	CAA-CBA-CGA-O2A
22	B	613	CLA	C11-C12-C13-C15
22	B	615	CLA	C6-C7-C8-C10
22	B	615	CLA	C12-C13-C15-C16
22	C	506	CLA	C11-C10-C8-C7
22	C	506	CLA	C12-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C7
22	C	511	CLA	C6-C7-C8-C10
22	C	512	CLA	C11-C12-C13-C15
22	D	404	CLA	C6-C7-C8-C10
22	b	604	CLA	C6-C7-C8-C10
22	b	610	CLA	C11-C12-C13-C15
22	b	612	CLA	C12-C13-C15-C16
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C12-C13-C15-C16
22	c	512	CLA	C12-C13-C15-C16
30	c	518	DGD	O6D-C5D-C6D-O5D
22	B	616	CLA	C2B-C3B-CAB-CBB
22	b	607	CLA	C2B-C3B-CAB-CBB
22	c	503	CLA	C2B-C3B-CAB-CBB
24	B	618	BCR	C23-C24-C25-C26
24	b	618	BCR	C23-C24-C25-C26
24	d	406	BCR	C23-C24-C25-C26
22	C	506	CLA	C2-C1-O2A-CGA
22	D	402	CLA	C2-C1-O2A-CGA
22	c	507	CLA	C2-C1-O2A-CGA
22	c	512	CLA	C2-C1-O2A-CGA
22	c	513	CLA	C2-C1-O2A-CGA
28	A	414	SQD	C9-C10-C11-C12
32	b	625	STE	C7-C8-C9-C10
28	a	411	SQD	O47-C7-C8-C9
27	a	414	LMG	C37-C38-C39-C40
32	C	519	STE	C11-C12-C13-C14
28	A	412	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	603	CLA	C15-C16-C17-C18
29	D	408	LHG	O10-C23-O8-C6
27	d	410	LMG	O7-C10-C11-C12
27	m	101	LMG	O8-C28-C29-C30
32	H	103	STE	C11-C12-C13-C14
32	C	520	STE	C1-C2-C3-C4
32	C	519	STE	C5-C6-C7-C8
22	a	403	CLA	CBD-CGD-O2D-CED
22	C	512	CLA	C14-C13-C15-C16
22	a	403	CLA	C11-C12-C13-C14
22	b	604	CLA	C11-C10-C8-C9
22	b	614	CLA	C11-C10-C8-C9
22	c	507	CLA	C6-C7-C8-C9
30	o	301	DGD	O1G-C1A-C2A-C3A
27	A	411	LMG	C7-C8-C9-O8
28	b	620	SQD	O6-C44-C45-C46
22	B	602	CLA	C1A-C2A-CAA-CBA
22	C	503	CLA	C4B-C3B-CAB-CBB
22	C	512	CLA	C1A-C2A-CAA-CBA
22	b	607	CLA	C4B-C3B-CAB-CBB
32	D	413	STE	O1-C1-C2-C3
22	b	611	CLA	C4-C3-C5-C6
27	m	101	LMG	C14-C15-C16-C17
28	b	620	SQD	C11-C10-C9-C8
30	H	102	DGD	C5A-C6A-C7A-C8A
24	B	617	BCR	C6-C7-C8-C9
30	C	516	DGD	O6D-C1D-O3G-C3G
22	B	613	CLA	CAA-CBA-CGA-O2A
27	b	623	LMG	O7-C10-C11-C12
27	c	521	LMG	O1-C7-C8-O7
28	A	412	SQD	O6-C44-C45-O47
29	D	411	LHG	O7-C5-C6-O8
32	D	413	STE	O2-C1-C2-C3
29	A	413	LHG	C15-C16-C17-C18
29	D	411	LHG	C13-C14-C15-C16
32	b	625	STE	C2-C3-C4-C5
28	A	412	SQD	O47-C7-C8-C9
30	C	515	DGD	O2G-C1B-C2B-C3B
27	Y	101	LMG	C39-C40-C41-C42
29	d	409	LHG	C9-C10-C11-C12
32	c	520	STE	C14-C15-C16-C17
22	c	502	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
27	A	411	LMG	C18-C19-C20-C21
29	L	101	LHG	C27-C28-C29-C30
30	c	518	DGD	CAA-CBA-CCA-CDA
22	B	601	CLA	C15-C16-C17-C18
28	a	411	SQD	C5-C6-S-O7
28	b	620	SQD	C5-C6-S-O7
30	A	415	DGD	CCA-CDA-CEA-CFA
22	C	502	CLA	C11-C12-C13-C15
22	b	604	CLA	C12-C13-C15-C16
32	b	626	STE	C1-C2-C3-C4
32	C	520	STE	O1-C1-C2-C3
29	e	101	LHG	C17-C18-C19-C20
30	o	301	DGD	CEB-CFB-CGB-CHB
22	d	403	CLA	C4C-C3C-CAC-CBC
22	C	501	CLA	C2A-CAA-CBA-CGA
32	c	522	STE	C7-C8-C9-C10
29	a	410	LHG	C25-C26-C27-C28
32	d	412	STE	C11-C10-C9-C8
22	B	612	CLA	CBA-CGA-O2A-C1
34	f	101	HEM	CAD-CBD-CGD-O1D
28	F	102	SQD	C34-C35-C36-C37
30	h	103	DGD	O1B-C1B-C2B-C3B
22	b	609	CLA	C13-C15-C16-C17
22	b	605	CLA	C2-C3-C5-C6
28	B	621	SQD	C11-C10-C9-C8
29	l	101	LHG	C9-C10-C11-C12
28	f	102	SQD	O10-C23-C24-C25
27	A	411	LMG	C30-C31-C32-C33
22	B	606	CLA	C14-C13-C15-C16
22	C	502	CLA	C14-C13-C15-C16
22	C	511	CLA	C11-C12-C13-C14
22	D	402	CLA	C11-C12-C13-C14
22	D	404	CLA	C6-C7-C8-C9
22	D	404	CLA	C11-C10-C8-C9
22	b	601	CLA	C6-C7-C8-C9
22	d	403	CLA	C11-C12-C13-C14
27	b	623	LMG	O10-C28-C29-C30
22	c	501	CLA	CBD-CGD-O2D-CED
27	a	414	LMG	C36-C37-C38-C39
24	h	101	BCR	C11-C12-C13-C35
22	C	505	CLA	O1D-CGD-O2D-CED
22	B	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	B	610	CLA	C15-C16-C17-C18
30	c	516	DGD	O1B-C1B-C2B-C3B
27	b	623	LMG	C8-C7-O1-C1
30	C	515	DGD	C5D-C6D-O5D-C1E
30	c	517	DGD	O1A-C1A-C2A-C3A
27	M	101	LMG	C29-C30-C31-C32
27	c	521	LMG	C35-C36-C37-C38
32	M	103	STE	C6-C7-C8-C9
22	B	601	CLA	C10-C11-C12-C13
22	b	611	CLA	C15-C16-C17-C18
30	C	515	DGD	CDB-CEB-CFB-CGB
22	B	610	CLA	CAD-CBD-CGD-O2D
22	b	607	CLA	CAD-CBD-CGD-O2D
22	b	613	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CAD-CBD-CGD-O2D
22	d	405	CLA	CAD-CBD-CGD-O2D
28	a	411	SQD	C14-C15-C16-C17
22	C	512	CLA	C15-C16-C17-C18
27	Y	101	LMG	C16-C17-C18-C19
22	d	403	CLA	C2-C1-O2A-CGA
29	a	410	LHG	O8-C23-C24-C25
30	c	516	DGD	O2G-C1B-C2B-C3B
22	b	615	CLA	C13-C15-C16-C17
29	d	408	LHG	C7-C8-C9-C10
22	B	606	CLA	C11-C10-C8-C7
30	A	415	DGD	O1B-C1B-C2B-C3B
28	a	411	SQD	C13-C14-C15-C16
27	a	414	LMG	C10-C11-C12-C13
22	B	613	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

100 monomers are involved in 130 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	C	511	CLA	1	0
22	c	509	CLA	2	0
22	b	616	CLA	2	0
27	A	411	LMG	1	0
30	c	517	DGD	1	0
32	M	104	STE	1	0
22	B	607	CLA	1	0
32	d	412	STE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	405	BCR	2	0
26	A	410	PL9	1	0
24	d	406	BCR	2	0
26	a	409	PL9	4	0
32	I	101	STE	2	0
22	C	509	CLA	1	0
35	V	201	HEC	2	0
22	b	604	CLA	2	0
22	c	511	CLA	2	0
32	c	520	STE	2	0
29	D	411	LHG	3	0
22	B	614	CLA	1	0
30	o	301	DGD	3	0
24	b	618	BCR	2	0
22	c	507	CLA	1	0
22	B	605	CLA	1	0
22	c	512	CLA	1	0
29	A	413	LHG	3	0
27	D	410	LMG	1	0
29	a	410	LHG	1	0
29	e	101	LHG	2	0
24	B	619	BCR	1	0
22	A	406	CLA	1	0
29	l	101	LHG	1	0
22	d	404	CLA	1	0
32	B	627	STE	2	0
28	f	102	SQD	2	0
28	B	621	SQD	1	0
24	K	102	BCR	2	0
22	a	402	CLA	1	0
22	B	601	CLA	4	0
22	c	510	CLA	2	0
22	b	602	CLA	2	0
22	C	512	CLA	2	0
24	h	101	BCR	1	0
24	t	101	BCR	2	0
26	D	406	PL9	1	0
22	C	513	CLA	1	0
22	b	601	CLA	2	0
22	D	402	CLA	1	0
24	k	102	BCR	1	0
22	B	611	CLA	1	0

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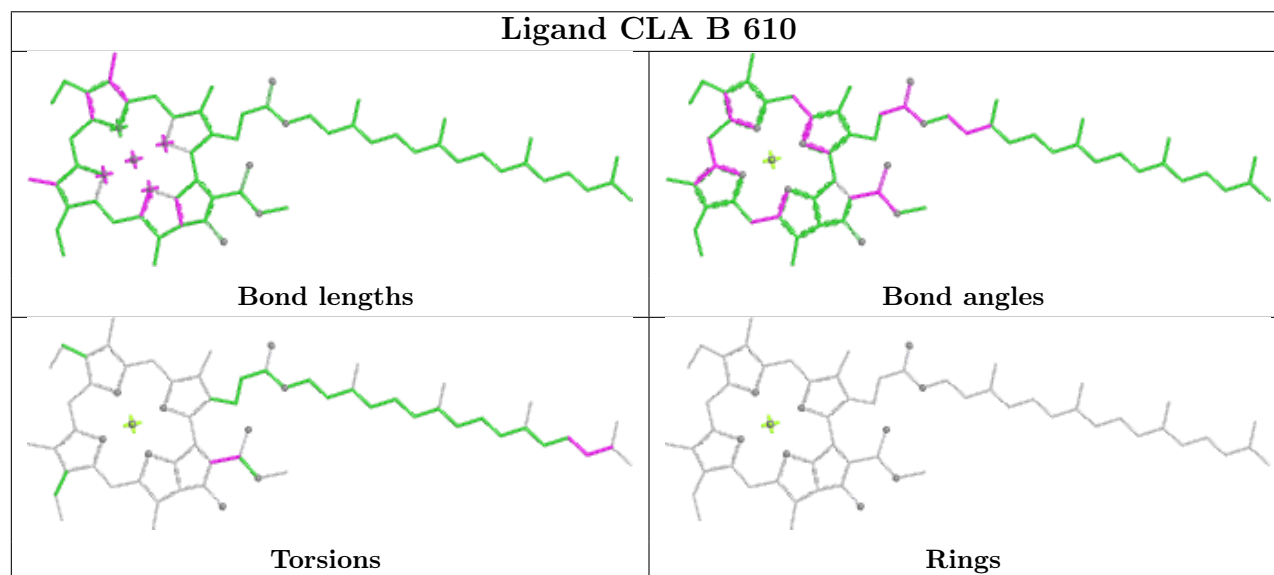
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22	b	614	CLA	1	0
24	b	619	BCR	1	0
29	D	408	LHG	1	0
22	b	610	CLA	1	0
27	m	101	LMG	1	0
29	d	408	LHG	1	0
28	A	414	SQD	2	0
22	B	602	CLA	1	0
22	B	606	CLA	2	0
26	d	407	PL9	1	0
22	b	605	CLA	1	0
32	D	413	STE	1	0
22	b	606	CLA	2	0
24	H	101	BCR	3	0
34	f	101	HEM	6	0
32	b	622	STE	1	0
23	A	405	PHO	1	0
24	c	515	BCR	1	0
29	L	101	LHG	1	0
27	M	101	LMG	2	0
24	C	514	BCR	1	0
22	b	615	CLA	3	0
22	C	508	CLA	1	0
32	B	624	STE	1	0
22	c	513	CLA	1	0
22	B	604	CLA	1	0
35	v	201	HEC	2	0
28	b	620	SQD	1	0
24	T	101	BCR	2	0
30	A	415	DGD	5	0
22	c	501	CLA	2	0
30	C	516	DGD	1	0
32	H	103	STE	1	0
22	D	404	CLA	1	0
22	C	502	CLA	1	0
22	a	405	CLA	1	0
32	B	620	STE	1	0
22	B	612	CLA	1	0
22	C	510	CLA	1	0
34	F	101	HEM	1	0
24	c	514	BCR	1	0
22	C	506	CLA	1	0

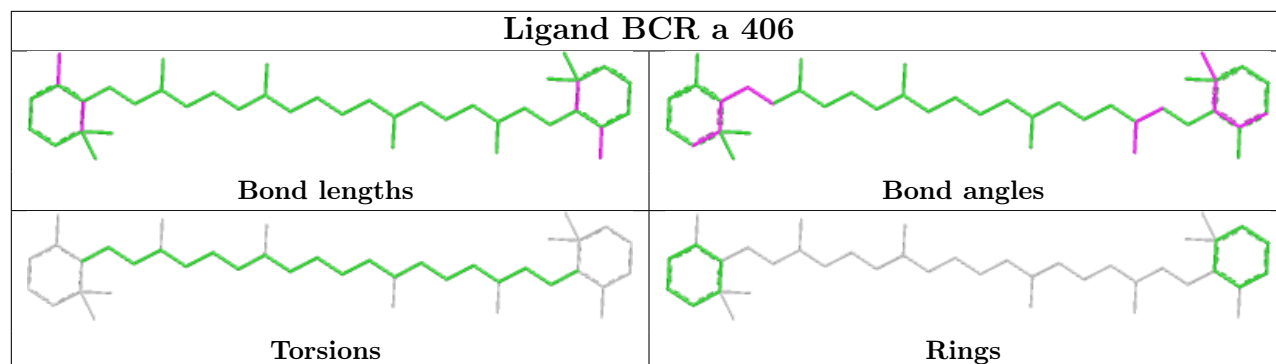
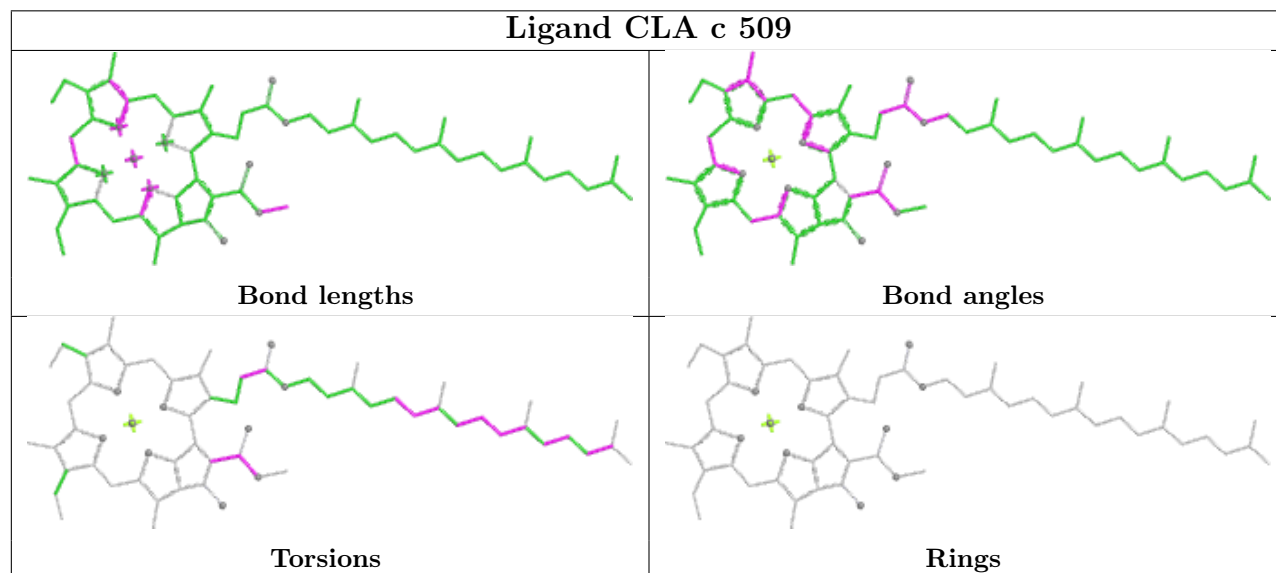
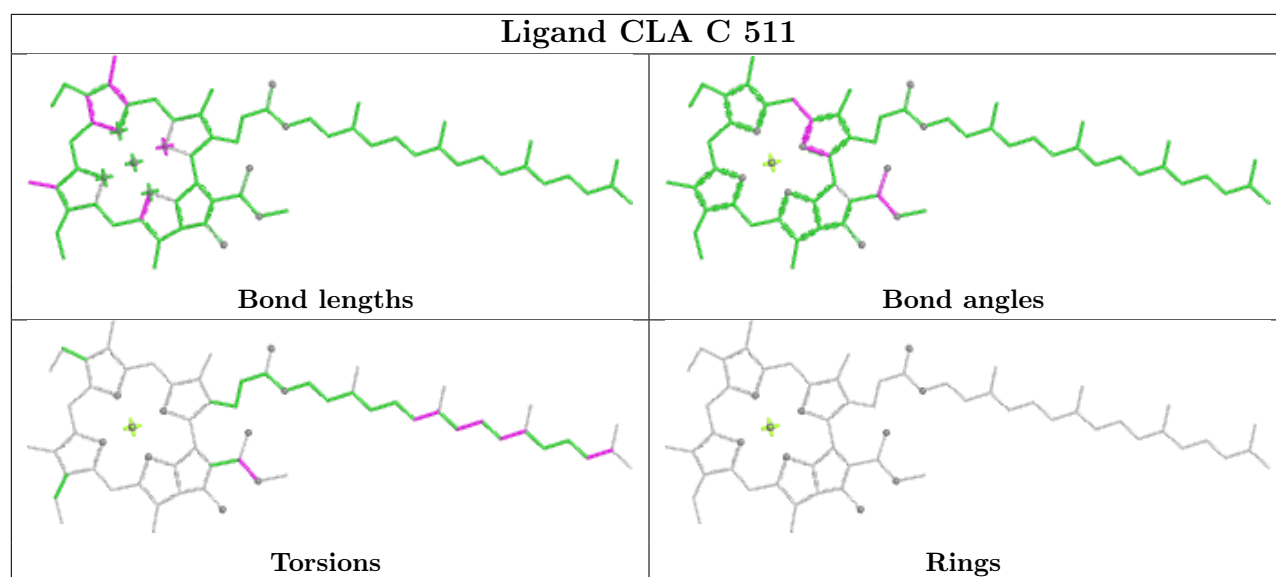
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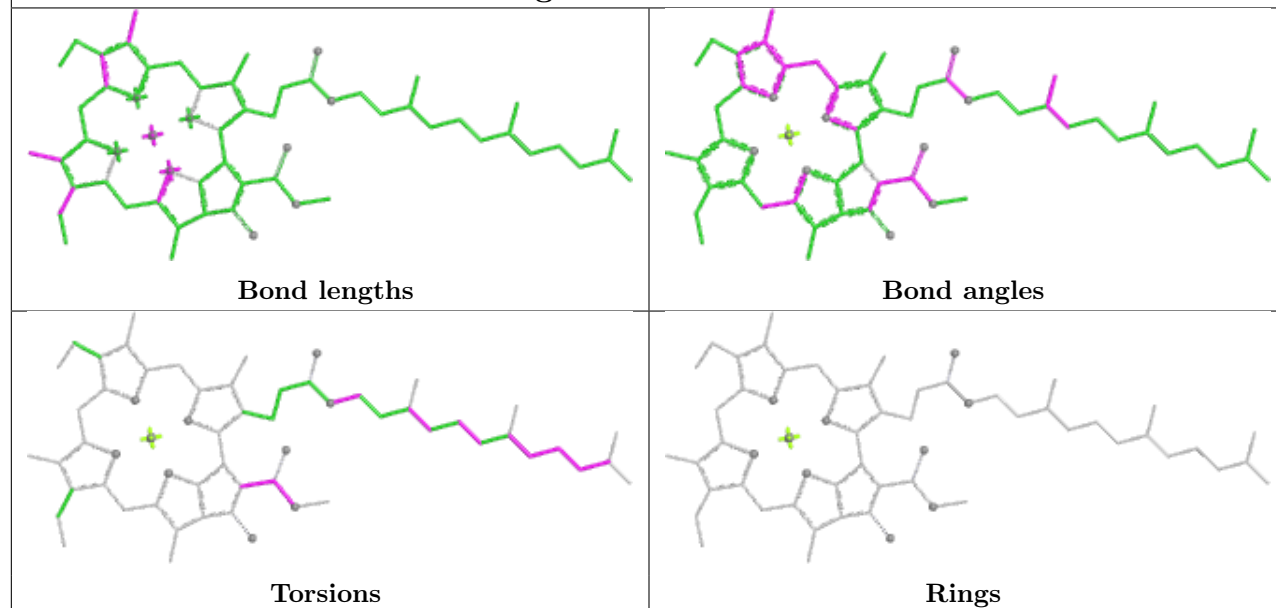
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	616	CLA	1	0
22	C	507	CLA	1	0
22	C	501	CLA	2	0
22	D	403	CLA	1	0
30	c	518	DGD	1	0
22	c	506	CLA	1	0
22	b	612	CLA	1	0
22	c	503	CLA	2	0

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.

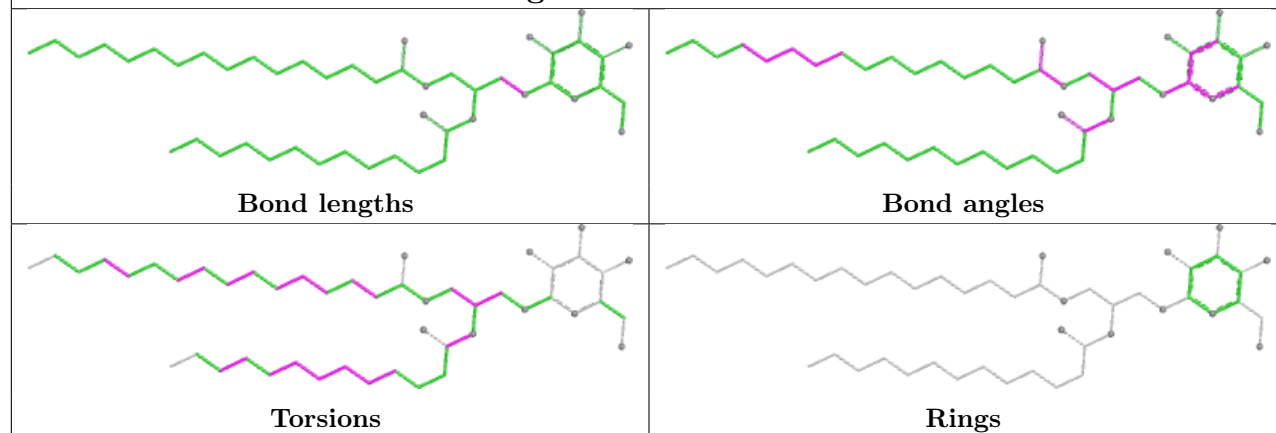




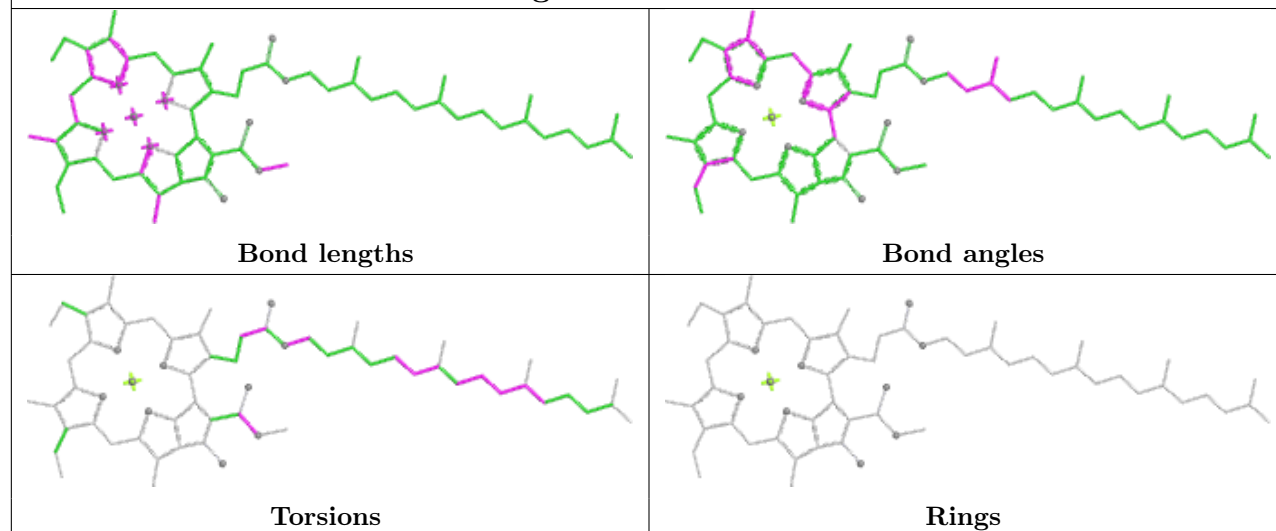
Ligand CLA b 616

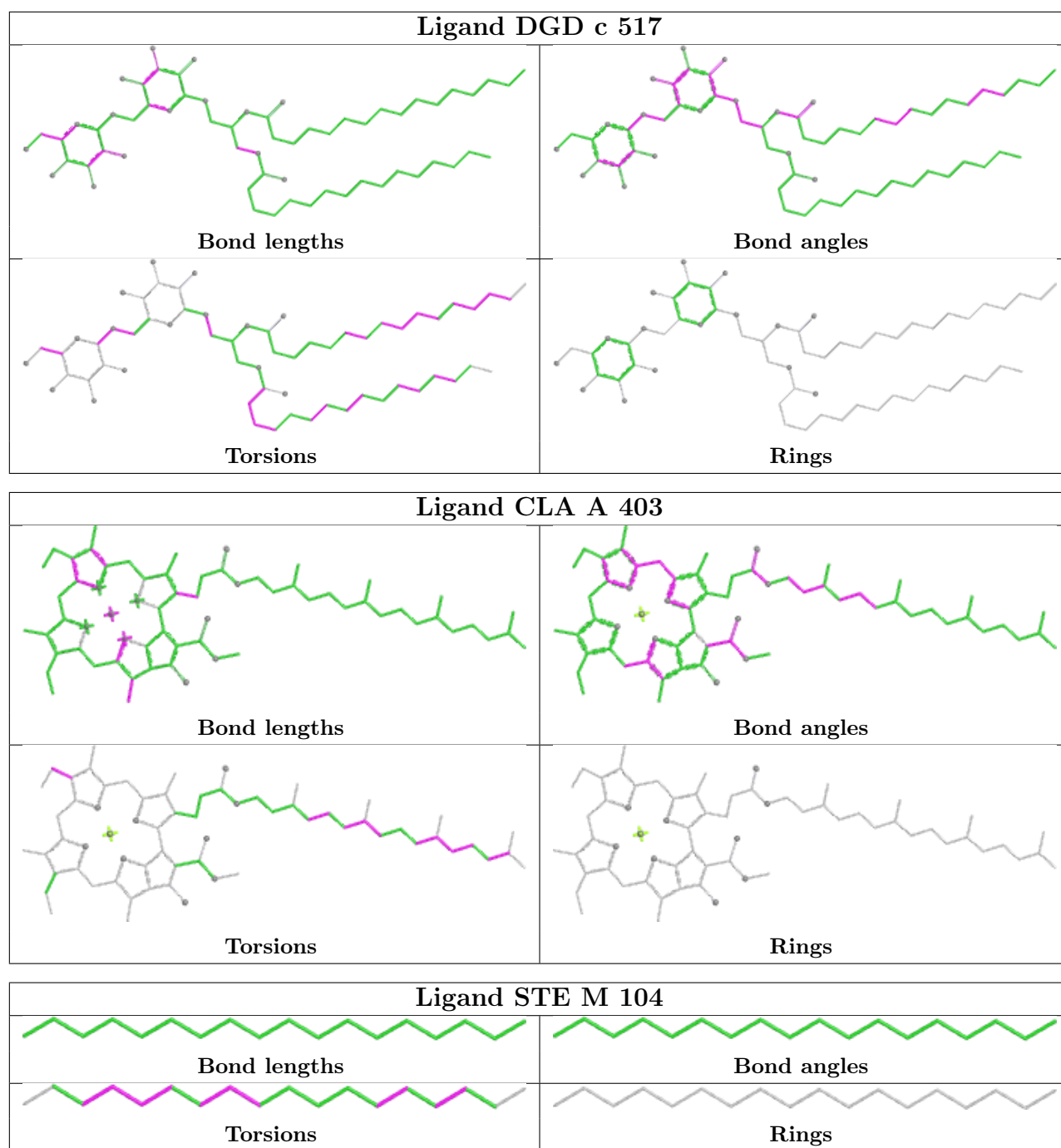


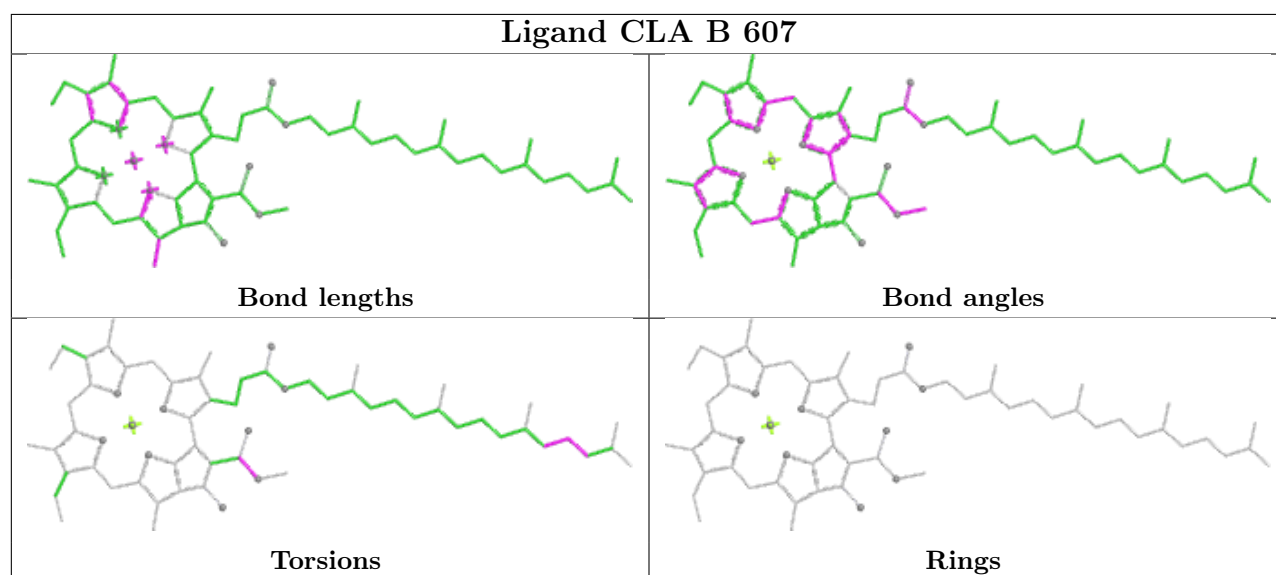
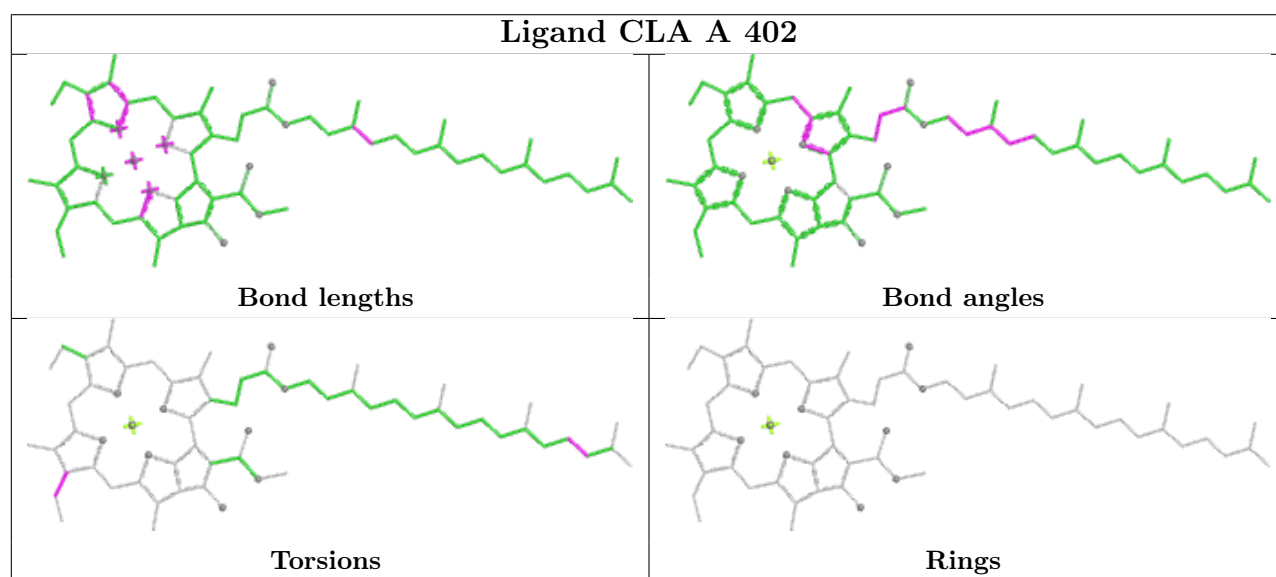
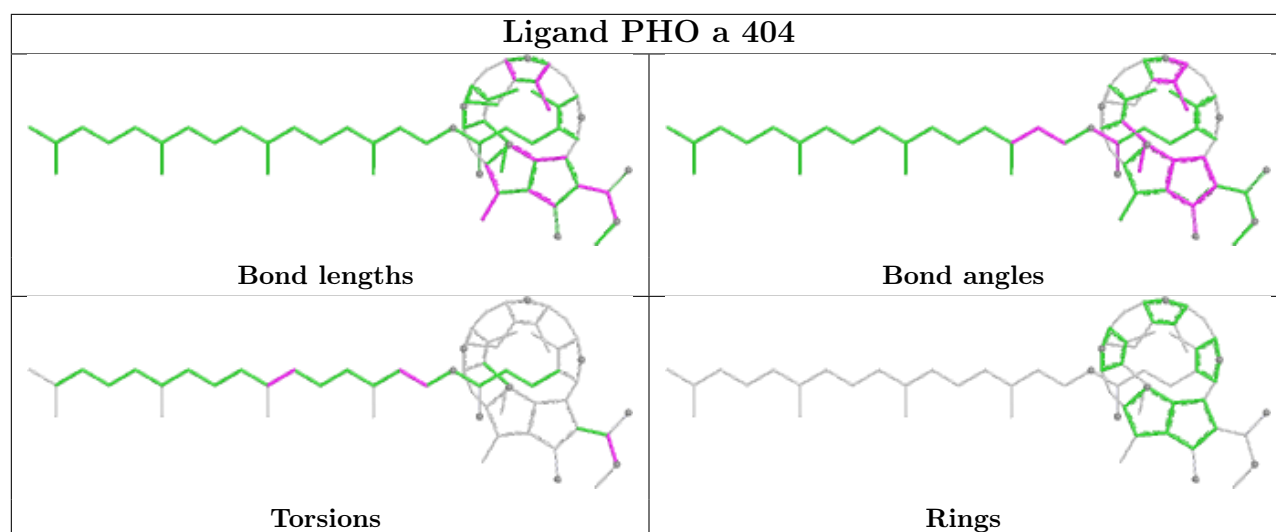
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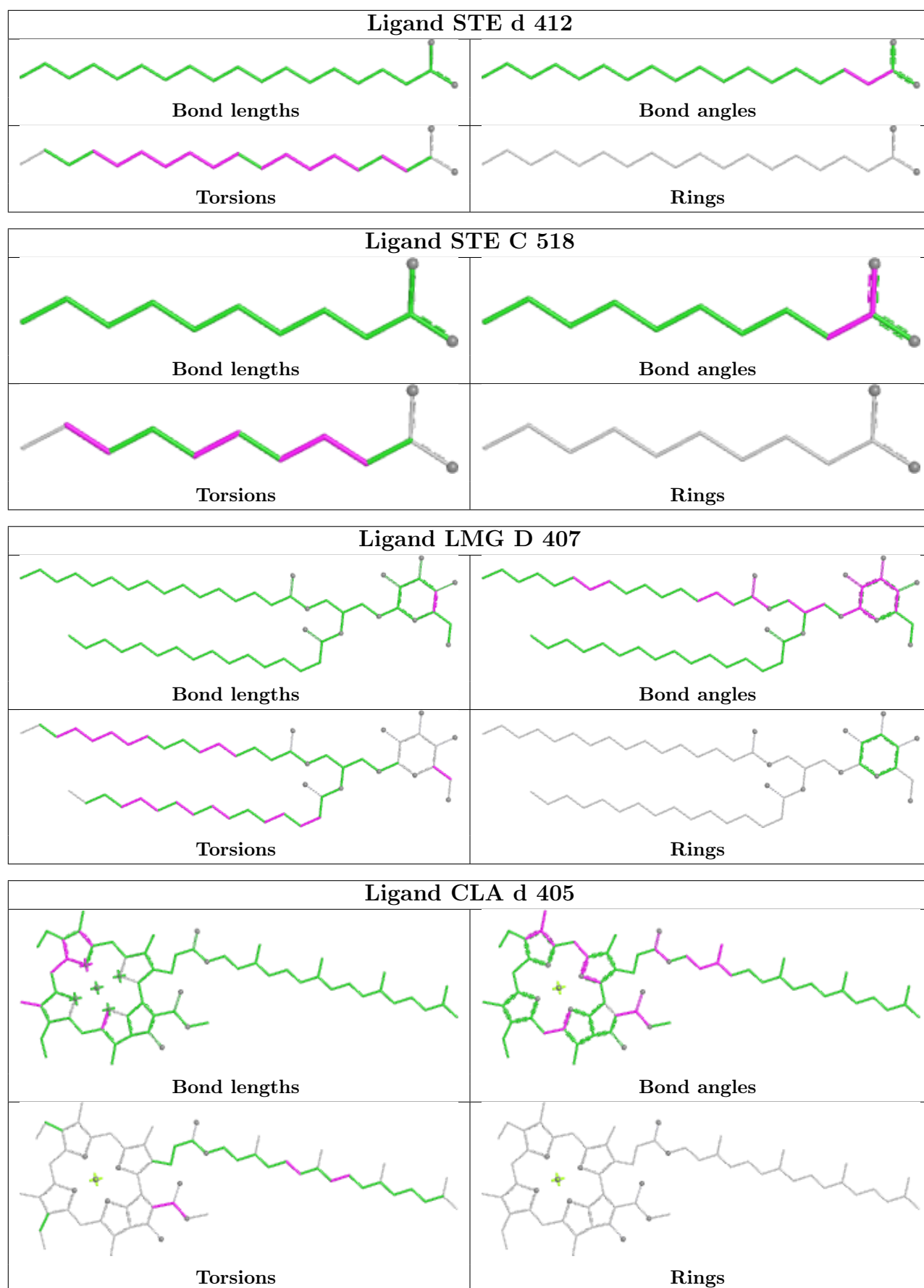


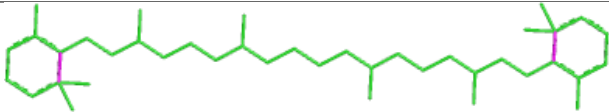
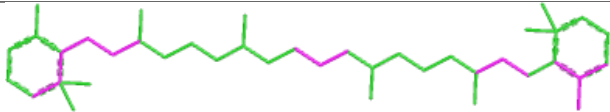
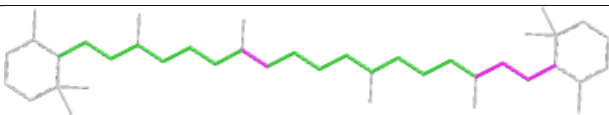
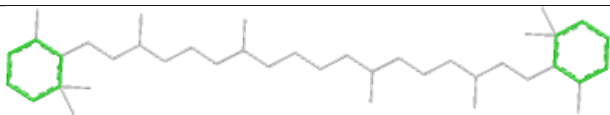
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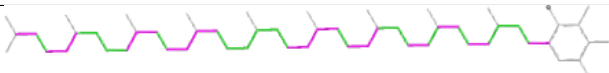


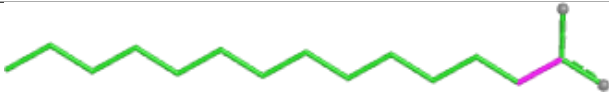
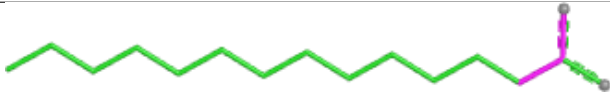
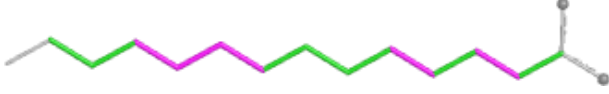
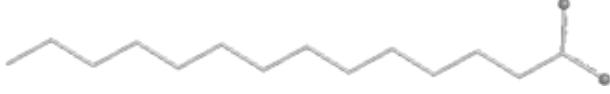


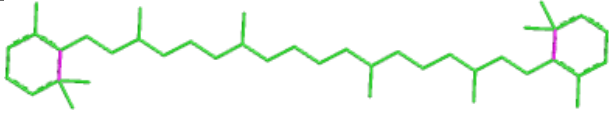
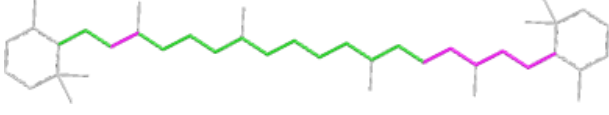
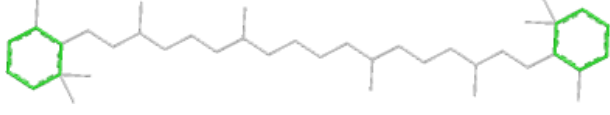


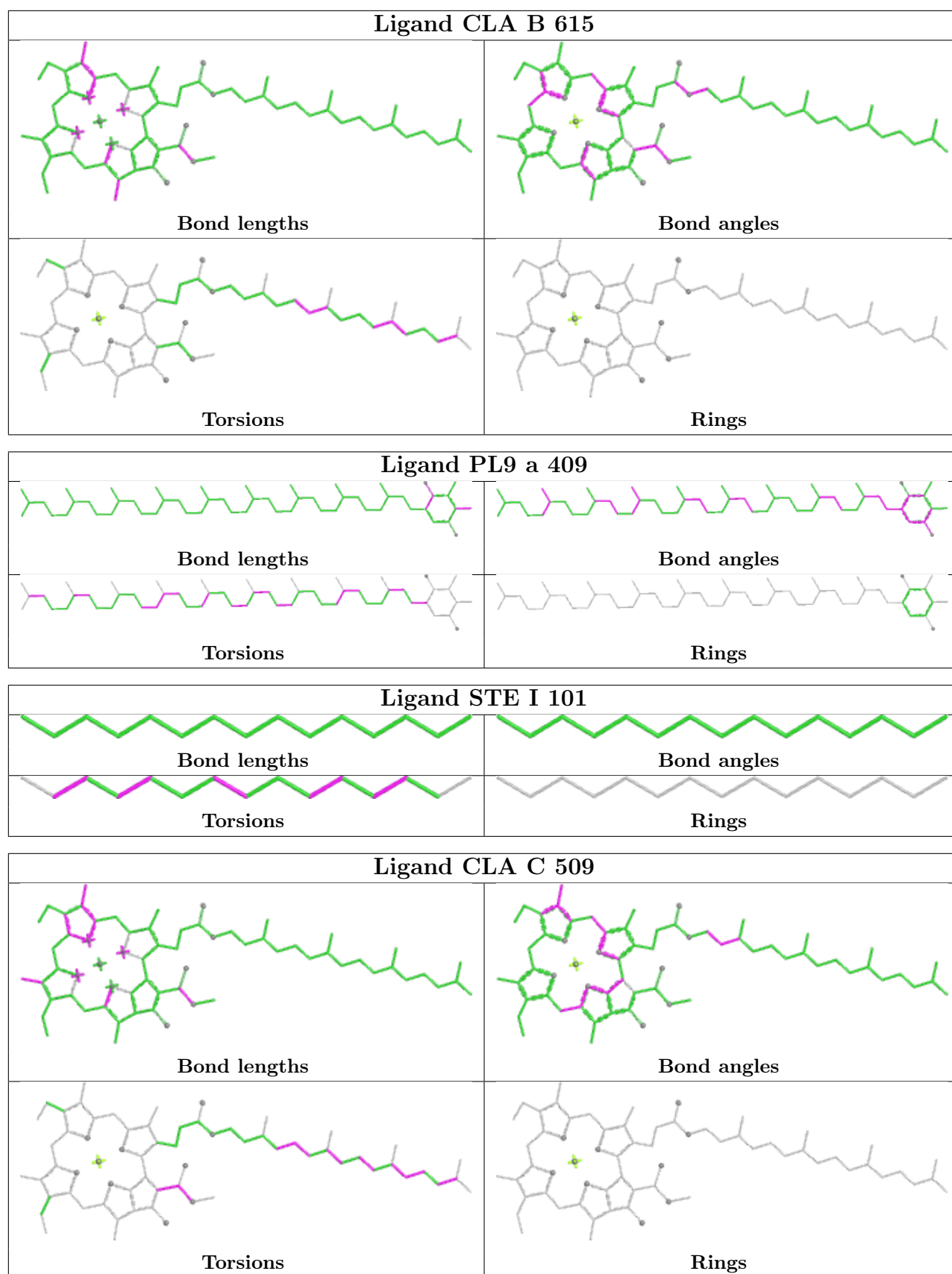


Ligand BCR D 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

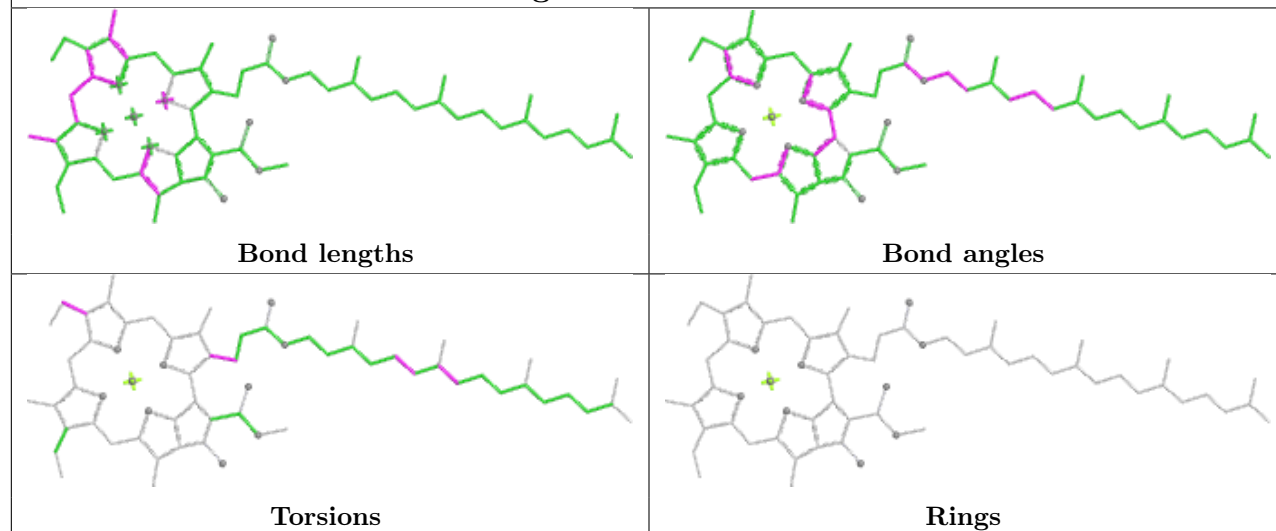
Ligand PL9 A 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

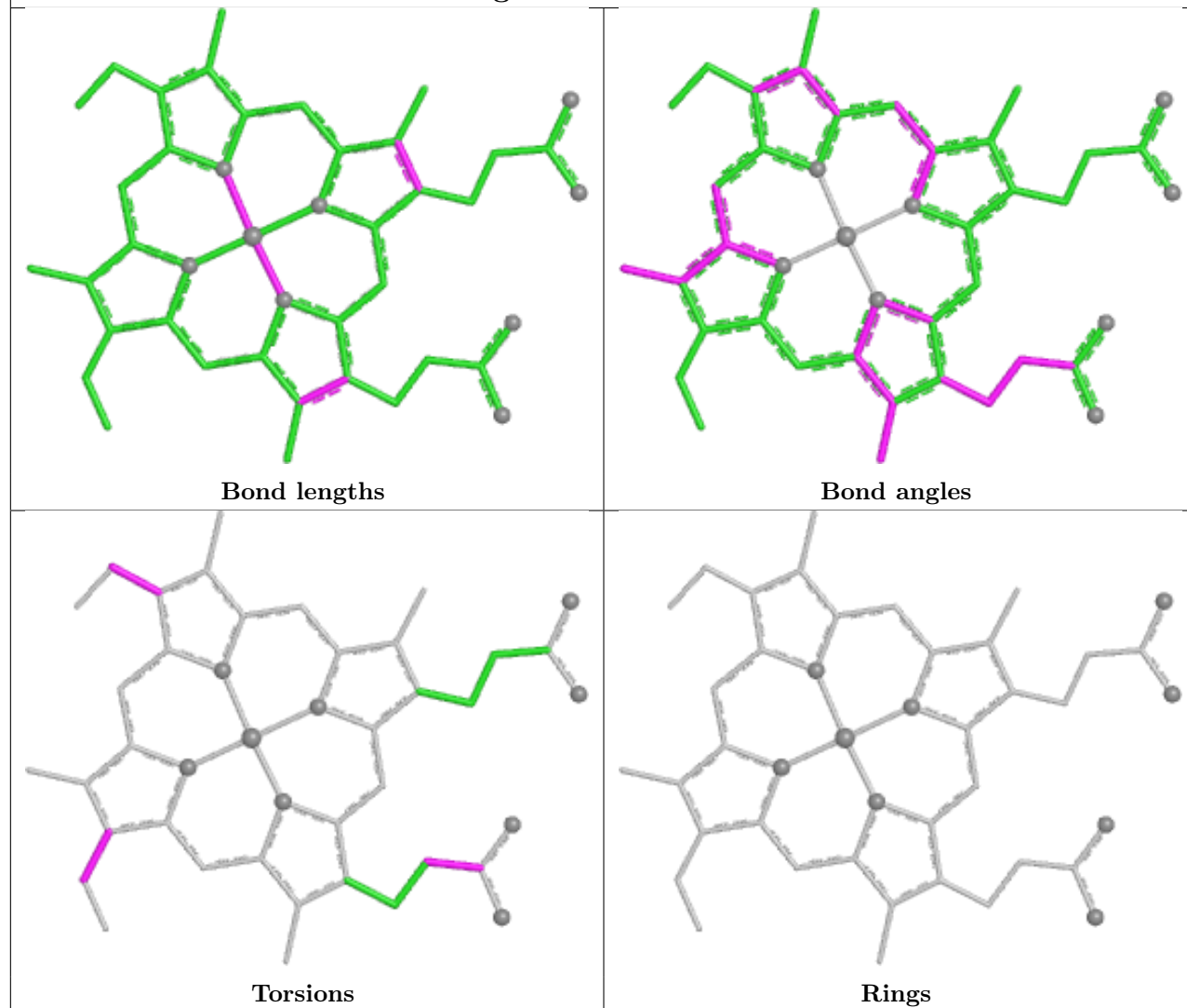
Ligand BCR d 406	
	
Bond lengths	Bond angles
	
Torsions	Rings

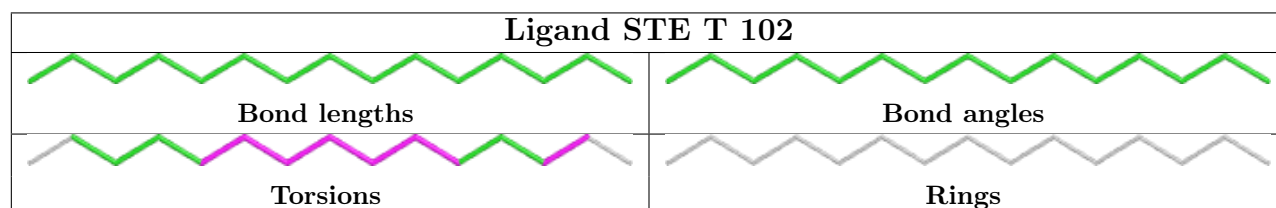
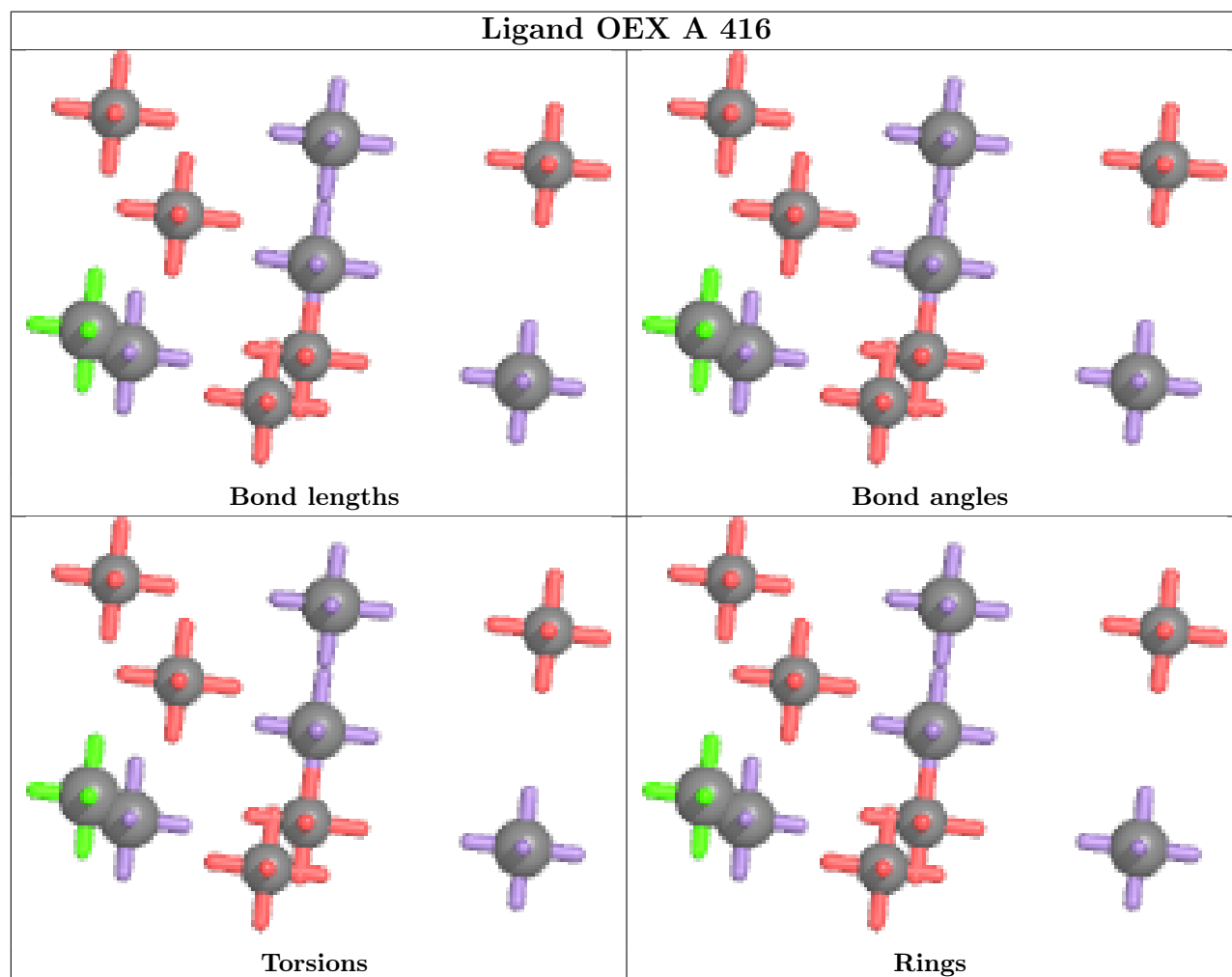
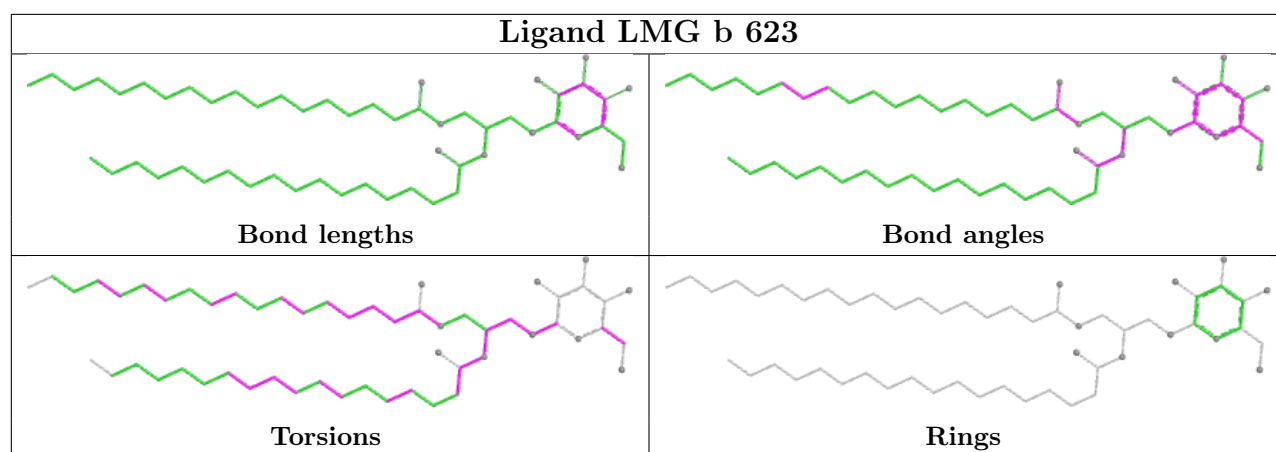


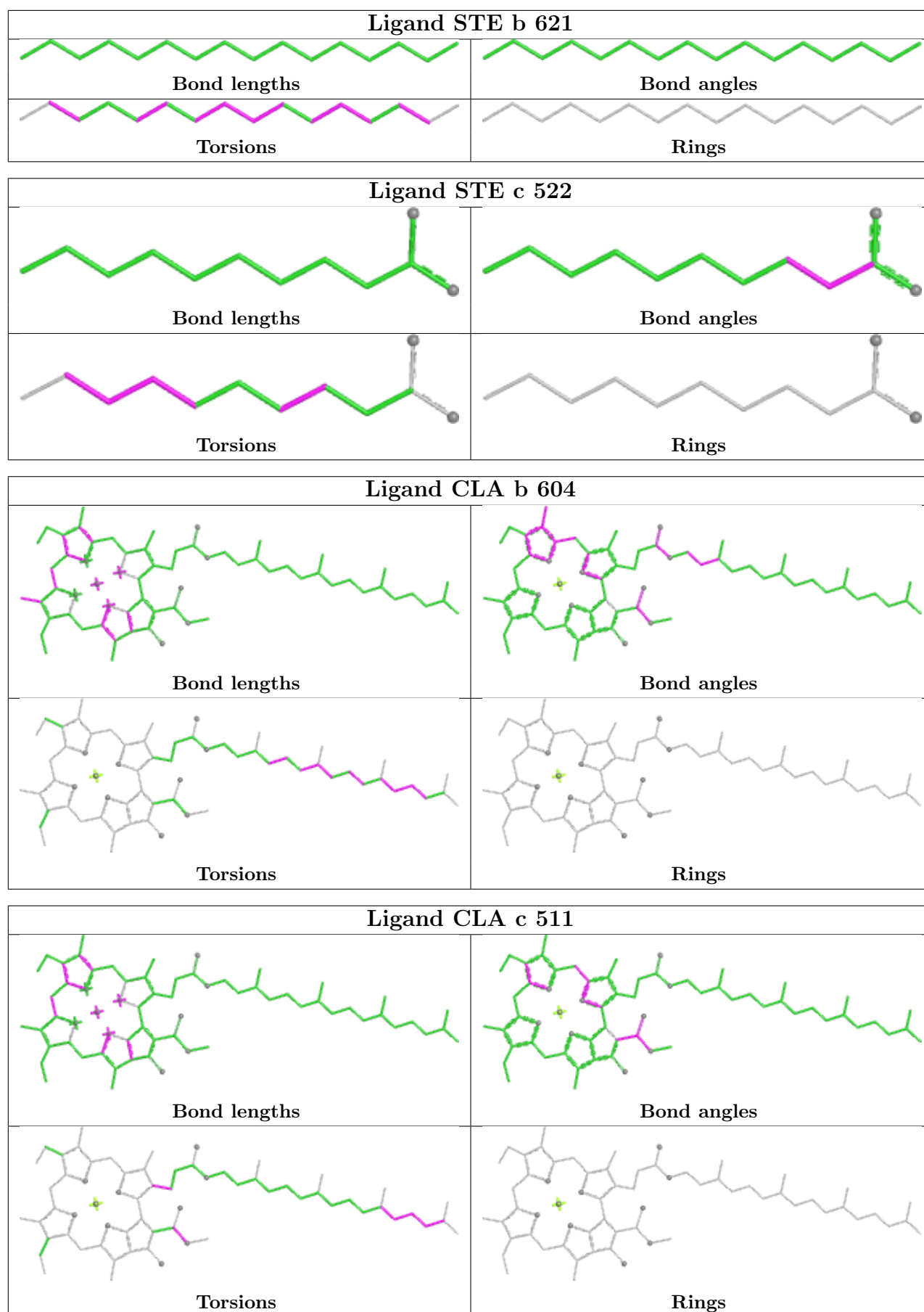
Ligand CLA C 503

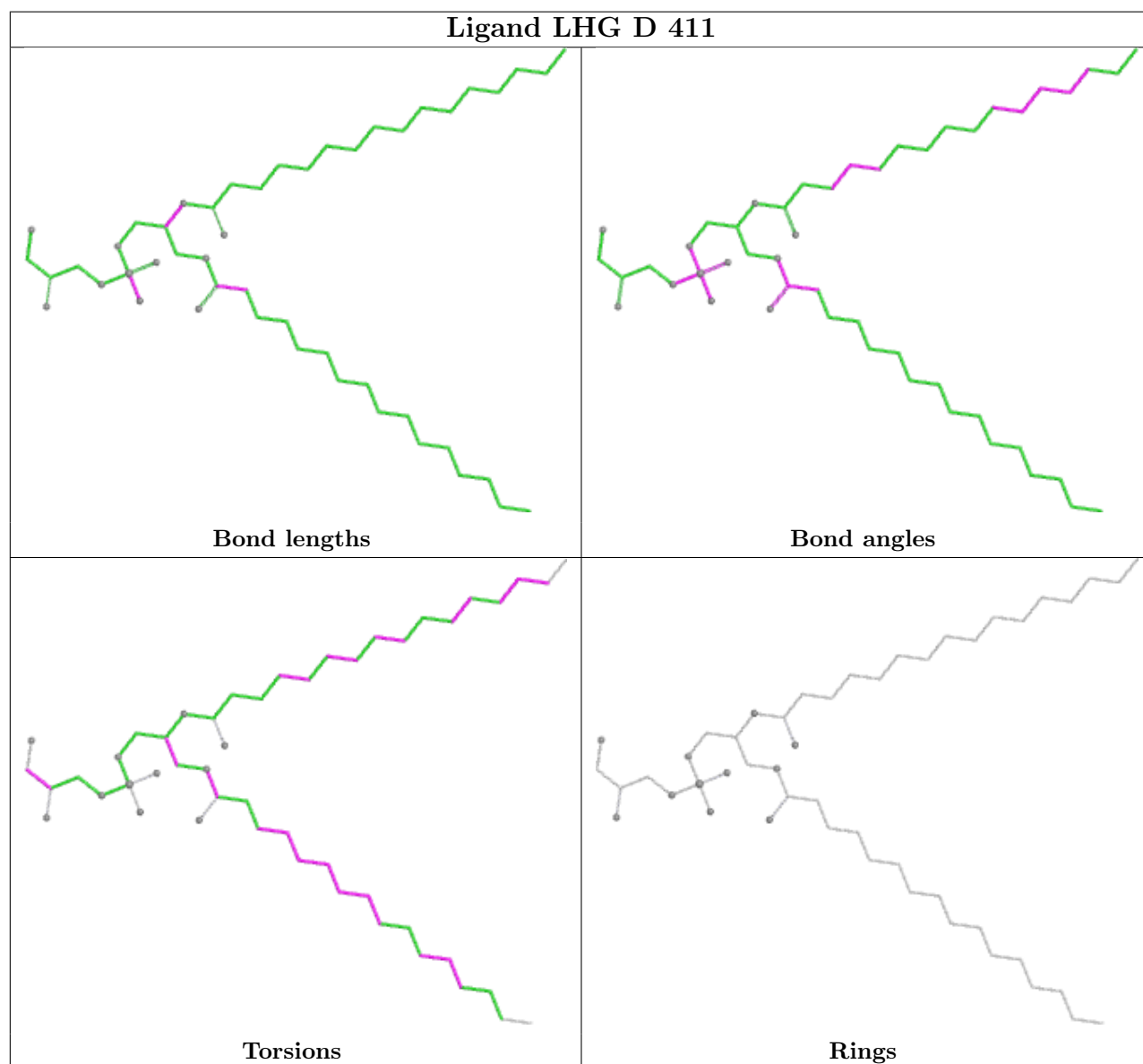
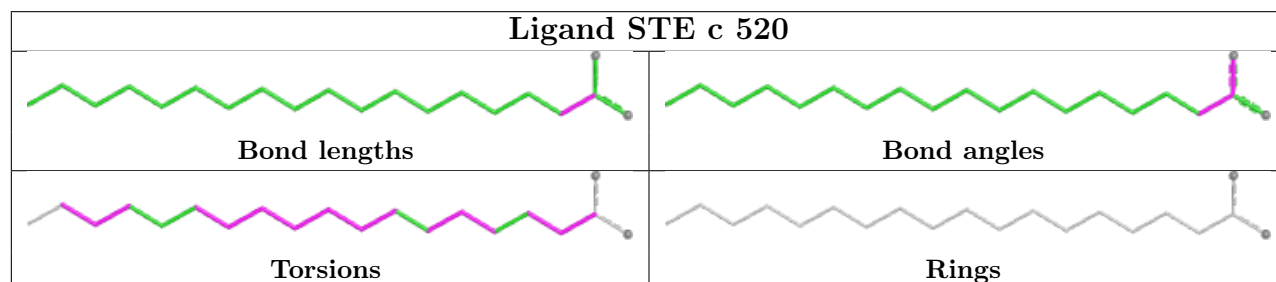
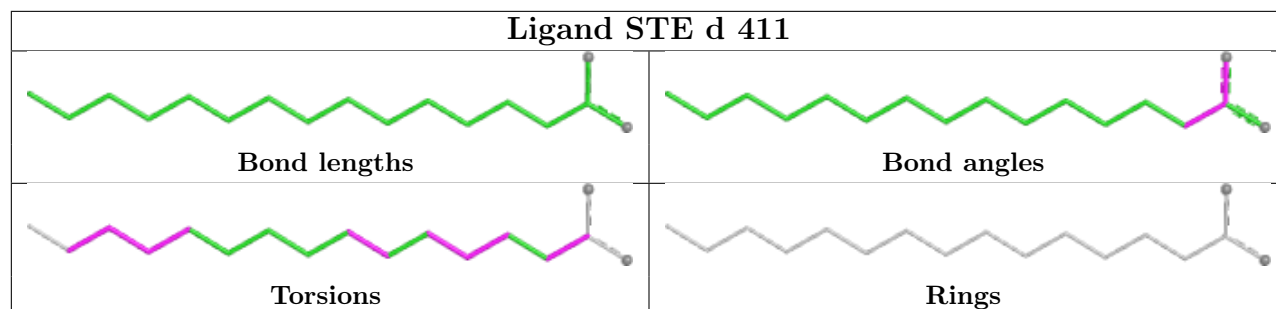


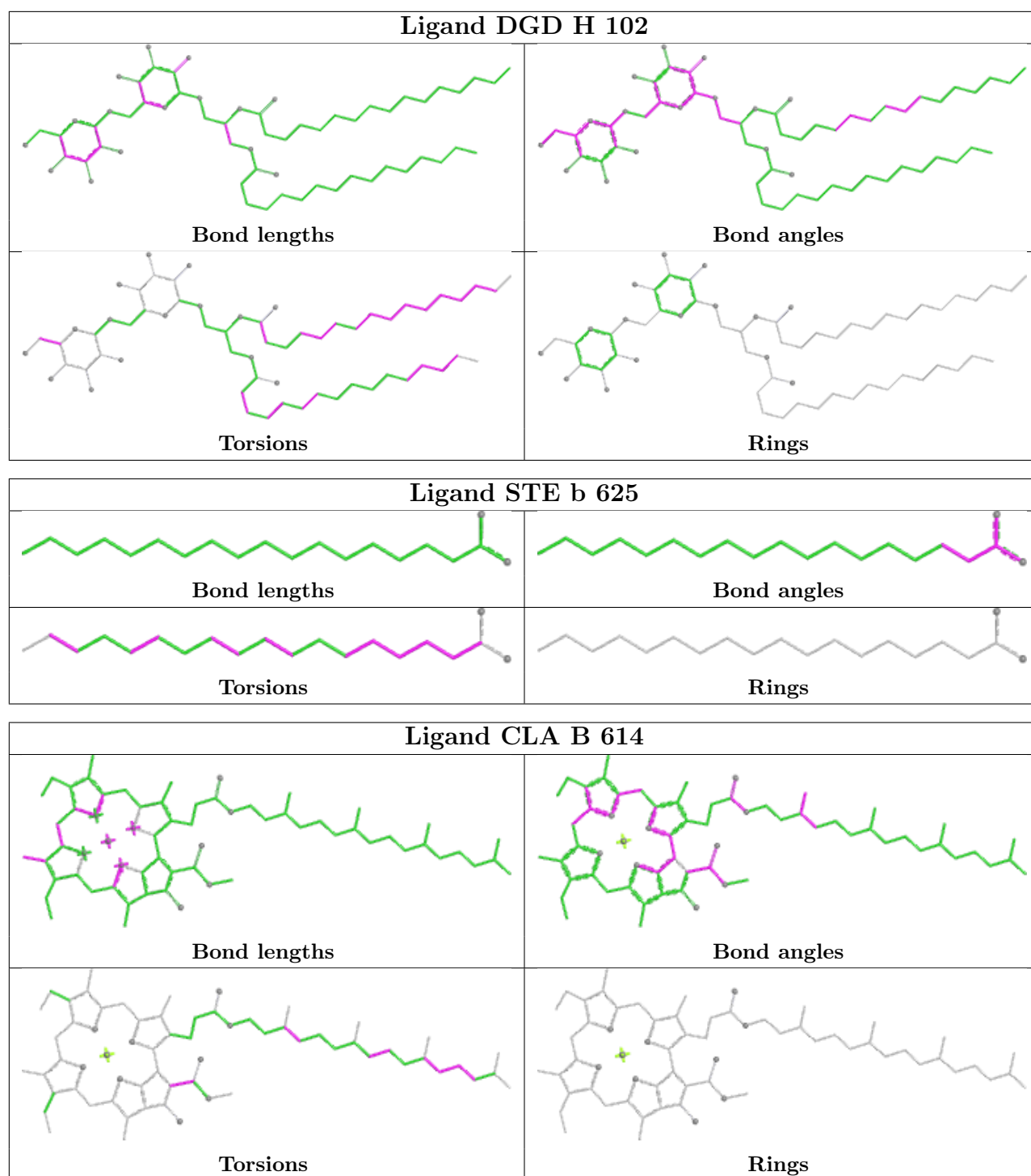
Ligand HEC V 201

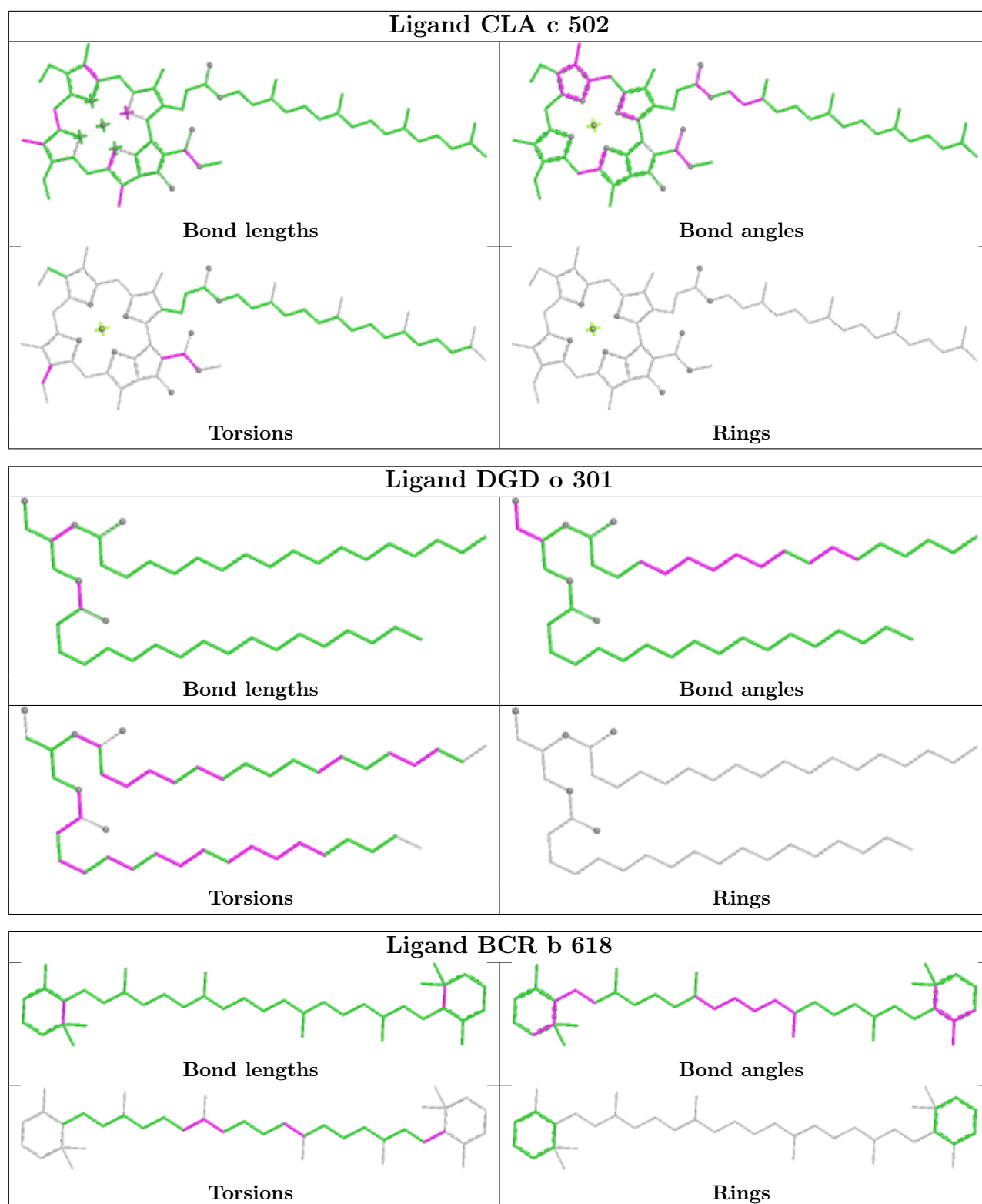




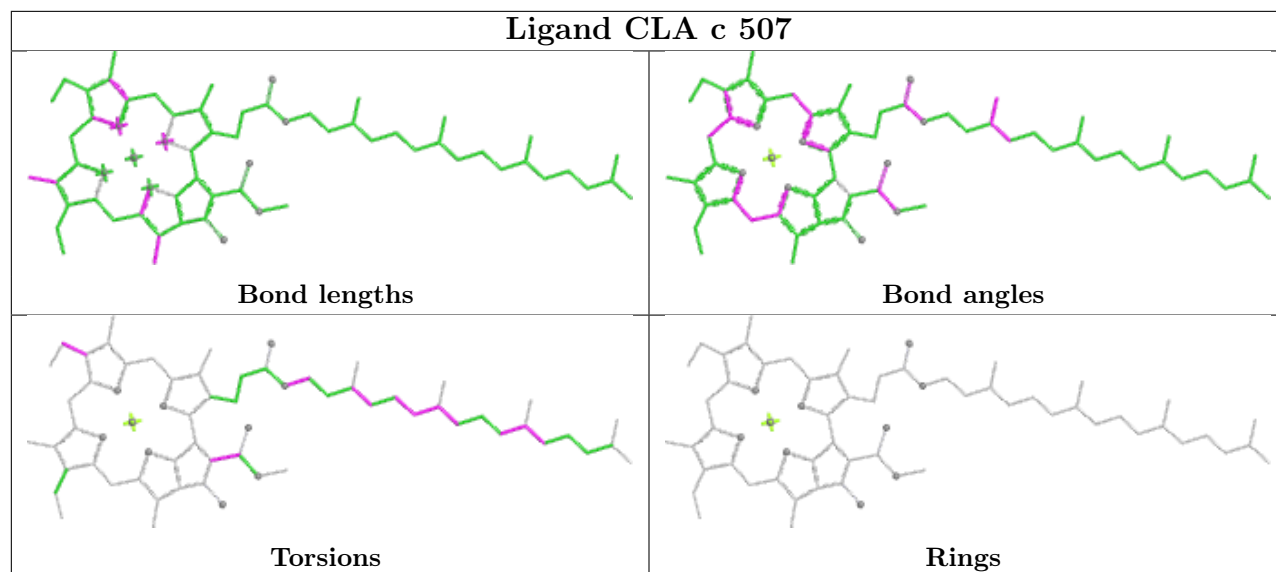




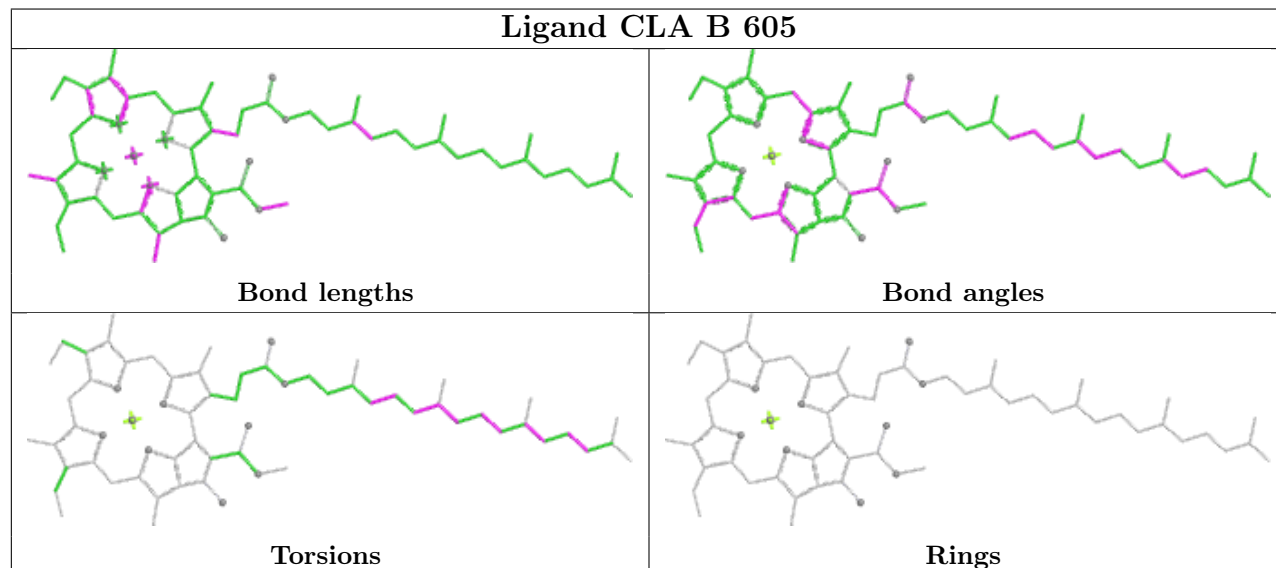




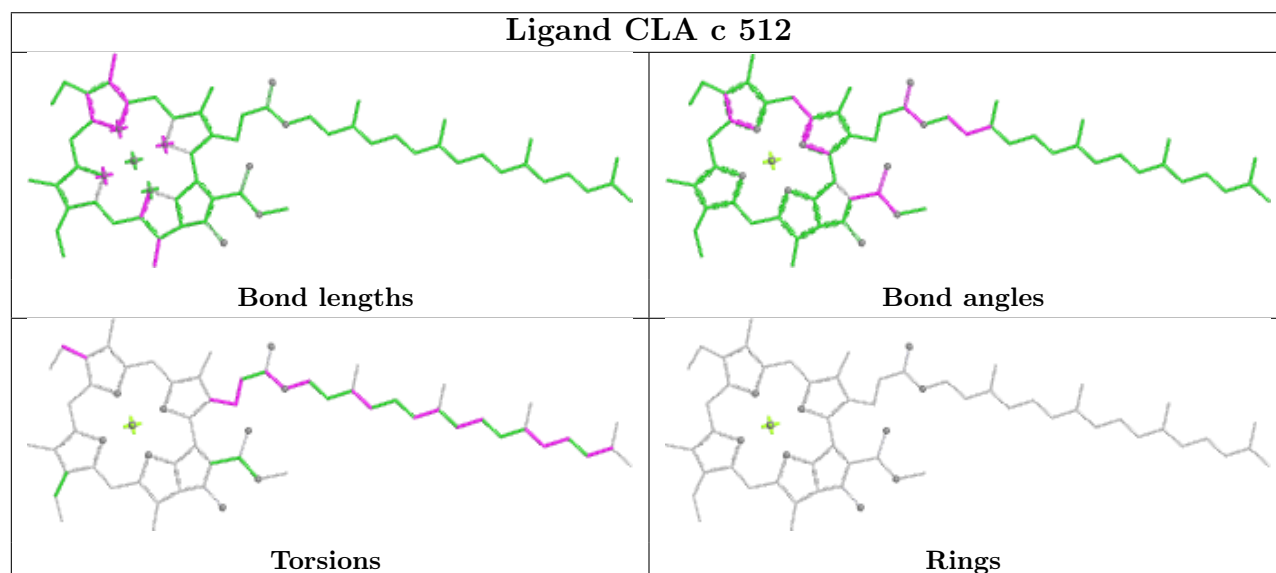
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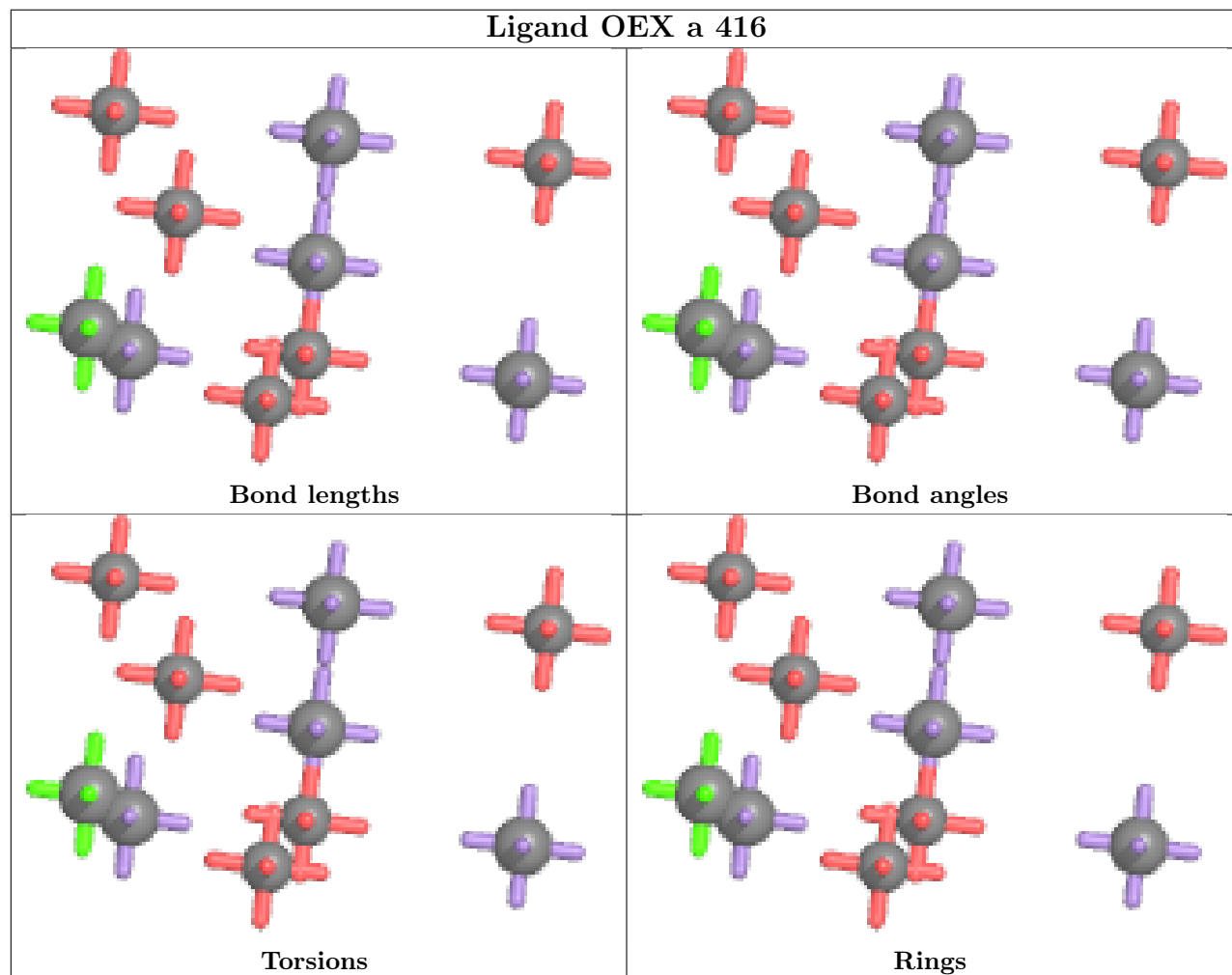
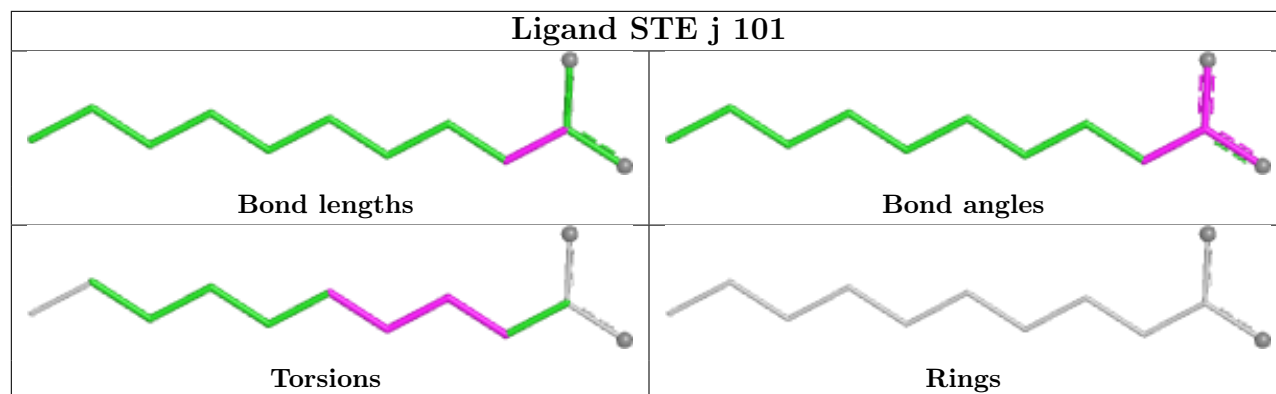


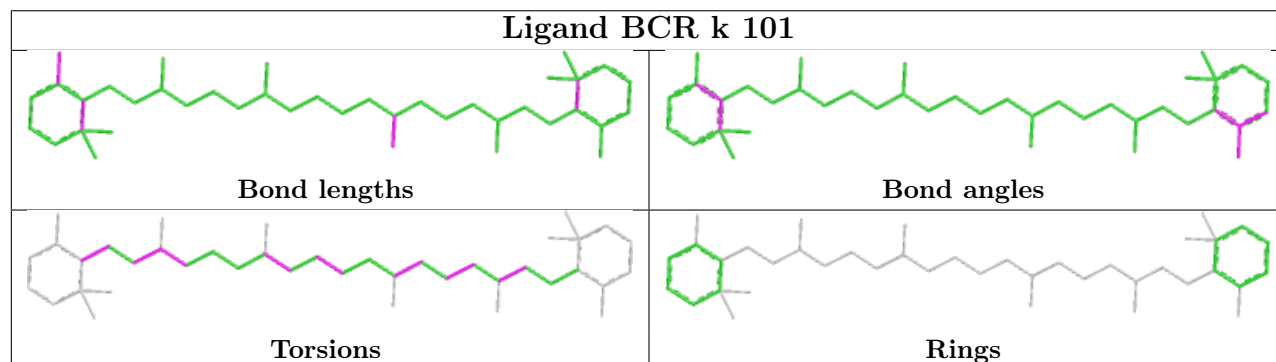
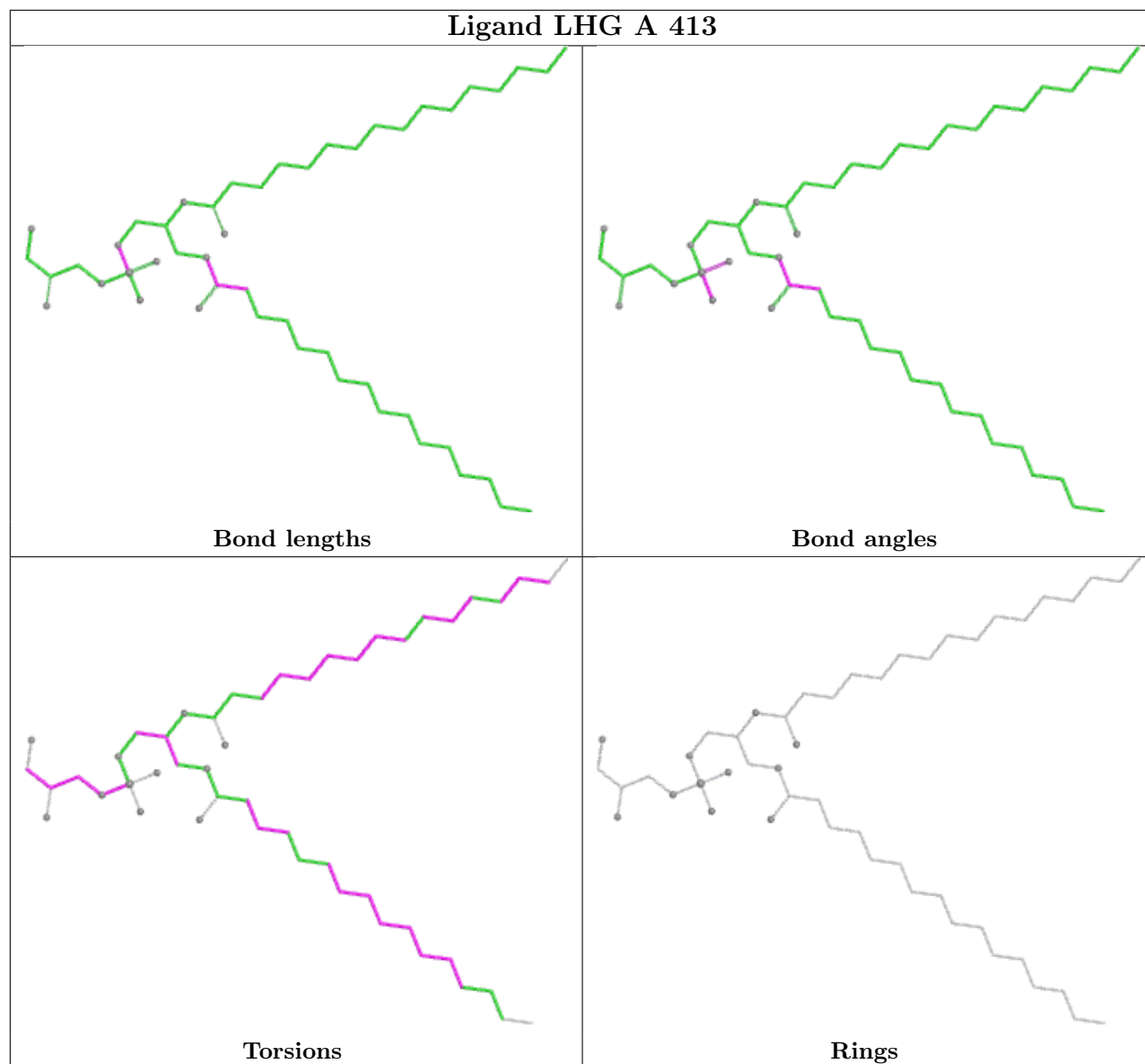
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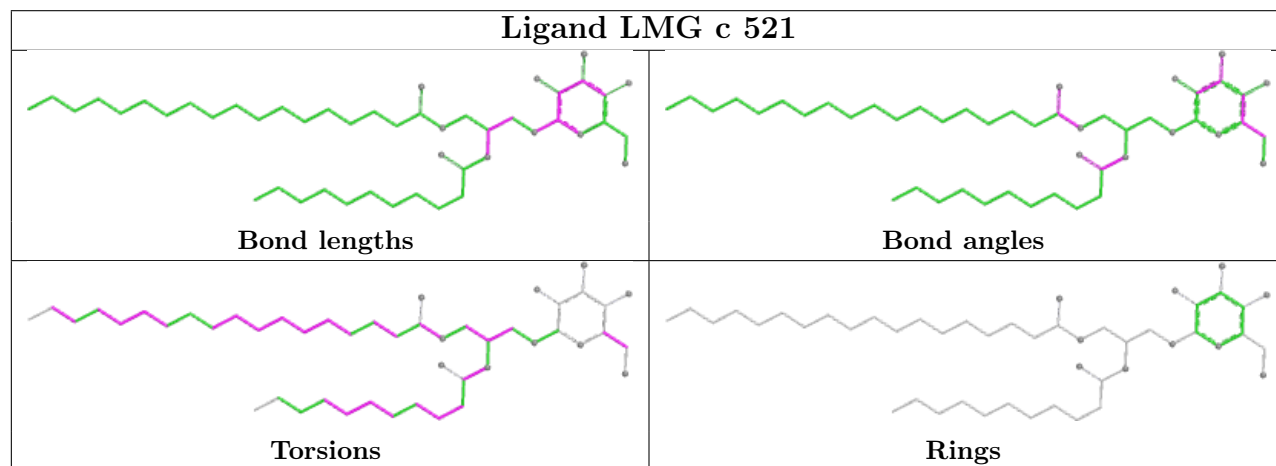
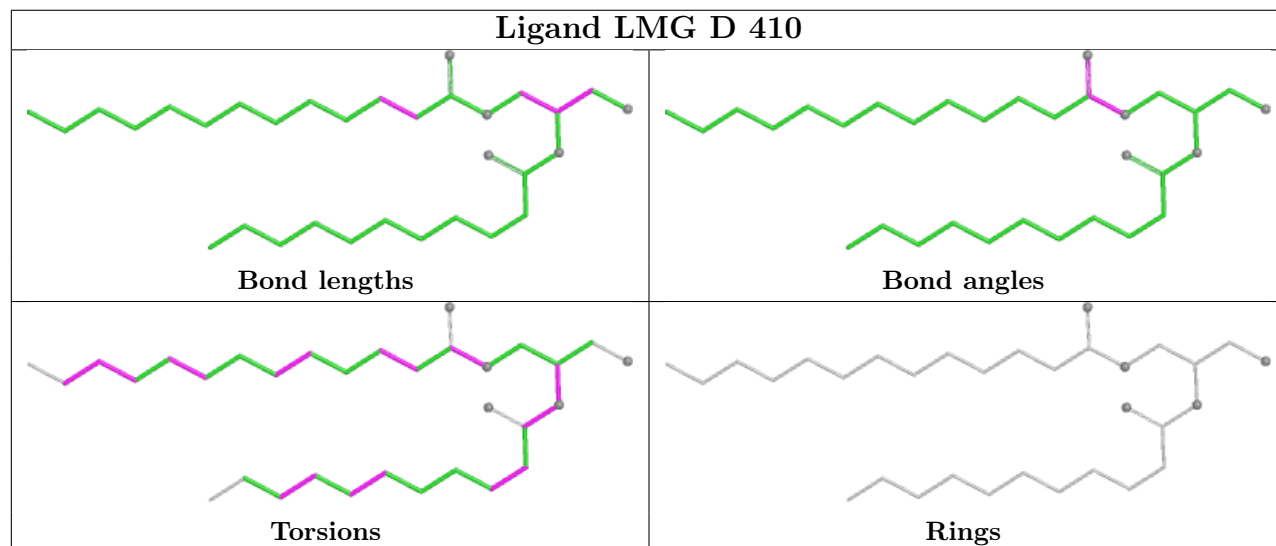
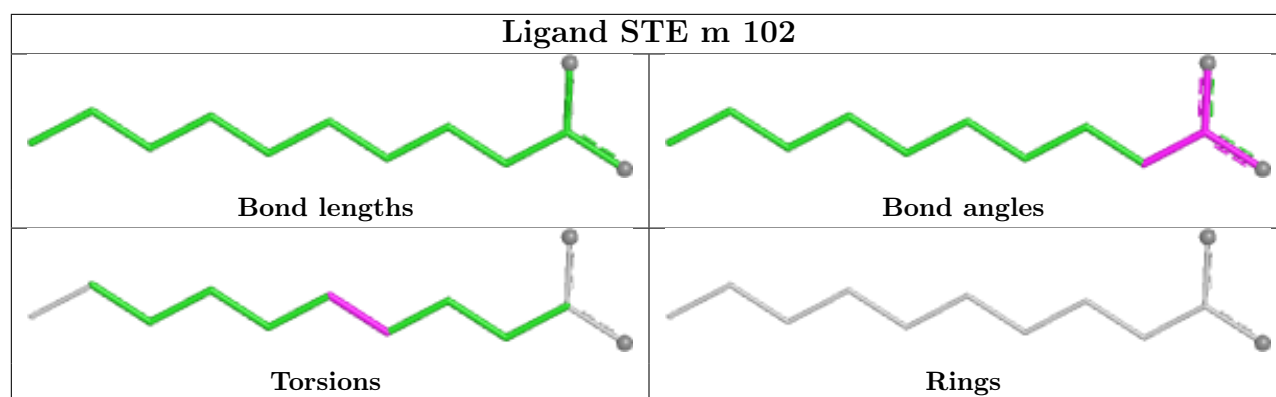


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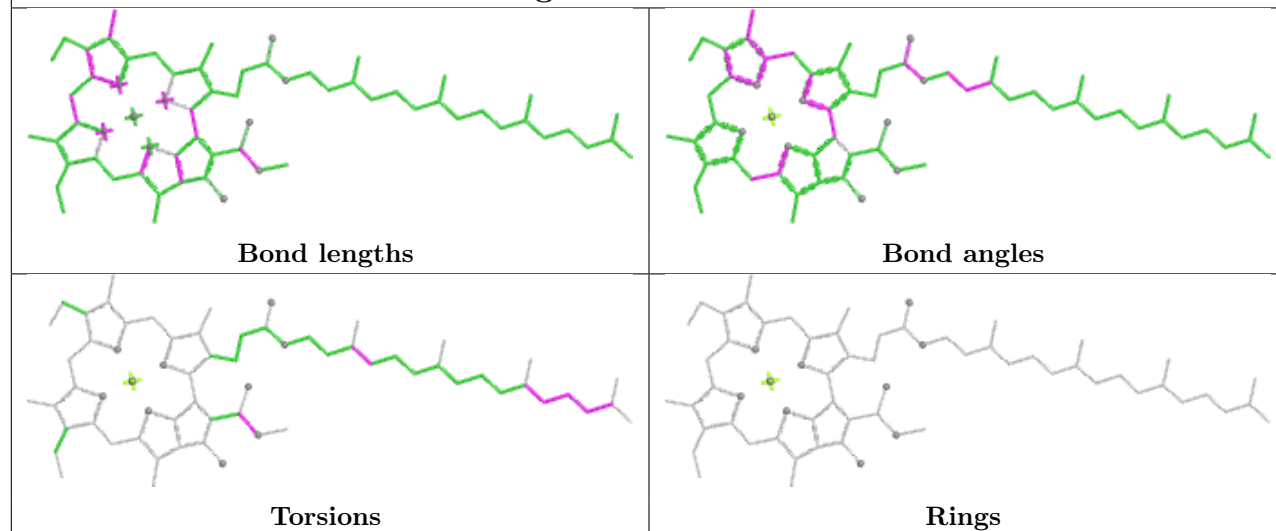




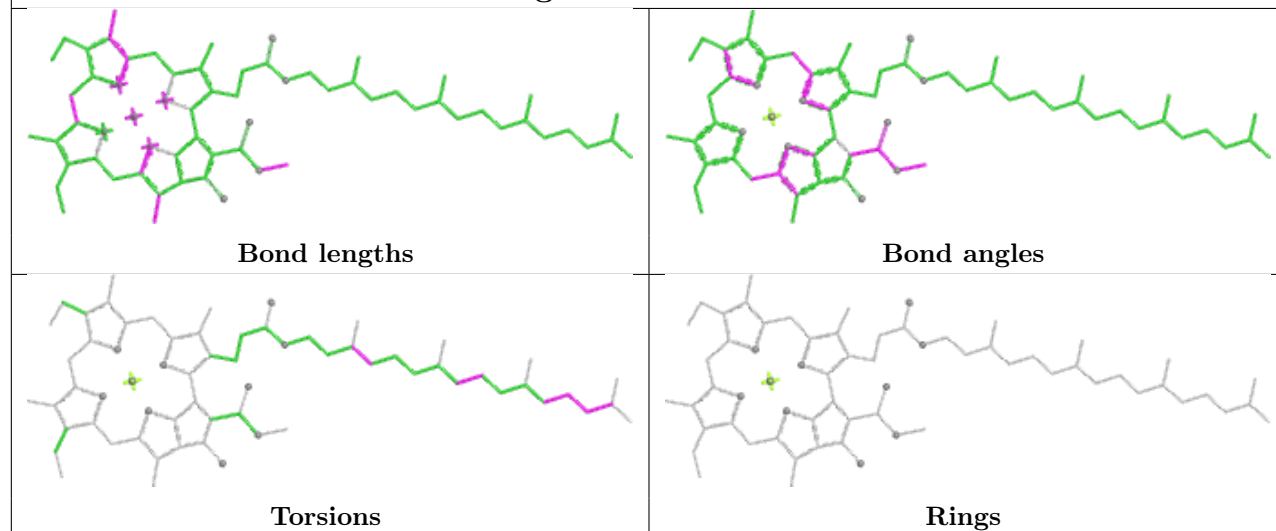


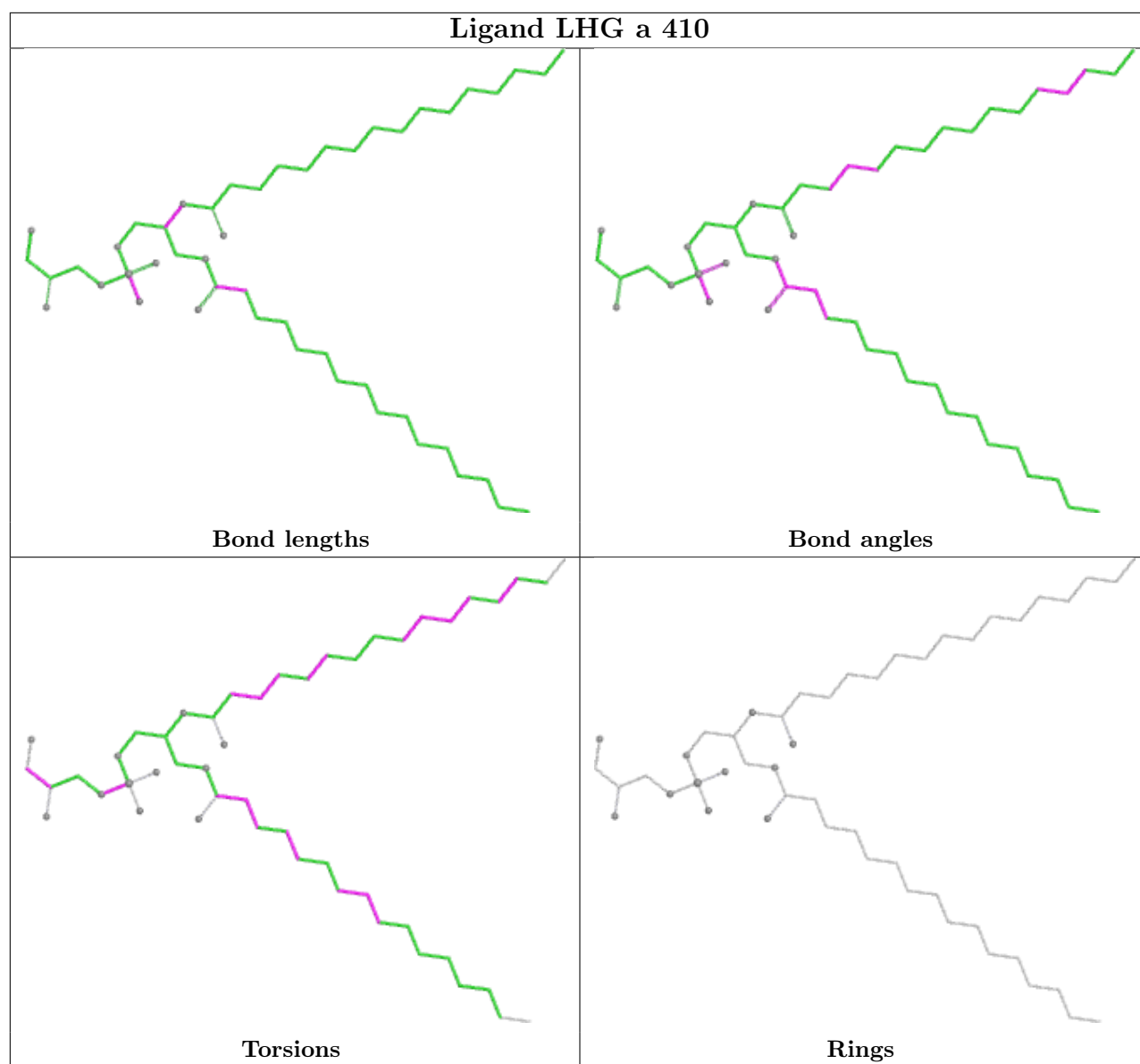


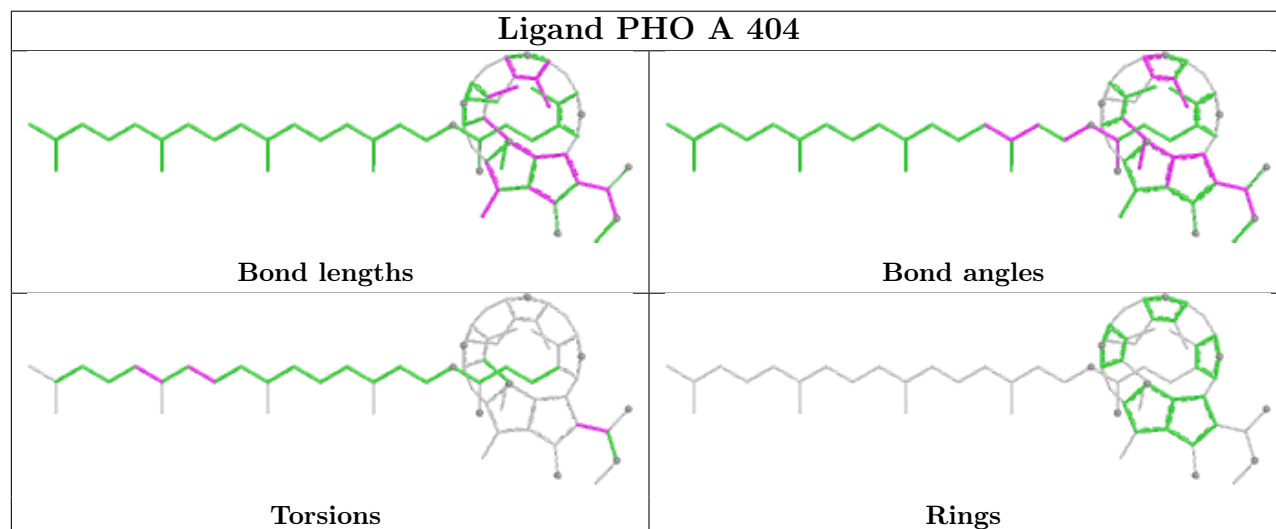
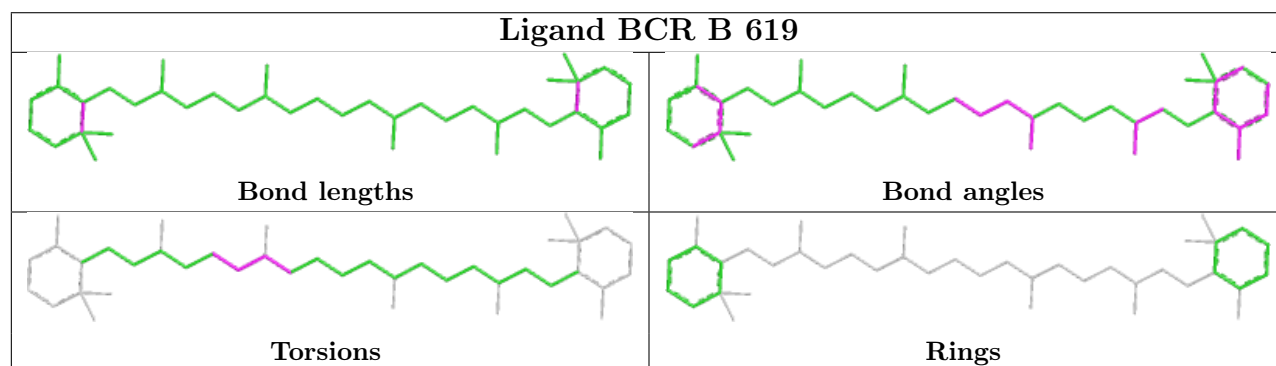
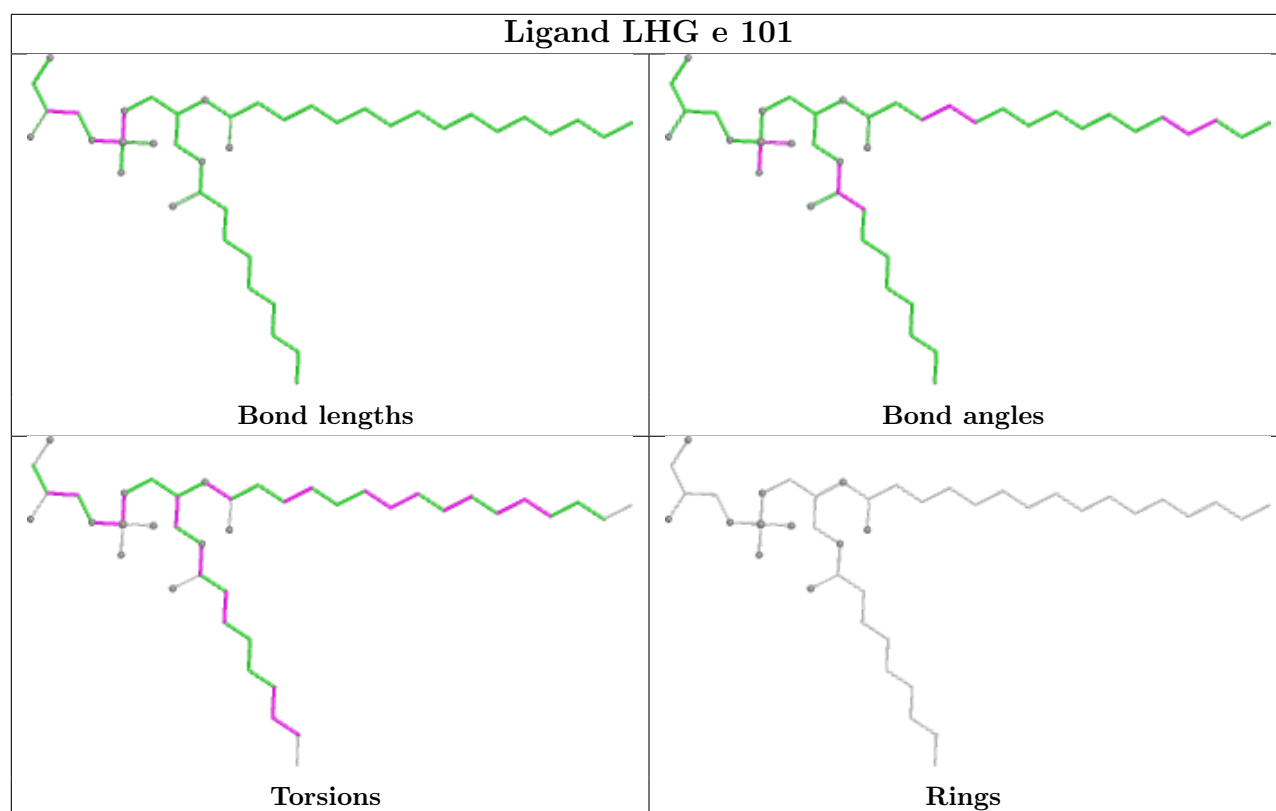
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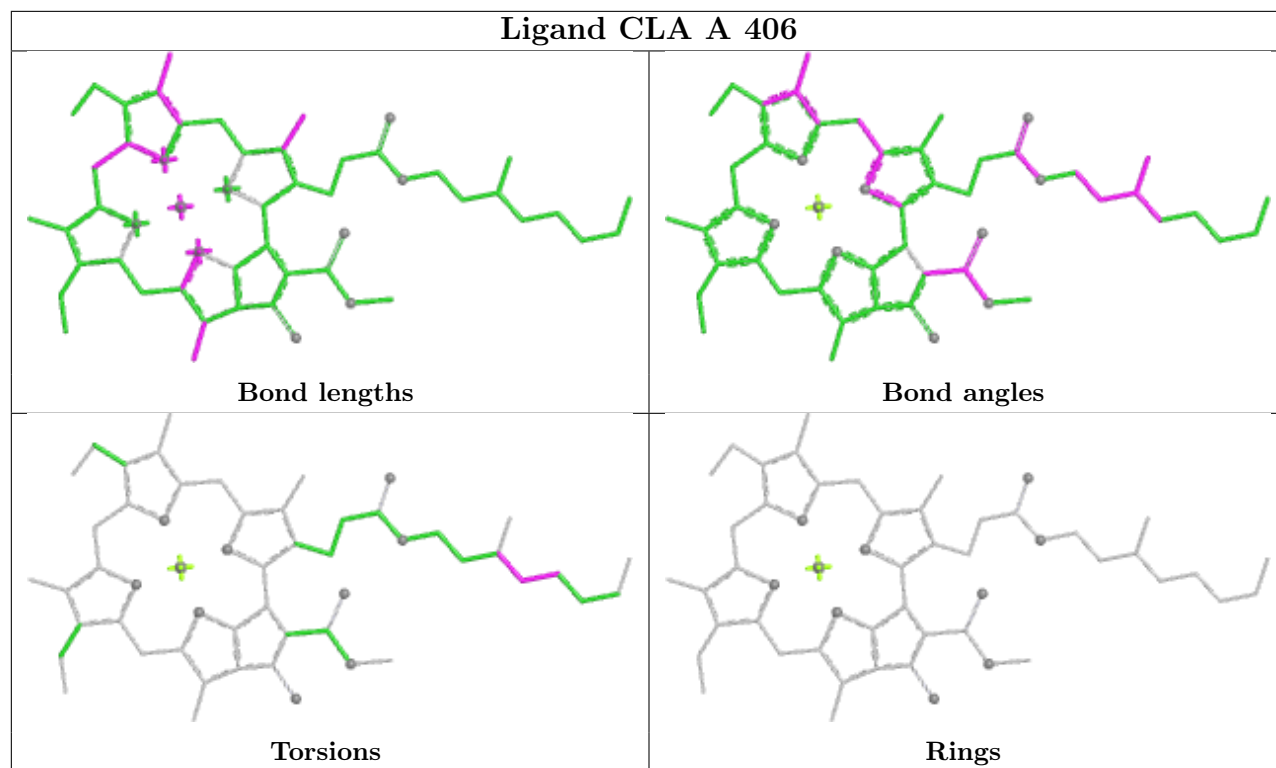


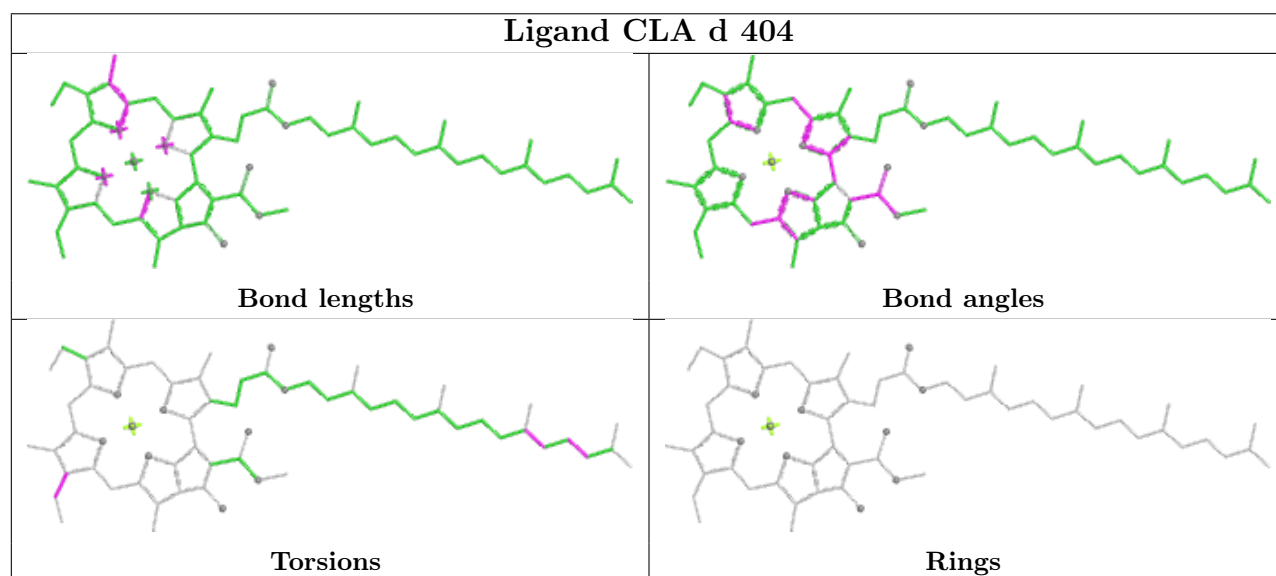
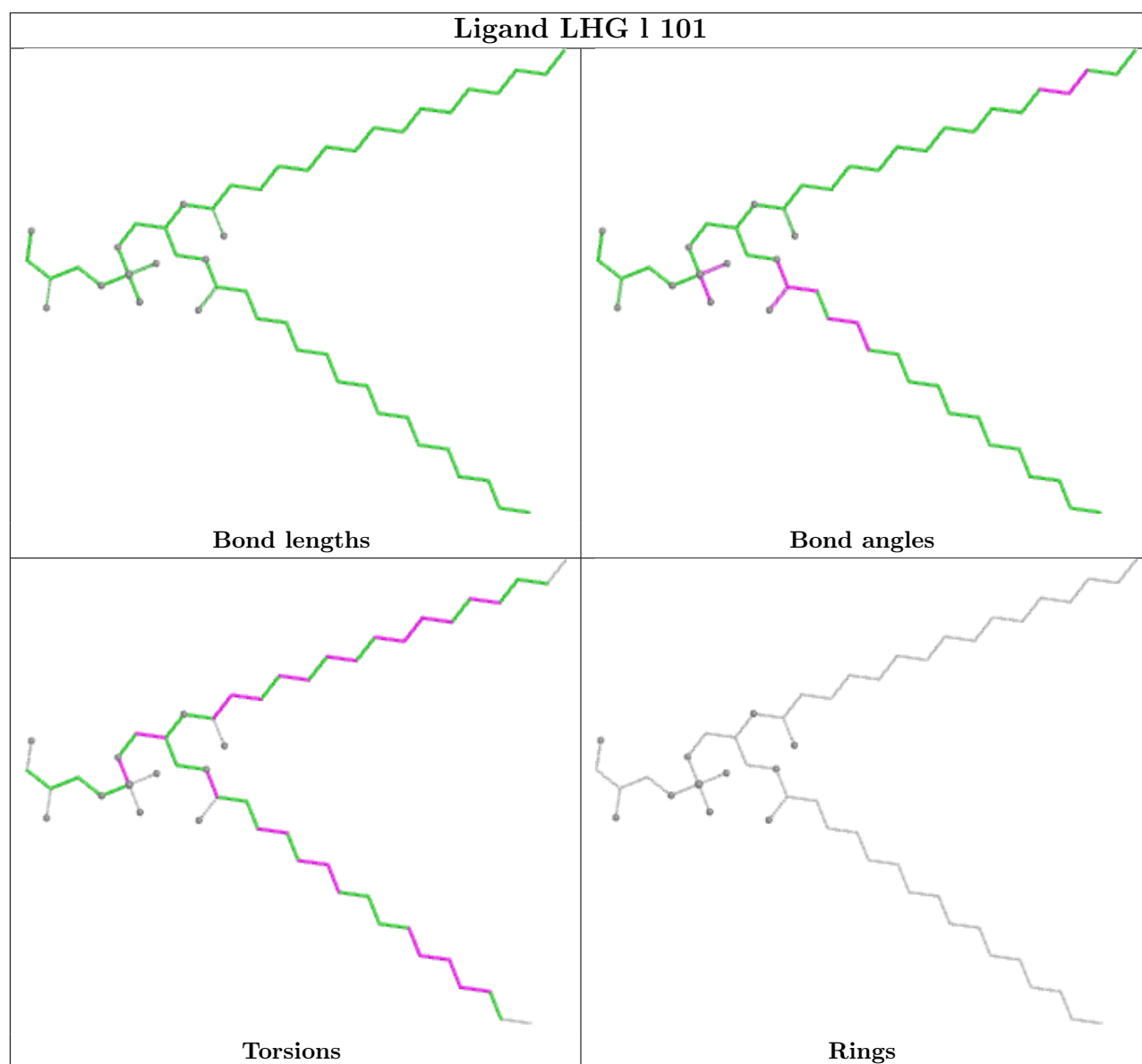
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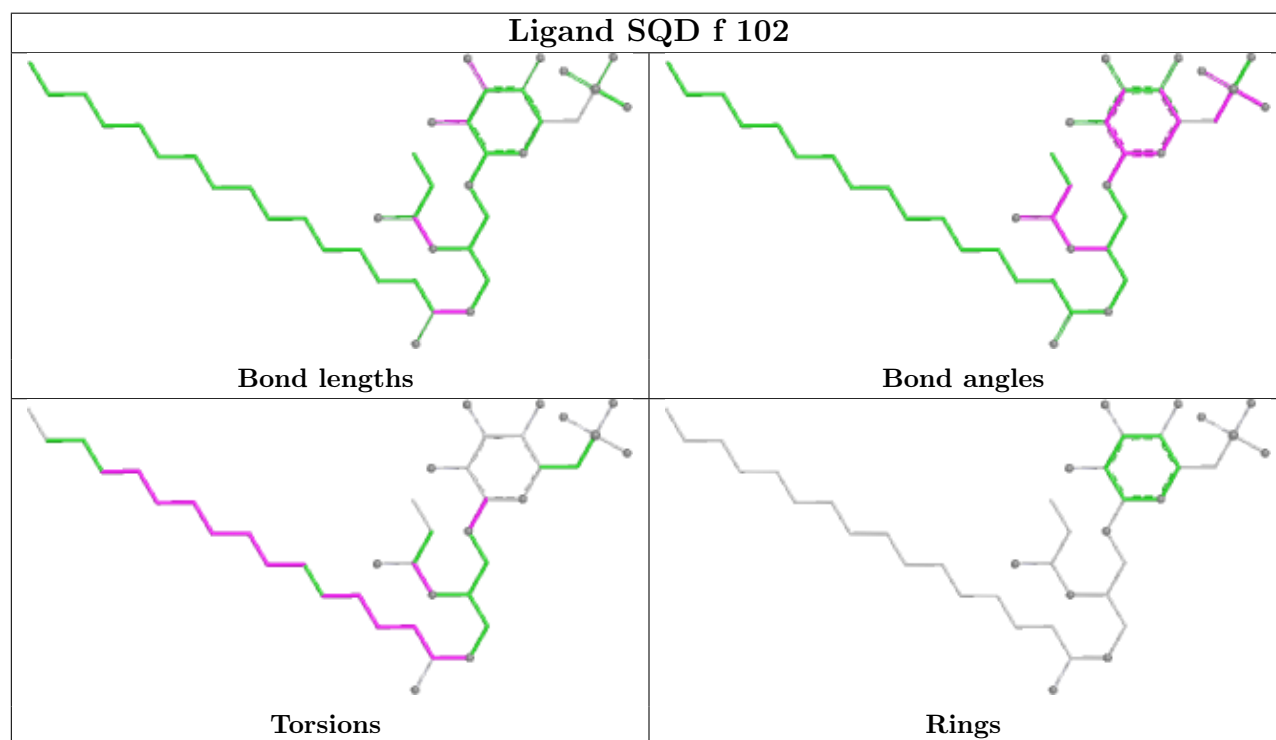
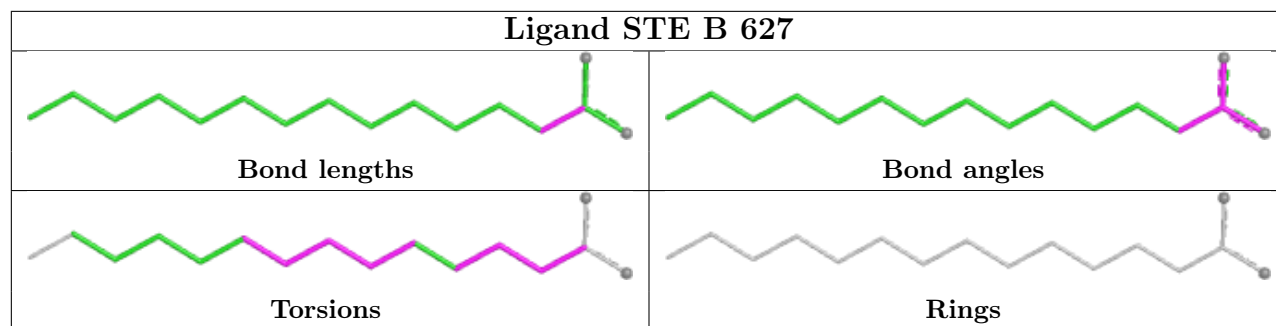


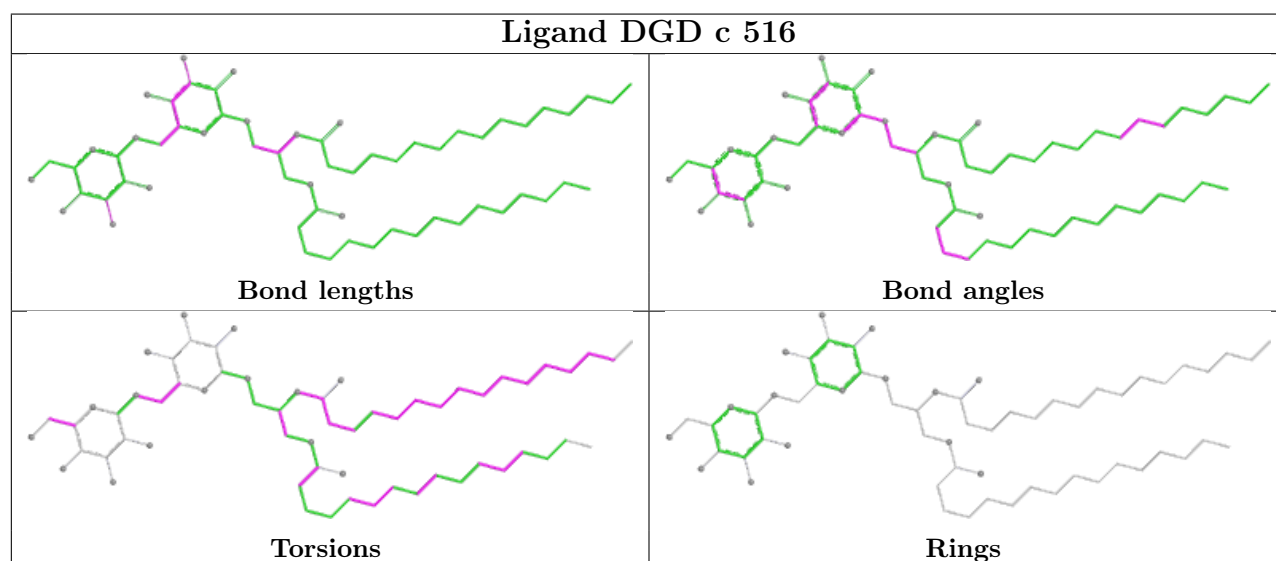
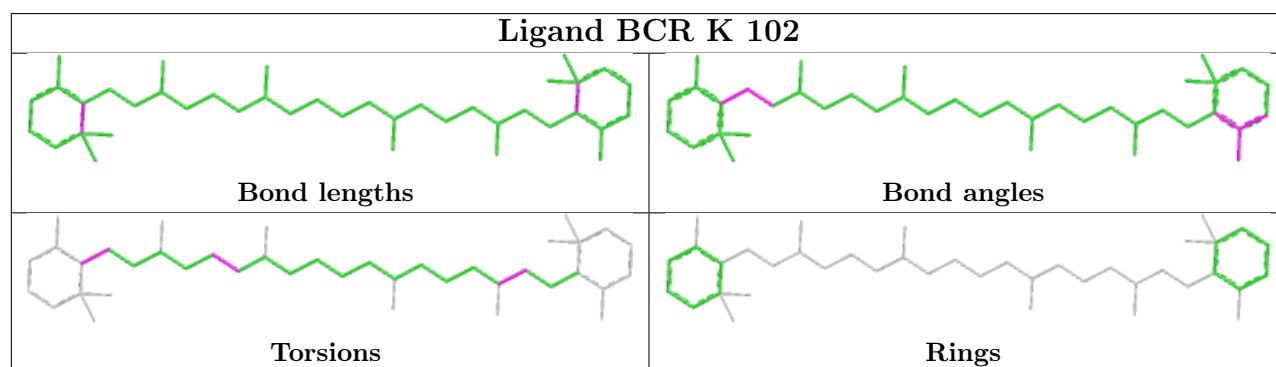
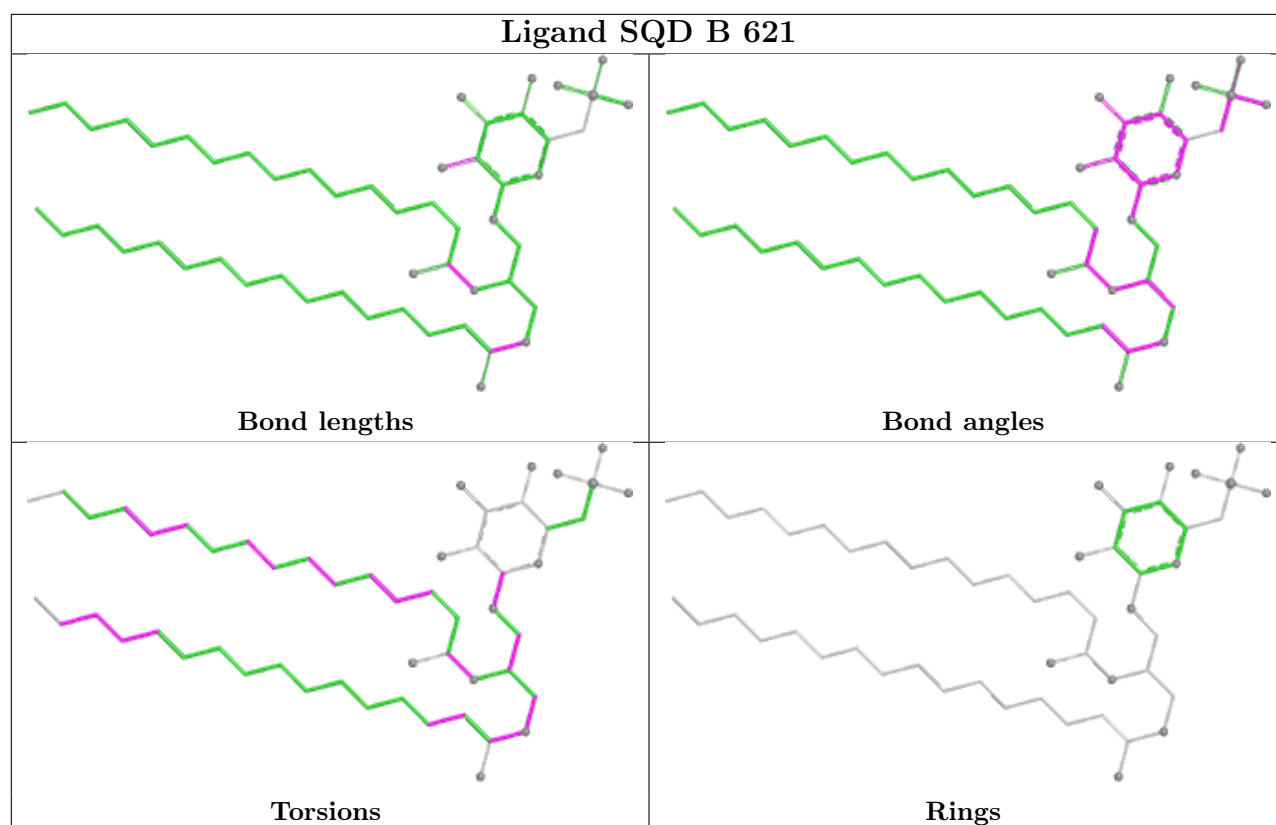


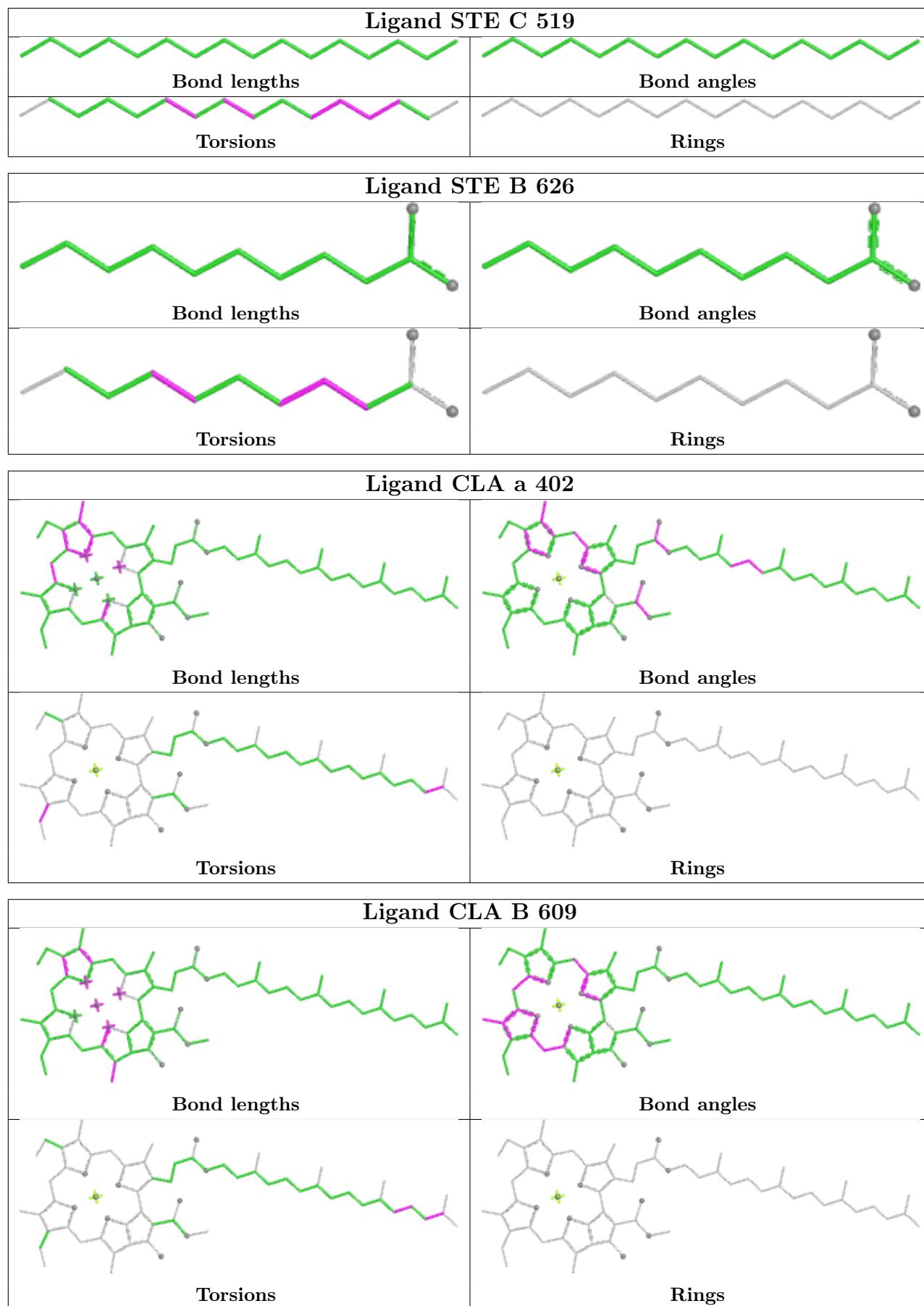


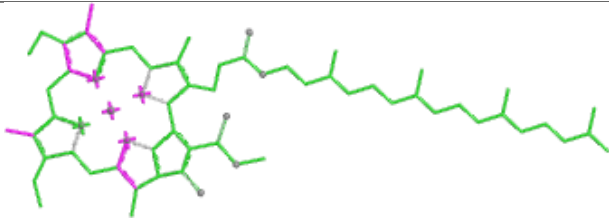
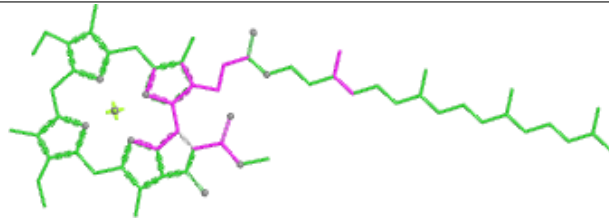
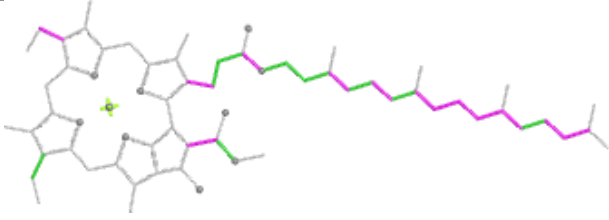
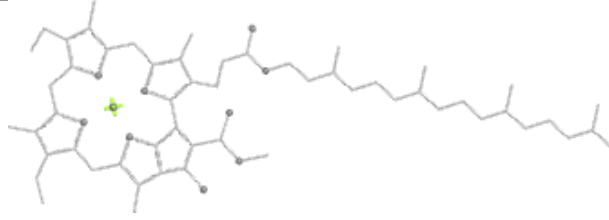


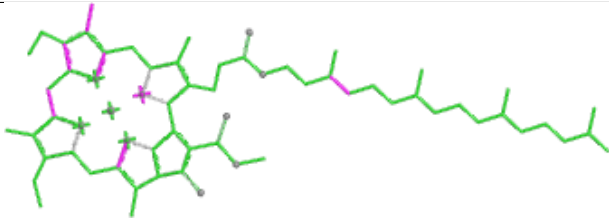
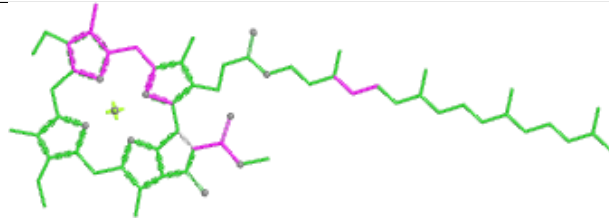
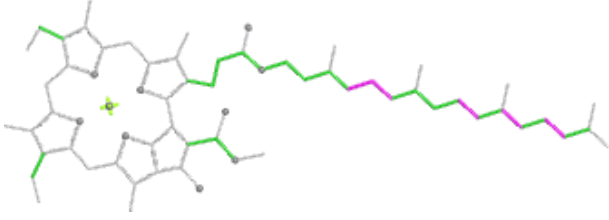
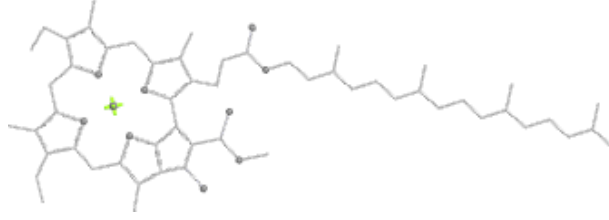


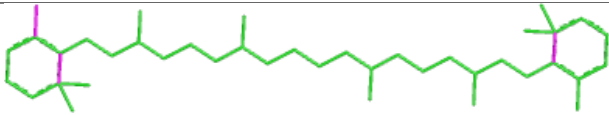
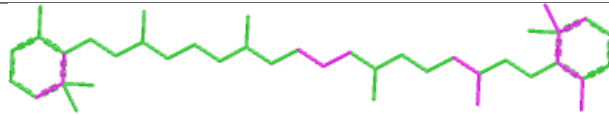
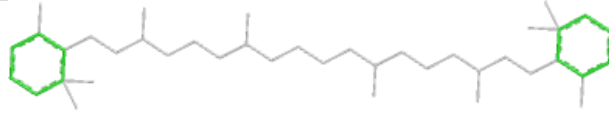


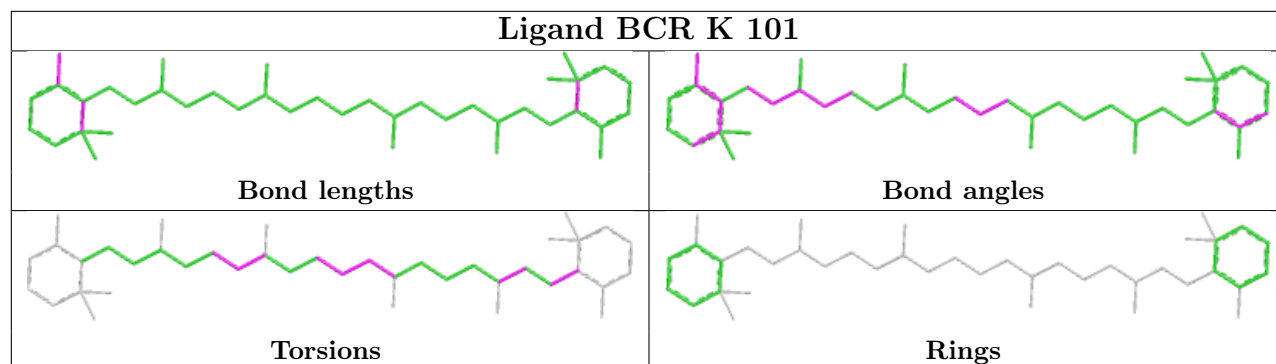
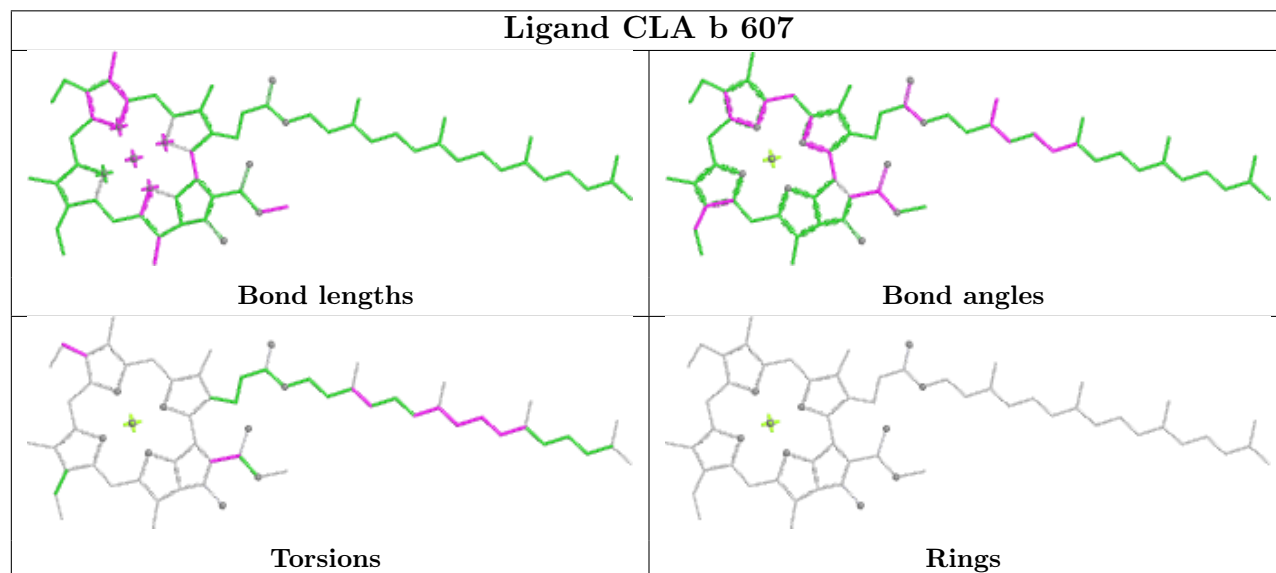
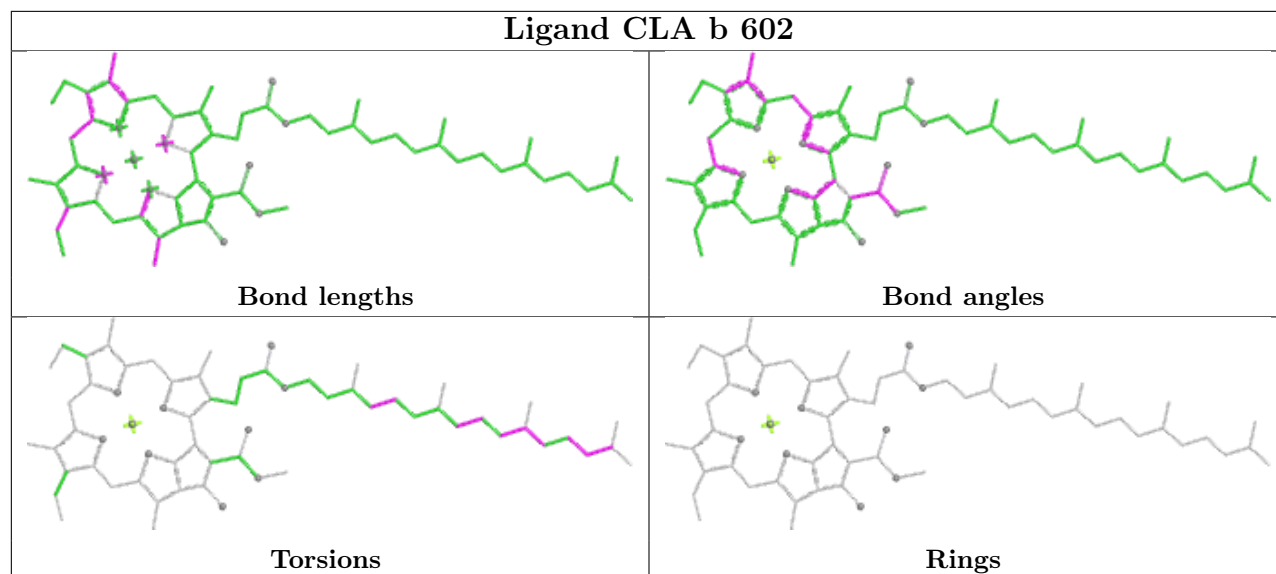


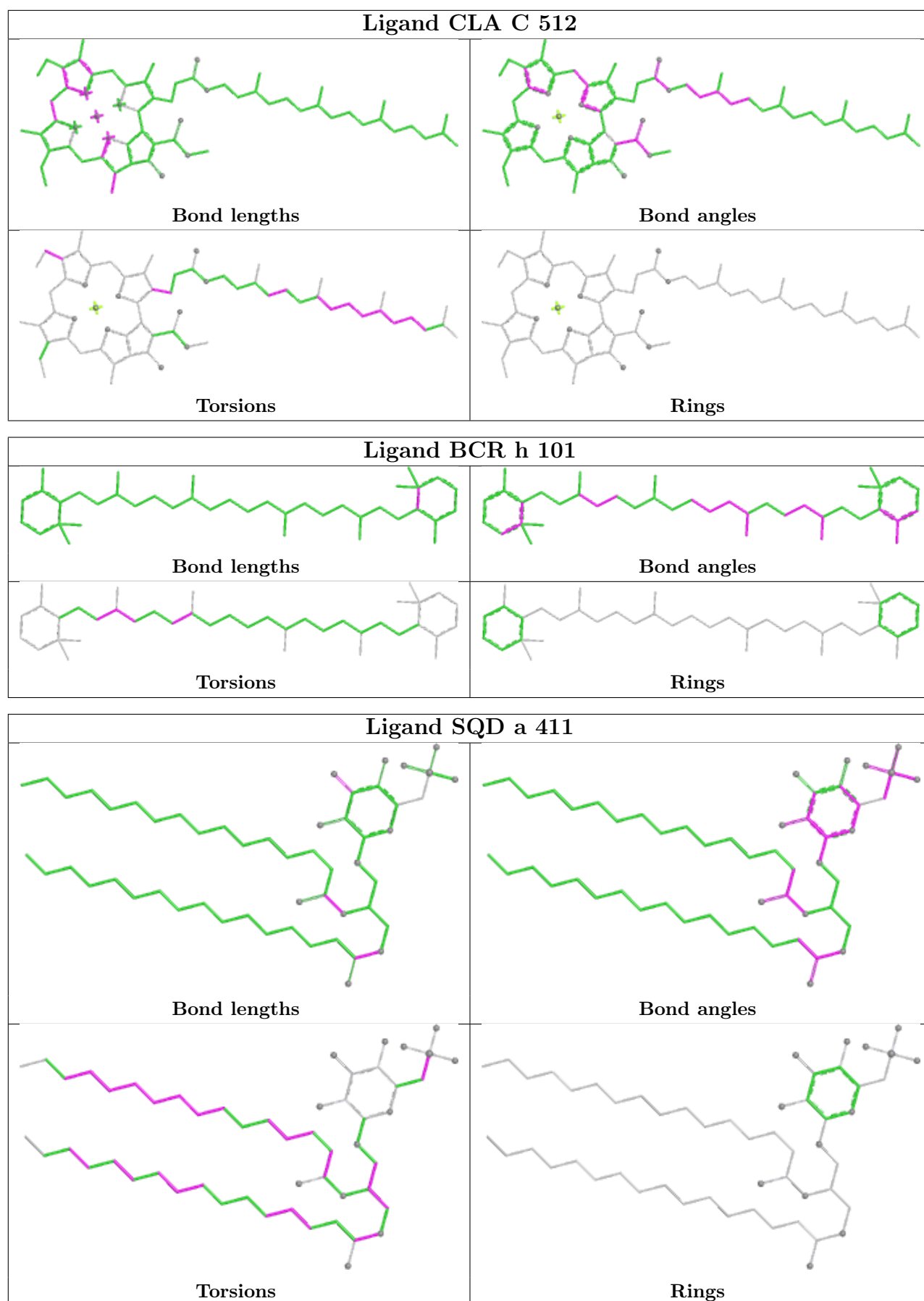


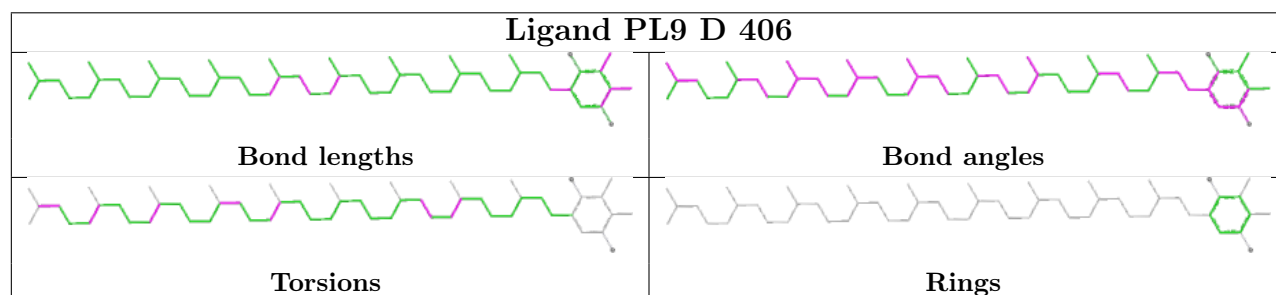
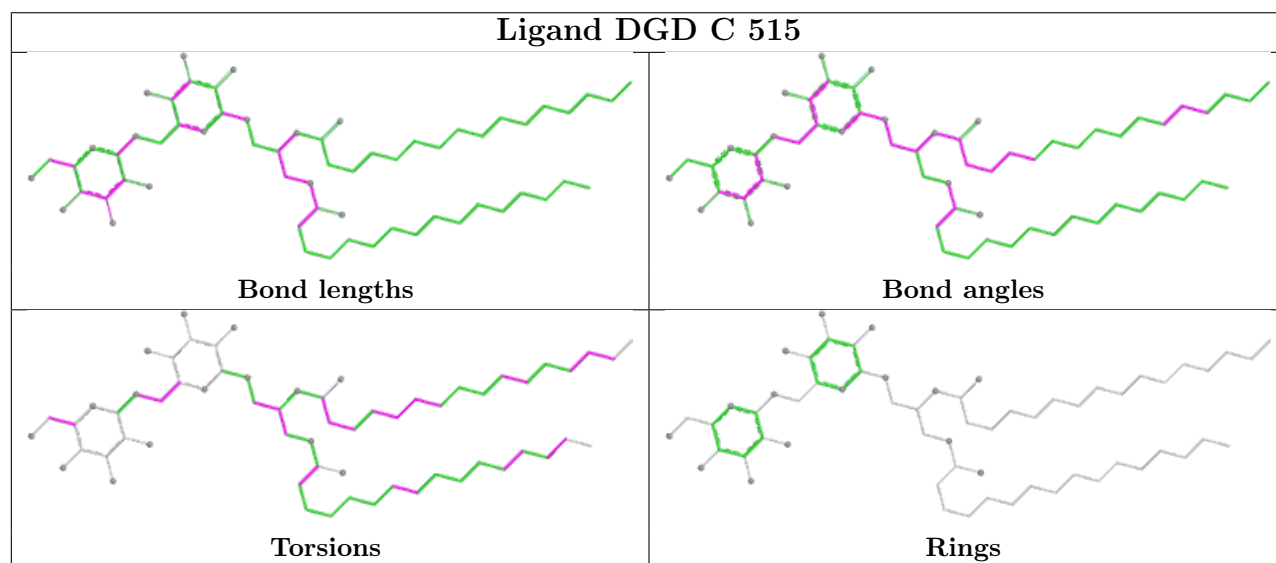
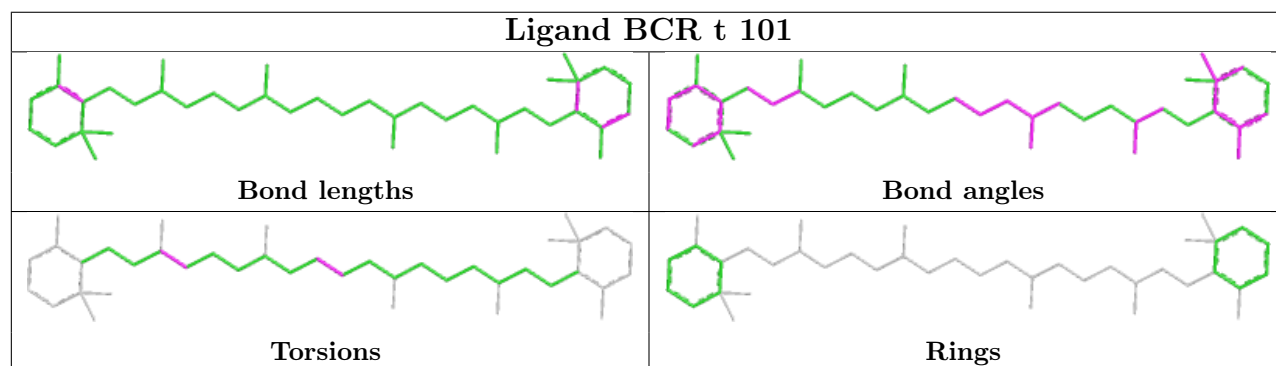
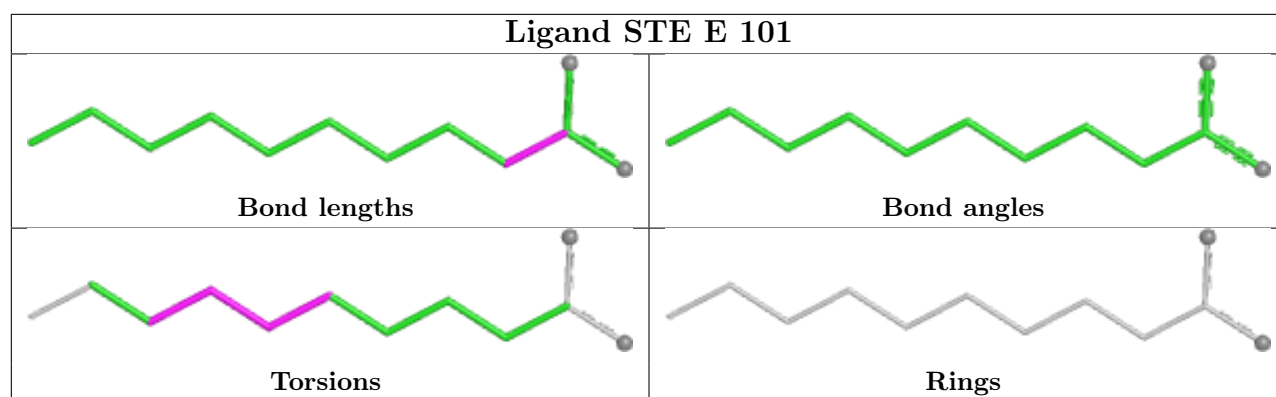
Ligand CLA B 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

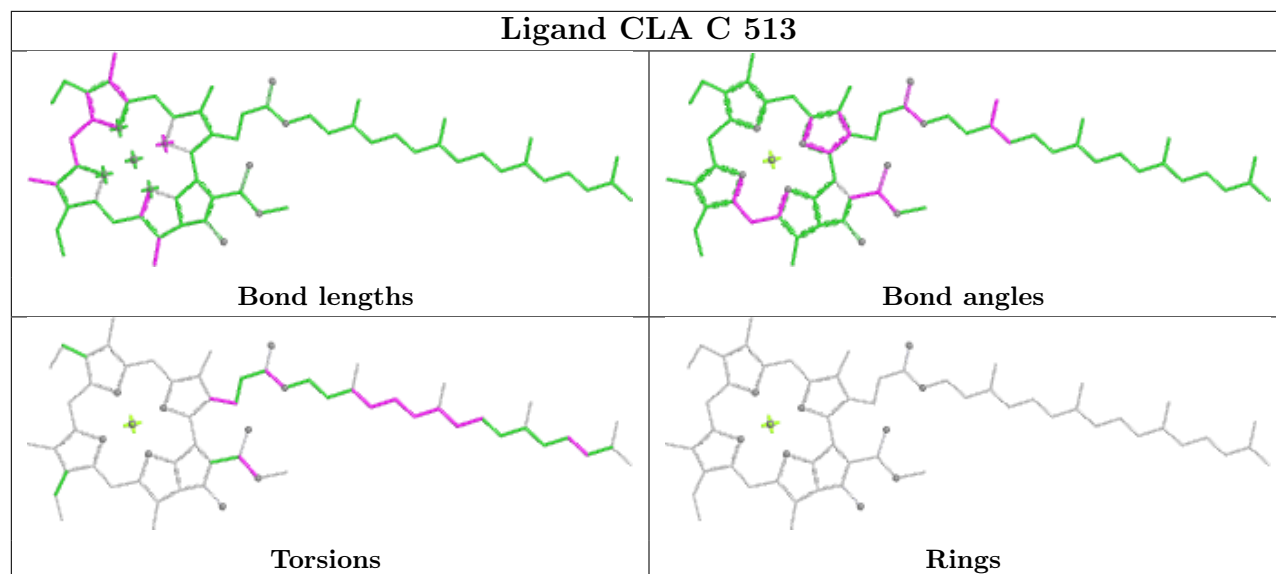
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



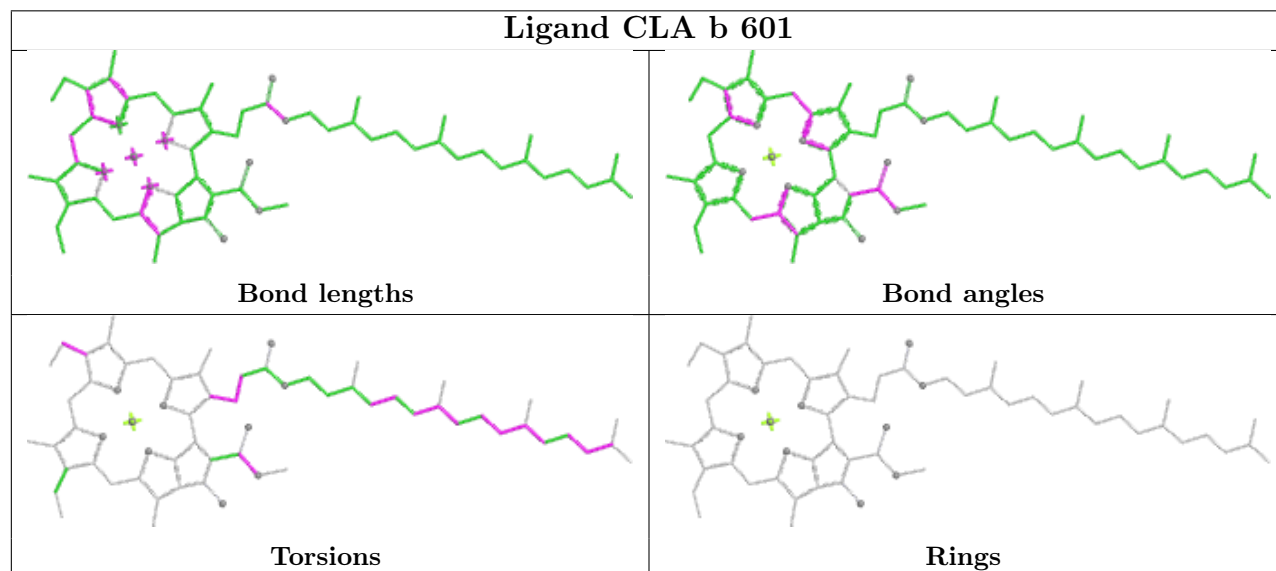




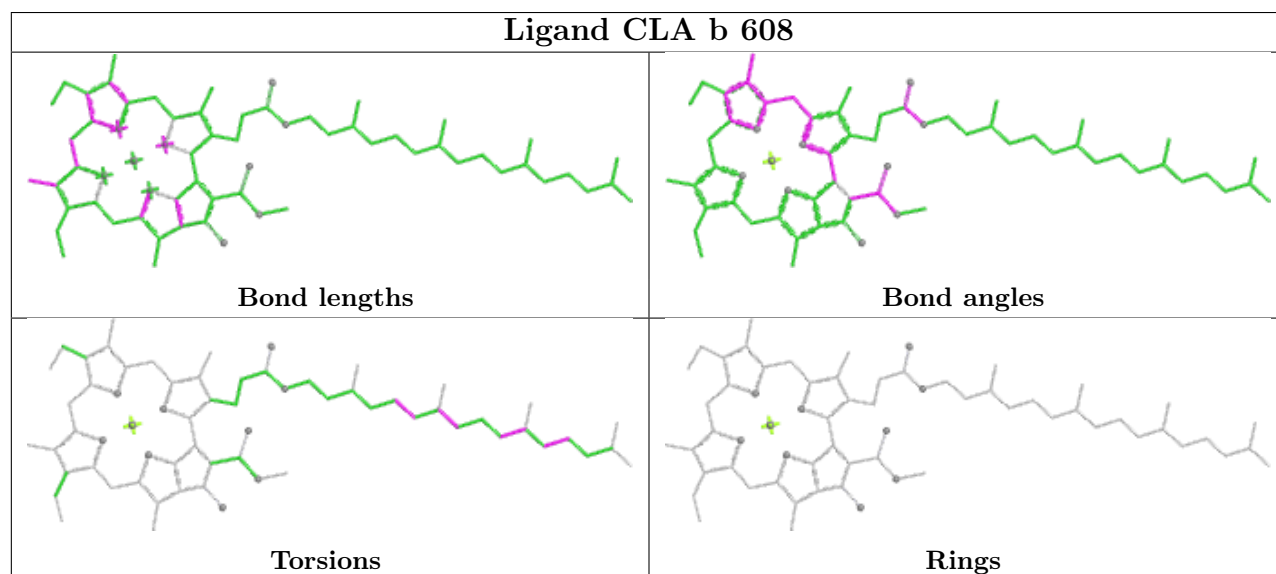
Ligand CLA C 513

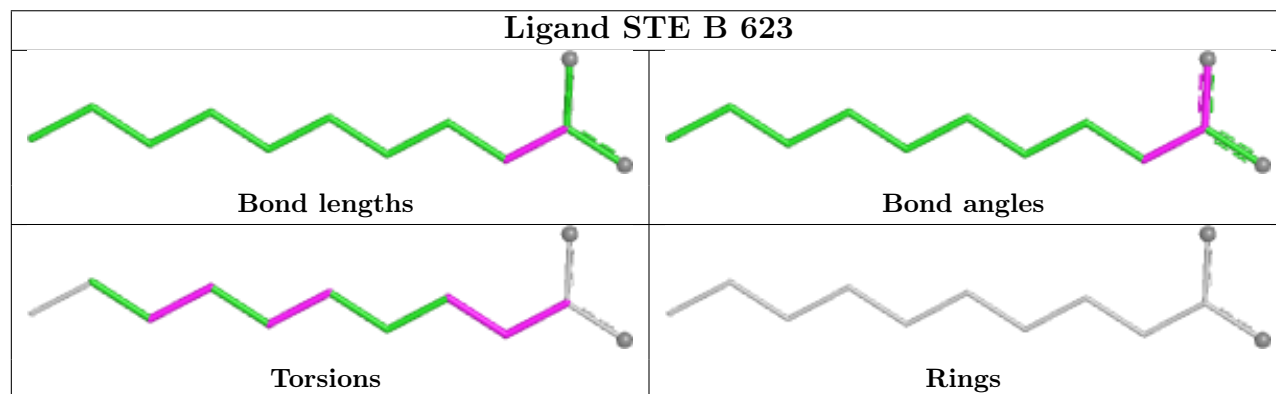
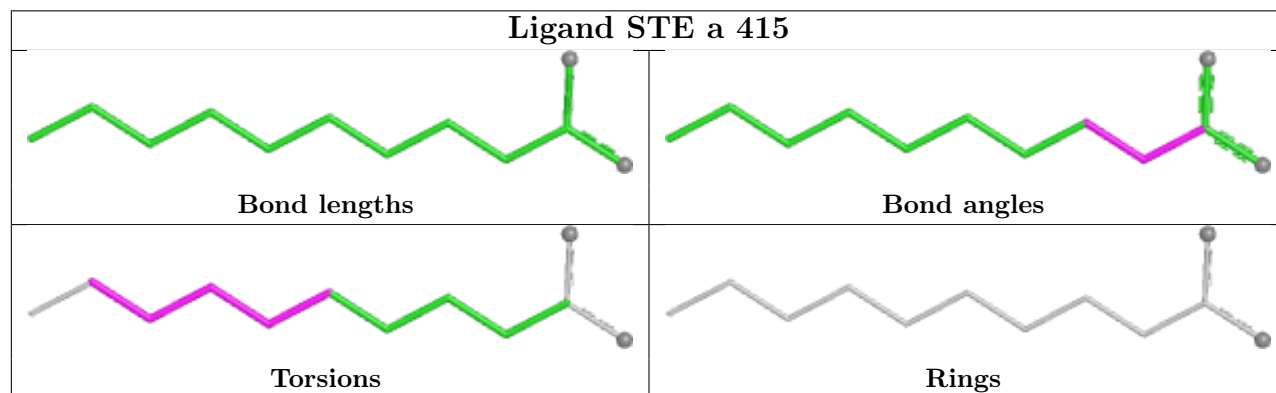
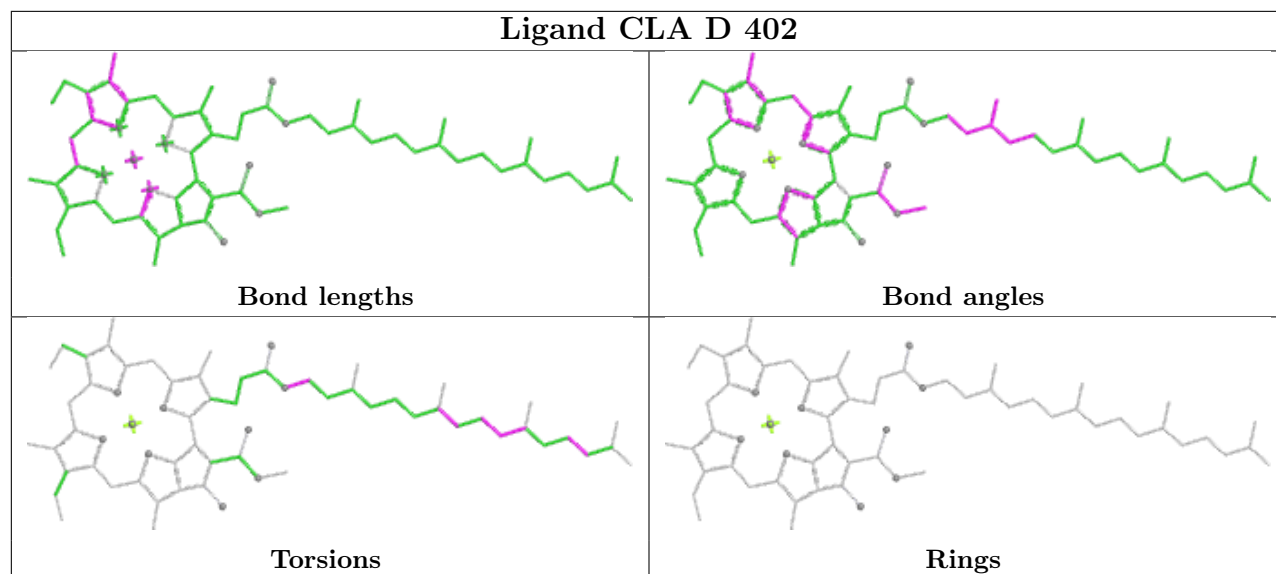


Ligand CLA b 601

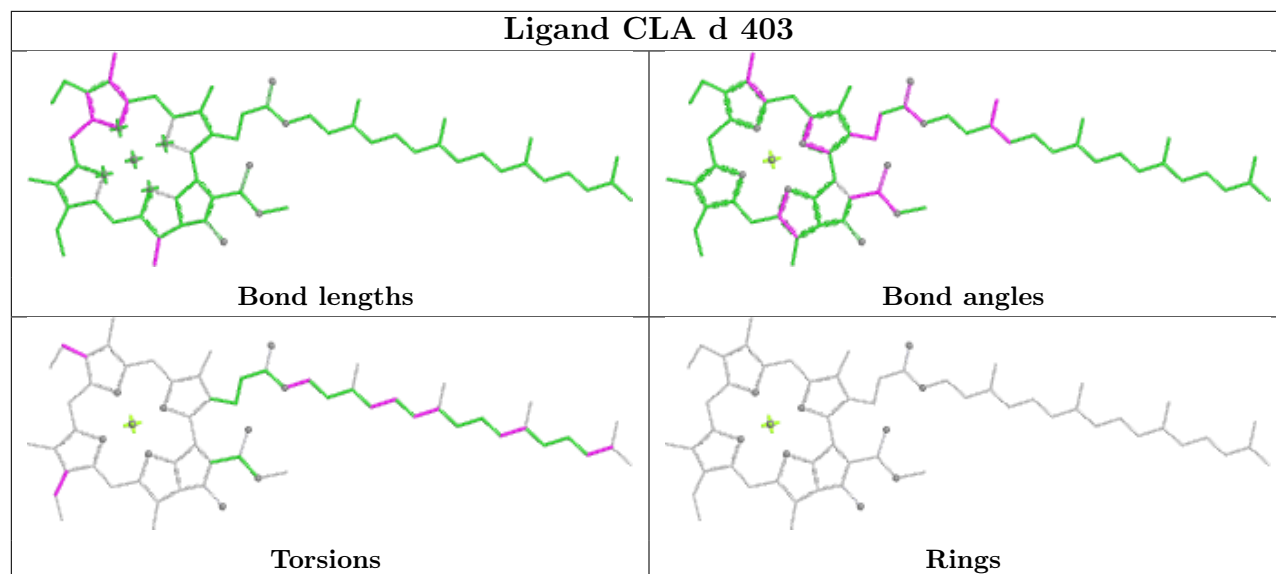


Ligand CLA b 608

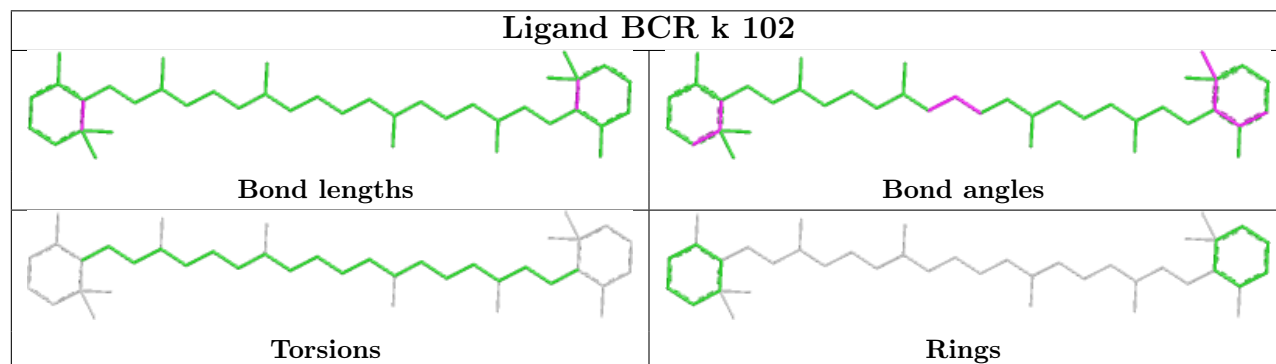




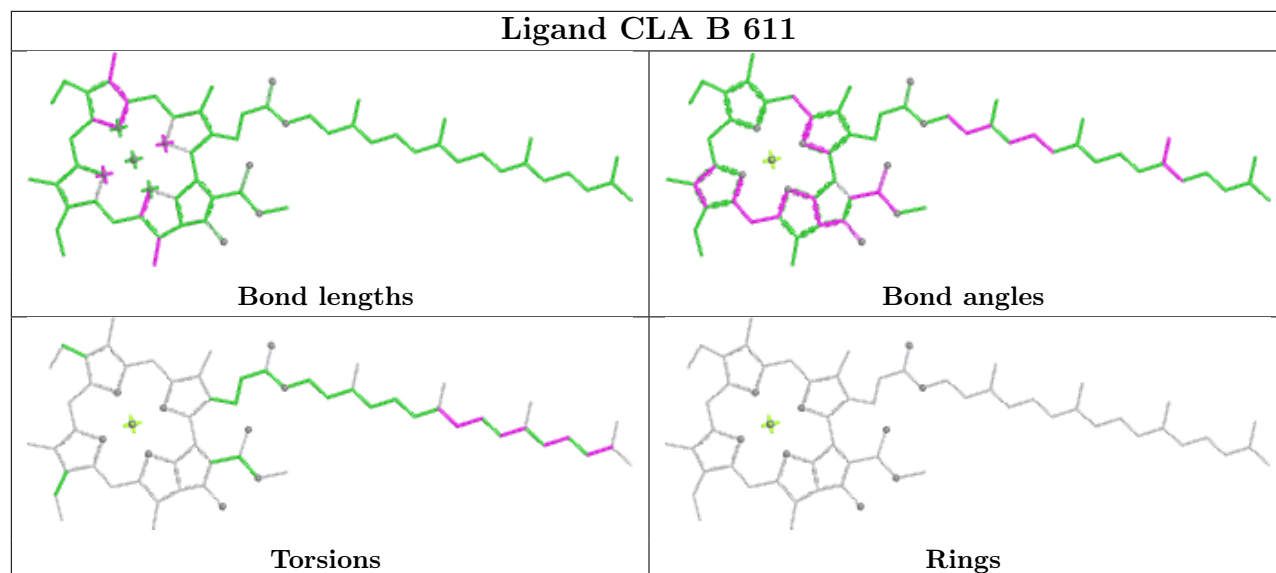
Ligand CLA d 403



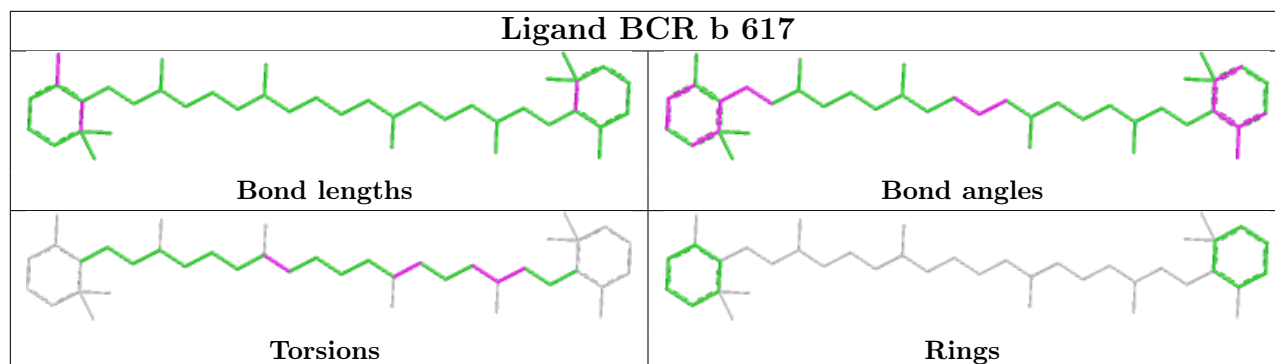
Ligand BCR k 102



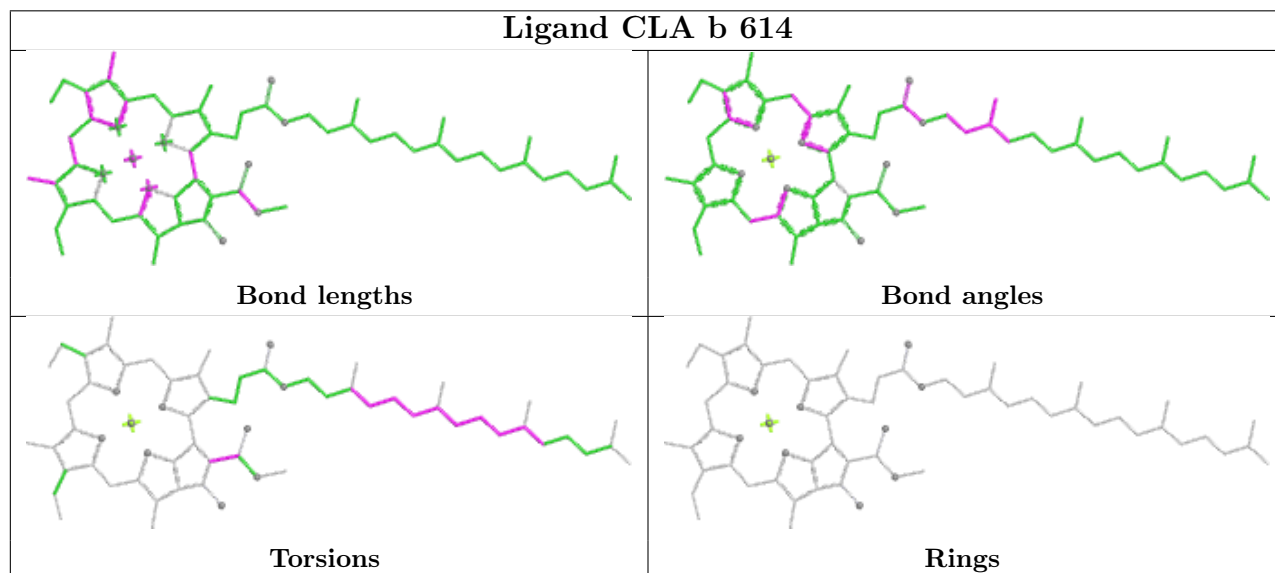
Ligand CLA B 611



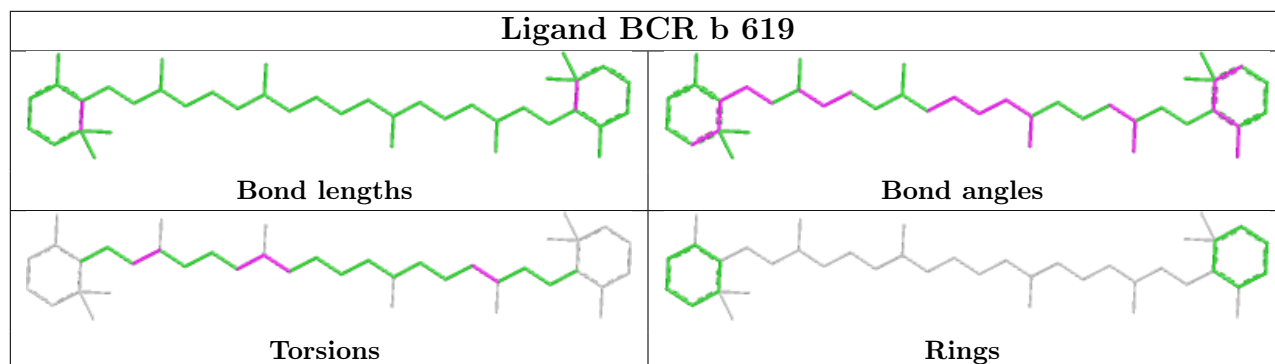
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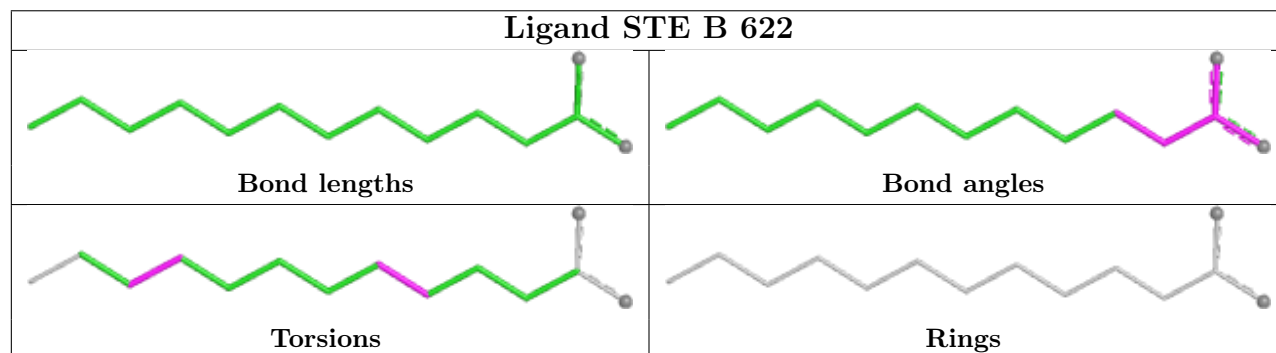
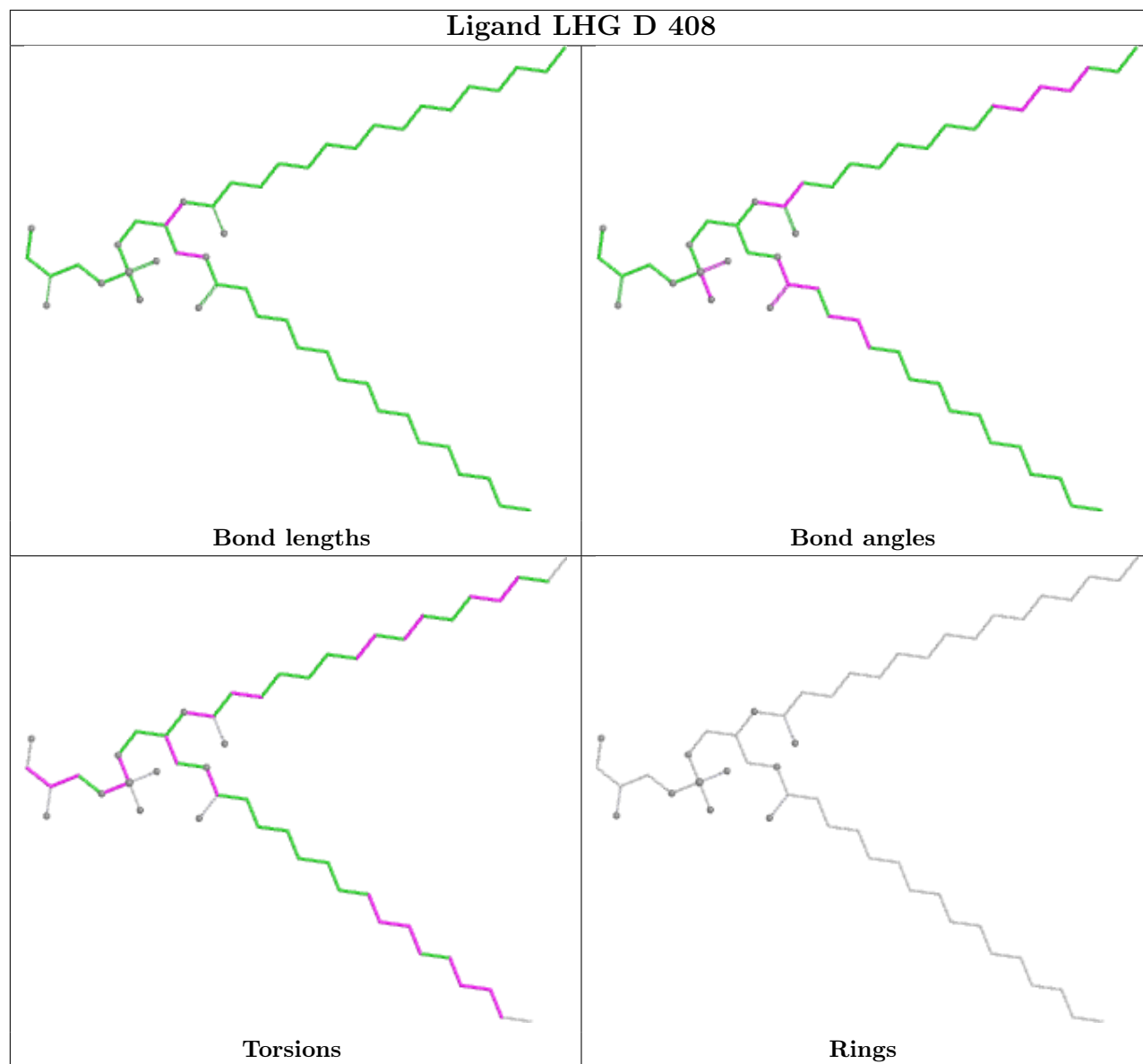


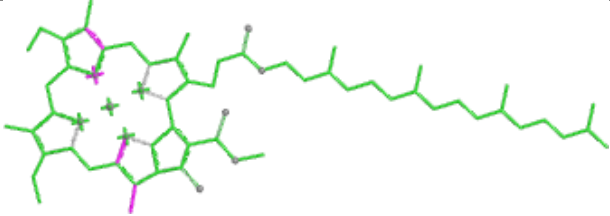
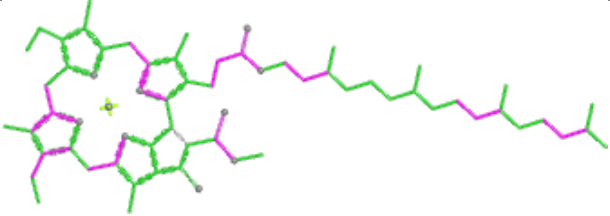
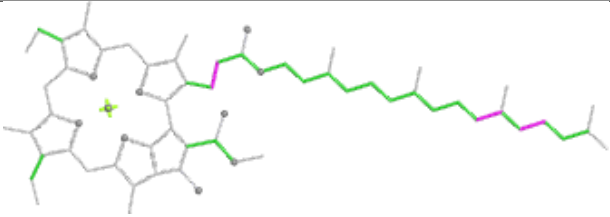
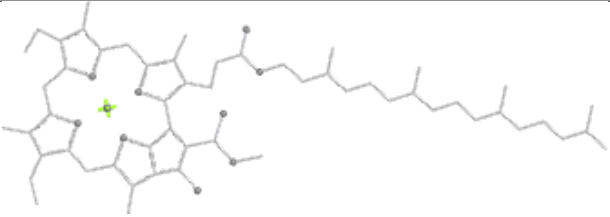
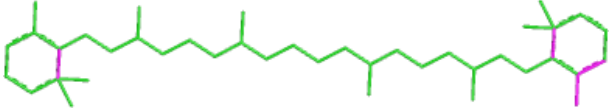
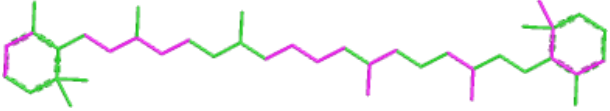
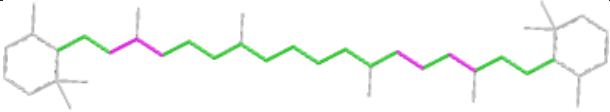
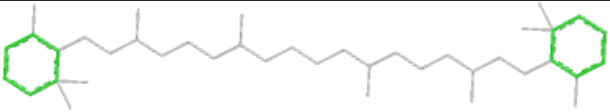
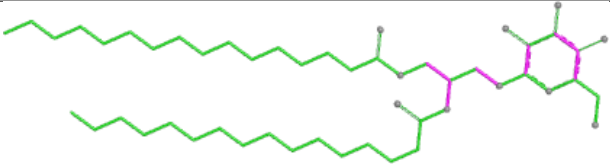
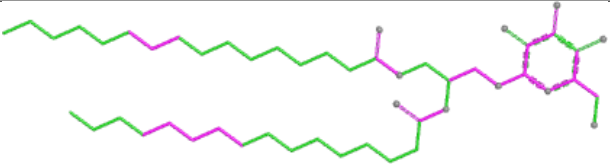
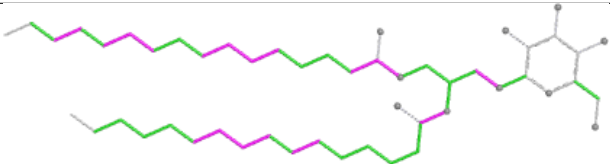
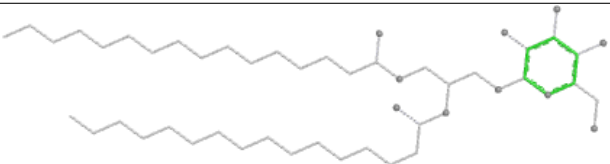
Ligand CLA b 614

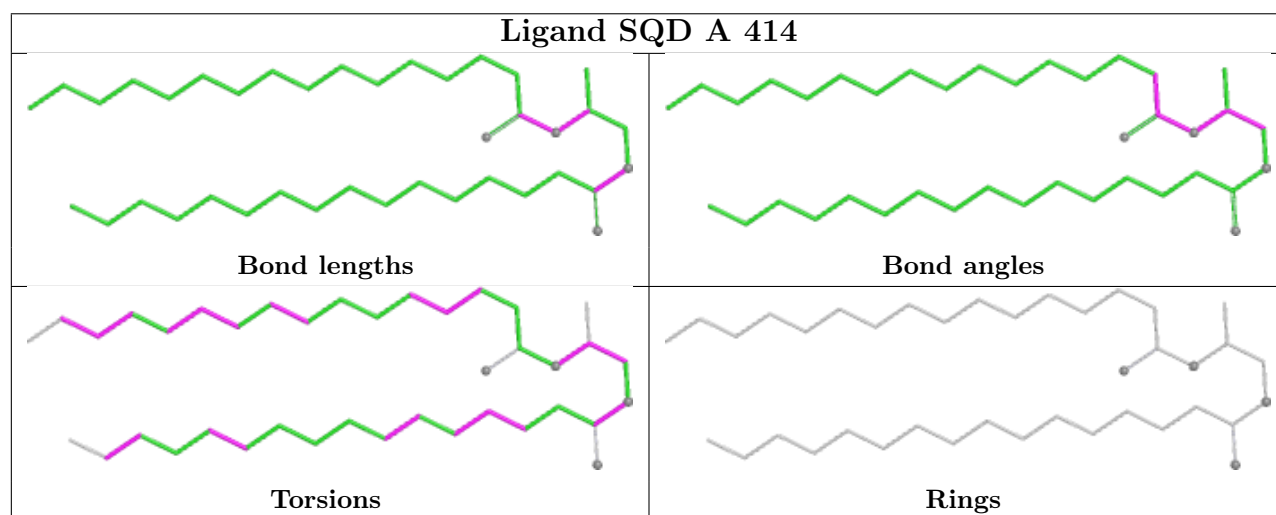
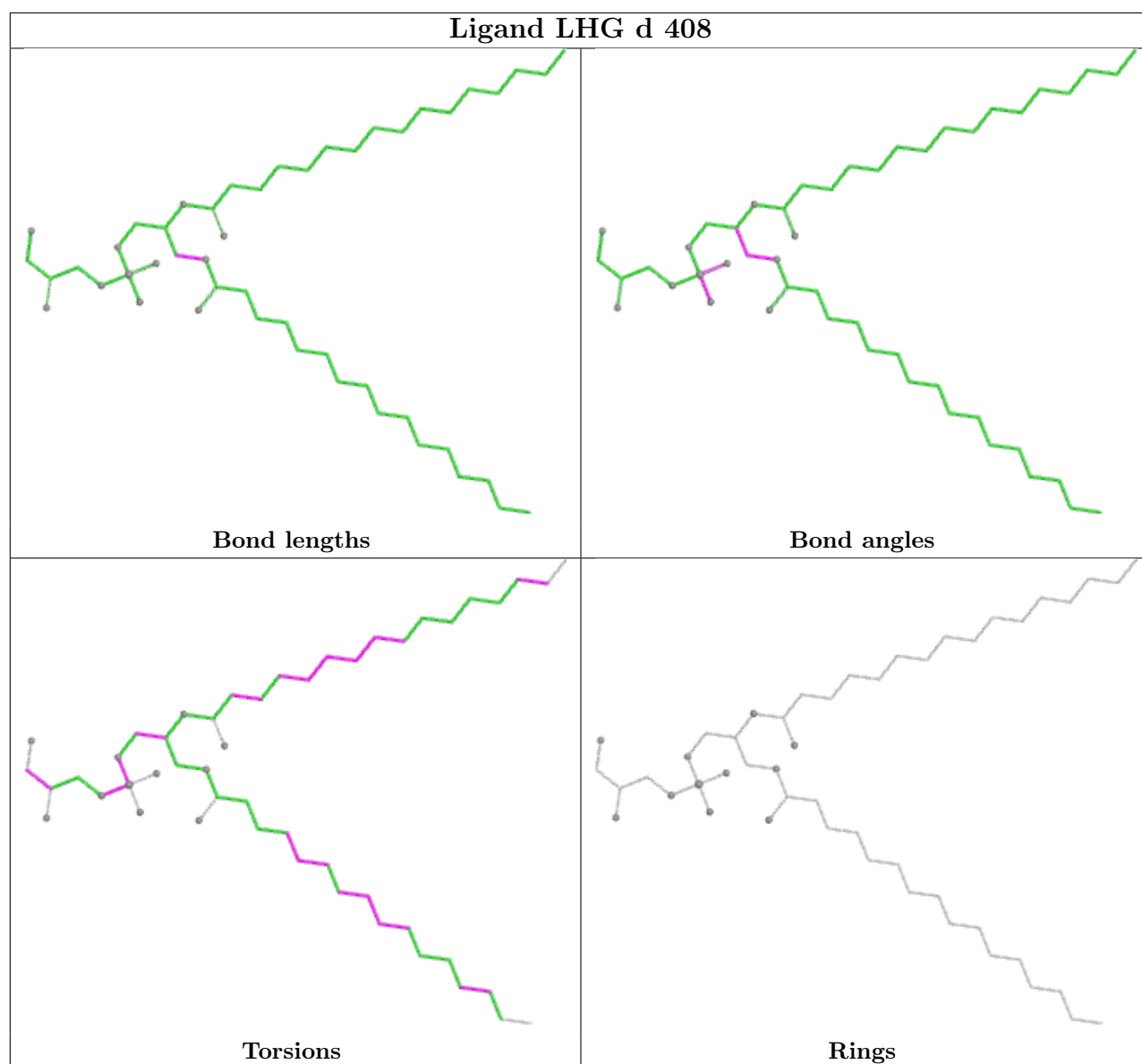


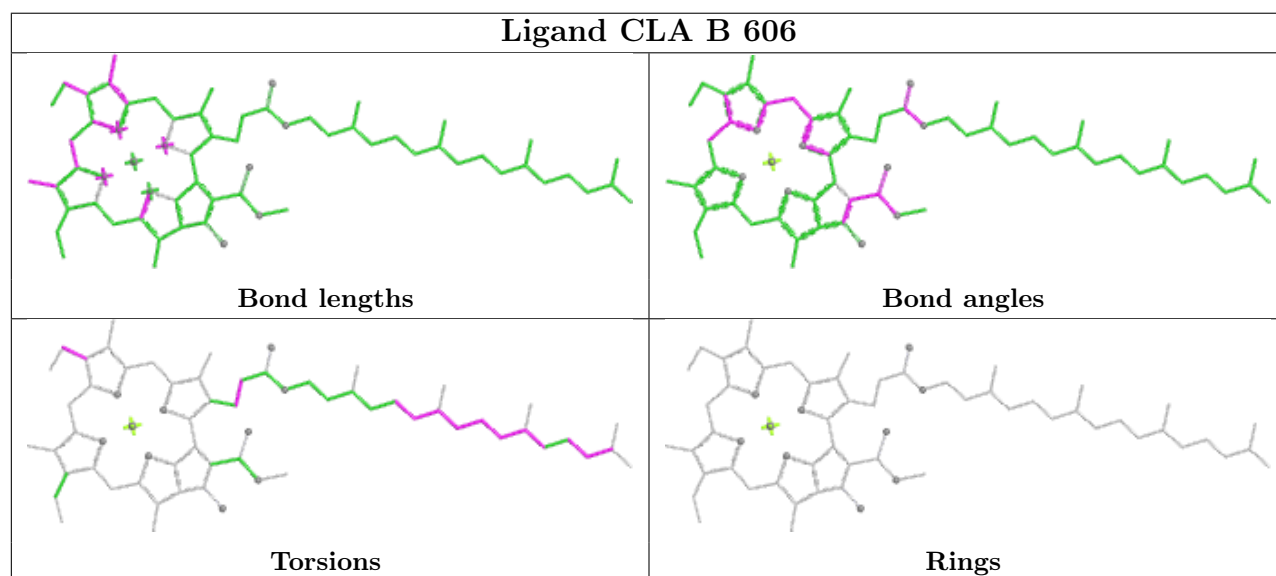
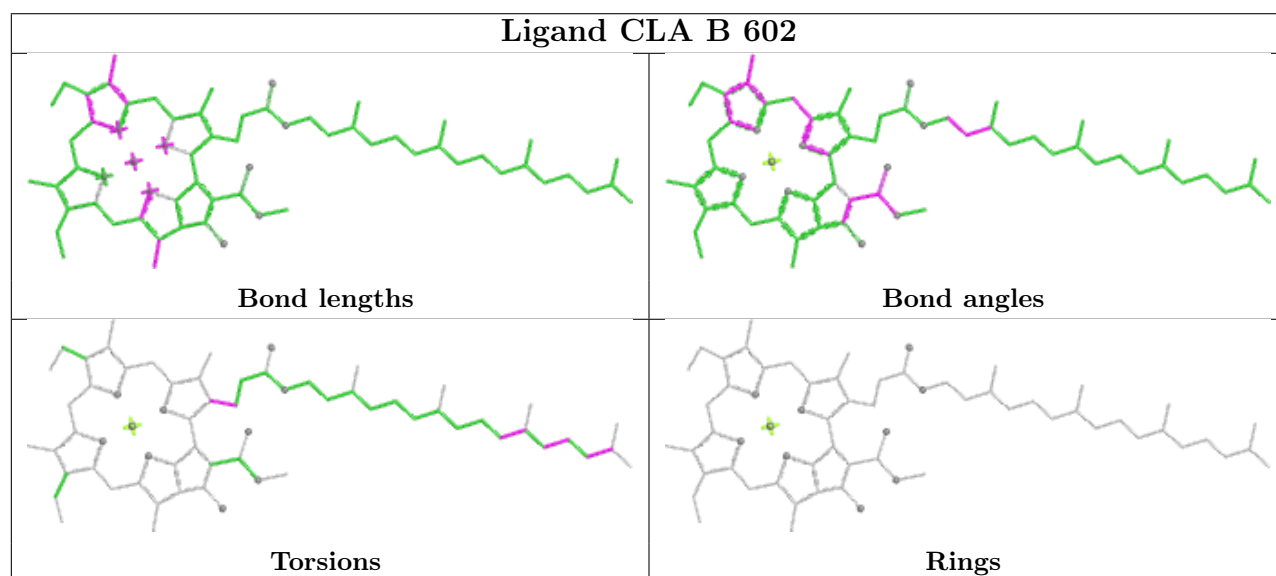
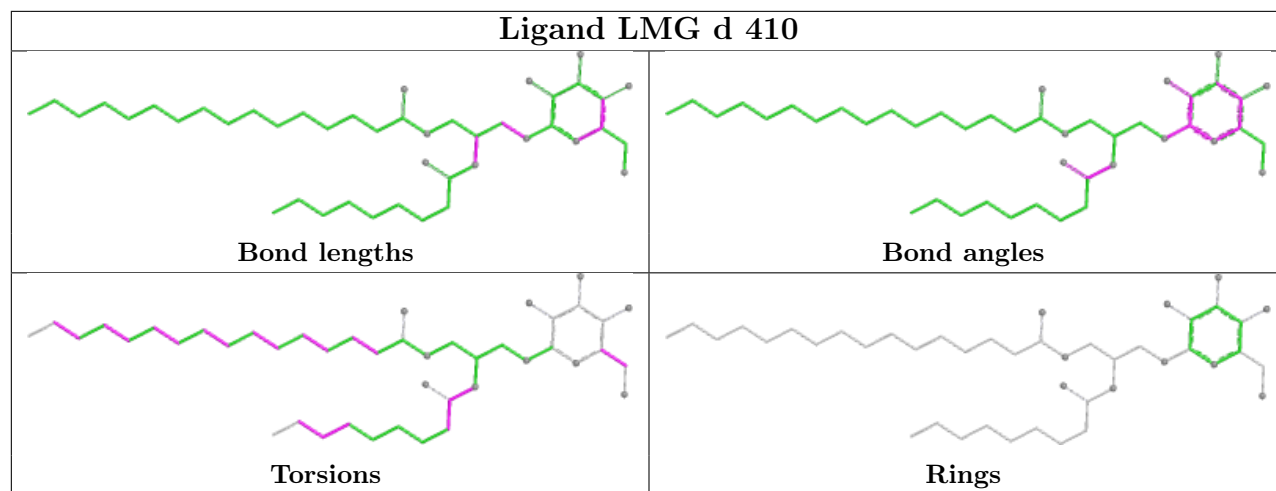
Ligand BCR b 619

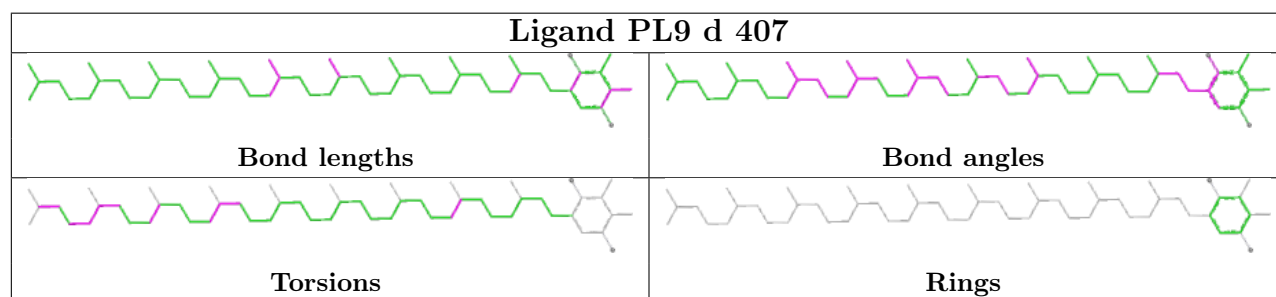
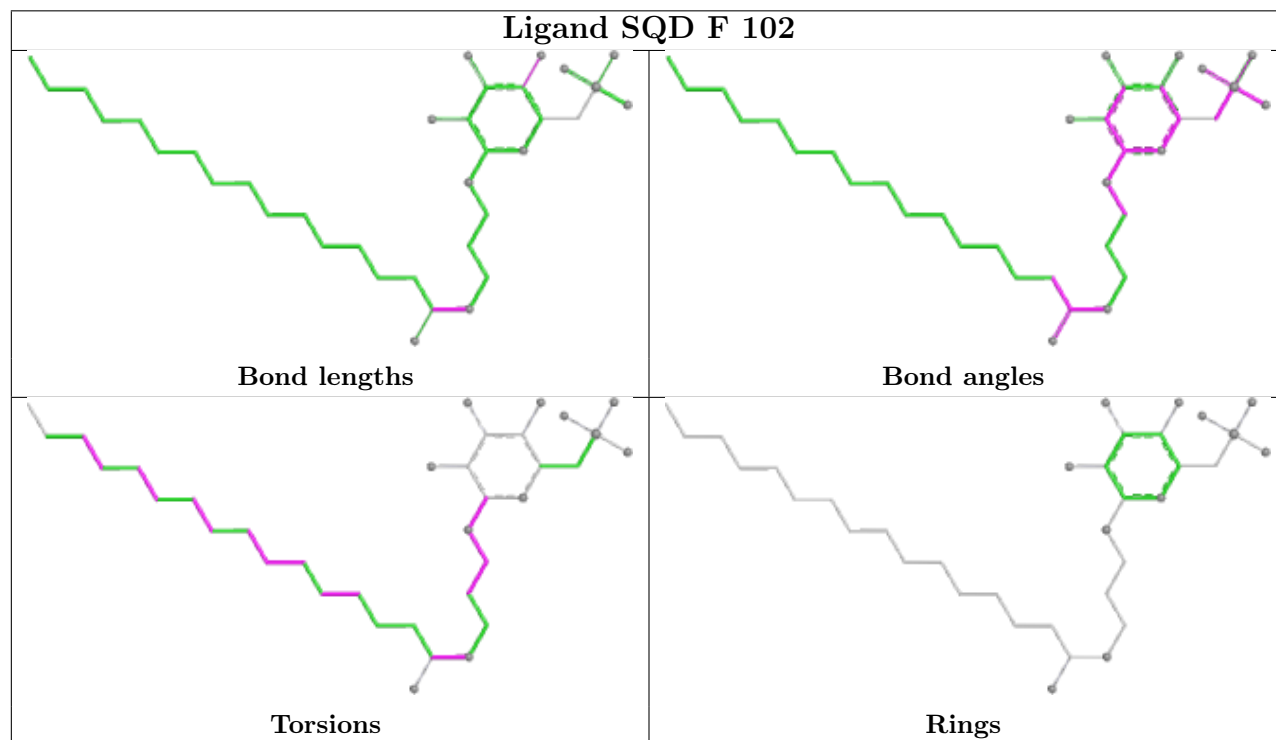
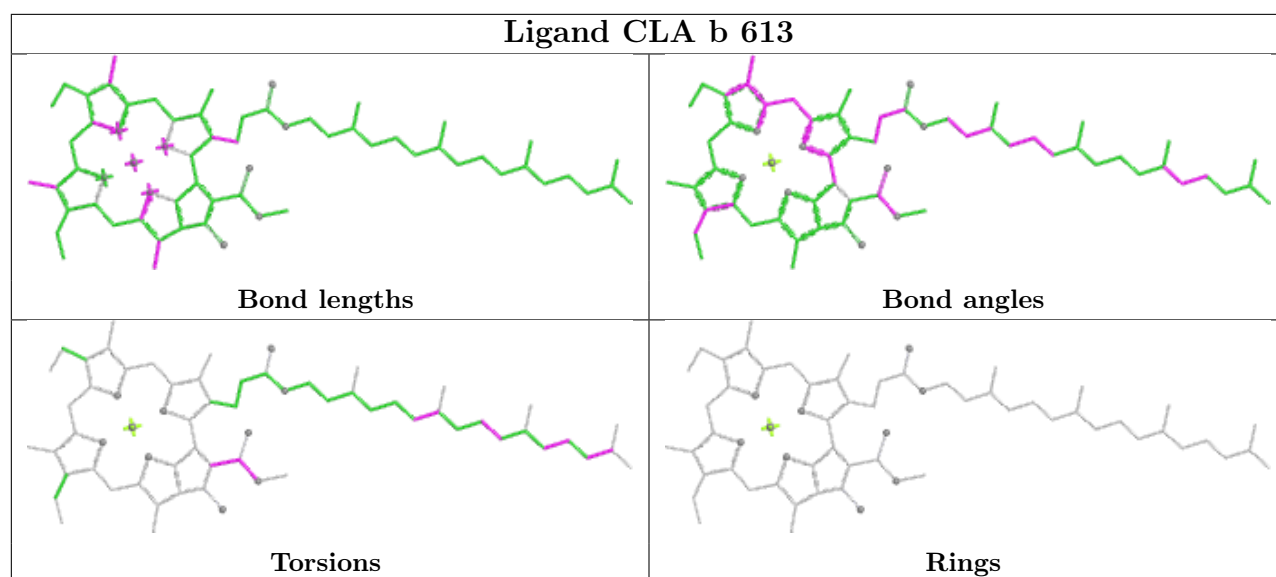


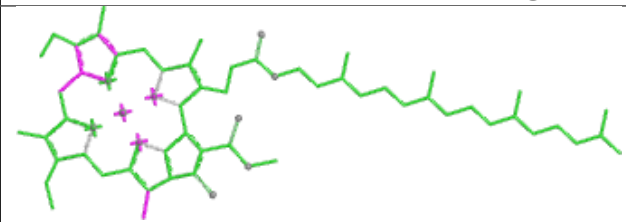
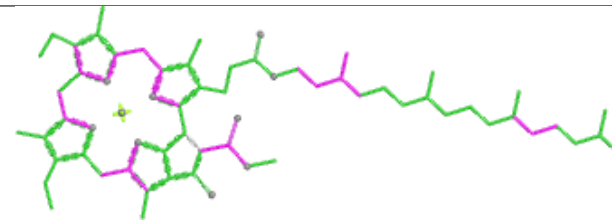
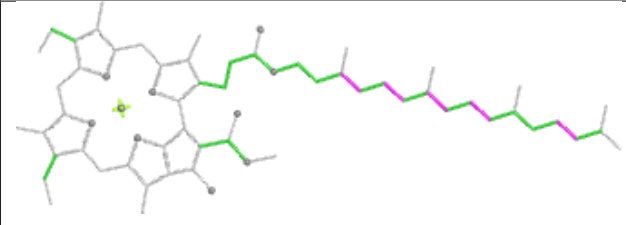
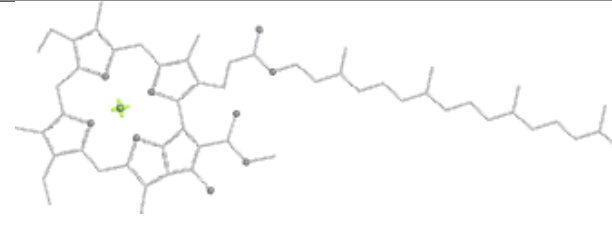
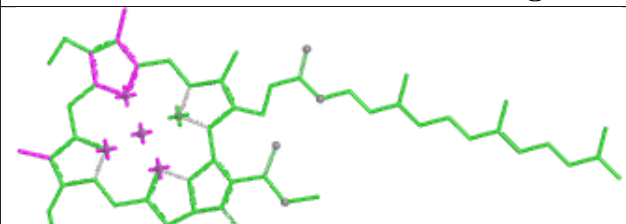
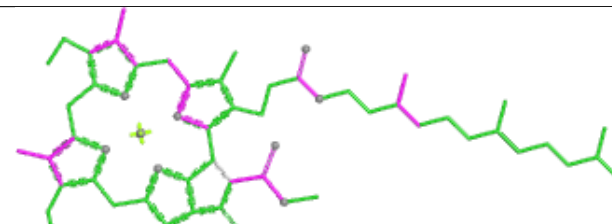
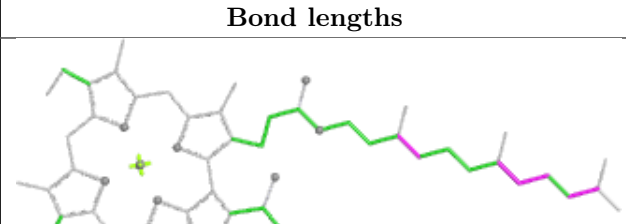
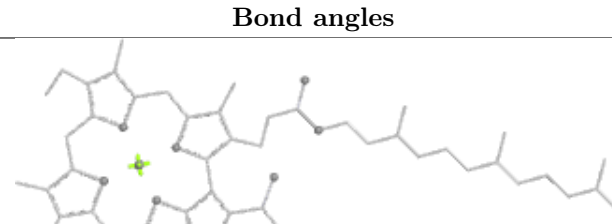
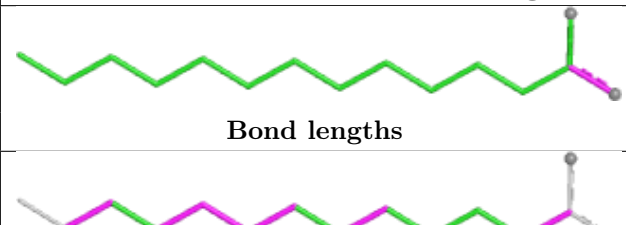
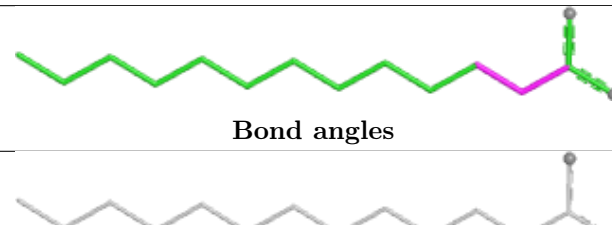


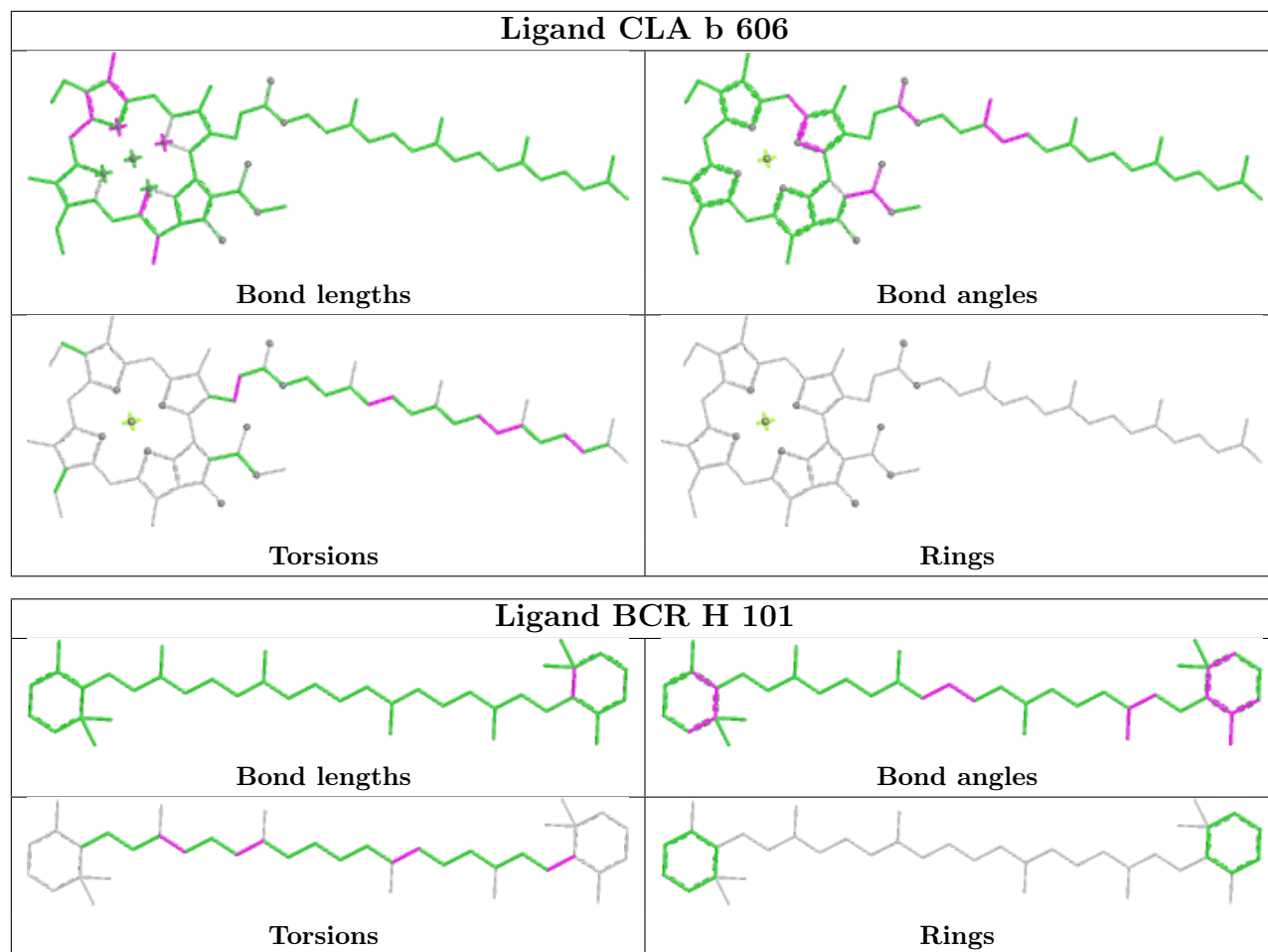
Ligand CLA b 610	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG m 101	
 Bond lengths	 Bond angles
 Torsions	 Rings



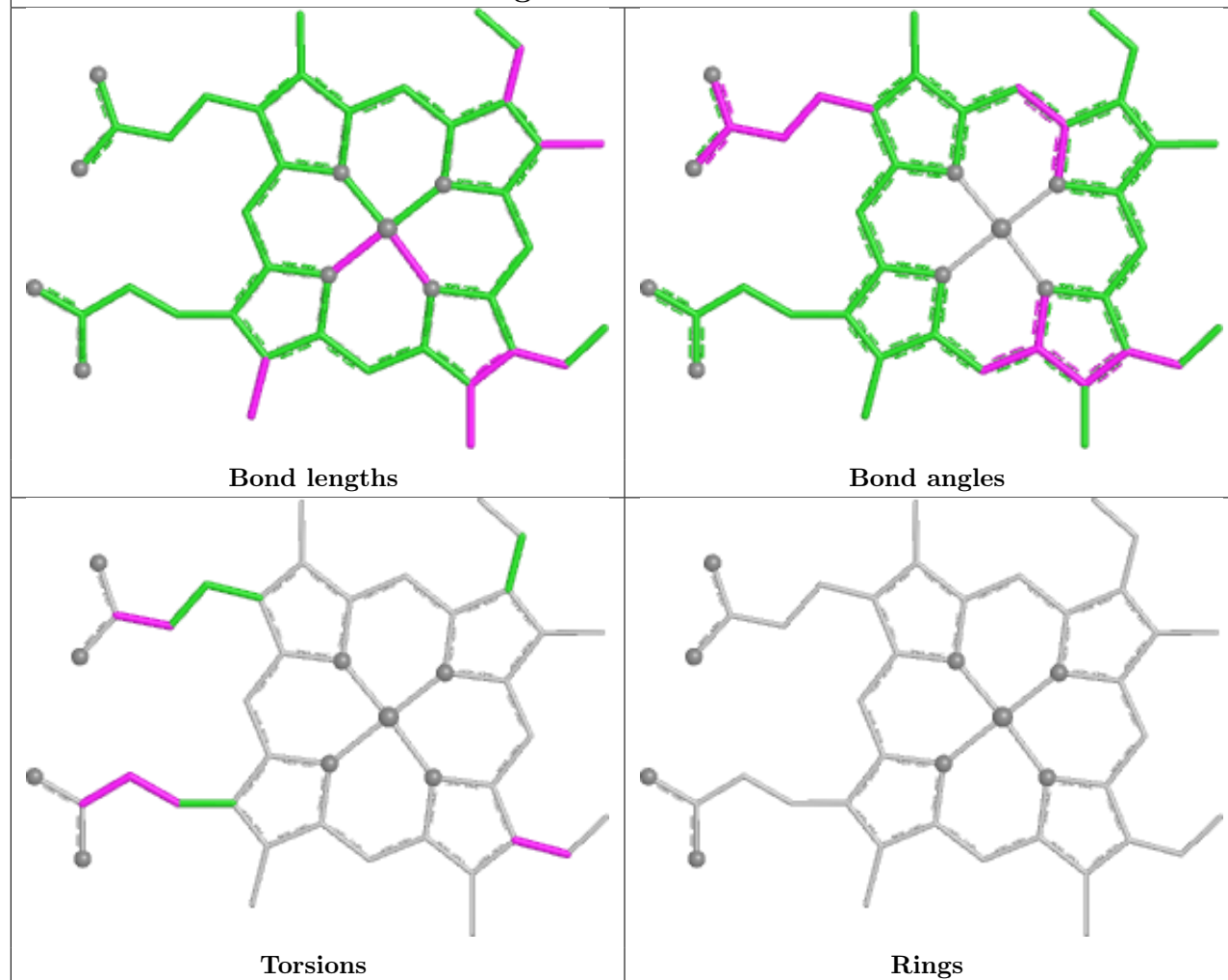




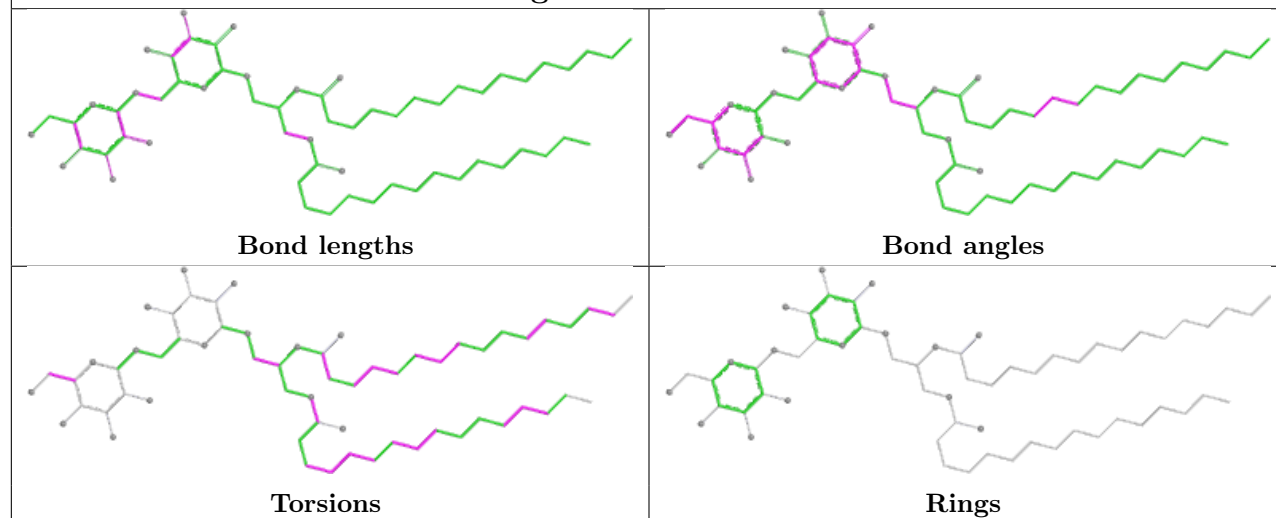
Ligand CLA b 605	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA c 504	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand STE D 413	
	
Bond lengths	Bond angles
	
Torsions	Rings

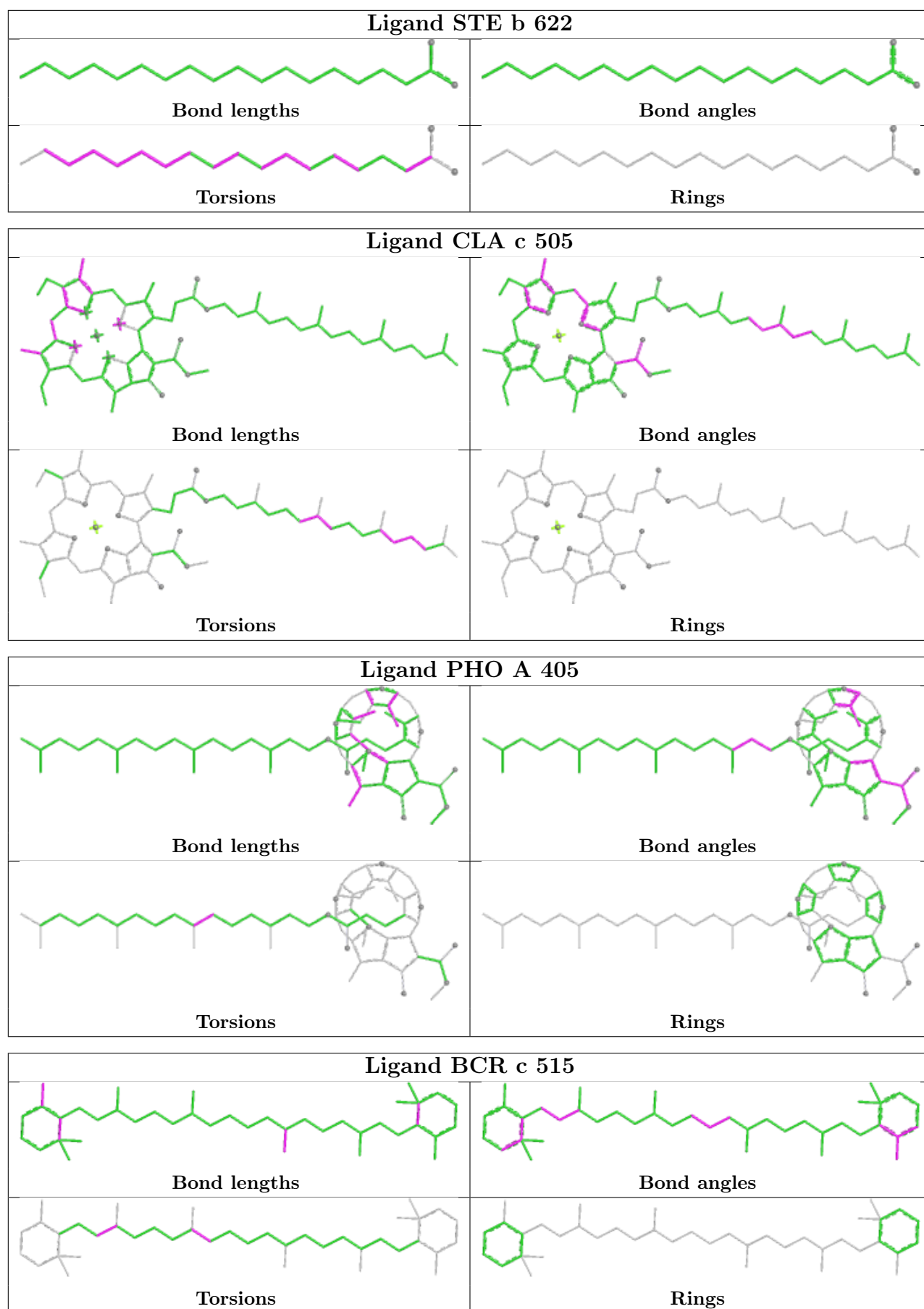


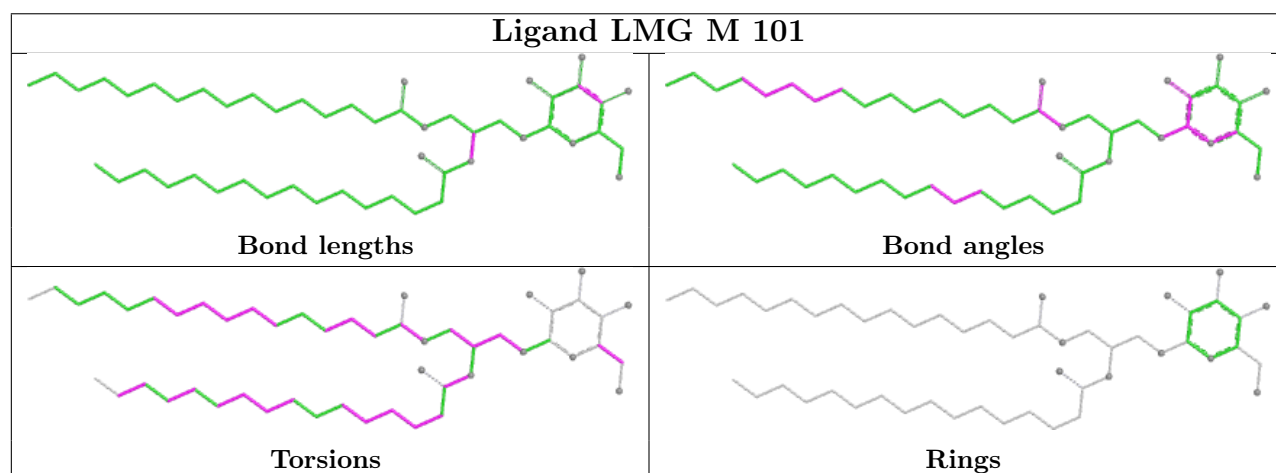
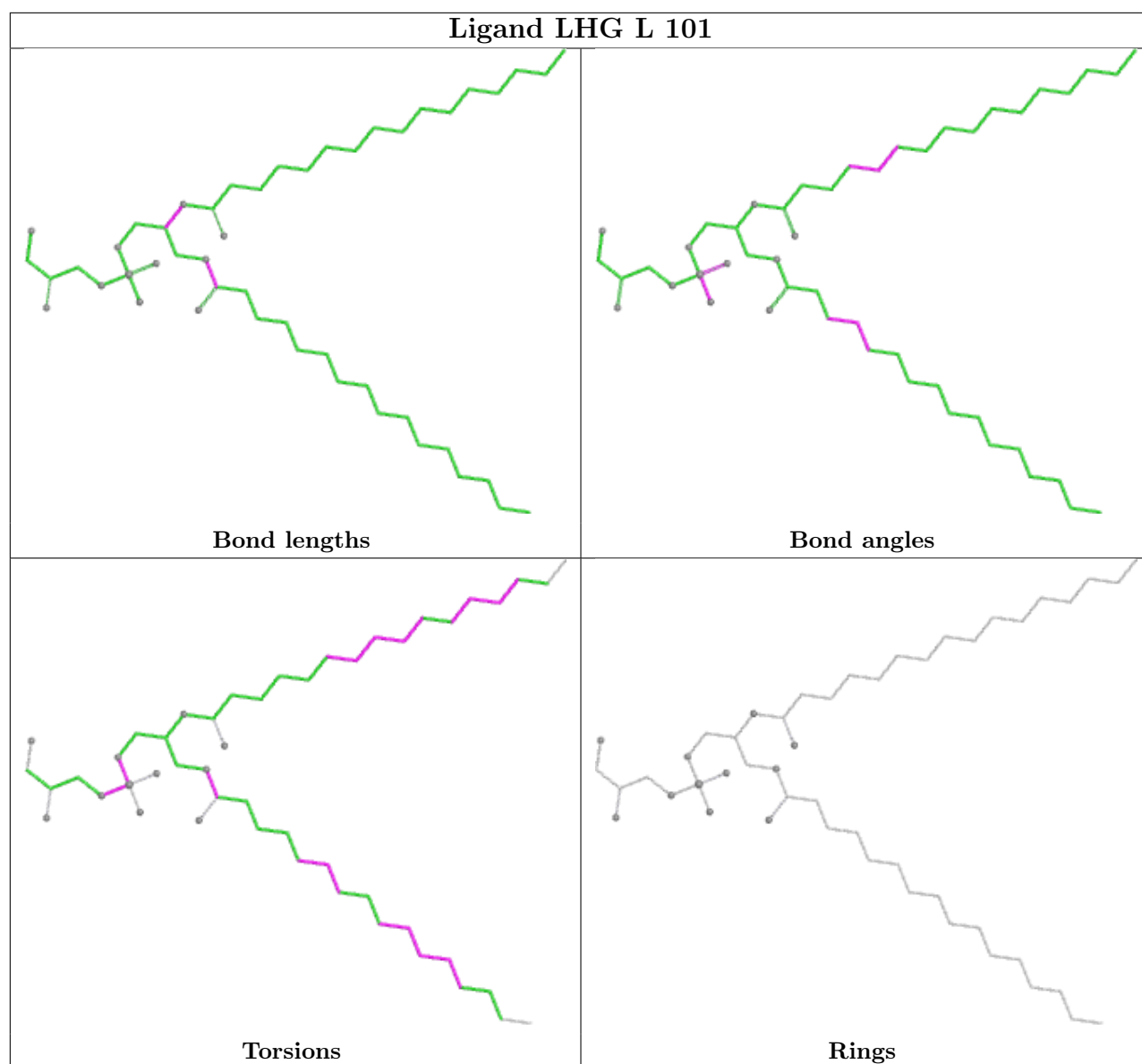
Ligand HEM f 101

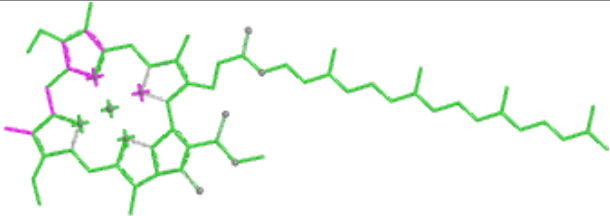
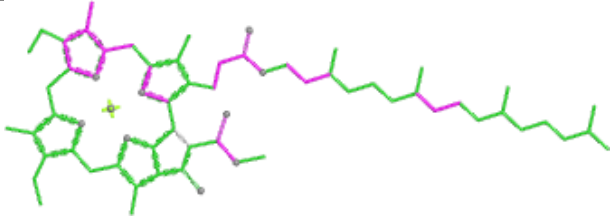
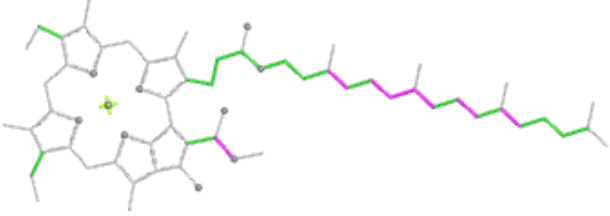
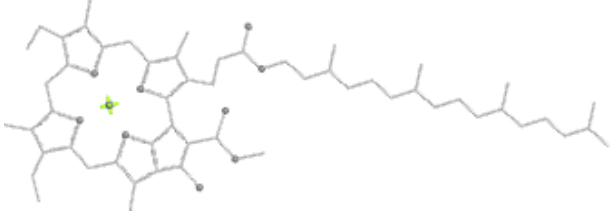
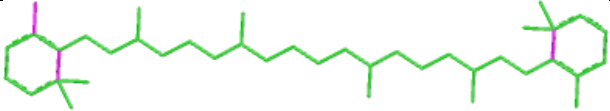
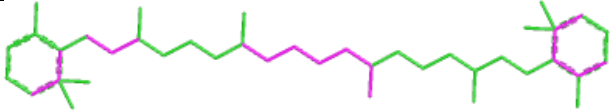
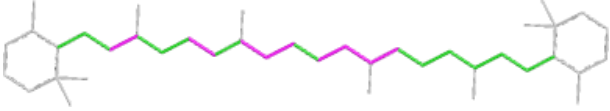
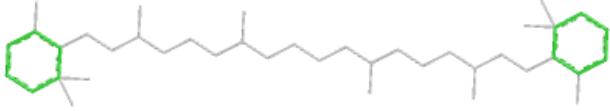
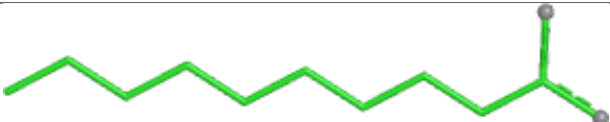
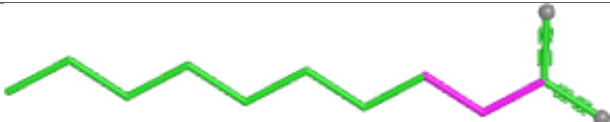
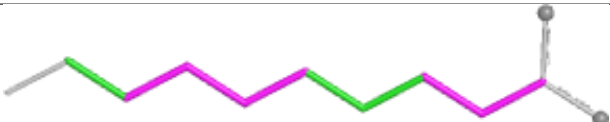
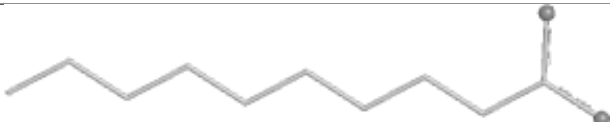


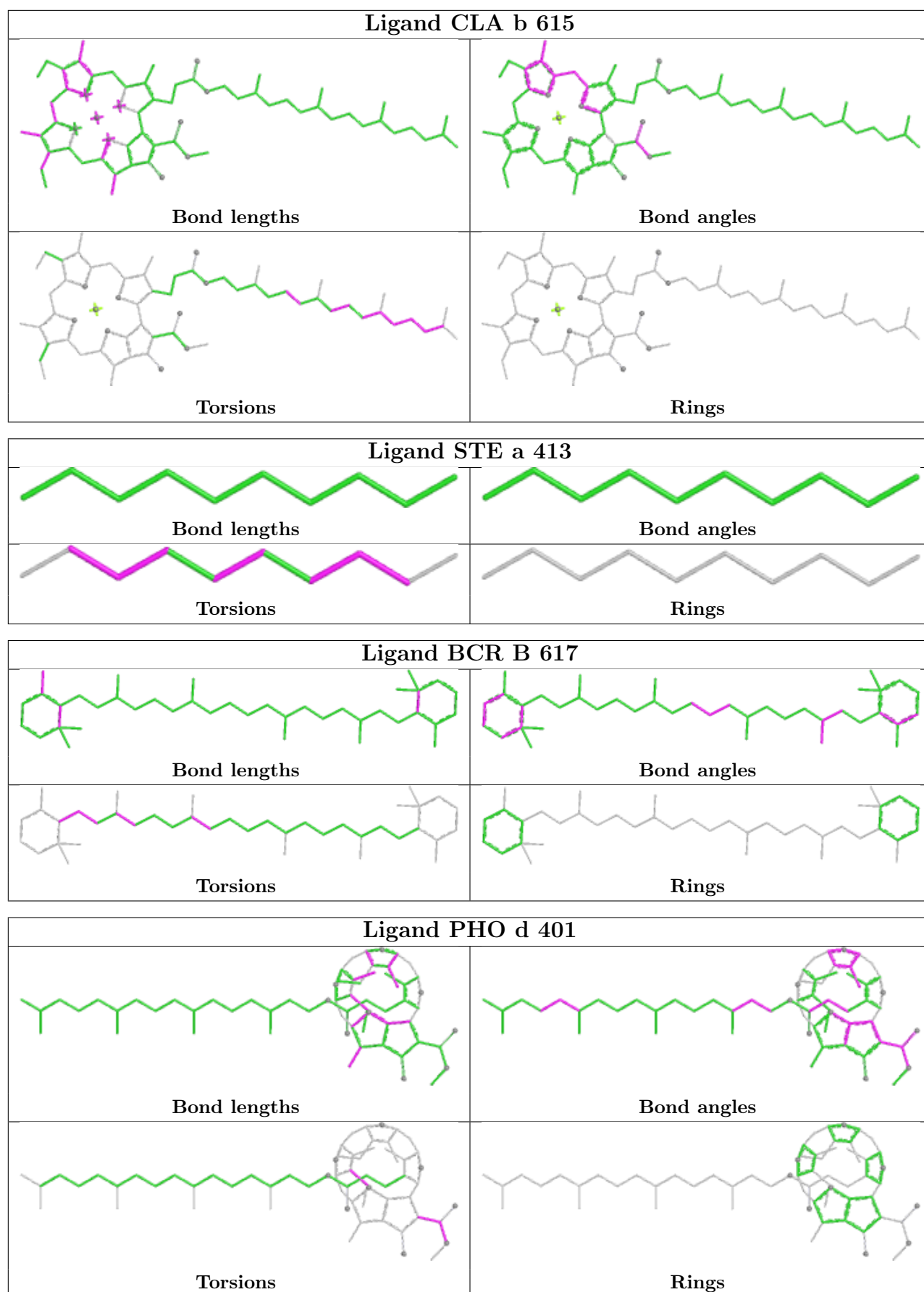
Ligand DGD h 103

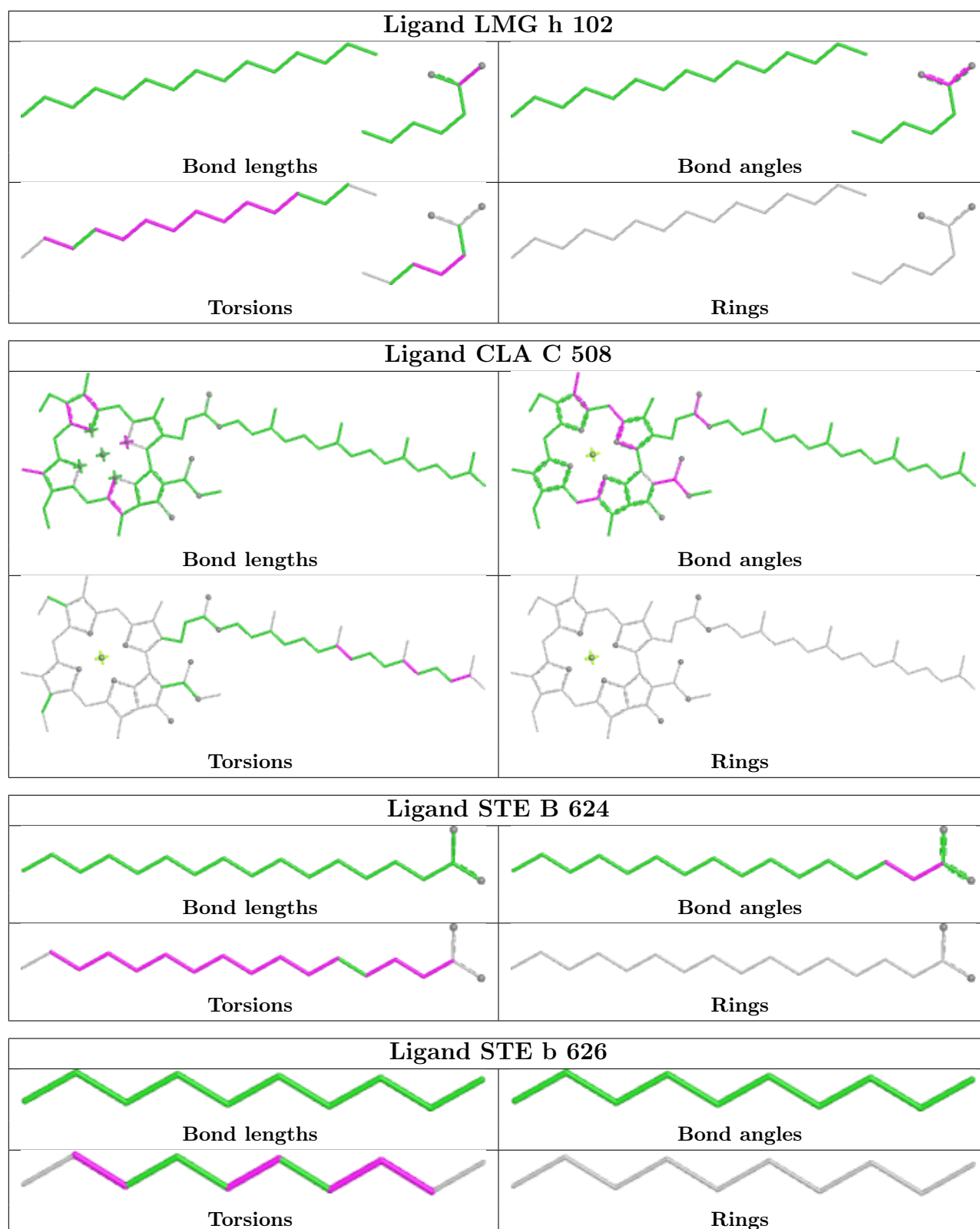


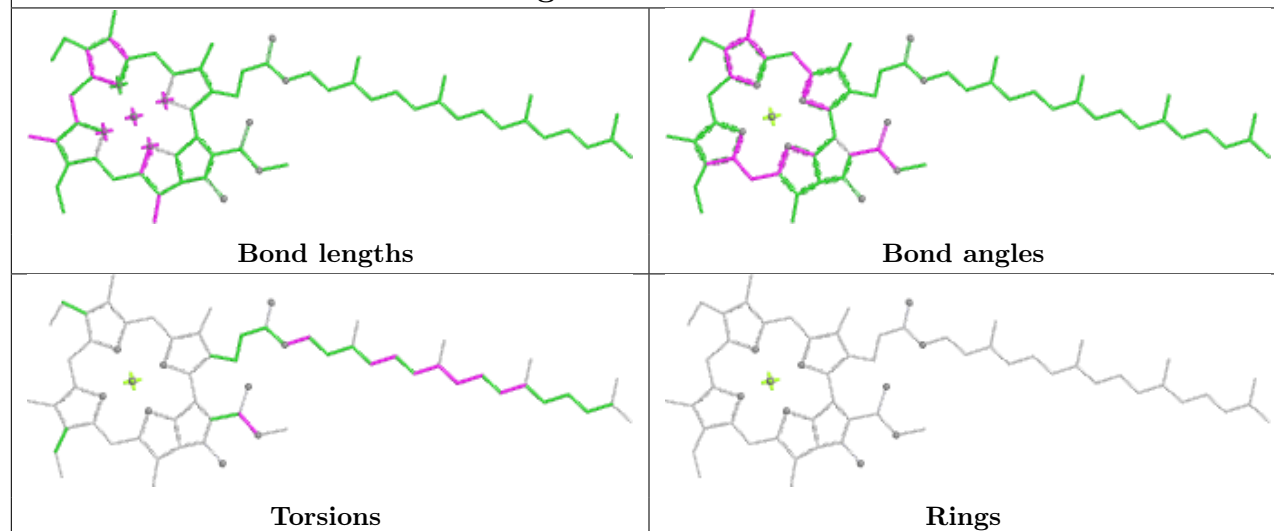
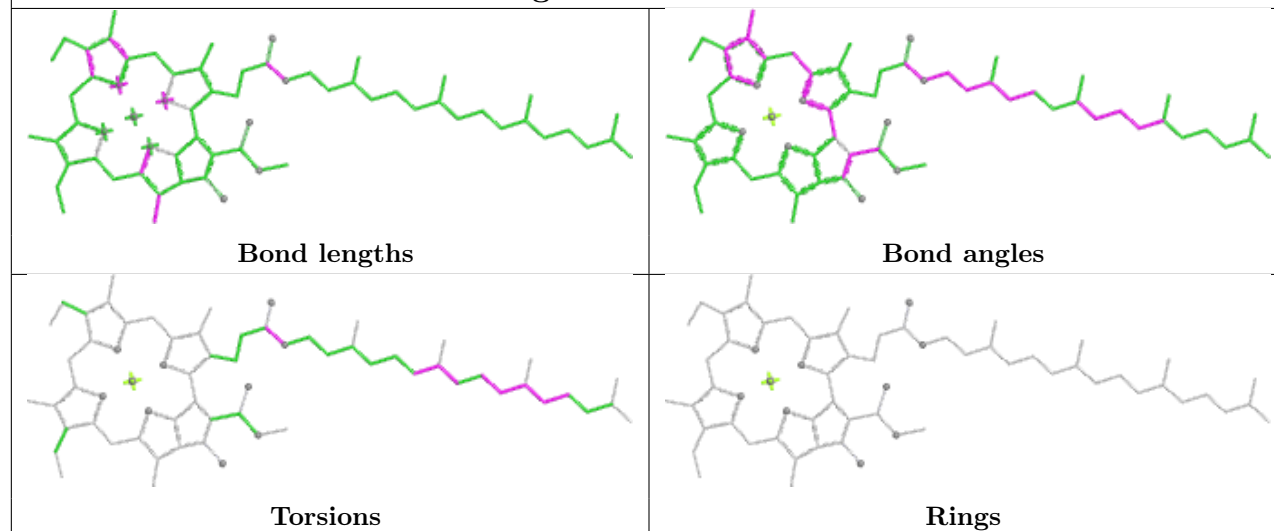




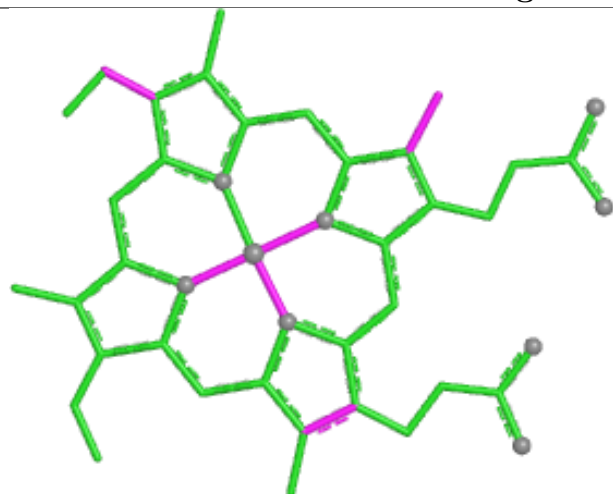
Ligand CLA C 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR C 514	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE C 520	
 Bond lengths	 Bond angles
 Torsions	 Rings



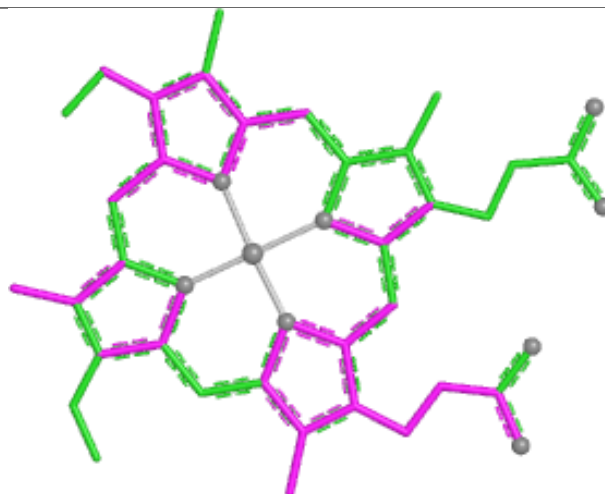


Ligand CLA c 513**Ligand CLA B 604**

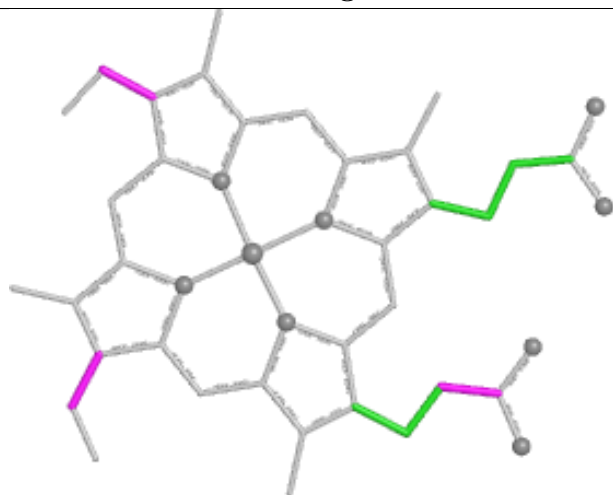
Ligand HEC v 201



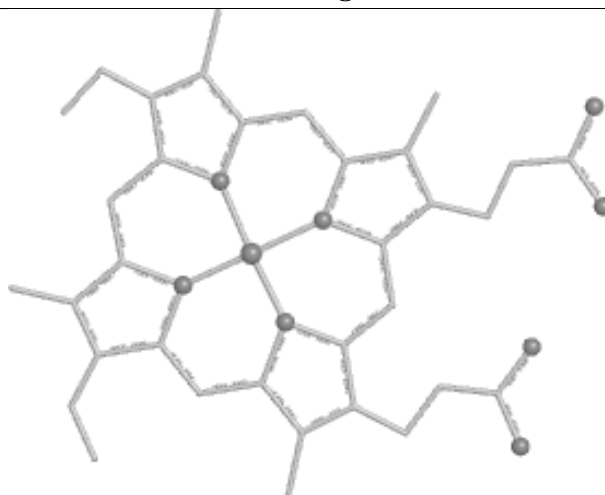
Bond lengths



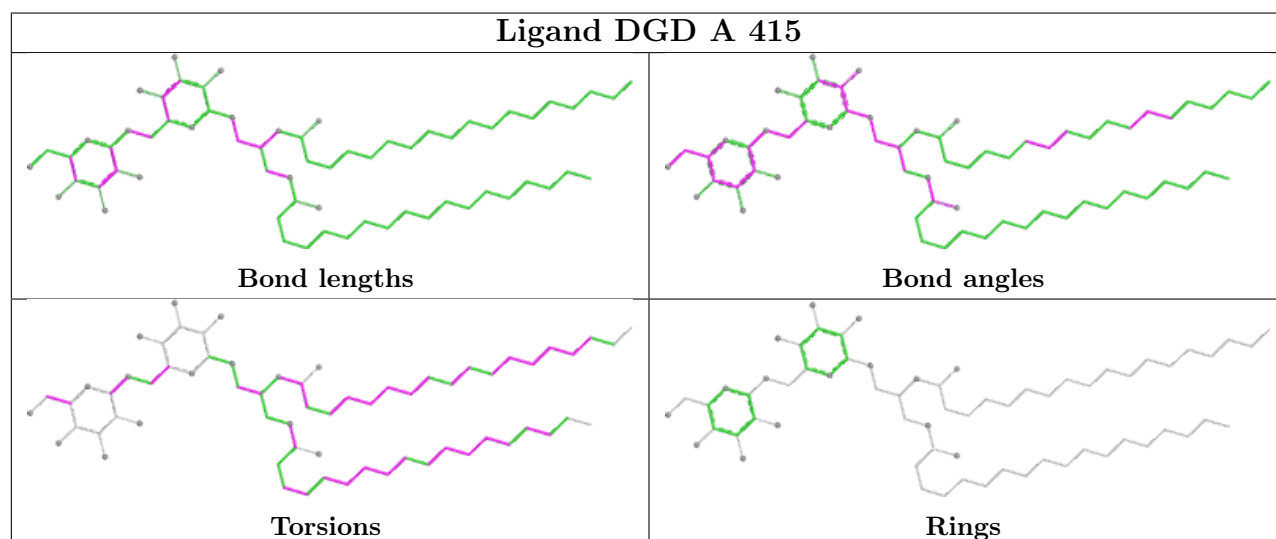
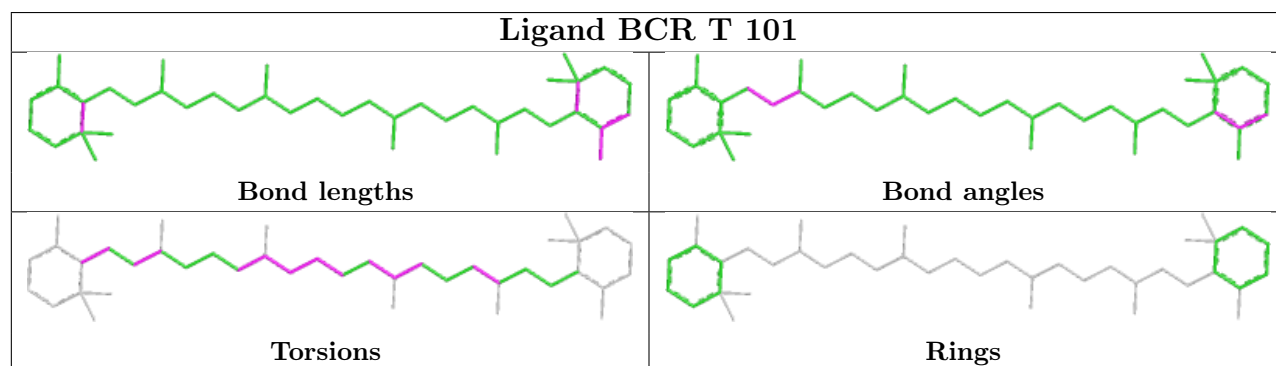
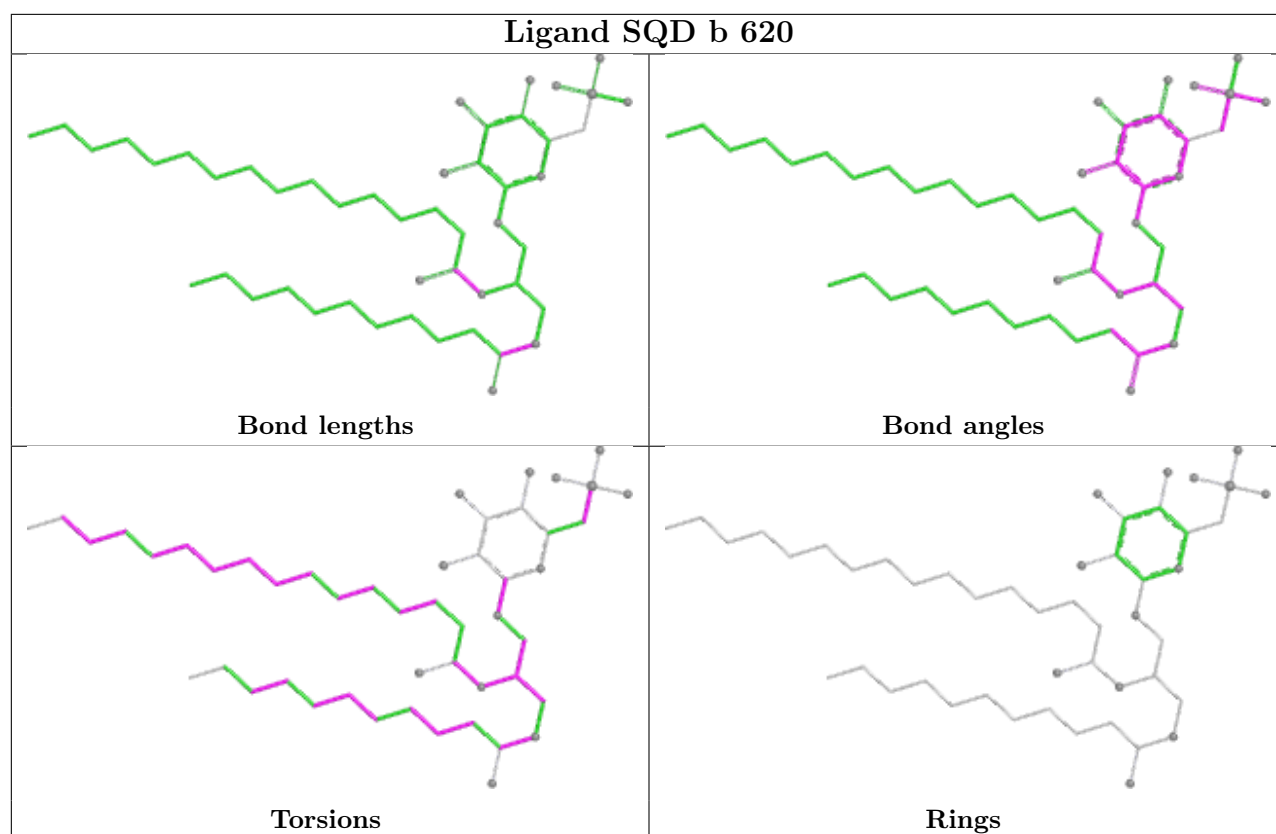
Bond angles

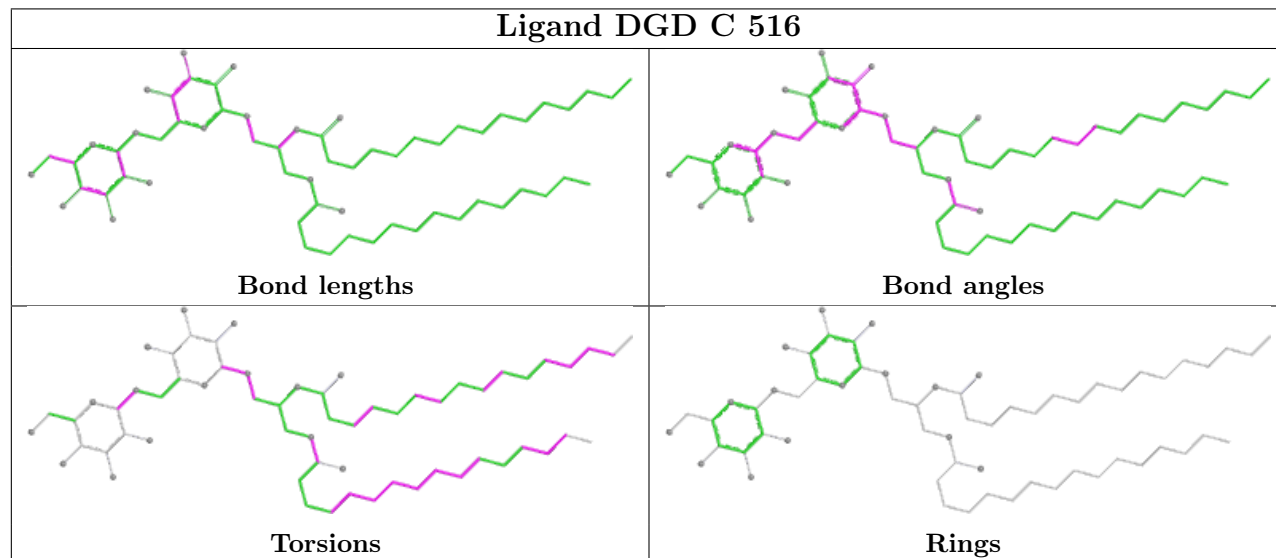
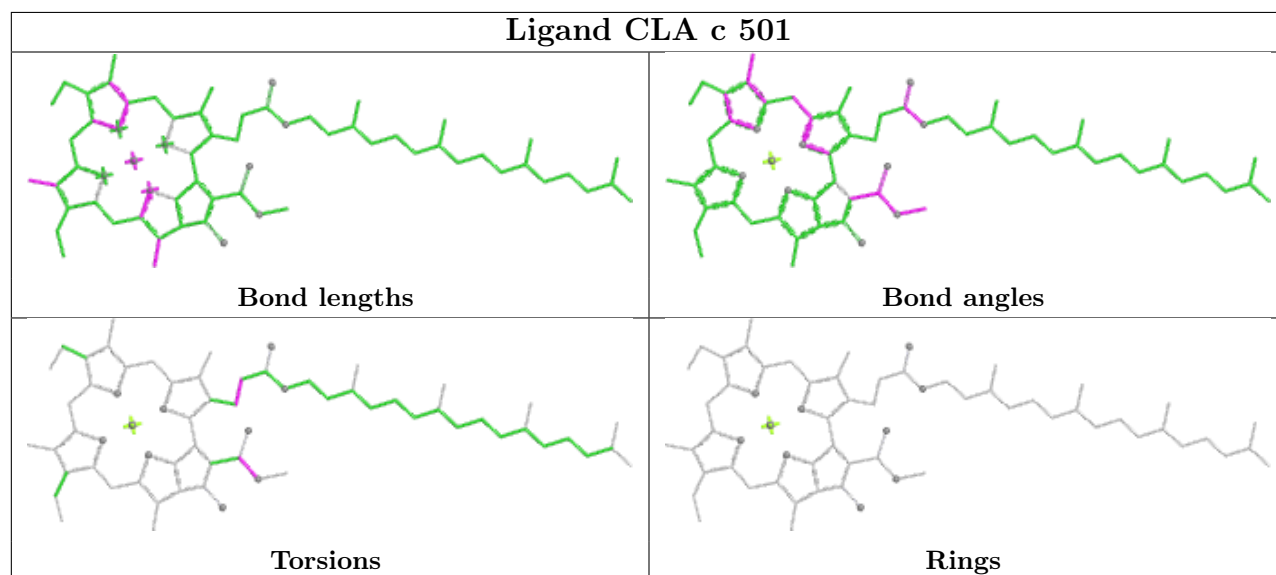
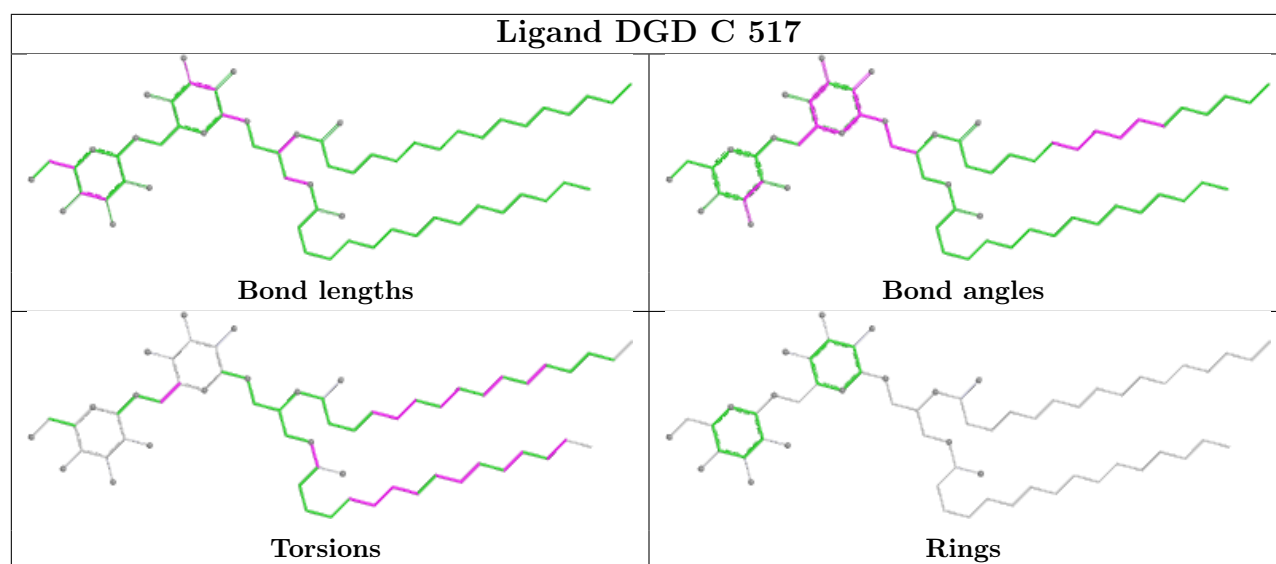


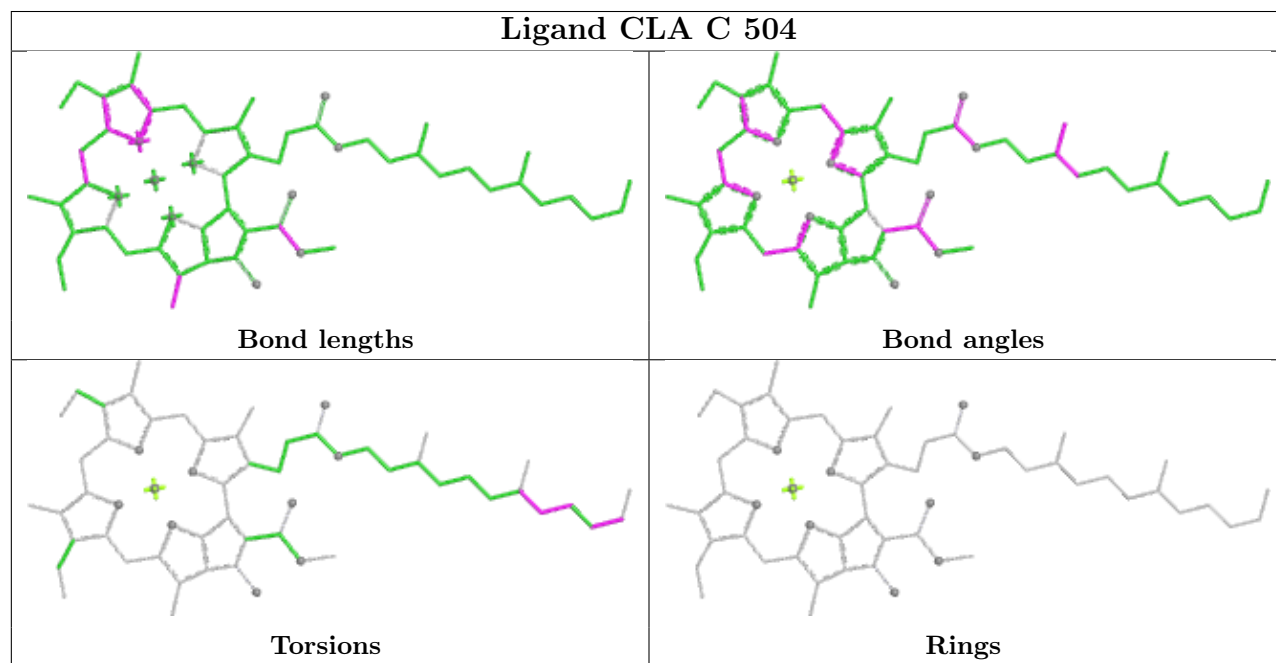
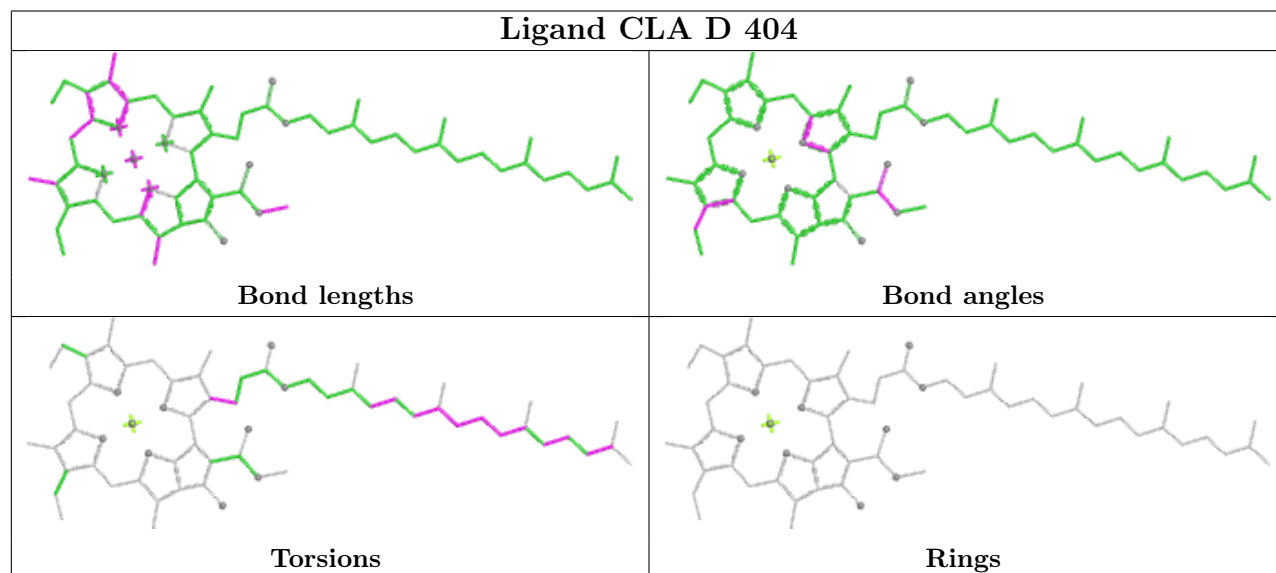
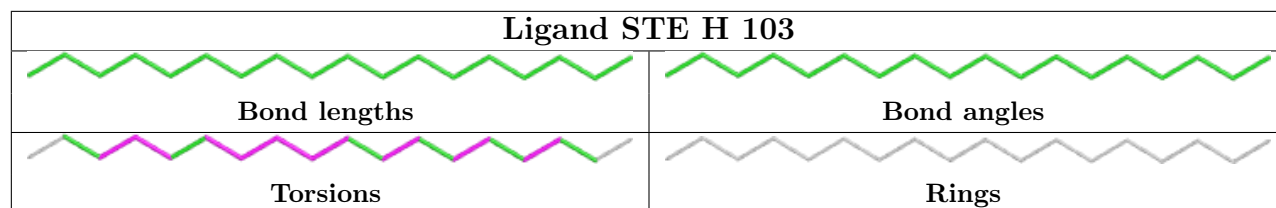
Torsions

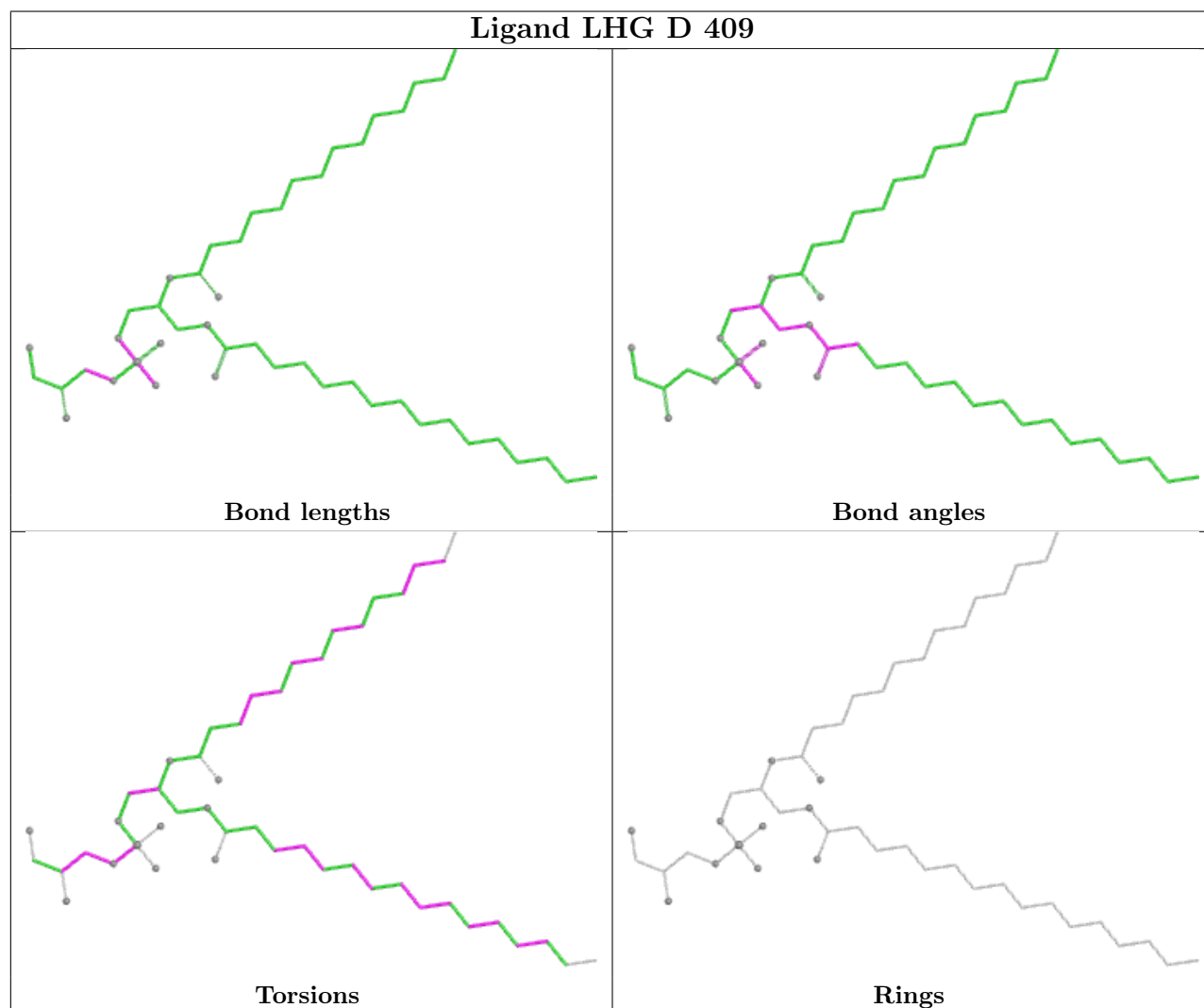
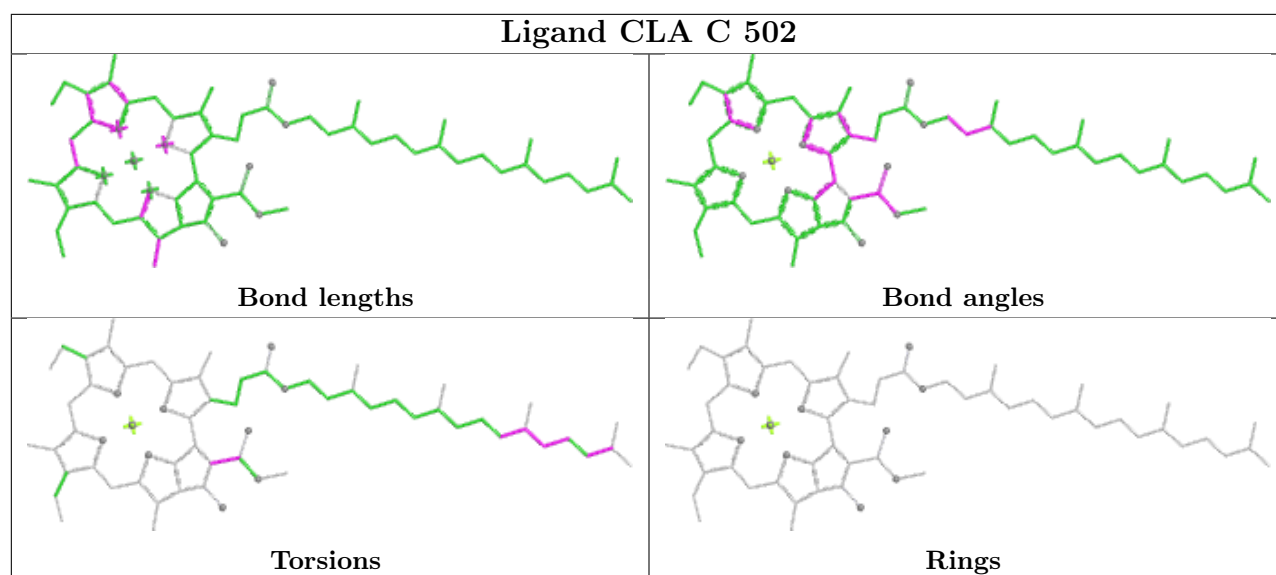


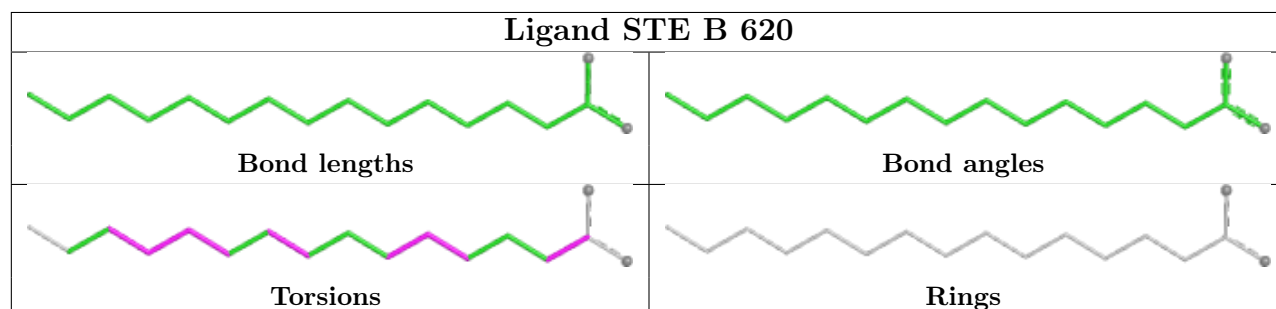
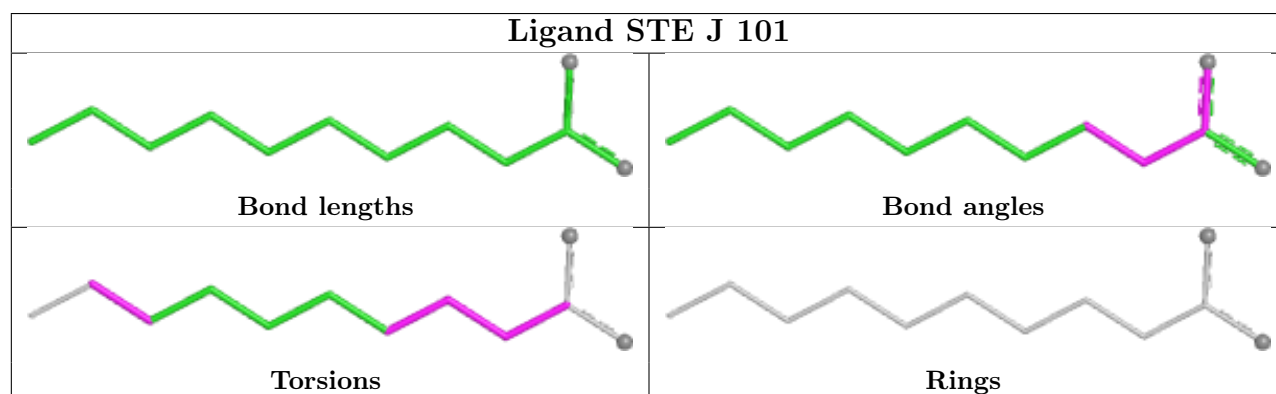
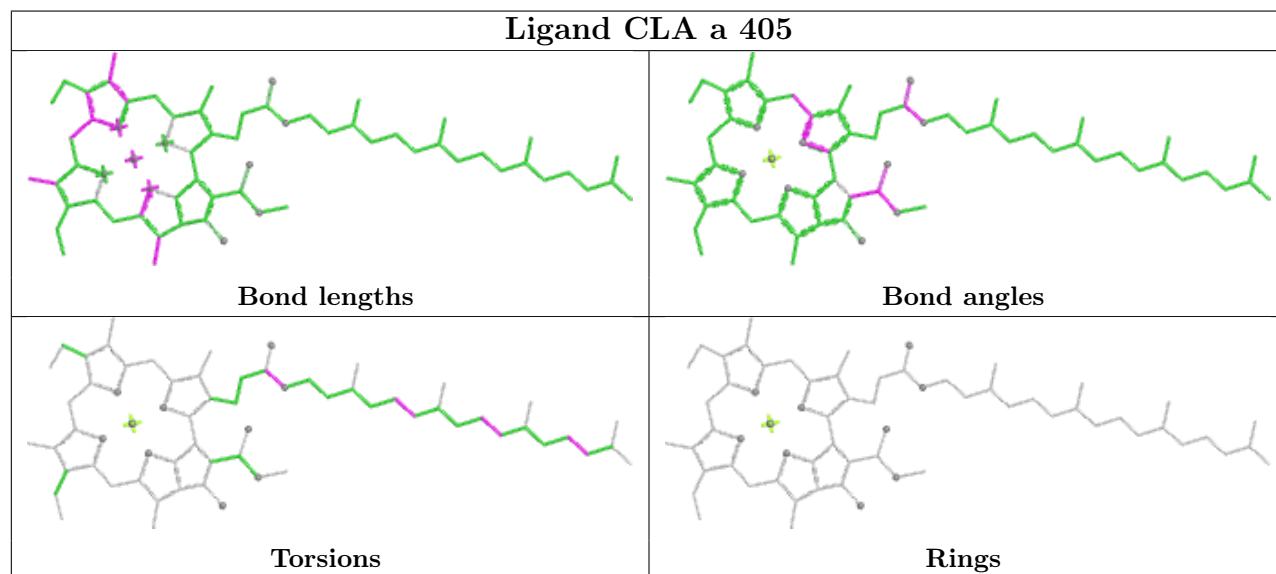
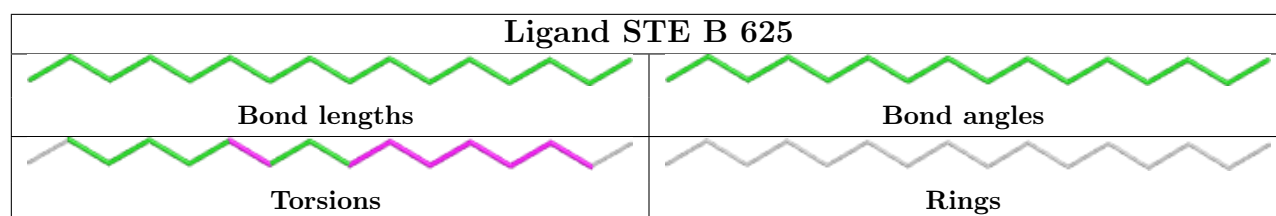
Rings

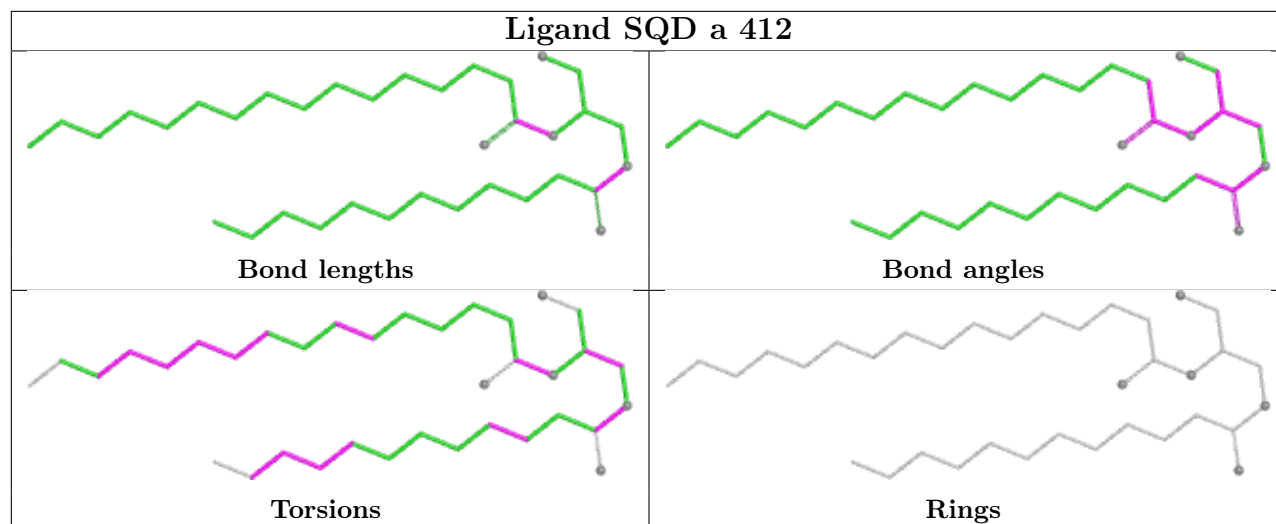
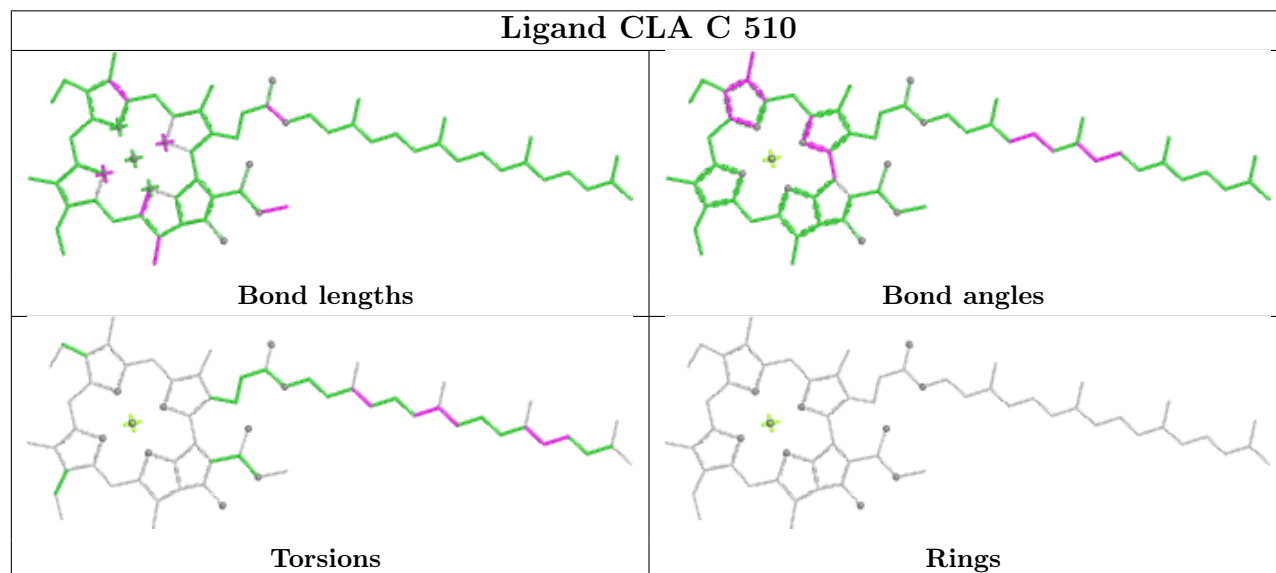
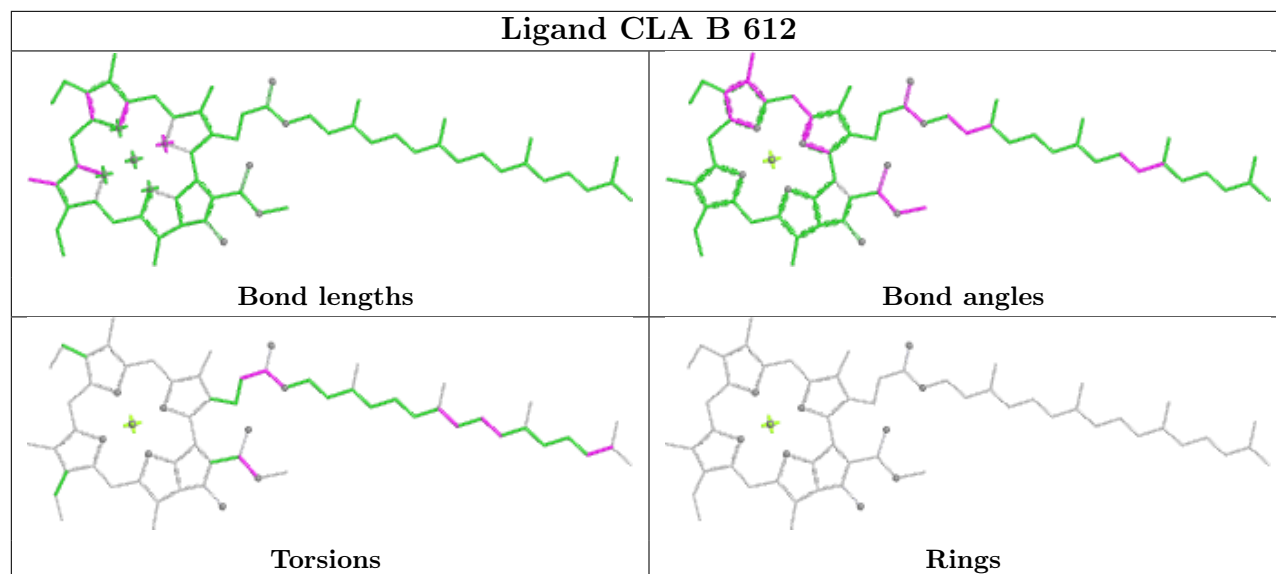


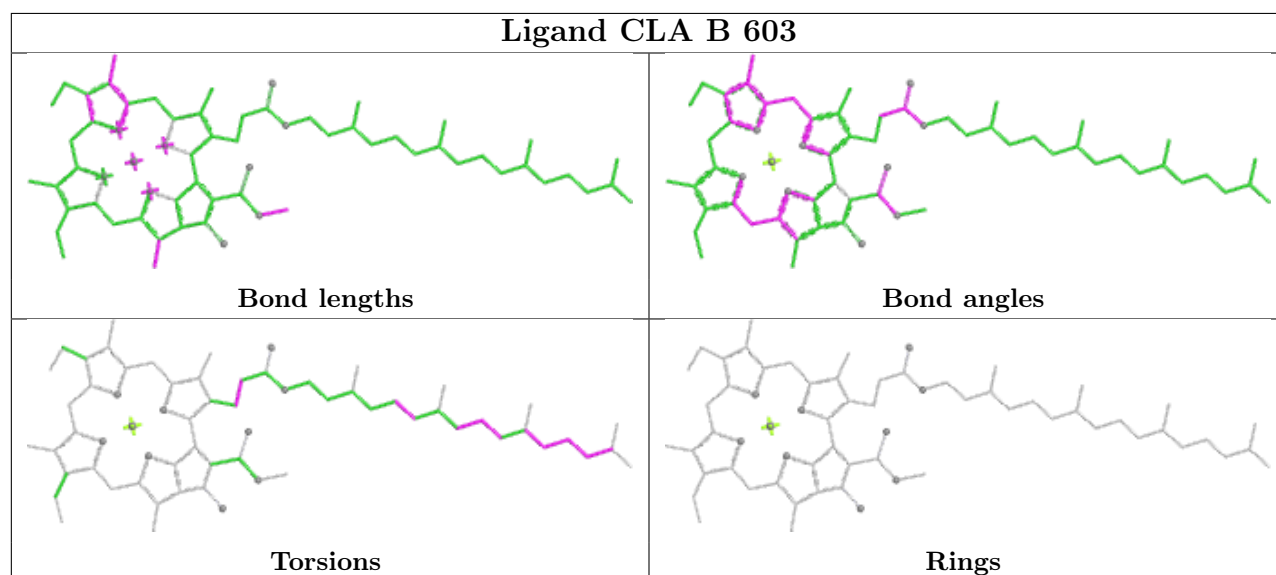
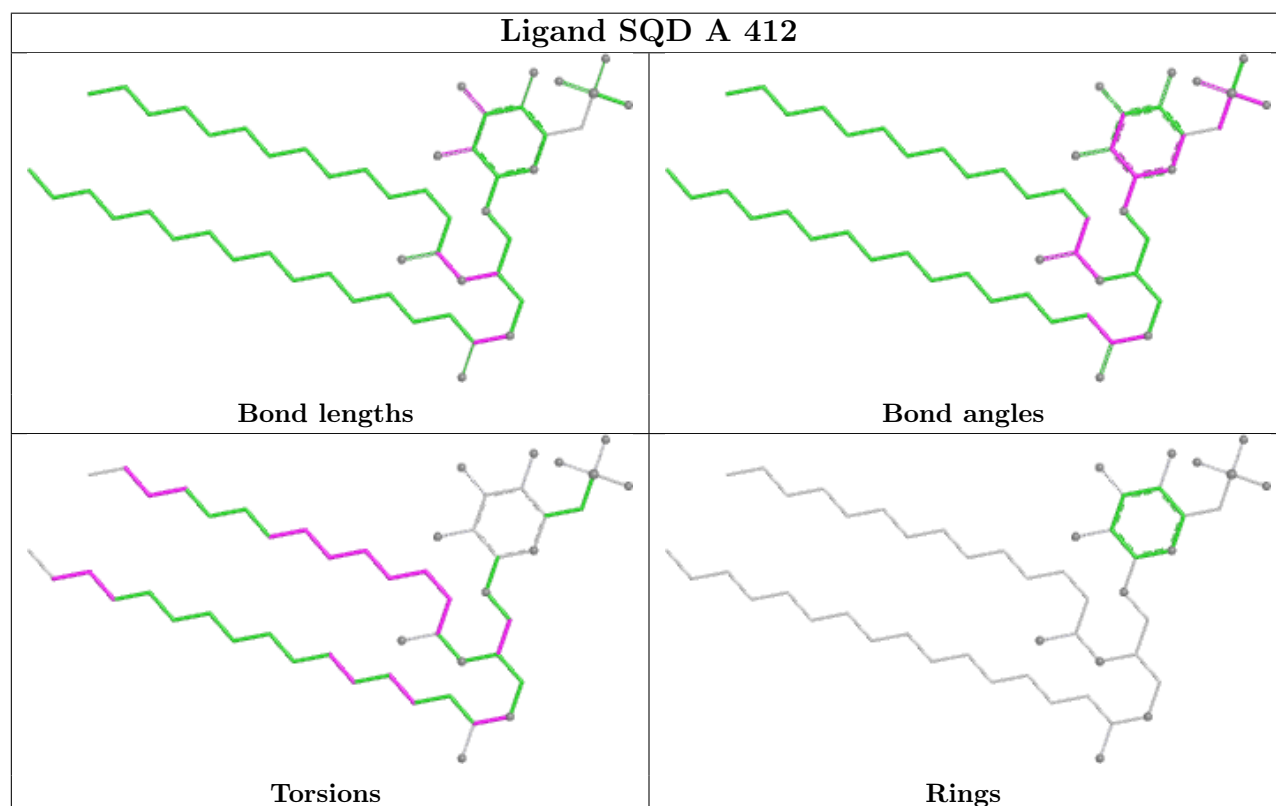
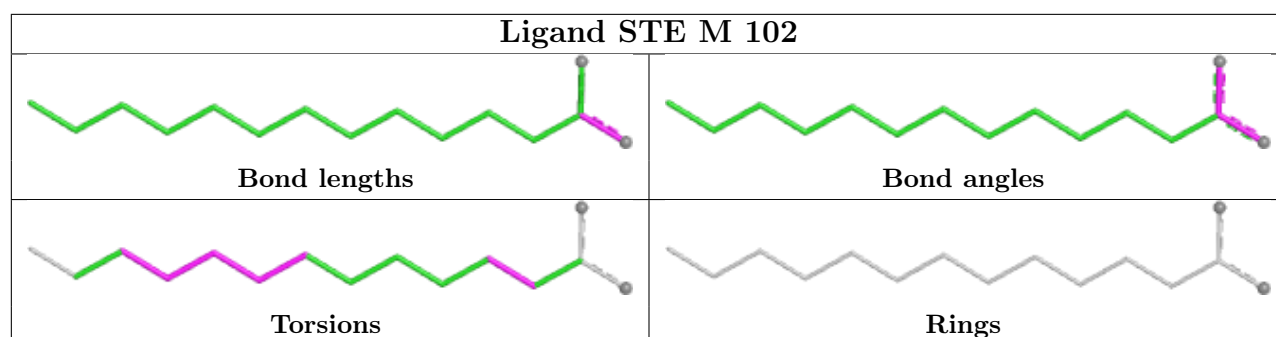


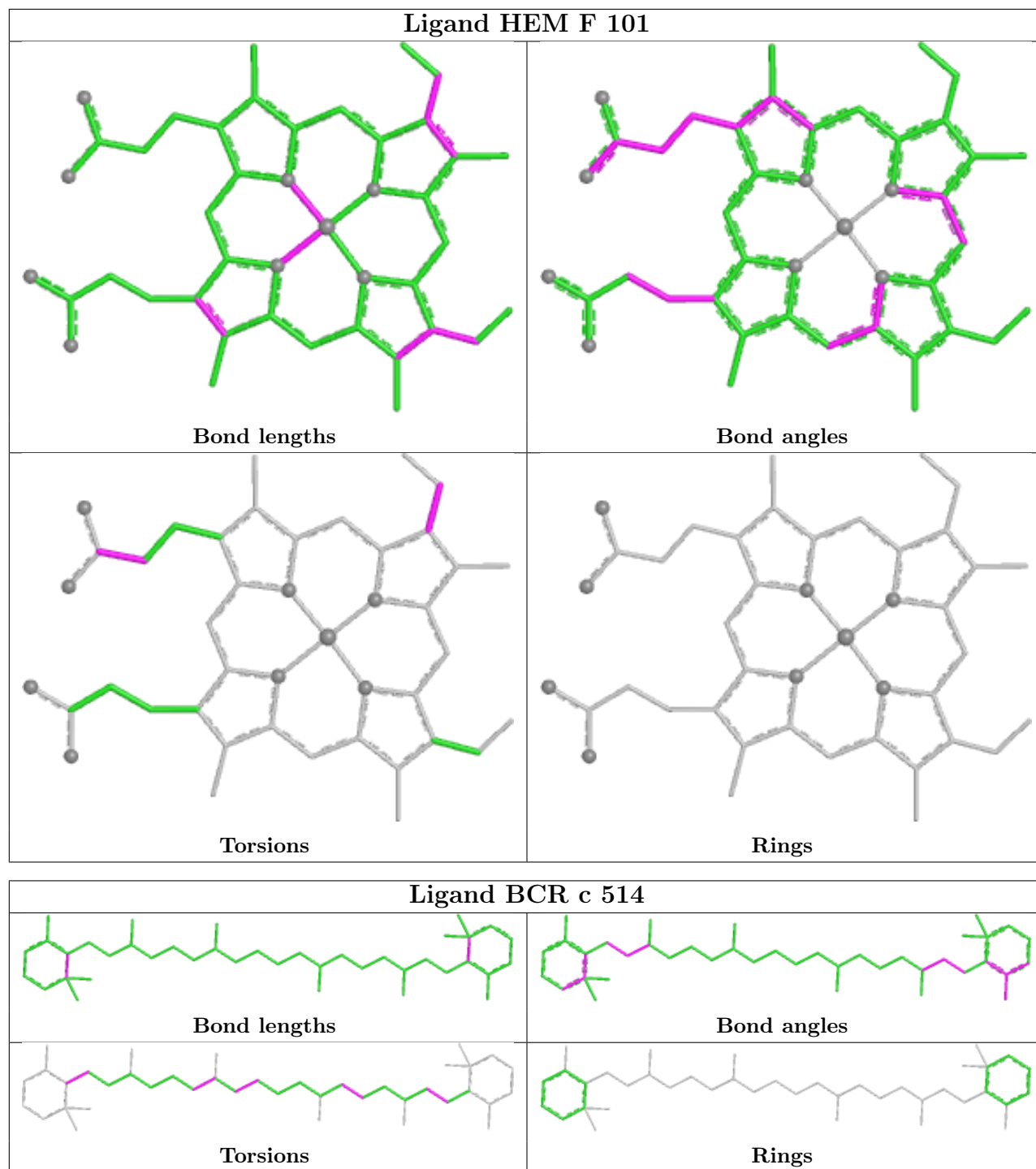


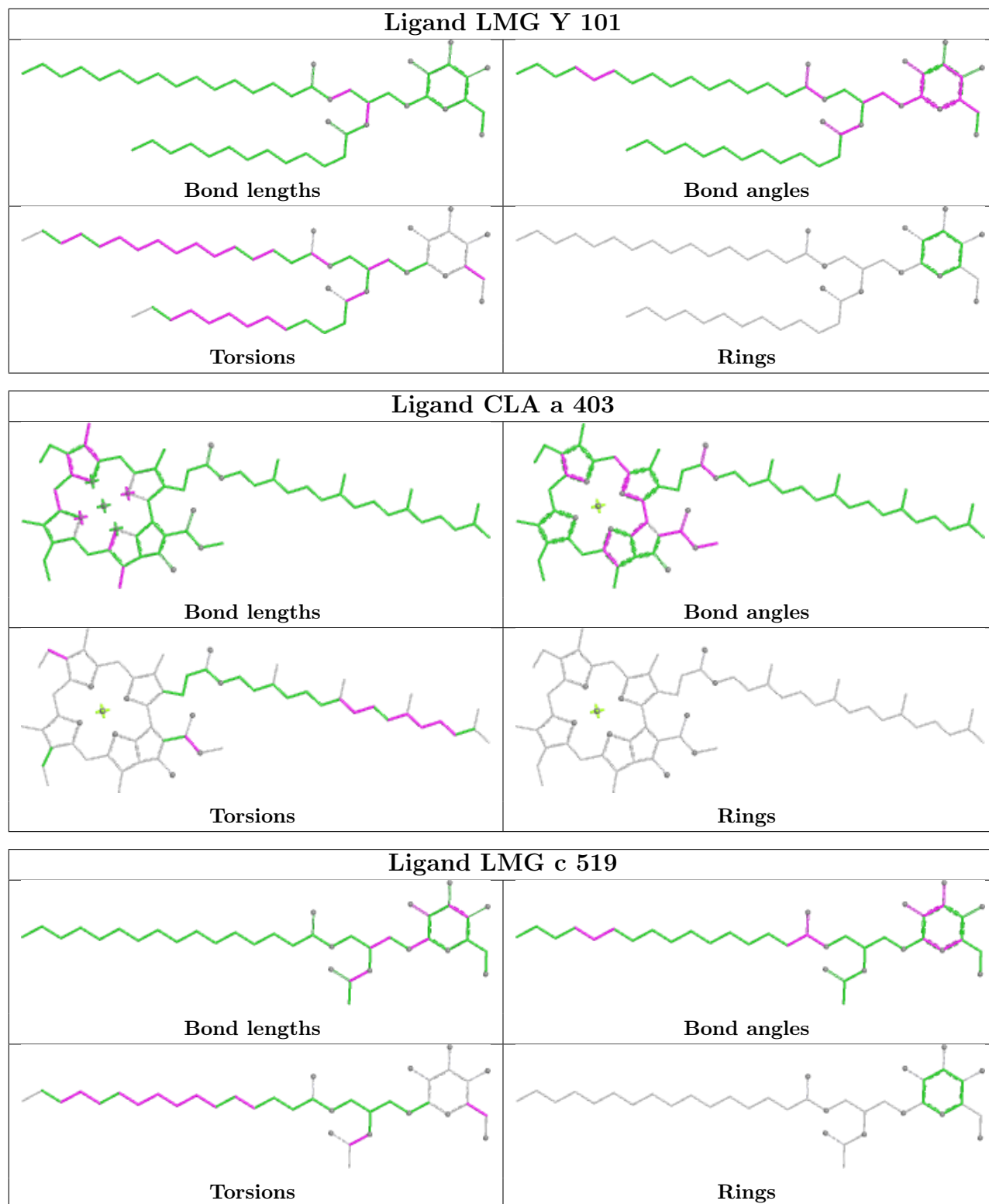


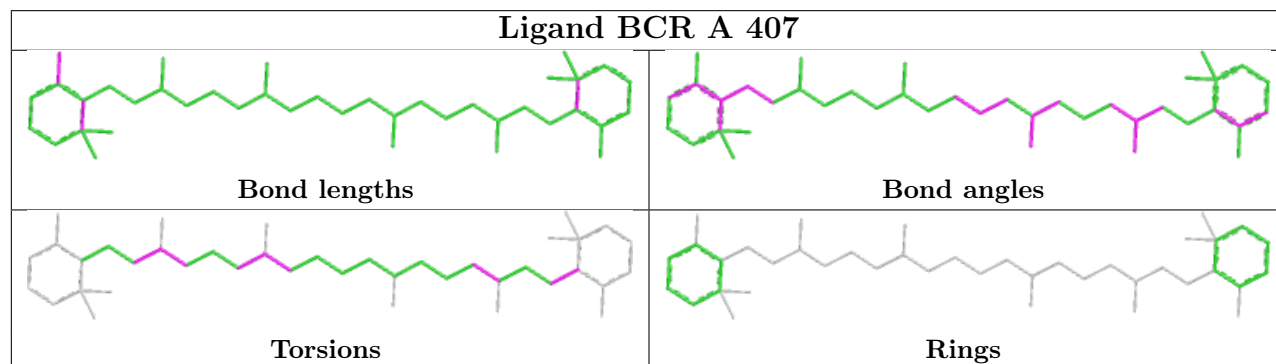
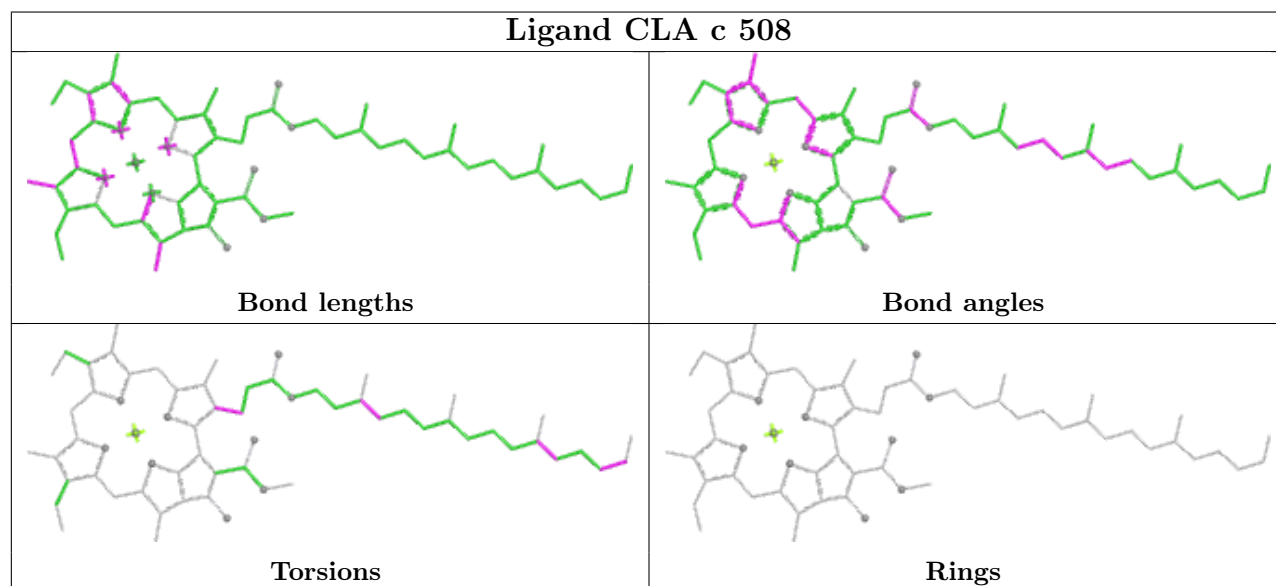
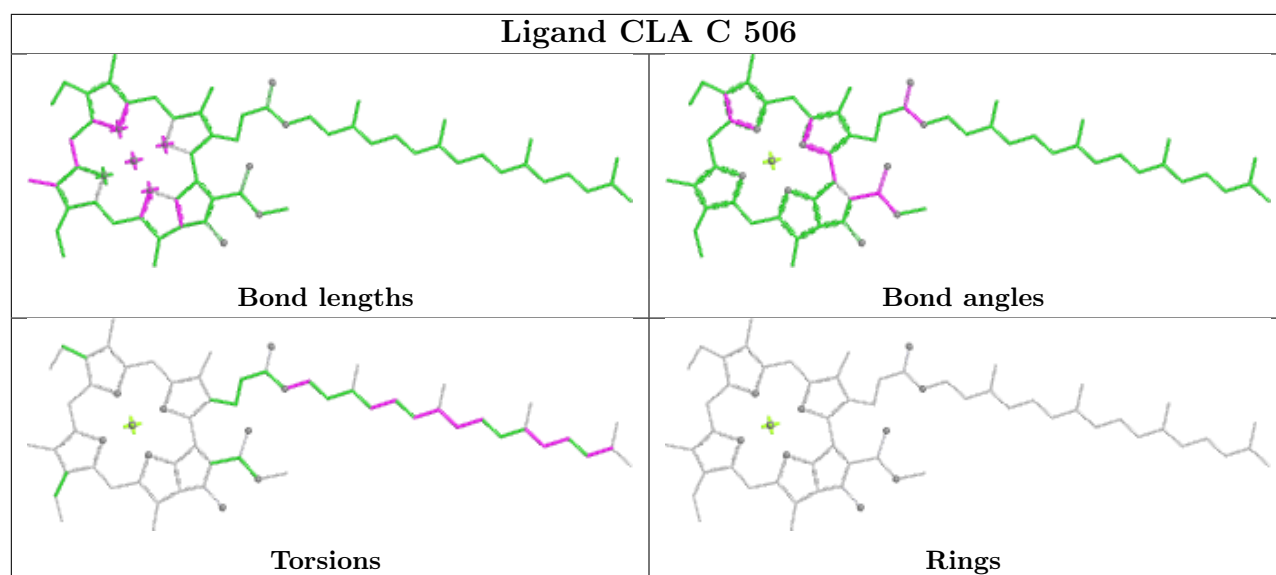


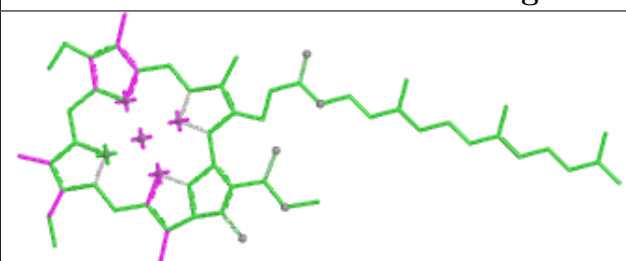
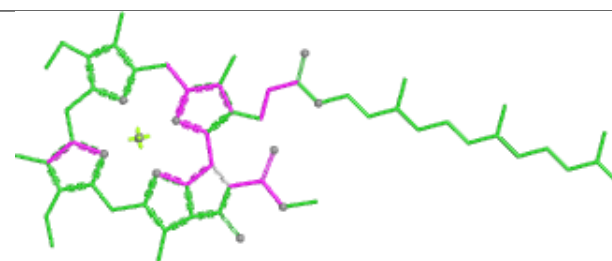
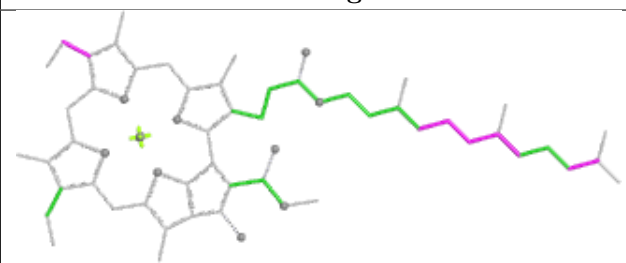
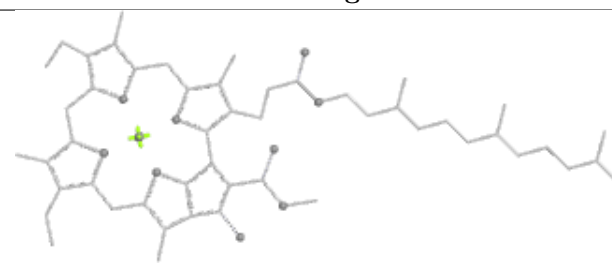


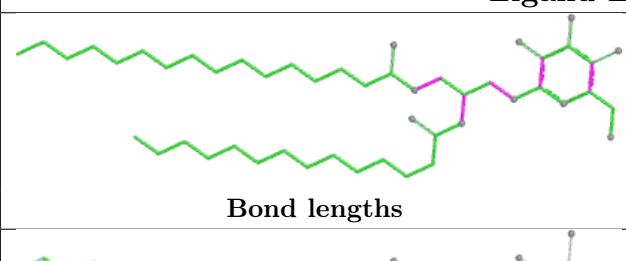
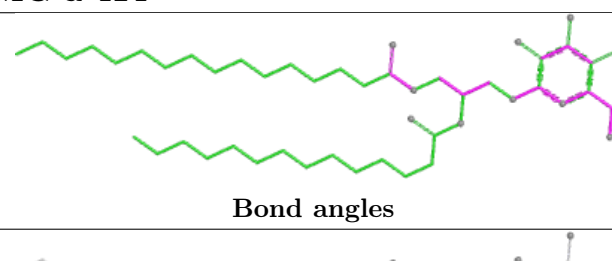
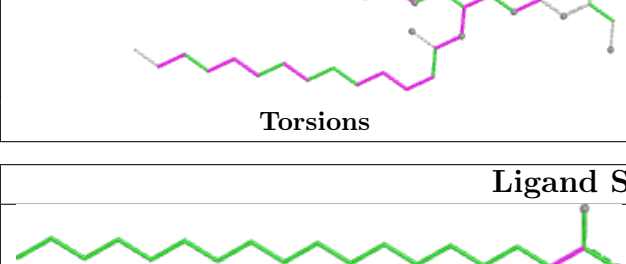


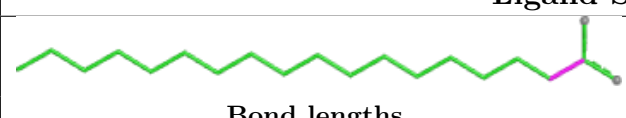




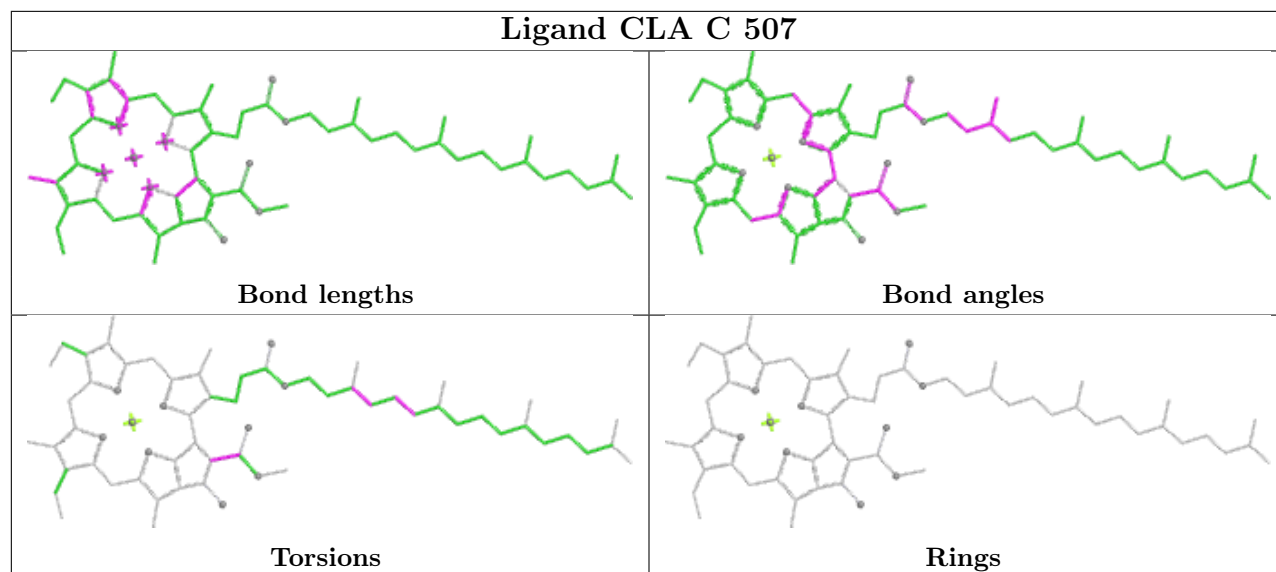


Ligand CLA B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

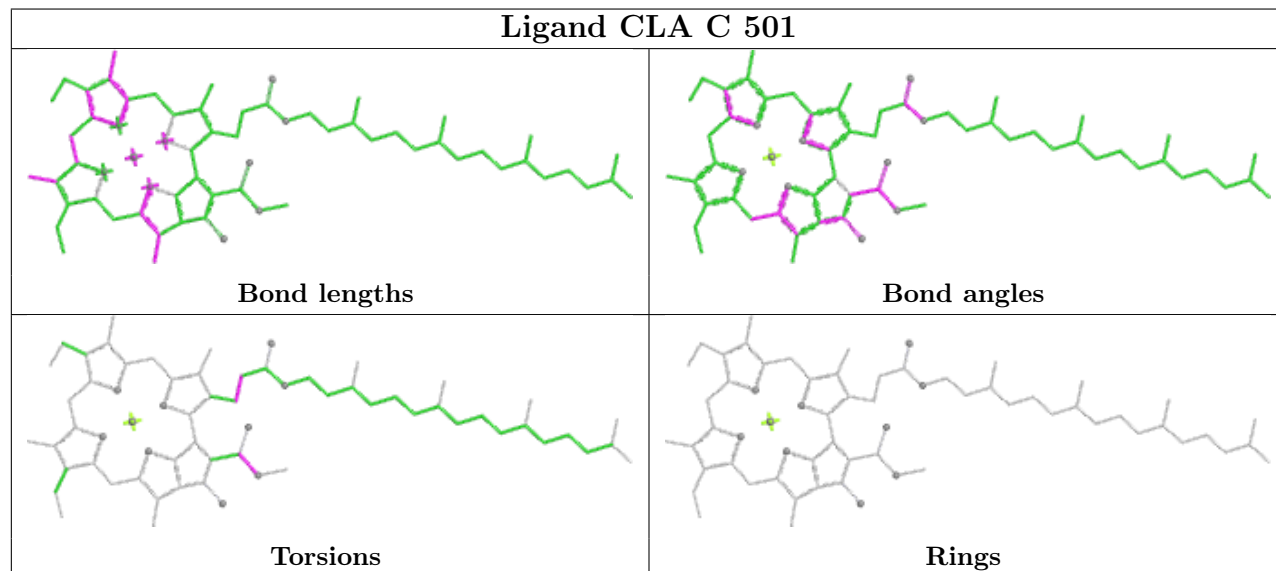
Ligand LMG a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

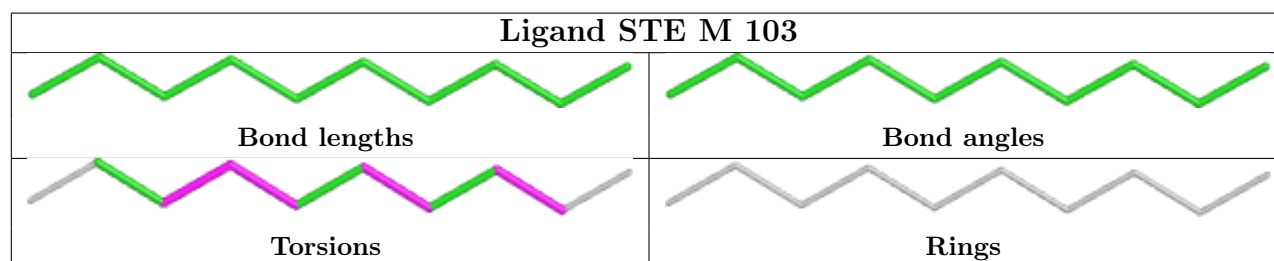
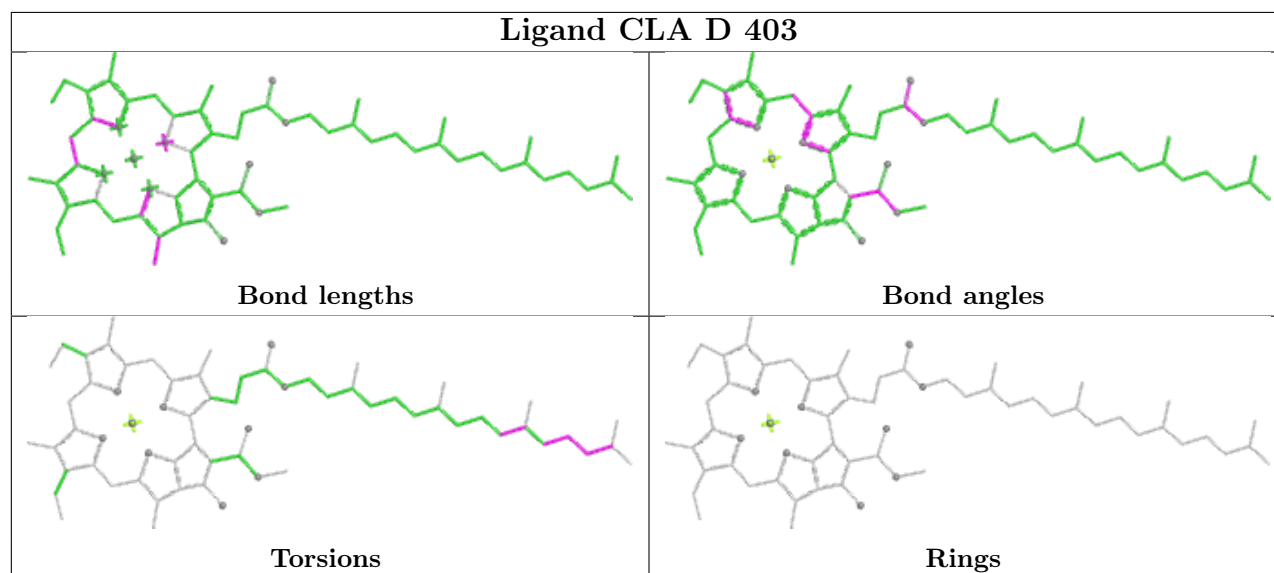
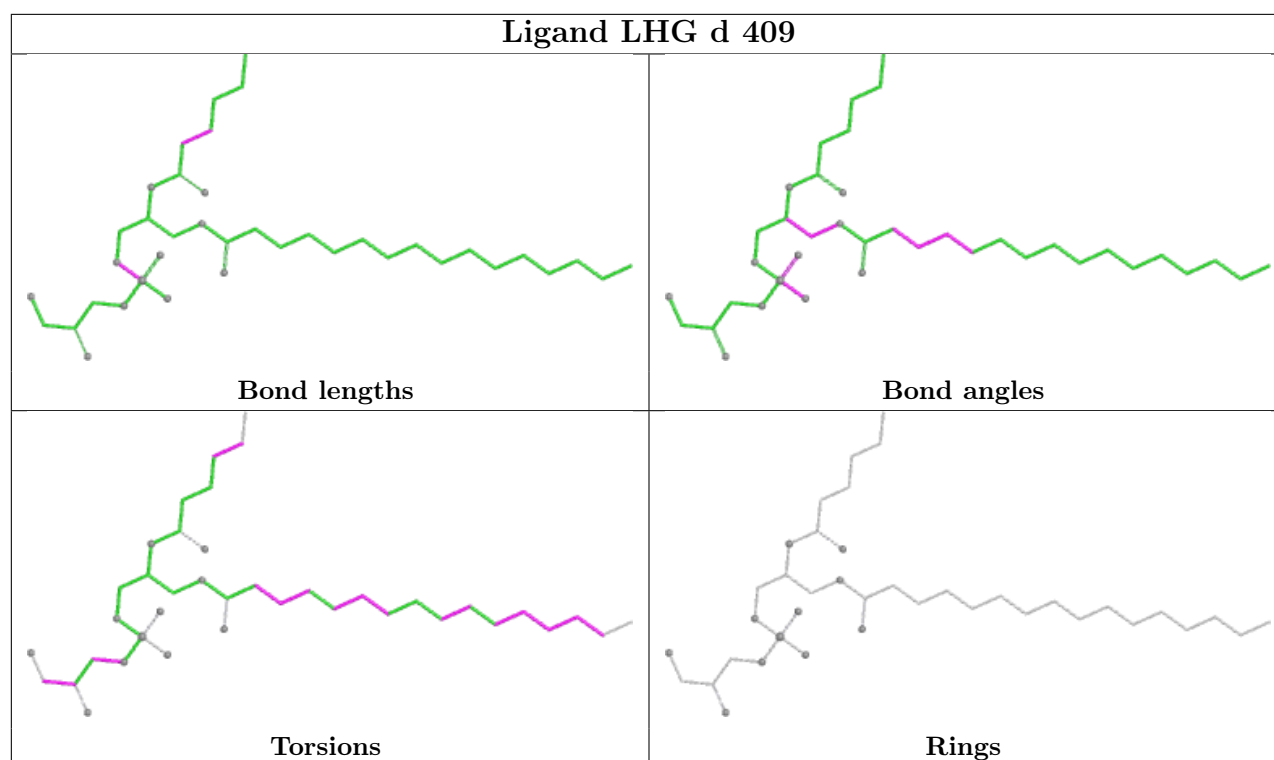
Ligand STE D 412	
	
Bond lengths	Bond angles
	
Torsions	Rings

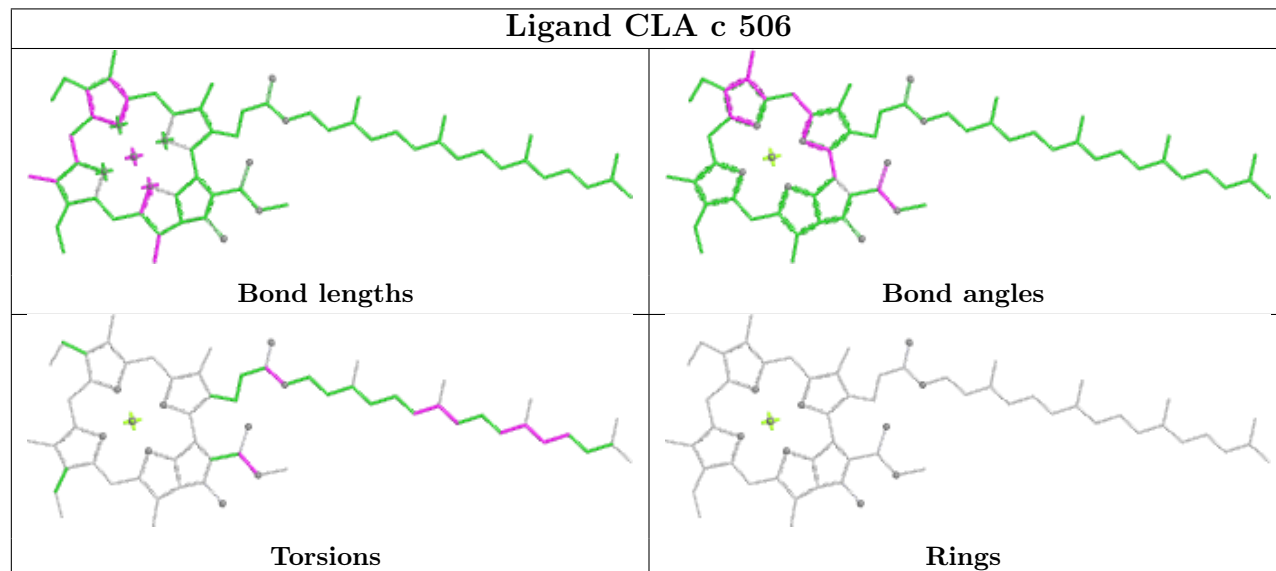
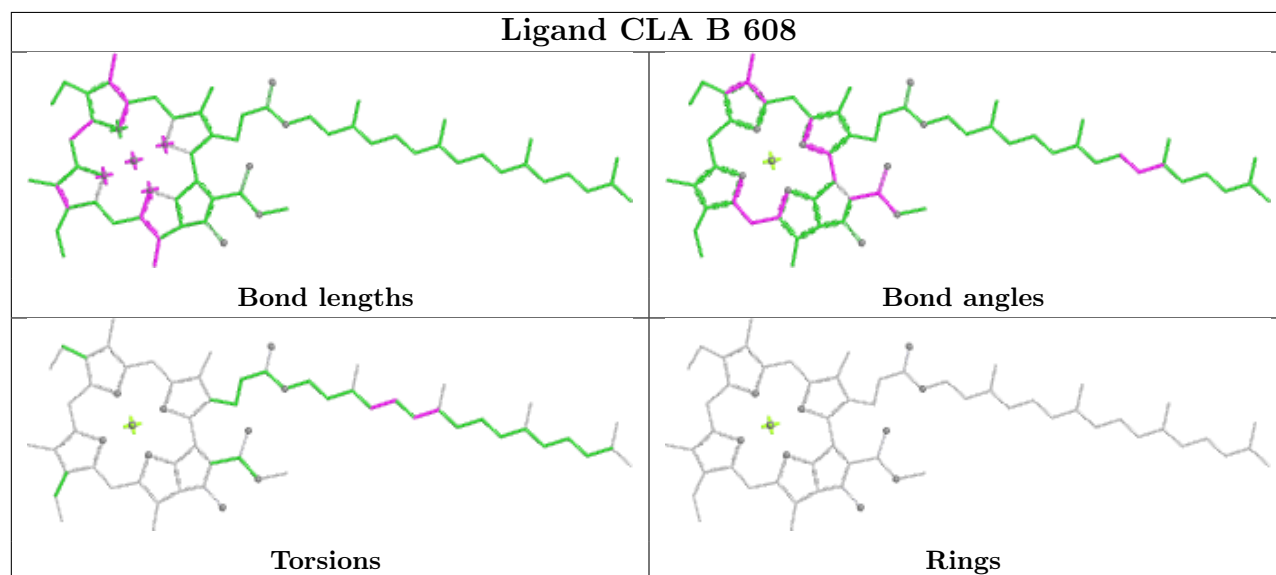
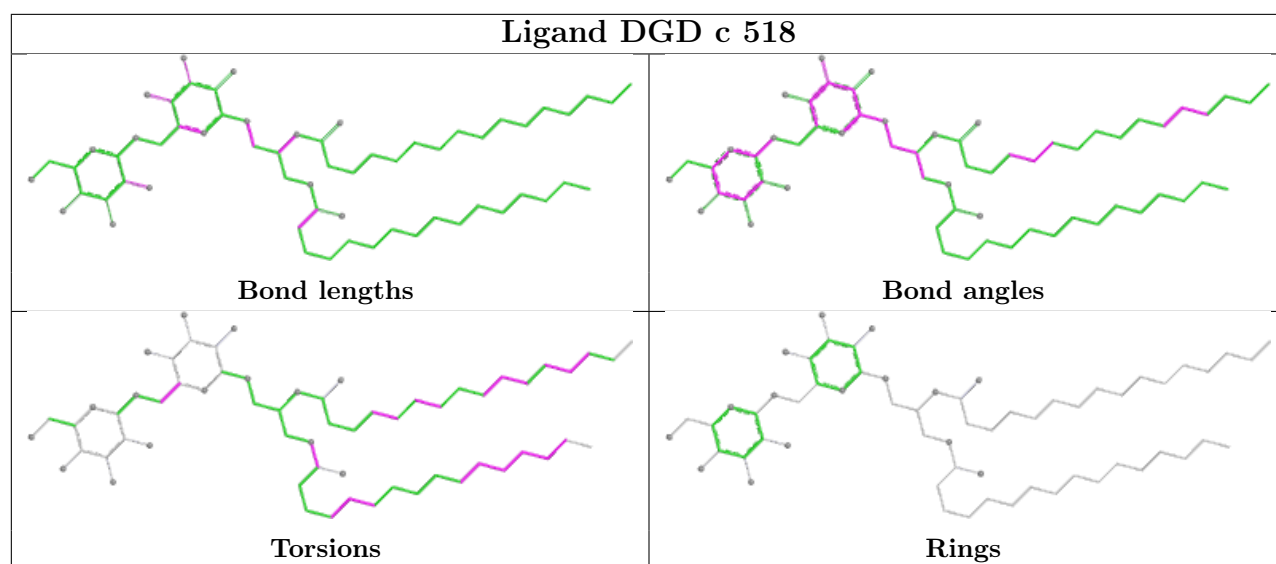
Ligand CLA C 507



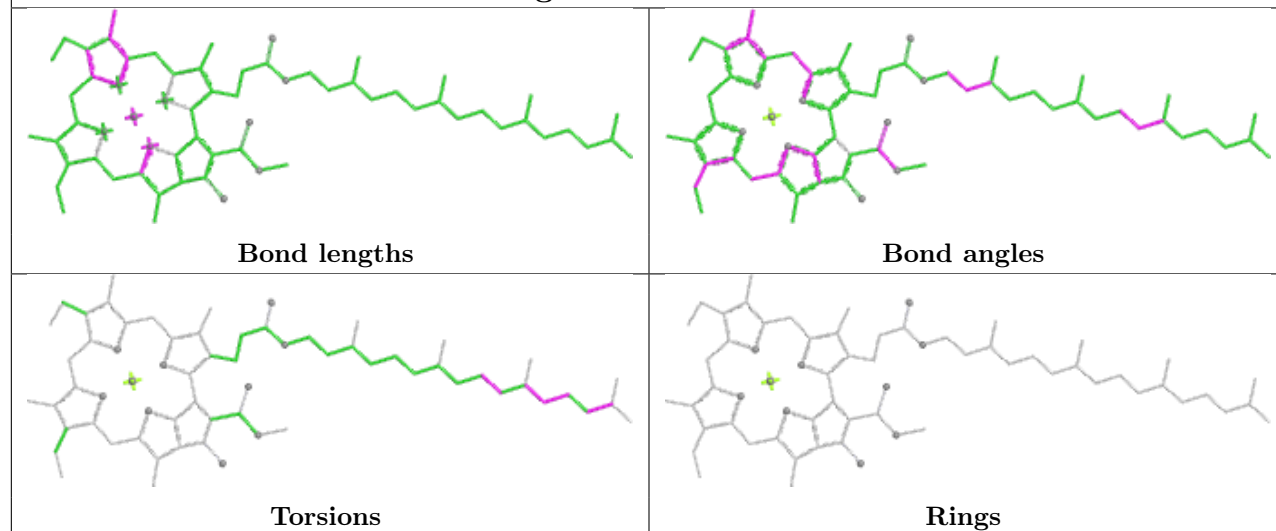
Ligand CLA C 501



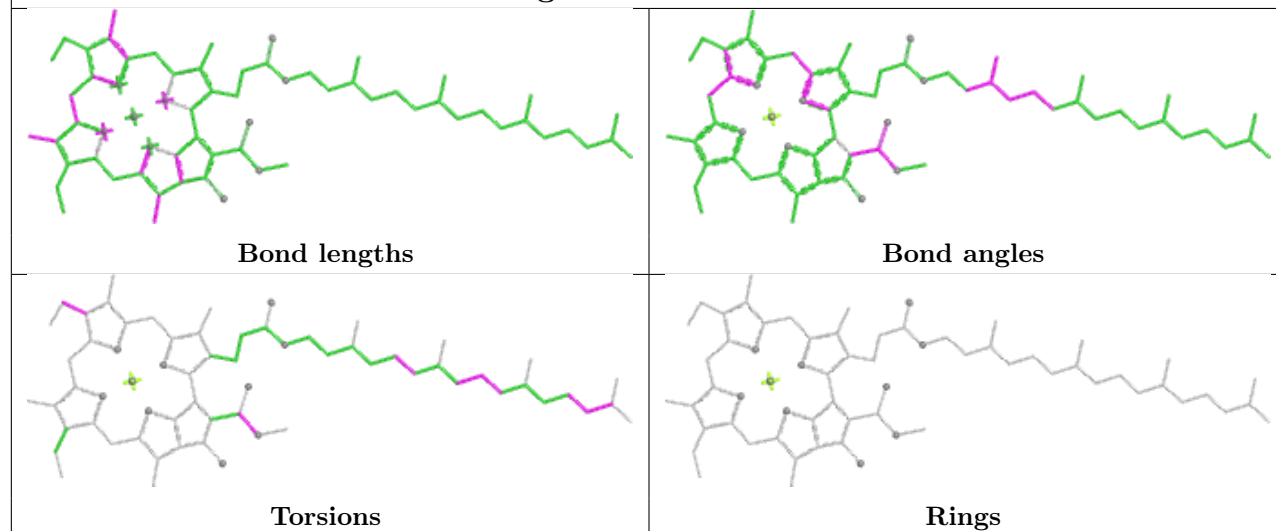




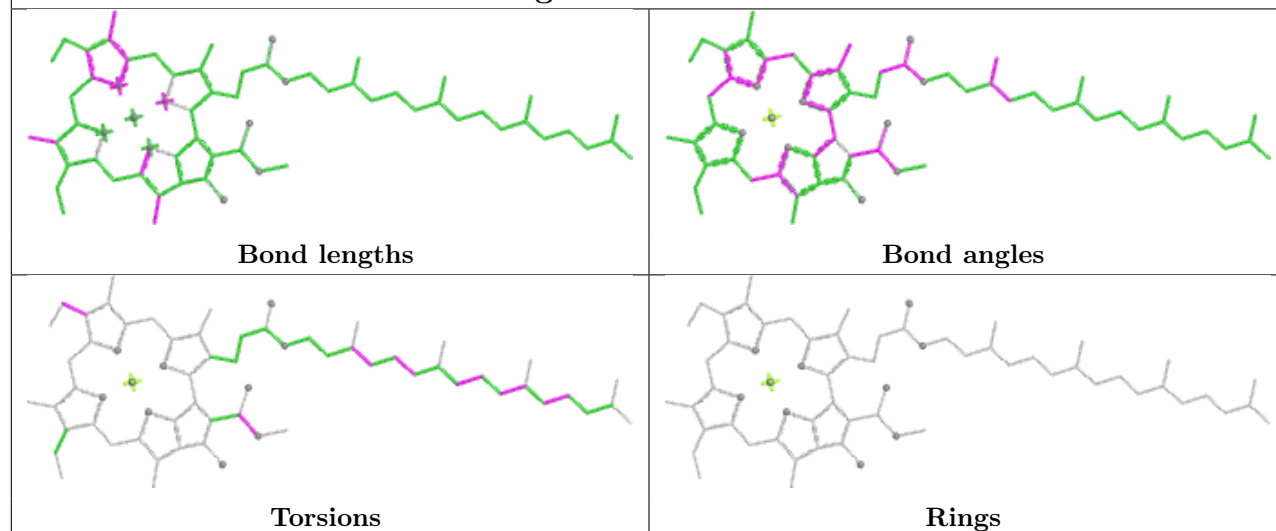
Ligand CLA b 612



Ligand CLA c 503



Ligand CLA b 603



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.58	0 100 100	23, 31, 52, 80	0
1	a	334/344 (97%)	-0.49	3 (0%) 81 83	22, 33, 60, 76	0
2	B	505/510 (99%)	-0.42	4 (0%) 82 84	18, 35, 63, 92	4 (0%)
2	b	505/510 (99%)	-0.27	6 (1%) 76 78	24, 39, 72, 109	0
3	C	442/461 (95%)	-0.39	0 100 100	16, 38, 54, 83	1 (0%)
3	c	451/461 (97%)	-0.26	3 (0%) 84 86	20, 42, 62, 92	2 (0%)
4	D	341/352 (96%)	-0.57	1 (0%) 90 91	22, 32, 51, 84	0
4	d	341/352 (96%)	-0.41	0 100 100	23, 36, 58, 86	1 (0%)
5	E	82/84 (97%)	0.15	2 (2%) 59 62	31, 55, 72, 78	1 (1%)
5	e	82/84 (97%)	0.25	1 (1%) 76 78	42, 63, 79, 91	0
6	F	34/45 (75%)	-0.07	0 100 100	37, 45, 70, 93	0
6	f	34/45 (75%)	0.08	0 100 100	45, 53, 84, 96	0
7	H	65/66 (98%)	-0.25	2 (3%) 51 53	32, 43, 61, 73	0
7	h	63/66 (95%)	0.02	2 (3%) 50 52	43, 52, 62, 76	0
8	I	35/38 (92%)	-0.38	0 100 100	31, 40, 68, 84	0
8	i	35/38 (92%)	-0.21	0 100 100	33, 42, 78, 84	0
9	J	36/40 (90%)	-0.00	0 100 100	36, 52, 82, 96	0
9	j	36/40 (90%)	0.18	1 (2%) 55 57	41, 55, 89, 101	0
10	K	37/46 (80%)	-0.01	0 100 100	44, 55, 74, 77	0
10	k	37/46 (80%)	0.18	0 100 100	48, 59, 72, 78	0
11	L	37/37 (100%)	-0.64	0 100 100	25, 32, 65, 71	0
11	l	36/37 (97%)	-0.56	0 100 100	26, 32, 72, 86	0
12	M	32/36 (88%)	-0.55	0 100 100	27, 36, 56, 69	0
12	m	31/36 (86%)	-0.54	0 100 100	28, 36, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.27	2 (0%) 82 84	25, 42, 79, 134	1 (0%)
13	o	244/272 (89%)	-0.24	1 (0%) 88 90	23, 42, 81, 114	0
14	R	28/41 (68%)	0.81	1 (3%) 46 48	60, 76, 85, 102	0
14	r	28/41 (68%)	1.45	5 (17%) 3 4	68, 98, 119, 133	0
15	T	29/32 (90%)	-0.60	0 100 100	27, 33, 60, 76	0
15	t	29/32 (90%)	-0.45	1 (3%) 48 50	27, 34, 75, 94	0
16	U	97/134 (72%)	-0.26	0 100 100	31, 44, 68, 89	0
16	u	97/134 (72%)	-0.32	0 100 100	31, 42, 58, 81	0
17	V	137/163 (84%)	-0.38	0 100 100	31, 42, 58, 73	0
17	v	137/163 (84%)	-0.12	0 100 100	33, 49, 69, 87	0
18	X	38/41 (92%)	-0.10	0 100 100	41, 53, 72, 82	0
18	x	39/41 (95%)	0.22	2 (5%) 33 35	48, 62, 91, 107	0
19	Y	27/46 (58%)	0.96	2 (7%) 20 22	54, 75, 91, 101	0
19	y	30/46 (65%)	0.74	1 (3%) 49 51	62, 75, 90, 101	0
20	Z	62/62 (100%)	0.71	3 (4%) 35 37	55, 72, 119, 128	0
20	z	62/62 (100%)	0.65	1 (1%) 70 73	61, 75, 108, 125	0
All	All	5293/5700 (92%)	-0.28	44 (0%) 82 84	16, 40, 75, 134	10 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.7
15	t	30	THR	3.9
18	x	40	SER	3.5
20	Z	62	VAL	3.4
20	z	33	TRP	3.3
2	b	495	PHE	3.1
19	Y	22	LEU	3.0
14	r	20	VAL	3.0
2	b	486	LEU	2.9
13	O	60	ARG	2.9
9	j	6	GLY	2.9
14	r	14	LEU	2.9
7	H	41	PHE	2.8
2	b	499	VAL	2.7
13	O	59	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	495	PHE	2.6
7	h	64	ALA	2.6
19	Y	25	ILE	2.5
2	B	479[A]	PHE	2.5
5	e	79	PHE	2.5
2	b	488	PRO	2.5
20	Z	33	TRP	2.4
14	r	18	TRP	2.4
14	r	19	ALA	2.4
1	a	249	VAL	2.3
7	h	41	PHE	2.3
2	B	499	VAL	2.3
3	c	134	ILE	2.3
19	y	42	ARG	2.3
5	E	79	PHE	2.2
18	x	37	VAL	2.2
7	H	65	LEU	2.2
14	R	29	LYS	2.2
5	E	74	GLN	2.2
2	B	127	ARG	2.2
1	a	250	ALA	2.1
2	b	490	GLN	2.1
20	Z	34	ASP	2.1
1	a	248	ILE	2.1
3	c	147	PHE	2.1
14	r	3	TRP	2.1
3	c	23	ALA	2.1
4	D	12	ARG	2.0
2	b	84	THR	2.0

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

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	0.95	0.07	40,48,60,60	0
15	FME	T	1	10/11	0.95	0.08	27,46,62,62	0
15	FME	t	1	10/11	0.95	0.07	29,43,65,65	0
12	FME	m	1	10/11	0.96	0.07	35,43,58,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	i	1	10/11	0.96	0.10	39,48,60,60	0
12	FME	M	1	10/11	0.96	0.08	39,53,66,71	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	STE	b	626	10/20	0.74	0.20	45,57,66,79	0
32	STE	b	625	20/20	0.76	0.17	45,67,80,91	0
32	STE	I	101	15/20	0.76	0.19	43,60,76,80	0
26	PL9	a	409	55/55	0.77	0.18	44,72,88,94	0
29	LHG	A	413	49/49	0.77	0.15	48,83,110,124	0
32	STE	E	101	12/20	0.77	0.18	52,76,90,92	0
32	STE	m	102	12/20	0.78	0.19	49,64,81,90	0
32	STE	j	101	12/20	0.79	0.14	42,57,69,72	0
27	LMG	h	102	23/55	0.79	0.19	47,65,83,88	0
32	STE	c	522	12/20	0.80	0.13	58,71,85,89	0
26	PL9	A	410	55/55	0.80	0.16	46,66,88,93	0
29	LHG	e	101	42/49	0.80	0.15	64,84,110,118	0
32	STE	a	415	12/20	0.81	0.14	45,68,76,82	0
32	STE	C	519	16/20	0.81	0.14	45,58,76,76	0
32	STE	a	413	10/20	0.81	0.15	40,65,68,69	0
32	STE	H	103	18/20	0.82	0.18	54,82,92,98	0
32	STE	B	625	16/20	0.82	0.14	37,64,85,88	0
32	STE	B	627	16/20	0.82	0.19	39,47,69,72	0
27	LMG	c	521	48/55	0.83	0.15	50,77,103,106	0
27	LMG	b	623	55/55	0.84	0.15	46,71,92,102	0
32	STE	d	412	20/20	0.84	0.13	47,65,79,80	0
30	DGD	o	301	44/66	0.84	0.14	38,58,81,95	0
22	CLA	b	601	65/65	0.84	0.12	46,66,84,89	0
32	STE	b	621	16/20	0.85	0.14	41,52,70,71	0
32	STE	b	622	20/20	0.85	0.12	37,59,81,84	0
32	STE	D	413	15/20	0.85	0.17	33,40,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	SQD	a	412	36/54	0.85	0.14	32,66,92,99	0
27	LMG	D	410	32/55	0.86	0.13	36,58,75,85	0
28	SQD	f	102	41/54	0.86	0.14	57,92,112,114	0
32	STE	T	102	15/20	0.86	0.14	52,65,79,81	0
32	STE	b	624	16/20	0.86	0.14	44,61,82,89	0
30	DGD	A	415	66/66	0.86	0.11	47,63,79,89	0
27	LMG	A	411	48/55	0.87	0.11	43,58,72,79	0
32	STE	c	520	20/20	0.87	0.12	43,58,91,99	0
28	SQD	A	414	39/54	0.87	0.13	44,62,91,95	0
32	STE	d	411	17/20	0.87	0.13	44,57,65,77	0
32	STE	J	101	12/20	0.87	0.12	46,58,69,77	0
32	STE	B	620	17/20	0.87	0.11	35,52,71,82	0
27	LMG	Y	101	48/55	0.87	0.12	32,67,84,92	0
32	STE	M	103	10/20	0.88	0.13	36,47,60,69	0
32	STE	B	626	12/20	0.88	0.14	57,69,80,85	0
28	SQD	b	620	49/54	0.88	0.10	43,59,84,98	0
32	STE	B	623	12/20	0.88	0.11	37,49,69,82	0
24	BCR	K	101	40/40	0.88	0.12	44,58,74,78	0
28	SQD	B	621	54/54	0.89	0.10	42,65,90,100	0
32	STE	M	104	18/20	0.89	0.11	35,52,79,82	0
27	LMG	c	519	37/55	0.89	0.11	40,63,78,78	0
32	STE	B	624	18/20	0.89	0.10	38,60,76,78	0
24	BCR	k	101	40/40	0.90	0.10	43,60,72,77	0
32	STE	C	520	12/20	0.90	0.10	35,49,59,59	0
27	LMG	m	101	51/55	0.90	0.10	35,54,76,95	0
22	CLA	B	601	65/65	0.90	0.10	32,62,87,99	0
27	LMG	a	414	49/55	0.90	0.10	30,59,83,100	0
32	STE	B	622	14/20	0.90	0.10	39,49,62,66	0
32	STE	C	518	12/20	0.90	0.11	45,56,65,67	0
32	STE	M	102	15/20	0.90	0.12	33,50,71,73	0
30	DGD	C	516	62/66	0.91	0.10	31,52,95,110	0
28	SQD	F	102	36/54	0.91	0.11	45,74,95,99	0
24	BCR	c	514	40/40	0.91	0.10	41,60,71,72	0
24	BCR	h	101	40/40	0.91	0.09	34,52,73,80	0
32	STE	D	412	20/20	0.91	0.10	36,52,75,78	0
27	LMG	M	101	51/55	0.91	0.09	32,49,73,81	0
22	CLA	c	512	65/65	0.91	0.10	38,54,82,93	0
22	CLA	C	513	65/65	0.91	0.10	39,61,91,95	0
24	BCR	K	102	40/40	0.91	0.09	36,54,68,73	0
30	DGD	H	102	62/66	0.92	0.09	30,47,59,66	0
30	DGD	h	103	62/66	0.92	0.09	27,47,63,72	0
22	CLA	c	513	65/65	0.92	0.10	39,65,104,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	B	618	40/40	0.92	0.07	23,39,49,53	0
24	BCR	D	405	40/40	0.92	0.10	23,46,83,85	0
24	BCR	d	406	40/40	0.92	0.11	30,52,86,93	0
24	BCR	H	101	40/40	0.93	0.08	33,48,66,72	0
24	BCR	K	103	40/40	0.93	0.10	37,51,65,66	0
29	LHG	d	409	39/49	0.93	0.09	28,41,68,74	0
24	BCR	T	101	40/40	0.93	0.07	25,37,49,51	0
28	SQD	a	411	54/54	0.93	0.10	40,62,96,97	0
24	BCR	C	514	40/40	0.93	0.09	25,39,50,58	0
24	BCR	c	515	40/40	0.93	0.09	25,44,55,64	0
22	CLA	C	503	65/65	0.94	0.07	31,41,50,62	0
24	BCR	A	407	40/40	0.94	0.07	25,35,44,44	0
22	CLA	C	510	65/65	0.94	0.07	25,43,59,61	0
24	BCR	b	617	40/40	0.94	0.07	24,41,52,54	0
24	BCR	b	618	40/40	0.94	0.07	23,39,52,56	0
24	BCR	b	619	40/40	0.94	0.07	31,46,61,65	0
24	BCR	B	619	40/40	0.94	0.07	27,43,59,67	0
22	CLA	c	505	65/65	0.94	0.08	24,40,64,67	0
29	LHG	D	409	47/49	0.94	0.10	24,51,77,89	0
29	LHG	a	410	49/49	0.94	0.10	32,52,70,77	0
22	CLA	c	509	65/65	0.94	0.08	31,47,67,72	0
22	CLA	c	511	65/65	0.94	0.09	37,52,68,71	0
27	LMG	d	410	44/55	0.94	0.09	32,54,88,100	0
22	CLA	C	512	65/65	0.94	0.09	35,53,82,90	0
24	BCR	k	102	40/40	0.94	0.09	42,53,69,69	0
30	DGD	c	517	62/66	0.94	0.08	30,50,87,88	0
28	SQD	A	412	52/54	0.94	0.09	35,58,85,88	0
22	CLA	C	509	65/65	0.95	0.08	25,46,61,69	0
27	LMG	D	407	51/55	0.95	0.09	23,55,83,89	0
22	CLA	d	405	65/65	0.95	0.09	29,48,81,89	0
23	PHO	d	401	64/64	0.95	0.07	23,38,47,59	0
22	CLA	B	615	65/65	0.95	0.07	20,37,57,63	0
24	BCR	B	617	40/40	0.95	0.06	26,38,56,56	0
22	CLA	C	511	65/65	0.95	0.08	28,48,63,72	0
22	CLA	B	616	60/65	0.95	0.10	25,38,88,95	0
22	CLA	C	502	65/65	0.95	0.07	27,40,52,54	0
22	CLA	a	403	65/65	0.95	0.09	24,41,88,95	0
22	CLA	B	606	65/65	0.95	0.07	23,36,64,71	0
22	CLA	b	606	65/65	0.95	0.08	23,39,67,75	0
22	CLA	b	609	65/65	0.95	0.08	29,44,61,69	0
22	CLA	b	614	65/65	0.95	0.07	23,39,71,79	0
22	CLA	b	615	65/65	0.95	0.07	25,39,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	a	406	40/40	0.95	0.06	19,33,49,50	0
22	CLA	b	616	60/65	0.95	0.08	26,43,84,91	0
22	CLA	c	503	65/65	0.95	0.07	32,42,53,59	0
22	CLA	c	504	60/65	0.95	0.07	29,44,74,85	0
22	CLA	C	504	59/65	0.95	0.07	30,42,77,79	0
22	CLA	c	506	65/65	0.95	0.09	31,49,95,99	0
22	CLA	c	507	65/65	0.95	0.08	29,44,58,67	0
29	LHG	D	411	49/49	0.95	0.08	30,45,61,73	0
22	CLA	c	508	64/65	0.95	0.08	29,44,87,101	0
22	CLA	C	505	65/65	0.95	0.08	20,40,69,72	0
22	CLA	c	510	65/65	0.95	0.07	30,47,62,65	0
24	BCR	t	101	40/40	0.95	0.06	26,37,50,54	0
30	DGD	C	515	62/66	0.95	0.10	18,39,69,77	0
22	CLA	C	506	65/65	0.95	0.09	28,45,78,89	0
30	DGD	C	517	62/66	0.95	0.08	26,47,73,79	0
26	PL9	D	406	55/55	0.95	0.06	21,33,47,53	0
22	CLA	C	508	65/65	0.95	0.07	26,42,91,97	0
30	DGD	c	518	62/66	0.95	0.08	26,52,78,83	0
26	PL9	d	407	55/55	0.95	0.06	22,34,41,47	0
22	CLA	b	608	65/65	0.96	0.07	23,42,61,66	0
22	CLA	B	609	65/65	0.96	0.07	26,38,59,66	0
22	CLA	b	610	65/65	0.96	0.08	24,37,50,55	0
22	CLA	b	611	65/65	0.96	0.06	19,35,52,60	0
22	CLA	b	612	65/65	0.96	0.07	17,34,48,58	0
22	CLA	b	613	65/65	0.96	0.07	19,35,66,78	0
22	CLA	B	610	65/65	0.96	0.07	19,33,44,50	0
22	CLA	C	507	65/65	0.96	0.07	21,39,57,60	0
22	CLA	B	611	65/65	0.96	0.06	20,31,51,54	0
22	CLA	c	501	65/65	0.96	0.06	28,40,52,55	0
22	CLA	c	502	65/65	0.96	0.07	30,42,59,62	0
22	CLA	B	612	65/65	0.96	0.07	21,32,45,58	0
22	CLA	B	614	65/65	0.96	0.08	20,37,67,77	0
22	CLA	A	402	65/65	0.96	0.06	17,27,45,49	0
22	CLA	B	604	65/65	0.96	0.07	19,32,70,84	0
22	CLA	C	501	65/65	0.96	0.06	19,35,46,56	0
22	CLA	a	402	65/65	0.96	0.06	20,30,42,55	0
22	CLA	B	605	65/65	0.96	0.07	18,31,47,49	0
29	LHG	L	101	49/49	0.96	0.07	26,43,57,64	0
22	CLA	a	405	65/65	0.96	0.08	18,37,74,82	0
22	CLA	A	403	65/65	0.96	0.08	22,34,95,103	0
22	CLA	b	602	65/65	0.96	0.08	26,43,62,65	0
29	LHG	l	101	49/49	0.96	0.07	25,46,58,60	0

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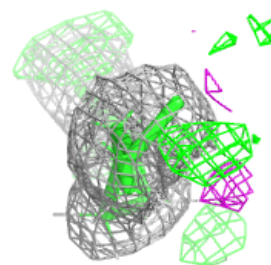
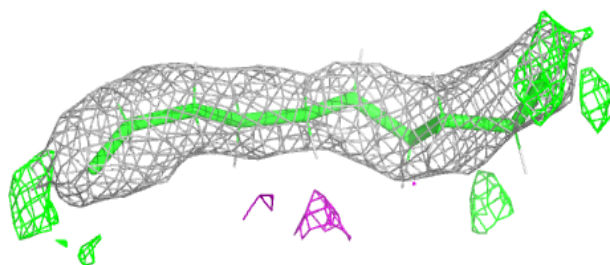
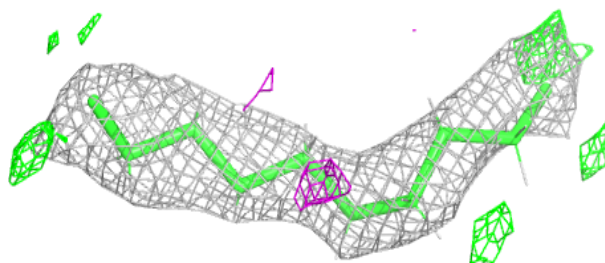
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	603	65/65	0.96	0.07	19,36,61,68	0
22	CLA	d	403	65/65	0.96	0.07	18,35,54,59	0
22	CLA	d	404	65/65	0.96	0.06	18,30,45,53	0
22	CLA	b	604	65/65	0.96	0.07	21,34,68,80	0
23	PHO	A	404	64/64	0.96	0.06	17,28,42,48	0
30	DGD	c	516	62/66	0.96	0.08	22,43,76,81	0
23	PHO	A	405	64/64	0.96	0.06	22,32,42,46	0
23	PHO	a	404	64/64	0.96	0.06	20,31,38,44	0
22	CLA	b	605	65/65	0.96	0.06	21,34,48,52	0
22	CLA	B	608	65/65	0.96	0.06	20,34,55,59	0
33	BCT	d	402	4/4	0.96	0.07	32,38,45,52	0
22	CLA	B	603	65/65	0.97	0.07	17,32,65,67	0
22	CLA	b	607	65/65	0.97	0.07	17,36,64,75	0
29	LHG	d	408	49/49	0.97	0.07	22,42,57,67	0
22	CLA	B	602	65/65	0.97	0.06	23,35,53,66	0
22	CLA	B	613	65/65	0.97	0.07	18,31,66,75	0
22	CLA	D	402	65/65	0.97	0.06	17,27,53,64	0
22	CLA	D	403	65/65	0.97	0.06	19,28,49,59	0
29	LHG	D	408	49/49	0.97	0.07	23,42,56,61	0
22	CLA	D	404	65/65	0.97	0.07	24,41,96,106	0
33	BCT	D	401	4/4	0.97	0.07	22,26,32,35	0
22	CLA	B	607	65/65	0.97	0.07	15,35,60,62	0
34	HEM	F	101	43/43	0.97	0.08	37,48,61,62	0
34	HEM	f	101	43/43	0.97	0.09	45,58,77,83	0
25	CL	a	408	1/1	0.98	0.09	28,28,28,28	0
22	CLA	A	406	54/65	0.98	0.05	19,31,64,72	0
35	HEC	V	201	43/43	0.98	0.06	20,34,42,43	0
35	HEC	v	201	43/43	0.98	0.06	28,36,49,53	0
31	OEX	a	416	10/10	0.99	0.03	25,26,31,31	0
21	FE2	a	401	1/1	0.99	0.03	35,35,35,35	0
25	CL	A	408	1/1	0.99	0.03	28,28,28,28	0
25	CL	a	407	1/1	0.99	0.03	28,28,28,28	0
21	FE2	A	401	1/1	0.99	0.02	26,26,26,26	0
25	CL	A	409	1/1	1.00	0.02	31,31,31,31	0
31	OEX	A	416	10/10	1.00	0.02	22,26,29,31	0

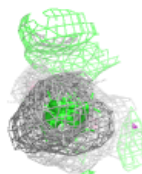
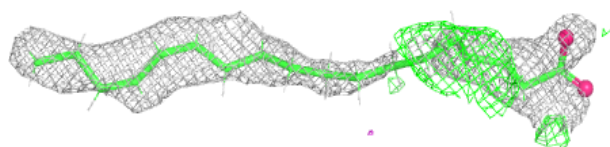
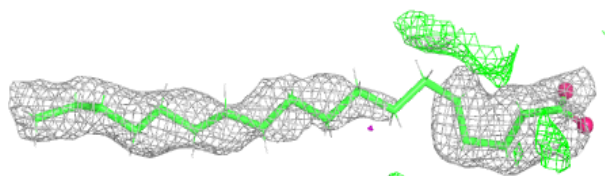
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE 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)

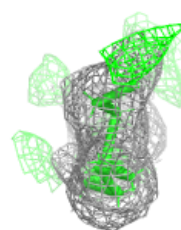
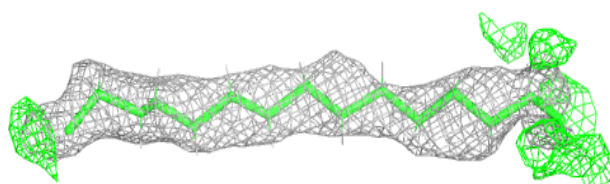
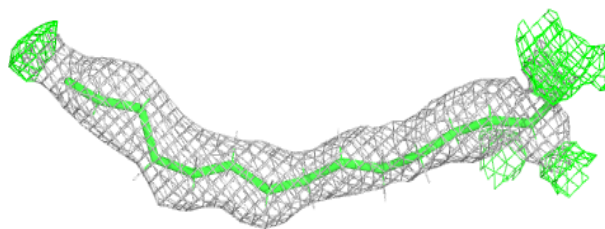
**Electron density around STE b 625:**

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

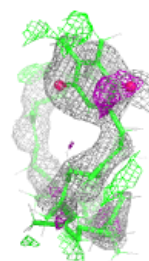
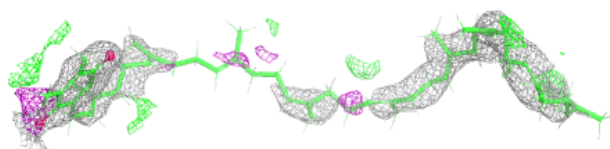
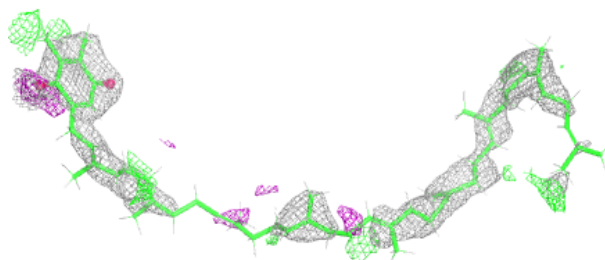


Electron density around STE I 101:

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

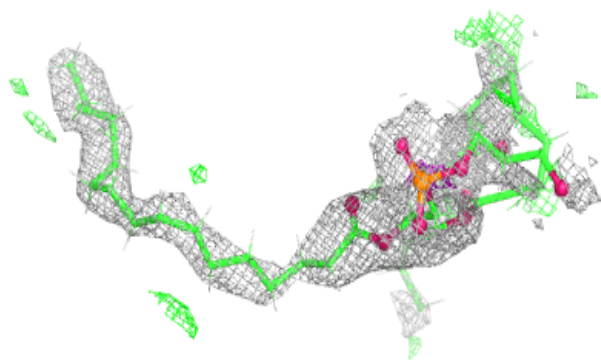
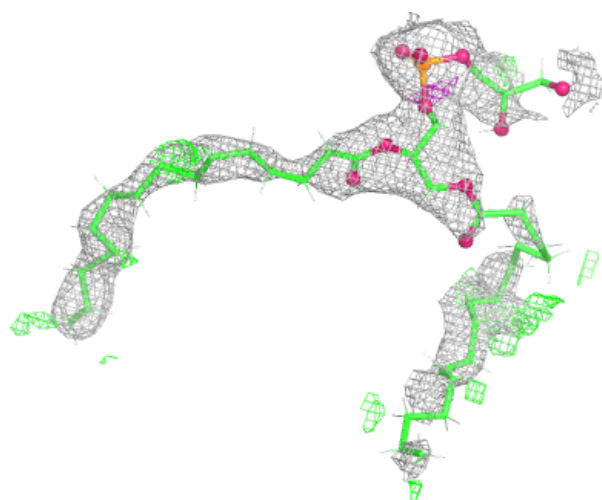
**Electron density around PL9 a 409:**

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



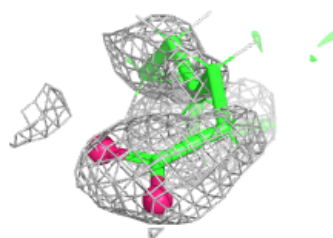
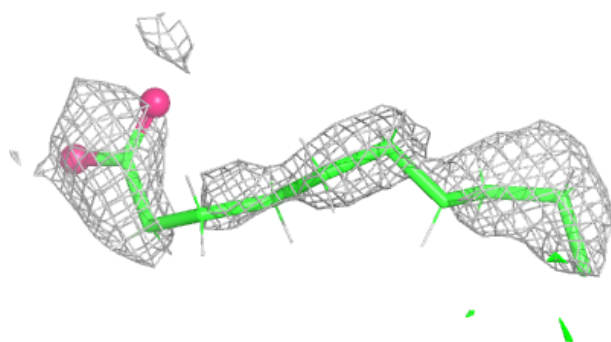
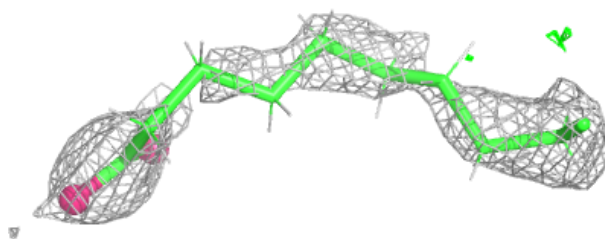
Electron density around LHG A 413:

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

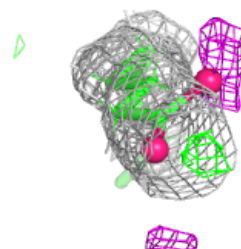
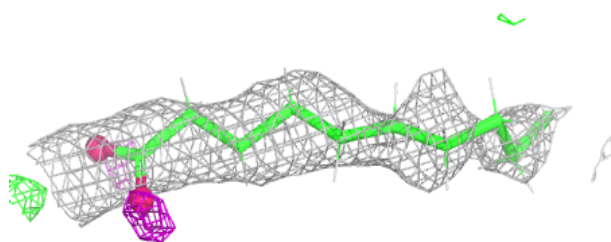
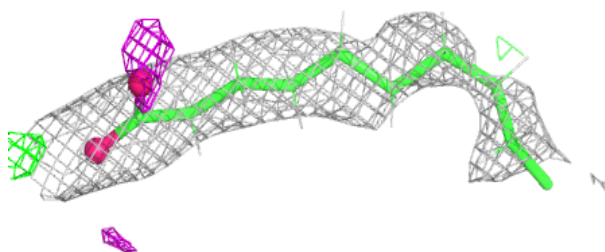


Electron density around STE E 101:

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

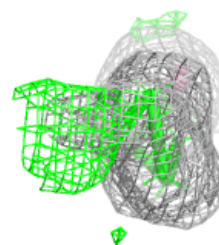
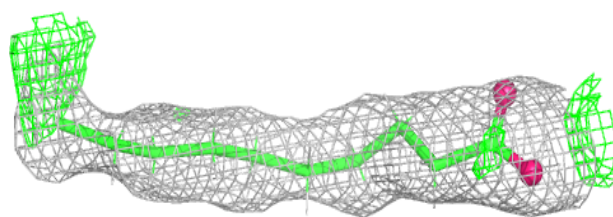
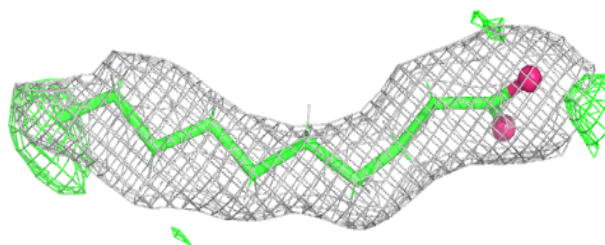
**Electron density around STE m 102:**

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

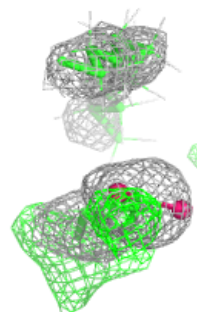
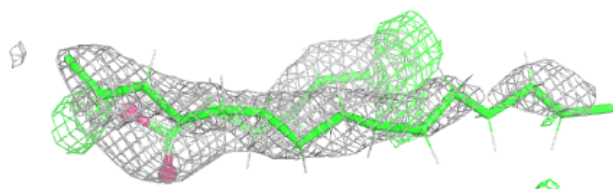
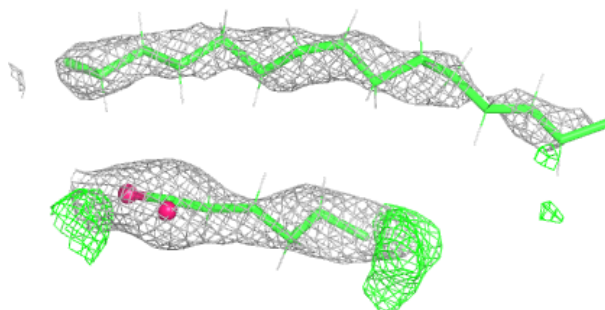


Electron density around STE j 101:

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and green (positive)

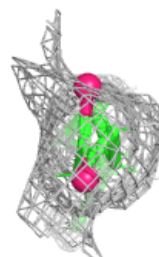
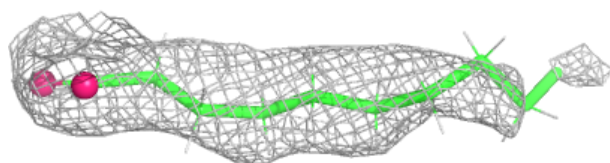
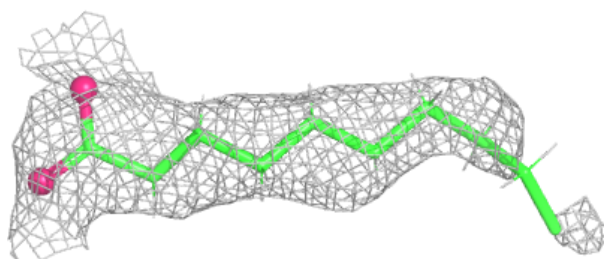
**Electron density around LMG h 102:**

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and green (positive)

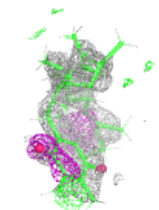
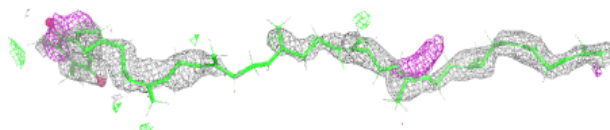
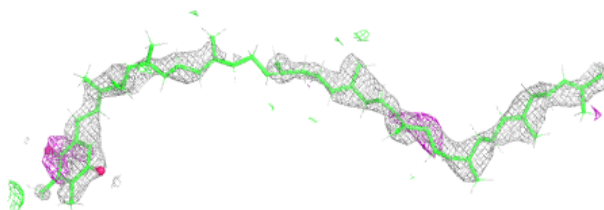


Electron density around STE c 522:

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and green (positive)

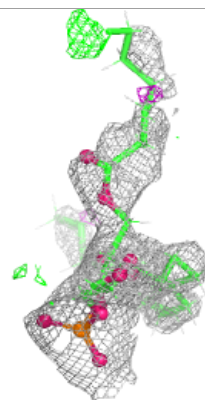
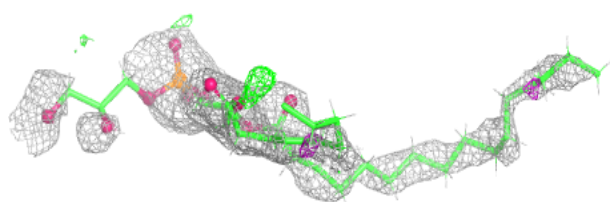
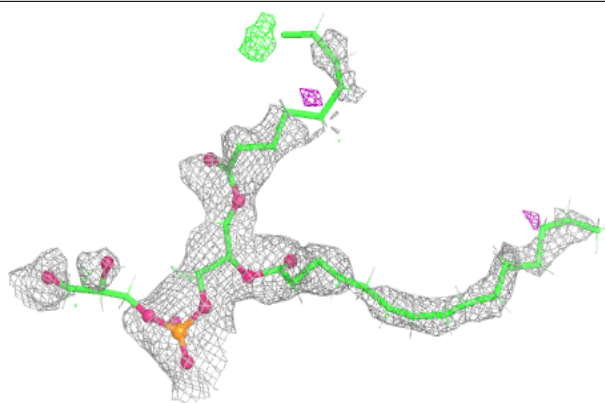
**Electron density around PL9 A 410:**

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and green (positive)

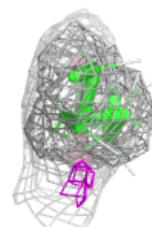
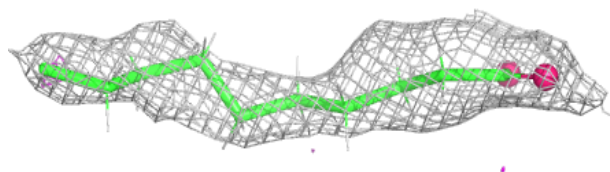
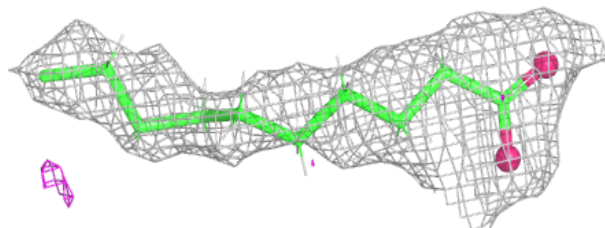


Electron density around LHG e 101:

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

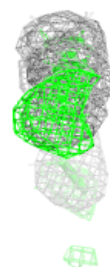
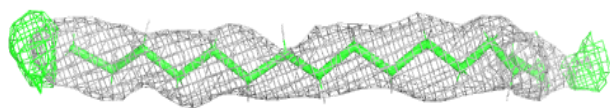
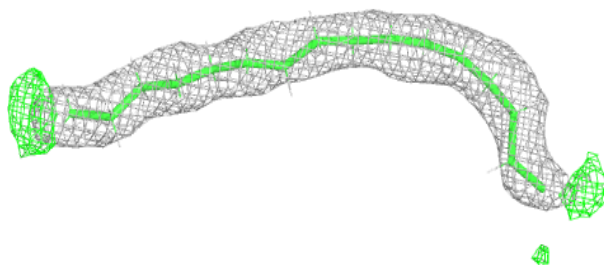
**Electron density around STE a 415:**

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

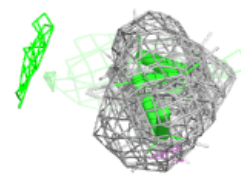
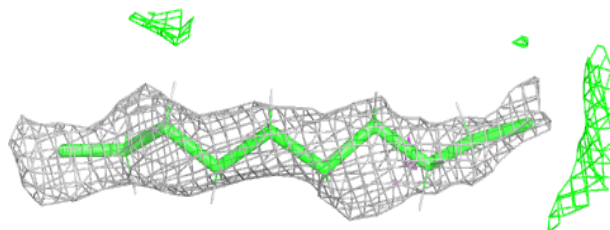
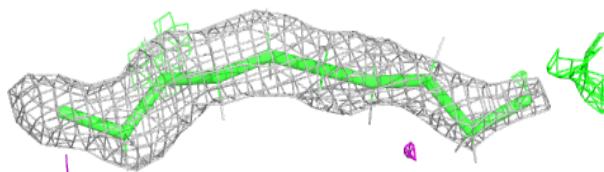


Electron density around STE C 519:

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

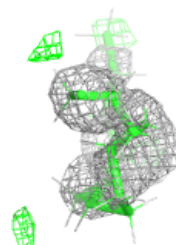
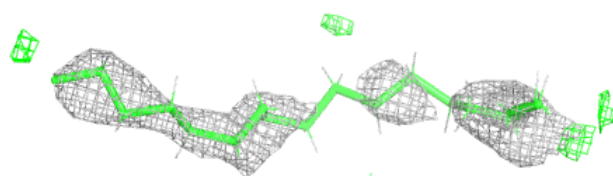
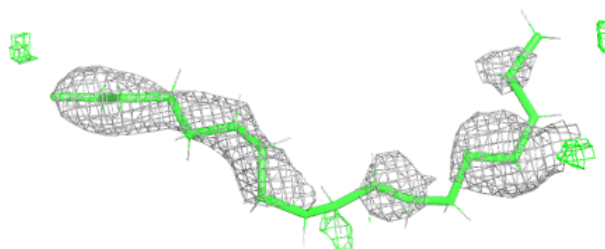
**Electron density around STE a 413:**

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

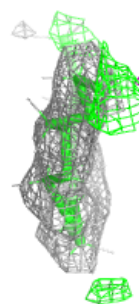
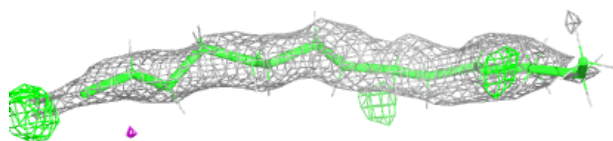


Electron density around STE H 103:

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

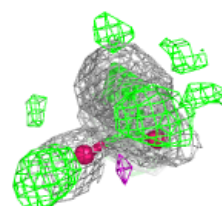
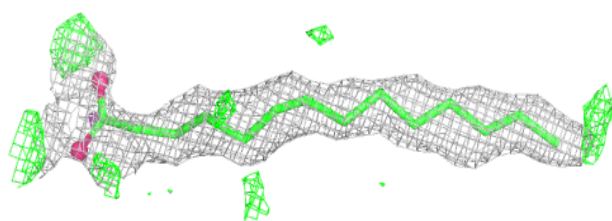
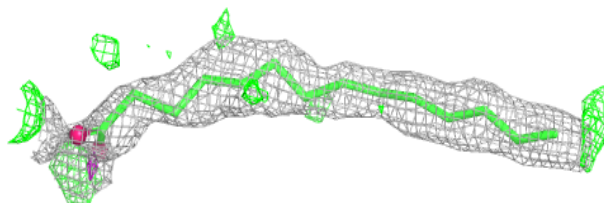
**Electron density around STE B 625:**

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

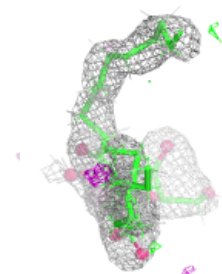
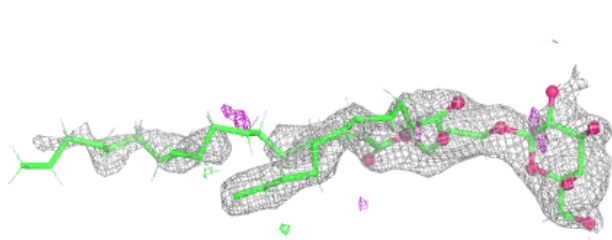
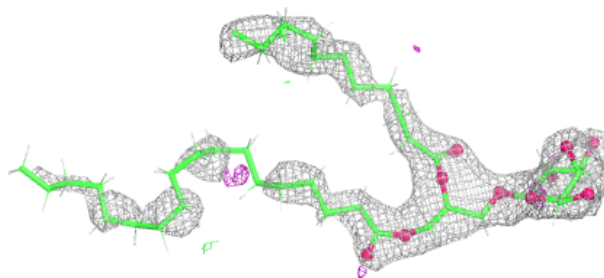


Electron density around STE B 627:

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

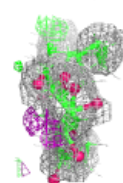
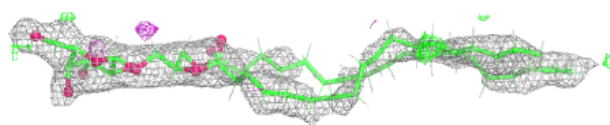
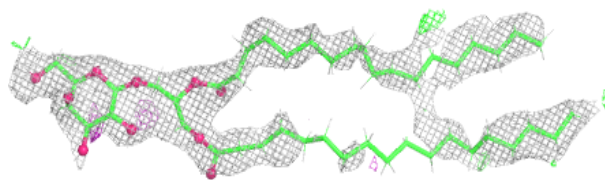
**Electron density around LMG c 521:**

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

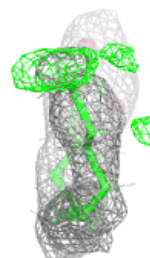
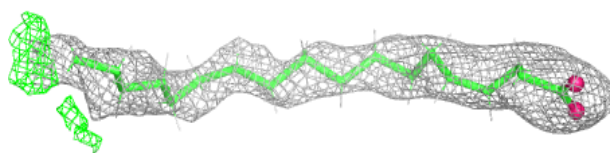
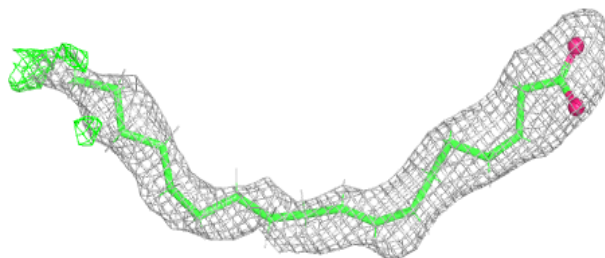


Electron density around LMG b 623:

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

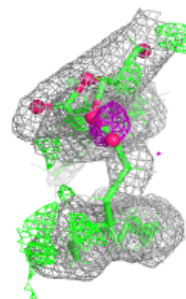
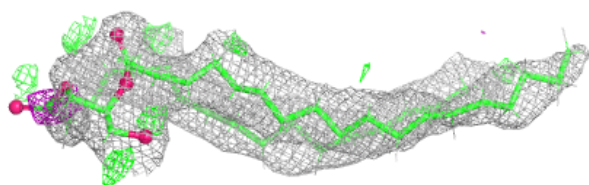
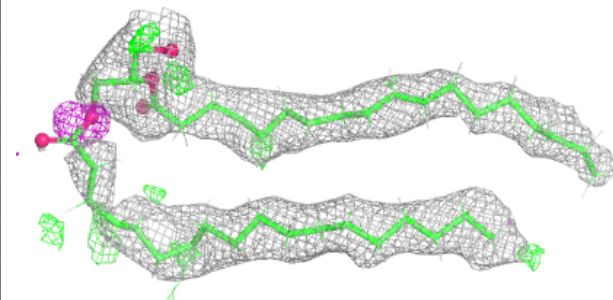
**Electron density around STE d 412:**

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



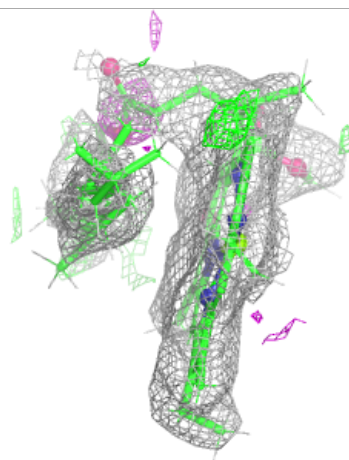
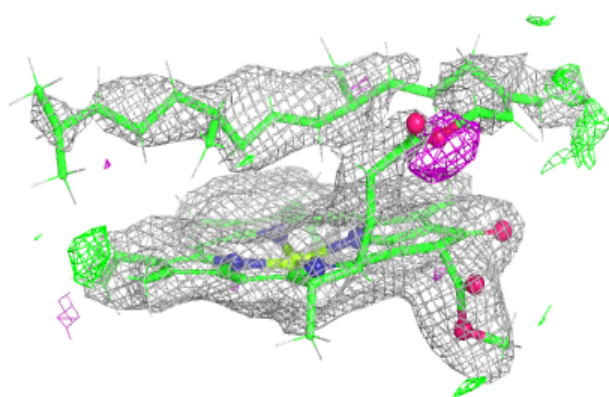
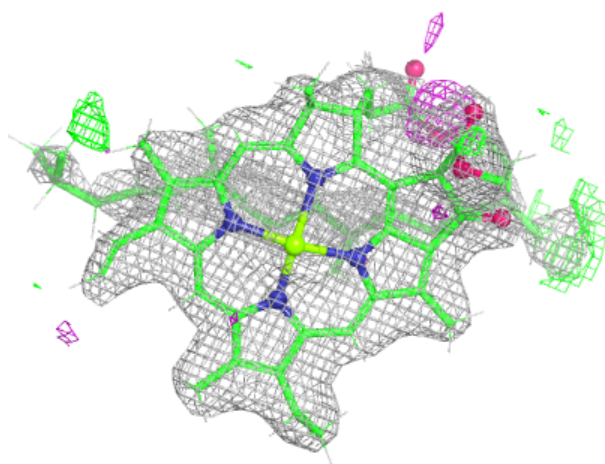
Electron density around DGD o 301:

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



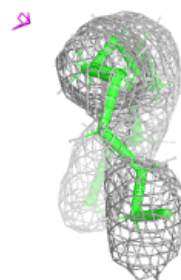
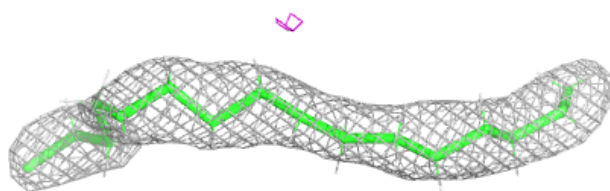
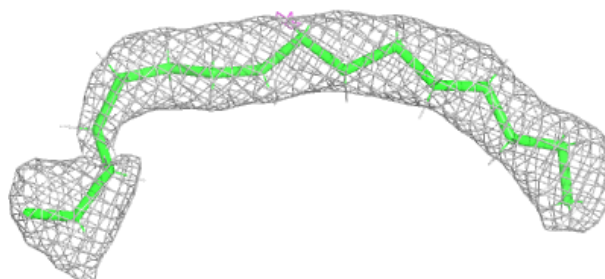
Electron density around CLA b 601:

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

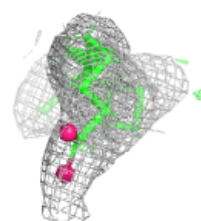
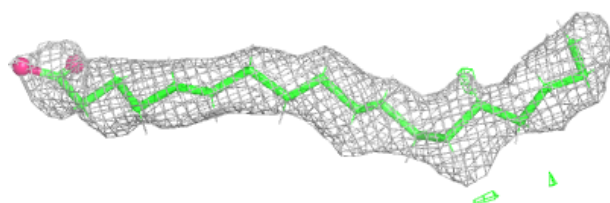
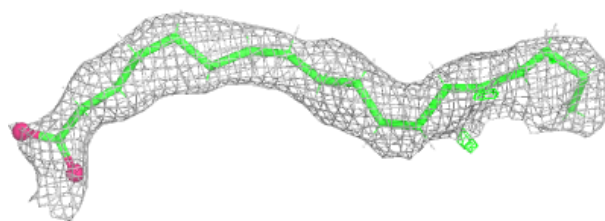


Electron density around STE b 621:

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

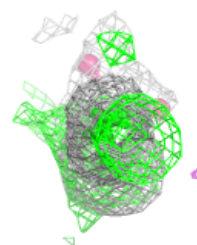
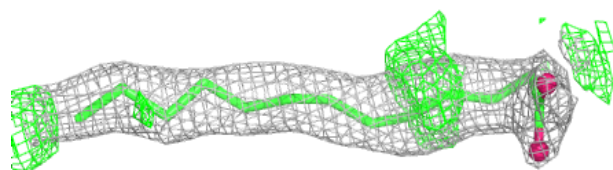
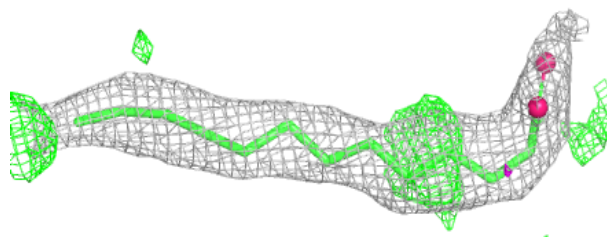
**Electron density around STE b 622:**

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

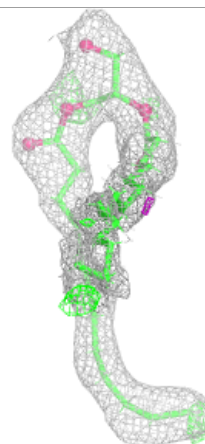
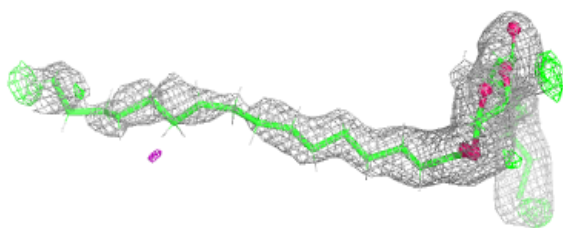
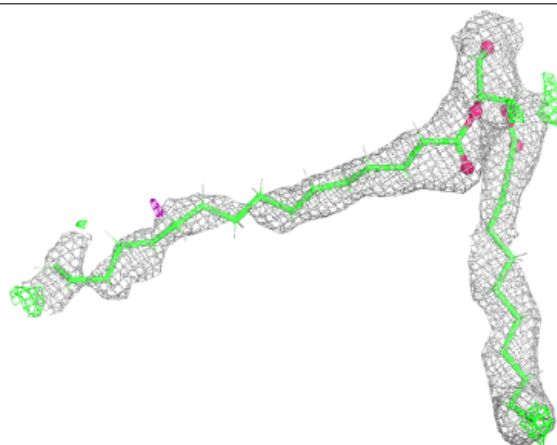


Electron density around STE D 413:

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

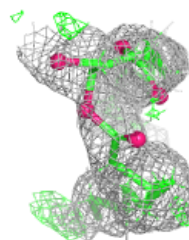
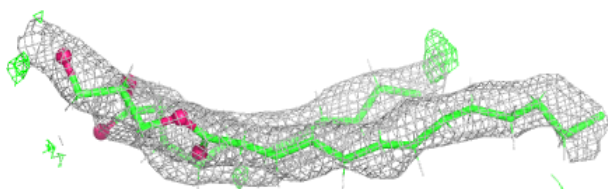
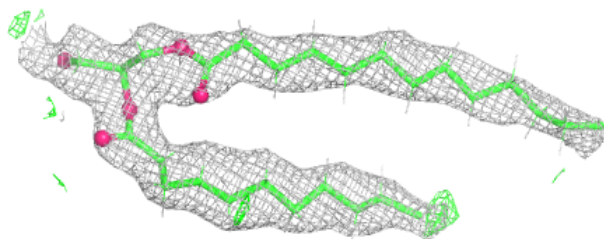
**Electron density around SQD a 412:**

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

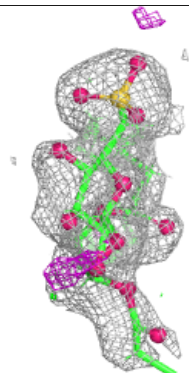
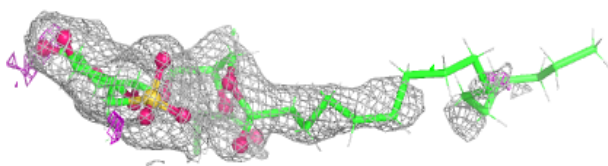
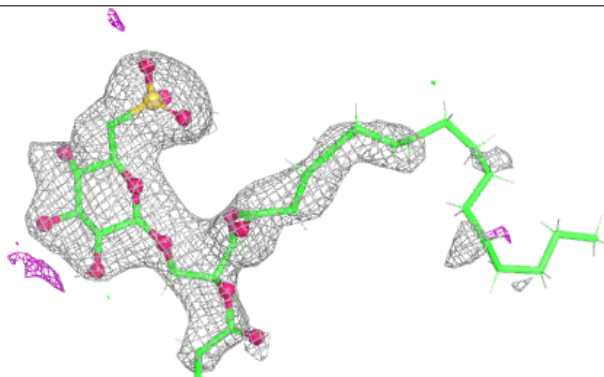


Electron density around LMG D 410:

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

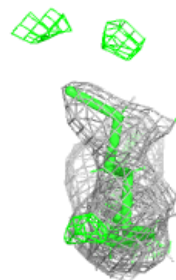
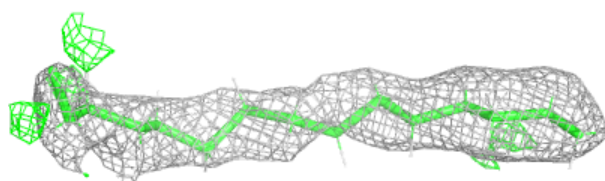
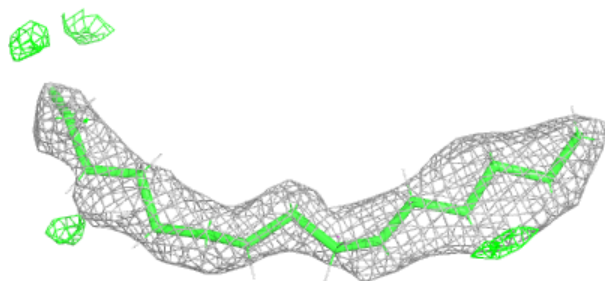
**Electron density around SQD f 102:**

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

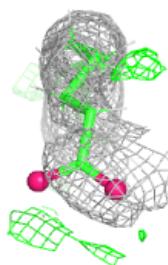
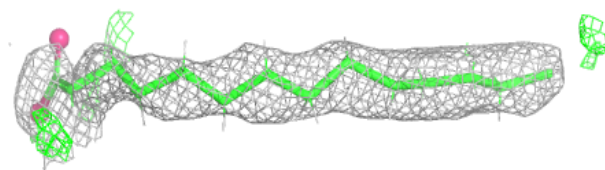
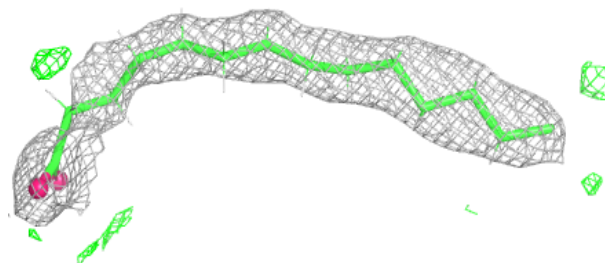


Electron density around STE T 102:

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

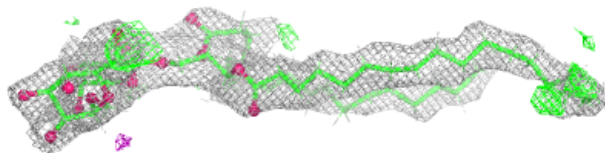
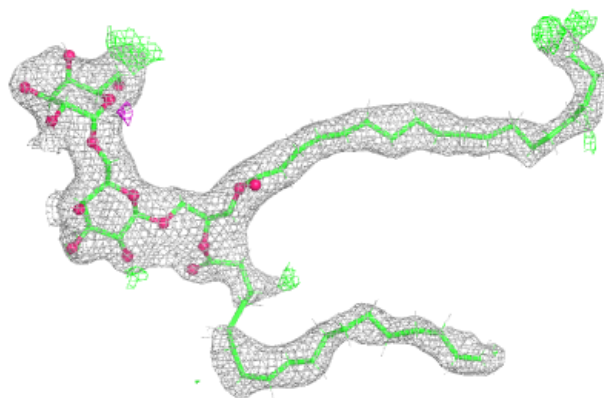
**Electron density around STE b 624:**

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

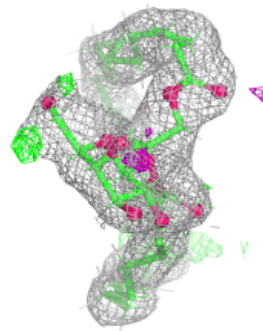
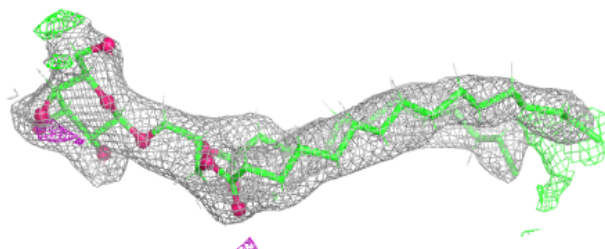
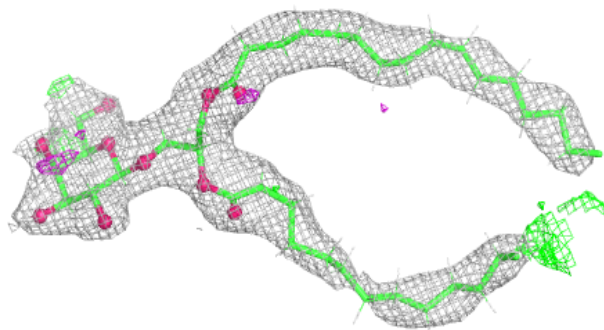


Electron density around DGD A 415:

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

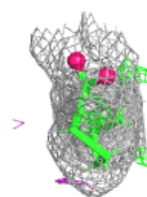
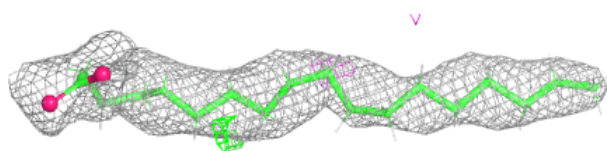
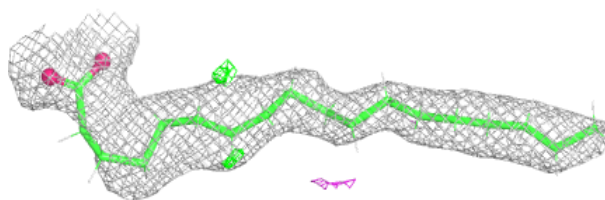
**Electron density around LMG A 411:**

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

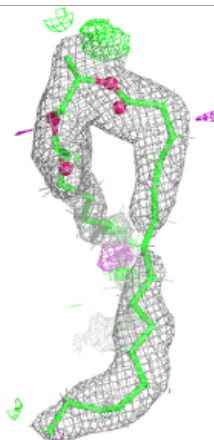
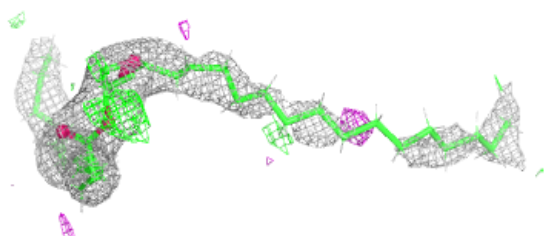
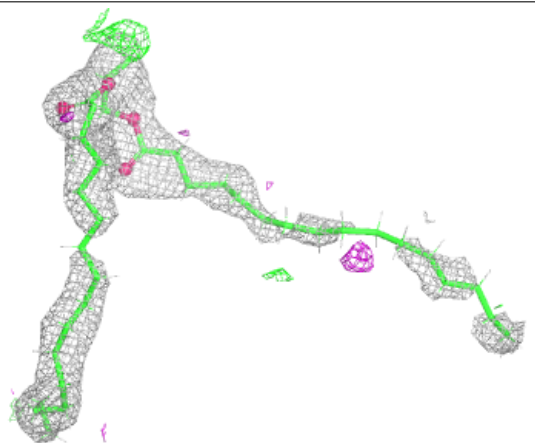


Electron density around STE c 520:

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

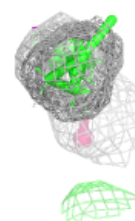
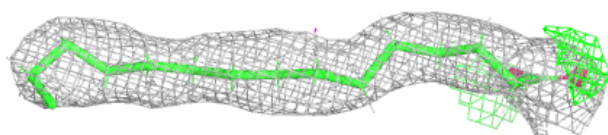
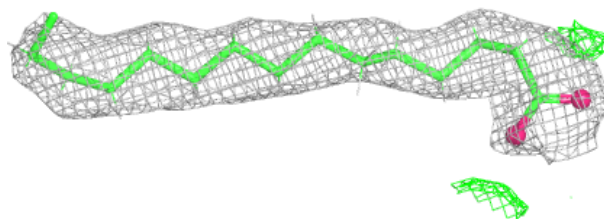
**Electron density around SQD A 414:**

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

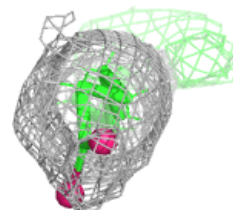
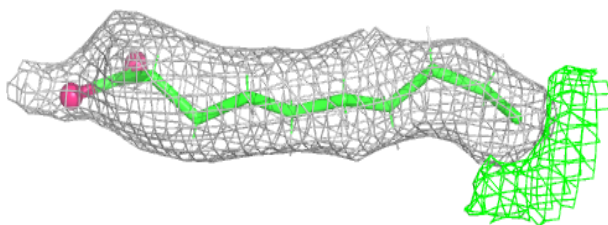
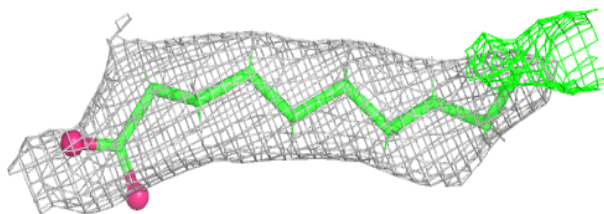


Electron density around STE d 411:

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

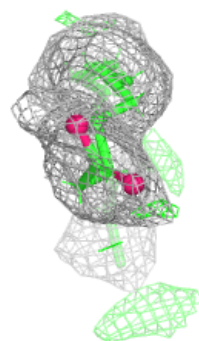
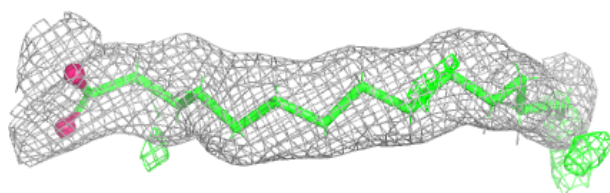
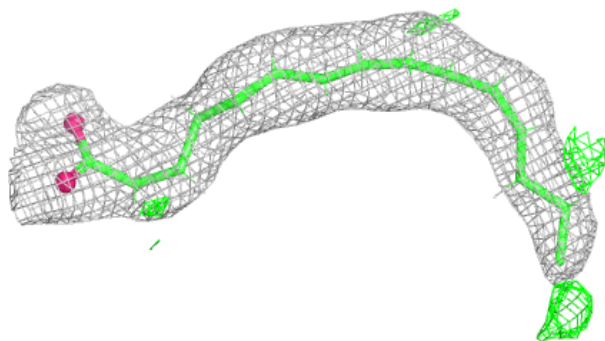
**Electron density around STE J 101:**

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



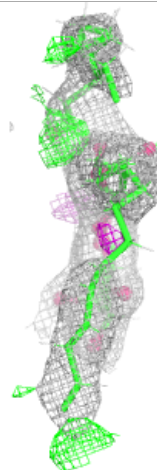
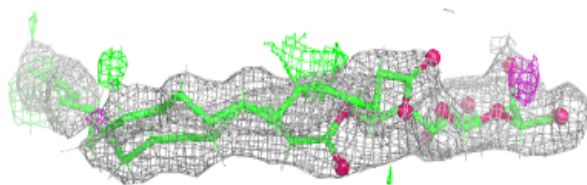
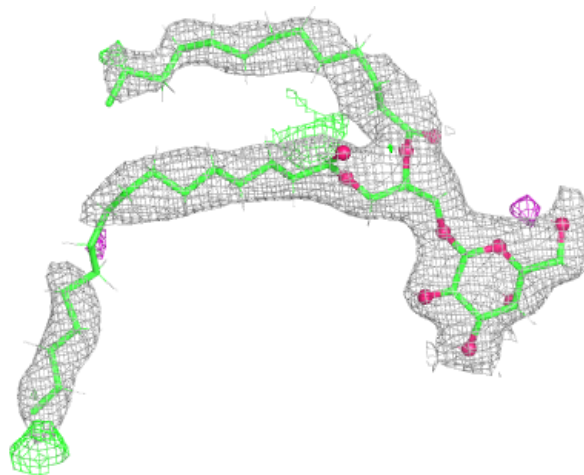
Electron density around STE B 620:

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



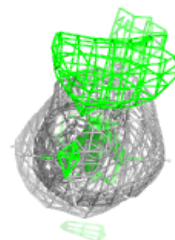
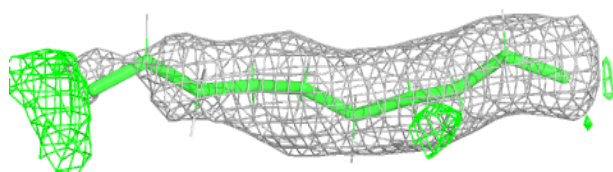
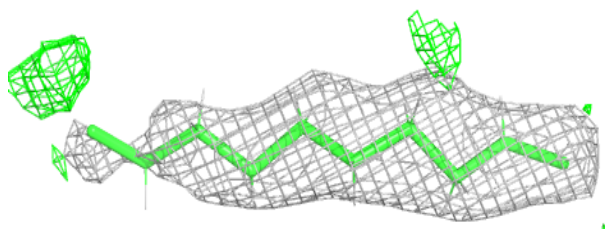
Electron density around LMG Y 101:

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

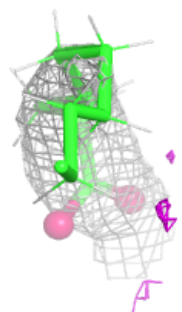
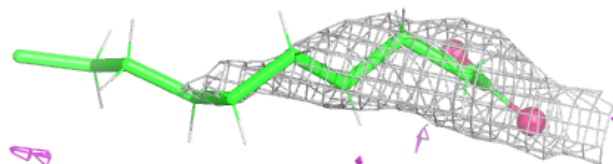
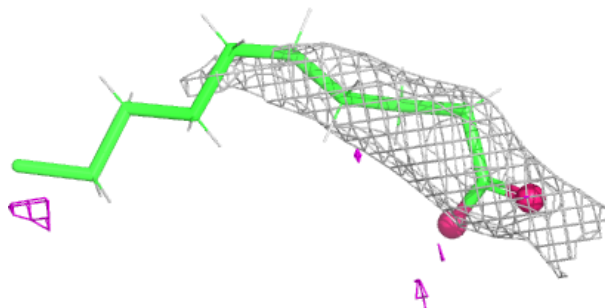


Electron density around STE M 103:

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

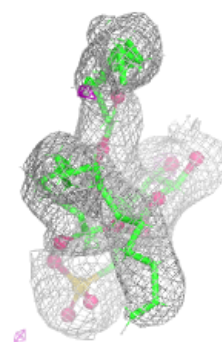
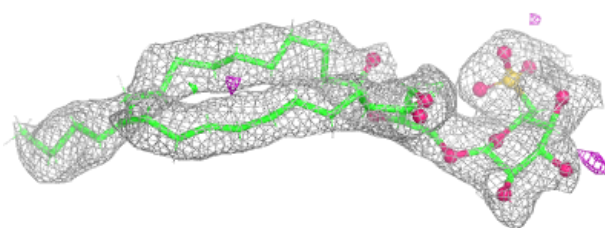
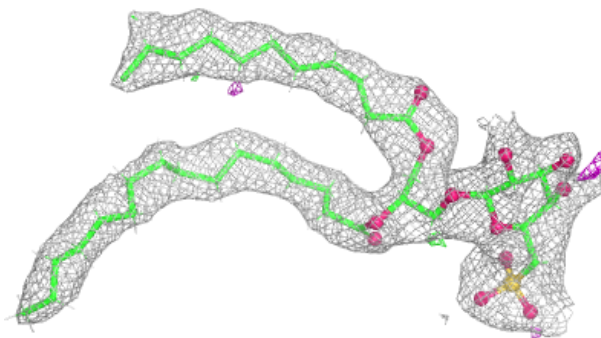
**Electron density around STE B 626:**

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

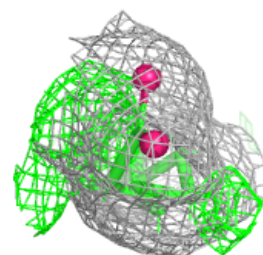
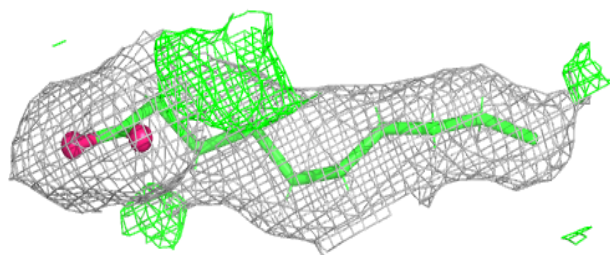
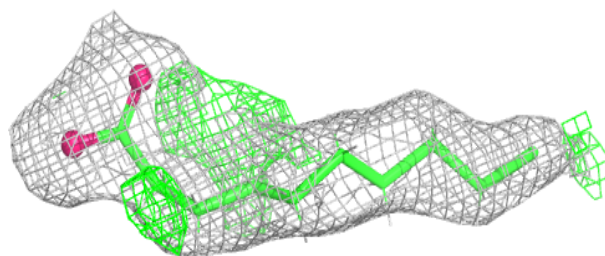


Electron density around SQD b 620:

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

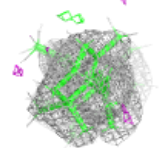
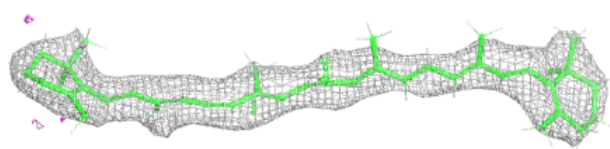
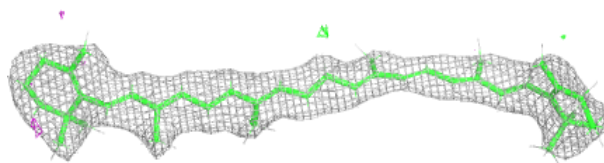
**Electron density around STE B 623:**

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

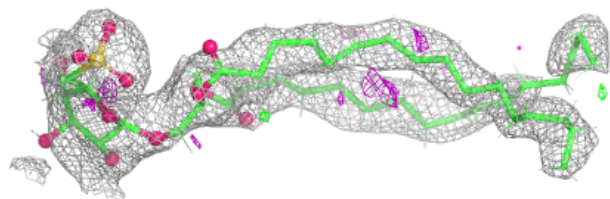
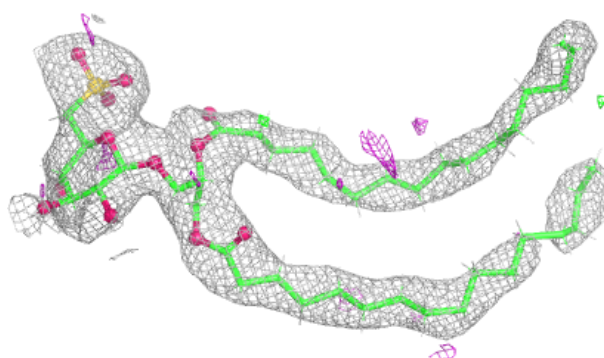


Electron density around BCR K 101:

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

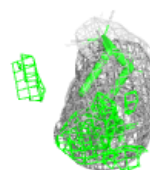
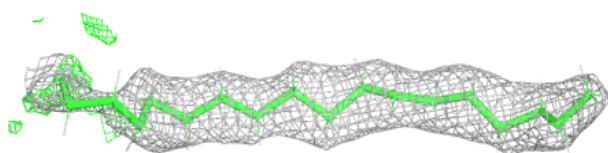
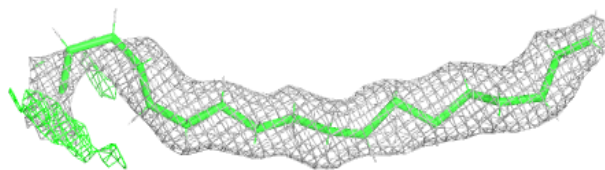
**Electron density around SQD B 621:**

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

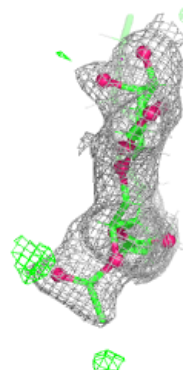
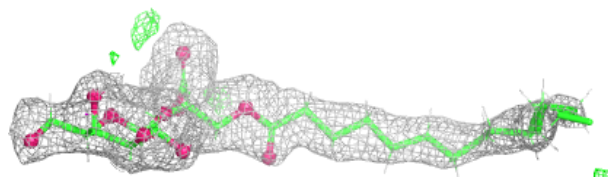
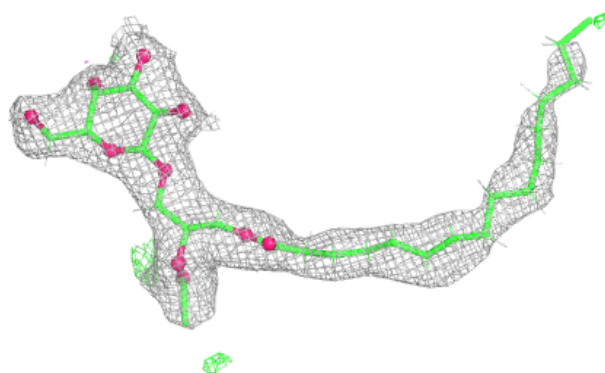


Electron density around STE M 104:

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

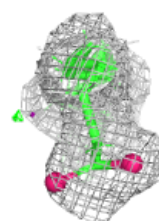
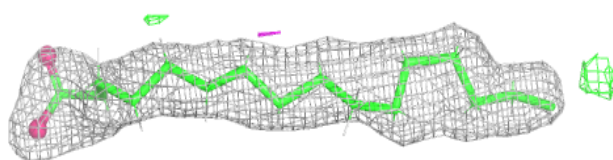
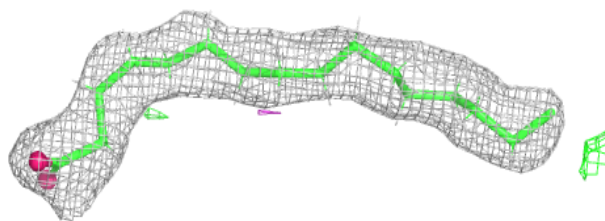
**Electron density around LMG c 519:**

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

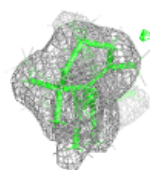
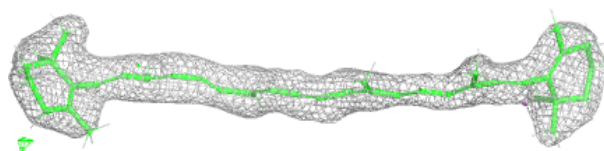
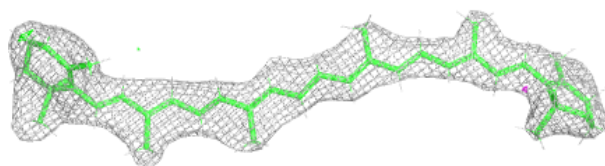


Electron density around STE B 624:

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

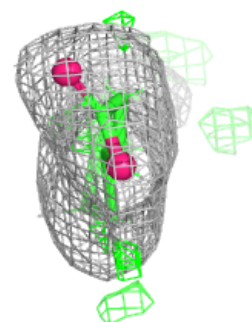
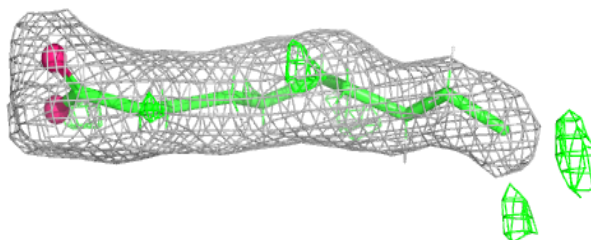
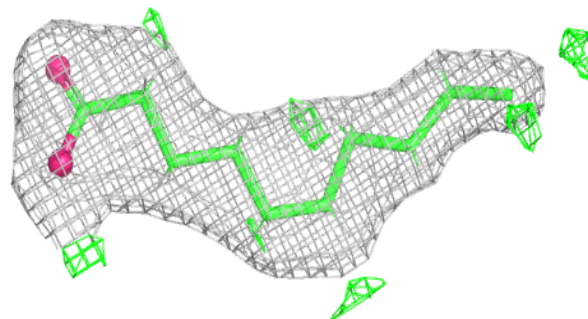
**Electron density around BCR k 101:**

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

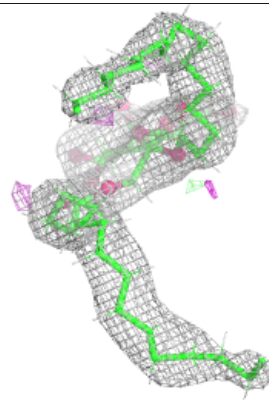
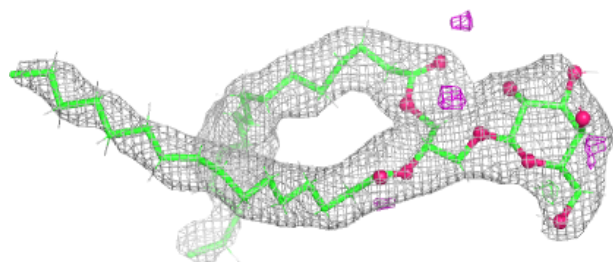
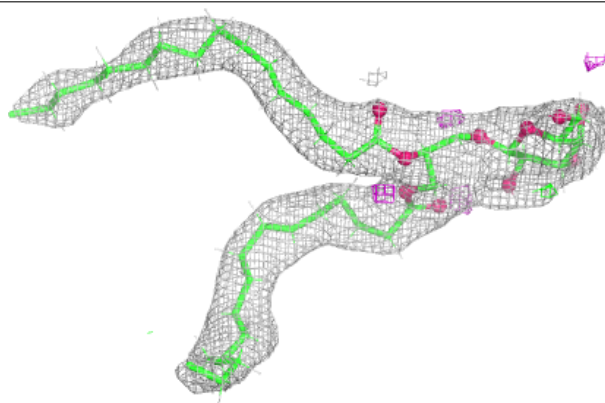


Electron density around STE C 520:

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

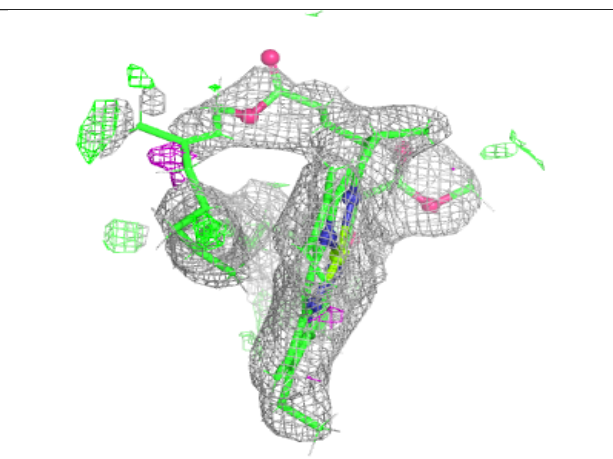
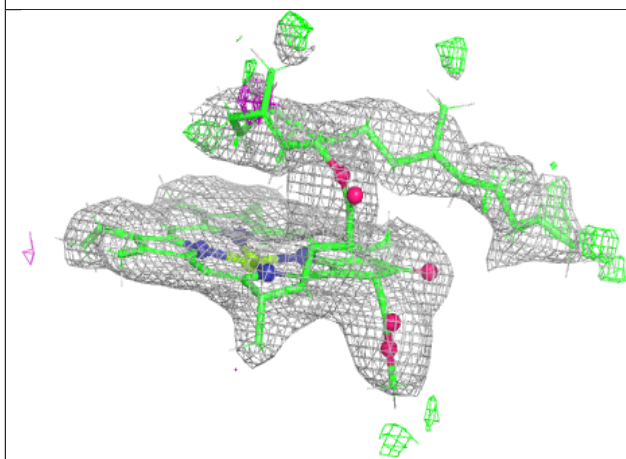
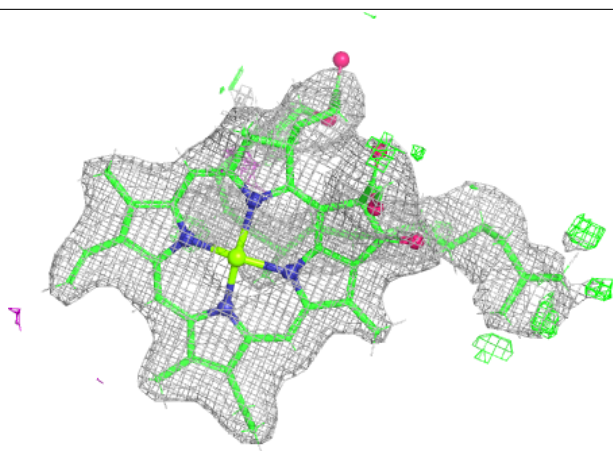
**Electron density around LMG m 101:**

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

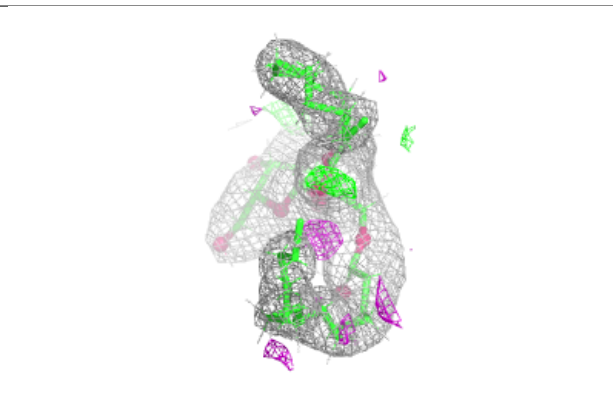
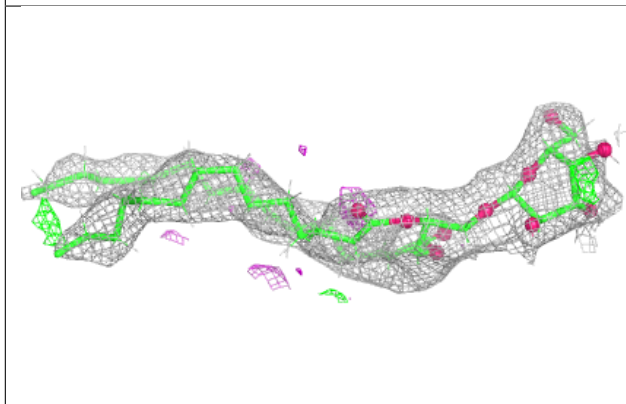
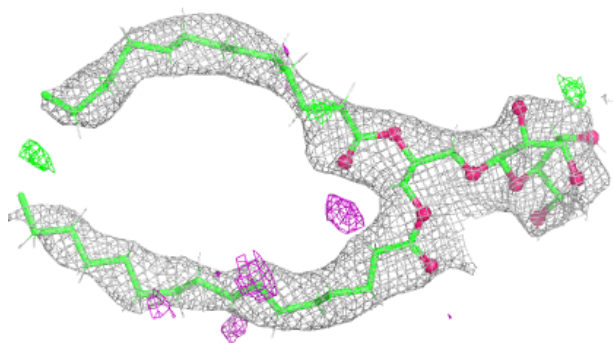


Electron density around CLA B 601:

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

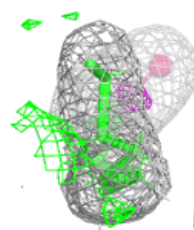
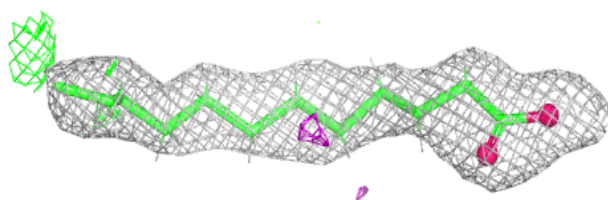
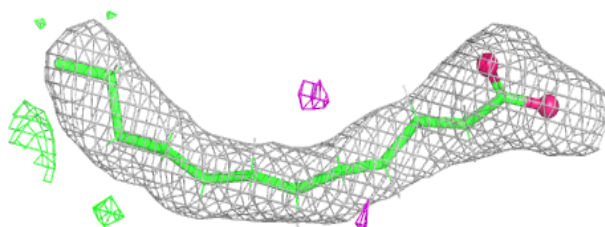
**Electron density around LMG a 414:**

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

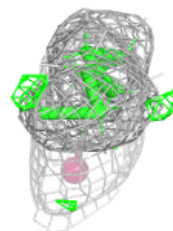
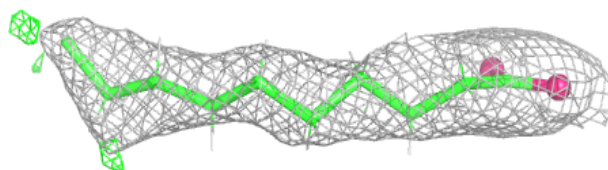
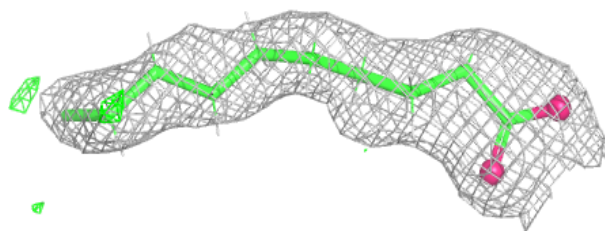


Electron density around STE B 622:

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

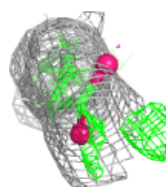
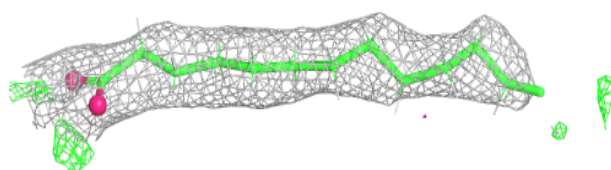
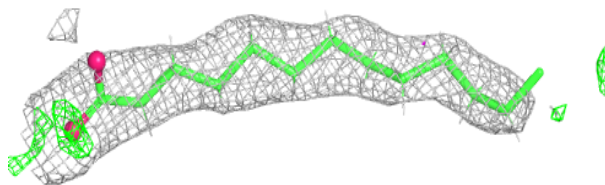
**Electron density around STE C 518:**

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

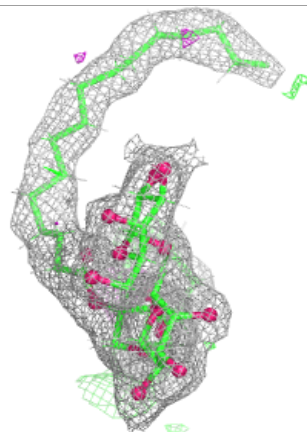
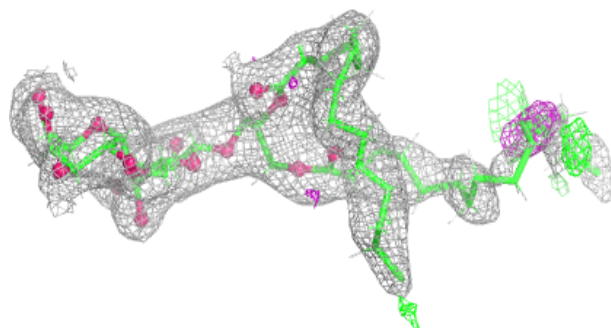
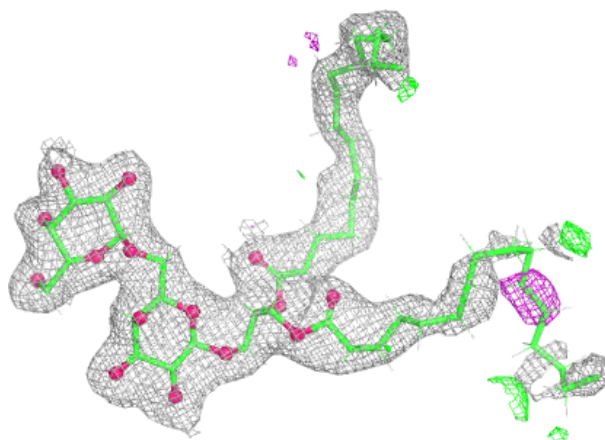


Electron density around STE M 102:

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

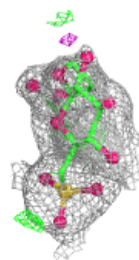
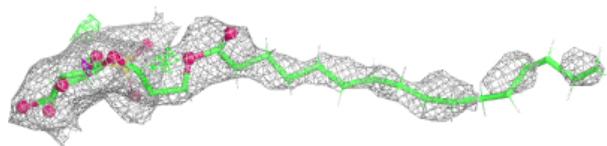
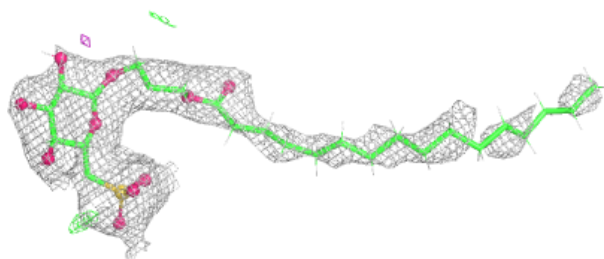
**Electron density around DGD C 516:**

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

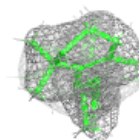
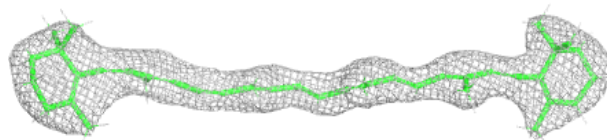
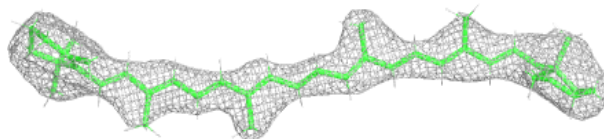


Electron density around SQD F 102:

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

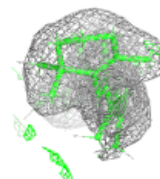
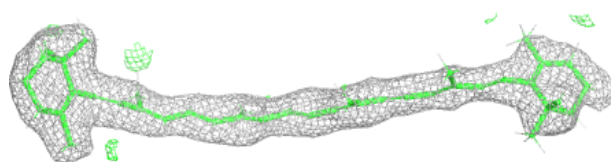
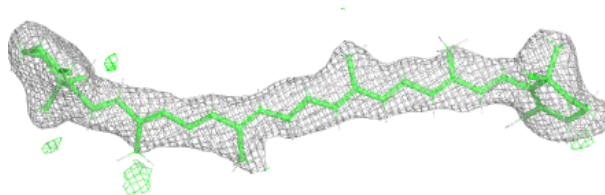
**Electron density around BCR c 514:**

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

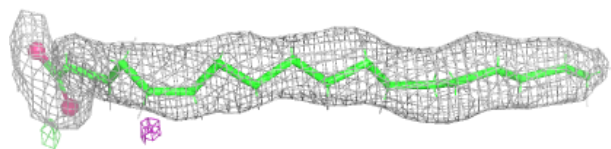
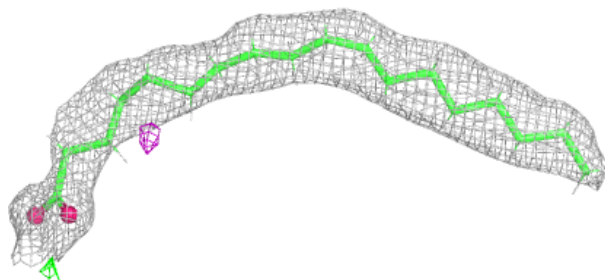


Electron density around BCR h 101:

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

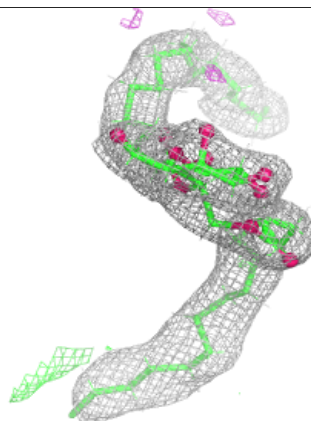
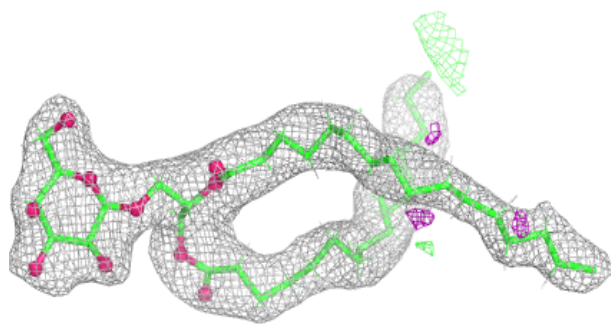
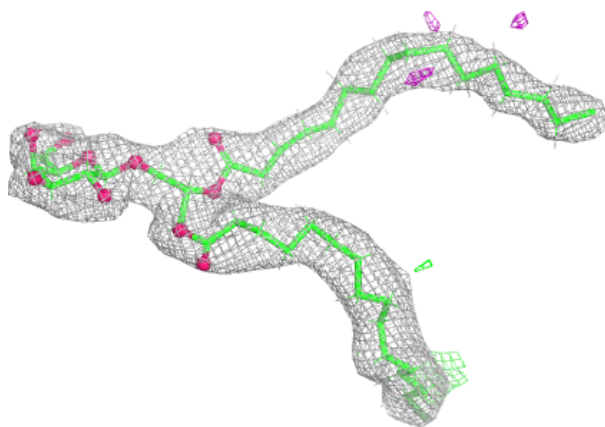
**Electron density around STE D 412:**

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



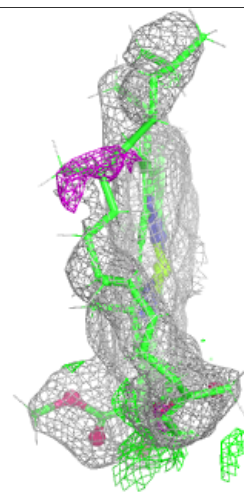
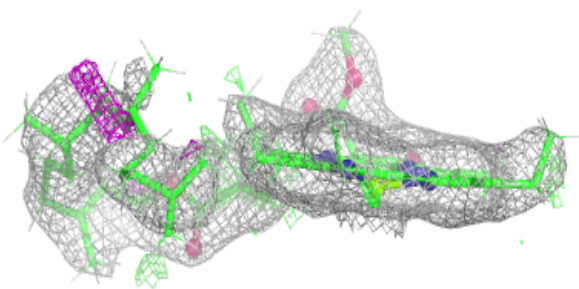
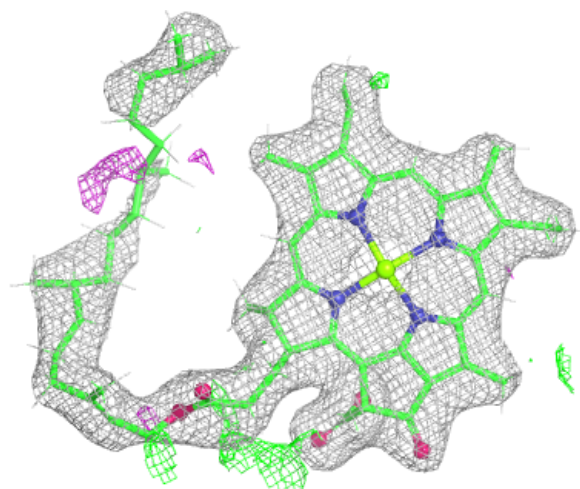
Electron density around LMG M 101:

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



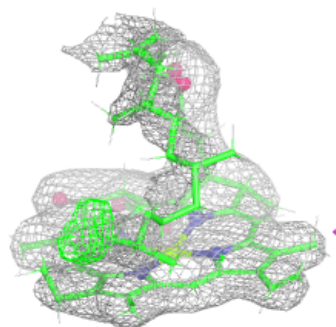
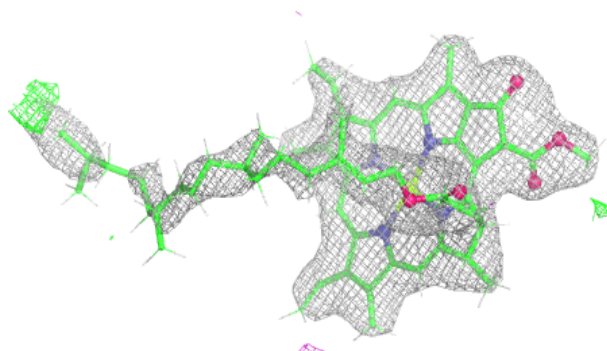
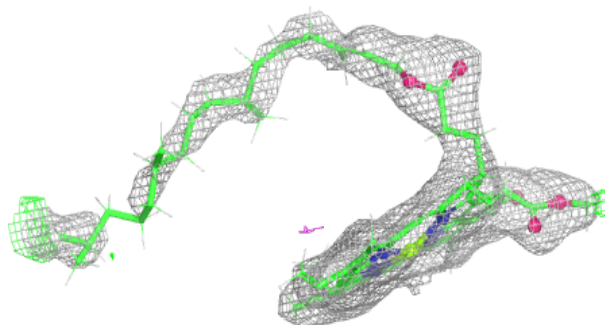
Electron density around CLA c 512:

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

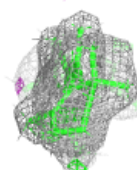
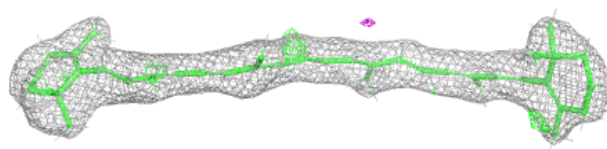
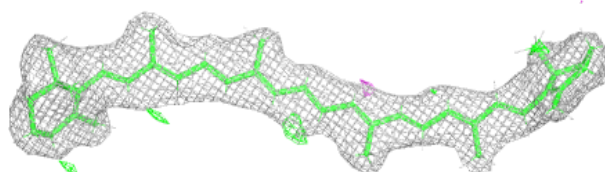


Electron density around CLA C 513:

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

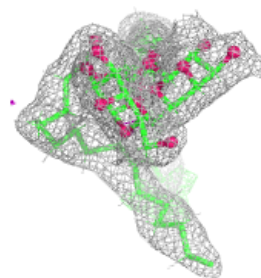
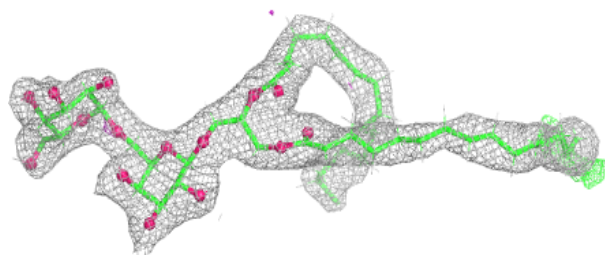
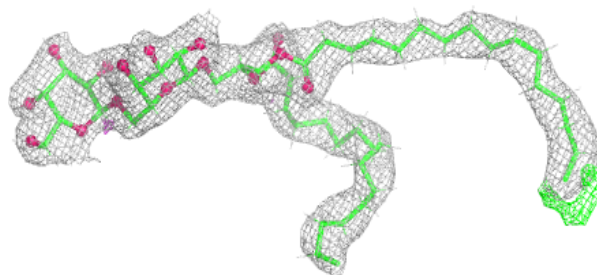
**Electron density around BCR K 102:**

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

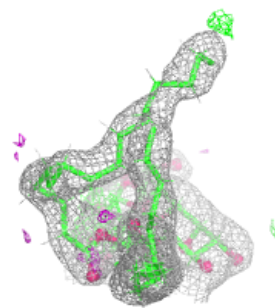
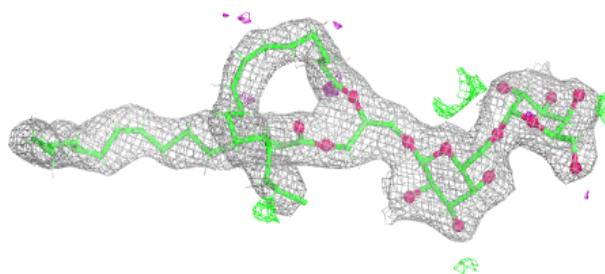
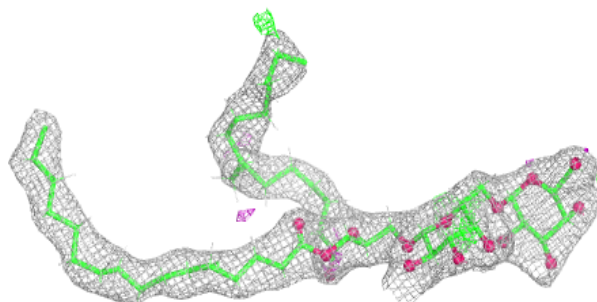


Electron density around DGD H 102:

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

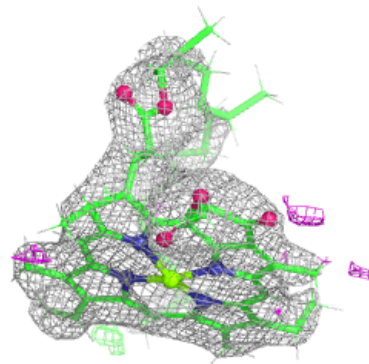
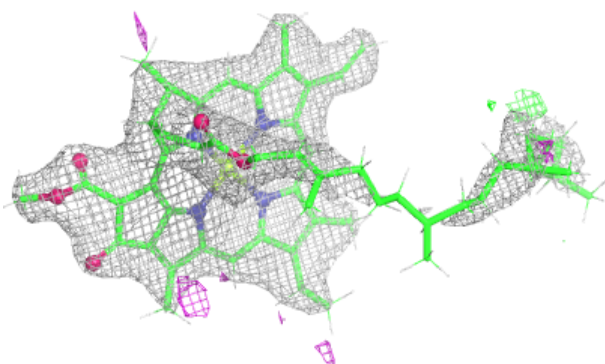
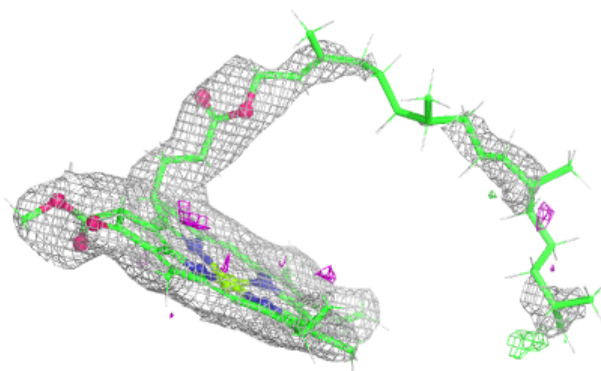
**Electron density around DGD h 103:**

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

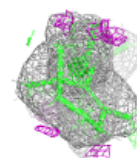
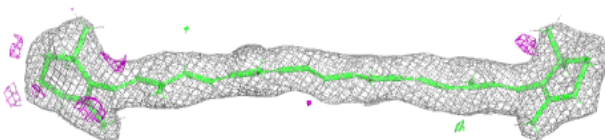
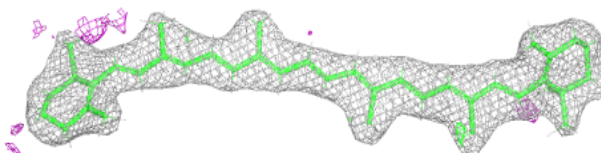


Electron density around CLA c 513:

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

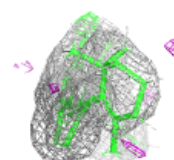
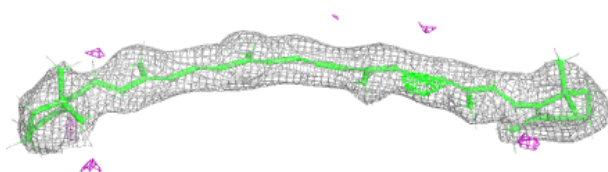
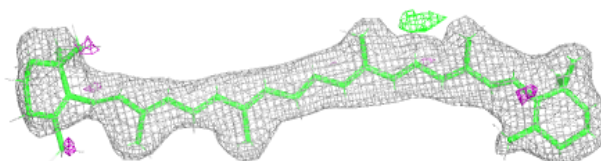
**Electron density around BCR B 618:**

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

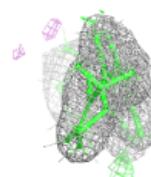
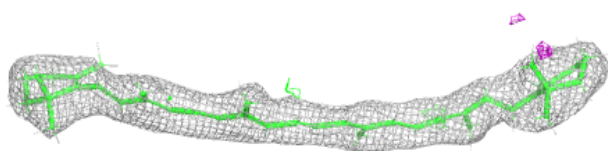
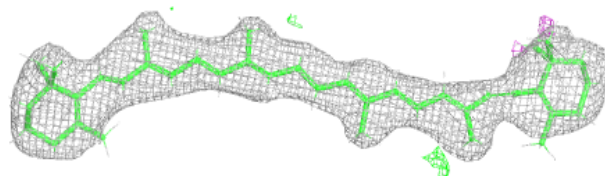


Electron density around BCR D 405:

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

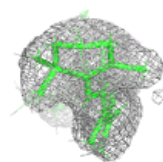
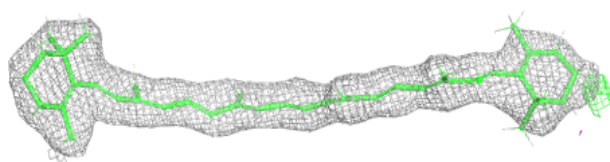
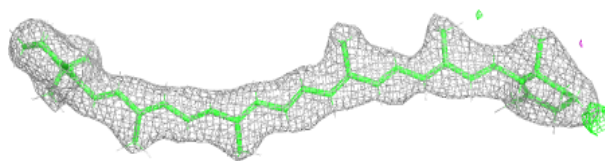
**Electron density around BCR d 406:**

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

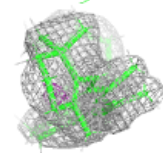
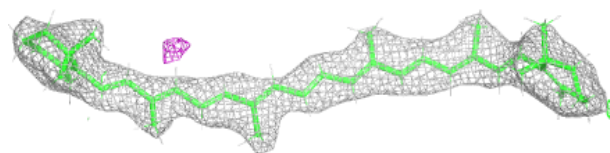
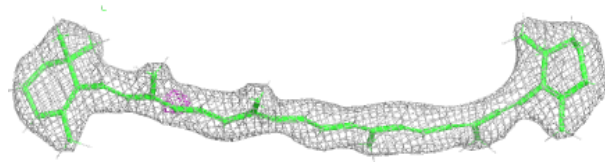


Electron density around BCR H 101:

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

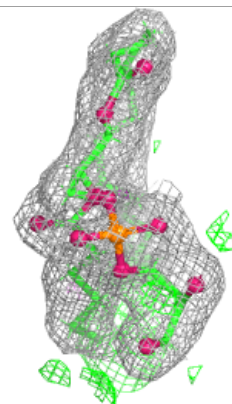
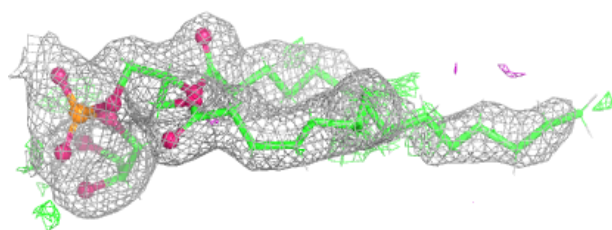
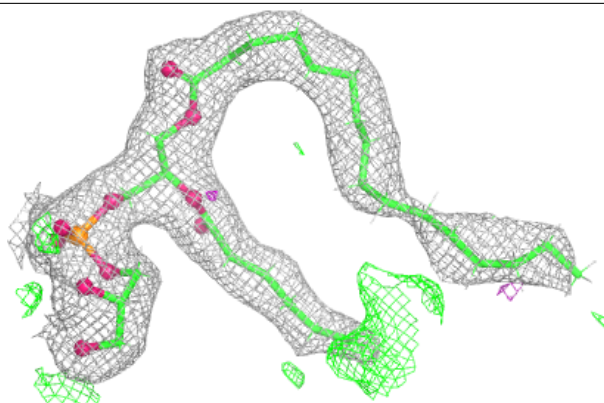
**Electron density around BCR K 103:**

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

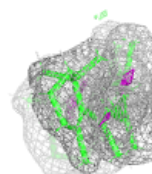
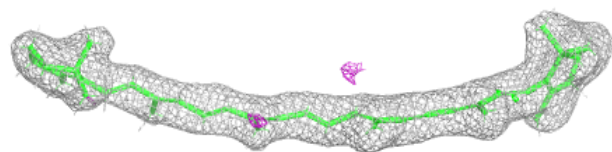
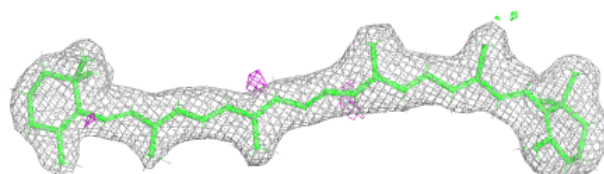


Electron density around LHG d 409:

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

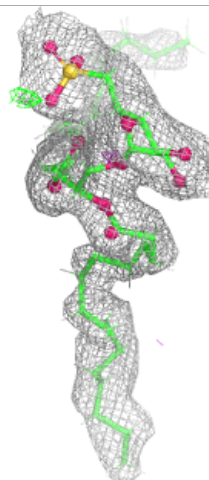
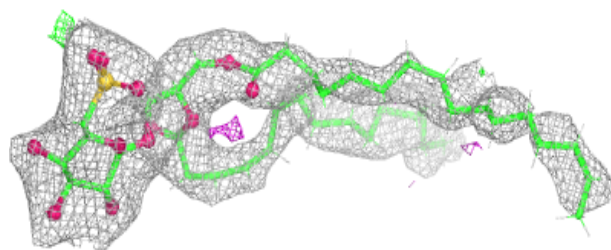
**Electron density around BCR T 101:**

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



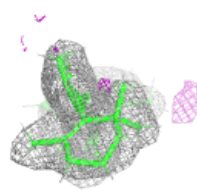
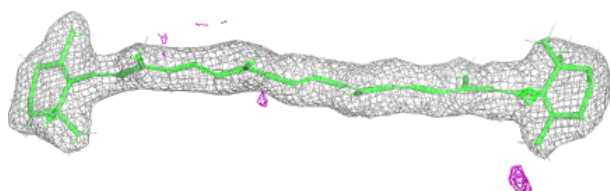
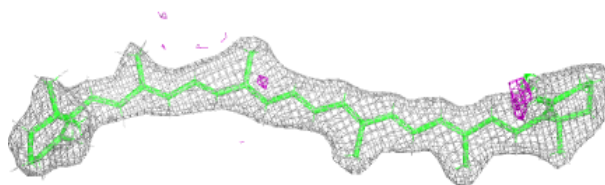
Electron density around SQD a 411:

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

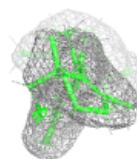
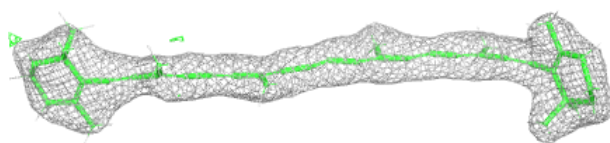
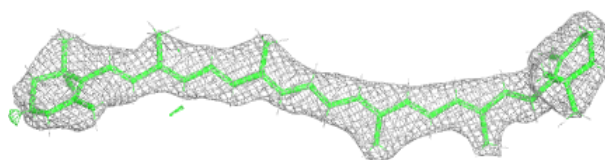


Electron density around BCR C 514:

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

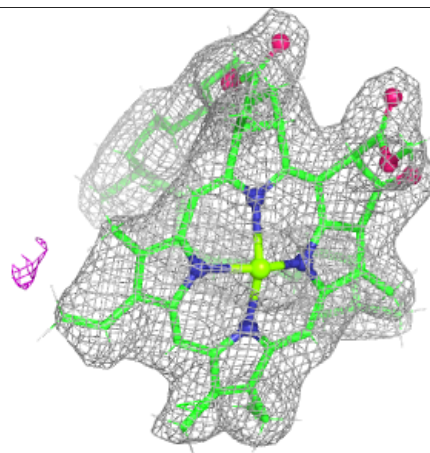
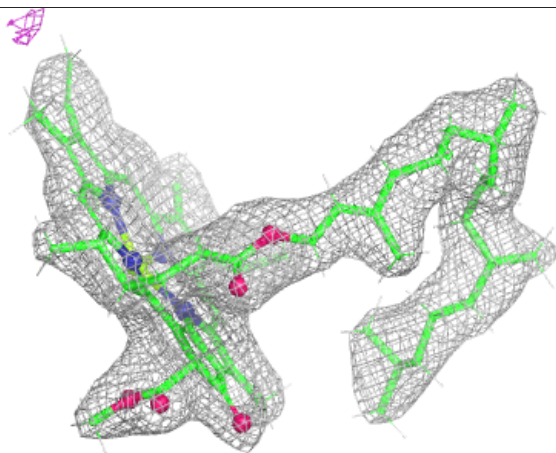
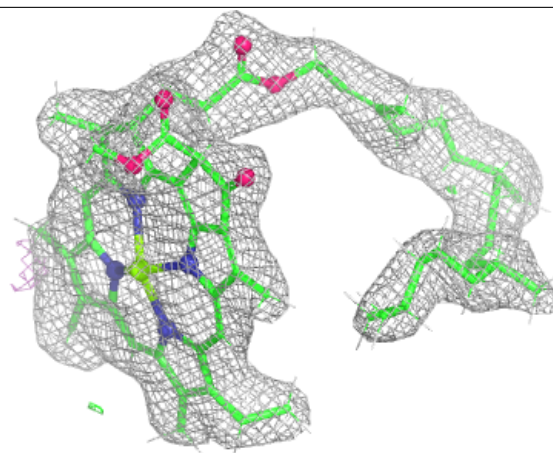
**Electron density around BCR c 515:**

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

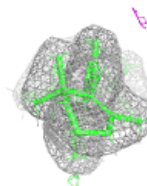
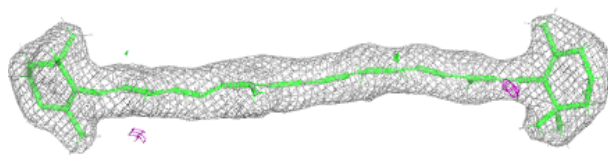
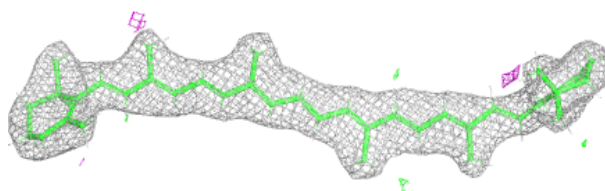


Electron density around CLA C 503:

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

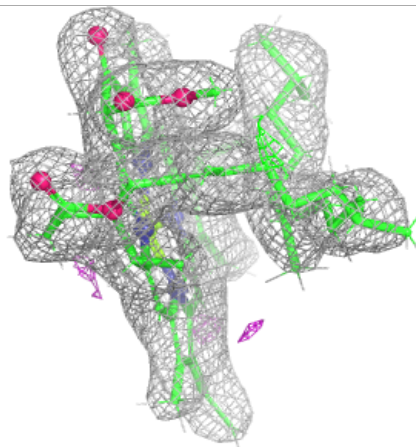
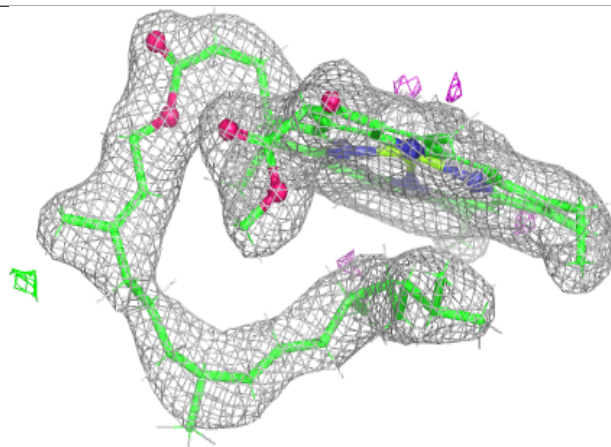
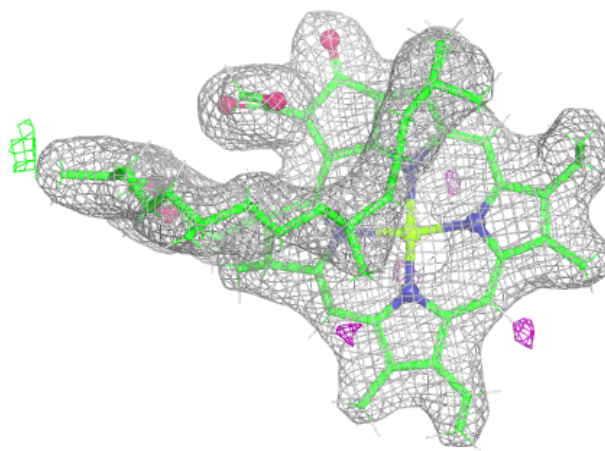
**Electron density around BCR A 407:**

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



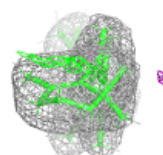
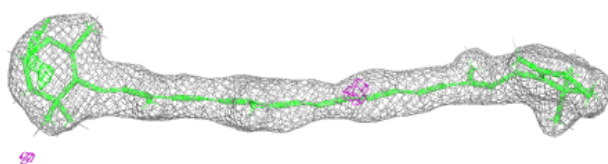
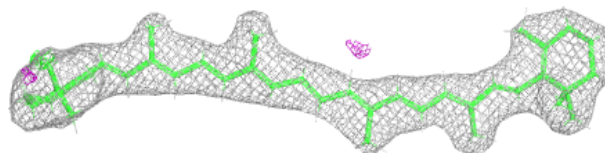
Electron density around CLA C 510:

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

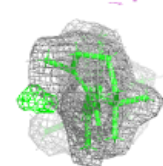
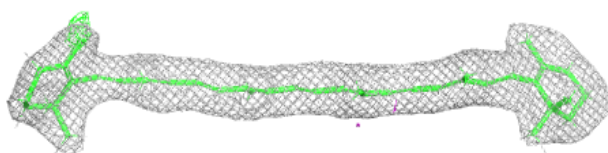
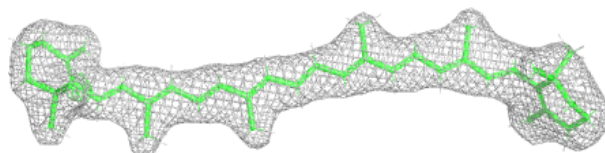


Electron density around BCR b 617:

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

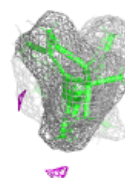
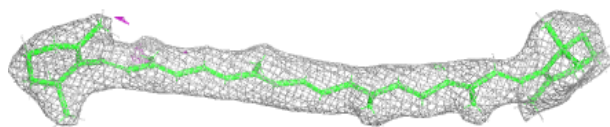
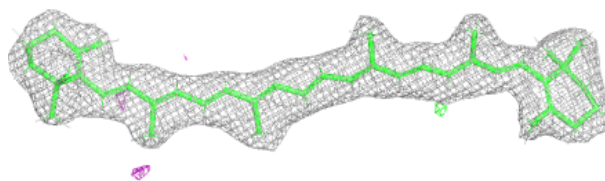
**Electron density around BCR b 618:**

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

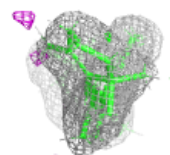
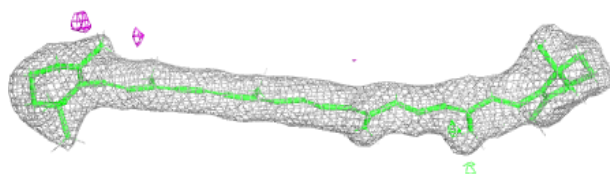
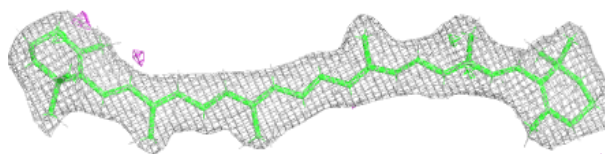


Electron density around BCR b 619:

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

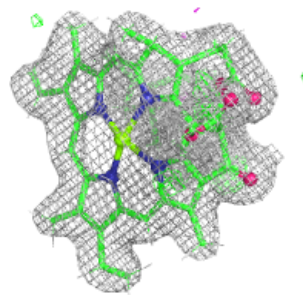
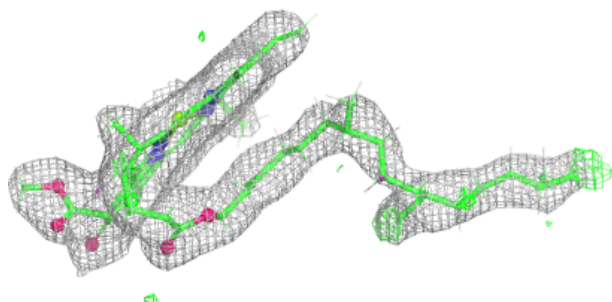
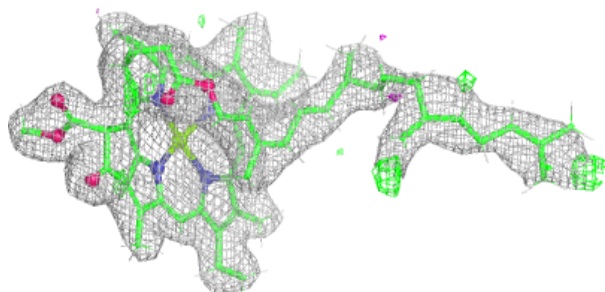
**Electron density around BCR B 619:**

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

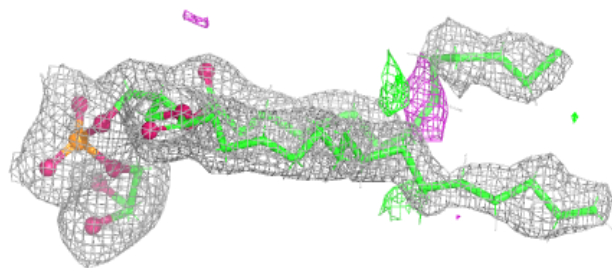
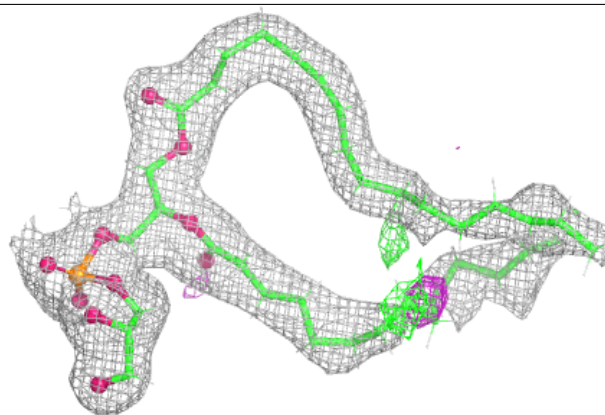


Electron density around CLA c 505:

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

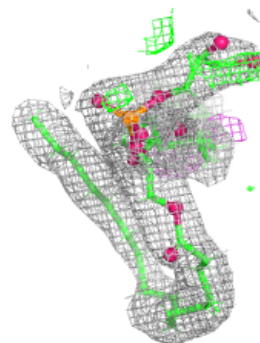
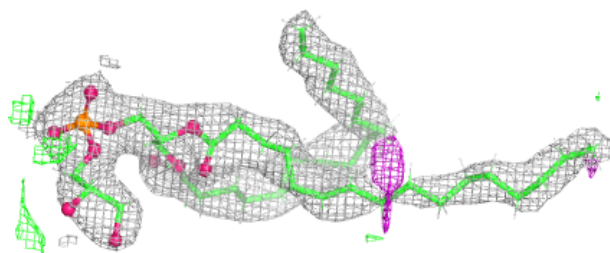
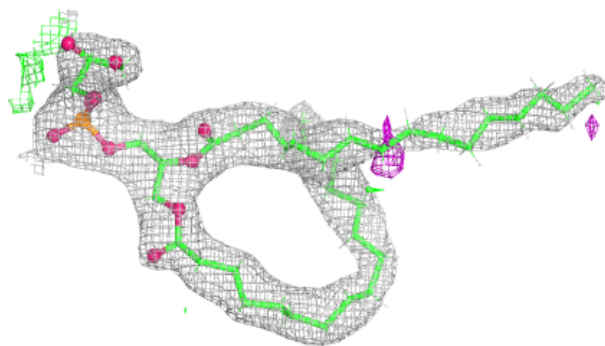
**Electron density around LHG D 409:**

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



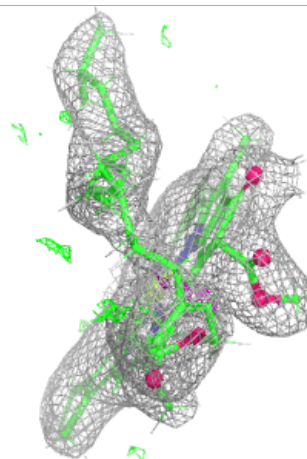
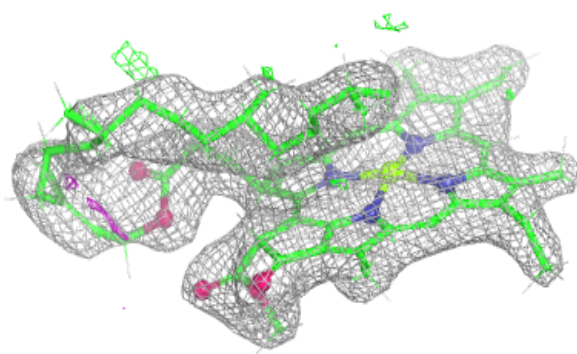
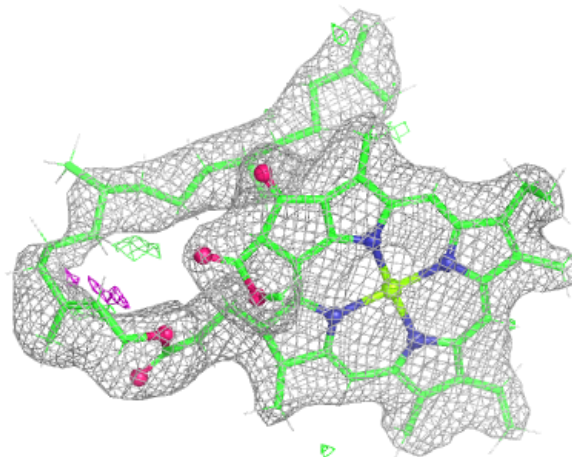
Electron density around LHG a 410:

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



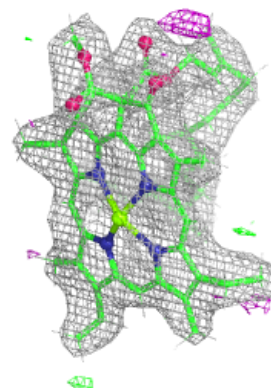
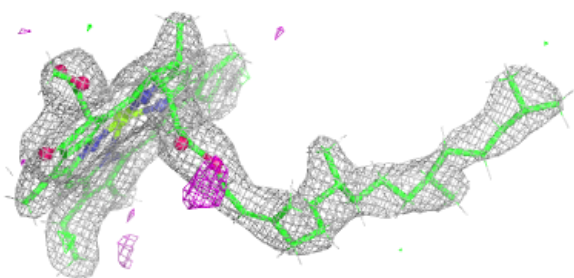
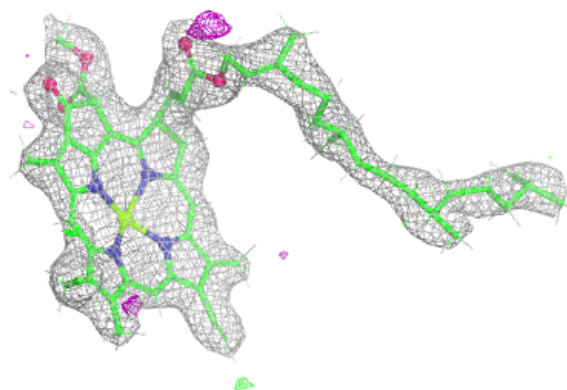
Electron density around CLA c 509:

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

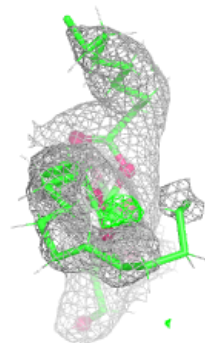
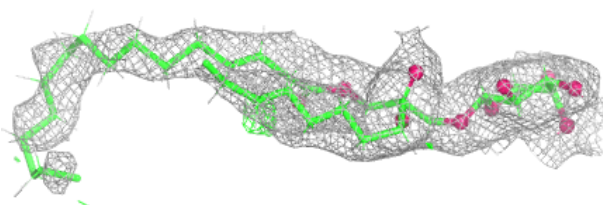
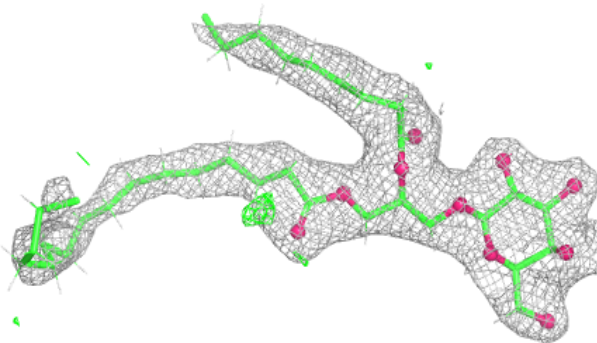


Electron density around CLA c 511:

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

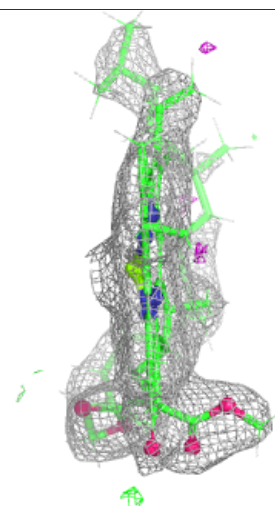
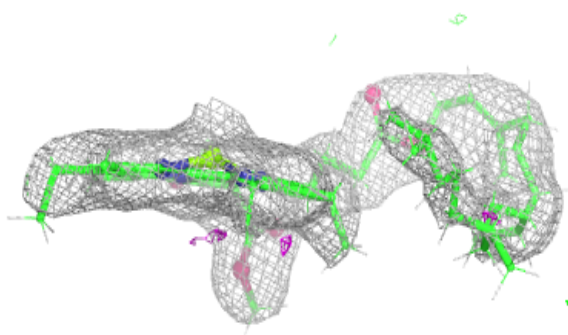
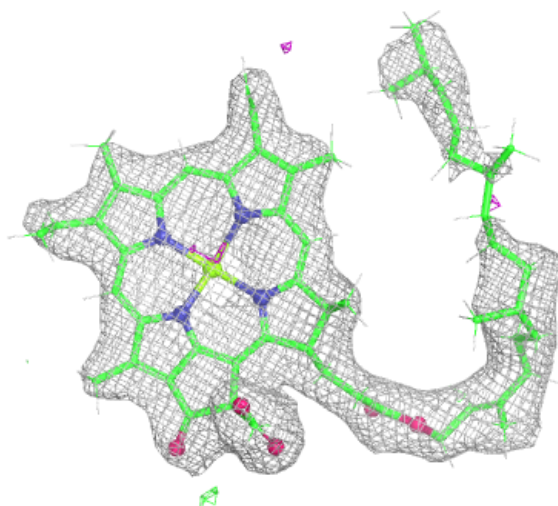
**Electron density around LMG d 410:**

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



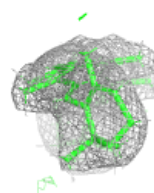
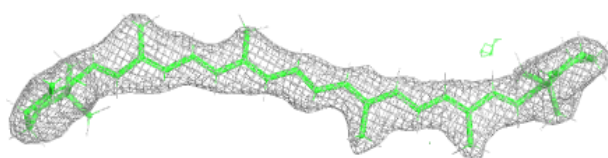
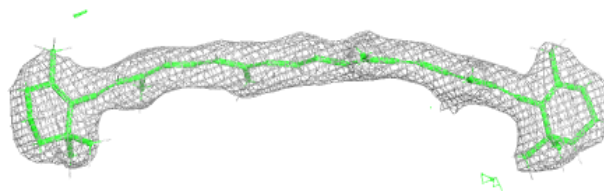
Electron density around CLA C 512:

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

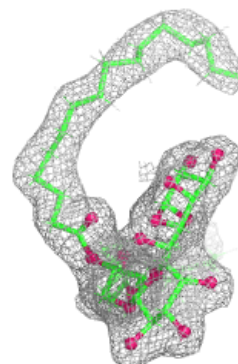
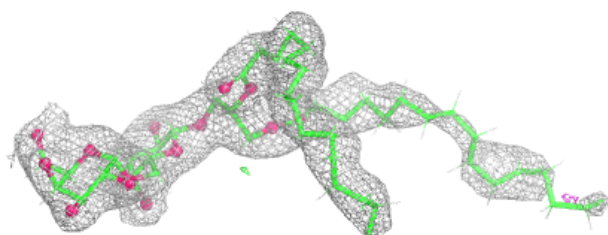
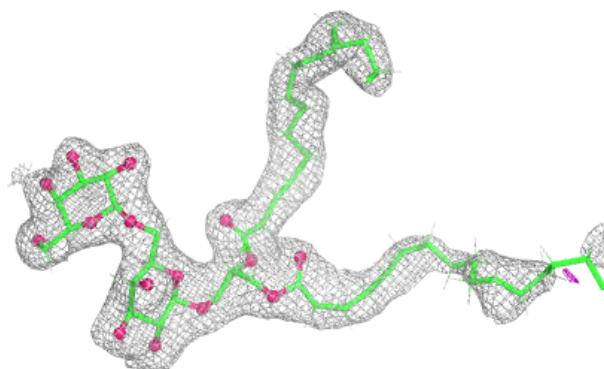


Electron density around BCR k 102:

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

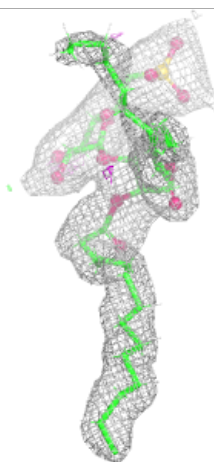
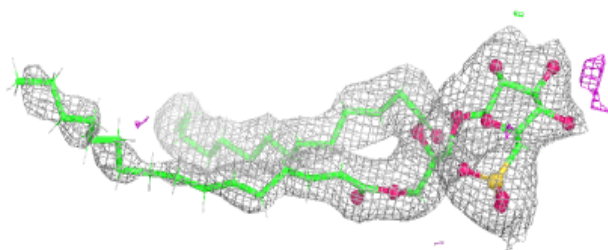
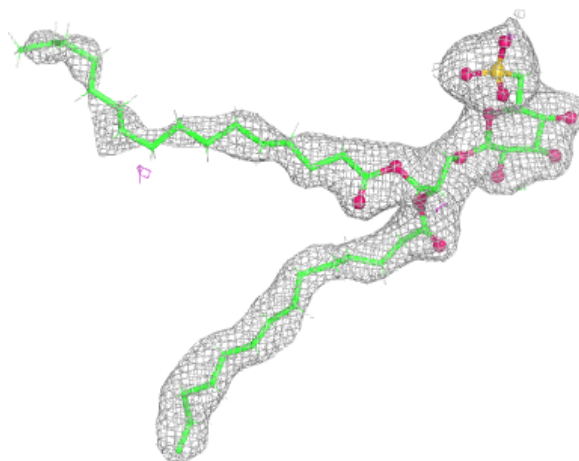
**Electron density around DGD c 517:**

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



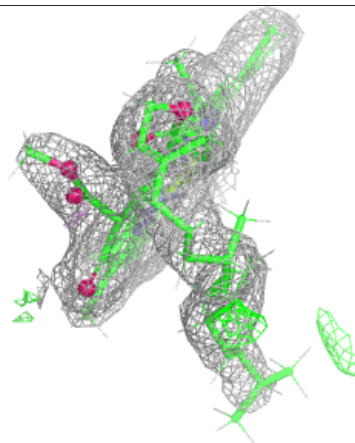
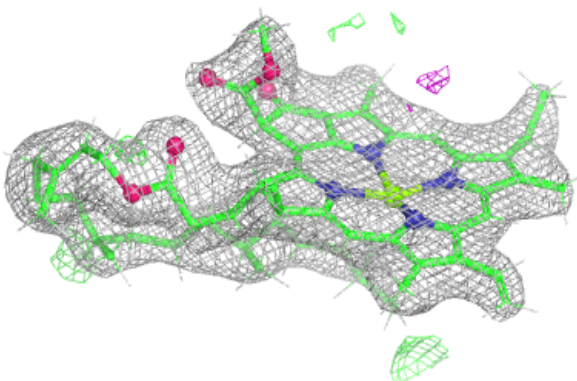
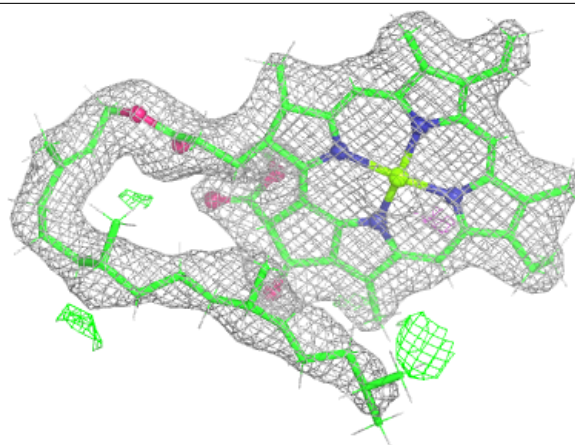
Electron density around SQD A 412:

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

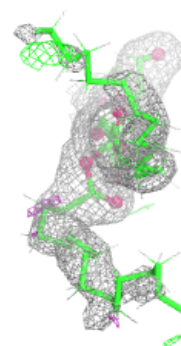
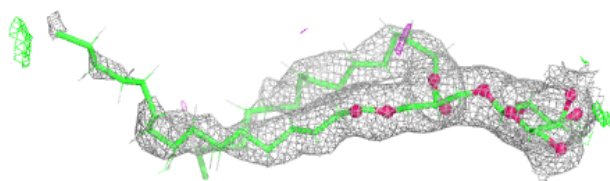
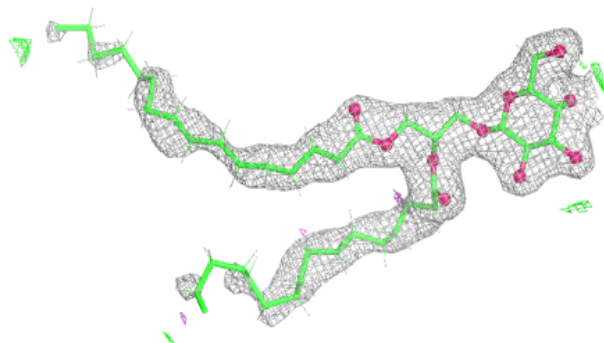


Electron density around CLA C 509:

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

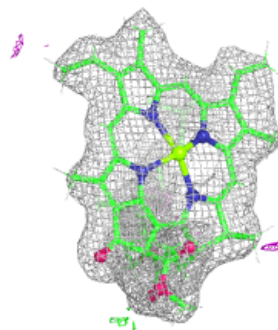
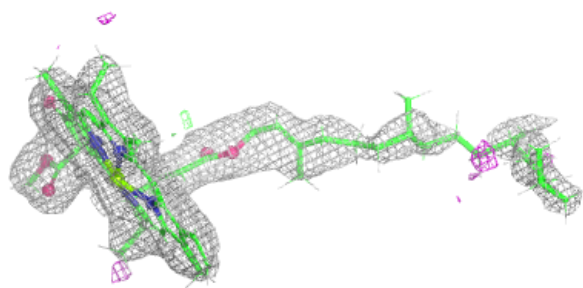
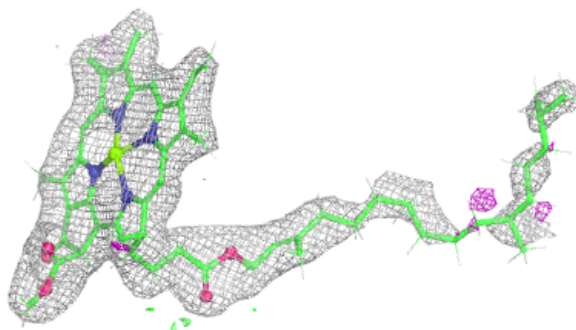
**Electron density around LMG D 407:**

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



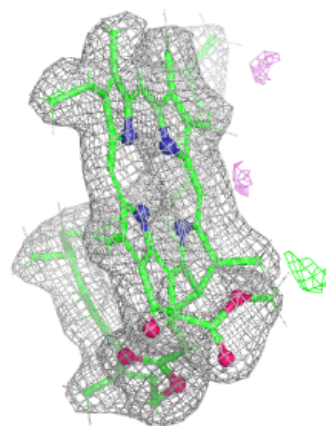
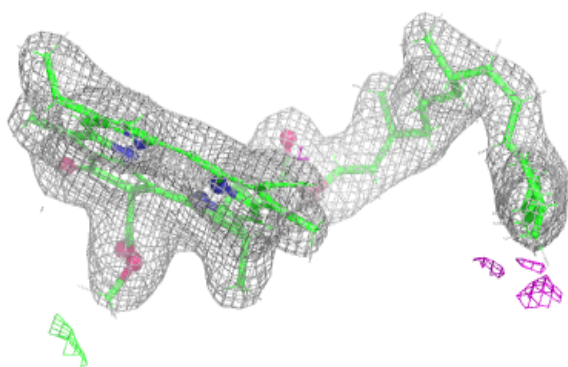
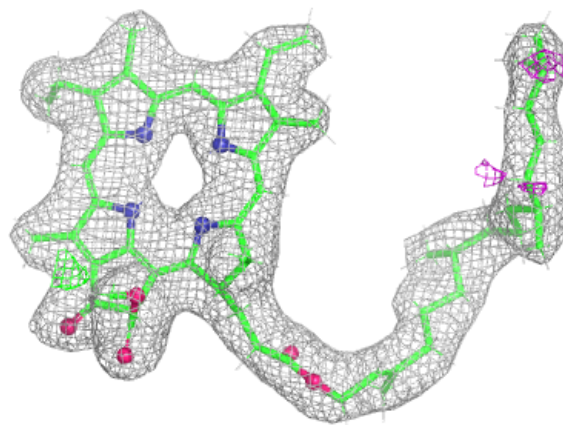
Electron density around CLA d 405:

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



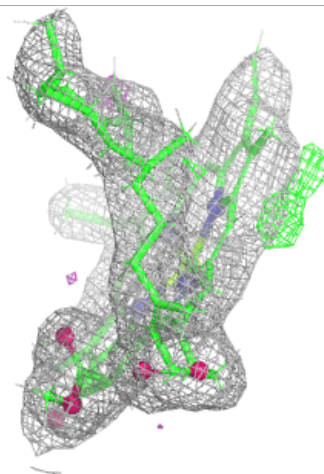
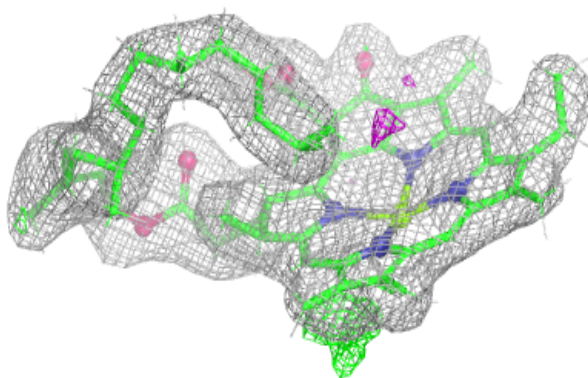
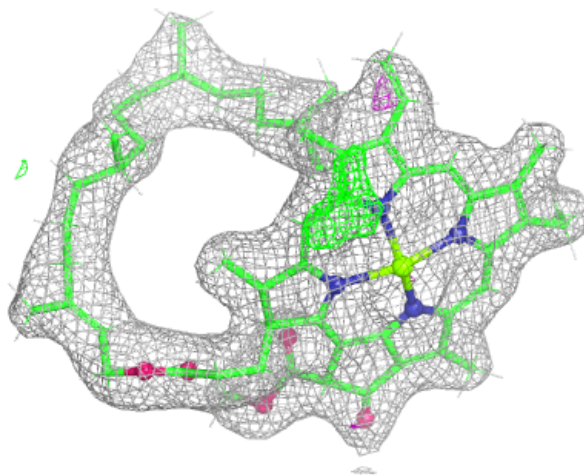
Electron density around PHO d 401:

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



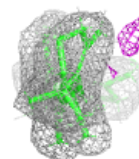
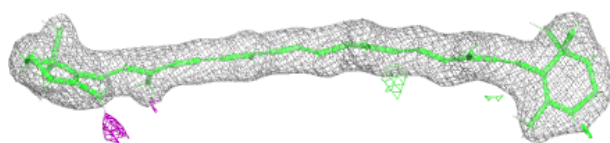
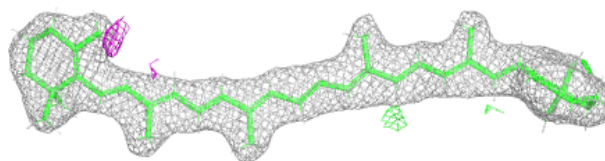
Electron density around CLA B 615:

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

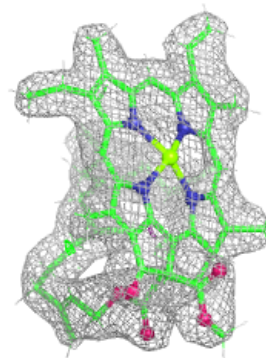
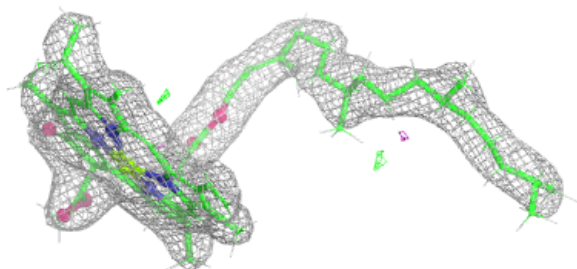
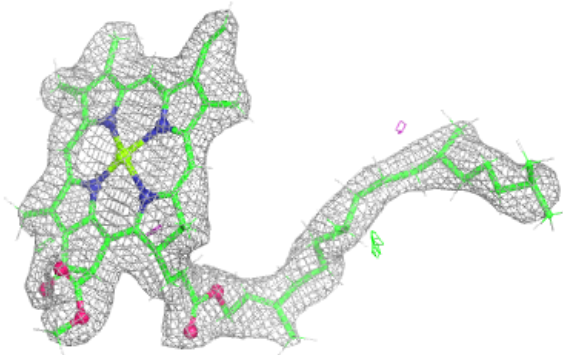


Electron density around BCR B 617:

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

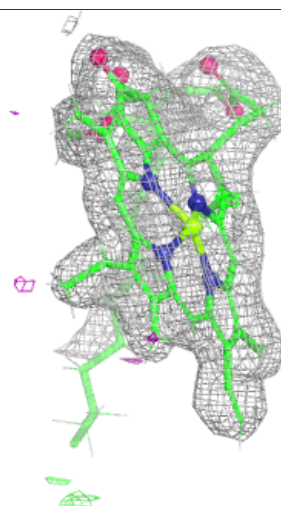
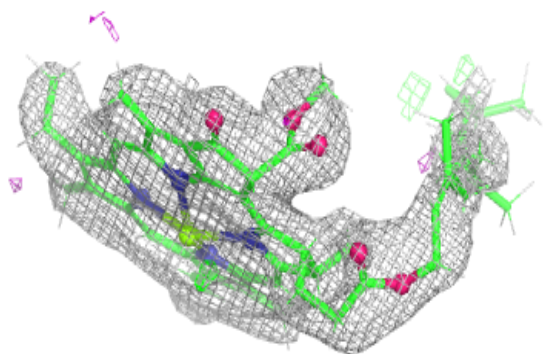
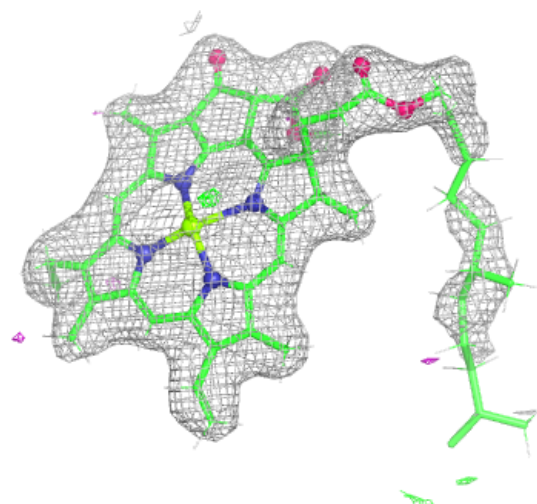
**Electron density around CLA C 511:**

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



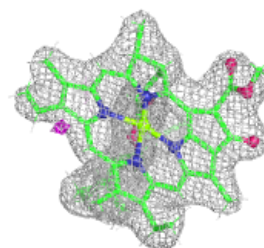
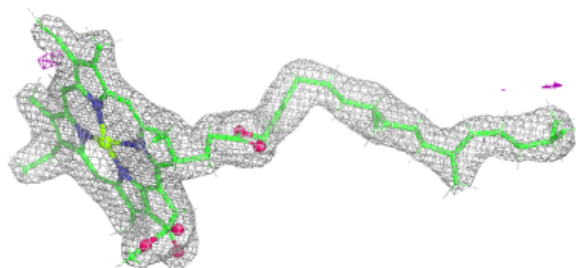
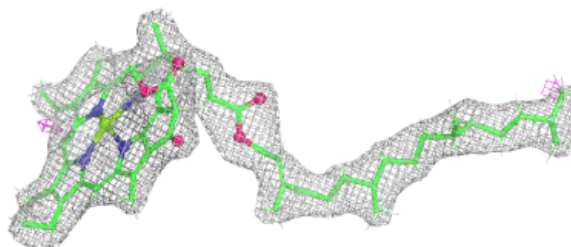
Electron density around CLA B 616:

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

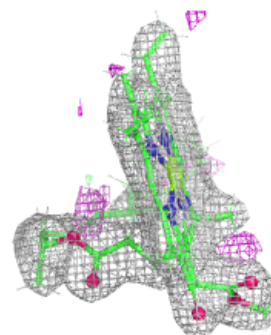
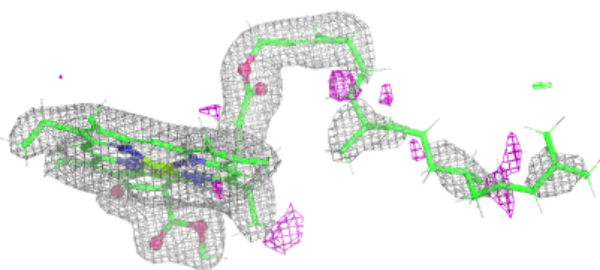
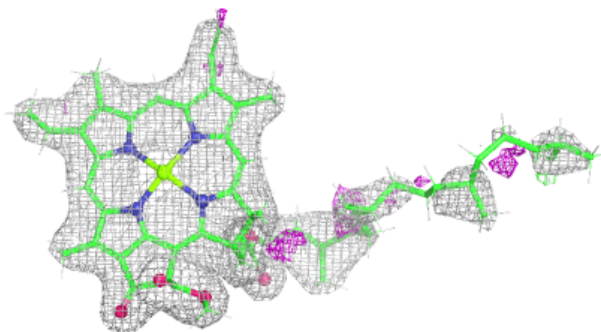


Electron density around CLA C 502:

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

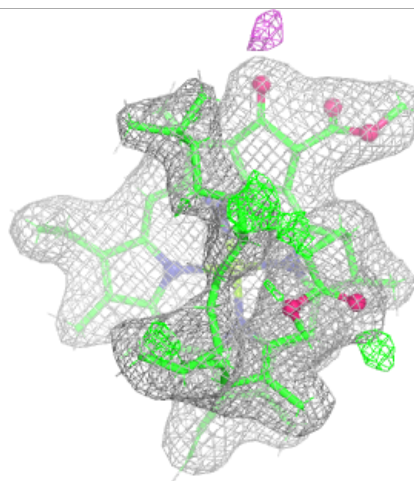
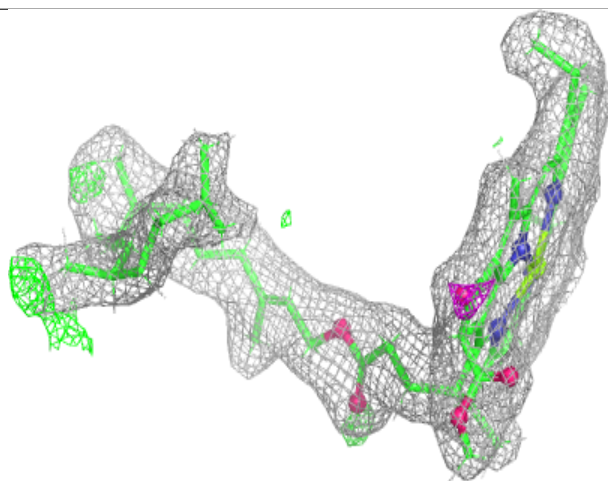
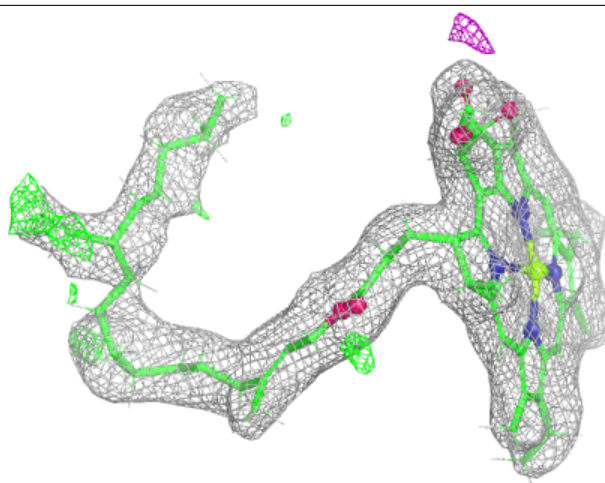
**Electron density around CLA a 403:**

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



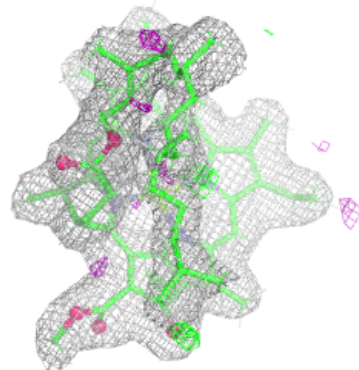
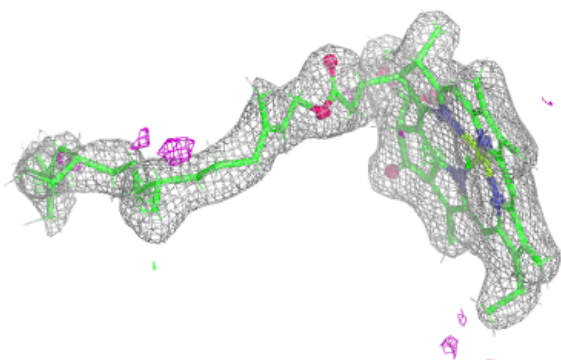
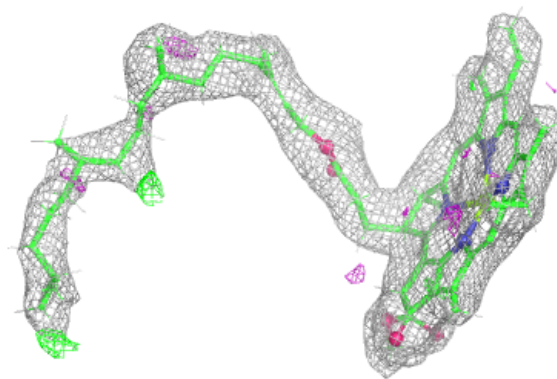
Electron density around CLA B 606:

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

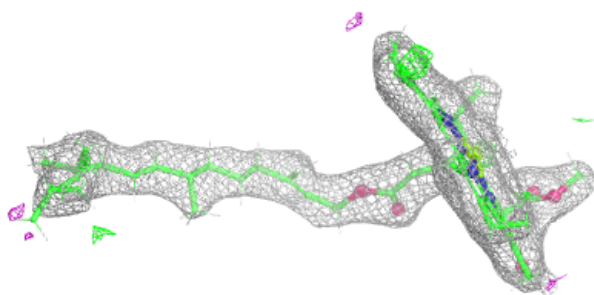
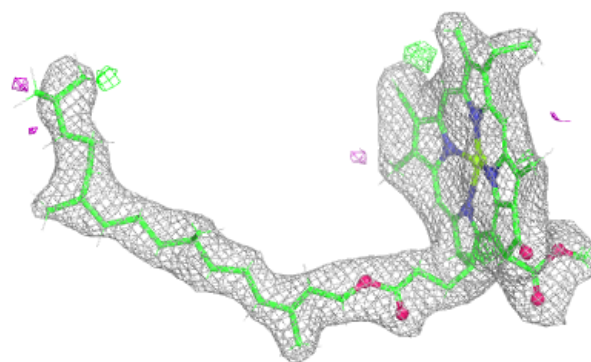


Electron density around CLA b 606:

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

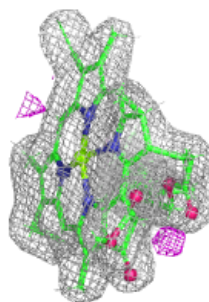
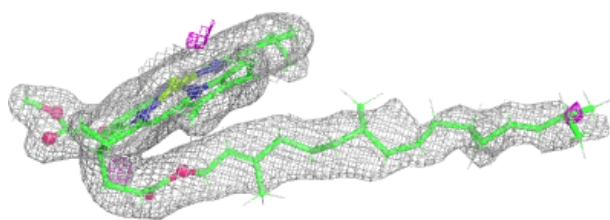
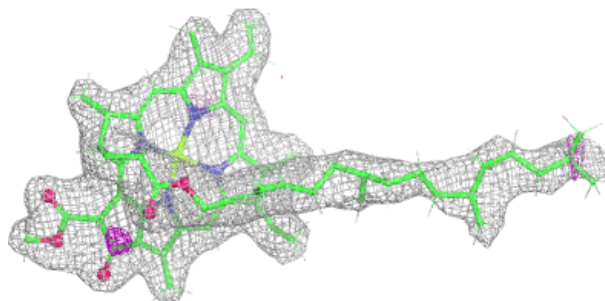
**Electron density around CLA b 609:**

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



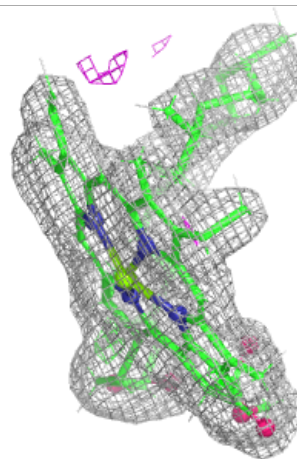
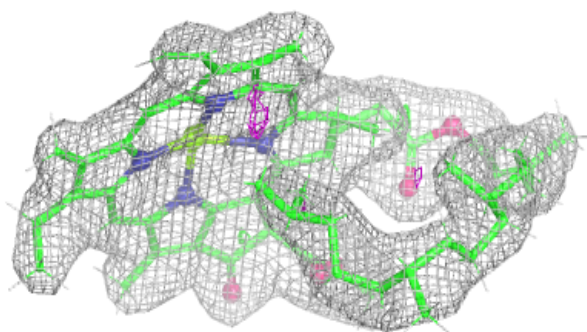
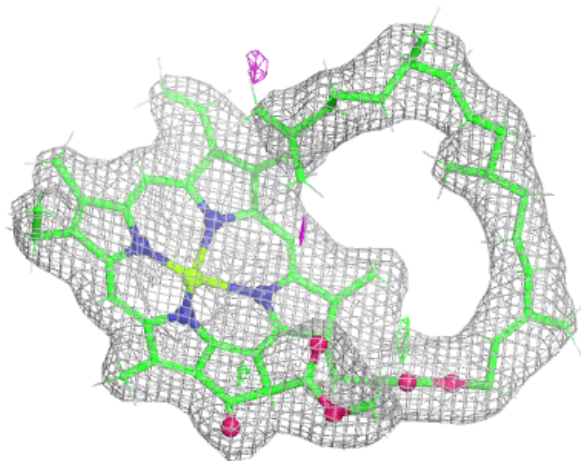
Electron density around CLA b 614:

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



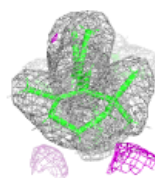
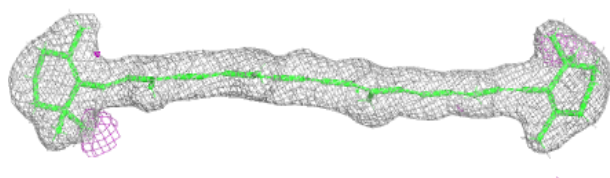
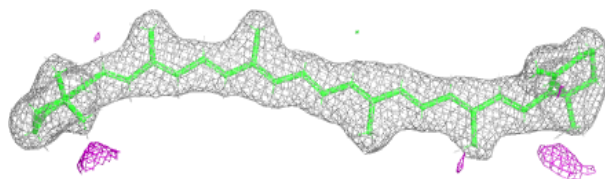
Electron density around CLA b 615:

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



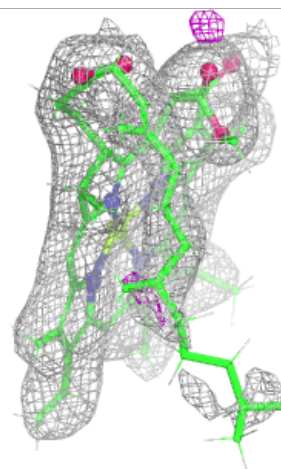
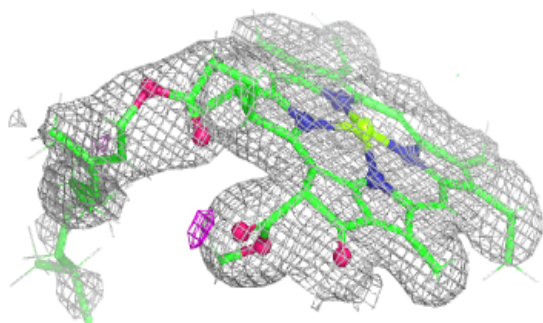
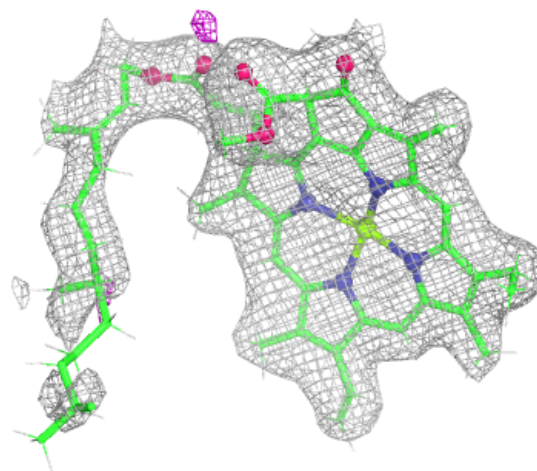
Electron density around BCR a 406:

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



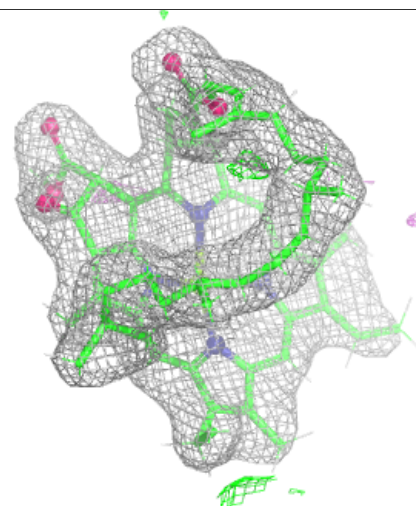
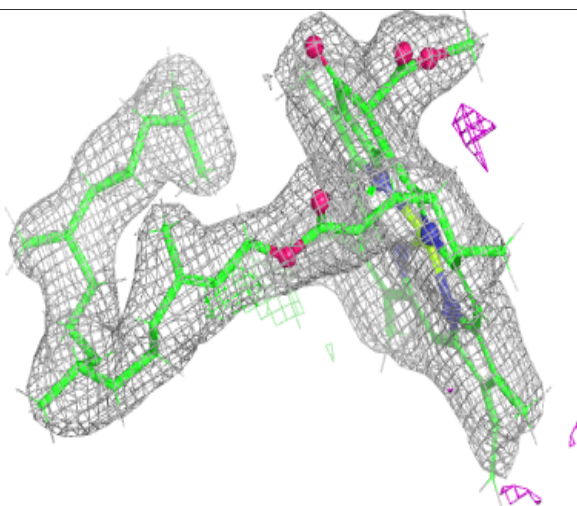
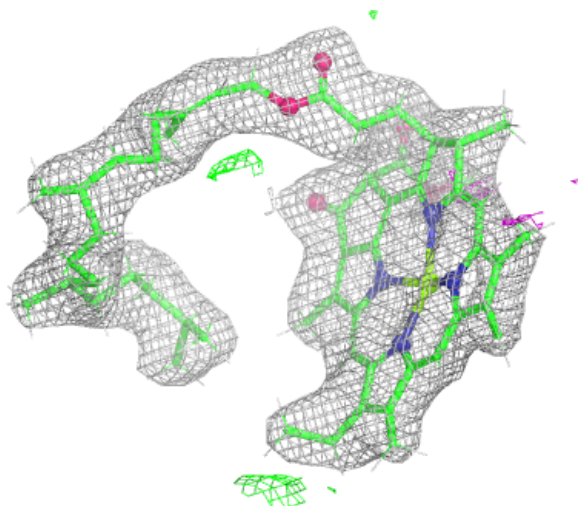
Electron density around CLA b 616:

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



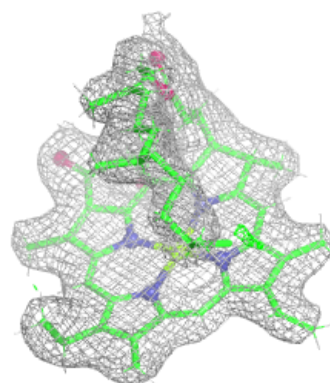
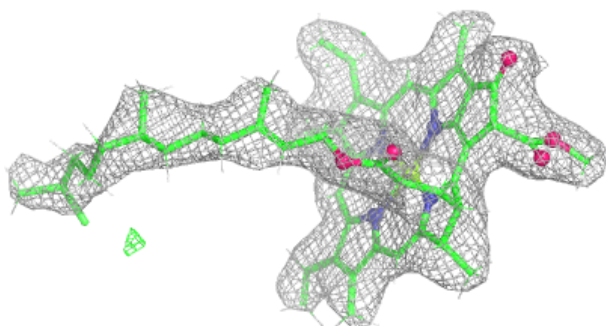
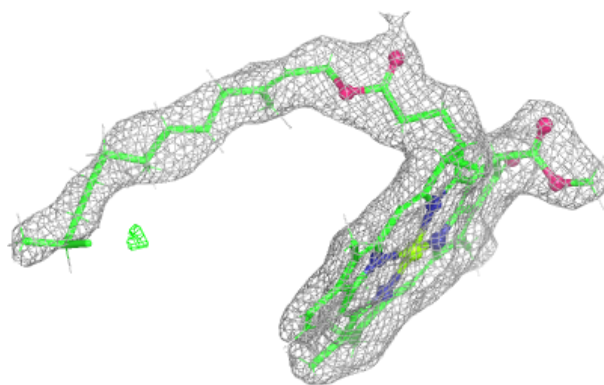
Electron density around CLA c 503:

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

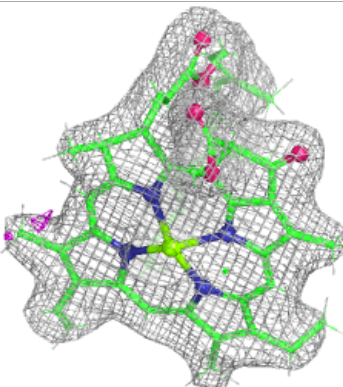
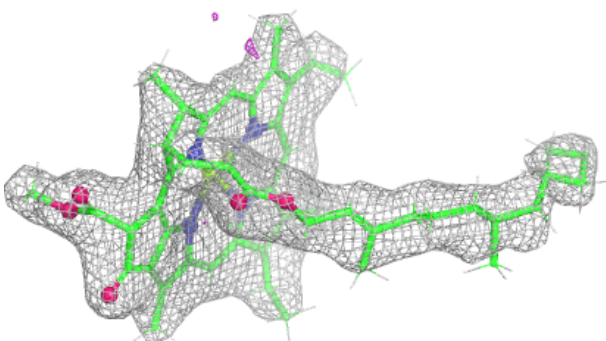
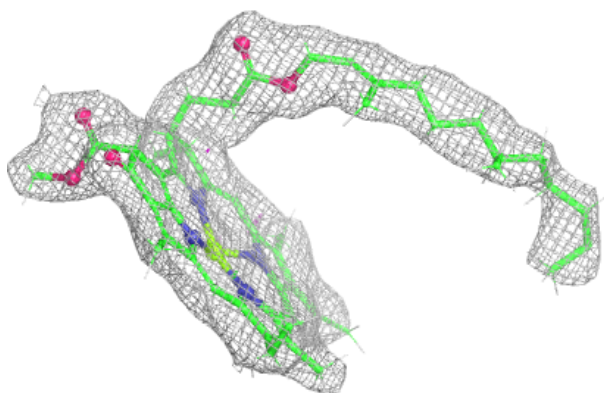


Electron density around CLA c 504:

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

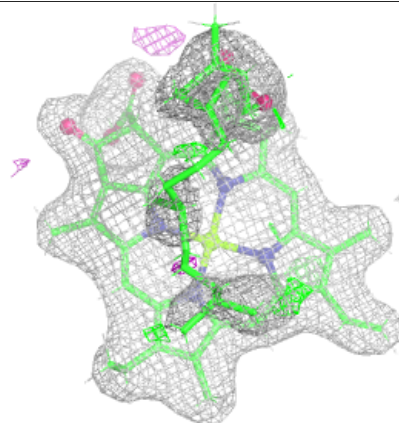
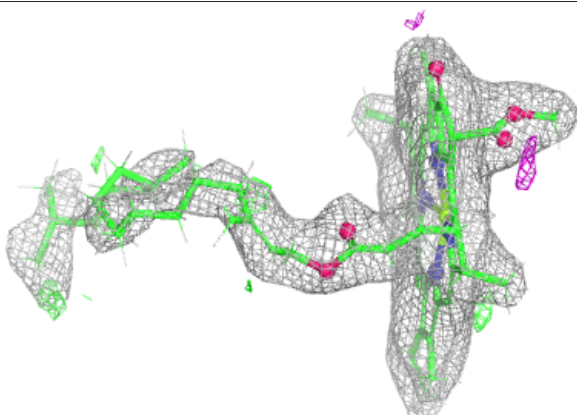
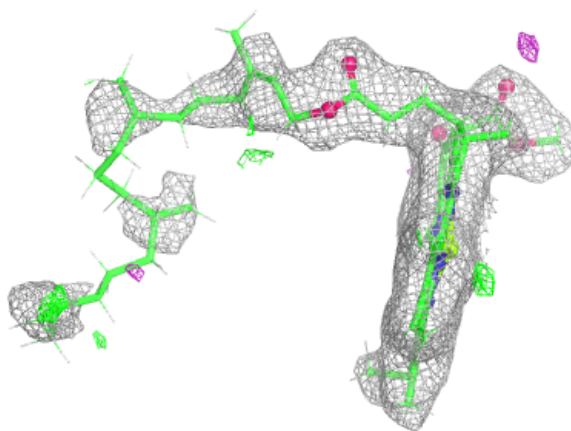
**Electron density around CLA C 504:**

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



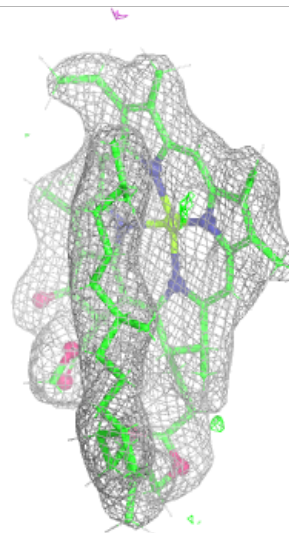
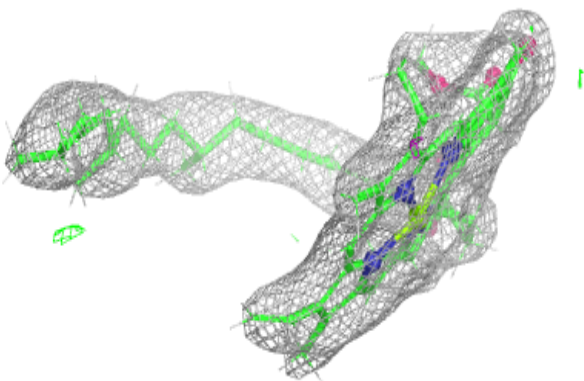
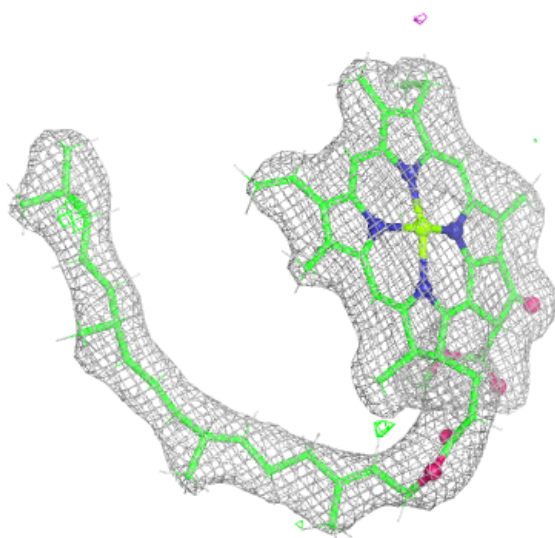
Electron density around CLA c 506:

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



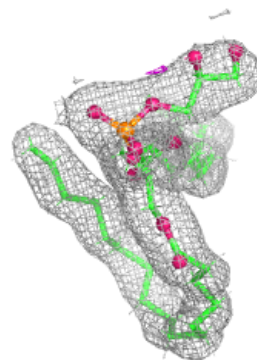
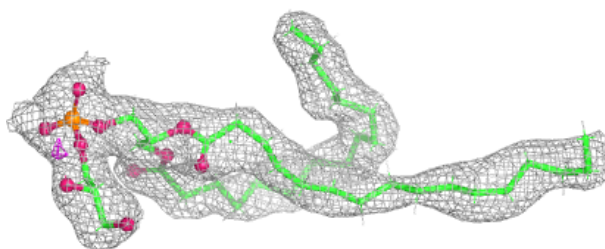
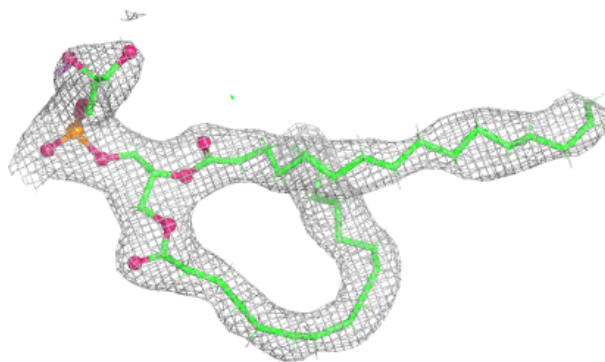
Electron density around CLA c 507:

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

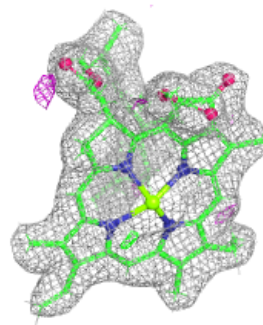
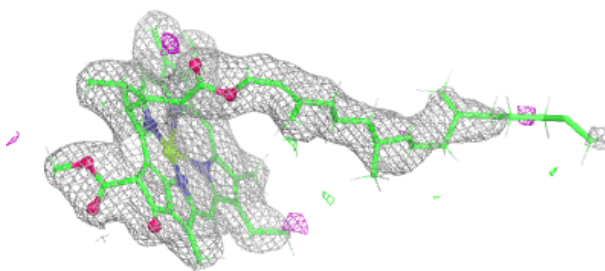
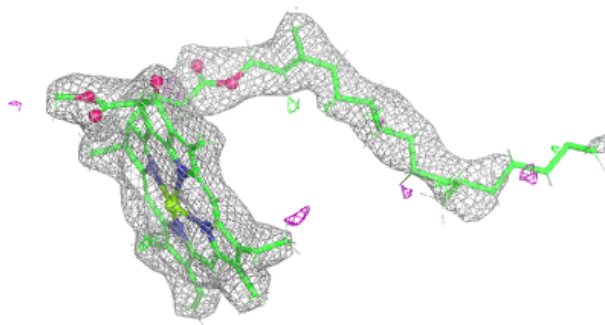


Electron density around LHG D 411:

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

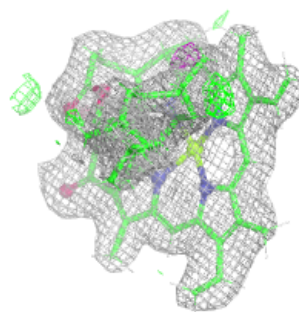
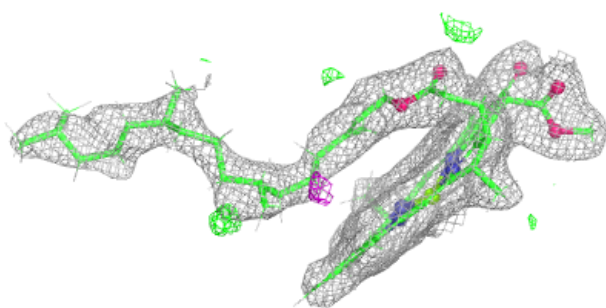
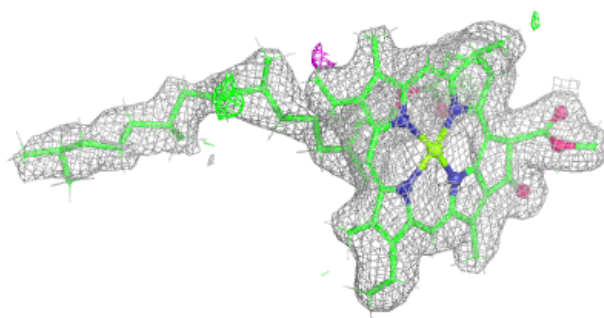
**Electron density around CLA c 508:**

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



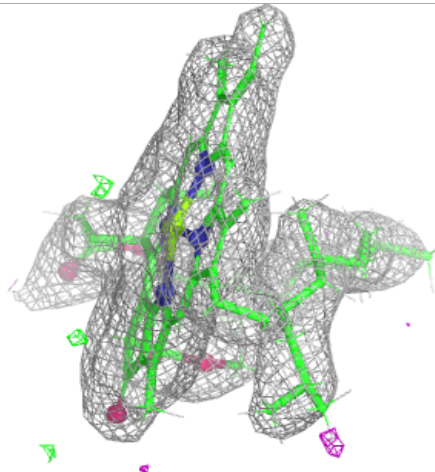
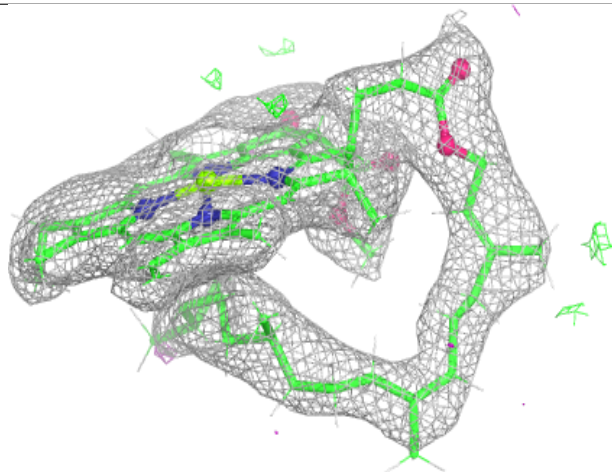
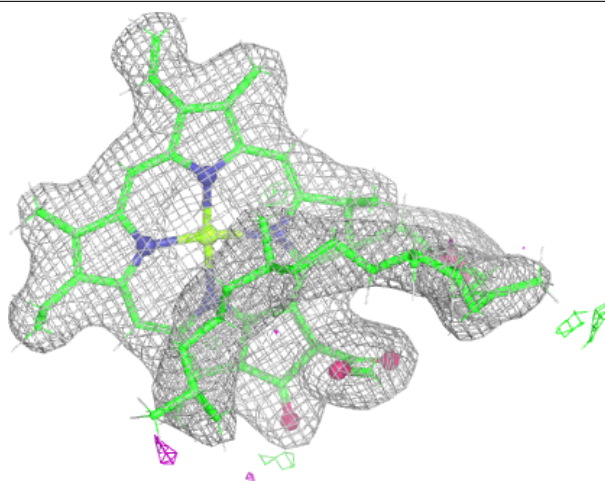
Electron density around CLA C 505:

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



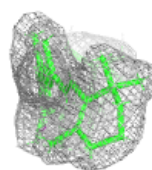
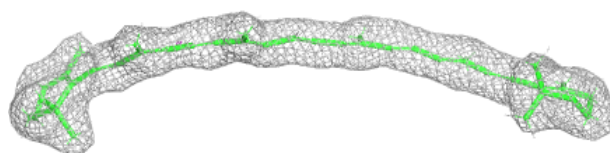
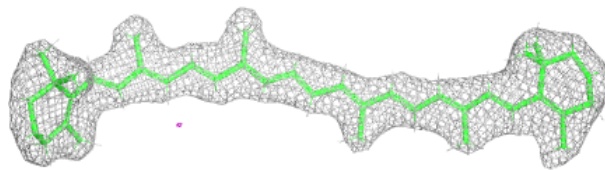
Electron density around CLA c 510:

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

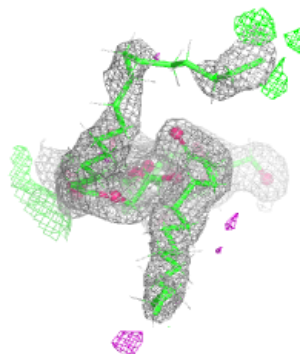
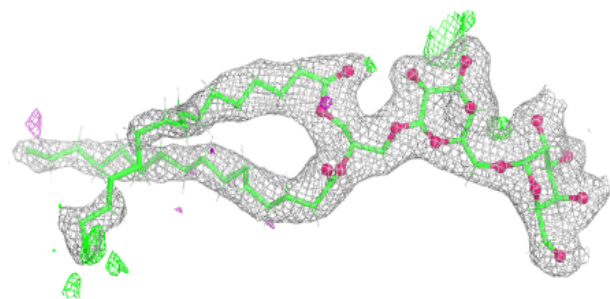
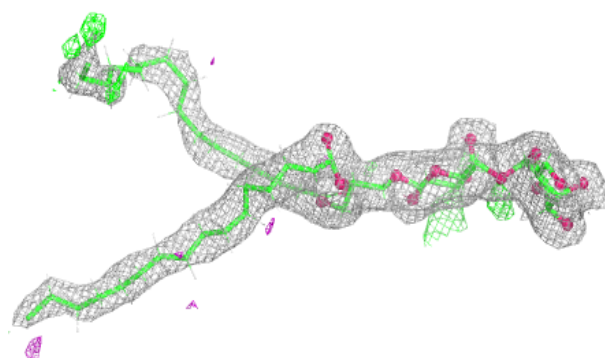


Electron density around BCR t 101:

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

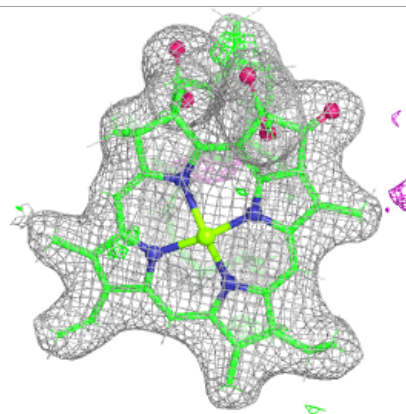
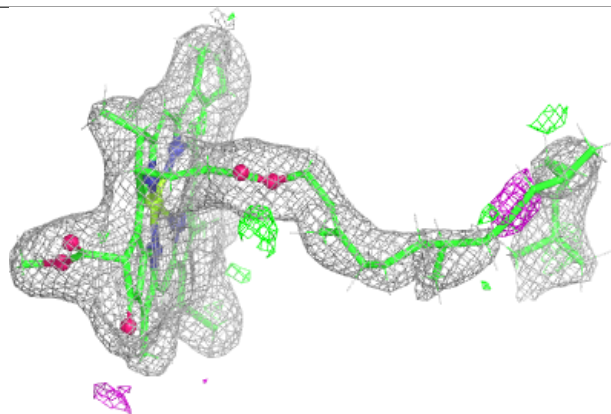
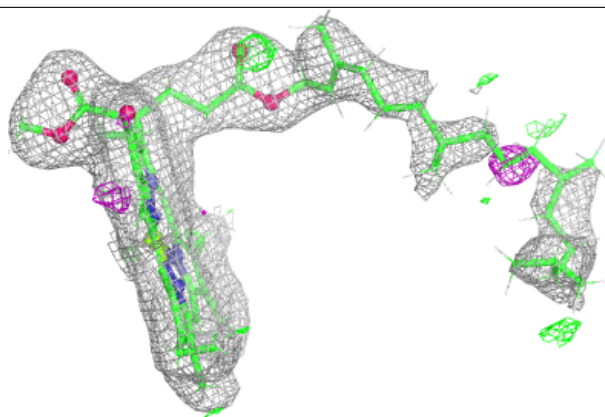
**Electron density around DGD C 515:**

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

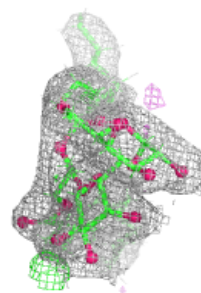
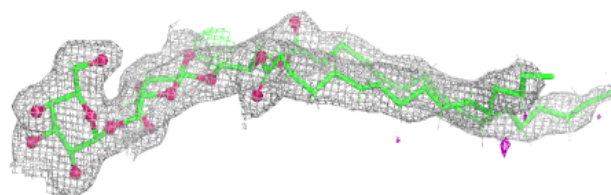
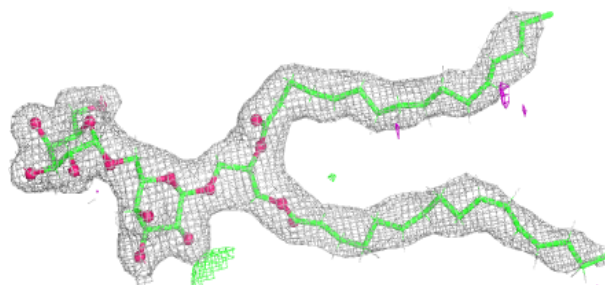


Electron density around CLA C 506:

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

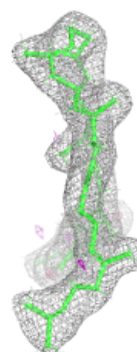
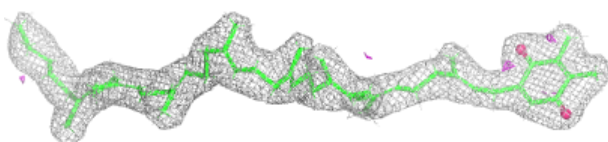
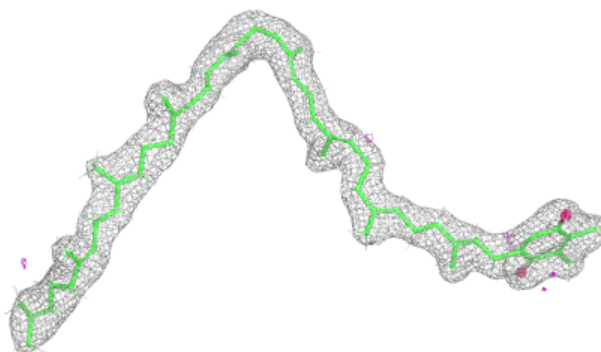
**Electron density around DGD C 517:**

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

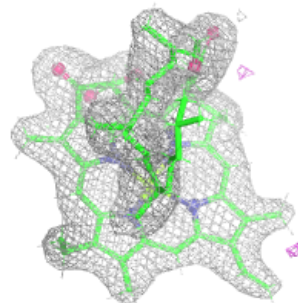
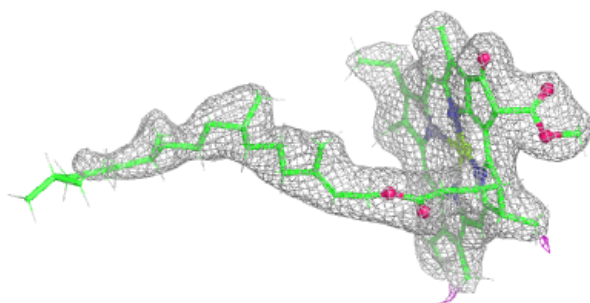
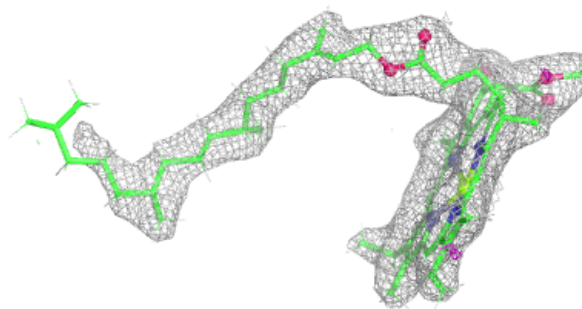


Electron density around PL9 D 406:

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

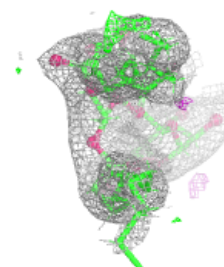
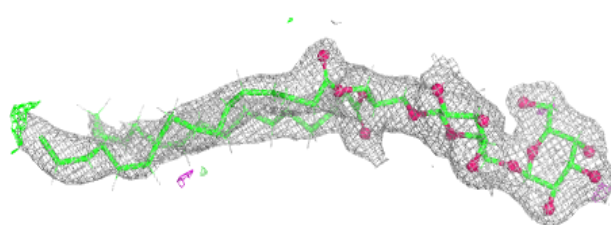
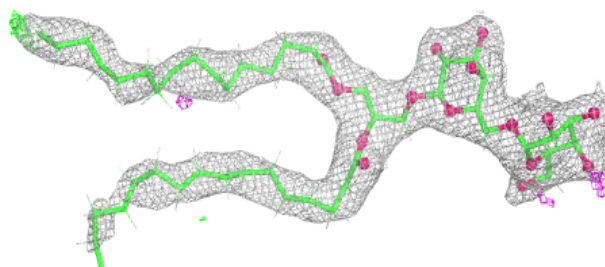
**Electron density around CLA C 508:**

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

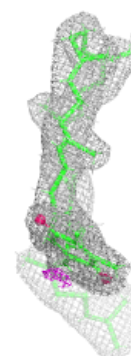
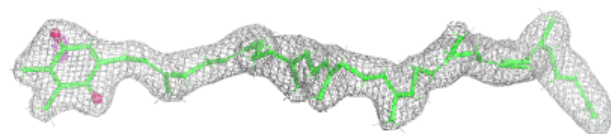
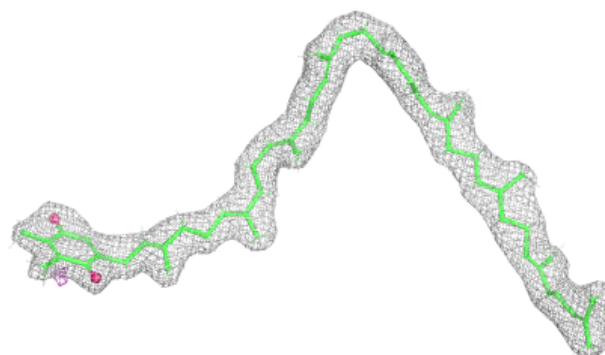


Electron density around DGD c 518:

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

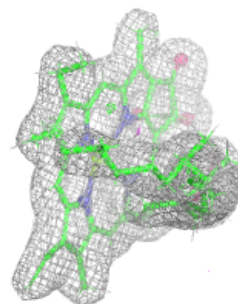
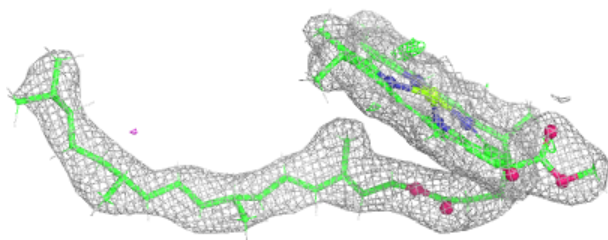
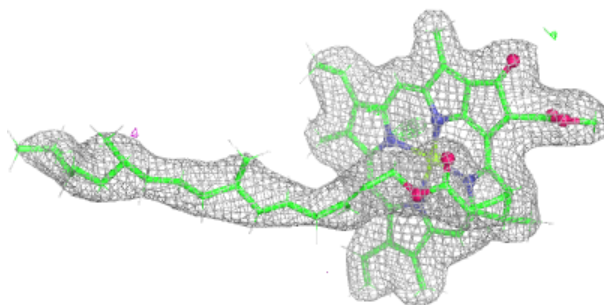
**Electron density around PL9 d 407:**

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

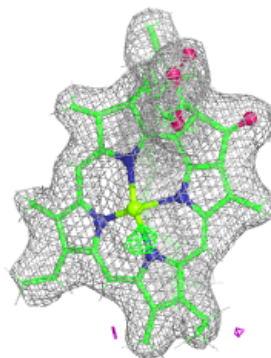
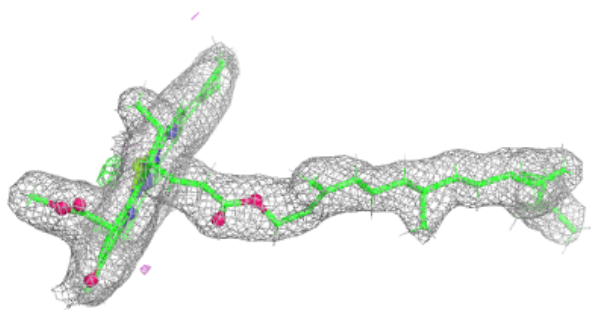
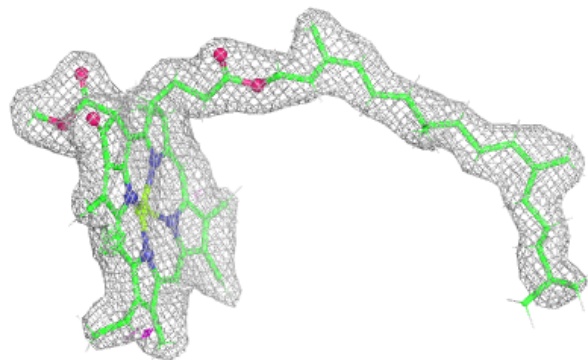


Electron density around CLA b 608:

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

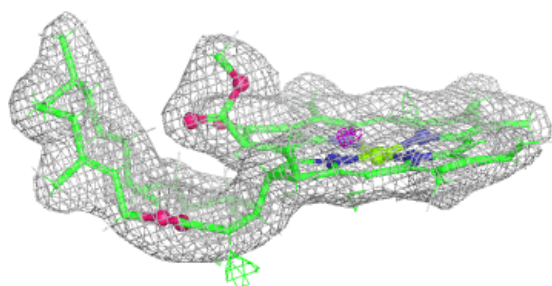
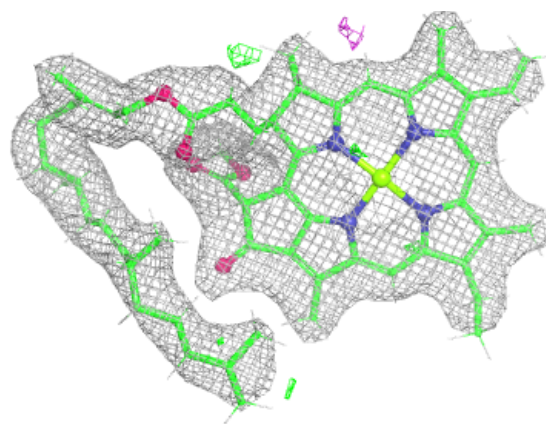
**Electron density around CLA B 609:**

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



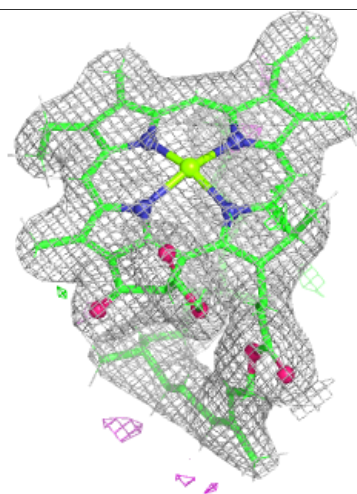
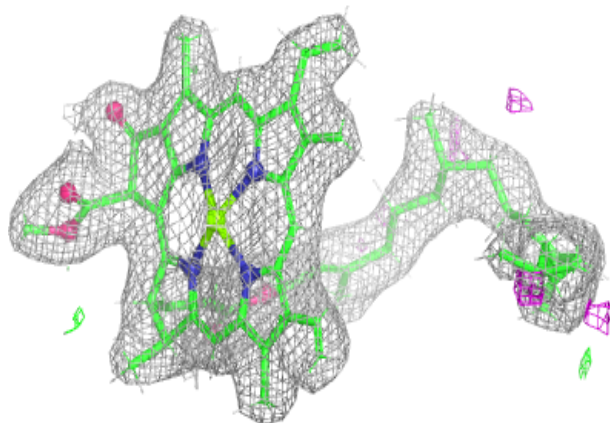
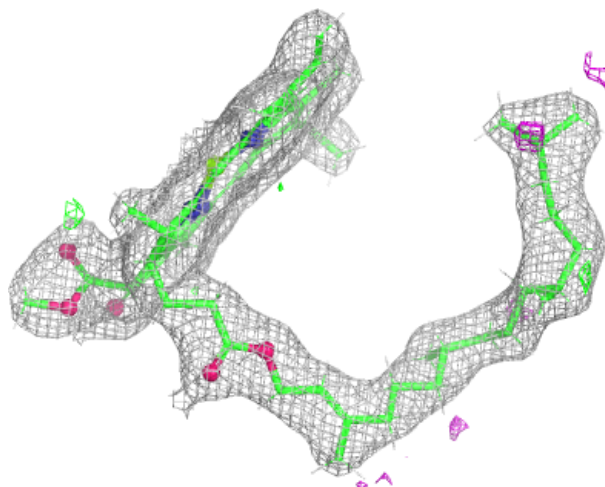
Electron density around CLA b 610:

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



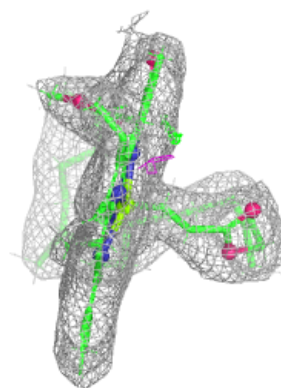
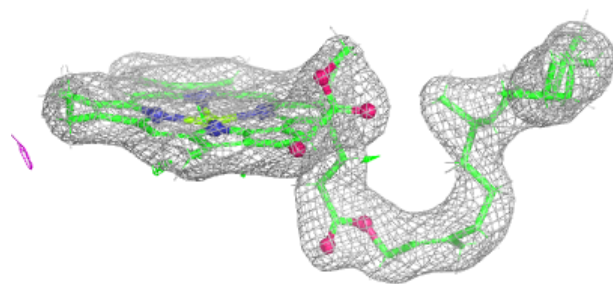
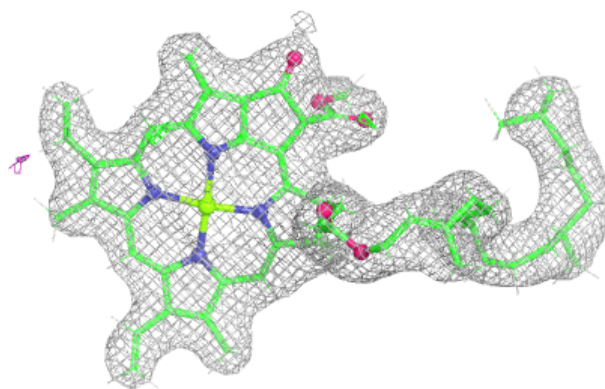
Electron density around CLA b 611:

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



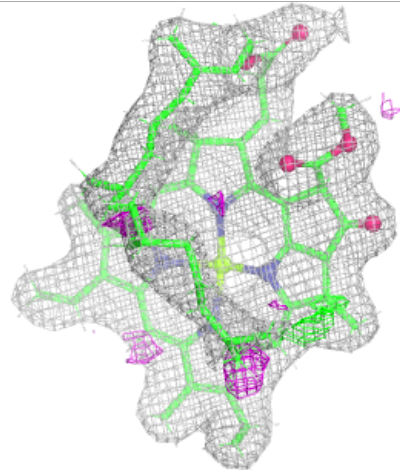
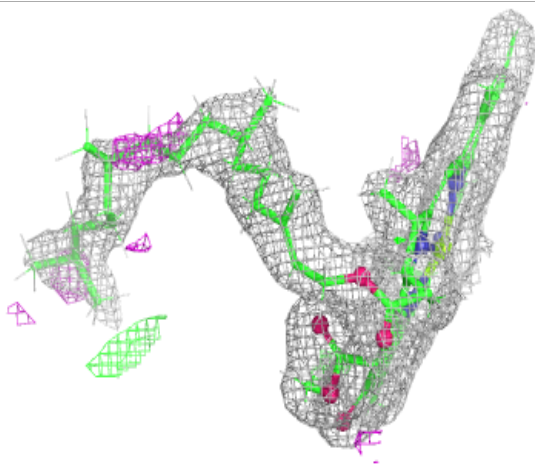
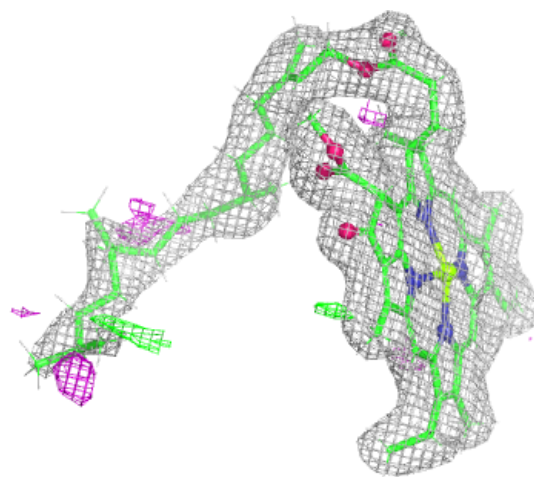
Electron density around CLA b 612:

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



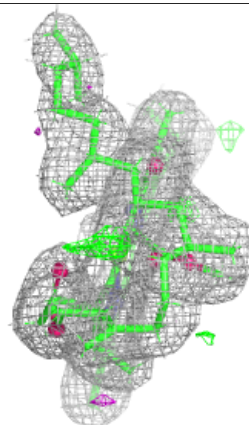
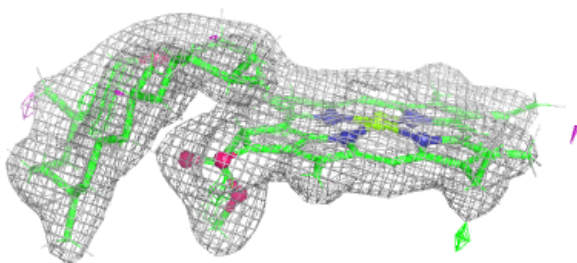
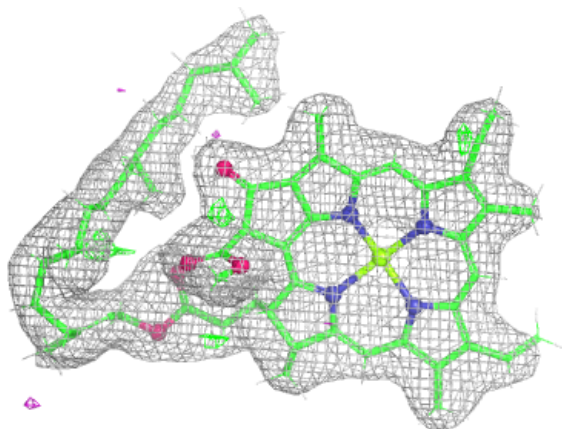
Electron density around CLA b 613:

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



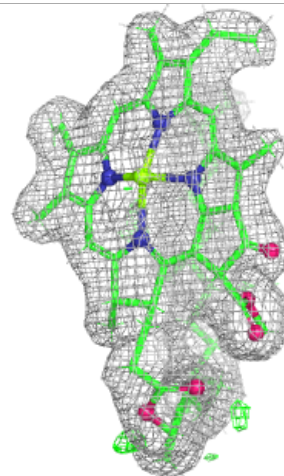
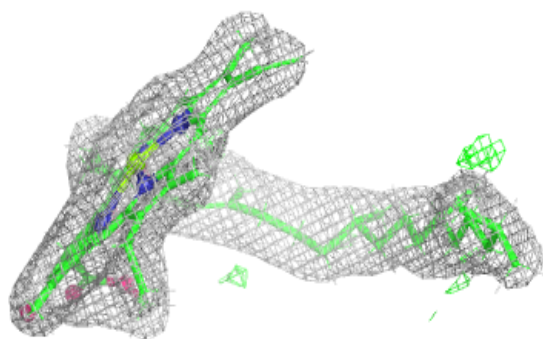
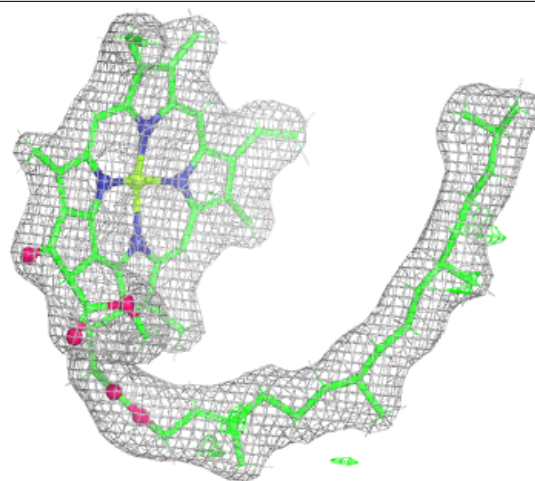
Electron density around CLA B 610:

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



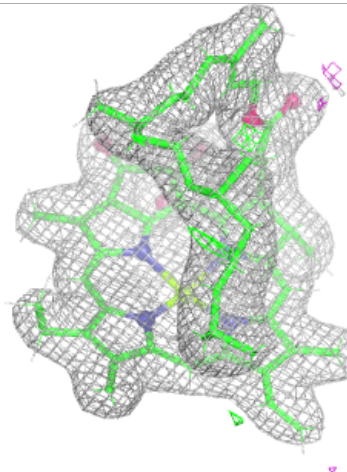
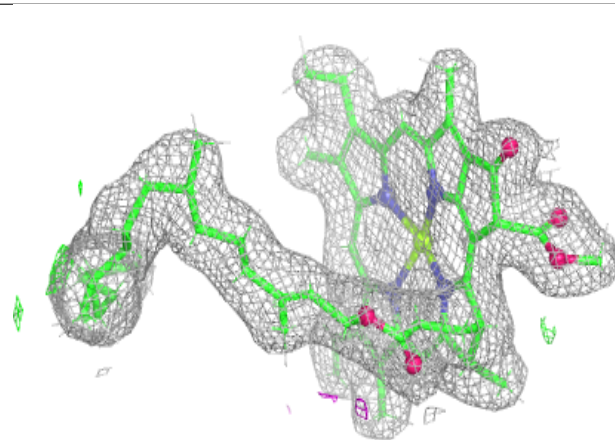
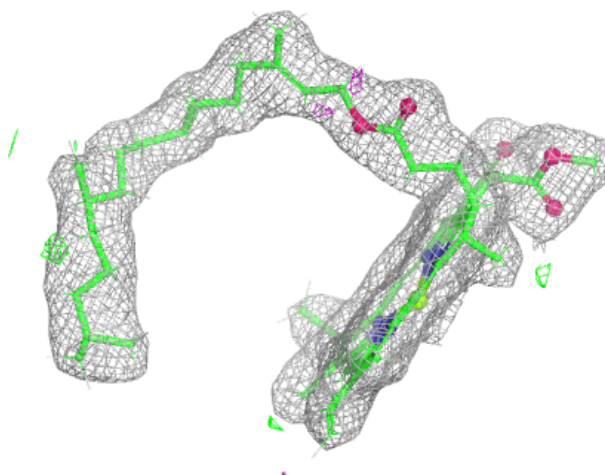
Electron density around CLA C 507:

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



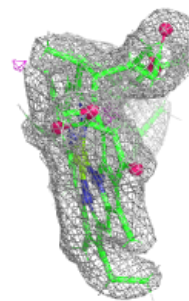
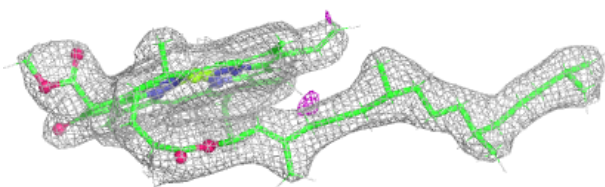
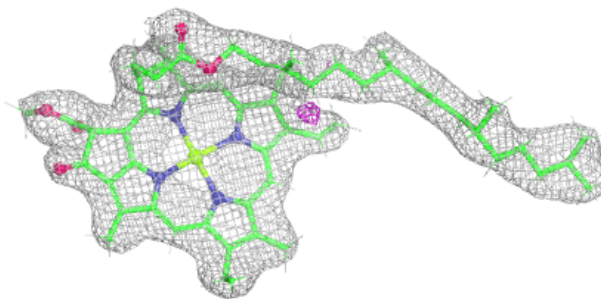
Electron density around CLA B 611:

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

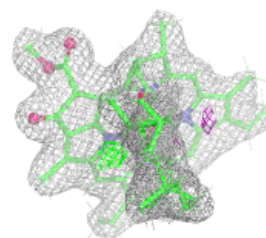
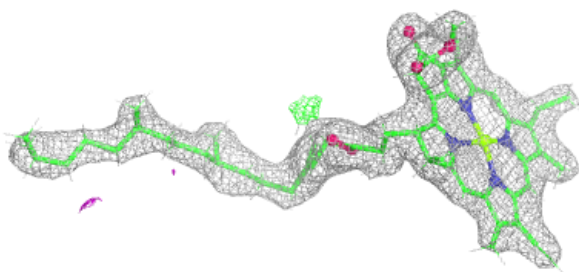
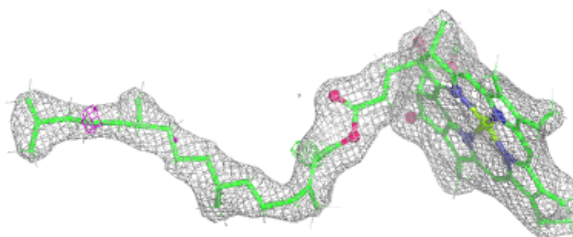


Electron density around CLA c 501:

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

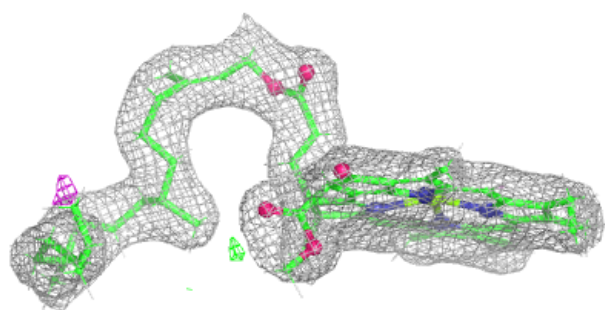
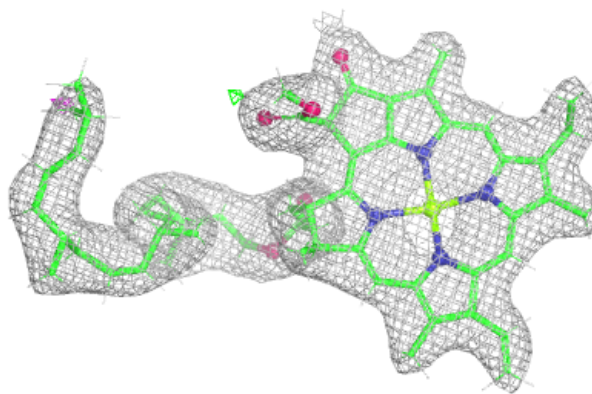
**Electron density around CLA c 502:**

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

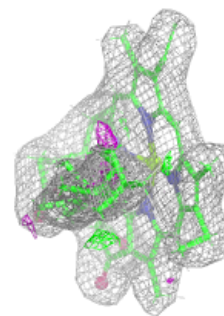
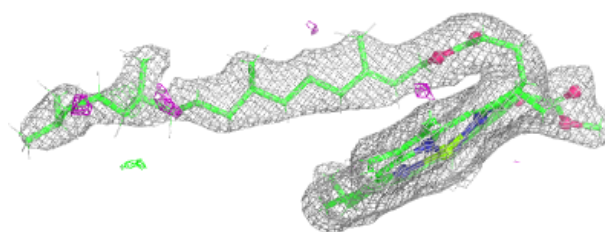
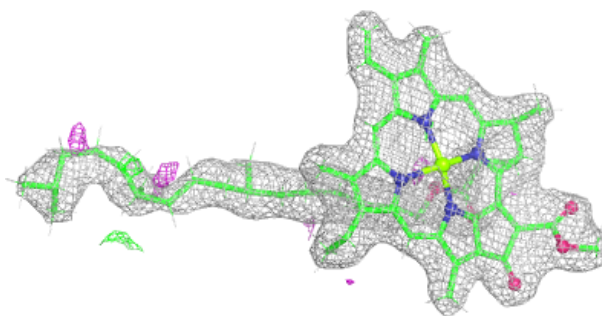


Electron density around CLA B 612:

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

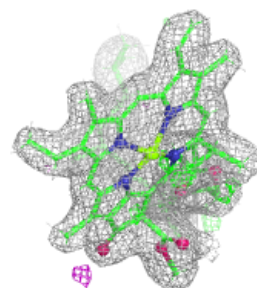
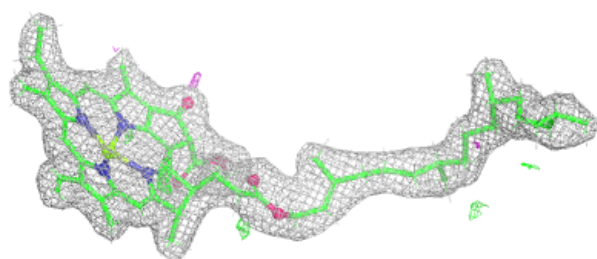
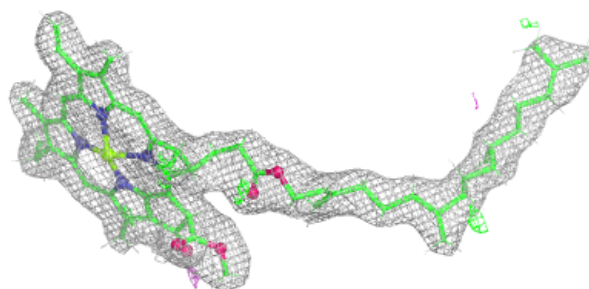
**Electron density around CLA B 614:**

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

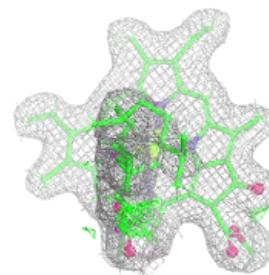
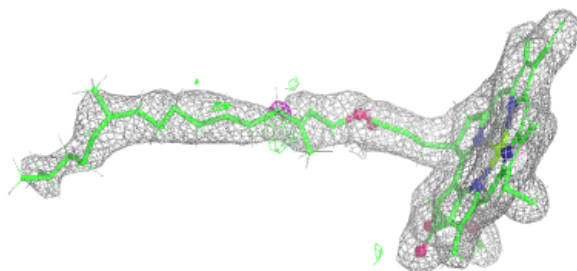
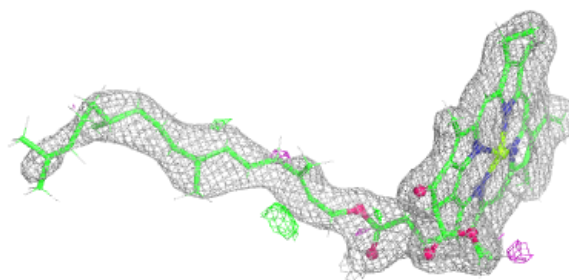


Electron density around CLA A 402:

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

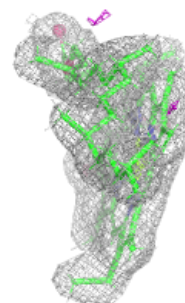
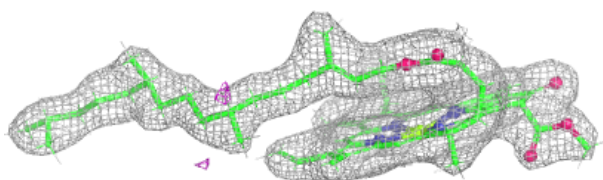
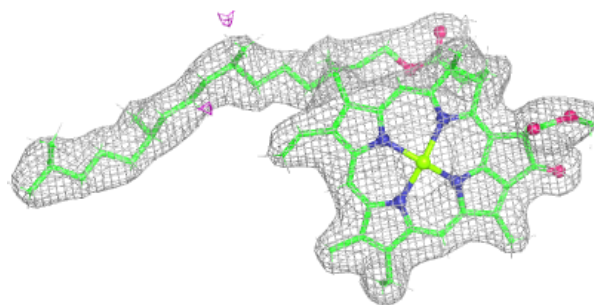
**Electron density around CLA B 604:**

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

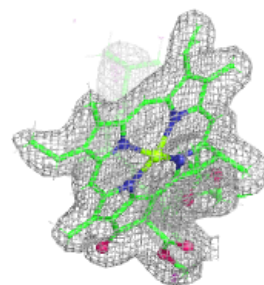
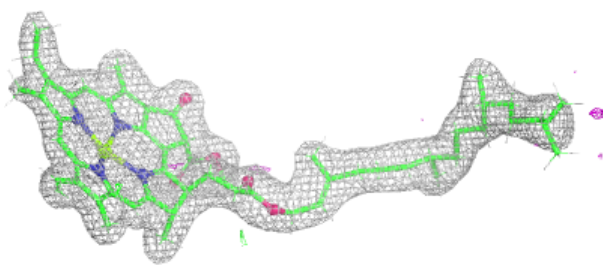
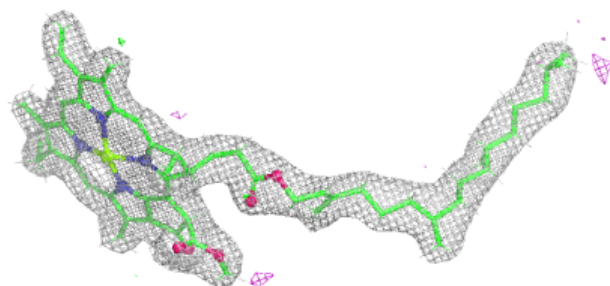


Electron density around CLA C 501:

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

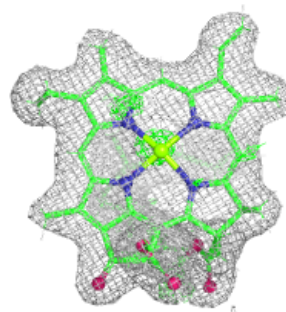
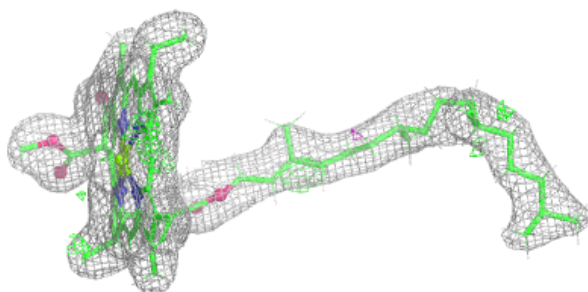
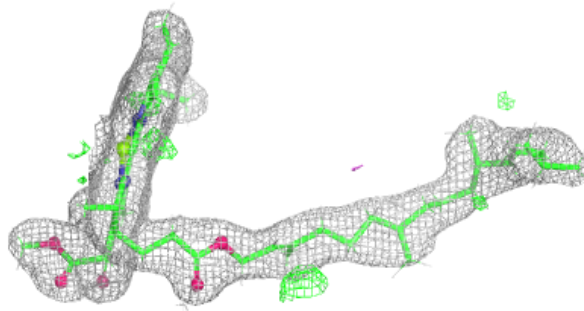
**Electron density around CLA a 402:**

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



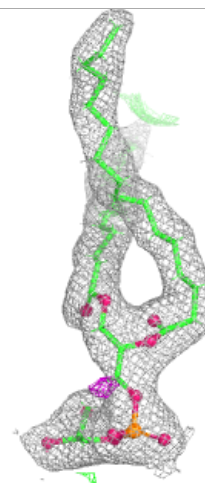
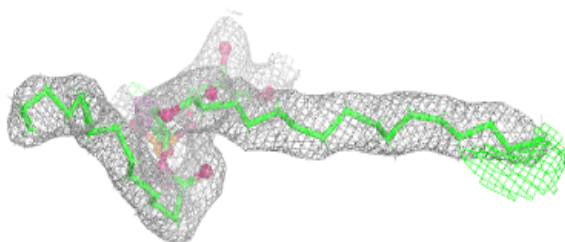
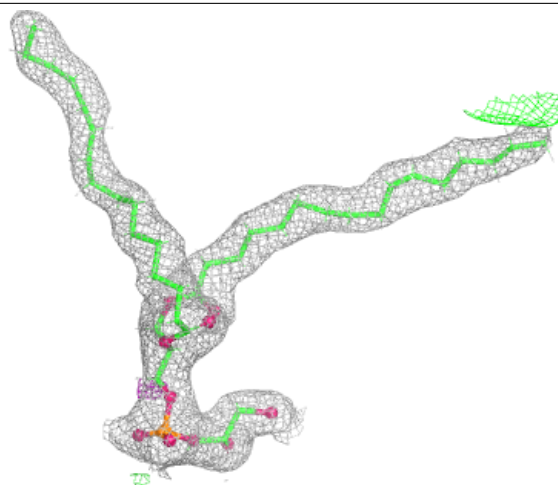
Electron density around CLA B 605:

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



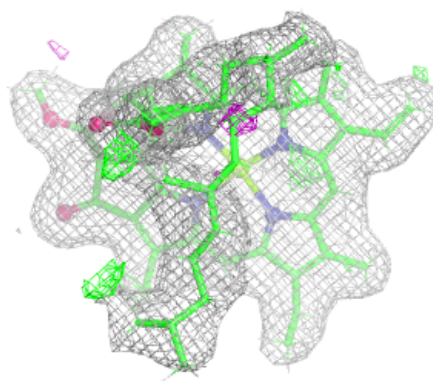
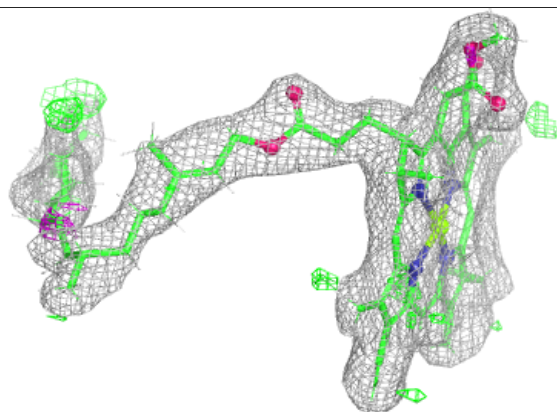
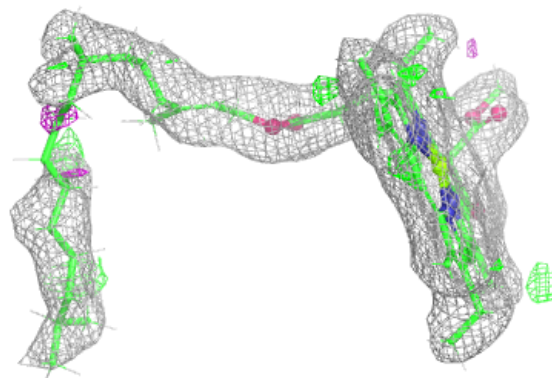
Electron density around LHG L 101:

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

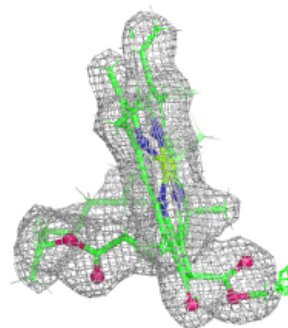
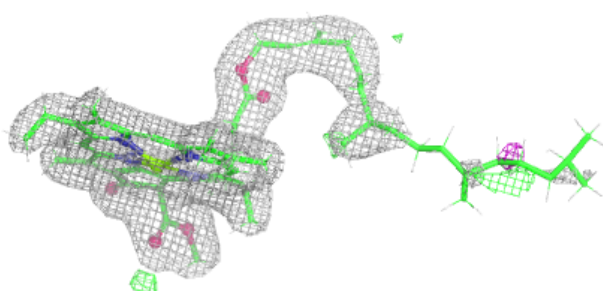
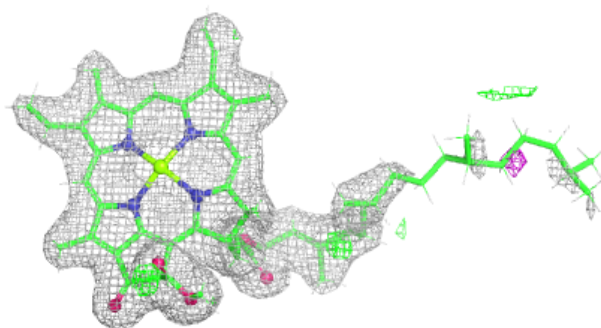


Electron density around CLA a 405:

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

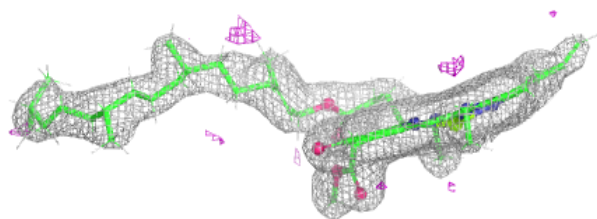
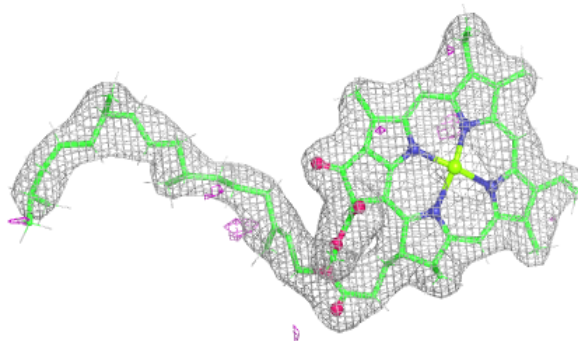
**Electron density around CLA A 403:**

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



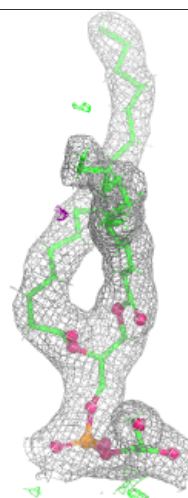
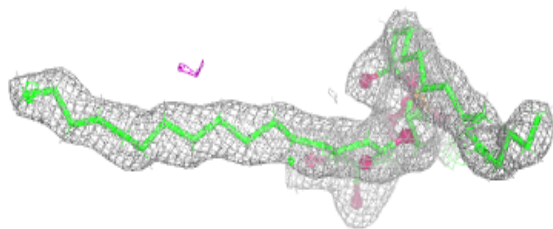
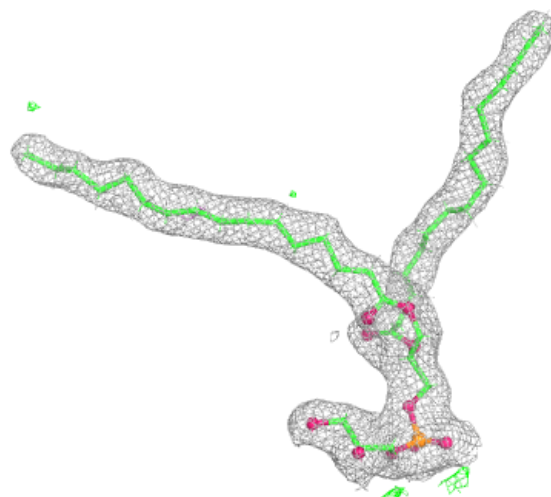
Electron density around CLA b 602:

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



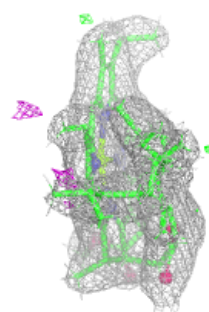
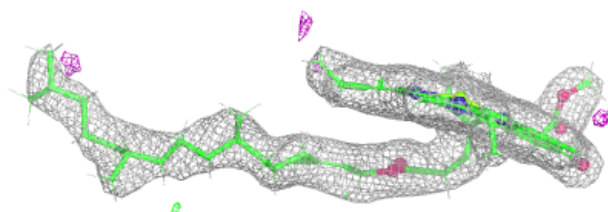
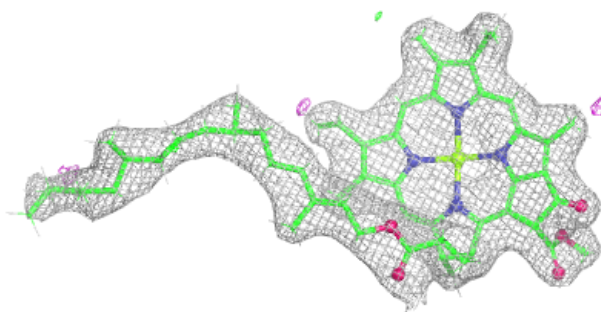
Electron density around LHG 1 101:

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

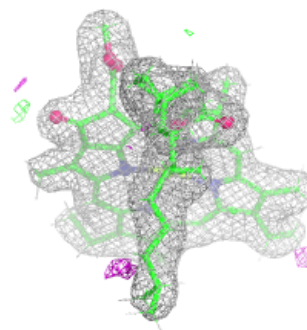
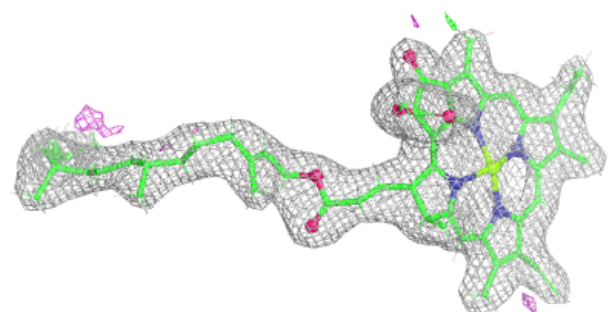
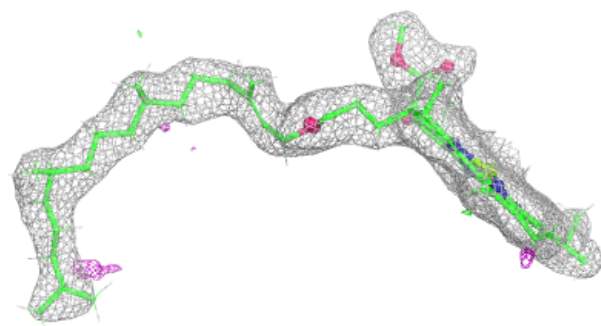


Electron density around CLA b 603:

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

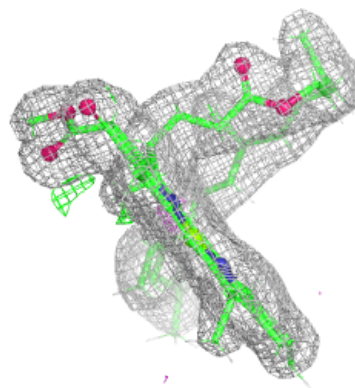
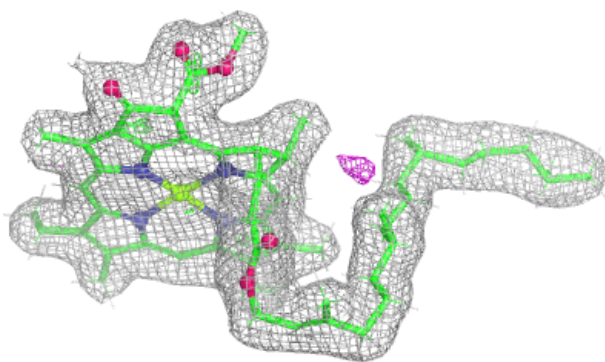
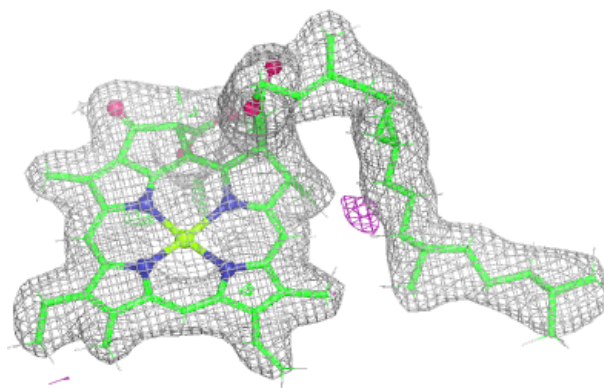
**Electron density around CLA d 403:**

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

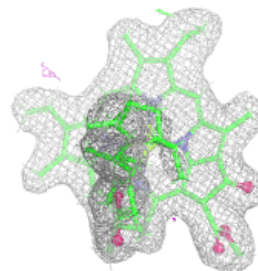
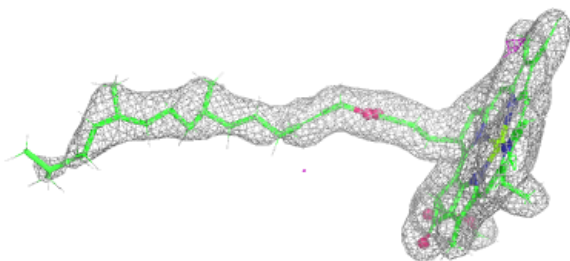
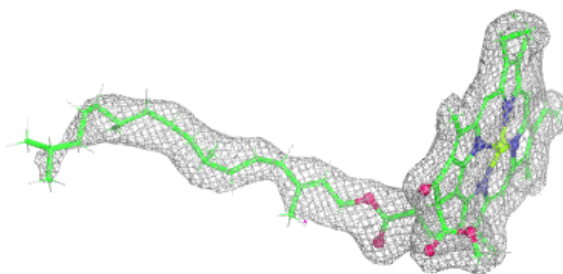


Electron density around CLA d 404:

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

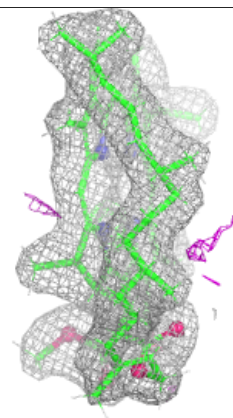
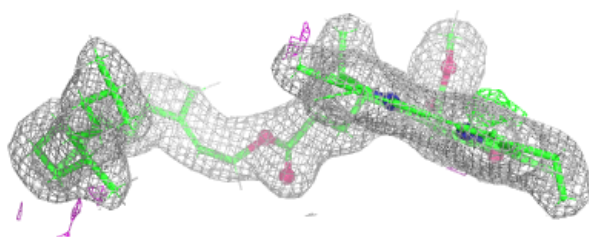
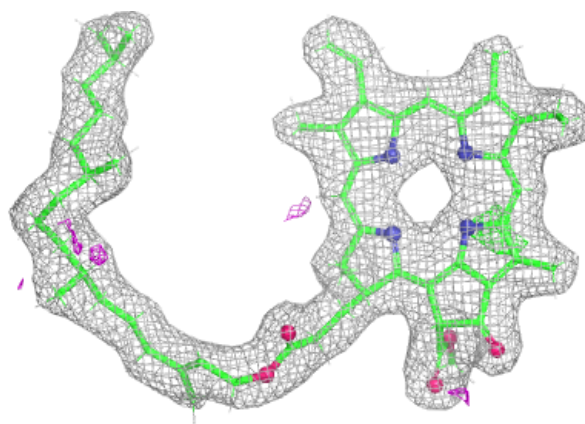
**Electron density around CLA b 604:**

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

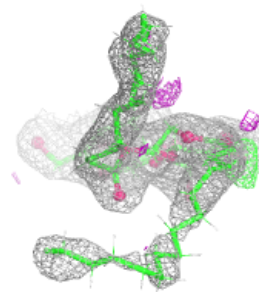
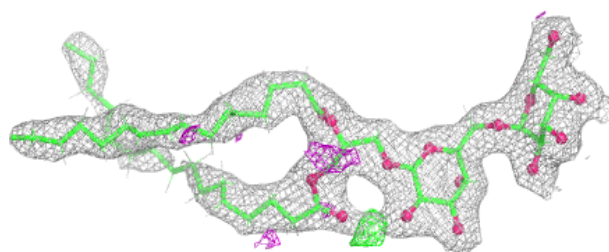
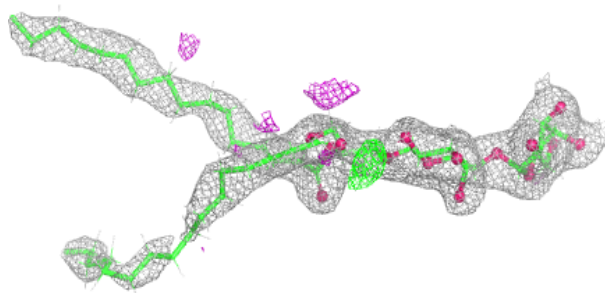


Electron density around PHO A 404:

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

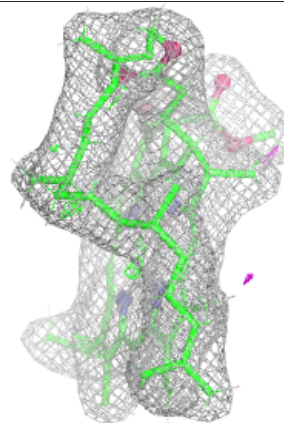
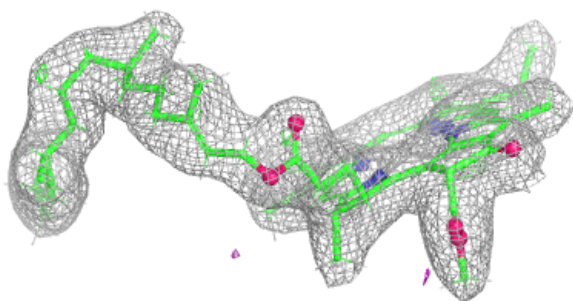
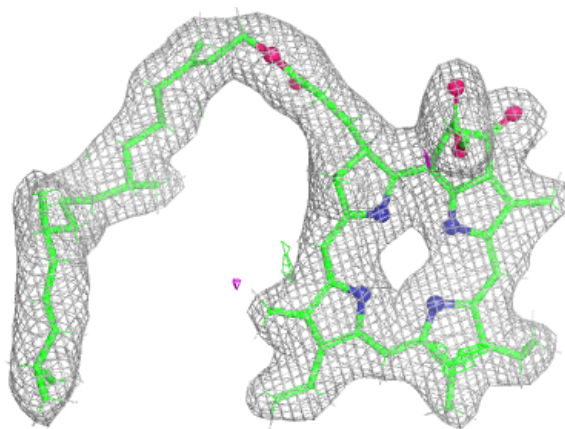
**Electron density around DGD c 516:**

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



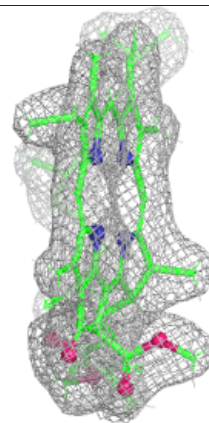
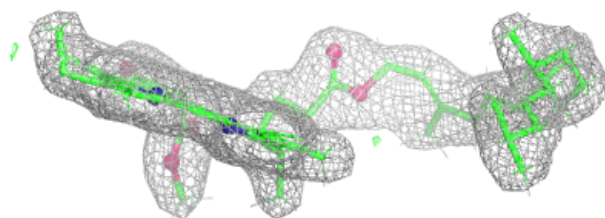
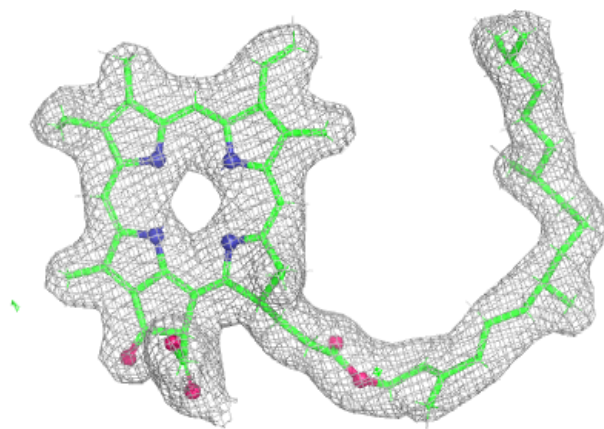
Electron density around PHO A 405:

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

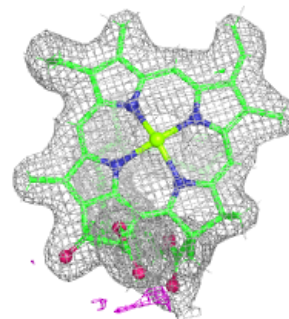
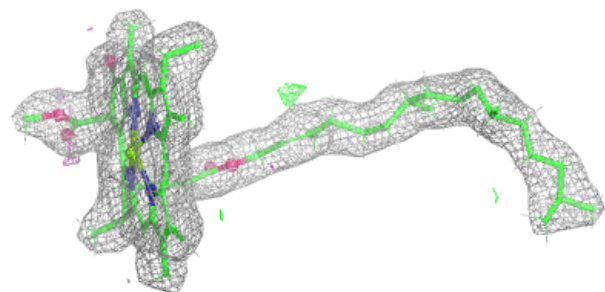
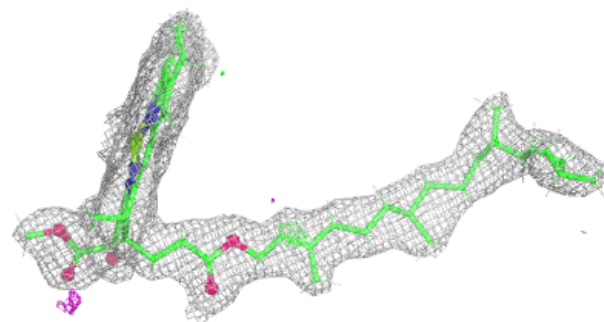


Electron density around PHO a 404:

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

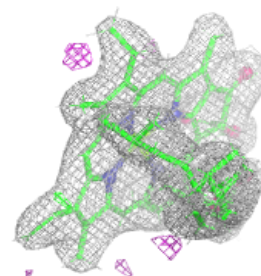
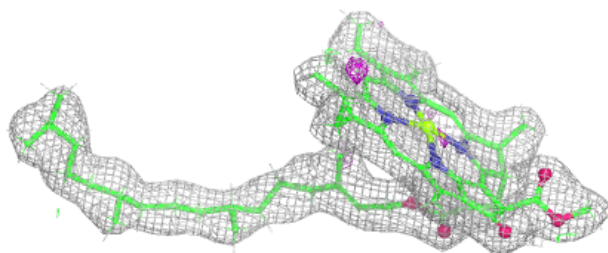
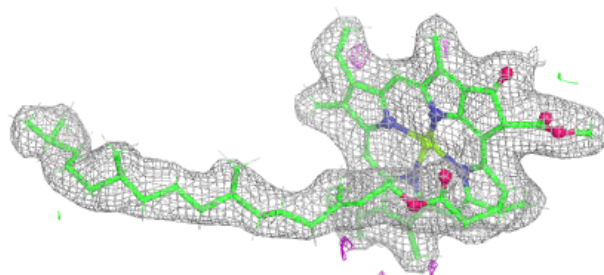
**Electron density around CLA b 605:**

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

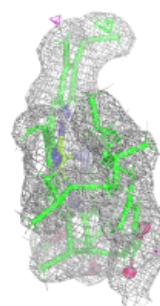
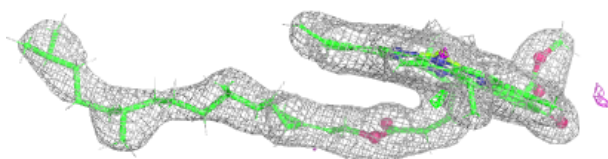
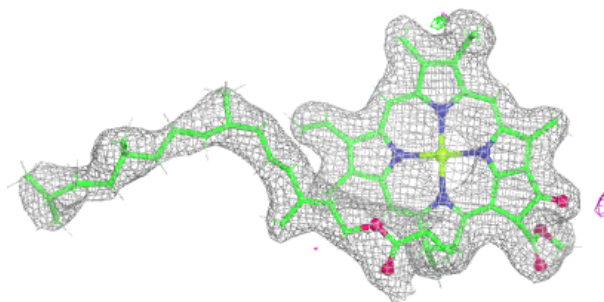


Electron density around CLA B 608:

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

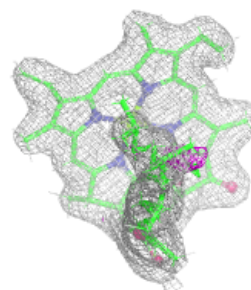
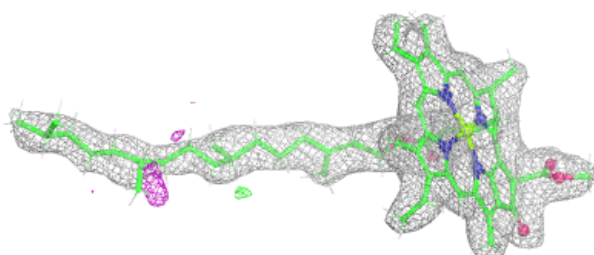
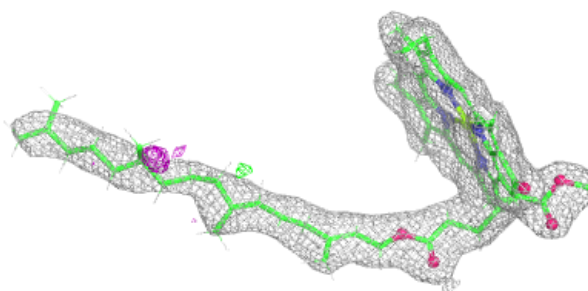
**Electron density around CLA B 603:**

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

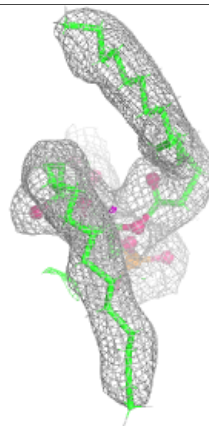
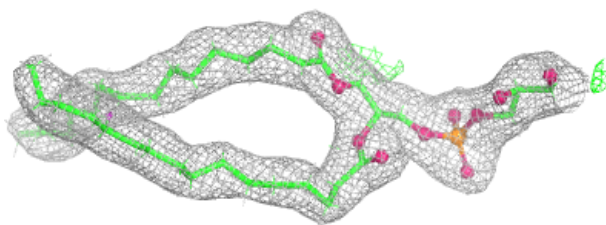
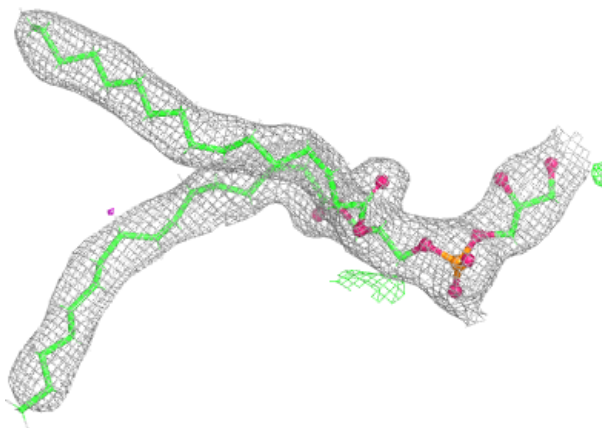


Electron density around CLA b 607:

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

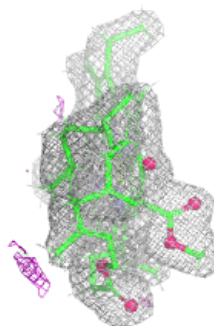
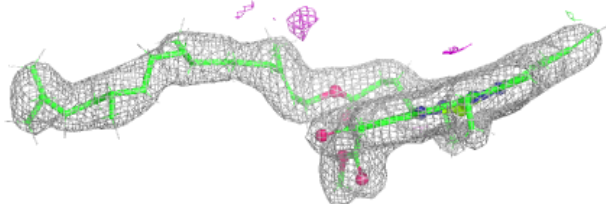
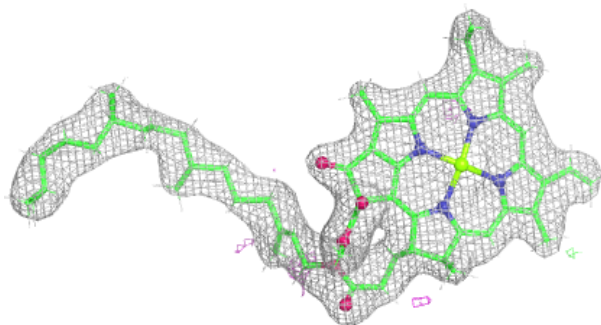
**Electron density around LHG d 408:**

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



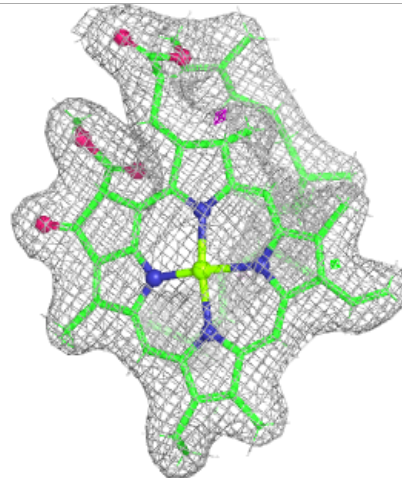
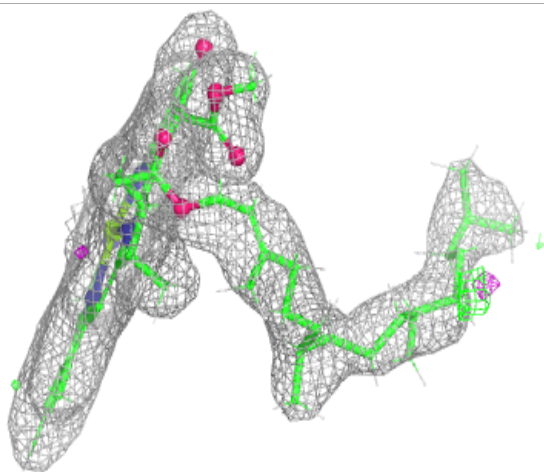
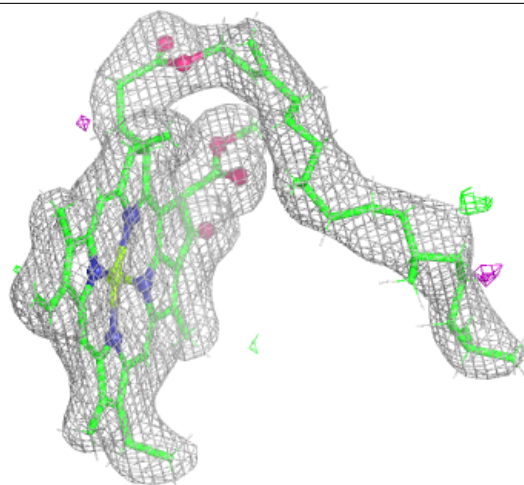
Electron density around CLA B 602:

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



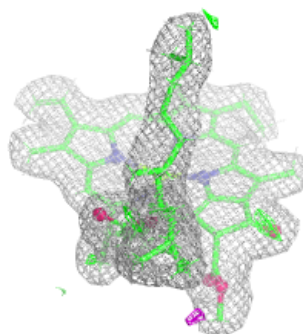
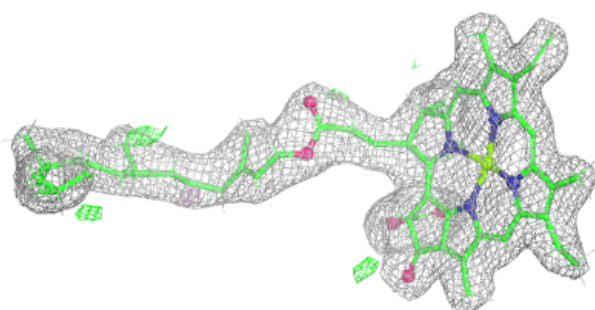
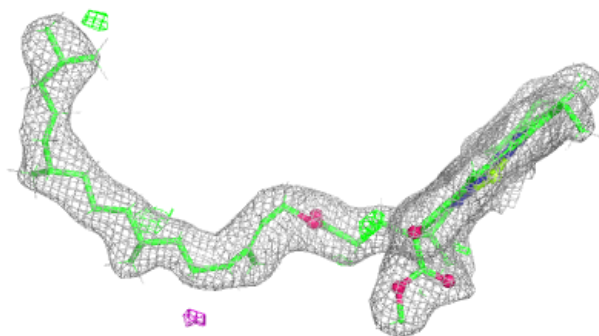
Electron density around CLA B 613:

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

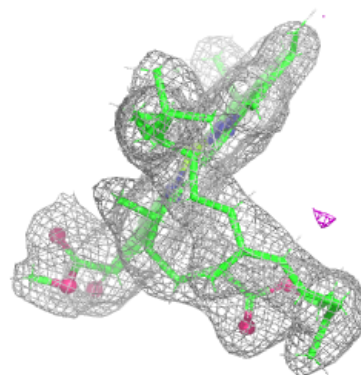
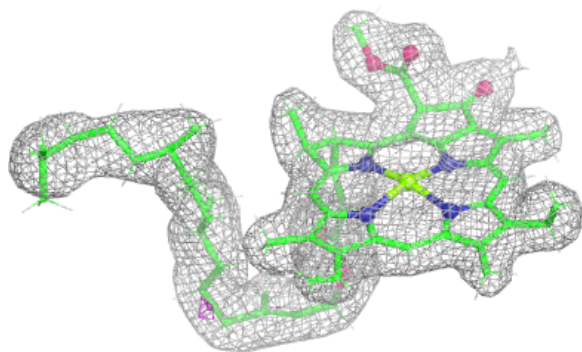
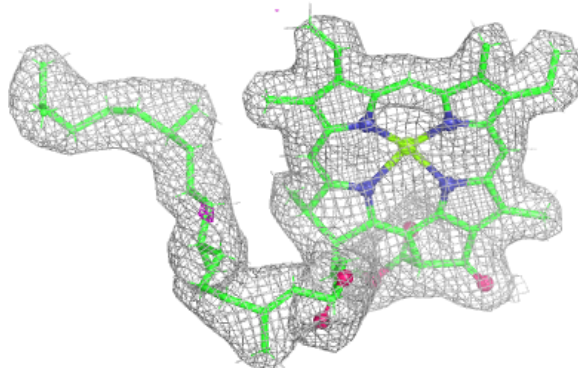


Electron density around CLA D 402:

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

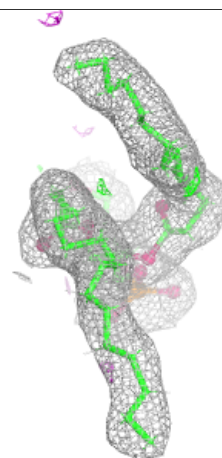
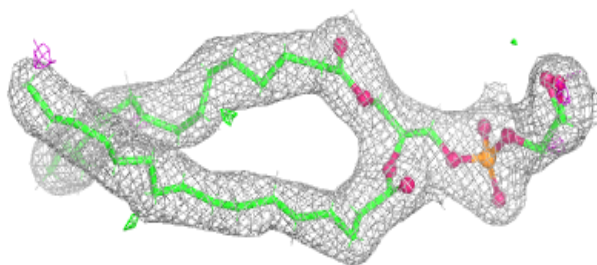
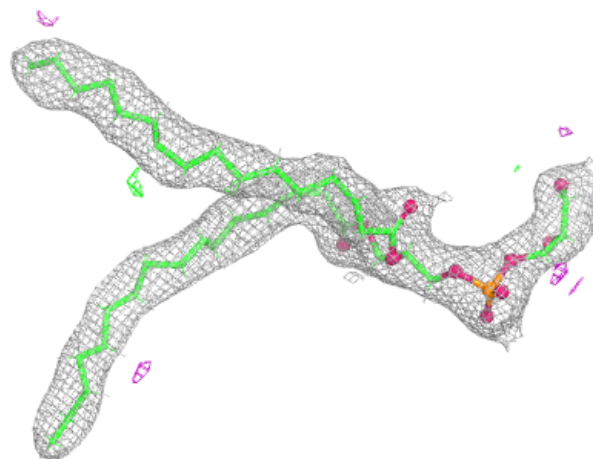
**Electron density around CLA D 403:**

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



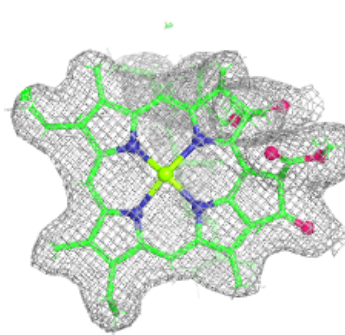
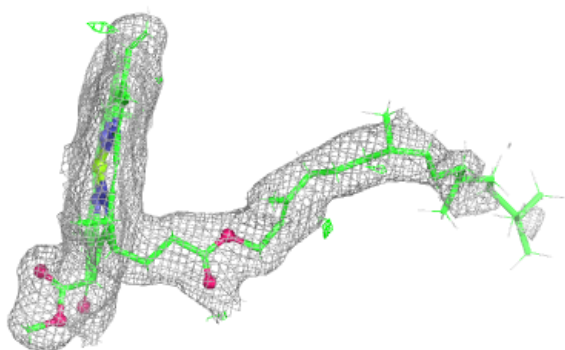
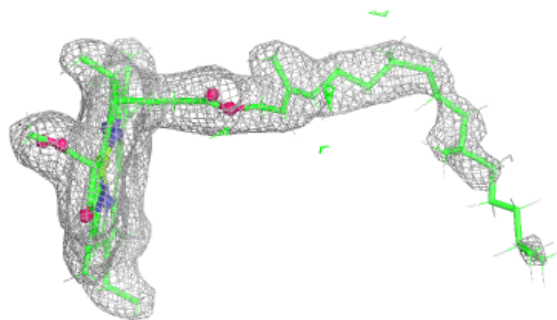
Electron density around LHG D 408:

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

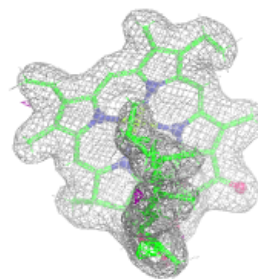
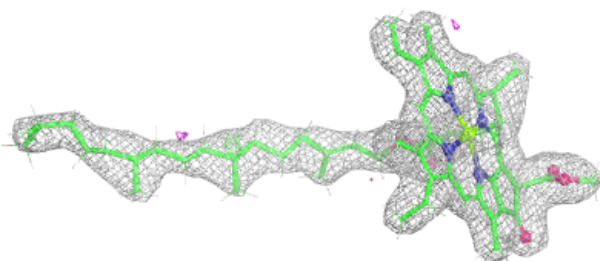
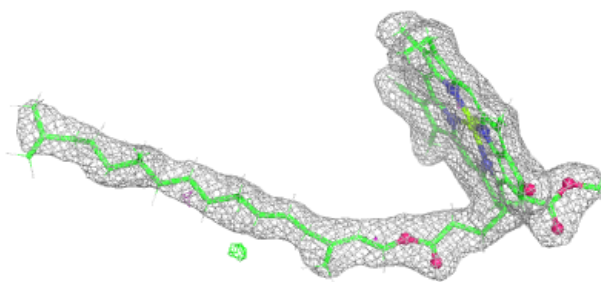


Electron density around CLA D 404:

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

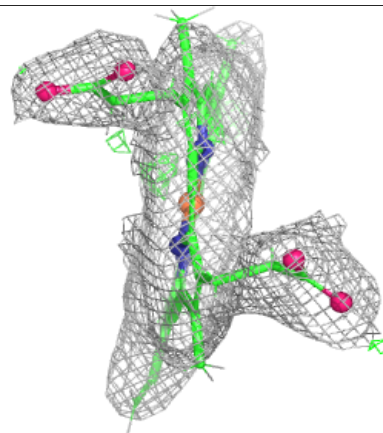
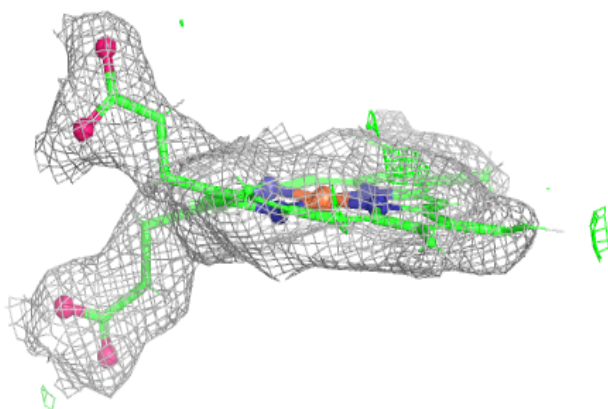
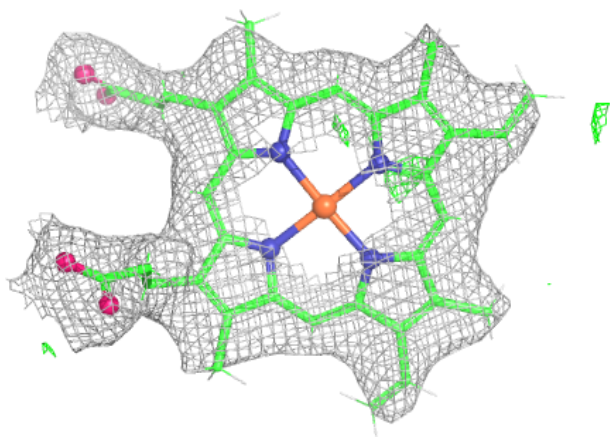
**Electron density around CLA B 607:**

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



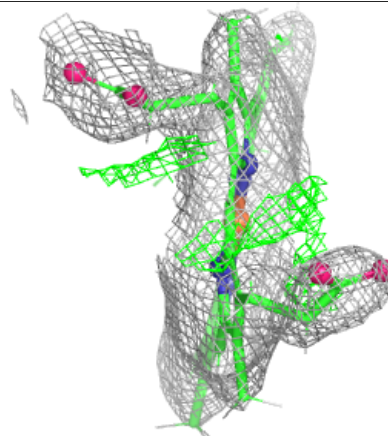
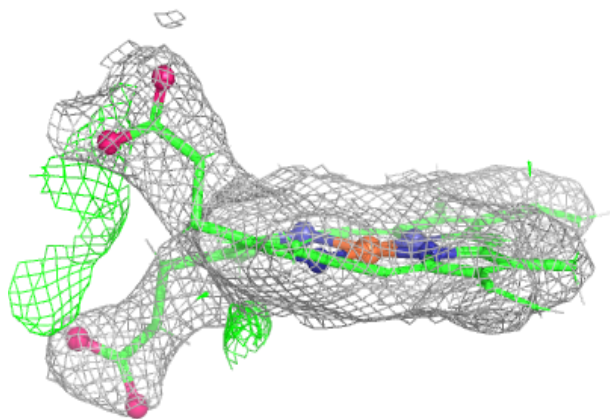
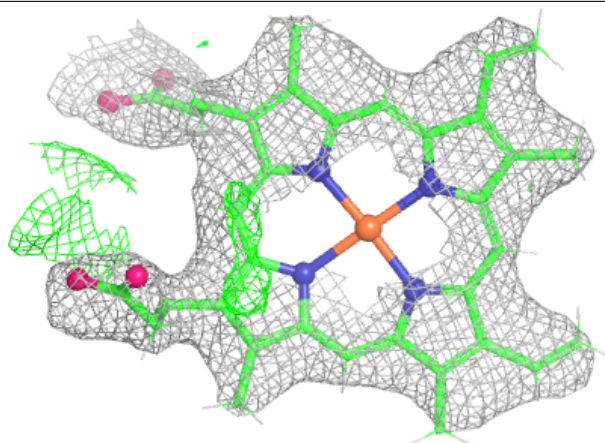
Electron density around HEM F 101:

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



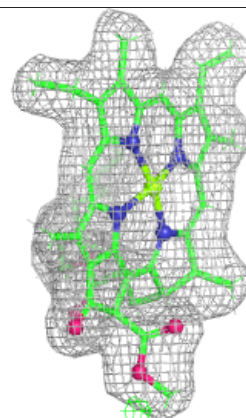
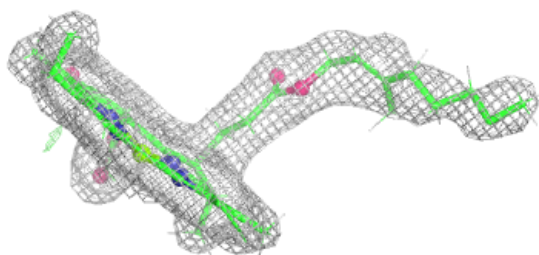
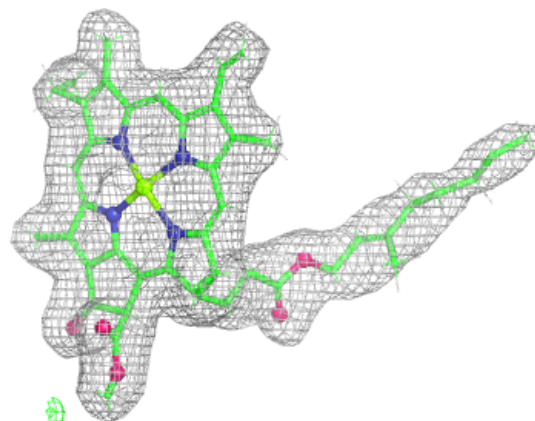
Electron density around HEM f 101:

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



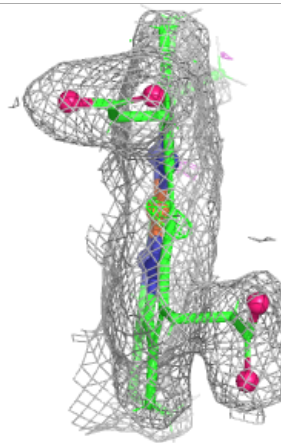
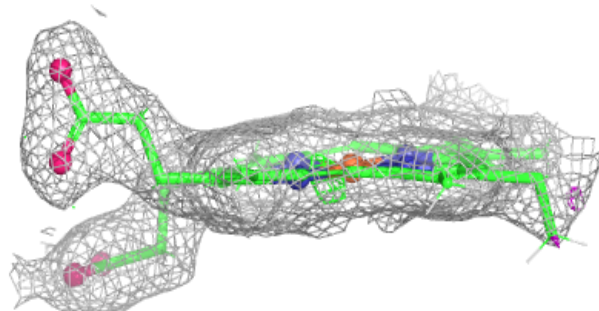
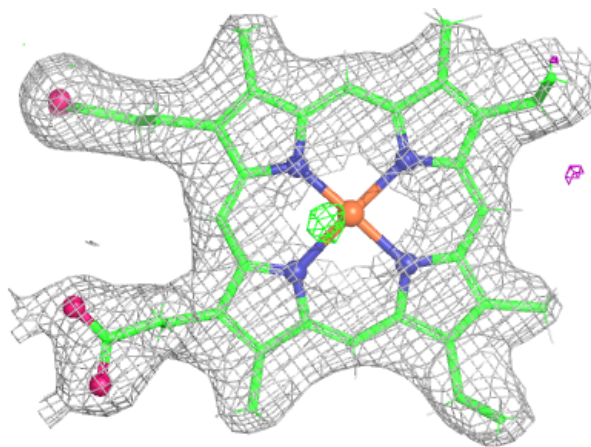
Electron density around CLA A 406:

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



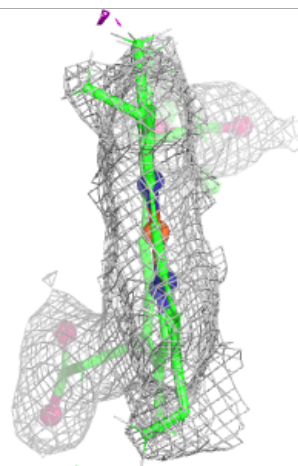
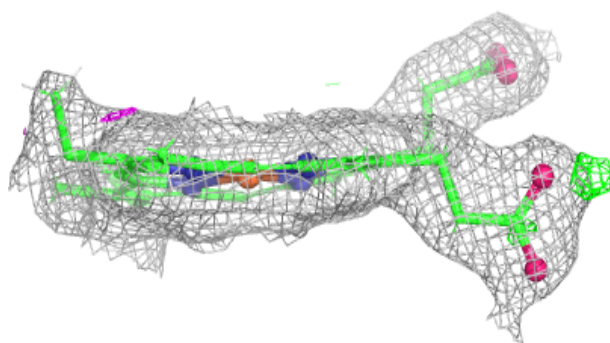
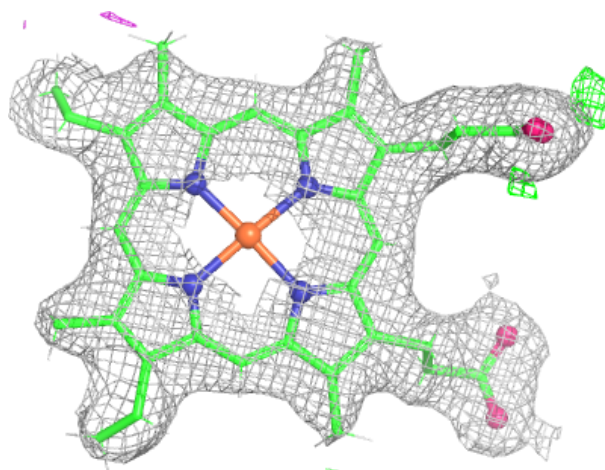
Electron density around HEC V 201:

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



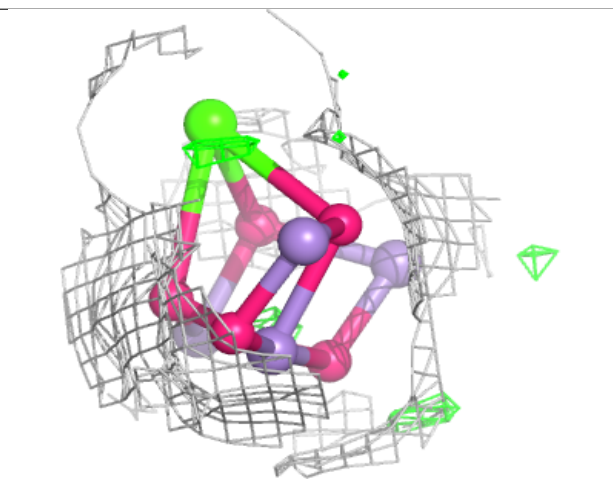
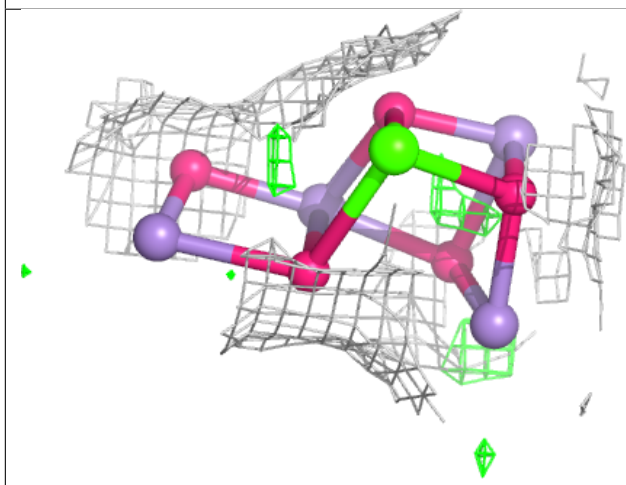
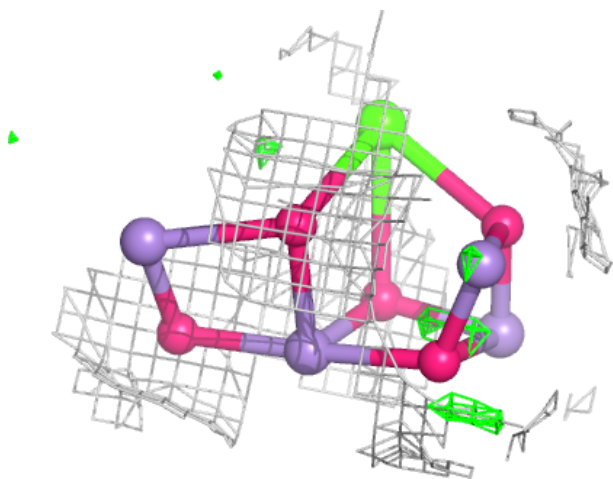
Electron density around HEC v 201:

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



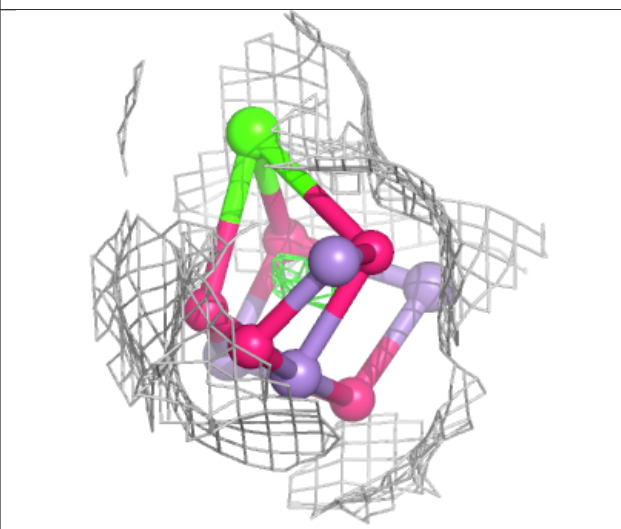
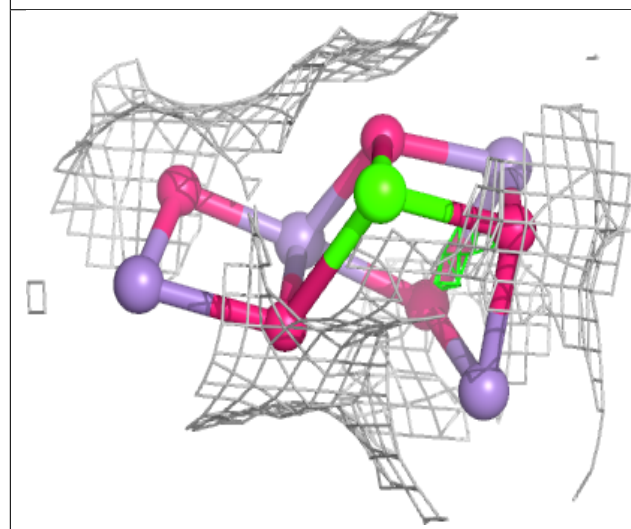
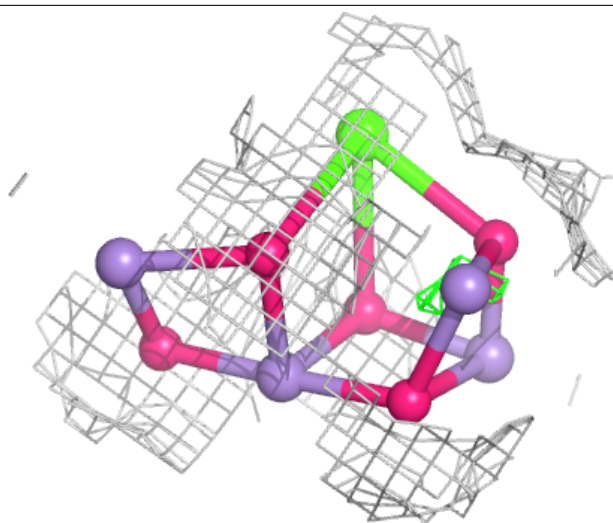
Electron density around OEX a 416:

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



Electron density around OEX A 416:

$2mF_o-DF_c$ (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.