



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:02 PM EDT

PDB ID : 6W1T / pdb_00006w1t
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution
Authors : Ibrahim, M.; Fransson, T.; Chatterjee, R.; Cheah, M.H.; Hussein, R.; Lassalle, L.; Sutherlin, K.D.; Young, I.D.; Fuller, F.D.; Gul, S.; Kim, I.-S.; Simon, P.S.; de Lichtenberg, C.; Chernev, P.; Bogacz, I.; Pham, C.; Orville, A.M.; Saichek, N.; Northen, T.R.; Batyuk, A.; Carbajo, S.; Alonso-Mori, R.; Tono, K.; Owada, S.; Bhowmick, A.; Bolotovskii, R.; Mendez, D.; Moriarty, N.W.; Holton, J.M.; Dobbek, H.; Brewster, A.S.; Adams, P.D.; Sauter, N.K.; Bergmann, U.; Zouni, A.; Messinger, J.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2020-03-04
Resolution : 2.01 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)

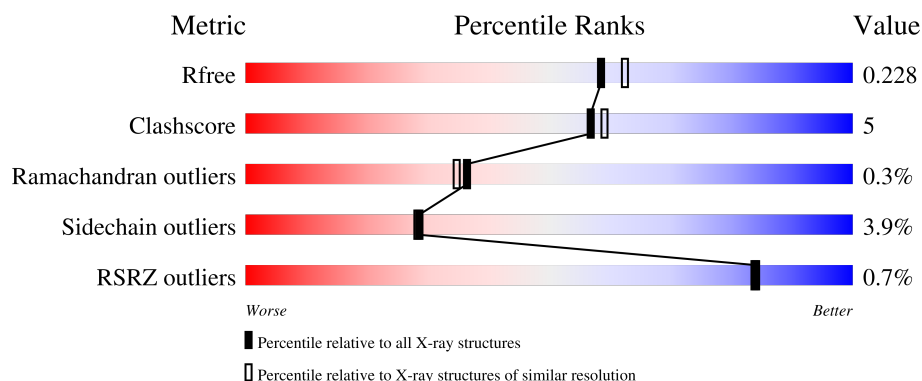
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

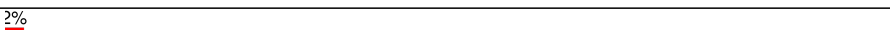
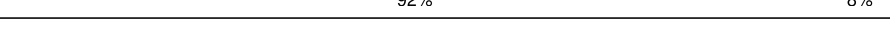
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

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CCP4 : 9.0.015 (Gargrove)
 Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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Mol	Chain	Length	Quality of chain
2	B	506	
2	b	506	
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	40	

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Mol	Chain	Length	Quality of chain
14	r	40	
15	T	30	
15	t	30	
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	F	101	X	-	-	-
35	HEC	V	201	X	-	-	-
35	HEC	f	101	X	-	-	-
35	HEC	v	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 105978 atoms, of which 52553 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	60	0
			6031	2014	2942	509	547	19			
1	a	334	Total	C	H	N	O	S	0	60	0
			6019	2011	2933	509	547	19			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	505	Total	C	H	N	O	S	0	5	0
			7864	2631	3859	666	695	13			
2	b	505	Total	C	H	N	O	S	0	0	0
			7800	2610	3822	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	10	0
			6876	2283	3397	580	602	14			
3	c	451	Total	C	H	N	O	S	0	10	0
			7021	2324	3468	596	619	14			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	341	Total	C	H	N	O	S	0	1	0
			5350	1806	2624	445	463	12			
4	d	341	Total	C	H	N	O	S	0	2	0
			5362	1810	2630	445	465	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	0	1	0
			1316	436	650	107	123			
5	e	82	Total	C	H	N	O	0	0	0
			1311	434	647	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
			556	187	281	45	42			
6	f	34	Total	C	H	N	O	0	0	0
			556	187	281	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
			3698	1168	1828	313	385			
13	o	244	Total	C	H	N	O	0	0	0
			3718	1170	1844	317	383			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	R	34	Total	C	H	N	O	0	0	0
			569	184	298	47	40			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	r	31	Total	C	H	N	O	0	0	0
			493	162	253	42	36			

- 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
			1546	491	772	129	154			
16	u	97	Total	C	H	N	O	0	0	0
			1546	491	772	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
			2132	675	1068	177	208	4		
17	v	137	Total	C	H	N	O	S	0	0
			2132	675	1068	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			

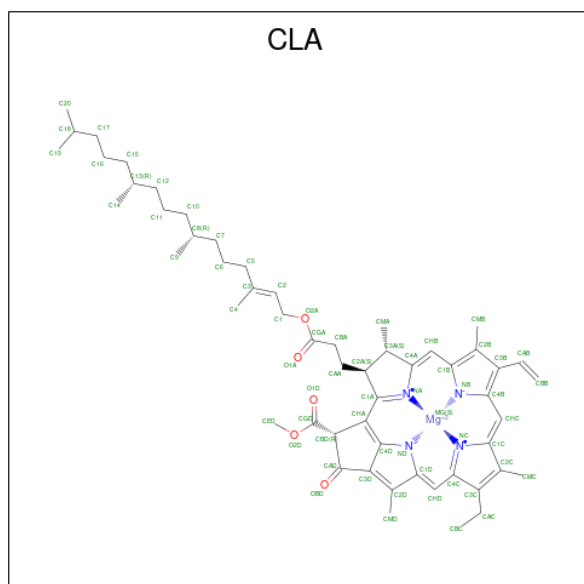
- Molecule 20 is a protein called Photosystem II reaction center protein Z.

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 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	A	1	Total 102	C 44	H 48	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	C	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0

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

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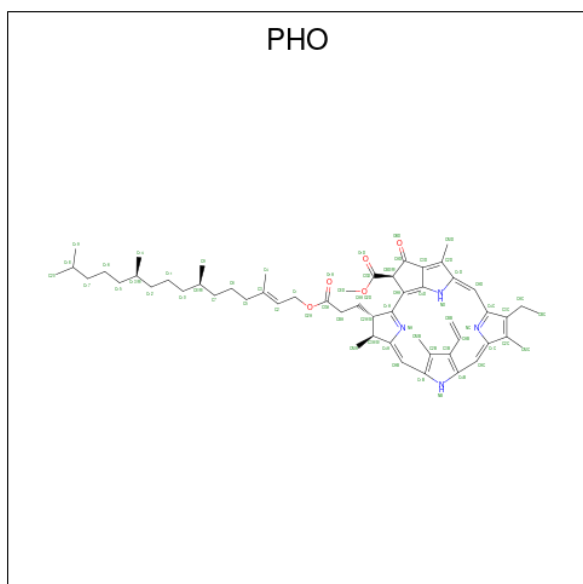
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	b	1	Total 137	C 55	H 72	Mg 1	N 4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

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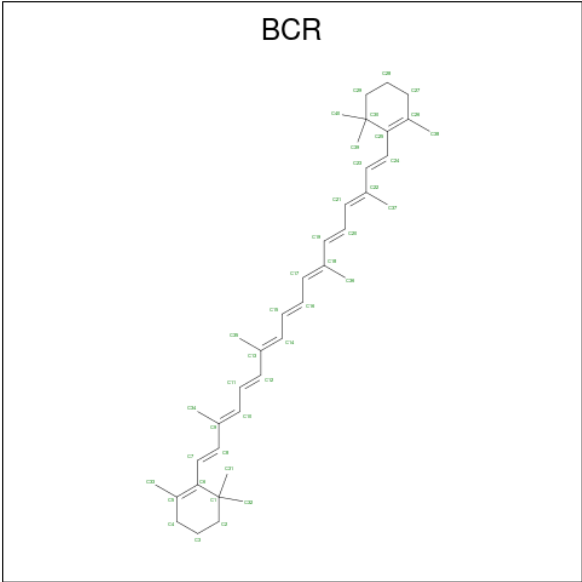
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	c	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0	0
22	d	1	Total 137	C 55	H 72	Mg 1	N 4	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	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	T	1	Total	C	H	0	0
			96	40	56		
24	Y	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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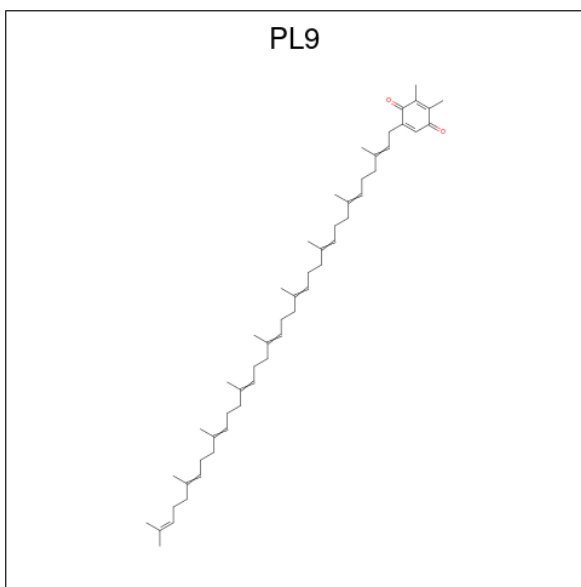
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	b	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	c	1	Total	C	H	0	0
			96	40	56		
24	d	1	Total	C	H	0	0
			96	40	56		
24	k	1	Total	C	H	0	0
			96	40	56		
24	t	1	Total	C	H	0	0
			96	40	56		
24	x	1	Total	C	H	0	0
			96	40	56		

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

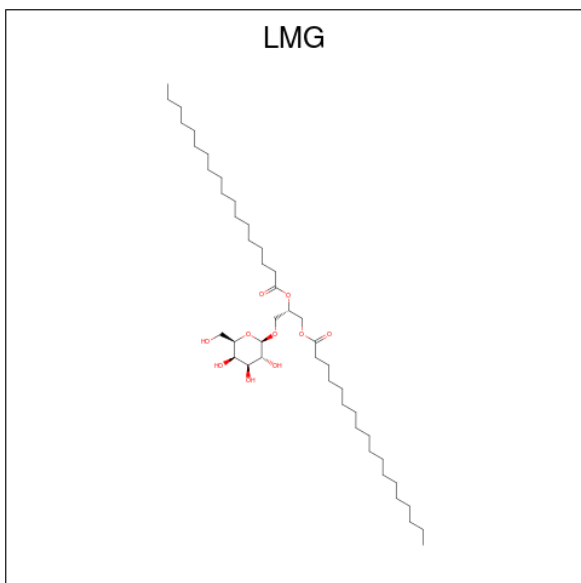
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	2	Total	Cl	0	0
			2	2		
25	a	2	Total	Cl	0	0
			2	2		

- 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) (labeled as "Ligand of Interest" by depositor).



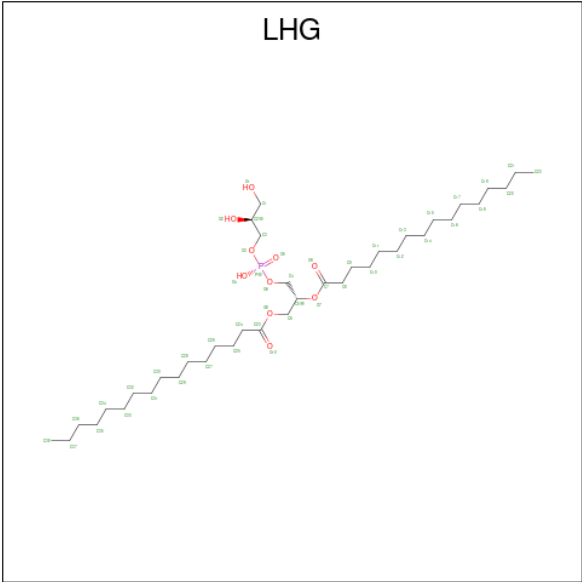
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	H	O	0	0
			135	53	80	2		
26	D	1	Total	C	H	O	0	0
			135	53	80	2		
26	a	1	Total	C	H	O	0	0
			135	53	80	2		
26	d	1	Total	C	H	O	0	0
			135	53	80	2		

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



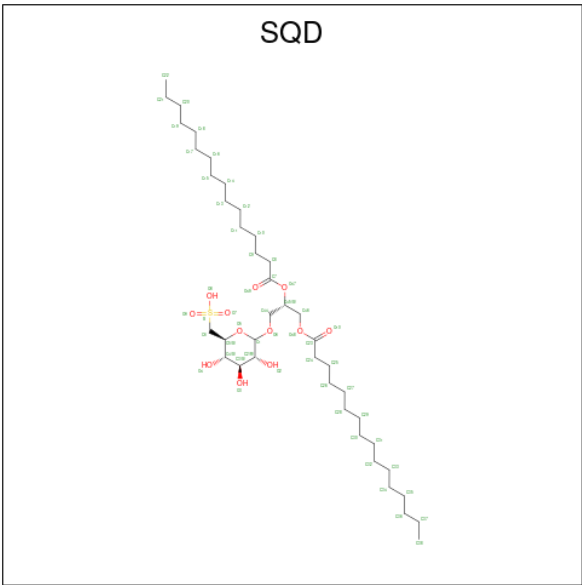
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	H	O	0	0
			113	38	65	10		
27	C	1	Total	C	H	O	0	0
			113	38	65	10		
27	D	1	Total	C	H	O	0	0
			122	41	71	10		
27	D	1	Total	C	H	O	0	0
			78	27	45	6		
27	D	1	Total	C	H	O	0	0
			68	24	40	4		
27	M	1	Total	C	H	O	0	0
			120	41	69	10		
27	a	1	Total	C	H	O	0	0
			138	45	83	10		
27	b	1	Total	C	H	O	0	0
			140	45	85	10		
27	c	1	Total	C	H	O	0	0
			78	27	41	10		
27	c	1	Total	C	H	O	0	0
			116	38	68	10		
27	c	1	Total	C	H	O	0	0
			117	39	68	10		
27	d	1	Total	C	H	O	0	0
			101	34	57	10		
27	m	1	Total	C	H	O	0	0
			120	41	69	10		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



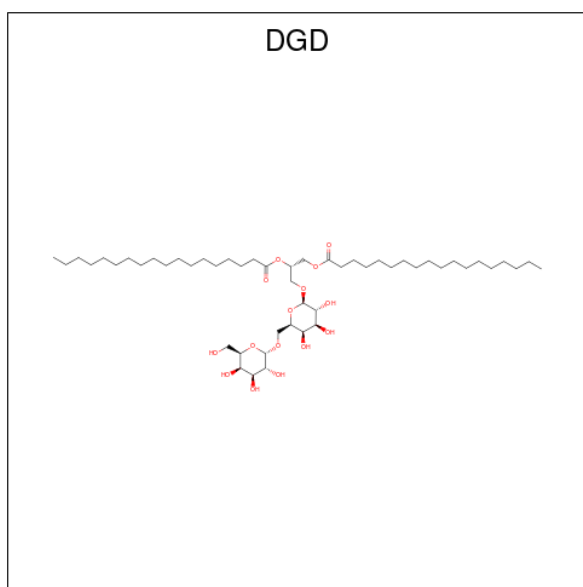
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	A	1	Total	C	H	O	P	0	0
			112	36	65	10	1		
28	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
28	B	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	D	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	E	1	Total	C	H	O	P	0	0
			122	38	73	10	1		
28	a	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			121	38	72	10	1		
28	d	1	Total	C	H	O	P	0	0
			88	28	49	10	1		
28	e	1	Total	C	H	O	P	0	0
			97	31	55	10	1		
28	l	1	Total	C	H	O	P	0	0
			122	38	73	10	1		

- Molecule 29 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



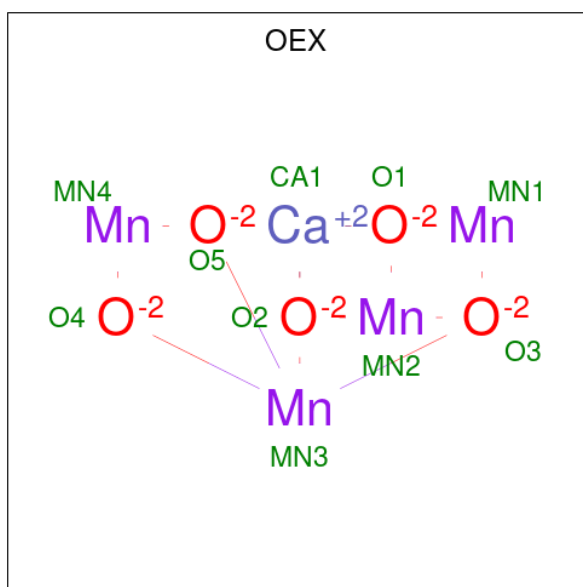
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
29	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
29	A	1	Total	C	H	O		0	0
			104	35	65	4			
29	B	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	D	1	Total	C	H	O	S	0	0
			81	25	45	10	1		
29	a	1	Total	C	H	O	S	0	0
			131	41	77	12	1		
29	a	1	Total	C	H	O		0	0
			92	31	56	5			
29	b	1	Total	C	H	O	S	0	0
			114	36	65	12	1		
29	f	1	Total	C	H	O	S	0	0
			89	28	48	12	1		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



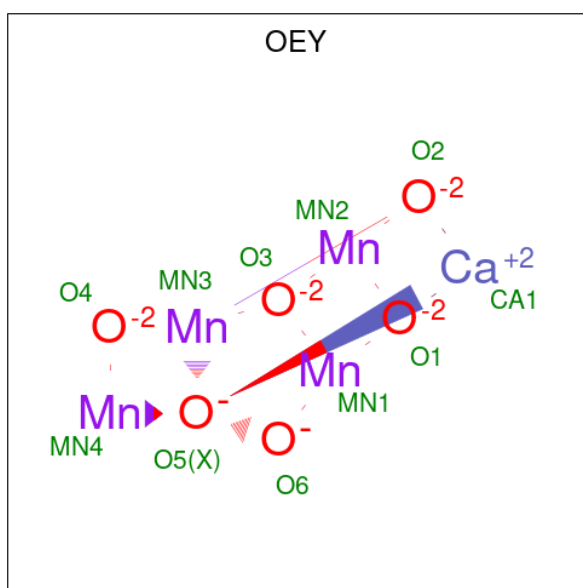
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	C	H	O	0	0
			160	51	94	15		
30	C	1	Total	C	H	O	0	0
			143	47	81	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	C	1	Total	C	H	O	0	0
			142	47	80	15		
30	H	1	Total	C	H	O	0	0
			142	47	80	15		
30	c	1	Total	C	H	O	0	0
			140	47	78	15		
30	c	1	Total	C	H	O	0	0
			138	47	76	15		
30	c	1	Total	C	H	O	0	0
			142	47	80	15		
30	h	1	Total	C	H	O	0	0
			139	47	77	15		

- Molecule 31 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



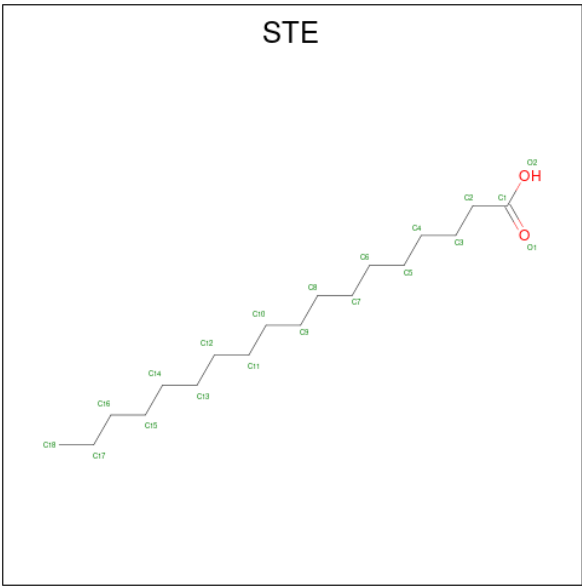
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
31	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 32 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



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

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C H O 43 15 26 2	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	B	1	Total C H 47 16 31	0	0
33	B	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	C	1	Total C H 47 16 31	0	0
33	C	1	Total C H O 28 10 16 2	0	0
33	D	1	Total C H O 55 18 35 2	0	0
33	H	1	Total C H 53 18 35	0	0
33	I	1	Total C H 41 15 26	0	0
33	J	1	Total C H O 28 10 16 2	0	0
33	M	1	Total C H O 37 13 22 2	0	0
33	M	1	Total C H 26 10 16	0	0

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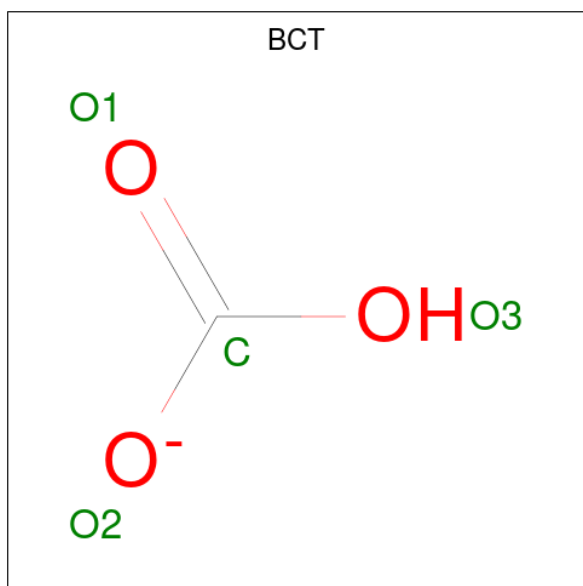
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	R	1	Total C H O 28 10 16 2	0	0
33	T	1	Total C H 44 15 29	0	0
33	Z	1	Total C H 20 8 12	0	0
33	a	1	Total C H 26 10 16	0	0
33	a	1	Total C H O 28 10 16 2	0	0
33	a	1	Total C H 41 15 26	0	0
33	b	1	Total C H 47 16 31	0	0
33	b	1	Total C H O 55 18 35 2	0	0
33	b	1	Total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

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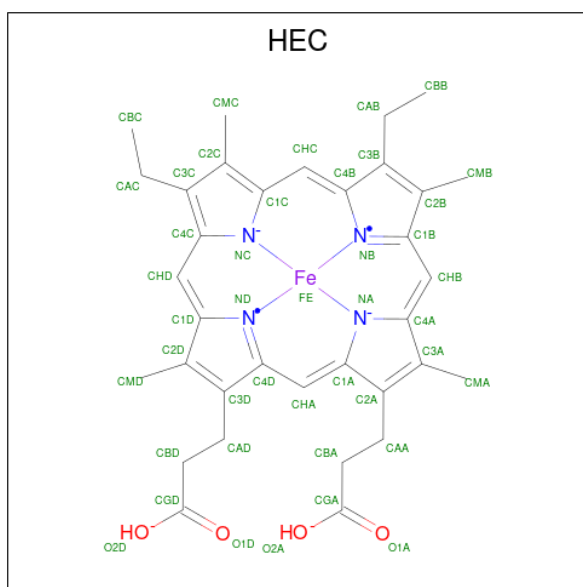
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	t	1	Total	C	H	O	0	0
			46	16	28	2		

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



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

- Molecule 35 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
35	F	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
35	V	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
35	f	1	Total 75	C 34	Fe 1	H 32	N 4	O 4	0	0
35	v	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	146	Total O 146 146	0	8
36	B	211	Total O 211 211	0	0
36	C	185	Total O 185 185	0	0
36	D	129	Total O 129 129	0	0
36	E	34	Total O 34 34	0	0
36	F	13	Total O 13 13	0	0
36	H	33	Total O 33 33	0	0
36	I	11	Total O 11 11	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	J	15	Total 15	O 15	0	0
36	K	9	Total 9	O 9	0	0
36	L	9	Total 9	O 9	0	0
36	M	5	Total 5	O 5	0	0
36	O	104	Total 104	O 104	0	0
36	R	13	Total 13	O 13	0	0
36	T	15	Total 15	O 15	0	0
36	U	51	Total 51	O 51	0	0
36	V	70	Total 70	O 70	0	0
36	X	11	Total 11	O 11	0	0
36	Y	2	Total 2	O 2	0	0
36	Z	5	Total 5	O 5	0	0
36	a	130	Total 130	O 130	0	8
36	b	215	Total 215	O 215	0	0
36	c	190	Total 190	O 190	0	0
36	d	122	Total 122	O 122	0	0
36	e	30	Total 30	O 30	0	0
36	f	9	Total 9	O 9	0	0
36	h	22	Total 22	O 22	0	0
36	i	9	Total 9	O 9	0	0
36	j	10	Total 10	O 10	0	0

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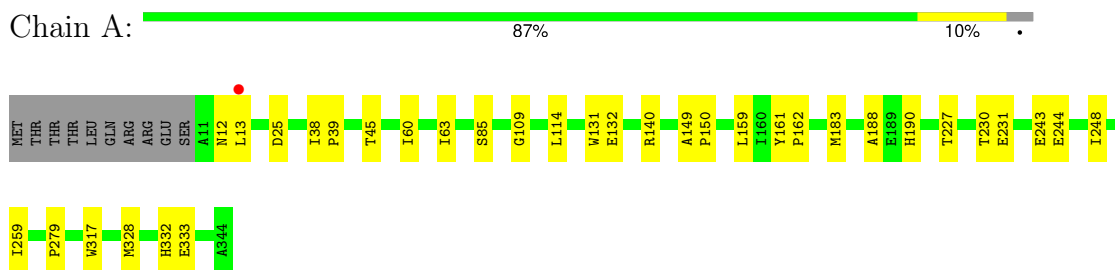
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	k	10	Total 10	O 10	0	0
36	l	9	Total 9	O 9	0	0
36	m	8	Total 8	O 8	0	0
36	o	103	Total 103	O 103	0	0
36	r	2	Total 2	O 2	0	0
36	t	11	Total 11	O 11	0	0
36	u	66	Total 66	O 66	0	0
36	v	58	Total 58	O 58	0	0
36	x	10	Total 10	O 10	0	0
36	y	6	Total 6	O 6	0	0
36	z	6	Total 6	O 6	0	0

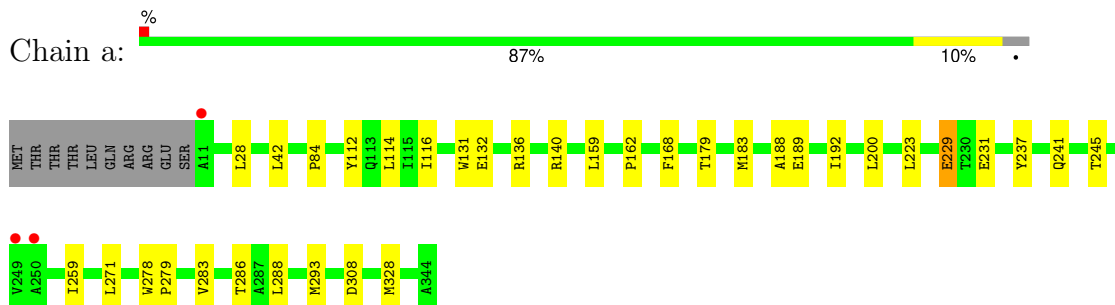
3 Residue-property plots [i](#)

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

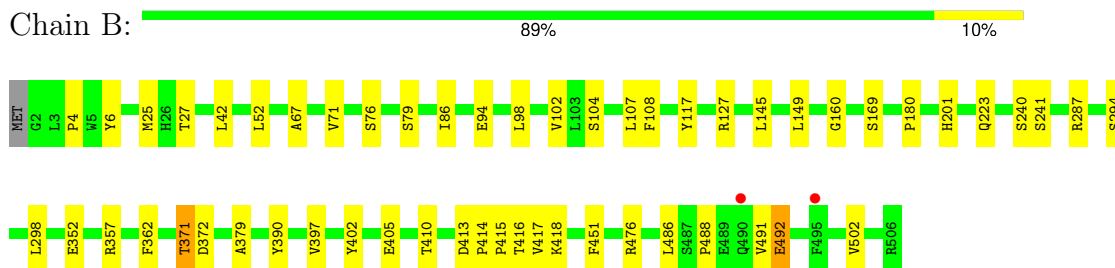
- Molecule 1: Photosystem II protein D1 1



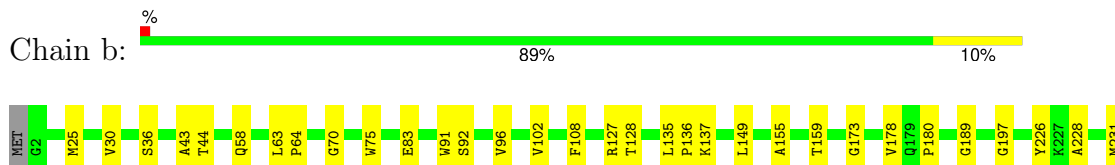
- Molecule 1: Photosystem II protein D1 1

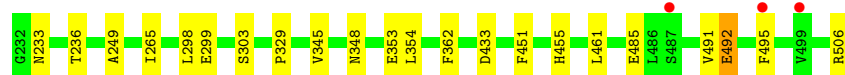


- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein





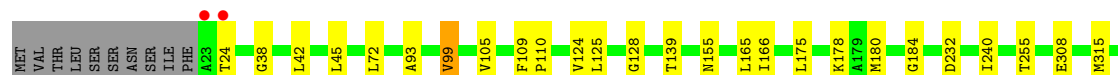
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 9% .



- Molecule 4: Photosystem II D2 protein

Chain D: 88% 8% .



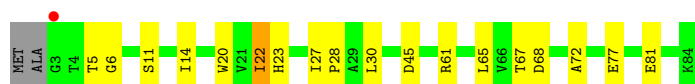
- Molecule 4: Photosystem II D2 protein

Chain d: 85% 11% . .

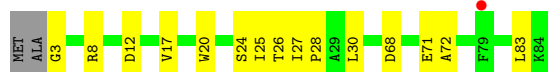
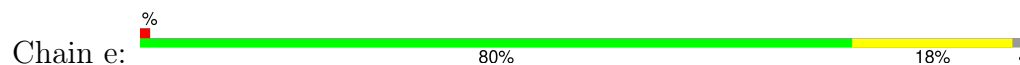


- Molecule 5: Cytochrome b559 subunit alpha

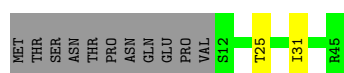
Chain E: 76% 20% . .



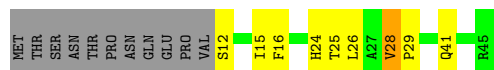
- Molecule 5: Cytochrome b559 subunit alpha



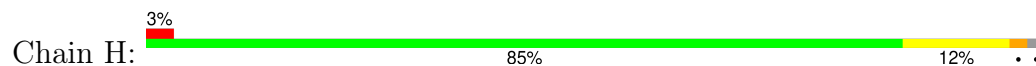
- Molecule 6: Cytochrome b559 subunit beta



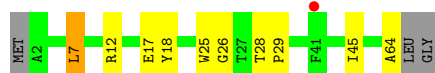
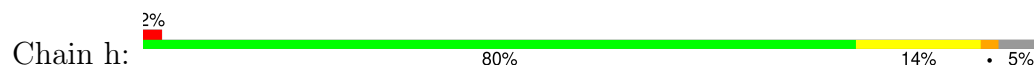
- Molecule 6: Cytochrome b559 subunit beta



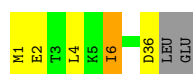
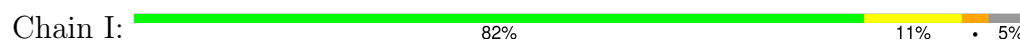
- Molecule 7: Photosystem II reaction center protein H



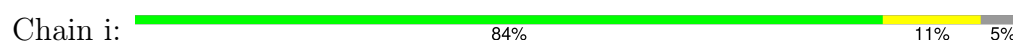
- Molecule 7: Photosystem II reaction center protein H

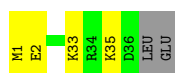


- Molecule 8: Photosystem II reaction center protein I

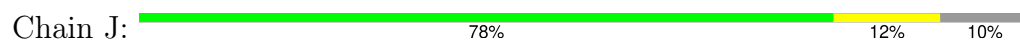


- Molecule 8: Photosystem II reaction center protein I

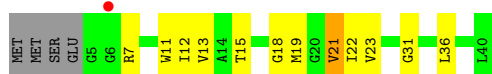




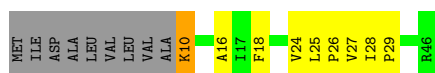
• Molecule 9: Photosystem II reaction center protein J



• Molecule 9: Photosystem II reaction center protein J



• Molecule 10: Photosystem II reaction center protein K



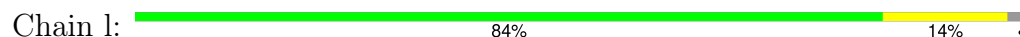
• Molecule 10: Photosystem II reaction center protein K



• Molecule 11: Photosystem II reaction center protein L



• Molecule 11: Photosystem II reaction center protein L



• Molecule 12: Photosystem II reaction center protein M

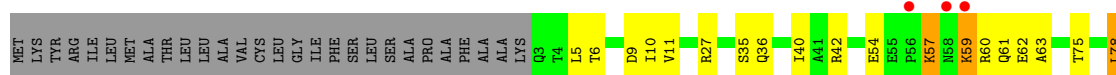
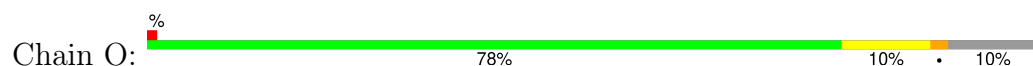




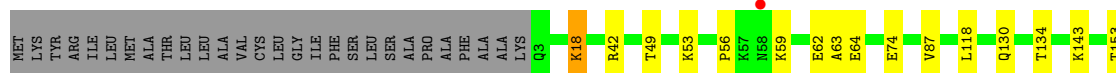
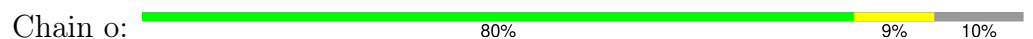
- Molecule 12: Photosystem II reaction center protein M



- Molecule 13: Photosystem II manganese-stabilizing polypeptide



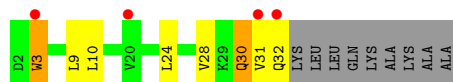
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



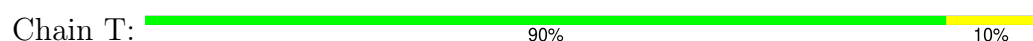
- Molecule 14: Photosystem II protein Y



- Molecule 14: Photosystem II protein Y

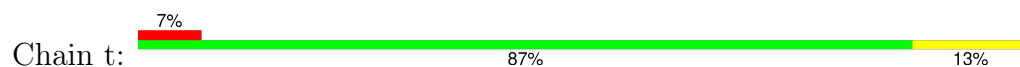


- Molecule 15: Photosystem II reaction center protein T

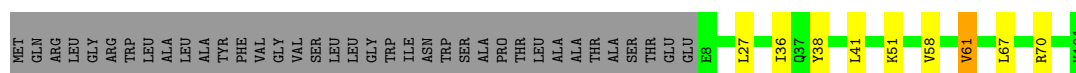




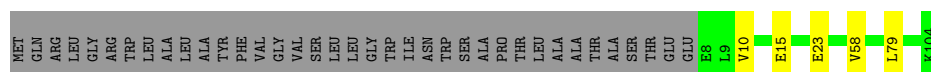
- Molecule 15: Photosystem II reaction center protein T



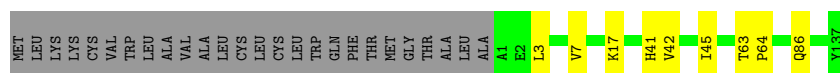
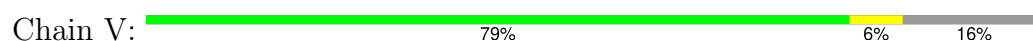
- Molecule 16: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Photosystem II 12 kDa extrinsic protein



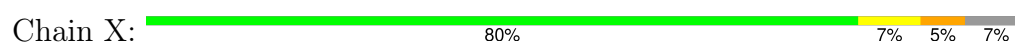
- Molecule 17: Cytochrome c-550



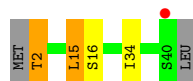
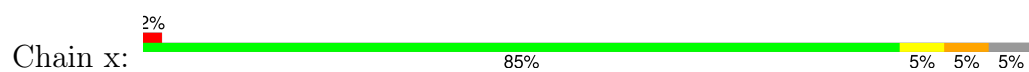
- Molecule 17: Cytochrome c-550



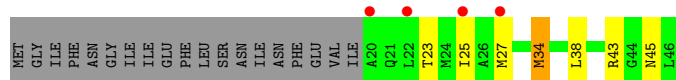
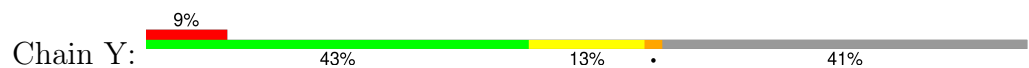
- Molecule 18: Photosystem II reaction center X protein



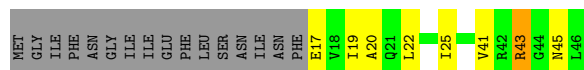
- Molecule 18: Photosystem II reaction center X protein



- Molecule 19: Photosystem II reaction center protein Ycf12



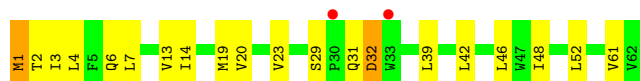
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.04Å 221.92Å 308.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.59 – 2.01 33.59 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.59-2.01) 86.9 (33.59-2.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.57 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.175 , 0.228 0.175 , 0.228	Depositor DCC
R_{free} test set	4767 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	105978	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.57	0/3187	0.63	0/4342
1	a	0.53	0/3184	0.63	1/4338 (0.0%)
2	B	0.60	0/4161	0.67	0/5669
2	b	0.56	0/4118	0.65	0/5611
3	C	0.57	0/3621	0.66	2/4930 (0.0%)
3	c	0.53	0/3693	0.64	0/5026
4	D	0.64	0/2820	0.70	0/3840
4	d	0.60	0/2829	0.68	0/3852
5	E	0.50	0/688	0.60	0/940
5	e	0.45	0/683	0.61	0/932
6	F	0.49	0/284	0.62	0/387
6	f	0.48	0/284	0.66	0/387
7	H	0.58	0/523	0.65	0/713
7	h	0.50	0/511	0.62	0/697
8	I	0.56	0/293	0.64	0/396
8	i	0.55	0/293	0.61	0/396
9	J	0.44	0/263	0.64	0/356
9	j	0.43	0/263	0.57	0/356
10	K	0.44	0/303	0.61	0/416
10	k	0.45	0/303	0.55	0/416
11	L	0.61	0/311	0.66	0/422
11	l	0.63	0/303	0.66	0/412
12	M	0.62	0/249	0.70	0/341
12	m	0.56	0/244	0.72	0/334
13	O	0.57	0/1904	0.65	0/2585
13	o	0.58	0/1905	0.65	0/2583
14	R	0.41	0/277	0.54	0/380
14	r	0.32	0/246	0.52	0/339
15	T	0.63	0/257	0.66	0/349
15	t	0.67	0/255	0.63	0/346
16	U	0.50	0/785	0.60	0/1064
16	u	0.52	0/785	0.66	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	V	0.56	0/1085	0.68	0/1473
17	v	0.52	0/1085	0.61	0/1473
18	X	0.46	0/284	0.57	0/384
18	x	0.42	0/289	0.51	0/391
19	Y	0.48	0/197	0.57	0/264
19	y	0.40	0/219	0.54	0/294
20	Z	0.39	0/490	0.58	0/669
20	z	0.33	0/488	0.48	0/666
All	All	0.56	0/43962	0.65	3/59833 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
17	V	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	88	LEU	CA-C-N	5.36	123.62	120.24
3	C	88	LEU	C-N-CA	5.36	123.62	120.24
1	a	131	TRP	CA-CB-CG	-5.03	104.05	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190[A]	HIS	Mainchain
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	3089	2942	2956	19	0
1	a	3086	2933	2947	19	0
2	B	4005	3859	3867	35	0
2	b	3978	3822	3836	34	0
3	C	3479	3397	3383	23	0
3	c	3553	3468	3466	33	0
4	D	2726	2624	2632	20	0
4	d	2732	2630	2638	32	0
5	E	666	650	651	13	0
5	e	664	647	648	11	0
6	F	275	281	282	2	0
6	f	275	281	282	8	0
7	H	510	532	532	5	0
7	h	498	518	518	7	0
8	I	296	311	311	1	0
8	i	296	311	311	1	0
9	J	257	268	268	4	0
9	j	257	268	268	9	0
10	K	293	305	305	9	0
10	k	293	305	305	6	0
11	L	304	316	316	3	0
11	l	296	304	304	1	0
12	M	256	269	269	6	0
12	m	251	267	267	7	0
13	O	1870	1828	1830	19	0
13	o	1874	1844	1846	11	0
14	R	271	298	298	3	0
14	r	240	253	250	6	0
15	T	258	261	261	0	0
15	t	256	256	256	4	0
16	U	774	772	773	6	0
16	u	774	772	773	1	0
17	V	1064	1068	1073	2	0
17	v	1064	1068	1073	12	0
18	X	281	312	312	4	0
18	x	286	316	314	3	0
19	Y	196	217	217	4	0
19	y	218	241	241	4	0
20	Z	479	516	516	9	0
20	z	477	509	509	10	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	184	192	192	1	0
22	B	1035	1139	1139	17	0
22	C	839	922	922	13	0
22	D	195	216	216	5	0
22	a	130	144	144	1	0
22	b	1035	1139	1139	19	0
22	c	839	919	919	15	0
22	d	260	288	288	3	0
23	A	128	148	148	1	0
23	a	64	74	74	1	0
23	d	64	74	74	2	0
24	A	40	56	56	1	0
24	B	120	168	168	9	0
24	C	120	168	168	4	0
24	D	40	56	56	2	0
24	H	40	56	56	4	0
24	T	40	56	56	4	0
24	Y	40	56	56	2	0
24	a	40	56	56	1	0
24	b	120	168	168	5	0
24	c	120	168	168	2	0
24	d	40	56	56	7	0
24	k	40	56	56	0	0
24	t	40	56	56	4	0
24	x	40	56	56	0	0
25	A	2	0	0	0	0
25	a	2	0	0	0	0
26	A	55	80	80	8	0
26	D	55	80	80	0	0
26	a	55	80	80	4	0
26	d	55	80	80	0	0
27	A	48	65	66	0	0
27	C	48	65	66	0	0
27	D	112	156	157	0	0
27	M	51	69	72	0	0
27	a	55	83	86	0	0
27	b	55	85	86	2	0
27	c	134	177	181	3	0
27	d	44	57	58	0	0
27	m	51	69	72	2	0
28	A	47	65	67	0	0
28	B	98	146	148	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	D	49	73	74	0	0
28	E	49	73	74	3	0
28	a	49	72	74	1	0
28	d	88	121	125	0	0
28	e	42	55	57	0	0
28	l	49	73	74	0	0
29	A	91	136	136	1	0
29	B	54	77	77	2	0
29	D	36	45	46	0	0
29	a	90	133	132	3	0
29	b	49	65	65	1	0
29	f	41	48	48	1	0
30	A	66	94	95	1	0
30	C	186	241	246	1	0
30	H	62	80	81	0	0
30	c	186	234	246	1	0
30	h	62	77	79	1	0
31	A	10	0	0	0	0
31	a	10	0	0	0	0
32	A	11	0	0	1	0
32	a	11	0	0	1	0
33	B	57	89	86	3	0
33	C	40	63	60	0	0
33	D	20	35	35	3	0
33	H	18	35	35	0	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	M	25	38	38	1	0
33	R	12	16	16	0	0
33	T	15	29	26	1	0
33	Z	8	12	12	0	0
33	a	37	58	58	0	0
33	b	96	168	165	6	0
33	c	20	35	35	0	0
33	d	57	96	96	4	0
33	j	12	16	16	0	0
33	k	12	16	16	0	0
33	l	18	35	35	0	0
33	m	12	16	16	0	0
33	t	32	48	48	2	0
34	D	4	1	1	0	0
34	a	4	1	1	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	F	43	32	32	5	0
35	V	43	30	30	2	0
35	f	43	32	32	5	0
35	v	43	30	30	3	0
36	A	146	0	0	3	0
36	B	211	0	0	8	0
36	C	185	0	0	1	0
36	D	129	0	0	2	0
36	E	34	0	0	1	0
36	F	13	0	0	1	0
36	H	33	0	0	0	0
36	I	11	0	0	0	0
36	J	15	0	0	2	0
36	K	9	0	0	1	0
36	L	9	0	0	0	0
36	M	5	0	0	2	0
36	O	104	0	0	3	0
36	R	13	0	0	0	0
36	T	15	0	0	0	0
36	U	51	0	0	1	0
36	V	70	0	0	0	0
36	X	11	0	0	0	0
36	Y	2	0	0	0	0
36	Z	5	0	0	1	0
36	a	130	0	0	3	0
36	b	215	0	0	3	0
36	c	190	0	0	9	0
36	d	122	0	0	3	0
36	e	30	0	0	2	0
36	f	9	0	0	1	0
36	h	22	0	0	1	0
36	i	9	0	0	0	0
36	j	10	0	0	1	0
36	k	10	0	0	1	0
36	l	9	0	0	0	0
36	m	8	0	0	2	0
36	o	103	0	0	2	0
36	r	2	0	0	0	0
36	t	11	0	0	1	0
36	u	66	0	0	0	0
36	v	58	0	0	2	0
36	x	10	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	y	6	0	0	2	0
36	z	6	0	0	0	0
All	All	53425	52553	52660	482	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:v:40:CYS:SG	35:v:201:HEC:CAC	2.04	1.44
3:c:315:MET:SD	36:c:768:HOH:O	2.23	0.94
32:A:417[B]:OEY:O5	32:A:417[B]:OEY:O6	1.92	0.88
5:e:71:GLU:OE1	36:e:201:HOH:O	1.91	0.86
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.58	0.86
30:c:517:DGD:O1A	36:c:601:HOH:O	1.91	0.86
1:A:25:ASP:OD1	36:A:501:HOH:O	1.94	0.84
35:F:101:HEC:HBC3	35:F:101:HEC:HHD	1.59	0.84
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.59	0.83
16:U:58:VAL:O	16:U:61:VAL:HG22	1.80	0.82
3:c:391[A]:ARG:NE	36:c:603:HOH:O	2.14	0.81
3:c:391[A]:ARG:NH1	36:c:602:HOH:O	2.13	0.80
35:V:201:HEC:HMC1	35:V:201:HEC:HBC3	1.64	0.80
17:v:40:CYS:SG	35:v:201:HEC:C3C	2.70	0.78
2:B:410:THR:O	36:B:701:HOH:O	2.01	0.78
7:h:64:ALA:O	36:h:201:HOH:O	2.01	0.76
6:f:12:SER:N	36:f:201:HOH:O	2.19	0.75
24:t:101:BCR:H321	24:t:101:BCR:HC8	1.69	0.74
26:A:410:PL9:H361	6:F:25:THR:HG21	1.69	0.74
10:K:24:VAL:HG13	19:Y:25:ILE:HD13	1.69	0.73
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.72	0.72
9:J:5:GLY:N	36:J:201:HOH:O	2.23	0.72
3:C:141:GLU:OE1	36:C:601:HOH:O	2.08	0.71
3:C:143:TYR:CE1	22:C:513:CLA:HED3	2.25	0.71
12:m:30:GLU:OE2	36:m:201:HOH:O	2.09	0.70
4:d:246:MET:HE3	4:d:264:LYS:CG	2.22	0.69
24:d:406:BCR:H331	24:d:406:BCR:C8	2.23	0.69
4:d:126:MET:HE3	4:d:143:ALA:O	1.93	0.68
24:D:405:BCR:H23C	24:D:405:BCR:H392	1.76	0.68
10:K:10:LYS:NZ	36:K:101:HOH:O	2.20	0.67
27:b:623:LMG:O5	36:b:701:HOH:O	2.13	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:GLY:O	3:C:156:LYS:NZ	2.27	0.67
3:c:391[B]:ARG:NH2	36:c:606:HOH:O	2.27	0.66
3:C:279:LEU:HD12	22:C:509:CLA:HED2	1.77	0.66
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.79	0.65
2:B:371:THR:HG23	2:B:372:ASP:O	1.96	0.65
33:t:102:STE:O2	36:t:201:HOH:O	2.13	0.65
24:C:514:BCR:H331	24:C:514:BCR:C8	2.26	0.64
2:B:223:GLN:OE1	36:B:703:HOH:O	2.15	0.64
13:O:35:SER:OG	13:O:36:GLN:N	2.27	0.64
13:o:62:GLU:OE1	13:o:63:ALA:N	2.31	0.64
33:B:624:STE:O1	36:B:704:HOH:O	2.15	0.63
6:f:24:HIS:O	6:f:28:VAL:HG13	1.98	0.63
2:b:102:VAL:HG21	22:b:606:CLA:H141	1.81	0.63
19:y:43:ARG:NH2	36:y:101:HOH:O	2.31	0.62
3:C:279:LEU:CD1	22:C:509:CLA:HED2	2.29	0.62
4:D:209:LEU:HD23	4:D:209:LEU:C	2.24	0.62
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.62
2:b:492:GLU:OE2	2:b:495:PHE:CE1	2.53	0.62
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.35	0.61
9:j:15:THR:HG22	9:j:19:MET:HE2	1.81	0.61
4:d:267:LEU:C	4:d:267:LEU:HD23	2.25	0.61
2:B:145:LEU:HD22	22:B:604:CLA:H193	1.82	0.61
13:O:27:ARG:O	13:O:27:ARG:HG2	2.00	0.61
24:T:101:BCR:H321	24:T:101:BCR:HC8	1.82	0.60
4:d:272:LEU:C	4:d:272:LEU:HD23	2.27	0.60
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.82	0.60
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.82	0.60
22:C:513:CLA:HBB1	22:C:513:CLA:HMB3	1.83	0.60
5:e:30:LEU:HD11	35:f:101:HEC:CBB	2.31	0.60
3:c:342:MET:SD	3:c:356[B]:MET:HE2	2.42	0.60
36:A:585:HOH:O	13:O:107:THR:HG21	2.01	0.59
5:e:26:THR:HB	35:f:101:HEC:HBB2	1.84	0.59
20:Z:51:VAL:O	20:Z:54:VAL:O	2.20	0.59
26:A:410:PL9:H152	28:E:101:LHG:H381	1.83	0.59
20:z:32:ASP:OD1	20:z:32:ASP:N	2.36	0.58
24:b:618:BCR:H331	24:b:618:BCR:C8	2.32	0.58
2:B:169:SER:O	7:H:65:LEU:HD22	2.03	0.58
22:B:607:CLA:H193	11:L:27:LEU:HD11	1.84	0.58
3:C:45:LEU:HD22	3:C:138:GLU:HG2	1.86	0.58
12:m:4:ASN:ND2	27:m:101:LMG:O10	2.32	0.58
10:k:23:ASP:OD2	36:k:201:HOH:O	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:622:STE:O2	36:b:702:HOH:O	2.17	0.58
8:i:33:LYS:O	8:i:35:LYS:NZ	2.37	0.57
2:B:357:ARG:NE	36:B:702:HOH:O	2.10	0.57
24:d:406:BCR:H331	24:d:406:BCR:HC8	1.85	0.57
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.18	0.57
22:c:504:CLA:H91	22:c:508:CLA:C17	2.34	0.57
5:E:22[A]:ILE:HG23	5:E:23:HIS:ND1	2.19	0.57
22:C:509:CLA:HBB1	22:C:509:CLA:HMB1	1.87	0.57
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.86	0.57
3:c:406:SER:HA	3:c:420:VAL:HG23	1.85	0.57
4:d:246:MET:HE3	4:d:264:LYS:HG3	1.87	0.57
22:c:504:CLA:H142	22:c:508:CLA:H121	1.86	0.57
23:A:405:PHO:HBC3	4:D:279:LEU:HD22	1.86	0.57
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.87	0.57
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.20	0.56
2:b:30:VAL:HG12	22:b:605:CLA:HHD	1.88	0.56
2:b:345:VAL:HG13	2:b:353:GLU:OE2	2.05	0.56
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.88	0.56
2:B:352:GLU:OE1	36:B:705:HOH:O	2.18	0.56
24:B:618:BCR:H331	24:B:618:BCR:C8	2.35	0.56
20:Z:31:GLN:NE2	36:Z:201:HOH:O	2.38	0.56
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.87	0.56
22:D:403:CLA:HBB1	22:D:403:CLA:HMB3	1.88	0.56
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.06	0.56
3:C:406:SER:HA	3:C:420:VAL:HG23	1.88	0.56
29:b:620:SQD:O9	36:b:703:HOH:O	2.18	0.55
3:c:178:LYS:NZ	3:c:184:GLY:O	2.39	0.55
13:O:133:VAL:C	13:O:134:THR:HG23	2.31	0.55
2:b:155:ALA:HB1	27:b:623:LMG:H122	1.89	0.54
5:e:68:ASP:O	5:e:72:ALA:HB2	2.07	0.54
17:v:40:CYS:SG	35:v:201:HEC:CBC	2.90	0.54
22:b:602:CLA:H43	7:h:45:ILE:HG22	1.89	0.54
24:B:619:BCR:H331	24:B:619:BCR:C8	2.37	0.54
9:j:18:GLY:O	9:j:22:ILE:HD13	2.07	0.54
24:Y:101:BCR:H322	20:Z:17:PHE:CE2	2.43	0.54
9:j:36:LEU:O	36:j:201:HOH:O	2.18	0.54
13:o:164:LEU:HD13	13:o:188:LYS:O	2.08	0.53
2:b:127:ARG:NH1	7:h:18:TYR:O	2.41	0.53
2:B:117:TYR:HA	11:L:1:MET:HE1	1.89	0.53
13:O:59:LYS:O	13:O:61:GLN:N	2.41	0.53
3:c:232:ASP:OD2	36:c:604:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B:624:STE:C1	36:B:704:HOH:O	2.57	0.53
2:b:249:ALA:HB2	22:b:604:CLA:HBC3	1.91	0.52
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.91	0.52
29:a:412:SQD:C23	36:a:514:HOH:O	2.56	0.52
17:v:104:MET:HA	17:v:107:LEU:HD22	1.91	0.52
2:b:44:THR:HG22	33:b:621:STE:H41	1.92	0.52
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.45	0.52
13:O:54:GLU:O	13:O:63:ALA:HB3	2.09	0.52
29:a:412:SQD:C46	36:a:514:HOH:O	2.58	0.52
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.52
1:a:283:VAL:HA	1:a:286:THR:HG22	1.92	0.52
18:X:3:ILE:HG13	18:X:3:ILE:O	2.10	0.51
20:z:1:MET:HB3	20:z:4:LEU:HD23	1.92	0.51
6:f:16:PHE:H	14:r:30:GLN:HE22	1.59	0.51
3:c:166:ILE:HG21	22:c:512:CLA:H202	1.91	0.51
22:C:505:CLA:HBC2	24:C:515:BCR:H341	1.93	0.51
20:Z:52:LEU:O	20:Z:56:VAL:HG23	2.10	0.51
22:b:604:CLA:HAB	22:b:611:CLA:H191	1.93	0.51
24:H:101:BCR:H331	24:H:101:BCR:C8	2.39	0.51
10:K:18:PHE:HE2	20:Z:9:LEU:HD21	1.75	0.51
35:F:101:HEC:HBC3	35:F:101:HEC:CHD	2.34	0.51
5:e:30:LEU:HD11	35:f:101:HEC:HBB3	1.93	0.51
33:D:412:STE:H92	18:X:16:SER:HB3	1.93	0.51
4:d:179:PHE:HA	4:d:182:LEU:HD22	1.93	0.51
9:j:19:MET:O	9:j:23:VAL:HG23	2.10	0.51
22:B:610:CLA:HHC	22:B:610:CLA:CBB	2.41	0.50
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.46	0.50
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.93	0.50
12:M:5:GLN:O	36:M:201:HOH:O	2.20	0.50
22:b:606:CLA:H142	22:b:606:CLA:H102	1.92	0.50
35:f:101:HEC:CBB	35:f:101:HEC:HHC	2.41	0.50
10:k:26:PRO:O	10:k:29:PRO:HD2	2.11	0.50
15:t:15:ALA:HB2	24:t:101:BCR:H14C	1.93	0.50
18:x:2:THR:N	36:x:202:HOH:O	2.44	0.50
3:C:213:LEU:HG	22:C:506:CLA:H193	1.93	0.50
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.41	0.50
29:a:412:SQD:H461	36:a:514:HOH:O	2.11	0.50
18:x:15:LEU:HD23	36:x:209:HOH:O	2.12	0.50
22:B:604:CLA:HBD	22:B:605:CLA:H43	1.94	0.50
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.12	0.50
14:r:30:GLN:N	14:r:31:VAL:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:615:CLA:HHC	22:b:615:CLA:HBB1	1.94	0.49
24:D:405:BCR:H331	24:D:405:BCR:C8	2.41	0.49
5:e:20:TRP:O	5:e:24:SER:OG	2.12	0.49
2:B:414:PRO:O	2:B:418:LYS:HG3	2.12	0.49
22:c:501:CLA:H192	22:c:507:CLA:HBB1	1.93	0.49
20:z:19:MET:O	20:z:23:VAL:HG23	2.12	0.49
1:A:230:THR:HG21	11:L:8:GLN:NE2	2.27	0.49
3:c:391[B]:ARG:HA	3:c:391[B]:ARG:HE	1.76	0.49
10:k:18:PHE:HE2	20:z:13:VAL:HG21	1.78	0.49
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.94	0.49
22:B:604:CLA:H42	22:B:605:CLA:H42	1.95	0.49
5:E:68:ASP:O	5:E:72:ALA:HB2	2.12	0.49
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.95	0.49
26:A:410:PL9:H152	28:E:101:LHG:C38	2.42	0.48
10:K:24:VAL:CG1	19:Y:25:ILE:HD13	2.39	0.48
24:b:619:BCR:H331	24:b:619:BCR:C8	2.41	0.48
3:c:45:LEU:HA	3:c:139:THR:HG22	1.94	0.48
13:o:18:LYS:NZ	13:o:74:GLU:OE1	2.43	0.48
22:a:404:CLA:HMA2	27:c:523:LMG:H142	1.94	0.48
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.95	0.48
22:B:613:CLA:HBB1	22:B:613:CLA:HMB1	1.96	0.48
2:b:492:GLU:OE1	5:e:3:GLY:N	2.46	0.48
22:D:404:CLA:HMB1	22:D:404:CLA:HBB1	1.94	0.48
1:a:112:TYR:O	1:a:116:ILE:HG12	2.13	0.48
4:d:16:ASP:OD1	33:d:413:STE:H183	2.14	0.48
12:m:32:GLN:C	36:m:205:HOH:O	2.56	0.48
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.48	0.48
2:B:102:VAL:HA	24:B:618:BCR:C40	2.44	0.48
2:b:249:ALA:CB	22:b:604:CLA:HBC3	2.43	0.48
2:b:102:VAL:HG11	22:b:606:CLA:H142	1.96	0.48
4:d:194:ASN:HA	4:d:295:SER:OG	2.13	0.48
6:F:31:ILE:HG13	35:F:101:HEC:HMC1	1.95	0.47
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.49	0.47
5:e:17:VAL:HG23	9:j:7:ARG:HD3	1.96	0.47
20:z:3:ILE:HG22	20:z:7:LEU:HD23	1.95	0.47
1:A:227:THR:HB	1:A:231:GLU:HG3	1.97	0.47
2:B:27:THR:HG22	2:B:107:LEU:CD1	2.44	0.47
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.96	0.47
22:b:604:CLA:H42	22:b:605:CLA:H2	1.96	0.47
3:c:315:MET:CE	3:c:365:TRP:HZ3	2.27	0.47
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:15:THR:HG22	9:J:19:MET:HE2	1.96	0.47
13:O:57:LYS:NZ	36:O:301:HOH:O	2.29	0.47
10:k:17:ILE:HD11	20:z:6:GLN:HG2	1.97	0.47
7:H:6:TRP:CZ2	7:H:10:ILE:HD11	2.50	0.47
15:t:29:ILE:HD12	15:t:29:ILE:H	1.80	0.47
2:B:502:VAL:HG22	2:B:502:VAL:O	2.15	0.46
12:M:31:SER:HB2	12:m:32:GLN:OE1	2.16	0.46
3:c:315:MET:CE	36:c:768:HOH:O	2.60	0.46
2:B:287:ARG:HD3	36:B:709:HOH:O	2.14	0.46
2:B:397:VAL:HG12	2:B:417:VAL:HG11	1.97	0.46
3:c:38:GLY:HA3	22:c:511:CLA:HMD2	1.96	0.46
3:c:391[B]:ARG:CZ	36:c:606:HOH:O	2.61	0.46
26:a:409:PL9:H402	4:d:38:PHE:CD1	2.50	0.46
9:J:5:GLY:N	36:J:205:HOH:O	2.49	0.46
13:O:27:ARG:HG3	13:O:27:ARG:HH11	1.81	0.46
12:M:30:GLU:HA	12:M:30:GLU:OE1	2.15	0.46
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.51	0.46
23:d:402:PHO:H3A	22:d:403:CLA:H142	1.97	0.46
7:h:28:THR:HB	7:h:29:PRO:HD3	1.96	0.46
5:E:22[A]:ILE:HD12	5:E:23:HIS:CE1	2.50	0.46
2:b:58:GLN:C	2:b:329:PRO:HB3	2.41	0.46
2:B:67:ALA:HA	2:B:71:VAL:O	2.16	0.46
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.51	0.46
35:f:101:HEC:HBB3	35:f:101:HEC:HHC	1.98	0.46
3:c:42:LEU:HD21	22:c:511:CLA:H2A	1.96	0.46
4:d:209:LEU:HD23	4:d:209:LEU:C	2.41	0.46
5:e:8:ARG:NH2	5:e:12:ASP:OD2	2.43	0.46
13:o:53:LYS:NZ	13:o:232:GLU:OE1	2.49	0.46
14:r:28:VAL:O	14:r:31:VAL:CB	2.63	0.46
4:D:170:ALA:HB1	4:D:171:PRO:HD2	1.97	0.46
22:c:513:CLA:C4B	24:c:514:BCR:H383	2.45	0.46
3:c:180:MET:HE1	27:c:522:LMG:HC72	1.98	0.46
2:B:413:ASP:OD2	2:B:416:THR:OG1	2.27	0.45
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.80	0.45
28:a:410:LHG:O4	4:d:141:TYR:OH	2.18	0.45
2:b:228:ALA:HB2	33:b:627:STE:H62	1.98	0.45
2:b:189:GLY:O	2:b:197:GLY:HA3	2.16	0.45
22:B:606:CLA:H93	22:B:606:CLA:H112	1.78	0.45
24:B:619:BCR:H383	24:B:619:BCR:H23C	1.98	0.45
29:f:102:SQD:C7	14:r:32:GLN:CB	2.94	0.45
4:d:13:GLY:N	36:d:510:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.45
1:a:229:GLU:CD	1:a:229:GLU:H	2.25	0.45
24:C:514:BCR:H371	24:C:514:BCR:H24C	1.72	0.45
16:U:27:LEU:HD13	16:U:61:VAL:HG13	1.99	0.45
22:c:504:CLA:H91	22:c:508:CLA:H172	1.97	0.45
4:d:49:LEU:HD13	24:d:406:BCR:C15	2.45	0.45
9:j:18:GLY:O	9:j:21:VAL:HG13	2.17	0.45
1:A:159:LEU:C	1:A:162[A]:PRO:HD2	2.42	0.45
3:C:344:SER:O	13:O:75:THR:HG22	2.17	0.45
4:D:246:MET:HE2	4:D:246:MET:HA	1.99	0.45
4:D:272:LEU:C	4:D:272:LEU:HD23	2.42	0.45
16:U:36:ILE:O	16:U:36:ILE:HG22	2.16	0.45
17:v:76:MET:HE1	17:v:115:ILE:HD12	1.98	0.45
17:v:99:ASP:N	17:v:99:ASP:OD1	2.49	0.45
2:B:414:PRO:N	2:B:415:PRO:HD2	2.31	0.45
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.99	0.45
17:V:41:HIS:HA	17:V:45:ILE:O	2.17	0.45
24:d:406:BCR:H402	9:j:21:VAL:HG21	1.98	0.45
9:J:19:MET:O	9:J:23:VAL:HG23	2.16	0.45
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.05	0.45
20:Z:2:THR:HG22	20:Z:3:ILE:N	2.31	0.45
22:b:614:CLA:H192	27:m:101:LMG:H421	1.99	0.45
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.51	0.44
24:H:101:BCR:H331	24:H:101:BCR:HC8	1.99	0.44
10:K:25:LEU:HD22	24:Y:101:BCR:H332	2.00	0.44
19:y:22:LEU:HA	19:y:25:ILE:HG22	1.99	0.44
24:B:618:BCR:H15C	24:B:618:BCR:H351	1.83	0.44
22:b:615:CLA:H161	7:h:7:LEU:HD11	1.99	0.44
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.44
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.52	0.44
2:B:241:SER:HB3	22:B:612:CLA:HED3	2.00	0.44
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.53	0.44
3:C:180:MET:HG2	3:C:199:ILE:O	2.18	0.44
3:c:315:MET:HE3	3:c:365:TRP:CZ3	2.52	0.44
3:c:367:GLU:N	3:c:368:PRO:CD	2.81	0.44
14:r:24:LEU:HD13	14:r:24:LEU:C	2.42	0.44
19:y:17:GLU:O	19:y:20:ALA:HB3	2.17	0.44
24:t:101:BCR:H23C	24:t:101:BCR:H382	2.00	0.44
20:z:3:ILE:O	20:z:7:LEU:HD23	2.18	0.44
26:A:410:PL9:H371	36:F:211:HOH:O	2.17	0.44
5:E:30:LEU:HD12	35:F:101:HEC:HMC3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:U:70:ARG:HD2	36:U:213:HOH:O	2.18	0.44
4:d:233:ARG:NH1	36:d:506:HOH:O	2.43	0.44
13:o:194:LYS:NZ	36:o:309:HOH:O	2.50	0.44
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.99	0.44
1:a:84:PRO:HA	1:a:112:TYR:CG	2.53	0.44
26:A:410:PL9:C15	28:E:101:LHG:H381	2.46	0.44
5:E:22[A]:ILE:HG23	5:E:23:HIS:HD1	1.83	0.44
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.44
26:A:410:PL9:H513	36:D:629:HOH:O	2.17	0.43
13:O:5:LEU:HD12	13:O:10:ILE:HD11	2.00	0.43
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.00	0.43
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.00	0.43
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	2.00	0.43
2:b:43:ALA:HB1	33:b:621:STE:H72	2.01	0.43
10:K:27:VAL:HG12	10:K:27:VAL:O	2.18	0.43
17:v:69:ILE:HD12	17:v:120:LEU:HD12	2.00	0.43
2:B:145:LEU:CD2	22:B:604:CLA:H193	2.47	0.43
22:b:609:CLA:H141	22:b:609:CLA:H172	2.00	0.43
5:e:25:ILE:HD12	5:e:25:ILE:N	2.34	0.43
10:k:18:PHE:CE2	20:z:13:VAL:HG21	2.53	0.43
2:B:160:GLY:HA3	2:B:180:PRO:HB3	2.00	0.43
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.00	0.43
4:d:56:THR:HG22	36:e:213:HOH:O	2.19	0.43
24:T:101:BCR:HC7	24:T:101:BCR:H331	1.81	0.43
24:b:618:BCR:H331	24:b:618:BCR:HC8	2.00	0.43
3:c:315:MET:CE	3:c:366:LEU:HD13	2.48	0.43
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.00	0.43
2:B:149[A]:LEU:HD21	22:B:606:CLA:HBB2	2.01	0.43
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.43
24:B:618:BCR:H24C	24:B:618:BCR:H371	1.77	0.43
13:O:93:LEU:O	13:O:128:SER:HA	2.19	0.43
22:b:609:CLA:HBB1	22:b:609:CLA:HMB3	2.00	0.43
24:d:406:BCR:C8	24:d:406:BCR:C33	2.96	0.43
15:t:29:ILE:HD12	15:t:29:ILE:N	2.33	0.43
3:C:178:LYS:NZ	3:C:184:GLY:O	2.50	0.43
13:O:27:ARG:NH1	36:O:304:HOH:O	2.41	0.43
2:b:226:TYR:HA	2:b:231:MET:HG3	2.00	0.43
17:v:41:HIS:HA	17:v:45:ILE:O	2.19	0.43
22:C:509:CLA:H141	22:C:509:CLA:H171	2.00	0.43
2:b:299:GLU:O	2:b:303:SER:HB2	2.18	0.43
29:A:414:SQD:H383	22:b:606:CLA:H93	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:610:CLA:HHC	22:B:610:CLA:HBB1	2.01	0.42
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.01	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.42
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.42
33:M:102:STE:O1	36:M:202:HOH:O	2.21	0.42
3:c:315:MET:CE	3:c:365:TRP:CZ3	3.02	0.42
12:m:9:ILE:HG13	12:m:13:LEU:HD22	2.01	0.42
20:z:1:MET:CB	20:z:4:LEU:HD23	2.49	0.42
2:B:52:LEU:HD12	13:o:59:LYS:HE2	2.01	0.42
2:B:413:ASP:OD1	36:B:706:HOH:O	2.21	0.42
3:C:50:LEU:O	3:C:54:VAL:HG23	2.19	0.42
3:C:62:PHE:C	3:C:62:PHE:CD1	2.95	0.42
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.83	0.42
4:D:307:GLU:HG3	36:D:530:HOH:O	2.18	0.42
5:E:65:LEU:O	5:E:67:THR:HG23	2.19	0.42
24:T:101:BCR:H382	24:T:101:BCR:H23C	2.01	0.42
3:c:155:ASN:OD1	3:c:255:THR:HG22	2.19	0.42
6:f:26:LEU:O	6:f:29:PRO:HD2	2.19	0.42
2:B:201:HIS:HB2	22:B:602:CLA:CHB	2.50	0.42
33:D:412:STE:H172	18:X:21:LEU:HD21	2.01	0.42
10:K:18:PHE:CE2	20:Z:9:LEU:HD21	2.54	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.89	0.42
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.00	0.42
1:a:192:ILE:HG13	1:a:293:MET:HE1	2.02	0.42
3:c:128:GLY:HA3	22:c:513:CLA:C3C	2.49	0.42
2:B:25:MET:HE1	2:B:108:PHE:CD1	2.54	0.42
22:C:509:CLA:H91	22:C:509:CLA:H112	1.81	0.42
30:C:518:DGD:O1A	30:C:518:DGD:HA41	2.19	0.42
14:R:5:VAL:HG12	14:R:9:LEU:HD12	2.01	0.42
20:Z:55:GLY:HA2	20:Z:58:ASN:CB	2.49	0.42
3:c:93:ALA:HB1	3:c:99:VAL:HG21	2.02	0.42
22:c:504:CLA:H92	22:c:504:CLA:H62	1.85	0.42
4:d:42:TYR:CZ	6:f:25:THR:HG23	2.55	0.42
13:o:143:LYS:HE3	36:o:359:HOH:O	2.20	0.42
5:E:14:ILE:O	5:E:20:TRP:NE1	2.50	0.42
35:F:101:HEC:HBB2	35:F:101:HEC:HMB3	2.00	0.42
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.01	0.42
1:a:237:TYR:HB2	1:a:245:THR:HG21	2.00	0.42
17:v:78:ASN:OD1	17:v:96:ARG:NH1	2.49	0.42
22:B:601:CLA:H92	24:H:101:BCR:H21C	2.01	0.42
24:H:101:BCR:H11C	24:H:101:BCR:H341	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:608:CLA:H141	22:b:608:CLA:H161	1.88	0.42
3:c:318:LEU:C	3:c:318:LEU:HD23	2.45	0.42
15:t:8:PHE:CE2	33:t:103:STE:H151	2.54	0.42
1:A:332[B]:HIS:O	1:A:333[B]:GLU:C	2.63	0.42
8:I:2:GLU:O	8:I:6:ILE:HG12	2.20	0.42
23:a:403:PHO:CMB	23:a:403:PHO:HBB1	2.50	0.42
26:a:409:PL9:C49	4:d:39:PRO:HG3	2.50	0.42
2:b:92:SER:O	2:b:96:VAL:HG23	2.20	0.42
22:b:610:CLA:H151	22:b:610:CLA:H203	2.02	0.42
24:d:406:BCR:HC8	24:d:406:BCR:C33	2.49	0.42
14:r:3:TRP:CD1	14:r:3:TRP:C	2.98	0.42
5:E:45:ASP:OD2	14:R:4:ARG:NH2	2.47	0.42
3:c:352:GLY:O	3:c:355[A]:THR:HG22	2.19	0.42
22:d:404:CLA:H43	22:d:404:CLA:O1A	2.20	0.42
17:v:103:LYS:NZ	36:v:308:HOH:O	2.53	0.42
26:A:410:PL9:H471	26:A:410:PL9:H451	1.91	0.42
10:K:25:LEU:N	10:K:26:PRO:CD	2.82	0.42
2:b:91:TRP:HE1	33:b:622:STE:H111	1.84	0.42
2:b:298:LEU:HD23	2:b:298:LEU:HA	1.88	0.42
24:A:407:BCR:H24C	24:A:407:BCR:H371	1.78	0.41
2:B:104:SER:OG	29:B:623:SQD:H221	2.20	0.41
5:E:6:GLY:HA2	36:E:218:HOH:O	2.20	0.41
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.02	0.41
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.54	0.41
3:c:315:MET:HE2	3:c:365:TRP:HZ3	1.85	0.41
9:j:11:TRP:CZ2	9:j:12:ILE:HD11	2.55	0.41
22:B:607:CLA:H191	28:B:622:LHG:H142	2.02	0.41
22:B:616:CLA:O1A	22:B:616:CLA:C2	2.67	0.41
2:b:36:SER:OG	24:b:618:BCR:H362	2.19	0.41
4:d:134:ARG:HG2	33:d:411:STE:O1	2.21	0.41
7:h:25:TRP:O	7:h:26:GLY:C	2.63	0.41
10:k:25:LEU:N	10:k:26:PRO:CD	2.82	0.41
1:A:114:LEU:C	1:A:114:LEU:HD23	2.45	0.41
24:B:619:BCR:H383	24:B:619:BCR:C23	2.50	0.41
29:B:623:SQD:H383	29:B:623:SQD:H352	1.86	0.41
1:a:245:THR:HB	4:d:265:ARG:HE	1.85	0.41
1:A:183[B]:MET:HA	22:A:402:CLA:HMD1	2.02	0.41
30:A:415:DGD:HD5	2:b:75:TRP:HB3	2.01	0.41
2:B:488:PRO:O	2:B:492:GLU:HB2	2.21	0.41
3:C:128:GLY:HA3	22:C:513:CLA:C3C	2.51	0.41
4:D:90:LEU:HD23	4:D:90:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:22[A]:ILE:HG13	14:R:19:ALA:CB	2.51	0.41
10:K:28:ILE:N	10:K:29:PRO:CD	2.83	0.41
20:Z:6:GLN:O	20:Z:7:LEU:HD23	2.20	0.41
22:c:512:CLA:H203	27:c:522:LMG:H442	2.02	0.41
22:C:505:CLA:HBC2	24:C:515:BCR:C34	2.50	0.41
24:a:405:BCR:C8	24:a:405:BCR:H331	2.51	0.41
33:b:627:STE:H61	33:d:413:STE:H92	2.02	0.41
3:c:175:LEU:HD22	22:c:501:CLA:C3D	2.51	0.41
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.56	0.41
4:d:103:ARG:NH2	36:d:518:HOH:O	2.54	0.41
4:d:279:LEU:HD22	23:d:402:PHO:HBC3	2.02	0.41
4:d:291:LEU:HD11	30:h:101:DGD:CGB	2.50	0.41
35:V:201:HEC:HMC1	35:V:201:HEC:CBC	2.44	0.41
1:a:114:LEU:C	1:a:114:LEU:HD23	2.45	0.41
1:a:189[B]:GLU:OE1	32:a:418[B]:OEY:O6	2.38	0.41
2:b:159:THR:O	2:b:180:PRO:HB3	2.21	0.41
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.20	0.41
19:Y:34:MET:O	19:Y:38:LEU:HG	2.21	0.41
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.02	0.41
20:z:48:ILE:O	20:z:52:LEU:HG	2.21	0.41
4:D:13:GLY:O	4:D:17:ILE:HG12	2.21	0.41
22:D:403:CLA:HBA1	22:D:403:CLA:C4A	2.50	0.41
24:b:618:BCR:H15C	24:b:618:BCR:H351	1.79	0.41
24:d:406:BCR:H20C	24:d:406:BCR:H361	1.90	0.41
13:o:42:ARG:O	13:o:241:ALA:HA	2.21	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.03	0.41
1:A:161[B]:TYR:HB3	1:A:162[B]:PRO:HD3	2.03	0.41
3:C:135:ARG:O	3:C:135:ARG:HD3	2.20	0.41
16:U:27:LEU:HD13	16:U:61:VAL:CG1	2.51	0.41
18:X:11:PHE:O	18:X:15:LEU:HD23	2.21	0.41
1:a:278:TRP:HB3	1:a:279:PRO:HD3	2.03	0.41
22:b:612:CLA:HBB1	22:b:612:CLA:HMB1	2.03	0.41
22:c:507:CLA:H92	22:c:507:CLA:H61	1.95	0.41
22:B:604:CLA:H142	33:B:620:STE:H142	2.02	0.41
3:C:126:GLY:O	3:C:130:VAL:HG13	2.21	0.41
17:V:41:HIS:O	17:V:42:VAL:C	2.64	0.41
1:a:308:ASP:OD1	1:a:308:ASP:C	2.64	0.41
2:b:63:LEU:N	2:b:64:PRO:HD2	2.36	0.41
2:b:135:LEU:N	2:b:136:PRO:CD	2.84	0.41
2:b:433:ASP:OD1	2:b:433:ASP:C	2.64	0.41
3:c:109:PHE:N	3:c:110:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:391[A]:ARG:CD	36:c:603:HOH:O	2.64	0.41
22:c:509:CLA:H142	22:c:509:CLA:H111	1.85	0.41
1:A:140:ARG:HB2	4:D:220:ASN:HA	2.03	0.40
2:B:4:PRO:HB2	2:B:6:TYR:CE1	2.56	0.40
2:B:451:PHE:CD1	2:B:451:PHE:C	2.98	0.40
22:B:605:CLA:H143	22:B:610:CLA:HMA2	2.02	0.40
4:D:38:PHE:N	4:D:39:PRO:CD	2.84	0.40
3:c:334:PRO:HA	13:o:153:THR:OG1	2.21	0.40
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.51	0.40
26:A:410:PL9:H422	26:A:410:PL9:H401	1.89	0.40
24:B:619:BCR:C23	24:B:619:BCR:C38	2.98	0.40
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.93	0.40
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.40
13:O:193:THR:HG21	13:O:220:LEU:HD12	2.02	0.40
1:a:132:GLU:O	1:a:136:ARG:HG2	2.21	0.40
2:b:233:ASN:C	2:b:233:ASN:OD1	2.64	0.40
19:y:17:GLU:HB3	36:y:102:HOH:O	2.19	0.40
1:A:45:THR:HG23	22:D:403:CLA:H191	2.03	0.40
36:A:503:HOH:O	4:D:243:THR:HG22	2.21	0.40
22:D:404:CLA:C4B	33:D:412:STE:H151	2.52	0.40
12:M:8:LEU:HD11	33:T:102:STE:H111	2.03	0.40
26:a:409:PL9:H251	22:d:403:CLA:H141	2.03	0.40
24:c:516:BCR:H15C	24:c:516:BCR:H351	1.98	0.40
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.57	0.40
24:B:618:BCR:H361	24:B:618:BCR:H20C	1.78	0.40
4:D:209:LEU:C	4:D:209:LEU:CD2	2.94	0.40
4:d:267:LEU:C	4:d:267:LEU:CD2	2.93	0.40
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.21	0.40
13:o:173:ALA:C	13:o:175:PRO:HD3	2.46	0.40
24:t:101:BCR:H11C	24:t:101:BCR:H341	1.97	0.40
22:C:501:CLA:CAD	22:C:503:CLA:H12	2.52	0.40
22:C:513:CLA:C4	22:C:513:CLA:O2A	2.70	0.40
13:O:27:ARG:HG3	36:O:304:HOH:O	2.22	0.40
24:T:101:BCR:H20C	24:T:101:BCR:H361	1.92	0.40
26:a:409:PL9:H302	4:d:45:LEU:HD22	2.04	0.40
22:b:615:CLA:H2	22:b:616:CLA:HBB2	2.04	0.40
22:c:506:CLA:O1A	22:c:506:CLA:C2	2.69	0.40
33:d:412:STE:H71	18:x:16:SER:HB3	2.03	0.40
7:h:17:GLU:O	7:h:18:TYR:C	2.61	0.40
11:l:2:GLU:N	11:l:3:PRO:CD	2.84	0.40
17:v:57:GLU:OE1	36:v:301:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	36	35
1	a	391/344 (114%)	387 (99%)	3 (1%)	1 (0%)	36	35
2	B	508/506 (100%)	497 (98%)	10 (2%)	1 (0%)	43	42
2	b	503/506 (99%)	491 (98%)	12 (2%)	0	100	100
3	C	450/461 (98%)	440 (98%)	9 (2%)	1 (0%)	43	42
3	c	459/461 (100%)	443 (96%)	15 (3%)	1 (0%)	43	42
4	D	339/352 (96%)	329 (97%)	10 (3%)	0	100	100
4	d	340/352 (97%)	331 (97%)	9 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	30 (94%)	2 (6%)	0	100	100
7	H	63/66 (96%)	58 (92%)	4 (6%)	1 (2%)	7	3
7	h	61/66 (92%)	57 (93%)	4 (7%)	0	100	100
8	I	34/38 (90%)	33 (97%)	1 (3%)	0	100	100
8	i	34/38 (90%)	31 (91%)	3 (9%)	0	100	100
9	J	34/40 (85%)	32 (94%)	2 (6%)	0	100	100
9	j	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/46 (76%)	34 (97%)	0	1 (3%)	3	1
10	k	35/46 (76%)	35 (100%)	0	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	M	31/36 (86%)	30 (97%)	1 (3%)	0	100	100
12	m	30/36 (83%)	28 (93%)	2 (7%)	0	100	100
13	O	243/272 (89%)	227 (93%)	12 (5%)	4 (2%)	7	3
13	o	242/272 (89%)	233 (96%)	8 (3%)	1 (0%)	30	27
14	R	32/40 (80%)	30 (94%)	2 (6%)	0	100	100
14	r	29/40 (72%)	27 (93%)	2 (7%)	0	100	100
15	T	28/30 (93%)	28 (100%)	0	0	100	100
15	t	28/30 (93%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	92 (97%)	3 (3%)	0	100	100
16	u	95/134 (71%)	93 (98%)	2 (2%)	0	100	100
17	V	135/163 (83%)	129 (96%)	5 (4%)	1 (1%)	18	14
17	v	135/163 (83%)	129 (96%)	6 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	37 (100%)	0	0	100	100
19	Y	25/46 (54%)	23 (92%)	1 (4%)	1 (4%)	2	0
19	y	28/46 (61%)	25 (89%)	2 (7%)	1 (4%)	2	1
20	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
20	z	60/62 (97%)	55 (92%)	3 (5%)	2 (3%)	3	1
All	All	5374/5686 (94%)	5216 (97%)	141 (3%)	17 (0%)	36	35

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
10	K	16	ALA
13	O	60	ARG
17	V	64	PRO
3	c	416	SER
13	O	62	GLU
20	z	2	THR
7	H	26	GLY
13	O	59	LYS
19	Y	43	ARG
19	y	43	ARG
2	B	294	SER
13	O	133	VAL

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Mol	Chain	Res	Type
13	o	56	PRO
1	a	259	ILE
20	z	61	VAL
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	320/280 (114%)	313 (98%)	7 (2%)	45	50
1	a	319/280 (114%)	310 (97%)	9 (3%)	38	41
2	B	408/404 (101%)	396 (97%)	12 (3%)	37	40
2	b	402/404 (100%)	393 (98%)	9 (2%)	45	50
3	C	353/362 (98%)	345 (98%)	8 (2%)	44	49
3	c	361/362 (100%)	351 (97%)	10 (3%)	38	41
4	D	277/283 (98%)	270 (98%)	7 (2%)	42	45
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	35
5	E	72/73 (99%)	66 (92%)	6 (8%)	10	7
5	e	71/73 (97%)	70 (99%)	1 (1%)	59	66
6	F	28/39 (72%)	28 (100%)	0	100	100
6	f	28/39 (72%)	26 (93%)	2 (7%)	13	10
7	H	54/55 (98%)	52 (96%)	2 (4%)	30	30
7	h	53/55 (96%)	51 (96%)	2 (4%)	29	29
8	I	32/34 (94%)	29 (91%)	3 (9%)	8	5
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	25
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	29 (97%)	1 (3%)	33	34
10	k	30/37 (81%)	23 (77%)	7 (23%)	1	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	31 (91%)	3 (9%)	9	6
12	M	28/32 (88%)	27 (96%)	1 (4%)	31	31
12	m	28/32 (88%)	26 (93%)	2 (7%)	13	10
13	O	206/228 (90%)	199 (97%)	7 (3%)	32	33
13	o	207/228 (91%)	199 (96%)	8 (4%)	28	28
14	R	28/32 (88%)	24 (86%)	4 (14%)	3	2
14	r	23/32 (72%)	19 (83%)	4 (17%)	2	1
15	T	26/26 (100%)	24 (92%)	2 (8%)	12	8
15	t	25/26 (96%)	25 (100%)	0	100	100
16	U	84/112 (75%)	81 (96%)	3 (4%)	31	31
16	u	84/112 (75%)	81 (96%)	3 (4%)	31	31
17	V	117/138 (85%)	113 (97%)	4 (3%)	32	33
17	v	117/138 (85%)	111 (95%)	6 (5%)	21	19
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	12
18	x	31/34 (91%)	28 (90%)	3 (10%)	8	5
19	Y	19/37 (51%)	17 (90%)	2 (10%)	6	4
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%)	42 (82%)	9 (18%)	2	1
All	All	4444/4642 (96%)	4273 (96%)	171 (4%)	28	29

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	13	LEU
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	243	GLU
1	A	244	GLU
1	A	248	ILE
2	B	76	SER
2	B	79	SER
2	B	86	ILE

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Mol	Chain	Res	Type
2	B	98	LEU
2	B	127	ARG
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	405	GLU
2	B	476	ARG
2	B	486	LEU
2	B	492	GLU
3	C	130	VAL
3	C	141	GLU
3	C	200	THR
3	C	240	ILE
3	C	255	THR
3	C	273	SER
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	154	VAL
4	D	259	ILE
4	D	264	LYS
4	D	272	LEU
4	D	295	SER
4	D	345	VAL
5	E	5	THR
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
5	E	81	GLU
7	H	20	LYS
7	H	65	LEU
8	I	4	LEU
8	I	6	ILE
8	I	36	ASP
9	J	24	ILE
10	K	10	LYS
12	M	25	LEU
13	O	57	LYS
13	O	78	LEU
13	O	107	THR
13	O	134	THR

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Mol	Chain	Res	Type
13	O	135	SER
13	O	198	SER
13	O	214	THR
14	R	10	LEU
14	R	21	ARG
14	R	29	LYS
14	R	32	GLN
15	T	25	GLU
15	T	29	ILE
16	U	51	LYS
16	U	61	VAL
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	17	LYS
17	V	86	GLN
18	X	3	ILE
18	X	15	LEU
19	Y	34	MET
19	Y	45	ASN
20	Z	2	THR
20	Z	15	LEU
20	Z	19	MET
20	Z	32	ASP
20	Z	35	ARG
20	Z	46	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	231	GLU
1	a	271	LEU
1	a	288	LEU
2	b	83	GLU
2	b	128	THR
2	b	137	LYS
2	b	149	LEU
2	b	236	THR
2	b	362	PHE
2	b	485	GLU

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Mol	Chain	Res	Type
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	99	VAL
3	c	105	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	354[A]	GLU
3	c	354[B]	GLU
4	d	90	LEU
4	d	182	LEU
4	d	233	ARG
4	d	259	ILE
4	d	291	LEU
4	d	293	LEU
4	d	307	GLU
4	d	321	LEU
4	d	329	MET
5	e	83	LEU
6	f	15	ILE
6	f	28	VAL
7	h	7	LEU
7	h	12	ARG
8	i	2	GLU
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
10	k	24	VAL
10	k	25	LEU
10	k	27	VAL
10	k	30	VAL
10	k	35	LEU
11	l	7	ARG
11	l	21	LEU
11	l	30	LEU
12	m	13	LEU
12	m	16	LEU
13	o	18	LYS

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Mol	Chain	Res	Type
13	o	49	THR
13	o	64	GLU
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	134	THR
13	o	207	ARG
14	r	3	TRP
14	r	9	LEU
14	r	10	LEU
14	r	30	GLN
16	u	10	VAL
16	u	15	GLU
16	u	23	GLU
17	v	2	GLU
17	v	52	LEU
17	v	57	GLU
17	v	90	GLU
17	v	107	LEU
17	v	110	LYS
18	x	2	THR
18	x	15	LEU
18	x	34	ILE
19	y	19	ILE
19	y	41	VAL
19	y	45	ASN
20	z	1	MET
20	z	14	ILE
20	z	20	VAL
20	z	29	SER
20	z	31	GLN
20	z	32	ASP
20	z	39	LEU
20	z	42	LEU
20	z	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
2	B	179	GLN
2	B	331	ASN

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Mol	Chain	Res	Type
2	B	374	ASN
2	B	394	GLN
2	B	497	GLN
3	C	385	GLN
3	C	415	ASN
4	D	236	ASN
4	D	334	GLN
11	L	8	GLN
13	O	88	ASN
13	O	155	ASN
13	O	219	GLN
14	R	22	ASN
16	U	37	GLN
17	V	86	GLN
18	X	38	GLN
20	Z	31	GLN
1	a	199	GLN
1	a	234	ASN
2	b	179	GLN
3	c	201	ASN
3	c	322	GLN
3	c	378	ASN
4	d	350	ASN
5	e	82	GLN
7	h	59	ASN
13	o	80	GLN
13	o	155	ASN
14	r	30	GLN
17	v	106	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	0.95	0	8,9,11	1.06	1 (12%)
15	FME	T	1	15	8,9,10	1.04	1 (12%)	8,9,11	1.46	1 (12%)
12	FME	m	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.97	0
12	FME	M	1	12	8,9,10	1.10	1 (12%)	8,9,11	0.97	0
15	FME	t	1	15	8,9,10	1.54	1 (12%)	8,9,11	0.86	1 (12%)
8	FME	i	1	8	8,9,10	1.16	1 (12%)	8,9,11	1.10	1 (12%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	t	1	FME	CA-N	-3.67	1.41	1.46
8	i	1	FME	CA-N	-2.58	1.42	1.46
15	T	1	FME	CA-N	-2.38	1.43	1.46
12	M	1	FME	CA-N	-2.22	1.43	1.46
12	m	1	FME	CA-N	-2.20	1.43	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.64	118.51	125.32
8	i	1	FME	CA-N-CN	-2.13	119.54	122.82
15	t	1	FME	CB-CA-N	2.10	114.35	110.52
8	I	1	FME	C-CA-N	2.01	113.37	109.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	m	1	FME	O-C-CA-CB
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	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 191 ligands modelled in this entry, 6 are monoatomic - leaving 185 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
27	LMG	m	101	-	51,51,55	0.95	2 (3%)	59,59,63	1.48	8 (13%)
24	BCR	b	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.50	9 (16%)
22	CLA	D	404	4	69,73,73	1.69	11 (15%)	82,113,113	1.16	4 (4%)
33	STE	R	101	-	11,11,19	0.98	0	11,11,19	0.93	0
31	OEX	A	416[A]	1,36,3	0,14,14	-	-	-	-	-
22	CLA	b	615	2	69,73,73	1.65	10 (14%)	82,113,113	1.58	11 (13%)
28	LHG	B	622	-	48,48,48	0.92	3 (6%)	51,54,54	1.29	5 (9%)
27	LMG	M	101	-	51,51,55	1.03	4 (7%)	59,59,63	1.55	9 (15%)
22	CLA	B	607	36	69,73,73	1.13	7 (10%)	82,113,113	1.29	8 (9%)
24	BCR	H	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.35	8 (14%)

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	10 (14%)	82,113,113	1.40	9 (10%)
33	STE	D	412	-	19,19,19	0.55	0	19,19,19	1.34	2 (10%)
33	STE	b	625	-	19,19,19	0.73	0	19,19,19	0.82	0
33	STE	t	103	-	17,17,19	0.63	0	17,17,19	1.12	1 (5%)
33	STE	a	413	-	9,9,19	0.56	0	8,8,19	0.53	0
26	PL9	A	410	-	55,55,55	1.24	6 (10%)	68,69,69	1.42	12 (17%)
33	STE	c	521	-	19,19,19	0.66	0	19,19,19	0.94	0
24	BCR	D	405	-	41,41,41	1.22	3 (7%)	56,56,56	1.39	10 (17%)
27	LMG	c	523	-	49,49,55	0.85	1 (2%)	57,57,63	1.29	6 (10%)
22	CLA	B	614	2	69,73,73	1.06	5 (7%)	82,113,113	1.31	9 (10%)
22	CLA	C	508	3	69,73,73	1.50	10 (14%)	82,113,113	1.51	11 (13%)
27	LMG	D	410	-	31,31,55	1.14	3 (9%)	33,33,63	1.12	2 (6%)
22	CLA	B	610	36	69,73,73	1.46	11 (15%)	82,113,113	1.39	9 (10%)
32	OEY	A	417[B]	1,36,3	0,16,16	-	-	-	-	-
22	CLA	c	501	3	69,73,73	1.15	7 (10%)	82,113,113	1.41	9 (10%)
24	BCR	a	405	-	41,41,41	1.01	3 (7%)	56,56,56	1.28	5 (8%)
22	CLA	b	616	2	64,68,73	1.16	7 (10%)	76,107,113	1.39	8 (10%)
30	DGD	C	519	-	63,63,67	1.23	6 (9%)	77,77,81	1.33	8 (10%)
22	CLA	c	512	3	69,73,73	1.12	8 (11%)	82,113,113	1.34	7 (8%)
28	LHG	A	412	-	46,46,48	1.18	5 (10%)	49,52,54	1.40	7 (14%)
22	CLA	B	612	2	69,73,73	1.30	8 (11%)	82,113,113	1.53	12 (14%)
29	SQD	D	408	-	34,36,54	1.00	3 (8%)	42,45,65	2.17	10 (23%)
22	CLA	B	601	36	69,73,73	1.30	8 (11%)	82,113,113	1.47	7 (8%)
24	BCR	d	406	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	6 (10%)
22	CLA	C	506	3	69,73,73	1.56	9 (13%)	82,113,113	1.18	6 (7%)
23	PHO	A	404	-	58,69,69	1.82	12 (20%)	55,99,99	1.74	12 (21%)
28	LHG	d	409	-	38,38,48	1.04	2 (5%)	41,44,54	1.18	4 (9%)
33	STE	b	621	-	15,15,19	0.42	0	14,14,19	0.80	0
33	STE	a	414	-	11,11,19	0.89	0	11,11,19	1.07	1 (9%)
22	CLA	C	503	3	69,73,73	1.30	7 (10%)	82,113,113	1.76	11 (13%)
24	BCR	B	619	-	41,41,41	1.18	3 (7%)	56,56,56	1.36	5 (8%)
29	SQD	a	412	-	35,35,54	1.11	2 (5%)	37,37,65	1.63	5 (13%)
33	STE	j	101	-	11,11,19	0.98	1 (9%)	11,11,19	1.11	2 (18%)
28	LHG	e	101	-	41,41,48	0.95	3 (7%)	44,47,54	1.32	5 (11%)
33	STE	C	521	-	11,11,19	0.80	0	11,11,19	1.22	1 (9%)
24	BCR	c	515	-	41,41,41	1.27	4 (9%)	56,56,56	1.44	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	A	411	-	48,48,55	1.10	5 (10%)	56,56,63	1.34	7 (12%)
30	DGD	H	102	-	63,63,67	1.41	12 (19%)	77,77,81	1.42	9 (11%)
24	BCR	A	407	-	41,41,41	1.15	4 (9%)	56,56,56	1.47	11 (19%)
24	BCR	x	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	8 (14%)
22	CLA	d	405	4	69,73,73	1.37	10 (14%)	82,113,113	1.21	9 (10%)
22	CLA	A	402	1	69,73,73	1.27	7 (10%)	82,113,113	1.24	10 (12%)
33	STE	B	625	-	15,15,19	0.48	0	14,14,19	0.62	0
30	DGD	h	101	-	63,63,67	1.18	7 (11%)	77,77,81	1.37	9 (11%)
22	CLA	c	503	3	69,73,73	1.23	9 (13%)	82,113,113	1.27	6 (7%)
33	STE	T	102	-	14,14,19	0.49	0	13,13,19	0.65	0
22	CLA	b	607	36	69,73,73	1.20	8 (11%)	82,113,113	1.18	8 (9%)
33	STE	d	412	-	19,19,19	0.81	1 (5%)	19,19,19	1.15	2 (10%)
29	SQD	A	413	-	50,52,54	1.10	7 (14%)	60,63,65	1.98	9 (15%)
30	DGD	c	518	-	63,63,67	1.24	10 (15%)	77,77,81	1.38	9 (11%)
22	CLA	C	505	3	69,73,73	1.27	8 (11%)	82,113,113	1.30	7 (8%)
24	BCR	c	514	-	41,41,41	1.18	3 (7%)	56,56,56	1.34	7 (12%)
24	BCR	C	514	-	41,41,41	1.19	3 (7%)	56,56,56	1.41	10 (17%)
24	BCR	k	101	-	41,41,41	1.10	4 (9%)	56,56,56	1.11	4 (7%)
28	LHG	B	621	-	48,48,48	0.92	2 (4%)	51,54,54	1.14	2 (3%)
26	PL9	D	406	-	55,55,55	1.61	8 (14%)	68,69,69	1.72	16 (23%)
22	CLA	b	614	2	69,73,73	1.26	8 (11%)	82,113,113	1.45	10 (12%)
26	PL9	a	409	-	55,55,55	1.13	5 (9%)	68,69,69	1.63	13 (19%)
22	CLA	B	616	2	64,68,73	1.39	7 (10%)	76,107,113	1.48	8 (10%)
27	LMG	a	416	-	55,55,55	1.06	2 (3%)	63,63,63	1.36	7 (11%)
28	LHG	D	409	-	48,48,48	1.14	3 (6%)	51,54,54	1.26	6 (11%)
33	STE	k	102	-	11,11,19	0.82	0	11,11,19	1.12	1 (9%)
22	CLA	C	512	3	69,73,73	1.20	6 (8%)	82,113,113	1.32	11 (13%)
22	CLA	C	511	3	69,73,73	1.48	11 (15%)	82,113,113	1.37	7 (8%)
22	CLA	b	604	2	69,73,73	1.19	6 (8%)	82,113,113	1.56	16 (19%)
24	BCR	b	618	-	41,41,41	1.21	3 (7%)	56,56,56	1.27	9 (16%)
22	CLA	c	510	3	69,73,73	1.41	8 (11%)	82,113,113	1.35	9 (10%)
22	CLA	C	501	3	69,73,73	1.38	9 (13%)	82,113,113	1.40	6 (7%)
33	STE	l	102	-	17,17,19	0.38	0	16,16,19	0.91	0
22	CLA	c	507	36	69,73,73	1.16	6 (8%)	82,113,113	1.40	12 (14%)
22	CLA	c	513	3	69,73,73	1.27	10 (14%)	82,113,113	1.18	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	C	516	-	41,41,41	1.20	3 (7%)	56,56,56	1.20	4 (7%)
22	CLA	b	611	2	69,73,73	1.25	7 (10%)	82,113,113	1.34	10 (12%)
33	STE	b	624	-	15,15,19	0.82	0	15,15,19	1.00	1 (6%)
24	BCR	b	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	6 (10%)
33	STE	M	102	-	14,14,19	0.61	0	14,14,19	1.16	0
22	CLA	b	613	2	69,73,73	1.15	7 (10%)	82,113,113	1.25	5 (6%)
22	CLA	B	609	2	69,73,73	1.51	9 (13%)	82,113,113	1.43	11 (13%)
22	CLA	C	502	3	69,73,73	1.29	9 (13%)	82,113,113	1.35	11 (13%)
22	CLA	C	509	3	69,73,73	1.25	8 (11%)	82,113,113	1.46	9 (10%)
22	CLA	B	602	2	69,73,73	1.36	8 (11%)	82,113,113	1.25	10 (12%)
24	BCR	T	101	-	41,41,41	1.09	3 (7%)	56,56,56	1.41	7 (12%)
33	STE	M	103	-	9,9,19	0.44	0	8,8,19	0.82	0
27	LMG	c	520	-	37,37,55	1.22	5 (13%)	45,45,63	1.36	8 (17%)
27	LMG	C	520	-	48,48,55	0.86	3 (6%)	56,56,63	1.36	8 (14%)
22	CLA	b	608	2	69,73,73	1.23	7 (10%)	82,113,113	1.26	11 (13%)
33	STE	d	411	-	16,16,19	0.63	0	16,16,19	1.43	3 (18%)
34	BCT	D	401	21	3,3,3	0.95	0	2,3,3	3.63	2 (100%)
23	PHO	d	402	-	58,69,69	2.11	9 (15%)	55,99,99	1.73	10 (18%)
22	CLA	C	507	36	69,73,73	1.21	8 (11%)	82,113,113	1.57	10 (12%)
29	SQD	a	411	-	52,54,54	1.02	4 (7%)	62,65,65	1.84	11 (17%)
35	HEC	v	201	17	50,50,50	1.72	3 (6%)	68,82,82	1.36	7 (10%)
22	CLA	c	506	3	69,73,73	1.55	9 (13%)	82,113,113	1.33	9 (10%)
22	CLA	B	605	2	69,73,73	1.24	7 (10%)	82,113,113	1.39	10 (12%)
22	CLA	B	603	2	69,73,73	1.28	10 (14%)	82,113,113	1.60	11 (13%)
30	DGD	c	519	-	63,63,67	1.13	3 (4%)	77,77,81	1.38	8 (10%)
29	SQD	f	102	-	39,41,54	1.08	3 (7%)	49,52,65	2.00	11 (22%)
35	HEC	V	201	17	50,50,50	1.57	4 (8%)	68,82,82	1.19	4 (5%)
27	LMG	b	623	-	55,55,55	1.00	2 (3%)	63,63,63	1.50	8 (12%)
33	STE	B	626	-	11,11,19	0.98	0	11,11,19	0.85	0
35	HEC	f	101	5,6	50,50,50	1.71	6 (12%)	68,82,82	1.76	10 (14%)
33	STE	B	620	-	16,16,19	0.77	0	16,16,19	1.00	0
33	STE	Z	101	-	7,7,19	0.48	0	6,6,19	0.55	0
22	CLA	c	502	3	69,73,73	1.19	7 (10%)	82,113,113	1.30	8 (9%)
33	STE	b	626	-	9,9,19	0.51	0	8,8,19	0.55	0
29	SQD	A	414	-	38,38,54	1.03	4 (10%)	40,40,65	1.56	4 (10%)
30	DGD	C	517	-	63,63,67	1.30	10 (15%)	77,77,81	1.41	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	m	102	-	11,11,19	0.79	0	11,11,19	1.24	1 (9%)
34	BCT	a	408	21	3,3,3	1.33	0	2,3,3	3.58	2 (100%)
31	OEX	a	417[A]	1,36,3	0,14,14	-	-	-		
33	STE	C	522	-	15,15,19	0.49	0	14,14,19	0.65	0
24	BCR	B	617	-	41,41,41	1.15	4 (9%)	56,56,56	1.30	11 (19%)
22	CLA	c	505	3	69,73,73	1.28	11 (15%)	82,113,113	1.30	8 (9%)
28	LHG	a	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.50	8 (15%)
29	SQD	B	623	-	52,54,54	0.97	3 (5%)	62,65,65	1.84	14 (22%)
33	STE	B	624	-	11,11,19	0.83	0	11,11,19	1.31	1 (9%)
22	CLA	C	510	3	69,73,73	1.16	10 (14%)	82,113,113	1.39	7 (8%)
33	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.69	0
33	STE	J	101	-	11,11,19	0.66	0	11,11,19	1.36	2 (18%)
27	LMG	c	522	-	48,48,55	1.06	5 (10%)	56,56,63	1.28	4 (7%)
22	CLA	c	509	3	69,73,73	1.27	7 (10%)	82,113,113	1.47	7 (8%)
32	OXY	a	418[B]	1,36,3	0,16,16	-	-	-		
22	CLA	b	605	2	69,73,73	1.20	8 (11%)	82,113,113	1.51	15 (18%)
22	CLA	d	401	36	69,73,73	1.45	12 (17%)	82,113,113	1.42	11 (13%)
22	CLA	B	606	2	69,73,73	1.36	11 (15%)	82,113,113	1.46	13 (15%)
22	CLA	b	609	2	69,73,73	1.34	8 (11%)	82,113,113	1.51	11 (13%)
35	HEC	F	101	5,6	50,50,50	1.63	4 (8%)	68,82,82	1.54	11 (16%)
23	PHO	a	403	-	58,69,69	1.93	10 (17%)	55,99,99	1.59	10 (18%)
22	CLA	C	504	36	63,67,73	1.18	6 (9%)	74,105,113	1.33	10 (13%)
22	CLA	b	601	36	69,73,73	1.26	9 (13%)	82,113,113	1.29	5 (6%)
24	BCR	C	515	-	41,41,41	1.20	4 (9%)	56,56,56	1.32	9 (16%)
22	CLA	b	602	2	69,73,73	1.10	7 (10%)	82,113,113	1.45	12 (14%)
27	LMG	d	410	-	44,44,55	1.12	3 (6%)	52,52,63	1.30	7 (13%)
28	LHG	l	101	-	48,48,48	0.88	1 (2%)	51,54,54	1.31	7 (13%)
24	BCR	t	101	-	41,41,41	1.11	4 (9%)	56,56,56	1.44	12 (21%)
30	DGD	A	415	-	67,67,67	1.39	11 (16%)	81,81,81	1.34	9 (11%)
22	CLA	D	402	4	69,73,73	1.15	7 (10%)	82,113,113	1.36	8 (9%)
22	CLA	D	403	36	69,73,73	1.20	8 (11%)	82,113,113	1.29	6 (7%)
27	LMG	D	407	-	51,51,55	0.99	5 (9%)	59,59,63	1.25	4 (6%)
22	CLA	b	612	2	69,73,73	1.62	10 (14%)	82,113,113	1.32	9 (10%)
29	SQD	b	620	-	47,49,54	0.98	2 (4%)	57,60,65	1.92	14 (24%)
22	CLA	c	508	3	68,72,73	1.37	7 (10%)	80,111,113	1.38	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	STE	C	523	-	11,11,19	0.63	0	11,11,19	1.42	2 (18%)
22	CLA	b	610	36	69,73,73	1.44	9 (13%)	82,113,113	1.51	12 (14%)
22	CLA	B	613	2	69,73,73	1.32	9 (13%)	82,113,113	1.07	6 (7%)
33	STE	b	627	-	13,13,19	0.54	0	12,12,19	0.46	0
22	CLA	A	403	36	69,73,73	1.33	8 (11%)	82,113,113	1.27	7 (8%)
22	CLA	c	504	36	64,68,73	1.22	7 (10%)	76,107,113	1.29	10 (13%)
22	CLA	d	404	36	69,73,73	1.82	11 (15%)	82,113,113	1.46	11 (13%)
22	CLA	B	604	2	69,73,73	1.26	6 (8%)	82,113,113	1.56	6 (7%)
24	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.39	8 (14%)
22	CLA	B	608	2	69,73,73	1.07	5 (7%)	82,113,113	1.29	10 (12%)
30	DGD	C	518	-	63,63,67	1.22	8 (12%)	77,77,81	1.33	9 (11%)
22	CLA	c	511	3	69,73,73	1.47	10 (14%)	82,113,113	1.29	7 (8%)
26	PL9	d	407	-	55,55,55	1.60	10 (18%)	68,69,69	1.85	15 (22%)
30	DGD	c	517	-	63,63,67	1.21	9 (14%)	77,77,81	1.42	15 (19%)
22	CLA	A	406	1	58,62,73	1.34	7 (12%)	68,99,113	1.37	9 (13%)
22	CLA	d	403	4	69,73,73	1.29	8 (11%)	82,113,113	1.36	9 (10%)
27	LMG	D	411	-	26,26,55	0.67	0	26,26,63	1.25	1 (3%)
22	CLA	b	603	2	69,73,73	1.35	7 (10%)	82,113,113	1.37	13 (15%)
33	STE	I	101	-	14,14,19	0.58	0	13,13,19	0.53	0
24	BCR	c	516	-	41,41,41	1.14	3 (7%)	56,56,56	1.17	3 (5%)
28	LHG	d	408	-	48,48,48	0.98	1 (2%)	51,54,54	1.21	4 (7%)
33	STE	b	622	-	19,19,19	0.62	0	19,19,19	1.01	0
33	STE	d	413	-	19,19,19	0.54	0	19,19,19	1.01	0
22	CLA	b	606	2	69,73,73	1.72	9 (13%)	82,113,113	1.55	8 (9%)
23	PHO	A	405	-	58,69,69	1.95	12 (20%)	55,99,99	1.45	9 (16%)
24	BCR	B	618	-	41,41,41	1.16	2 (4%)	56,56,56	1.33	9 (16%)
22	CLA	B	611	2	69,73,73	1.33	7 (10%)	82,113,113	1.63	9 (10%)
22	CLA	C	513	3	69,73,73	1.15	5 (7%)	82,113,113	1.41	6 (7%)
33	STE	t	102	-	13,13,19	0.73	0	13,13,19	1.34	2 (15%)
28	LHG	E	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.27	5 (9%)
22	CLA	B	615	2	69,73,73	1.26	9 (13%)	82,113,113	1.28	9 (10%)
33	STE	a	415	-	14,14,19	0.40	0	13,13,19	0.73	0
22	CLA	a	404	1	69,73,73	1.58	8 (11%)	82,113,113	1.33	11 (13%)

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	m	101	-	-	24/46/66/70	0/1/1/1
24	BCR	b	617	-	-	7/29/63/63	0/2/2/2
22	CLA	D	404	4	-	9/39/115/115	-
33	STE	R	101	-	-	4/9/9/17	-
22	CLA	b	615	2	-	7/39/115/115	-
28	LHG	B	622	-	-	18/53/53/53	-
27	LMG	M	101	-	-	23/46/66/70	0/1/1/1
22	CLA	B	607	36	-	4/39/115/115	-
24	BCR	H	101	-	-	6/29/63/63	0/2/2/2
22	CLA	a	402	1	-	6/39/115/115	-
33	STE	D	412	-	-	9/17/17/17	-
33	STE	b	625	-	-	9/17/17/17	-
33	STE	t	103	-	-	8/15/15/17	-
33	STE	a	413	-	-	3/7/7/17	-
26	PL9	A	410	-	-	25/53/73/73	0/1/1/1
33	STE	c	521	-	-	7/17/17/17	-
24	BCR	D	405	-	-	6/29/63/63	0/2/2/2
27	LMG	c	523	-	-	20/44/64/70	0/1/1/1
22	CLA	B	614	2	-	15/39/115/115	-
22	CLA	C	508	3	-	8/39/115/115	-
27	LMG	D	410	-	-	15/33/33/70	-
22	CLA	B	610	36	-	5/39/115/115	-
22	CLA	c	501	3	-	2/39/115/115	-
24	BCR	a	405	-	-	1/29/63/63	0/2/2/2
22	CLA	b	616	2	-	7/33/109/115	-
30	DGD	C	519	-	-	11/51/91/95	0/2/2/2
22	CLA	c	512	3	-	20/39/115/115	-
28	LHG	A	412	-	-	18/51/51/53	-
22	CLA	B	612	2	-	6/39/115/115	-
29	SQD	D	408	-	-	12/28/48/69	0/1/1/1
22	CLA	B	601	36	-	13/39/115/115	-
24	BCR	d	406	-	-	8/29/63/63	0/2/2/2
22	CLA	C	506	3	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	A	404	-	-	0/37/103/103	0/5/6/6
28	LHG	d	409	-	-	13/43/43/53	-
33	STE	b	621	-	-	8/13/13/17	-
33	STE	a	414	-	-	3/9/9/17	-
22	CLA	C	503	3	-	3/39/115/115	-
24	BCR	B	619	-	-	4/29/63/63	0/2/2/2
29	SQD	a	412	-	-	17/37/37/69	-
33	STE	j	101	-	-	3/9/9/17	-
28	LHG	e	101	-	-	29/46/46/53	-
33	STE	C	521	-	-	7/9/9/17	-
24	BCR	c	515	-	-	5/29/63/63	0/2/2/2
27	LMG	A	411	-	-	21/43/63/70	0/1/1/1
30	DGD	H	102	-	-	16/51/91/95	0/2/2/2
24	BCR	A	407	-	-	8/29/63/63	0/2/2/2
24	BCR	x	101	-	-	5/29/63/63	0/2/2/2
22	CLA	d	405	4	-	11/39/115/115	-
22	CLA	A	402	1	-	5/39/115/115	-
33	STE	B	625	-	-	9/13/13/17	-
30	DGD	h	101	-	-	19/51/91/95	0/2/2/2
22	CLA	c	503	3	-	6/39/115/115	-
33	STE	T	102	-	-	11/12/12/17	-
22	CLA	b	607	36	-	13/39/115/115	-
33	STE	d	412	-	-	8/17/17/17	-
29	SQD	A	413	-	-	14/47/67/69	0/1/1/1
30	DGD	c	518	-	-	18/51/91/95	0/2/2/2
22	CLA	C	505	3	-	11/39/115/115	-
24	BCR	c	514	-	-	15/29/63/63	0/2/2/2
24	BCR	C	514	-	-	10/29/63/63	0/2/2/2
24	BCR	k	101	-	-	10/29/63/63	0/2/2/2
28	LHG	B	621	-	-	25/53/53/53	-
26	PL9	D	406	-	-	9/53/73/73	0/1/1/1
22	CLA	b	614	2	-	11/39/115/115	-
26	PL9	a	409	-	-	27/53/73/73	0/1/1/1
22	CLA	B	616	2	-	7/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	a	416	-	-	30/50/70/70	0/1/1/1
28	LHG	D	409	-	-	20/53/53/53	-
33	STE	k	102	-	-	6/9/9/17	-
22	CLA	C	512	3	-	13/39/115/115	-
22	CLA	C	511	3	-	4/39/115/115	-
22	CLA	b	604	2	-	7/39/115/115	-
24	BCR	b	618	-	-	6/29/63/63	0/2/2/2
22	CLA	c	510	3	-	10/39/115/115	-
22	CLA	C	501	3	-	3/39/115/115	-
33	STE	l	102	-	-	9/15/15/17	-
22	CLA	c	507	36	-	6/39/115/115	-
22	CLA	c	513	3	-	6/39/115/115	-
24	BCR	C	516	-	-	9/29/63/63	0/2/2/2
22	CLA	b	611	2	-	6/39/115/115	-
33	STE	b	624	-	-	7/13/13/17	-
24	BCR	b	619	-	-	0/29/63/63	0/2/2/2
33	STE	M	102	-	-	5/12/12/17	-
22	CLA	b	613	2	-	9/39/115/115	-
22	CLA	B	609	2	-	5/39/115/115	-
22	CLA	C	502	3	-	5/39/115/115	-
22	CLA	C	509	3	-	11/39/115/115	-
22	CLA	B	602	2	-	5/39/115/115	-
24	BCR	T	101	-	-	7/29/63/63	0/2/2/2
33	STE	M	103	-	-	2/7/7/17	-
27	LMG	c	520	-	-	11/31/51/70	0/1/1/1
27	LMG	C	520	-	-	12/43/63/70	0/1/1/1
22	CLA	b	608	2	-	1/39/115/115	-
33	STE	d	411	-	-	5/14/14/17	-
23	PHO	d	402	-	-	0/37/103/103	0/5/6/6
22	CLA	C	507	36	-	10/39/115/115	-
29	SQD	a	411	-	-	23/49/69/69	0/1/1/1
35	HEC	v	201	17	1/1/7/7	4/14/54/54	-
22	CLA	c	506	3	-	16/39/115/115	-
22	CLA	B	605	2	-	9/39/115/115	-
22	CLA	B	603	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	DGD	c	519	-	-	13/51/91/95	0/2/2/2
35	HEC	V	201	17	1/1/7/7	6/14/54/54	-
29	SQD	f	102	-	-	11/36/56/69	0/1/1/1
27	LMG	b	623	-	-	21/50/70/70	0/1/1/1
35	HEC	f	101	5,6	1/1/7/7	6/14/54/54	-
33	STE	B	626	-	-	5/9/9/17	-
33	STE	B	620	-	-	5/14/14/17	-
33	STE	Z	101	-	-	2/5/5/17	-
22	CLA	c	502	3	-	4/39/115/115	-
33	STE	b	626	-	-	4/7/7/17	-
29	SQD	A	414	-	-	21/39/39/69	-
30	DGD	C	517	-	-	24/51/91/95	0/2/2/2
33	STE	m	102	-	-	4/9/9/17	-
33	STE	C	522	-	-	5/13/13/17	-
24	BCR	B	617	-	-	8/29/63/63	0/2/2/2
22	CLA	c	505	3	-	10/39/115/115	-
28	LHG	a	410	-	-	23/53/53/53	-
29	SQD	B	623	-	-	24/49/69/69	0/1/1/1
33	STE	B	624	-	-	3/9/9/17	-
22	CLA	C	510	3	-	8/39/115/115	-
33	STE	H	103	-	-	10/15/15/17	-
33	STE	J	101	-	-	6/9/9/17	-
27	LMG	c	522	-	-	24/43/63/70	0/1/1/1
22	CLA	c	509	3	-	9/39/115/115	-
22	CLA	b	605	2	-	5/39/115/115	-
22	CLA	d	401	36	-	12/39/115/115	-
22	CLA	B	606	2	-	9/39/115/115	-
22	CLA	b	609	2	-	8/39/115/115	-
35	HEC	F	101	5,6	1/1/7/7	6/14/54/54	-
23	PHO	a	403	-	-	1/37/103/103	0/5/6/6
22	CLA	C	504	36	-	6/32/108/115	-
22	CLA	b	601	36	-	14/39/115/115	-
24	BCR	C	515	-	-	5/29/63/63	0/2/2/2
22	CLA	b	602	2	-	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	d	410	-	-	10/39/59/70	0/1/1/1
28	LHG	l	101	-	-	15/53/53/53	-
24	BCR	t	101	-	-	6/29/63/63	0/2/2/2
30	DGD	A	415	-	-	20/55/95/95	0/2/2/2
22	CLA	D	402	4	-	6/39/115/115	-
22	CLA	D	403	36	-	5/39/115/115	-
27	LMG	D	407	-	-	15/46/66/70	0/1/1/1
22	CLA	b	612	2	-	3/39/115/115	-
29	SQD	b	620	-	-	21/44/64/69	0/1/1/1
22	CLA	c	508	3	-	9/38/114/115	-
33	STE	C	523	-	-	3/9/9/17	-
22	CLA	b	610	36	-	5/39/115/115	-
22	CLA	B	613	2	-	10/39/115/115	-
33	STE	b	627	-	-	5/11/11/17	-
22	CLA	A	403	36	-	9/39/115/115	-
22	CLA	c	504	36	-	7/33/109/115	-
22	CLA	d	404	36	-	2/39/115/115	-
22	CLA	B	604	2	-	7/39/115/115	-
24	BCR	Y	101	-	-	6/29/63/63	0/2/2/2
22	CLA	B	608	2	-	1/39/115/115	-
30	DGD	C	518	-	-	22/51/91/95	0/2/2/2
22	CLA	c	511	3	-	11/39/115/115	-
26	PL9	d	407	-	-	12/53/73/73	0/1/1/1
30	DGD	c	517	-	-	28/51/91/95	0/2/2/2
22	CLA	A	406	1	-	3/26/102/115	-
22	CLA	d	403	4	-	6/39/115/115	-
27	LMG	D	411	-	-	7/22/22/70	-
22	CLA	b	603	2	-	5/39/115/115	-
33	STE	I	101	-	-	3/12/12/17	-
24	BCR	c	516	-	-	3/29/63/63	0/2/2/2
28	LHG	d	408	-	-	18/53/53/53	-
33	STE	b	622	-	-	8/17/17/17	-
33	STE	d	413	-	-	8/17/17/17	-
22	CLA	b	606	2	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PHO	A	405	-	-	2/37/103/103	0/5/6/6
24	BCR	B	618	-	-	2/29/63/63	0/2/2/2
22	CLA	B	611	2	-	9/39/115/115	-
22	CLA	C	513	3	-	8/39/115/115	-
33	STE	t	102	-	-	3/11/11/17	-
28	LHG	E	101	-	-	23/53/53/53	-
22	CLA	B	615	2	-	9/39/115/115	-
33	STE	a	415	-	-	6/12/12/17	-
22	CLA	a	404	1	-	8/39/115/115	-

All (897) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	PHO	C1B-C2B	9.62	1.50	1.39
22	D	404	CLA	MG-NB	-9.28	1.87	2.05
22	b	606	CLA	MG-NA	9.01	2.27	2.06
23	a	403	PHO	C1B-C2B	8.94	1.49	1.39
23	d	402	PHO	C3B-C4B	8.35	1.49	1.41
23	A	405	PHO	C3B-C4B	8.31	1.49	1.41
22	a	404	CLA	MG-ND	-8.03	1.89	2.05
23	A	405	PHO	C1B-C2B	7.93	1.48	1.39
23	A	404	PHO	C1B-C2B	7.80	1.48	1.39
22	d	404	CLA	MG-NA	7.67	2.24	2.06
22	b	612	CLA	MG-NC	-7.66	1.88	2.06
35	v	201	HEC	C3D-C2D	7.52	1.53	1.36
35	f	101	HEC	C3D-C2D	7.20	1.52	1.36
35	F	101	HEC	C3D-C2D	7.16	1.52	1.36
22	c	511	CLA	MG-NA	7.08	2.23	2.06
22	B	610	CLA	MG-ND	-7.05	1.91	2.05
22	c	506	CLA	MG-NB	6.89	2.19	2.05
22	d	404	CLA	MG-NB	6.67	2.19	2.05
22	B	611	CLA	MG-NA	6.62	2.22	2.06
22	C	506	CLA	MG-ND	-6.61	1.92	2.05
35	V	201	HEC	C3D-C2D	6.37	1.50	1.36
22	b	615	CLA	MG-NB	6.34	2.18	2.05
22	c	510	CLA	MG-NA	6.31	2.21	2.06
22	B	616	CLA	MG-NA	6.24	2.21	2.06
26	d	407	PL9	C6-C1	-6.24	1.38	1.48
22	B	609	CLA	MG-NA	6.11	2.20	2.06
26	D	406	PL9	C7-C3	-5.79	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	604	CLA	MG-NC	5.76	2.20	2.06
22	b	611	CLA	MG-NB	5.68	2.17	2.05
22	C	505	CLA	MG-NA	5.62	2.19	2.06
22	C	508	CLA	MG-NA	5.53	2.19	2.06
22	B	606	CLA	MG-NA	5.34	2.19	2.06
22	b	610	CLA	MG-ND	-5.24	1.95	2.05
22	d	401	CLA	MG-NB	5.10	2.15	2.05
22	c	509	CLA	C1D-ND	5.02	1.44	1.37
23	a	403	PHO	C3B-C4B	5.01	1.46	1.41
22	C	508	CLA	MG-ND	5.00	2.15	2.05
22	c	506	CLA	MG-ND	-4.99	1.95	2.05
22	B	609	CLA	MG-NB	-4.94	1.96	2.05
23	a	403	PHO	C1D-C2D	4.93	1.45	1.39
22	C	506	CLA	MG-NA	4.91	2.17	2.06
22	B	602	CLA	C1D-ND	4.84	1.44	1.37
35	V	201	HEC	FE-ND	4.84	2.09	1.94
22	b	615	CLA	MG-NA	4.83	2.17	2.06
22	C	502	CLA	MG-NA	4.81	2.17	2.06
22	C	503	CLA	MG-NA	4.80	2.17	2.06
22	b	609	CLA	MG-NA	4.80	2.17	2.06
22	C	511	CLA	MG-NB	-4.78	1.96	2.05
28	D	409	LHG	O7-C5	-4.78	1.35	1.46
22	B	605	CLA	MG-NB	4.77	2.15	2.05
22	b	612	CLA	MG-NB	4.76	2.15	2.05
24	c	515	BCR	C1-C6	-4.74	1.47	1.53
22	A	403	CLA	MG-NB	-4.73	1.96	2.05
24	Y	101	BCR	C30-C25	-4.73	1.47	1.53
22	b	610	CLA	C1D-ND	4.73	1.44	1.37
22	b	606	CLA	MG-NB	-4.73	1.96	2.05
24	B	618	BCR	C30-C25	-4.66	1.47	1.53
22	C	511	CLA	MG-NA	4.65	2.17	2.06
22	b	614	CLA	MG-ND	-4.65	1.96	2.05
30	C	519	DGD	O2G-C2G	-4.64	1.35	1.46
22	b	615	CLA	MG-ND	-4.61	1.96	2.05
22	C	507	CLA	MG-NA	4.56	2.17	2.06
22	B	613	CLA	MG-ND	-4.55	1.96	2.05
22	C	501	CLA	MG-NA	4.54	2.17	2.06
24	C	515	BCR	C1-C6	-4.54	1.48	1.53
22	c	508	CLA	MG-NA	4.50	2.17	2.06
22	d	405	CLA	MG-NA	4.49	2.16	2.06
22	A	406	CLA	C1D-ND	4.49	1.43	1.37
23	A	404	PHO	C3B-C4B	4.47	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	MG-NC	4.46	2.16	2.06
22	A	406	CLA	MG-ND	-4.45	1.97	2.05
24	H	101	BCR	C30-C25	-4.42	1.48	1.53
22	A	402	CLA	MG-NC	4.42	2.16	2.06
22	d	404	CLA	MG-ND	-4.35	1.97	2.05
22	b	603	CLA	MG-NA	4.33	2.16	2.06
22	C	501	CLA	MG-NB	-4.31	1.97	2.05
22	d	405	CLA	MG-NB	-4.30	1.97	2.05
22	b	606	CLA	MG-ND	4.29	2.14	2.05
22	d	403	CLA	C4B-NB	4.29	1.43	1.37
35	f	101	HEC	FE-ND	4.28	2.08	1.94
22	C	509	CLA	C1D-ND	4.28	1.43	1.37
24	D	405	BCR	C30-C25	-4.25	1.48	1.53
30	C	519	DGD	O5D-C1E	4.24	1.47	1.40
30	c	517	DGD	O2G-C2G	-4.20	1.36	1.46
22	b	609	CLA	MG-ND	-4.20	1.97	2.05
22	c	513	CLA	MG-ND	-4.17	1.97	2.05
26	D	406	PL9	C3-C4	-4.15	1.43	1.49
26	d	407	PL9	C53-C6	-4.14	1.42	1.50
24	c	514	BCR	C1-C6	-4.13	1.48	1.53
35	F	101	HEC	FE-NC	4.11	2.08	1.95
22	c	507	CLA	MG-ND	4.08	2.13	2.05
22	b	610	CLA	MG-NB	-4.05	1.97	2.05
30	c	519	DGD	O3G-C3G	-4.05	1.36	1.43
28	A	412	LHG	O3-C3	-4.02	1.29	1.44
24	C	516	BCR	C30-C25	-3.97	1.48	1.53
24	C	514	BCR	C1-C6	-3.96	1.48	1.53
22	b	603	CLA	C4B-NB	3.92	1.43	1.37
22	b	604	CLA	MG-NC	3.89	2.15	2.06
23	d	402	PHO	CMC-C2C	-3.89	1.44	1.50
22	a	402	CLA	MG-NA	3.89	2.15	2.06
28	B	621	LHG	O7-C5	-3.86	1.37	1.46
22	c	508	CLA	MG-NB	3.84	2.13	2.05
22	C	501	CLA	C1D-ND	3.82	1.42	1.37
22	a	402	CLA	MG-NC	3.80	2.15	2.06
24	B	617	BCR	C1-C6	-3.79	1.48	1.53
22	c	505	CLA	MG-ND	3.79	2.13	2.05
22	c	501	CLA	MG-NB	-3.76	1.98	2.05
26	D	406	PL9	C26-C24	-3.75	1.43	1.51
22	c	501	CLA	C1D-ND	3.75	1.42	1.37
22	c	509	CLA	MG-NB	3.75	2.13	2.05
22	b	606	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	402	CLA	MG-ND	-3.74	1.98	2.05
22	C	509	CLA	MG-NB	-3.73	1.98	2.05
29	b	620	SQD	O48-C23	3.71	1.44	1.33
27	a	416	LMG	C4-C5	3.71	1.60	1.53
24	B	619	BCR	C1-C6	-3.71	1.49	1.53
30	A	415	DGD	C3E-C2E	3.71	1.62	1.52
35	v	201	HEC	FE-NA	3.71	2.07	1.95
28	a	410	LHG	C24-C23	3.70	1.61	1.50
30	C	518	DGD	C4D-C3D	3.69	1.61	1.52
22	b	612	CLA	MG-ND	-3.69	1.98	2.05
28	A	412	LHG	P-O6	3.69	1.73	1.59
24	C	514	BCR	C30-C25	-3.68	1.49	1.53
22	C	506	CLA	C1D-ND	3.68	1.42	1.37
22	a	404	CLA	C1D-ND	3.68	1.42	1.37
24	d	406	BCR	C30-C25	-3.68	1.49	1.53
22	B	609	CLA	C1D-ND	3.67	1.42	1.37
22	C	511	CLA	MG-ND	3.66	2.13	2.05
22	B	601	CLA	C1D-ND	3.66	1.42	1.37
24	b	619	BCR	C1-C6	-3.66	1.49	1.53
23	d	402	PHO	C1D-C2D	3.66	1.43	1.39
30	A	415	DGD	C3G-C2G	3.65	1.62	1.50
22	a	404	CLA	MG-NB	-3.65	1.98	2.05
27	c	520	LMG	C1-C2	3.65	1.63	1.52
22	c	502	CLA	MG-NB	-3.64	1.98	2.05
22	B	605	CLA	C1B-C2B	3.63	1.51	1.43
22	b	607	CLA	MG-NA	3.62	2.14	2.06
22	B	603	CLA	MG-ND	3.62	2.13	2.05
22	B	602	CLA	MG-NA	3.62	2.14	2.06
22	C	513	CLA	MG-NA	3.61	2.14	2.06
22	B	602	CLA	C4B-NB	3.61	1.42	1.37
22	d	404	CLA	C1D-ND	3.61	1.42	1.37
22	c	511	CLA	MG-NC	-3.59	1.97	2.06
24	k	101	BCR	C30-C25	-3.57	1.49	1.53
24	x	101	BCR	C30-C25	-3.57	1.49	1.53
22	B	612	CLA	C4B-NB	3.56	1.42	1.37
26	d	407	PL9	C31-C29	-3.54	1.44	1.51
22	D	404	CLA	C1D-ND	3.54	1.42	1.37
22	b	601	CLA	C1D-ND	3.53	1.42	1.37
22	d	401	CLA	MG-NC	3.52	2.14	2.06
22	A	403	CLA	C1D-ND	3.51	1.42	1.37
22	C	508	CLA	MG-NC	-3.49	1.98	2.06
22	c	510	CLA	C1D-ND	3.49	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	d	403	CLA	MG-ND	-3.49	1.98	2.05
24	c	516	BCR	C1-C6	-3.49	1.49	1.53
22	b	602	CLA	C1D-ND	3.48	1.42	1.37
22	B	601	CLA	MG-ND	-3.48	1.98	2.05
23	A	404	PHO	C4D-ND	-3.48	1.33	1.38
30	A	415	DGD	C4D-C3D	3.47	1.61	1.52
24	c	516	BCR	C30-C25	-3.47	1.49	1.53
30	H	102	DGD	O3G-C1D	3.47	1.46	1.40
30	H	102	DGD	C4E-C5E	3.46	1.60	1.53
24	b	617	BCR	C30-C25	-3.46	1.49	1.53
28	E	101	LHG	P-O6	3.46	1.72	1.59
22	B	613	CLA	C4B-NB	3.46	1.42	1.37
22	C	511	CLA	C1D-ND	3.45	1.42	1.37
22	c	504	CLA	MG-ND	-3.45	1.99	2.05
22	C	513	CLA	C1D-ND	3.44	1.42	1.37
22	b	605	CLA	MG-NB	-3.43	1.99	2.05
22	b	615	CLA	C1B-C2B	3.43	1.51	1.43
22	A	402	CLA	C4B-NB	3.43	1.42	1.37
22	b	607	CLA	C1B-NB	-3.42	1.33	1.37
22	B	613	CLA	CMD-C2D	-3.42	1.43	1.50
29	A	414	SQD	O47-C7	3.41	1.43	1.34
22	C	506	CLA	MG-NB	3.41	2.12	2.05
22	B	608	CLA	MG-NA	3.41	2.14	2.06
22	c	508	CLA	C1D-ND	3.41	1.42	1.37
30	H	102	DGD	O5D-C1E	3.40	1.45	1.40
22	B	601	CLA	C4B-NB	3.40	1.42	1.37
22	b	609	CLA	C1D-ND	3.40	1.42	1.37
22	b	601	CLA	C1B-C2B	3.40	1.51	1.43
22	c	504	CLA	C4B-NB	3.39	1.42	1.37
22	a	404	CLA	CMC-C2C	-3.39	1.43	1.50
24	c	514	BCR	C30-C25	-3.39	1.49	1.53
22	d	401	CLA	C1D-ND	3.37	1.42	1.37
30	A	415	DGD	C6E-C5E	3.36	1.63	1.51
24	b	618	BCR	C1-C6	-3.36	1.49	1.53
29	B	623	SQD	O48-C23	3.36	1.43	1.33
30	A	415	DGD	O5D-C6D	-3.34	1.37	1.43
22	B	615	CLA	C1D-ND	3.34	1.42	1.37
22	d	403	CLA	C1B-C2B	3.34	1.51	1.43
22	b	615	CLA	C1D-ND	3.34	1.42	1.37
22	b	605	CLA	C1B-C2B	3.33	1.51	1.43
30	c	518	DGD	C3E-C2E	3.33	1.61	1.52
22	c	503	CLA	C1D-ND	3.33	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	612	CLA	C1D-ND	3.32	1.42	1.37
29	a	412	SQD	O48-C23	3.32	1.43	1.33
24	B	617	BCR	C30-C25	-3.31	1.49	1.53
22	B	604	CLA	MG-NA	3.31	2.14	2.06
22	C	501	CLA	CHC-C1C	3.30	1.45	1.38
28	d	409	LHG	P-O6	3.30	1.72	1.59
29	a	412	SQD	O47-C7	3.29	1.43	1.34
24	b	617	BCR	C1-C6	-3.29	1.49	1.53
24	Y	101	BCR	C1-C6	-3.28	1.49	1.53
22	D	403	CLA	C1D-ND	3.27	1.42	1.37
22	b	612	CLA	C1D-ND	3.27	1.42	1.37
27	d	410	LMG	C4-C5	3.27	1.60	1.53
22	c	506	CLA	C1B-NB	-3.26	1.33	1.37
29	D	408	SQD	O48-C23	3.26	1.42	1.33
29	a	411	SQD	O48-C23	3.25	1.42	1.33
22	B	607	CLA	MG-NB	-3.25	1.99	2.05
30	c	519	DGD	O1G-C1G	-3.24	1.37	1.45
22	b	616	CLA	C1D-ND	3.23	1.42	1.37
30	C	518	DGD	C6E-C5E	3.23	1.62	1.51
22	B	603	CLA	C1D-ND	3.22	1.42	1.37
30	c	519	DGD	O2G-C2G	-3.22	1.39	1.46
22	b	613	CLA	C1B-NB	-3.22	1.33	1.37
27	D	410	LMG	C7-C8	3.21	1.58	1.51
27	c	522	LMG	C3-C2	3.20	1.60	1.52
35	v	201	HEC	FE-ND	3.20	2.04	1.94
22	b	603	CLA	C1D-ND	3.20	1.42	1.37
22	c	505	CLA	C4B-NB	3.20	1.42	1.37
22	D	404	CLA	MG-NC	3.20	2.13	2.06
30	c	518	DGD	C4D-C3D	3.20	1.60	1.52
24	c	515	BCR	C30-C25	-3.19	1.49	1.53
26	D	406	PL9	C30-C29	-3.19	1.42	1.50
23	a	403	PHO	C3D-C4D	3.19	1.45	1.41
23	A	404	PHO	CMC-C2C	-3.18	1.45	1.50
22	c	507	CLA	C1D-ND	3.18	1.42	1.37
24	C	516	BCR	C1-C6	-3.18	1.49	1.53
22	C	506	CLA	MG-NC	-3.17	1.98	2.06
22	B	615	CLA	C1B-C2B	3.17	1.50	1.43
26	a	409	PL9	C52-C5	-3.17	1.44	1.50
30	C	517	DGD	C6D-C5D	3.17	1.61	1.51
22	B	609	CLA	MG-ND	3.16	2.12	2.05
26	a	409	PL9	C53-C6	-3.15	1.44	1.50
22	b	613	CLA	MG-ND	-3.14	1.99	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	c	505	CLA	CHC-C1C	3.14	1.44	1.38
22	C	512	CLA	CMD-C2D	-3.14	1.44	1.50
22	C	503	CLA	MG-NC	3.14	2.13	2.06
24	A	407	BCR	C1-C6	-3.14	1.49	1.53
22	d	401	CLA	C4B-NB	3.14	1.42	1.37
29	A	414	SQD	O48-C23	3.13	1.42	1.33
22	B	607	CLA	C1D-ND	3.13	1.42	1.37
29	A	413	SQD	O48-C23	3.13	1.42	1.33
22	b	601	CLA	MG-NA	3.12	2.13	2.06
22	c	513	CLA	C1D-ND	3.12	1.42	1.37
22	C	509	CLA	MG-ND	3.12	2.12	2.05
22	C	512	CLA	MG-NA	3.11	2.13	2.06
22	B	603	CLA	MG-NA	3.11	2.13	2.06
22	A	403	CLA	C4B-NB	3.11	1.41	1.37
24	T	101	BCR	C30-C25	-3.11	1.49	1.53
26	d	407	PL9	C21-C19	-3.11	1.44	1.51
22	C	507	CLA	MG-NB	-3.09	1.99	2.05
23	A	404	PHO	C3D-C4D	3.09	1.45	1.41
29	B	623	SQD	O47-C7	3.08	1.43	1.34
22	B	614	CLA	C4B-NB	3.08	1.41	1.37
27	A	411	LMG	C4-C3	3.08	1.60	1.52
22	b	613	CLA	C1D-ND	3.07	1.41	1.37
24	d	406	BCR	C1-C6	-3.07	1.49	1.53
22	d	404	CLA	C1B-C2B	3.07	1.50	1.43
22	b	614	CLA	C1D-ND	3.07	1.41	1.37
22	c	509	CLA	C1B-C2B	3.05	1.50	1.43
22	b	615	CLA	C4B-NB	3.05	1.41	1.37
24	T	101	BCR	C1-C6	-3.05	1.49	1.53
22	b	603	CLA	MG-ND	-3.05	1.99	2.05
22	c	508	CLA	C1B-C2B	3.05	1.50	1.43
22	c	503	CLA	MG-NC	3.05	2.13	2.06
28	B	622	LHG	C24-C23	3.05	1.59	1.50
22	C	511	CLA	C4B-NB	3.05	1.41	1.37
22	C	511	CLA	C3B-C4B	3.04	1.51	1.42
22	C	504	CLA	C1D-ND	3.04	1.41	1.37
26	d	407	PL9	C3-C4	-3.04	1.44	1.49
30	C	517	DGD	O5D-C6D	-3.04	1.38	1.43
27	A	411	LMG	O1-C7	-3.04	1.38	1.43
22	b	610	CLA	C1B-C2B	3.03	1.50	1.43
22	a	404	CLA	C1B-C2B	3.03	1.50	1.43
22	D	403	CLA	MG-NA	3.03	2.13	2.06
24	b	618	BCR	C30-C25	-3.02	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	601	CLA	C4B-NB	3.01	1.41	1.37
22	b	608	CLA	CMB-C2B	-3.01	1.44	1.50
22	b	615	CLA	C3B-C4B	3.01	1.51	1.42
29	f	102	SQD	O48-C23	3.00	1.42	1.33
28	B	622	LHG	O7-C5	-3.00	1.39	1.46
22	A	402	CLA	MG-NB	-3.00	1.99	2.05
28	d	409	LHG	C24-C23	3.00	1.59	1.50
26	D	406	PL9	C6-C1	-2.99	1.43	1.48
30	c	517	DGD	C4D-C5D	2.99	1.59	1.53
22	D	404	CLA	C1B-NB	-2.98	1.33	1.37
22	B	611	CLA	C1B-C2B	2.98	1.50	1.43
22	d	404	CLA	C4B-NB	2.98	1.41	1.37
22	B	612	CLA	C1B-C2B	2.98	1.50	1.43
22	D	404	CLA	C1B-C2B	2.98	1.50	1.43
22	C	508	CLA	C1D-ND	2.98	1.41	1.37
28	D	409	LHG	C8-C7	-2.97	1.42	1.50
22	B	609	CLA	C4B-NB	2.97	1.41	1.37
22	B	615	CLA	CMB-C2B	-2.96	1.44	1.50
22	C	504	CLA	MG-NB	2.96	2.11	2.05
24	t	101	BCR	C30-C25	-2.96	1.50	1.53
22	B	610	CLA	C4B-NB	2.95	1.41	1.37
30	h	101	DGD	C4E-C5E	2.95	1.59	1.53
24	b	619	BCR	C30-C25	-2.94	1.50	1.53
22	b	615	CLA	CMB-C2B	-2.94	1.44	1.50
22	c	502	CLA	CMD-C2D	-2.93	1.44	1.50
22	D	402	CLA	CMD-C2D	-2.93	1.44	1.50
23	a	403	PHO	C3B-C2B	-2.92	1.36	1.40
30	C	518	DGD	O5D-C6D	-2.92	1.38	1.43
26	A	410	PL9	C6-C1	-2.92	1.43	1.48
22	d	401	CLA	CHC-C1C	2.92	1.44	1.38
22	C	505	CLA	C1B-C2B	2.91	1.50	1.43
30	h	101	DGD	O2D-C2D	-2.91	1.35	1.43
29	b	620	SQD	O47-C7	2.90	1.42	1.34
24	a	405	BCR	C1-C6	-2.90	1.50	1.53
22	B	601	CLA	C1B-C2B	2.90	1.49	1.43
24	x	101	BCR	C1-C6	-2.90	1.50	1.53
26	A	410	PL9	C37-C38	2.90	1.59	1.50
22	d	405	CLA	CMC-C2C	-2.89	1.44	1.50
22	b	615	CLA	CMD-C2D	-2.89	1.44	1.50
23	A	405	PHO	CMB-C2B	-2.88	1.45	1.51
22	B	604	CLA	C3B-C4B	2.88	1.51	1.42
22	d	403	CLA	MG-NA	2.88	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B	615	CLA	MG-NA	2.87	2.13	2.06
30	H	102	DGD	O2G-C2G	-2.87	1.39	1.46
24	D	405	BCR	C1-C6	-2.87	1.50	1.53
24	A	407	BCR	C33-C5	-2.87	1.46	1.50
22	c	513	CLA	C1B-C2B	2.87	1.49	1.43
22	B	613	CLA	C1B-C2B	2.87	1.49	1.43
22	c	511	CLA	C1B-C2B	2.87	1.49	1.43
22	C	505	CLA	C4B-NB	2.86	1.41	1.37
22	B	608	CLA	CMD-C2D	-2.86	1.44	1.50
22	B	603	CLA	CMB-C2B	-2.86	1.44	1.50
27	b	623	LMG	O6-C1	2.86	1.49	1.41
24	k	101	BCR	C1-C6	-2.85	1.50	1.53
23	A	405	PHO	C4D-CHA	2.85	1.43	1.39
22	A	402	CLA	C1D-ND	2.85	1.41	1.37
23	A	405	PHO	C1D-C2D	2.84	1.42	1.39
22	d	405	CLA	MG-ND	-2.84	2.00	2.05
22	d	404	CLA	C1B-NB	-2.84	1.34	1.37
22	B	616	CLA	C1B-NB	-2.84	1.34	1.37
22	D	402	CLA	CHC-C1C	2.83	1.44	1.38
22	C	511	CLA	C1B-C2B	2.83	1.49	1.43
22	b	605	CLA	MG-NA	2.82	2.13	2.06
23	A	404	PHO	C3B-C2B	-2.82	1.36	1.40
22	b	612	CLA	C1B-C2B	2.82	1.49	1.43
29	a	411	SQD	O47-C7	2.82	1.42	1.34
26	D	406	PL9	C5-C4	-2.81	1.37	1.47
22	B	601	CLA	CMB-C2B	-2.81	1.45	1.50
24	C	515	BCR	C30-C25	-2.81	1.50	1.53
22	A	406	CLA	MG-NB	-2.80	2.00	2.05
27	c	523	LMG	C4-C5	2.80	1.59	1.53
22	B	612	CLA	CHC-C1C	2.80	1.44	1.38
28	A	412	LHG	C8-C7	-2.80	1.42	1.50
22	b	612	CLA	CMC-C2C	-2.79	1.45	1.50
22	C	503	CLA	C4B-NB	2.79	1.41	1.37
29	f	102	SQD	O47-C7	2.79	1.42	1.34
22	c	506	CLA	CAC-C3C	-2.79	1.44	1.51
22	C	503	CLA	C1B-C2B	2.79	1.49	1.43
30	h	101	DGD	O2E-C2E	-2.79	1.36	1.43
30	H	102	DGD	C1E-C2E	2.79	1.60	1.52
24	t	101	BCR	C1-C6	-2.78	1.50	1.53
22	c	510	CLA	C4B-NB	2.78	1.41	1.37
22	B	610	CLA	C1D-ND	2.77	1.41	1.37
22	c	511	CLA	CHC-C1C	2.77	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	612	CLA	MG-NA	2.77	2.12	2.06
22	D	404	CLA	C4B-NB	2.77	1.41	1.37
30	C	518	DGD	O1G-C1G	-2.77	1.39	1.45
27	b	623	LMG	C3-C2	2.77	1.59	1.52
22	C	505	CLA	CHC-C1C	2.76	1.44	1.38
22	b	607	CLA	C1D-ND	2.76	1.41	1.37
22	C	509	CLA	C3B-C4B	2.76	1.50	1.42
30	H	102	DGD	O2D-C2D	-2.76	1.36	1.43
27	m	101	LMG	C4-C3	2.75	1.59	1.52
30	A	415	DGD	O3G-C1D	2.75	1.44	1.40
22	c	513	CLA	MG-NA	2.75	2.12	2.06
22	a	402	CLA	C1B-C2B	2.75	1.49	1.43
27	D	410	LMG	C9-C8	2.74	1.59	1.50
22	B	616	CLA	C1D-ND	2.74	1.41	1.37
22	B	606	CLA	CHC-C1C	2.74	1.44	1.38
22	C	504	CLA	C3B-C4B	2.74	1.50	1.42
22	B	610	CLA	MG-NA	2.74	2.12	2.06
22	b	603	CLA	CMC-C2C	-2.74	1.45	1.50
22	C	507	CLA	C1D-ND	2.74	1.41	1.37
22	c	510	CLA	MG-NC	-2.73	1.99	2.06
22	b	611	CLA	CMC-C2C	-2.73	1.45	1.50
26	A	410	PL9	C7-C3	-2.73	1.47	1.51
22	B	605	CLA	C1B-NB	-2.72	1.34	1.37
22	b	603	CLA	CMB-C2B	-2.72	1.45	1.50
22	c	512	CLA	C1D-ND	2.72	1.41	1.37
22	C	512	CLA	C1B-C2B	2.72	1.49	1.43
28	e	101	LHG	P-O6	2.71	1.70	1.59
22	A	402	CLA	C1B-C2B	2.71	1.49	1.43
22	d	405	CLA	MG-NC	-2.71	1.99	2.06
22	d	403	CLA	CMD-C2D	-2.71	1.45	1.50
22	A	403	CLA	CMD-C2D	-2.71	1.45	1.50
22	c	510	CLA	C1B-C2B	2.71	1.49	1.43
22	c	505	CLA	C1B-C2B	2.71	1.49	1.43
22	B	609	CLA	C1B-C2B	2.71	1.49	1.43
22	C	501	CLA	C4B-NB	2.70	1.41	1.37
22	b	608	CLA	C3B-C4B	2.70	1.50	1.42
22	C	510	CLA	C1B-NB	-2.69	1.34	1.37
23	d	402	PHO	CMD-C2D	-2.69	1.46	1.51
22	C	513	CLA	C1B-C2B	2.69	1.49	1.43
22	c	513	CLA	C4B-NB	2.69	1.41	1.37
23	A	404	PHO	C4D-CHA	2.69	1.43	1.39
30	C	517	DGD	C4E-C3E	2.68	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	403	PHO	C4D-ND	-2.68	1.34	1.38
22	C	502	CLA	MG-ND	2.68	2.11	2.05
22	C	510	CLA	O2A-CGA	2.68	1.41	1.33
22	d	405	CLA	CMD-C2D	-2.68	1.45	1.50
22	C	508	CLA	C1D-C2D	2.68	1.50	1.45
22	D	404	CLA	CMC-C2C	-2.68	1.45	1.50
30	h	101	DGD	C4D-C3D	2.68	1.59	1.52
22	B	606	CLA	C4B-NB	2.67	1.41	1.37
30	c	518	DGD	C4D-C5D	2.66	1.58	1.53
22	c	505	CLA	MG-NB	-2.66	2.00	2.05
24	B	619	BCR	C30-C25	-2.65	1.50	1.53
22	B	616	CLA	CMC-C2C	-2.65	1.45	1.50
26	d	407	PL9	C45-C44	-2.65	1.44	1.50
22	b	610	CLA	CMD-C2D	-2.65	1.45	1.50
22	c	510	CLA	CMB-C2B	-2.65	1.45	1.50
22	B	602	CLA	MG-ND	-2.64	2.00	2.05
22	B	606	CLA	MG-NC	2.64	2.12	2.06
22	C	502	CLA	C1B-C2B	2.64	1.49	1.43
30	C	519	DGD	O3G-C1D	-2.64	1.35	1.40
22	c	506	CLA	C1D-ND	2.63	1.41	1.37
29	A	413	SQD	O47-C7	2.63	1.41	1.34
22	d	401	CLA	C1B-C2B	2.63	1.49	1.43
22	B	612	CLA	C3B-C4B	2.63	1.50	1.42
22	c	508	CLA	C3B-C4B	2.63	1.50	1.42
28	E	101	LHG	O7-C5	-2.63	1.40	1.46
30	c	518	DGD	C6E-C5E	2.62	1.60	1.51
22	c	502	CLA	C1B-C2B	2.62	1.49	1.43
22	B	608	CLA	C1D-ND	2.62	1.41	1.37
22	c	507	CLA	MG-NC	-2.62	2.00	2.06
22	a	404	CLA	CMD-C2D	-2.62	1.45	1.50
22	B	604	CLA	CMC-C2C	-2.61	1.45	1.50
22	c	510	CLA	CHC-C1C	2.61	1.43	1.38
26	A	410	PL9	C25-C24	-2.61	1.44	1.50
30	H	102	DGD	C6E-C5E	2.61	1.60	1.51
22	c	505	CLA	MG-NA	2.60	2.12	2.06
22	B	611	CLA	CHC-C1C	2.60	1.43	1.38
22	B	612	CLA	C1B-NB	-2.59	1.34	1.37
27	d	410	LMG	O7-C8	-2.59	1.40	1.46
22	B	603	CLA	C1B-C2B	2.59	1.49	1.43
22	C	501	CLA	CMC-C2C	-2.59	1.45	1.50
22	B	616	CLA	C1B-C2B	2.59	1.49	1.43
22	C	507	CLA	CMB-C2B	-2.58	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	606	CLA	MG-NC	-2.58	2.00	2.06
22	b	611	CLA	C1B-C2B	2.58	1.49	1.43
22	B	601	CLA	MG-NA	2.58	2.12	2.06
23	A	405	PHO	CMD-C2D	-2.58	1.46	1.51
30	H	102	DGD	C4E-C3E	2.58	1.59	1.52
22	B	615	CLA	C4B-NB	2.58	1.41	1.37
22	C	512	CLA	MG-NC	-2.58	2.00	2.06
22	D	403	CLA	CMB-C2B	-2.57	1.45	1.50
22	b	602	CLA	CAC-C3C	-2.57	1.44	1.51
26	d	407	PL9	C27-C28	-2.57	1.42	1.50
30	C	517	DGD	O1G-C1A	2.57	1.40	1.33
30	C	518	DGD	O2G-C2G	-2.56	1.40	1.46
22	b	613	CLA	C4B-NB	2.56	1.41	1.37
22	b	607	CLA	CMD-C2D	-2.56	1.45	1.50
27	A	411	LMG	C4-C5	2.56	1.58	1.53
22	B	615	CLA	CHC-C4B	-2.56	1.33	1.39
27	c	522	LMG	O1-C1	2.56	1.44	1.40
22	B	605	CLA	CHC-C1C	2.56	1.43	1.38
22	C	510	CLA	C1D-ND	2.56	1.41	1.37
22	B	605	CLA	C3B-C4B	2.56	1.50	1.42
22	b	614	CLA	CAC-C3C	-2.55	1.44	1.51
22	c	506	CLA	CMC-C2C	-2.55	1.45	1.50
22	A	403	CLA	MG-NA	2.55	2.12	2.06
29	A	414	SQD	O47-C45	-2.55	1.42	1.47
22	B	616	CLA	MG-NC	-2.55	2.00	2.06
30	C	517	DGD	C3G-C2G	2.55	1.58	1.50
22	B	607	CLA	MG-NA	2.54	2.12	2.06
22	d	403	CLA	C1D-ND	2.54	1.41	1.37
22	D	403	CLA	C1B-NB	-2.54	1.34	1.37
22	B	611	CLA	CMC-C2C	-2.54	1.45	1.50
23	d	402	PHO	CAC-C3C	-2.54	1.47	1.51
22	c	508	CLA	CMD-C2D	-2.54	1.45	1.50
22	c	508	CLA	CHC-C1C	2.54	1.43	1.38
22	b	602	CLA	MG-NB	2.54	2.10	2.05
22	C	508	CLA	C3B-C4B	2.53	1.50	1.42
22	B	602	CLA	CMB-C2B	-2.53	1.45	1.50
29	a	411	SQD	O4-C4	-2.53	1.36	1.43
22	d	401	CLA	C1B-NB	-2.53	1.34	1.37
22	b	605	CLA	C3B-C4B	2.53	1.50	1.42
22	D	402	CLA	MG-NA	2.53	2.12	2.06
22	C	504	CLA	CMD-C2D	-2.53	1.45	1.50
22	b	606	CLA	C1B-C2B	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	A	415	DGD	C1E-C2E	2.52	1.59	1.52
22	b	608	CLA	C1B-C2B	2.52	1.49	1.43
22	D	402	CLA	MG-NB	-2.52	2.00	2.05
22	C	508	CLA	CHC-C1C	2.52	1.43	1.38
26	a	409	PL9	C6-C1	-2.52	1.44	1.48
30	A	415	DGD	O3D-C3D	-2.52	1.36	1.43
22	b	614	CLA	CMB-C2B	-2.51	1.45	1.50
22	B	606	CLA	C1D-ND	2.51	1.41	1.37
22	c	505	CLA	C3B-C4B	2.51	1.50	1.42
22	d	404	CLA	CMB-C2B	-2.51	1.45	1.50
30	C	517	DGD	C6E-C5E	2.51	1.60	1.51
35	f	101	HEC	FE-NA	2.51	2.03	1.95
22	c	507	CLA	C1B-NB	-2.51	1.34	1.37
22	B	610	CLA	C1B-C2B	2.50	1.49	1.43
23	A	404	PHO	CAC-C3C	-2.50	1.47	1.51
22	B	602	CLA	CHC-C1C	2.50	1.43	1.38
26	a	409	PL9	C3-C4	-2.50	1.45	1.49
22	c	512	CLA	C3B-C4B	2.50	1.50	1.42
22	A	406	CLA	CMD-C2D	-2.49	1.45	1.50
22	b	604	CLA	C1D-ND	2.49	1.41	1.37
22	C	502	CLA	CMB-C2B	-2.49	1.45	1.50
22	c	511	CLA	C3B-C4B	2.49	1.50	1.42
22	b	603	CLA	MG-NB	-2.49	2.00	2.05
22	b	612	CLA	CMB-C2B	-2.49	1.45	1.50
22	a	402	CLA	C3B-C4B	2.49	1.50	1.42
22	a	404	CLA	C4B-NB	2.48	1.41	1.37
22	C	505	CLA	C1B-NB	-2.48	1.34	1.37
22	c	504	CLA	C1B-C2B	2.47	1.48	1.43
22	D	402	CLA	CAA-C2A	-2.47	1.49	1.54
22	B	612	CLA	MG-ND	2.47	2.10	2.05
23	a	403	PHO	O2D-CGD	2.47	1.39	1.33
22	B	604	CLA	CHC-C1C	2.47	1.43	1.38
23	A	405	PHO	CMC-C2C	-2.47	1.46	1.50
22	d	405	CLA	C4B-NB	2.47	1.41	1.37
22	b	610	CLA	CHC-C4B	-2.47	1.33	1.39
24	A	407	BCR	C30-C25	-2.47	1.50	1.53
22	c	511	CLA	C1D-ND	2.47	1.41	1.37
22	B	613	CLA	CMC-C2C	-2.46	1.45	1.50
28	B	621	LHG	O1-C1	2.46	1.52	1.42
24	b	617	BCR	C33-C5	-2.46	1.47	1.50
24	A	407	BCR	C38-C26	-2.46	1.47	1.50
22	C	509	CLA	C1B-C2B	2.46	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	MG-NC	2.46	2.12	2.06
22	C	511	CLA	CMC-C2C	-2.46	1.45	1.50
22	b	614	CLA	CMC-C2C	-2.46	1.45	1.50
30	H	102	DGD	C3E-C2E	2.45	1.58	1.52
30	C	517	DGD	O2G-C1B	2.45	1.41	1.34
22	B	603	CLA	MG-NB	-2.45	2.00	2.05
22	C	507	CLA	C1B-NB	-2.45	1.34	1.37
22	D	404	CLA	CMB-C2B	-2.45	1.45	1.50
22	b	602	CLA	C3B-C4B	2.45	1.49	1.42
22	b	616	CLA	CMC-C2C	-2.45	1.45	1.50
30	h	101	DGD	C2A-C1A	-2.44	1.43	1.50
22	C	501	CLA	C1B-NB	-2.44	1.34	1.37
26	d	407	PL9	C7-C3	-2.44	1.48	1.51
27	A	411	LMG	C1-C2	2.44	1.59	1.52
24	a	405	BCR	C30-C25	-2.44	1.50	1.53
22	C	508	CLA	C1B-C2B	2.44	1.48	1.43
22	b	609	CLA	C1B-C2B	2.44	1.48	1.43
22	d	403	CLA	C3B-C4B	2.43	1.49	1.42
22	B	611	CLA	C1D-ND	2.43	1.41	1.37
22	b	601	CLA	CHC-C1C	2.43	1.43	1.38
22	C	507	CLA	C1B-C2B	2.43	1.48	1.43
22	b	608	CLA	MG-NB	-2.43	2.01	2.05
22	b	602	CLA	CMD-C2D	-2.43	1.45	1.50
22	d	401	CLA	CMB-C2B	-2.43	1.45	1.50
22	C	507	CLA	CMD-C2D	-2.43	1.45	1.50
23	A	404	PHO	CMA-C3A	-2.43	1.49	1.53
22	B	602	CLA	MG-NB	-2.43	2.01	2.05
22	B	606	CLA	CHC-C4B	-2.42	1.34	1.39
22	D	403	CLA	CHC-C1C	2.42	1.43	1.38
28	D	409	LHG	P-O3	2.42	1.68	1.59
22	d	404	CLA	MG-NC	-2.42	2.00	2.06
22	c	503	CLA	MG-NB	2.42	2.10	2.05
22	A	403	CLA	C1B-C2B	2.42	1.48	1.43
22	c	510	CLA	CMC-C2C	-2.42	1.45	1.50
22	b	616	CLA	C1B-C2B	2.41	1.48	1.43
23	A	404	PHO	C1D-C2D	2.41	1.42	1.39
22	b	616	CLA	CMB-C2B	-2.41	1.45	1.50
22	D	403	CLA	C3D-C4D	2.41	1.49	1.44
22	b	608	CLA	C1D-ND	2.41	1.41	1.37
22	b	604	CLA	C1B-C2B	2.41	1.48	1.43
28	A	412	LHG	O7-C7	2.41	1.41	1.34
35	V	201	HEC	CMB-C2B	2.41	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	PHO	C1D-ND	2.40	1.42	1.38
22	c	503	CLA	C1B-NB	-2.40	1.34	1.37
22	c	504	CLA	CMD-C2D	-2.40	1.45	1.50
27	M	101	LMG	O7-C8	-2.40	1.41	1.46
22	c	512	CLA	CHC-C1C	2.40	1.43	1.38
22	b	607	CLA	C1B-C2B	2.40	1.48	1.43
22	C	510	CLA	CMC-C2C	-2.40	1.45	1.50
30	c	518	DGD	O3G-C3G	-2.40	1.39	1.43
29	f	102	SQD	O3-C3	-2.40	1.37	1.43
22	c	507	CLA	MG-NB	-2.40	2.01	2.05
22	B	610	CLA	C3B-C4B	2.39	1.49	1.42
22	c	506	CLA	CHC-C1C	2.39	1.43	1.38
27	c	522	LMG	C4-C3	2.39	1.58	1.52
22	D	404	CLA	CMD-C2D	-2.39	1.45	1.50
24	B	617	BCR	C33-C5	-2.38	1.47	1.50
30	A	415	DGD	O5D-C1E	2.38	1.44	1.40
22	B	609	CLA	CMD-C2D	-2.38	1.45	1.50
30	C	517	DGD	C4D-C3D	2.38	1.58	1.52
22	b	601	CLA	O2A-CGA	2.37	1.40	1.33
22	c	503	CLA	C1B-C2B	2.37	1.48	1.43
22	C	512	CLA	CMC-C2C	-2.37	1.45	1.50
22	B	614	CLA	C1D-ND	2.36	1.41	1.37
22	B	610	CLA	MG-NB	-2.36	2.01	2.05
27	C	520	LMG	C4-C3	2.36	1.58	1.52
27	a	416	LMG	C7-C8	2.36	1.58	1.50
22	c	502	CLA	C4B-NB	2.36	1.41	1.37
22	c	501	CLA	MG-NA	2.36	2.11	2.06
22	c	503	CLA	C5-C3	-2.36	1.46	1.51
22	c	504	CLA	CHC-C1C	2.35	1.43	1.38
22	B	611	CLA	C1B-NB	-2.35	1.34	1.37
27	c	520	LMG	C3-C2	2.35	1.58	1.52
22	B	607	CLA	CMB-C2B	-2.35	1.45	1.50
22	B	615	CLA	C1D-C2D	2.35	1.50	1.45
22	b	605	CLA	CHC-C1C	2.35	1.43	1.38
22	B	606	CLA	C1B-C2B	2.35	1.48	1.43
22	b	614	CLA	MG-NB	2.35	2.10	2.05
35	f	101	HEC	CHB-C4A	-2.35	1.33	1.38
22	D	402	CLA	C1B-C2B	2.35	1.48	1.43
24	c	515	BCR	C33-C5	-2.35	1.47	1.50
22	c	505	CLA	CMB-C2B	-2.34	1.46	1.50
22	C	502	CLA	C1D-ND	2.34	1.40	1.37
22	D	404	CLA	CHC-C4B	-2.34	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	517	DGD	C6D-C5D	2.34	1.58	1.51
22	b	604	CLA	C3D-C4D	2.34	1.49	1.44
22	B	610	CLA	CHC-C1C	2.34	1.43	1.38
23	a	403	PHO	CAA-C2A	-2.34	1.49	1.54
22	b	601	CLA	C3B-C4B	2.34	1.49	1.42
23	a	403	PHO	CMB-C2B	-2.33	1.47	1.51
22	c	506	CLA	C1B-C2B	2.33	1.48	1.43
26	A	410	PL9	C7-C8	-2.33	1.46	1.50
27	M	101	LMG	C9-C8	2.33	1.58	1.50
22	c	511	CLA	C4B-NB	2.33	1.40	1.37
22	B	605	CLA	CMD-C2D	-2.33	1.46	1.50
23	d	402	PHO	CAA-C2A	-2.33	1.49	1.54
35	F	101	HEC	CMA-C3A	2.33	1.55	1.50
22	b	610	CLA	CMB-C2B	-2.33	1.46	1.50
22	B	602	CLA	C1B-C2B	2.32	1.48	1.43
22	B	609	CLA	C1B-NB	-2.32	1.34	1.37
27	m	101	LMG	C1-C2	2.32	1.59	1.52
22	B	610	CLA	CMA-C3A	-2.32	1.48	1.53
30	A	415	DGD	C4D-C5D	2.32	1.58	1.53
22	C	504	CLA	CHC-C1C	2.32	1.43	1.38
22	C	510	CLA	CMD-C2D	-2.32	1.46	1.50
22	B	603	CLA	CMC-C2C	-2.32	1.46	1.50
27	D	410	LMG	O8-C28	2.32	1.40	1.33
27	M	101	LMG	C29-C28	-2.31	1.44	1.50
30	c	517	DGD	O4D-C4D	-2.31	1.37	1.43
22	b	613	CLA	C1B-C2B	2.31	1.48	1.43
22	b	612	CLA	CHC-C1C	2.31	1.43	1.38
22	C	513	CLA	C3B-C4B	2.31	1.49	1.42
22	c	501	CLA	C1B-C2B	2.31	1.48	1.43
22	B	607	CLA	C3B-C4B	2.31	1.49	1.42
22	c	513	CLA	C3B-C4B	2.31	1.49	1.42
24	T	101	BCR	C38-C26	-2.31	1.47	1.50
22	b	615	CLA	CHC-C1C	2.30	1.43	1.38
22	d	401	CLA	C3B-C4B	2.30	1.49	1.42
22	c	509	CLA	MG-ND	-2.30	2.01	2.05
27	D	407	LMG	C7-C8	2.30	1.58	1.50
22	C	501	CLA	C3B-C4B	2.30	1.49	1.42
35	f	101	HEC	CMC-C2C	2.30	1.55	1.50
22	b	613	CLA	CMC-C2C	-2.30	1.46	1.50
30	c	517	DGD	O3E-C3E	-2.30	1.37	1.43
22	a	404	CLA	CHC-C4B	-2.30	1.34	1.39
27	c	520	LMG	C4-C3	2.30	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	C	502	CLA	CMC-C2C	-2.30	1.46	1.50
22	B	606	CLA	MG-ND	-2.30	2.01	2.05
24	t	101	BCR	C27-C26	-2.29	1.46	1.51
30	C	519	DGD	C6D-C5D	2.29	1.58	1.51
22	c	512	CLA	CMD-C2D	-2.29	1.46	1.50
22	c	507	CLA	C1B-C2B	2.29	1.48	1.43
27	D	407	LMG	C9-C8	2.29	1.58	1.50
22	C	504	CLA	C1B-NB	-2.29	1.34	1.37
24	C	516	BCR	C33-C5	-2.29	1.47	1.50
22	B	610	CLA	CMB-C2B	-2.29	1.46	1.50
30	H	102	DGD	C6D-C5D	2.28	1.58	1.51
22	c	502	CLA	C1D-ND	2.28	1.40	1.37
29	a	411	SQD	O2-C2	-2.28	1.37	1.43
24	a	405	BCR	C27-C26	-2.28	1.46	1.51
35	V	201	HEC	C1D-ND	-2.28	1.36	1.40
22	C	510	CLA	C1B-C2B	2.27	1.48	1.43
22	B	603	CLA	C3B-C4B	2.27	1.49	1.42
22	C	510	CLA	C4B-NB	2.27	1.40	1.37
22	A	402	CLA	CMD-C2D	-2.27	1.46	1.50
22	A	403	CLA	C3B-C4B	2.27	1.49	1.42
30	C	518	DGD	C6D-C5D	2.27	1.58	1.51
22	a	402	CLA	C4B-NB	2.27	1.40	1.37
30	c	517	DGD	C3G-C2G	2.27	1.57	1.50
27	c	520	LMG	O1-C1	2.26	1.44	1.40
22	b	601	CLA	C1D-C2D	2.26	1.49	1.45
22	a	402	CLA	C1D-ND	2.26	1.40	1.37
24	C	514	BCR	C38-C26	-2.26	1.47	1.50
22	b	614	CLA	C3B-C4B	2.26	1.49	1.42
22	c	505	CLA	MG-NC	2.26	2.11	2.06
30	h	101	DGD	O2G-C2G	-2.25	1.41	1.46
26	A	410	PL9	C3-C4	-2.25	1.46	1.49
23	A	405	PHO	C4D-ND	-2.25	1.35	1.38
22	B	611	CLA	C3B-C4B	2.25	1.49	1.42
30	h	101	DGD	C1E-C2E	2.25	1.59	1.52
22	a	402	CLA	MG-NB	2.25	2.10	2.05
22	A	406	CLA	C4B-NB	2.25	1.40	1.37
27	C	520	LMG	O7-C8	-2.25	1.41	1.46
22	d	401	CLA	MG-NA	-2.25	2.00	2.06
28	B	622	LHG	P-O4	-2.25	1.44	1.55
30	H	102	DGD	O6E-C1E	2.25	1.47	1.41
30	C	519	DGD	C6E-C5E	2.25	1.59	1.51
35	f	101	HEC	C3B-C2B	-2.24	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	403	CLA	C1B-C2B	2.24	1.48	1.43
22	C	501	CLA	C1B-C2B	2.24	1.48	1.43
30	C	517	DGD	O2E-C2E	-2.24	1.37	1.43
29	A	413	SQD	O47-C45	-2.24	1.41	1.46
22	B	607	CLA	CHC-C1C	2.24	1.43	1.38
29	A	413	SQD	O6-C44	-2.23	1.39	1.43
22	b	609	CLA	MG-NB	2.23	2.10	2.05
22	C	508	CLA	CMC-C2C	-2.23	1.46	1.50
22	D	403	CLA	CMD-C2D	-2.23	1.46	1.50
30	C	517	DGD	O3G-C3G	-2.23	1.39	1.43
23	A	405	PHO	C3B-C2B	-2.23	1.37	1.40
22	B	614	CLA	C1B-NB	-2.23	1.34	1.37
27	D	407	LMG	C4-C5	2.23	1.57	1.53
22	C	502	CLA	C3B-C4B	2.23	1.49	1.42
22	C	506	CLA	C4B-NB	2.23	1.40	1.37
22	c	506	CLA	CMD-C2D	-2.23	1.46	1.50
22	B	615	CLA	C3D-C4D	2.22	1.49	1.44
29	A	413	SQD	O2-C2	-2.22	1.37	1.43
22	C	511	CLA	CHC-C1C	2.22	1.42	1.38
22	c	504	CLA	CMC-C2C	-2.22	1.46	1.50
22	b	611	CLA	CHC-C1C	2.22	1.42	1.38
22	B	601	CLA	CMC-C2C	-2.22	1.46	1.50
22	c	503	CLA	CMC-C2C	-2.22	1.46	1.50
28	d	408	LHG	O6-C4	-2.22	1.36	1.44
29	D	408	SQD	O2-C2	-2.22	1.37	1.43
22	C	503	CLA	C1D-C2D	2.21	1.49	1.45
28	a	410	LHG	O7-C5	-2.21	1.41	1.46
22	b	604	CLA	MG-NB	-2.21	2.01	2.05
22	b	611	CLA	CMD-C2D	-2.21	1.46	1.50
22	B	613	CLA	MG-NC	2.21	2.11	2.06
22	b	613	CLA	CMB-C2B	-2.20	1.46	1.50
22	C	503	CLA	CMD-C2D	-2.20	1.46	1.50
22	b	609	CLA	C4B-NB	2.20	1.40	1.37
26	d	407	PL9	C51-C49	-2.20	1.44	1.50
22	B	609	CLA	C3B-C4B	2.20	1.49	1.42
23	d	402	PHO	C4D-CHA	2.20	1.42	1.39
22	d	405	CLA	C1B-C2B	2.20	1.48	1.43
27	d	410	LMG	O1-C1	2.20	1.43	1.40
28	l	101	LHG	O7-C5	-2.20	1.41	1.46
22	B	616	CLA	CMD-C2D	-2.20	1.46	1.50
22	C	510	CLA	C3D-C4D	2.20	1.49	1.44
22	c	505	CLA	C1D-ND	2.20	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	414	SQD	C46-C45	2.19	1.55	1.50
22	C	512	CLA	C3D-C4D	2.19	1.49	1.44
27	c	522	LMG	O7-C8	-2.19	1.41	1.46
22	b	616	CLA	CMD-C2D	-2.19	1.46	1.50
22	b	602	CLA	MG-NA	-2.19	2.01	2.06
22	a	402	CLA	C3D-C4D	2.19	1.49	1.44
22	d	404	CLA	C3B-C4B	2.19	1.49	1.42
24	D	405	BCR	C36-C18	-2.18	1.46	1.50
27	D	407	LMG	C6-C5	2.18	1.59	1.51
22	B	613	CLA	C3B-C4B	2.18	1.49	1.42
22	c	512	CLA	MG-NA	2.18	2.11	2.06
22	C	508	CLA	C3D-C4D	2.18	1.49	1.44
30	c	518	DGD	O3E-C3E	-2.18	1.37	1.43
30	H	102	DGD	O5D-C6D	2.18	1.47	1.43
22	c	505	CLA	CMC-C2C	-2.18	1.46	1.50
22	d	404	CLA	CHB-C1B	2.18	1.44	1.39
30	c	517	DGD	O2E-C2E	-2.17	1.37	1.43
29	D	408	SQD	O3-C3	-2.17	1.37	1.43
22	c	513	CLA	CMC-C2C	-2.17	1.46	1.50
22	b	601	CLA	CMC-C2C	-2.17	1.46	1.50
24	B	618	BCR	C27-C26	-2.17	1.47	1.51
22	c	503	CLA	C4B-NB	2.17	1.40	1.37
26	D	406	PL9	C46-C44	-2.17	1.46	1.51
22	c	509	CLA	C3D-C4D	2.17	1.49	1.44
22	B	608	CLA	C1B-C2B	2.17	1.48	1.43
30	c	518	DGD	C4E-C5E	2.17	1.57	1.53
22	b	616	CLA	CAC-C3C	-2.16	1.45	1.51
22	c	504	CLA	C3B-C4B	2.16	1.49	1.42
29	A	413	SQD	O4-C4	-2.16	1.37	1.43
22	B	613	CLA	MG-NB	-2.16	2.01	2.05
24	C	515	BCR	C38-C26	-2.16	1.47	1.50
22	d	405	CLA	CHC-C4B	-2.16	1.34	1.39
22	A	403	CLA	C4C-C3C	2.15	1.48	1.45
30	C	518	DGD	C1E-C2E	2.15	1.58	1.52
30	c	517	DGD	O3G-C3G	-2.15	1.40	1.43
22	b	608	CLA	CHC-C1C	2.15	1.42	1.38
22	b	604	CLA	C4B-NB	2.15	1.40	1.37
30	c	517	DGD	O1G-C1G	-2.15	1.40	1.45
22	C	511	CLA	CMD-C2D	-2.15	1.46	1.50
22	B	606	CLA	C3B-C4B	2.15	1.49	1.42
22	B	603	CLA	C1B-NB	-2.15	1.35	1.37
22	B	606	CLA	C3B-C2B	-2.15	1.33	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	A	412	LHG	C3-C2	2.15	1.58	1.51
22	B	614	CLA	CMC-C2C	-2.15	1.46	1.50
22	C	505	CLA	CMC-C2C	-2.14	1.46	1.50
22	b	612	CLA	C3B-C4B	2.14	1.49	1.42
22	b	614	CLA	C4B-NB	2.14	1.40	1.37
22	b	605	CLA	C1A-CHA	-2.14	1.34	1.43
22	A	402	CLA	C1D-C2D	2.14	1.49	1.45
28	e	101	LHG	C24-C23	2.14	1.56	1.50
22	C	502	CLA	C4B-NB	2.13	1.40	1.37
22	A	406	CLA	C1B-C2B	2.13	1.48	1.43
22	b	608	CLA	C1B-NB	-2.13	1.35	1.37
30	c	518	DGD	O3G-C1D	-2.13	1.36	1.40
22	D	402	CLA	C1C-NC	-2.13	1.34	1.37
23	A	405	PHO	CAC-C3C	-2.12	1.48	1.51
22	b	606	CLA	C3B-C4B	2.12	1.48	1.42
22	B	615	CLA	C1B-NB	-2.12	1.35	1.37
22	C	505	CLA	MG-NC	-2.12	2.01	2.06
22	b	611	CLA	O2D-CGD	2.12	1.38	1.33
22	c	511	CLA	C3D-C4D	2.12	1.49	1.44
22	c	513	CLA	MG-NB	2.12	2.10	2.05
22	c	512	CLA	C1B-C2B	2.12	1.48	1.43
22	C	509	CLA	C3D-C4D	2.12	1.49	1.44
22	b	607	CLA	MG-NC	2.12	2.11	2.06
23	A	405	PHO	C3A-C2A	-2.12	1.52	1.54
22	B	610	CLA	C1D-C2D	2.11	1.49	1.45
22	C	513	CLA	CHC-C4B	-2.11	1.34	1.39
24	t	101	BCR	C31-C1	-2.11	1.49	1.53
24	k	101	BCR	C36-C18	-2.11	1.46	1.50
24	k	101	BCR	C33-C5	-2.11	1.47	1.50
22	b	607	CLA	C3B-C4B	2.10	1.48	1.42
23	A	404	PHO	CMB-C2B	-2.10	1.47	1.51
22	c	501	CLA	MG-NC	-2.10	2.01	2.06
22	d	405	CLA	C3B-C4B	2.10	1.48	1.42
24	c	516	BCR	C38-C26	-2.10	1.47	1.50
27	M	101	LMG	O1-C7	-2.10	1.40	1.43
22	C	509	CLA	CMD-C2D	-2.10	1.46	1.50
28	e	101	LHG	O8-C23	2.10	1.39	1.33
27	D	407	LMG	O7-C10	2.10	1.40	1.34
22	C	506	CLA	C3D-C4D	2.10	1.48	1.44
22	d	401	CLA	CMC-C2C	-2.10	1.46	1.50
26	a	409	PL9	C46-C44	-2.10	1.47	1.51
22	B	607	CLA	MG-ND	2.09	2.09	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	b	610	CLA	C1C-NC	-2.09	1.34	1.37
22	C	510	CLA	C3B-C4B	2.09	1.48	1.42
22	B	606	CLA	CMB-C2B	-2.09	1.46	1.50
24	B	617	BCR	C38-C26	-2.09	1.47	1.50
22	b	602	CLA	C1B-C2B	2.09	1.48	1.43
22	B	601	CLA	C3B-C4B	2.09	1.48	1.42
22	c	513	CLA	CMD-C2D	-2.09	1.46	1.50
22	B	613	CLA	C5-C3	-2.09	1.47	1.51
22	b	610	CLA	MG-NA	2.09	2.11	2.06
23	a	403	PHO	C4D-CHA	2.09	1.42	1.39
22	b	605	CLA	C4B-NB	2.08	1.40	1.37
22	c	509	CLA	C4B-NB	2.08	1.40	1.37
22	A	406	CLA	CHC-C4B	-2.08	1.34	1.39
24	C	515	BCR	C33-C5	-2.08	1.47	1.50
22	b	605	CLA	CHC-C4B	-2.08	1.34	1.39
22	b	611	CLA	C3B-C4B	2.07	1.48	1.42
22	b	609	CLA	CMB-C2B	-2.07	1.46	1.50
22	c	512	CLA	CMB-C2B	-2.07	1.46	1.50
26	d	407	PL9	C46-C44	-2.07	1.47	1.51
29	A	413	SQD	O3-C3	-2.07	1.37	1.43
24	B	619	BCR	C31-C1	-2.07	1.49	1.53
22	c	501	CLA	CMC-C2C	-2.07	1.46	1.50
30	C	519	DGD	C4D-C3D	2.06	1.57	1.52
22	c	509	CLA	C3B-C4B	2.06	1.48	1.42
22	C	505	CLA	C1D-ND	2.06	1.40	1.37
22	C	511	CLA	CMB-C2B	-2.06	1.46	1.50
22	B	608	CLA	C3B-C4B	2.06	1.48	1.42
27	c	522	LMG	C1-C2	2.06	1.58	1.52
22	c	502	CLA	C3B-C4B	2.05	1.48	1.42
27	c	520	LMG	O2-C2	-2.05	1.37	1.43
27	A	411	LMG	O7-C8	-2.05	1.41	1.46
22	d	401	CLA	CMD-C2D	-2.05	1.46	1.50
22	b	609	CLA	O2D-CGD	2.05	1.38	1.33
33	j	101	STE	C2-C1	2.05	1.55	1.50
22	d	403	CLA	CHC-C4B	-2.05	1.34	1.39
22	C	503	CLA	C3B-C4B	2.05	1.48	1.42
22	c	502	CLA	CMB-C2B	-2.04	1.46	1.50
22	C	506	CLA	C1B-C2B	2.04	1.47	1.43
30	A	415	DGD	C3D-C2D	2.04	1.57	1.52
27	C	520	LMG	C4-C5	2.04	1.57	1.53
23	A	405	PHO	C1C-NC	-2.04	1.31	1.37
22	b	606	CLA	C3D-C4D	2.04	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	D	404	CLA	C1C-NC	-2.04	1.34	1.37
30	c	518	DGD	O4E-C4E	-2.04	1.37	1.43
22	b	606	CLA	CMB-C2B	-2.04	1.46	1.50
30	c	518	DGD	O3D-C3D	-2.03	1.37	1.43
22	c	511	CLA	C1D-C2D	2.03	1.49	1.45
24	c	514	BCR	C38-C26	-2.03	1.47	1.50
22	C	509	CLA	CMC-C2C	-2.03	1.46	1.50
22	B	604	CLA	MG-NB	2.03	2.09	2.05
22	C	510	CLA	CMB-C2B	-2.03	1.46	1.50
22	b	616	CLA	CHC-C4B	-2.02	1.34	1.39
22	B	605	CLA	CMC-C2C	-2.02	1.46	1.50
35	F	101	HEC	CMC-C2C	2.02	1.54	1.50
30	C	518	DGD	O6E-C5E	-2.02	1.39	1.44
24	b	618	BCR	C27-C26	-2.02	1.47	1.51
22	b	607	CLA	CHC-C1C	2.02	1.42	1.38
29	B	623	SQD	O4-C4	-2.02	1.38	1.43
22	B	614	CLA	CAA-C2A	-2.02	1.50	1.54
22	c	503	CLA	CHC-C1C	2.02	1.42	1.38
22	C	507	CLA	C3B-C4B	2.01	1.48	1.42
22	a	402	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	501	CLA	C4B-NB	2.01	1.40	1.37
24	c	515	BCR	C38-C26	-2.01	1.47	1.50
33	d	412	STE	C2-C1	2.01	1.55	1.50
22	c	513	CLA	CMB-C2B	-2.01	1.46	1.50
22	c	512	CLA	MG-NC	2.00	2.11	2.06
22	B	603	CLA	CMD-C2D	-2.00	1.46	1.50
22	C	506	CLA	CMB-C2B	-2.00	1.46	1.50
22	c	511	CLA	CMB-C2B	-2.00	1.46	1.50
26	D	406	PL9	C36-C37	-2.00	1.47	1.53
23	d	402	PHO	C4D-ND	-2.00	1.35	1.38

All (1257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	503	CLA	C4A-NA-C1A	10.48	111.46	106.68
22	B	604	CLA	C4A-NA-C1A	9.39	110.97	106.68
29	D	408	SQD	O6-C1-C2	8.87	121.75	108.27
22	B	611	CLA	C4A-NA-C1A	8.87	110.72	106.68
29	a	411	SQD	O6-C1-C2	8.84	121.69	108.27
22	C	507	CLA	C4A-NA-C1A	8.82	110.70	106.68
22	B	601	CLA	C4A-NA-C1A	8.77	110.68	106.68
22	b	615	CLA	C4A-NA-C1A	8.40	110.51	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	511	CLA	C4A-NA-C1A	8.04	110.35	106.68
22	b	606	CLA	C4A-NA-C1A	7.90	110.28	106.68
22	B	612	CLA	C4A-NA-C1A	7.79	110.23	106.68
22	C	513	CLA	C4A-NA-C1A	7.53	110.11	106.68
22	B	603	CLA	C4A-NA-C1A	7.49	110.09	106.68
22	c	509	CLA	C4A-NA-C1A	7.47	110.09	106.68
29	b	620	SQD	O6-C1-C2	7.34	119.42	108.27
22	b	609	CLA	C4A-NA-C1A	7.33	110.02	106.68
22	B	616	CLA	C4A-NA-C1A	7.23	109.98	106.68
22	B	609	CLA	C4A-NA-C1A	7.21	109.97	106.68
22	C	509	CLA	C4A-NA-C1A	7.11	109.92	106.68
22	b	601	CLA	C4A-NA-C1A	7.06	109.90	106.68
29	B	623	SQD	O6-C1-C2	6.98	118.87	108.27
23	A	404	PHO	C4D-CHA-CBD	-6.95	105.12	108.45
35	f	101	HEC	CAB-C3B-C4B	6.78	133.61	124.79
22	d	403	CLA	C4A-NA-C1A	6.62	109.70	106.68
22	b	614	CLA	C4A-NA-C1A	6.61	109.70	106.68
29	A	413	SQD	O6-C1-C2	6.59	118.28	108.27
22	B	606	CLA	C4A-NA-C1A	6.53	109.66	106.68
29	f	102	SQD	O6-C1-C2	6.53	118.19	108.27
22	b	604	CLA	C4A-NA-C1A	6.46	109.63	106.68
22	C	508	CLA	C4A-NA-C1A	6.43	109.61	106.68
22	d	404	CLA	C4A-NA-C1A	6.34	109.57	106.68
26	d	407	PL9	C7-C3-C4	6.33	122.12	116.91
22	c	510	CLA	C4A-NA-C1A	6.33	109.57	106.68
22	a	402	CLA	C4A-NA-C1A	6.31	109.56	106.68
22	b	616	CLA	C4A-NA-C1A	6.28	109.55	106.68
29	f	102	SQD	O7-S-C6	6.21	116.02	106.76
22	c	511	CLA	C4A-NA-C1A	6.20	109.51	106.68
29	A	413	SQD	O7-S-C6	5.96	115.66	106.76
26	a	409	PL9	C7-C3-C4	5.86	121.73	116.91
22	D	403	CLA	C4A-NA-C1A	5.85	109.35	106.68
22	C	505	CLA	C4A-NA-C1A	5.83	109.34	106.68
22	c	502	CLA	C4A-NA-C1A	5.82	109.33	106.68
29	a	412	SQD	O47-C7-C8	5.67	123.75	111.48
23	d	402	PHO	O1D-CGD-CBD	5.64	133.28	124.72
22	d	401	CLA	C4A-NA-C1A	5.62	109.24	106.68
22	c	501	CLA	O2D-CGD-O1D	-5.61	112.94	123.85
22	C	502	CLA	C4A-NA-C1A	5.57	109.22	106.68
22	c	506	CLA	C4A-NA-C1A	5.52	109.20	106.68
22	c	508	CLA	C4A-NA-C1A	5.51	109.19	106.68
22	B	615	CLA	C4A-NA-C1A	5.50	109.19	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	501	CLA	C4A-NA-C1A	5.44	109.16	106.68
29	A	414	SQD	C45-O47-C7	5.42	125.60	117.78
22	C	501	CLA	O2D-CGD-O1D	-5.31	113.52	123.85
23	a	403	PHO	C4D-CHA-CBD	-5.21	105.95	108.45
22	b	606	CLA	O2D-CGD-O1D	-5.20	113.72	123.85
29	a	412	SQD	O48-C23-O10	-5.18	110.67	123.63
22	c	505	CLA	C4A-NA-C1A	5.16	109.03	106.68
22	B	605	CLA	C4A-NA-C1A	5.08	109.00	106.68
29	A	413	SQD	O9-S-O7	-5.06	97.37	113.82
22	A	403	CLA	C4A-NA-C1A	5.06	108.99	106.68
22	D	404	CLA	C4A-NA-C1A	5.05	108.98	106.68
35	f	101	HEC	CAB-C3B-C2B	-5.04	118.30	127.56
26	d	407	PL9	C40-C39-C41	5.04	123.97	115.23
22	B	610	CLA	O2D-CGD-O1D	-4.99	114.14	123.85
22	C	510	CLA	O2D-CGD-O1D	-4.93	114.25	123.85
22	B	611	CLA	O2D-CGD-O1D	-4.90	114.30	123.85
22	C	501	CLA	C4A-NA-C1A	4.87	108.90	106.68
22	b	610	CLA	C4A-NA-C1A	4.82	108.88	106.68
29	A	413	SQD	C1-C2-C3	-4.80	99.91	110.01
22	b	602	CLA	C4A-NA-C1A	4.80	108.87	106.68
35	f	101	HEC	CHB-C1B-NB	4.78	129.57	124.42
28	A	412	LHG	O4-P-O5	4.77	134.64	112.44
22	B	607	CLA	C4A-NA-C1A	4.77	108.85	106.68
22	C	501	CLA	O2D-CGD-CBD	4.75	119.53	111.23
27	b	623	LMG	O1-C1-C2	-4.74	101.07	108.27
22	c	504	CLA	C4A-NA-C1A	4.70	108.82	106.68
23	d	402	PHO	C4D-CHA-CBD	-4.68	106.21	108.45
29	f	102	SQD	O9-S-O7	-4.68	98.62	113.82
34	D	401	BCT	O2-C-O1	4.66	131.60	119.68
22	D	402	CLA	C3B-C4B-NB	-4.60	106.43	110.53
29	A	413	SQD	C1-O5-C5	-4.59	104.75	113.72
35	f	101	HEC	CBD-CAD-C3D	-4.53	100.00	112.53
22	c	512	CLA	C3B-C4B-NB	-4.50	106.51	110.53
22	b	605	CLA	O2D-CGD-O1D	-4.50	115.09	123.85
22	b	611	CLA	O2D-CGD-CBD	4.50	119.09	111.23
22	c	512	CLA	C4A-NA-C1A	4.49	108.73	106.68
22	C	510	CLA	O2D-CGD-CBD	4.47	119.05	111.23
22	a	404	CLA	C4A-NA-C1A	4.47	108.72	106.68
22	C	512	CLA	C4A-NA-C1A	4.46	108.72	106.68
27	b	623	LMG	C1-O6-C5	-4.44	105.04	113.72
24	Y	101	BCR	C39-C30-C25	-4.44	103.28	110.24
22	c	513	CLA	C4A-NA-C1A	4.42	108.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	409	PL9	C7-C3-C2	-4.41	118.19	123.39
22	b	610	CLA	O2D-CGD-O1D	-4.37	115.34	123.85
28	E	101	LHG	O4-P-O5	4.37	132.78	112.44
35	F	101	HEC	CBD-CAD-C3D	-4.37	100.46	112.53
22	c	507	CLA	C4A-NA-C1A	4.36	108.67	106.68
22	a	402	CLA	C3B-C4B-NB	-4.36	106.64	110.53
22	B	608	CLA	O2D-CGD-O1D	-4.36	115.37	123.85
26	d	407	PL9	C7-C3-C2	-4.34	118.27	123.39
29	D	408	SQD	C1-O5-C5	-4.34	105.25	113.72
23	d	402	PHO	C2B-C1B-NB	-4.33	106.30	109.43
22	d	404	CLA	CMB-C2B-C1B	-4.31	118.86	125.42
34	a	408	BCT	O2-C-O1	4.31	130.70	119.68
29	B	623	SQD	O48-C23-C24	4.31	124.96	111.83
24	b	617	BCR	C2-C1-C6	4.29	116.67	110.44
28	e	101	LHG	O4-P-O5	4.27	132.32	112.44
29	A	413	SQD	O47-C7-C8	4.27	120.72	111.48
22	B	614	CLA	C3B-C4B-NB	-4.26	106.73	110.53
29	B	623	SQD	C1-O5-C5	-4.24	105.44	113.72
22	b	612	CLA	CHB-C4A-NA	4.22	130.49	124.40
28	a	410	LHG	O8-C23-O10	-4.21	113.09	123.63
22	b	607	CLA	C4A-NA-C1A	4.21	108.60	106.68
22	C	510	CLA	C4A-NA-C1A	4.20	108.59	106.68
28	a	410	LHG	O4-P-O5	4.19	131.96	112.44
22	C	508	CLA	CHD-C1D-ND	-4.19	118.90	124.80
28	d	409	LHG	O4-P-O5	4.19	131.94	112.44
28	B	622	LHG	O4-P-O5	4.17	131.85	112.44
28	d	408	LHG	O4-P-O5	4.15	131.76	112.44
22	C	510	CLA	C3B-C4B-NB	-4.15	106.83	110.53
22	D	402	CLA	C4A-NA-C1A	4.14	108.57	106.68
23	a	403	PHO	C2B-C1B-NB	-4.13	106.44	109.43
35	V	201	HEC	C1D-ND-C4D	4.12	110.09	105.21
28	D	409	LHG	O4-P-O5	4.12	131.60	112.44
22	b	602	CLA	O2D-CGD-CBD	4.11	118.42	111.23
22	b	602	CLA	O2D-CGD-O1D	-4.11	115.85	123.85
22	B	602	CLA	O2D-CGD-CBD	4.10	118.40	111.23
30	C	519	DGD	O3G-C3G-C2G	-4.06	100.93	110.82
22	b	603	CLA	O2D-CGD-O1D	-4.06	115.94	123.85
22	d	401	CLA	CHB-C4A-NA	4.05	130.24	124.40
27	M	101	LMG	O1-C1-C2	-4.04	102.14	108.27
22	c	503	CLA	C4A-NA-C1A	4.04	108.52	106.68
22	D	403	CLA	C3B-C4B-NB	-4.01	106.95	110.53
27	m	101	LMG	O7-C10-O9	-3.99	114.38	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	CHB-C4A-NA	3.98	130.15	124.40
30	C	519	DGD	O6D-C1D-O3G	-3.98	100.64	110.04
22	b	605	CLA	O1D-CGD-CBD	3.97	132.35	124.52
22	b	608	CLA	C3B-C4B-NB	-3.96	107.00	110.53
30	H	102	DGD	O3G-C3G-C2G	-3.95	101.22	110.82
29	D	408	SQD	O8-S-C6	3.95	113.59	105.97
22	A	406	CLA	O2D-CGD-O1D	-3.93	116.21	123.85
26	a	409	PL9	C35-C34-C36	3.92	122.03	115.23
22	B	614	CLA	O2D-CGD-O1D	-3.90	116.26	123.85
28	B	621	LHG	O4-P-O5	3.89	130.56	112.44
35	F	101	HEC	CMC-C2C-C1C	-3.88	119.50	125.42
28	l	101	LHG	O4-P-O5	3.88	130.51	112.44
22	B	607	CLA	C3B-C4B-NB	-3.88	107.07	110.53
22	B	611	CLA	O2D-CGD-CBD	3.87	118.00	111.23
22	b	613	CLA	C1-C2-C3	-3.87	119.86	126.20
24	B	619	BCR	C2-C1-C6	3.87	116.06	110.44
35	v	201	HEC	CHB-C1B-NB	3.85	128.57	124.42
22	c	509	CLA	O2A-CGA-O1A	-3.83	114.04	123.63
30	c	519	DGD	C3D-C4D-C5D	-3.82	103.30	110.23
22	C	503	CLA	C7-C6-C5	-3.82	103.08	113.26
23	d	402	PHO	C1-C2-C3	-3.81	119.95	126.20
22	C	506	CLA	C4A-NA-C1A	3.81	108.42	106.68
22	C	508	CLA	O2D-CGD-O1D	-3.80	116.46	123.85
29	f	102	SQD	C1-C2-C3	-3.79	102.03	110.01
35	v	201	HEC	C1D-ND-C4D	3.79	109.70	105.21
26	D	406	PL9	C30-C29-C31	-3.79	108.66	115.23
35	F	101	HEC	C1D-ND-C4D	3.77	109.67	105.21
22	C	513	CLA	O2D-CGD-O1D	-3.77	116.51	123.85
24	A	407	BCR	C27-C26-C25	3.76	127.79	122.70
22	b	613	CLA	CHB-C4A-NA	3.76	129.82	124.40
23	A	405	PHO	C2B-C1B-NB	-3.76	106.71	109.43
28	a	410	LHG	O8-C23-C24	3.76	123.29	111.83
26	D	406	PL9	C7-C3-C4	3.75	120.00	116.91
22	c	512	CLA	C1-C2-C3	-3.74	120.06	126.20
22	B	603	CLA	O2D-CGD-O1D	-3.74	116.57	123.85
29	A	414	SQD	O48-C23-C24	3.72	123.19	111.83
23	A	405	PHO	C3B-C4B-NB	-3.72	105.04	107.46
22	c	510	CLA	O2D-CGD-O1D	-3.72	116.61	123.85
24	T	101	BCR	C35-C13-C14	-3.72	116.80	122.82
29	b	620	SQD	O5-C5-C4	3.72	116.39	109.70
23	A	405	PHO	O1D-CGD-CBD	3.71	130.35	124.72
22	B	610	CLA	C4A-NA-C1A	3.70	108.37	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	605	CLA	C4-C3-C5	3.69	121.64	115.23
22	C	502	CLA	C3B-C4B-NB	-3.69	107.23	110.53
22	C	512	CLA	C1-C2-C3	-3.69	120.16	126.20
24	b	619	BCR	C29-C30-C25	3.68	115.79	110.44
30	C	517	DGD	C3D-C4D-C5D	-3.68	103.56	110.23
26	D	406	PL9	C27-C28-C29	-3.68	119.21	127.62
22	D	402	CLA	CED-O2D-CGD	3.67	124.25	115.92
27	a	416	LMG	C1-C2-C3	-3.66	102.31	110.01
22	c	504	CLA	CHB-C4A-NA	3.66	129.68	124.40
29	a	411	SQD	O47-C7-C8	3.66	119.40	111.48
29	b	620	SQD	O7-S-C6	3.65	112.21	106.76
22	C	503	CLA	O1D-CGD-CBD	3.65	131.72	124.52
22	B	603	CLA	C4-C3-C5	3.63	121.52	115.23
29	D	408	SQD	C1-C2-C3	-3.62	102.40	110.01
22	C	506	CLA	O2D-CGD-O1D	-3.60	116.83	123.85
26	A	410	PL9	C7-C3-C4	3.58	119.86	116.91
23	a	403	PHO	OBD-CAD-CBD	-3.58	120.57	125.82
22	C	507	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
22	B	604	CLA	C3B-C4B-NB	-3.57	107.34	110.53
22	C	508	CLA	C3B-C4B-NB	-3.57	107.34	110.53
26	d	407	PL9	C37-C38-C39	-3.57	119.46	127.62
22	b	615	CLA	C11-C10-C8	-3.57	104.11	115.97
22	B	604	CLA	CHB-C4A-NA	3.56	129.54	124.40
27	d	410	LMG	O1-C1-C2	-3.56	102.87	108.27
22	b	602	CLA	CHB-C4A-NA	3.56	129.53	124.40
22	C	501	CLA	C3B-C4B-NB	-3.55	107.36	110.53
22	C	509	CLA	C3B-C4B-NB	-3.55	107.36	110.53
23	A	405	PHO	O2D-CGD-O1D	-3.54	116.96	123.85
22	b	610	CLA	O1D-CGD-CBD	3.54	131.49	124.52
26	D	406	PL9	C42-C43-C44	-3.53	119.54	127.62
22	C	502	CLA	C4D-CHA-C1A	3.52	125.44	121.24
22	d	403	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
22	c	513	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
22	B	603	CLA	C5-C3-C2	-3.51	113.28	121.17
22	c	501	CLA	O2D-CGD-CBD	3.51	117.37	111.23
22	d	403	CLA	O2D-CGD-CBD	3.51	117.37	111.23
22	c	511	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
22	c	508	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
29	B	623	SQD	O7-S-C6	3.50	111.97	106.76
24	C	514	BCR	C2-C1-C6	3.49	115.51	110.44
24	c	515	BCR	C27-C26-C25	3.49	127.42	122.70
22	B	601	CLA	O2D-CGD-O1D	-3.49	117.06	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	614	CLA	O2A-CGA-O1A	-3.48	114.92	123.63
30	c	519	DGD	O3G-C3G-C2G	-3.48	102.35	110.82
26	D	406	PL9	C35-C34-C36	3.48	121.27	115.23
26	D	406	PL9	C20-C19-C21	3.47	121.25	115.23
30	C	518	DGD	O3G-C3G-C2G	-3.47	102.38	110.82
26	D	406	PL9	C36-C34-C33	-3.47	113.38	121.17
22	c	506	CLA	CHB-C4A-NA	3.46	129.39	124.40
22	B	616	CLA	CMB-C2B-C1B	-3.46	120.16	125.42
24	c	514	BCR	C33-C5-C6	-3.45	120.72	124.48
22	b	603	CLA	CMB-C2B-C1B	-3.45	120.16	125.42
29	a	411	SQD	C1-O5-C5	-3.44	107.00	113.72
22	b	615	CLA	O2D-CGD-CBD	3.43	117.23	111.23
22	A	403	CLA	CED-O2D-CGD	-3.43	108.14	115.92
29	b	620	SQD	C3-C4-C5	3.43	116.44	110.23
24	b	617	BCR	C27-C26-C25	3.42	127.33	122.70
22	b	602	CLA	C3B-C4B-NB	-3.42	107.48	110.53
22	c	503	CLA	C7-C6-C5	-3.41	104.16	113.26
30	C	517	DGD	O3G-C3G-C2G	-3.41	102.52	110.82
22	b	603	CLA	O2D-CGD-CBD	3.41	117.19	111.23
22	B	613	CLA	C1-C2-C3	-3.40	120.63	126.20
29	a	411	SQD	C1-C2-C3	-3.40	102.86	110.01
26	A	410	PL9	O1-C4-C3	-3.39	117.15	120.73
30	A	415	DGD	C4E-C3E-C2E	-3.38	104.89	110.83
29	b	620	SQD	C1-C2-C3	-3.37	102.92	110.01
22	c	512	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
22	b	610	CLA	O2A-CGA-O1A	-3.36	115.21	123.63
22	b	611	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
29	D	408	SQD	O9-S-C6	3.36	111.78	106.76
22	b	616	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
22	C	504	CLA	C3B-C4B-NB	-3.36	107.53	110.53
22	A	406	CLA	O2D-CGD-CBD	3.34	117.08	111.23
24	C	514	BCR	C33-C5-C6	-3.34	120.84	124.48
22	c	508	CLA	CHB-C4A-NA	3.34	129.22	124.40
29	a	411	SQD	O9-S-O7	-3.34	102.97	113.82
29	D	408	SQD	O48-C23-C24	3.33	121.99	111.83
22	B	612	CLA	C3B-C4B-NB	-3.33	107.56	110.53
26	d	407	PL9	C42-C43-C44	-3.32	120.02	127.62
33	t	102	STE	C3-C2-C1	-3.32	105.85	114.51
29	b	620	SQD	O48-C23-C24	3.29	121.87	111.83
23	A	404	PHO	OBD-CAD-CBD	-3.29	121.00	125.82
26	A	410	PL9	C20-C19-C21	3.29	120.93	115.23
22	b	612	CLA	CAC-C3C-C4C	3.29	129.07	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	b	623	LMG	O2-C2-C1	-3.29	102.25	110.08
22	C	503	CLA	C3B-C4B-NB	-3.28	107.60	110.53
22	b	610	CLA	CAC-C3C-C4C	3.28	129.06	124.79
22	A	406	CLA	C4-C3-C5	3.28	120.91	115.23
28	e	101	LHG	O8-C23-C24	3.27	121.82	111.83
22	B	606	CLA	C3B-C4B-NB	-3.27	107.61	110.53
27	M	101	LMG	C1-O6-C5	-3.27	107.33	113.72
35	f	101	HEC	C1D-ND-C4D	3.26	109.07	105.21
27	A	411	LMG	O6-C1-O1	-3.26	102.34	110.04
22	c	502	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
22	C	504	CLA	O2A-CGA-O1A	-3.25	115.51	123.63
24	c	516	BCR	C29-C30-C25	3.23	115.14	110.44
22	b	603	CLA	CHB-C1B-NB	3.23	128.90	124.05
22	b	604	CLA	O2D-CGD-O1D	-3.23	117.57	123.85
22	b	606	CLA	O2D-CGD-CBD	3.22	116.87	111.23
24	A	407	BCR	C2-C1-C6	3.21	115.11	110.44
22	b	605	CLA	CHB-C1B-NB	3.21	128.86	124.05
30	C	518	DGD	O6D-C1D-O3G	-3.20	102.47	110.04
22	B	602	CLA	C3B-C4B-NB	-3.20	107.67	110.53
29	b	620	SQD	O9-S-O7	-3.20	103.42	113.82
30	h	101	DGD	O3G-C3G-C2G	-3.20	103.04	110.82
24	H	101	BCR	C16-C15-C14	-3.20	116.98	123.52
22	b	611	CLA	CHD-C1D-ND	-3.19	120.31	124.80
24	B	617	BCR	C2-C1-C6	3.19	115.08	110.44
22	c	505	CLA	C3B-C4B-NB	-3.19	107.68	110.53
22	B	602	CLA	C4A-NA-C1A	3.19	108.13	106.68
24	t	101	BCR	C7-C8-C9	-3.19	121.52	126.23
24	C	515	BCR	C15-C16-C17	-3.19	117.00	123.52
24	C	514	BCR	C11-C10-C9	-3.18	122.82	127.28
26	A	410	PL9	C22-C23-C24	-3.17	120.36	127.62
22	c	503	CLA	C3B-C4B-NB	-3.17	107.70	110.53
24	c	515	BCR	C33-C5-C6	-3.16	121.03	124.48
30	H	102	DGD	C1E-O6E-C5E	3.15	119.88	113.72
22	C	504	CLA	C4-C3-C5	3.15	120.70	115.23
30	C	517	DGD	O6D-C1D-O3G	-3.15	102.61	110.04
24	T	101	BCR	C27-C26-C25	3.14	126.95	122.70
24	d	406	BCR	C38-C26-C25	-3.14	121.06	124.48
22	C	506	CLA	C3B-C4B-NB	-3.13	107.73	110.53
24	Y	101	BCR	C27-C26-C25	3.13	126.94	122.70
23	d	402	PHO	O2D-CGD-O1D	-3.13	117.76	123.85
29	b	620	SQD	O9-S-C6	3.13	111.43	106.76
22	c	508	CLA	O2D-CGD-CBD	3.11	116.67	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	504	CLA	C4A-NA-C1A	3.11	108.10	106.68
22	B	616	CLA	CMB-C2B-C3B	3.11	133.86	126.55
22	D	404	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
24	Y	101	BCR	C30-C25-C26	-3.11	118.39	122.64
22	b	601	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
24	T	101	BCR	C7-C8-C9	-3.10	121.64	126.23
23	d	402	PHO	C3B-C4B-NB	-3.10	105.44	107.46
22	d	401	CLA	CAC-C3C-C4C	3.10	128.82	124.79
33	D	412	STE	C3-C2-C1	-3.10	106.43	114.51
22	a	402	CLA	CMB-C2B-C1B	-3.10	120.71	125.42
22	c	506	CLA	CBC-CAC-C3C	-3.08	104.06	112.42
22	C	511	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
22	b	612	CLA	CHD-C1D-ND	-3.08	120.47	124.80
30	c	518	DGD	O3G-C1D-C2D	-3.08	103.60	108.27
22	B	610	CLA	O2A-CGA-O1A	-3.08	115.93	123.63
27	d	410	LMG	O2-C2-C1	-3.07	102.75	110.08
22	C	513	CLA	C3B-C4B-NB	-3.07	107.79	110.53
22	A	403	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
22	B	602	CLA	O2D-CGD-O1D	-3.07	117.88	123.85
22	B	605	CLA	C3B-C4B-NB	-3.07	107.79	110.53
30	c	517	DGD	O3G-C3G-C2G	-3.07	103.36	110.82
22	D	402	CLA	CMD-C2D-C1D	-3.06	119.34	124.73
24	d	406	BCR	C2-C1-C6	3.06	114.88	110.44
35	V	201	HEC	CBD-CAD-C3D	-3.06	104.08	112.53
22	B	603	CLA	O2A-CGA-O1A	-3.05	115.99	123.63
24	b	618	BCR	C15-C14-C13	-3.05	123.00	127.28
28	d	409	LHG	C26-C25-C24	3.05	124.33	113.13
23	A	404	PHO	CMB-C2B-C3B	3.05	130.77	124.68
22	C	503	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
22	b	615	CLA	C3B-C4B-NB	-3.04	107.81	110.53
24	b	617	BCR	C29-C30-C25	3.04	114.86	110.44
24	H	101	BCR	C29-C30-C25	3.04	114.85	110.44
22	B	611	CLA	C11-C12-C13	-3.03	105.88	115.97
27	m	101	LMG	O1-C7-C8	-3.03	103.44	110.82
22	B	614	CLA	C4A-NA-C1A	3.02	108.06	106.68
29	A	413	SQD	O47-C7-O49	-3.02	116.64	123.70
22	A	402	CLA	CHB-C4A-NA	3.02	128.76	124.40
22	d	404	CLA	O2D-CGD-CBD	3.02	116.51	111.23
22	a	404	CLA	C1D-ND-C4D	-3.02	104.19	106.31
29	B	623	SQD	O8-S-C6	3.02	111.80	105.97
22	c	507	CLA	CHD-C1D-ND	-3.02	120.55	124.80
27	C	520	LMG	O6-C1-O1	-3.02	102.91	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	605	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
27	m	101	LMG	C1-O6-C5	-3.00	107.85	113.72
27	m	101	LMG	O3-C3-C2	-3.00	103.30	110.38
27	a	416	LMG	O7-C10-O9	-3.00	116.70	123.70
22	c	511	CLA	C3B-C4B-NB	-3.00	107.86	110.53
24	c	515	BCR	C35-C13-C14	-2.99	117.97	122.82
29	B	623	SQD	C3-C4-C5	2.99	115.66	110.23
22	C	506	CLA	O1D-CGD-CBD	2.99	130.42	124.52
22	B	614	CLA	O1D-CGD-CBD	2.99	130.41	124.52
28	B	622	LHG	O8-C23-C24	2.99	120.95	111.83
22	d	401	CLA	C1D-ND-C4D	2.99	108.41	106.31
22	c	502	CLA	C3B-C4B-NB	-2.99	107.86	110.53
33	d	411	STE	O2-C1-C2	2.99	123.44	114.00
22	c	501	CLA	CED-O2D-CGD	-2.99	109.14	115.92
27	a	416	LMG	C9-C8-C7	-2.98	104.85	111.78
33	C	523	STE	C3-C2-C1	-2.97	106.75	114.51
30	H	102	DGD	C3E-C4E-C5E	-2.97	104.85	110.23
23	A	404	PHO	O2D-CGD-CBD	2.97	114.21	110.95
27	b	623	LMG	O6-C5-C6	2.96	113.77	106.44
22	B	612	CLA	CHD-C1D-ND	-2.96	120.64	124.80
22	b	605	CLA	C3B-C4B-NB	-2.95	107.89	110.53
26	a	409	PL9	C36-C34-C33	-2.95	114.54	121.17
29	A	414	SQD	O47-C45-C46	2.95	112.99	106.21
22	d	404	CLA	CHB-C4A-NA	2.94	128.65	124.40
26	A	410	PL9	C36-C34-C33	-2.94	114.57	121.17
28	B	622	LHG	O8-C23-O10	-2.94	116.28	123.63
24	a	405	BCR	C29-C30-C25	2.94	114.71	110.44
33	a	414	STE	C3-C2-C1	-2.94	106.84	114.51
27	D	407	LMG	O6-C1-O1	-2.93	103.11	110.04
22	C	513	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
22	B	611	CLA	CHB-C4A-NA	2.93	128.62	124.40
28	a	410	LHG	C11-C10-C9	-2.92	99.59	114.37
22	b	615	CLA	CHB-C4A-NA	2.92	128.61	124.40
22	C	509	CLA	CED-O2D-CGD	2.91	122.53	115.92
29	a	411	SQD	O9-S-C6	2.91	111.11	106.76
22	B	606	CLA	CHA-C1A-NA	-2.91	119.80	126.39
22	B	612	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
22	d	401	CLA	C2D-C1D-ND	-2.91	107.25	110.13
22	a	404	CLA	O2D-CGD-CBD	2.91	116.31	111.23
22	b	607	CLA	C1-O2A-CGA	2.91	123.68	116.65
22	B	615	CLA	CHC-C4B-NB	2.90	128.41	124.05
24	k	101	BCR	C33-C5-C6	-2.90	121.32	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	616	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
30	H	102	DGD	CDB-CCB-CBB	-2.90	99.73	114.37
27	m	101	LMG	C38-C37-C36	-2.89	99.74	114.37
30	c	518	DGD	O3G-C3G-C2G	-2.89	103.78	110.82
29	B	623	SQD	O5-C5-C4	2.89	114.91	109.70
22	B	612	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
24	H	101	BCR	C2-C1-C6	2.89	114.64	110.44
22	b	611	CLA	C4A-NA-C1A	2.89	108.00	106.68
22	A	402	CLA	C3B-C4B-NB	-2.89	107.95	110.53
22	B	603	CLA	CHD-C4C-NC	2.88	128.70	124.23
24	B	618	BCR	C29-C30-C25	2.88	114.62	110.44
24	d	406	BCR	C3-C4-C5	-2.88	108.93	114.06
22	B	606	CLA	C1-C2-C3	-2.88	121.48	126.20
23	A	404	PHO	C2D-C1D-ND	2.88	111.51	109.43
22	b	604	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
22	c	505	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
22	b	614	CLA	C3B-C4B-NB	-2.86	107.98	110.53
22	B	615	CLA	CAC-C3C-C4C	2.86	128.51	124.79
24	B	619	BCR	C3-C4-C5	-2.86	108.96	114.06
22	b	616	CLA	CHB-C4A-NA	2.86	128.52	124.40
24	C	514	BCR	C27-C26-C25	2.86	126.56	122.70
24	H	101	BCR	C27-C26-C25	2.86	126.56	122.70
22	C	509	CLA	CHB-C4A-NA	2.84	128.50	124.40
28	l	101	LHG	C20-C19-C18	-2.84	100.00	114.37
24	D	405	BCR	C24-C23-C22	-2.84	122.03	126.23
22	b	609	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
22	C	504	CLA	CHD-C1D-ND	-2.84	120.81	124.80
27	M	101	LMG	O3-C3-C2	-2.84	103.69	110.38
24	T	101	BCR	C38-C26-C27	-2.84	107.55	113.60
27	c	523	LMG	O6-C1-O1	-2.83	103.35	110.04
28	E	101	LHG	O8-C23-C24	2.83	120.46	111.83
26	d	407	PL9	C22-C23-C24	-2.83	121.15	127.62
23	A	404	PHO	C2B-C1B-NB	-2.83	107.39	109.43
22	b	613	CLA	C7-C6-C5	-2.83	105.73	113.26
22	C	507	CLA	O2D-CGD-CBD	2.82	116.17	111.23
22	c	511	CLA	O2D-CGD-CBD	2.82	116.16	111.23
22	C	505	CLA	CMB-C2B-C1B	-2.82	121.12	125.42
24	B	619	BCR	C29-C30-C25	2.82	114.53	110.44
24	b	619	BCR	C27-C26-C25	2.81	126.50	122.70
22	B	605	CLA	CHB-C4A-NA	2.81	128.46	124.40
22	d	405	CLA	C1-C2-C3	-2.81	121.59	126.20
30	h	101	DGD	O6E-C5E-C4E	2.81	114.76	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	C4-C3-C5	2.81	120.10	115.23
22	b	602	CLA	CHC-C1C-NC	2.80	128.53	124.31
22	C	512	CLA	CHB-C4A-NA	2.80	128.44	124.40
35	F	101	HEC	CAB-C3B-C4B	-2.80	121.15	124.79
22	D	402	CLA	CMD-C2D-C3D	2.80	134.10	127.69
22	b	614	CLA	CAC-C3C-C4C	2.80	128.43	124.79
35	F	101	HEC	CHB-C1B-NB	2.80	127.43	124.42
22	d	401	CLA	CMA-C3A-C4A	-2.79	104.26	111.77
22	B	610	CLA	O2D-CGD-CBD	2.79	116.11	111.23
29	B	623	SQD	O48-C23-O10	-2.79	116.64	123.63
22	B	609	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
22	a	404	CLA	CHB-C4A-NA	2.78	128.42	124.40
22	C	509	CLA	C1-C2-C3	-2.78	121.64	126.20
22	b	610	CLA	C2A-C1A-CHA	2.78	128.69	123.87
22	d	401	CLA	CHC-C1C-NC	2.78	128.50	124.31
22	B	606	CLA	C4-C3-C5	2.78	120.05	115.23
27	b	623	LMG	C3-C4-C5	-2.78	105.19	110.23
30	c	517	DGD	C8B-C7B-C6B	-2.78	100.33	114.37
22	C	507	CLA	C3B-C4B-NB	-2.77	108.05	110.53
22	C	513	CLA	CHB-C4A-NA	2.77	128.40	124.40
24	B	618	BCR	C35-C13-C14	-2.77	118.33	122.82
27	c	522	LMG	O3-C3-C2	-2.76	103.86	110.38
27	a	416	LMG	C1-O6-C5	-2.76	108.32	113.72
24	C	514	BCR	C15-C16-C17	-2.76	117.87	123.52
22	d	404	CLA	C3B-C4B-NB	-2.76	108.07	110.53
28	l	101	LHG	C11-C10-C9	-2.76	100.43	114.37
27	A	411	LMG	O3-C3-C2	-2.76	103.88	110.38
30	C	517	DGD	O5D-C6D-C5D	-2.76	103.21	109.42
29	a	411	SQD	O48-C23-C24	2.75	120.23	111.83
26	a	409	PL9	C37-C38-C39	-2.75	121.32	127.62
23	a	403	PHO	OBD-CAD-C3D	2.75	132.18	127.89
27	M	101	LMG	C31-C30-C29	-2.75	103.03	113.13
22	b	612	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
22	C	505	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
24	x	101	BCR	C27-C26-C25	2.74	126.41	122.70
22	b	611	CLA	CHD-C1D-C2D	2.74	131.18	125.49
22	b	611	CLA	C3B-C4B-NB	-2.74	108.08	110.53
29	b	620	SQD	O2-C2-C1	2.74	116.60	110.08
23	d	402	PHO	C3D-C4D-ND	2.73	111.21	107.71
33	m	102	STE	O2-C1-C2	2.73	122.63	114.00
22	b	610	CLA	C1-C2-C3	-2.73	121.72	126.20
29	B	623	SQD	O9-S-O7	-2.73	104.95	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	v	201	HEC	CHA-C4D-ND	2.73	127.36	124.42
26	D	406	PL9	C8-C7-C3	2.72	119.07	112.03
30	A	415	DGD	CDB-CCB-CBB	-2.72	100.59	114.37
26	D	406	PL9	C22-C23-C24	-2.72	121.39	127.62
22	b	602	CLA	C1-C2-C3	-2.72	121.74	126.20
24	D	405	BCR	C3-C4-C5	-2.72	109.20	114.06
29	f	102	SQD	O9-S-C6	2.72	110.81	106.76
22	c	507	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
30	C	518	DGD	O5D-C6D-C5D	-2.71	103.30	109.42
22	c	510	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
22	D	403	CLA	C17-C16-C15	-2.71	101.12	113.28
29	a	412	SQD	O49-C7-C8	-2.71	113.17	123.78
22	B	606	CLA	CGD-CBD-CAD	-2.71	102.07	110.85
22	b	609	CLA	C3B-C4B-NB	-2.71	108.11	110.53
22	b	608	CLA	CMB-C2B-C1B	-2.71	121.29	125.42
22	A	402	CLA	CHC-C4B-NB	2.71	128.11	124.05
24	c	515	BCR	C2-C1-C6	2.71	114.37	110.44
26	D	406	PL9	C40-C39-C38	-2.71	116.68	123.63
22	b	605	CLA	CMB-C2B-C1B	-2.71	121.30	125.42
22	B	612	CLA	C11-C12-C13	-2.70	106.98	115.97
27	c	520	LMG	C1-O6-C5	-2.70	108.44	113.72
22	c	507	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
24	b	619	BCR	C7-C8-C9	-2.70	122.24	126.23
22	a	404	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
26	D	406	PL9	C37-C38-C39	-2.70	121.44	127.62
24	c	516	BCR	C27-C26-C25	2.70	126.35	122.70
22	B	601	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
33	d	412	STE	O2-C1-O1	-2.70	116.40	123.33
22	A	402	CLA	CMB-C2B-C3B	2.70	132.89	126.55
22	c	507	CLA	CHB-C4A-NA	2.69	128.29	124.40
35	F	101	HEC	CBA-CAA-C2A	-2.69	105.08	112.53
22	b	615	CLA	C1-O2A-CGA	2.69	123.16	116.65
22	b	610	CLA	CHB-C4A-NA	2.69	128.28	124.40
30	c	518	DGD	O2D-C2D-C1D	-2.69	103.67	110.08
22	b	605	CLA	C4D-CHA-C1A	2.69	124.45	121.24
30	C	519	DGD	CDB-CCB-CBB	-2.68	100.84	114.37
22	B	613	CLA	CHA-C1A-NA	-2.68	120.33	126.39
22	b	610	CLA	CHA-C1A-NA	-2.67	120.35	126.39
23	a	403	PHO	O2A-CGA-O1A	-2.67	116.96	123.63
30	c	518	DGD	CBB-CAB-C9B	-2.67	100.89	114.37
22	b	615	CLA	C6-C5-C3	-2.67	106.97	113.47
22	B	601	CLA	C3B-C4B-NB	-2.67	108.15	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	m	101	LMG	O6-C1-O1	-2.67	103.74	110.04
24	x	101	BCR	C2-C1-C6	2.67	114.31	110.44
29	a	412	SQD	C46-O48-C23	2.66	126.86	117.12
22	d	404	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
30	C	517	DGD	C6B-C5B-C4B	-2.66	100.90	114.37
22	B	605	CLA	C7-C6-C5	-2.66	106.16	113.26
22	c	507	CLA	CMB-C2B-C3B	2.66	132.81	126.55
26	a	409	PL9	C20-C19-C21	2.66	119.85	115.23
22	C	508	CLA	C4D-C3D-CAD	-2.66	105.22	108.11
26	d	407	PL9	C20-C19-C21	2.66	119.84	115.23
22	A	406	CLA	CAA-CBA-CGA	-2.66	105.67	113.21
34	a	408	BCT	O3-C-O1	-2.65	112.89	119.68
22	B	610	CLA	O1D-CGD-CBD	2.65	129.75	124.52
22	C	508	CLA	CHB-C4A-NA	2.65	128.23	124.40
22	B	605	CLA	CHD-C1D-ND	-2.65	121.07	124.80
22	d	403	CLA	C4-C3-C5	2.65	119.83	115.23
30	c	519	DGD	O6D-C1D-O3G	-2.64	103.80	110.04
27	c	522	LMG	O6-C1-O1	-2.64	103.80	110.04
29	b	620	SQD	O8-S-C6	2.64	111.07	105.97
24	x	101	BCR	C38-C26-C25	-2.64	121.61	124.48
22	b	604	CLA	C6-C5-C3	-2.64	107.05	113.47
22	b	605	CLA	CHD-C1D-ND	-2.64	121.09	124.80
35	f	101	HEC	C3C-C4C-NC	-2.63	107.23	110.15
22	B	602	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
22	c	501	CLA	CHB-C4A-NA	2.63	128.20	124.40
22	B	608	CLA	C4A-NA-C1A	2.63	107.88	106.68
30	h	101	DGD	O2D-C2D-C1D	-2.63	103.80	110.08
22	C	508	CLA	CHD-C1D-C2D	2.63	130.96	125.49
28	D	409	LHG	O8-C23-C24	2.63	119.86	111.83
24	A	407	BCR	C35-C13-C14	-2.63	118.56	122.82
22	B	604	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
24	d	406	BCR	C24-C23-C22	-2.63	122.35	126.23
22	c	506	CLA	C3B-C4B-NB	-2.63	108.19	110.53
29	D	408	SQD	O9-S-O7	-2.62	105.29	113.82
24	c	514	BCR	C7-C8-C9	-2.62	122.35	126.23
33	j	101	STE	O2-C1-O1	-2.62	116.59	123.33
33	B	624	STE	C3-C2-C1	-2.62	107.67	114.51
22	c	513	CLA	CHB-C4A-NA	2.62	128.18	124.40
29	D	408	SQD	O5-C1-C2	-2.62	104.99	110.37
22	d	403	CLA	CHB-C4A-NA	2.62	128.18	124.40
27	D	407	LMG	O2-C2-C1	-2.62	103.83	110.08
22	c	512	CLA	CHB-C4A-NA	2.62	128.18	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	415	DGD	C3G-C2G-C1G	-2.62	105.68	111.78
22	c	501	CLA	C3B-C4B-NB	-2.62	108.19	110.53
27	C	520	LMG	O7-C10-O9	-2.62	117.59	123.70
22	d	404	CLA	CMB-C2B-C3B	2.61	132.70	126.55
22	b	612	CLA	CMD-C2D-C3D	2.61	133.68	127.69
26	A	410	PL9	C40-C39-C41	2.61	119.75	115.23
22	C	503	CLA	CHC-C4B-NB	2.61	127.96	124.05
28	l	101	LHG	C18-C17-C16	-2.60	101.20	114.37
24	c	514	BCR	C24-C23-C22	-2.60	122.38	126.23
35	F	101	HEC	C3C-C4C-NC	-2.60	107.27	110.15
22	A	402	CLA	C4A-NA-C1A	2.60	107.87	106.68
30	C	517	DGD	CDB-CCB-CBB	-2.60	101.22	114.37
22	c	507	CLA	O2A-CGA-O1A	-2.60	117.12	123.63
24	t	101	BCR	C15-C16-C17	-2.60	118.20	123.52
30	c	517	DGD	O6E-C5E-C4E	2.60	114.38	109.70
22	b	608	CLA	CMB-C2B-C3B	2.60	132.66	126.55
22	b	601	CLA	CHB-C4A-NA	2.60	128.15	124.40
22	B	614	CLA	CHC-C4B-NB	2.60	127.94	124.05
24	x	101	BCR	C29-C30-C25	2.60	114.21	110.44
22	c	501	CLA	O1D-CGD-CBD	2.59	129.63	124.52
22	B	614	CLA	C4-C3-C5	2.59	119.73	115.23
22	C	508	CLA	C4D-CHA-C1A	2.59	124.34	121.24
30	C	518	DGD	C3E-C4E-C5E	-2.59	105.53	110.23
22	b	604	CLA	CAC-C3C-C4C	2.59	128.16	124.79
22	b	604	CLA	C11-C12-C13	-2.59	107.36	115.97
24	b	617	BCR	C15-C16-C17	-2.59	118.22	123.52
24	a	405	BCR	C27-C26-C25	2.59	126.20	122.70
22	B	602	CLA	C1-C2-C3	-2.59	121.96	126.20
24	c	514	BCR	C27-C26-C25	2.59	126.20	122.70
35	F	101	HEC	CAD-C3D-C4D	2.59	129.21	124.70
22	b	602	CLA	CMB-C2B-C3B	2.59	132.63	126.55
22	C	513	CLA	O2D-CGD-CBD	2.58	115.75	111.23
22	b	614	CLA	C1-C2-C3	-2.58	121.97	126.20
26	a	409	PL9	C25-C24-C26	2.58	119.70	115.23
22	B	611	CLA	C9-C8-C10	-2.57	102.10	111.27
27	A	411	LMG	C1-O6-C5	-2.57	108.70	113.72
22	C	507	CLA	CHB-C4A-NA	2.57	128.11	124.40
27	c	520	LMG	C3-C4-C5	-2.57	105.57	110.23
24	b	619	BCR	C2-C1-C6	2.57	114.17	110.44
27	c	523	LMG	C38-C37-C36	-2.57	101.40	114.37
22	B	609	CLA	C6-C5-C3	2.56	119.72	113.47
23	A	405	PHO	C4D-CHA-CBD	-2.56	107.22	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	604	CLA	CMA-C3A-C4A	2.56	118.66	111.77
22	A	406	CLA	CHB-C4A-NA	2.56	128.10	124.40
24	C	514	BCR	C24-C23-C22	-2.56	122.45	126.23
24	B	617	BCR	C29-C30-C25	2.56	114.16	110.44
24	c	514	BCR	C15-C16-C17	-2.56	118.28	123.52
29	a	411	SQD	O8-S-C6	2.55	110.90	105.97
24	c	514	BCR	C11-C10-C9	-2.55	123.70	127.28
22	B	603	CLA	CHC-C1C-NC	2.55	128.15	124.31
22	d	401	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
22	B	606	CLA	C2A-C1A-CHA	2.55	128.29	123.87
30	H	102	DGD	O5D-C1E-C2E	2.54	112.14	108.27
24	A	407	BCR	C16-C15-C14	-2.54	118.31	123.52
30	c	517	DGD	O6D-C1D-O3G	-2.54	104.03	110.04
22	a	402	CLA	CAC-C3C-C4C	2.54	128.10	124.79
29	B	623	SQD	O47-C7-C8	2.54	116.97	111.48
22	B	613	CLA	C3B-C4B-NB	-2.54	108.27	110.53
24	t	101	BCR	C2-C1-C6	2.54	114.12	110.44
24	c	515	BCR	C7-C8-C9	-2.54	122.48	126.23
22	C	506	CLA	CHB-C4A-NA	2.53	128.06	124.40
24	B	618	BCR	C27-C26-C25	2.53	126.13	122.70
26	d	407	PL9	C8-C7-C3	2.53	118.57	112.03
24	D	405	BCR	C36-C18-C19	-2.53	114.22	118.09
24	d	406	BCR	C27-C26-C25	2.53	126.12	122.70
35	F	101	HEC	CAB-C3B-C2B	2.53	132.20	127.56
24	D	405	BCR	C27-C26-C25	2.52	126.11	122.70
24	B	619	BCR	C16-C15-C14	-2.52	118.36	123.52
24	B	618	BCR	C24-C23-C22	-2.52	122.50	126.23
22	b	607	CLA	CMB-C2B-C1B	-2.52	121.58	125.42
22	b	614	CLA	C4-C3-C5	2.52	119.60	115.23
29	f	102	SQD	C1-O5-C5	-2.51	108.81	113.72
22	b	609	CLA	CMB-C2B-C1B	-2.51	121.59	125.42
24	B	618	BCR	C7-C8-C9	-2.51	122.52	126.23
22	B	610	CLA	C1-C2-C3	-2.51	122.08	126.20
22	b	612	CLA	C1-C2-C3	-2.51	122.08	126.20
22	b	609	CLA	O1D-CGD-CBD	2.51	129.47	124.52
27	C	520	LMG	O1-C7-C8	-2.51	104.72	110.82
23	a	403	PHO	C3D-C4D-ND	2.51	110.92	107.71
22	B	609	CLA	C1D-ND-C4D	-2.51	104.55	106.31
24	H	101	BCR	C11-C10-C9	-2.51	123.76	127.28
24	A	407	BCR	C37-C22-C21	-2.51	118.76	122.82
26	A	410	PL9	C12-C13-C14	-2.51	121.89	127.62
30	c	517	DGD	CDB-CCB-CBB	-2.50	101.71	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	511	CLA	CHD-C1D-ND	-2.50	121.28	124.80
22	b	613	CLA	O2D-CGD-O1D	-2.50	118.97	123.85
24	B	617	BCR	C15-C14-C13	-2.50	123.77	127.28
22	C	510	CLA	C11-C10-C8	-2.50	107.65	115.97
22	b	606	CLA	CHB-C1B-NB	2.50	127.80	124.05
22	B	612	CLA	CMB-C2B-C3B	2.50	132.43	126.55
30	h	101	DGD	O5E-C6E-C5E	-2.50	102.82	111.33
22	C	505	CLA	CHB-C1B-NB	2.50	127.80	124.05
29	b	620	SQD	C45-O47-C7	2.50	123.78	117.80
22	C	512	CLA	C3B-C4B-NB	-2.50	108.30	110.53
29	A	413	SQD	O48-C23-C24	2.50	119.44	111.83
30	C	518	DGD	C1D-C2D-C3D	-2.49	104.77	110.01
26	d	407	PL9	C7-C8-C9	-2.49	122.54	126.83
29	A	414	SQD	O47-C7-C8	2.49	116.87	111.48
22	C	501	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
22	C	507	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
22	b	605	CLA	O1A-CGA-CBA	2.49	133.51	123.78
30	c	517	DGD	O3E-C3E-C2E	-2.49	104.51	110.38
27	c	520	LMG	O6-C1-O1	-2.49	104.17	110.04
26	D	406	PL9	C7-C3-C2	-2.49	120.46	123.39
22	B	616	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
28	e	101	LHG	O8-C23-O10	-2.48	117.41	123.63
35	v	201	HEC	CHD-C1D-ND	2.48	127.44	124.37
28	d	409	LHG	O8-C23-O10	-2.48	117.42	123.63
22	c	504	CLA	CMB-C2B-C1B	-2.48	121.64	125.42
23	A	405	PHO	CMB-C2B-C3B	2.48	129.64	124.68
22	d	401	CLA	CHD-C1D-C2D	2.48	130.65	125.49
22	B	615	CLA	CED-O2D-CGD	2.48	121.54	115.92
30	C	518	DGD	C6D-O5D-C1E	2.48	119.11	113.80
24	k	101	BCR	C27-C26-C25	2.48	126.05	122.70
24	A	407	BCR	C38-C26-C25	-2.48	121.78	124.48
27	d	410	LMG	O6-C1-O1	-2.48	104.19	110.04
22	B	603	CLA	C3B-C4B-NB	-2.48	108.32	110.53
22	C	511	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
23	A	405	PHO	C1-C2-C3	-2.47	122.14	126.20
33	b	624	STE	O2-C1-C2	2.47	121.81	114.00
33	d	412	STE	C3-C2-C1	-2.47	108.06	114.51
22	C	502	CLA	CHD-C1D-ND	-2.47	121.32	124.80
22	b	614	CLA	CMB-C2B-C1B	-2.47	121.66	125.42
26	D	406	PL9	C32-C33-C34	-2.47	121.97	127.62
22	D	403	CLA	C7-C6-C5	-2.47	106.69	113.26
28	D	409	LHG	C11-C10-C9	-2.47	101.90	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	b	608	CLA	CHA-C1A-NA	-2.46	120.81	126.39
26	a	409	PL9	C40-C39-C41	2.46	119.51	115.23
24	C	515	BCR	C27-C26-C25	2.46	126.03	122.70
22	a	402	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
30	C	517	DGD	O2D-C2D-C1D	-2.46	104.21	110.08
28	A	412	LHG	C27-C26-C25	-2.46	101.93	114.37
22	d	405	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
22	c	510	CLA	C3B-C4B-NB	-2.46	108.33	110.53
22	b	613	CLA	CHA-C1A-NA	-2.46	120.82	126.39
22	b	605	CLA	C4A-NA-C1A	2.46	107.80	106.68
24	k	101	BCR	C38-C26-C25	-2.46	121.80	124.48
22	B	608	CLA	O1D-CGD-CBD	2.46	129.36	124.52
28	l	101	LHG	O8-C23-C24	2.46	119.33	111.83
22	B	615	CLA	CHD-C1D-ND	-2.45	121.35	124.80
22	a	402	CLA	CMB-C2B-C3B	2.45	132.32	126.55
22	b	607	CLA	C3B-C4B-NB	-2.45	108.34	110.53
24	B	617	BCR	C3-C4-C5	-2.45	109.69	114.06
22	B	612	CLA	C4D-CHA-C1A	2.45	124.17	121.24
22	c	509	CLA	C3B-C4B-NB	-2.45	108.34	110.53
22	c	509	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
22	A	403	CLA	O2D-CGD-CBD	2.45	115.51	111.23
26	D	406	PL9	C50-C49-C48	-2.44	115.32	122.66
30	C	519	DGD	C1D-C2D-C3D	-2.44	104.87	110.01
30	A	415	DGD	O2D-C2D-C1D	-2.44	104.26	110.08
22	c	504	CLA	O1A-CGA-CBA	2.44	133.33	123.78
28	D	409	LHG	C20-C19-C18	-2.44	102.03	114.37
22	B	606	CLA	OBD-CAD-C3D	2.44	134.12	128.42
22	c	513	CLA	O2D-CGD-CBD	2.44	115.50	111.23
28	d	408	LHG	O8-C23-C24	2.44	119.27	111.83
22	B	607	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
22	b	610	CLA	C2C-C1C-NC	2.44	112.54	109.98
35	f	101	HEC	CHB-C1B-C2B	-2.44	121.18	125.03
24	T	101	BCR	C33-C5-C6	-2.44	121.83	124.48
22	b	603	CLA	CHB-C1B-C2B	-2.43	120.36	127.43
22	c	504	CLA	CHD-C1D-ND	-2.43	121.38	124.80
22	b	612	CLA	C11-C12-C13	-2.43	107.88	115.97
23	A	404	PHO	O2A-CGA-O1A	-2.43	117.54	123.63
22	B	611	CLA	C1-C2-C3	-2.43	122.22	126.20
24	x	101	BCR	C16-C15-C14	-2.43	118.55	123.52
30	C	517	DGD	O1G-C1A-C2A	-2.43	104.43	111.83
27	m	101	LMG	O1-C1-C2	-2.43	104.59	108.27
24	t	101	BCR	C33-C5-C6	-2.43	121.84	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	416	LMG	C7-O1-C1	2.43	119.00	113.80
24	b	617	BCR	C11-C10-C9	-2.42	123.88	127.28
26	d	407	PL9	C36-C34-C33	-2.42	115.73	121.17
22	D	404	CLA	CHC-C4B-NB	2.42	127.68	124.05
22	B	607	CLA	CHD-C1D-ND	-2.42	121.40	124.80
23	A	404	PHO	C4D-ND-C1D	-2.42	105.98	108.87
33	J	101	STE	C3-C2-C1	-2.42	108.20	114.51
22	b	615	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
22	b	603	CLA	C4A-NA-C1A	2.42	107.78	106.68
22	c	512	CLA	O1D-CGD-CBD	2.41	129.27	124.52
22	b	615	CLA	CHB-C1B-NB	2.41	127.67	124.05
30	A	415	DGD	C1D-C2D-C3D	-2.41	104.94	110.01
22	C	512	CLA	CAA-CBA-CGA	-2.41	106.37	113.21
30	h	101	DGD	C3D-C4D-C5D	-2.41	105.86	110.23
22	B	609	CLA	O2D-CGD-CBD	2.41	115.44	111.23
22	b	603	CLA	CMB-C2B-C3B	2.41	132.21	126.55
22	b	616	CLA	C3B-C4B-NB	-2.41	108.38	110.53
30	H	102	DGD	C3D-C4D-C5D	-2.40	105.87	110.23
28	A	412	LHG	O8-C6-C5	-2.40	101.46	108.40
22	b	615	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
29	f	102	SQD	O5-C1-O6	2.40	115.71	110.04
22	b	607	CLA	CHA-C1A-NA	-2.40	120.96	126.39
26	a	409	PL9	O2-C1-C6	2.40	124.29	120.48
27	c	520	LMG	O8-C28-O10	-2.40	117.63	123.63
22	B	608	CLA	C3B-C4B-NB	-2.39	108.39	110.53
22	C	512	CLA	CMB-C2B-C3B	2.39	132.18	126.55
22	c	510	CLA	CHB-C4A-NA	2.39	127.85	124.40
22	c	508	CLA	CHD-C4C-NC	2.39	127.93	124.23
22	B	607	CLA	CED-O2D-CGD	2.39	121.33	115.92
22	C	508	CLA	O2D-CGD-CBD	2.39	115.40	111.23
30	h	101	DGD	CDB-CCB-CBB	-2.39	102.31	114.37
24	B	617	BCR	C27-C26-C25	2.38	125.92	122.70
22	b	612	CLA	C4D-C3D-CAD	-2.38	105.52	108.11
24	Y	101	BCR	C12-C13-C14	-2.38	115.26	119.01
29	D	408	SQD	O48-C23-O10	-2.38	117.67	123.63
22	B	605	CLA	C1-C2-C3	2.38	130.10	126.20
22	B	616	CLA	CHD-C1D-ND	-2.38	121.45	124.80
22	b	614	CLA	C7-C6-C5	-2.38	106.93	113.26
28	E	101	LHG	C11-C10-C9	-2.37	102.36	114.37
35	v	201	HEC	CBD-CAD-C3D	-2.37	105.97	112.53
26	d	407	PL9	C12-C13-C14	-2.37	122.19	127.62
22	B	601	CLA	O2D-CGD-CBD	2.37	115.38	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	PHO	CBC-CAC-C3C	2.37	116.26	112.87
27	c	523	LMG	C1-O6-C5	-2.37	109.10	113.72
29	b	620	SQD	O47-C45-C46	2.37	116.83	108.34
22	D	402	CLA	C6-C5-C3	2.37	119.23	113.47
30	h	101	DGD	O3E-C3E-C2E	-2.36	104.80	110.38
26	D	406	PL9	C12-C13-C14	-2.36	122.21	127.62
22	A	406	CLA	C1-C2-C3	-2.36	122.32	126.20
23	A	404	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
35	f	101	HEC	CHA-C4D-ND	2.36	126.96	124.42
24	D	405	BCR	C2-C1-C6	2.36	113.86	110.44
22	B	612	CLA	C16-C15-C13	-2.36	108.14	115.97
22	b	609	CLA	C7-C6-C5	-2.36	106.98	113.26
22	d	405	CLA	CHA-C1A-NA	-2.36	121.06	126.39
33	k	102	STE	O2-C1-C2	2.35	121.44	114.00
33	C	521	STE	O2-C1-C2	2.35	121.44	114.00
22	b	609	CLA	CHB-C4A-NA	2.35	127.80	124.40
22	C	505	CLA	CHA-C1A-NA	-2.35	121.06	126.39
22	b	608	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
29	D	408	SQD	O5-C5-C4	2.35	113.93	109.70
22	b	604	CLA	C6-C7-C8	-2.35	108.16	115.97
24	x	101	BCR	C35-C13-C12	2.35	121.67	118.09
22	B	609	CLA	C3B-C4B-NB	-2.34	108.44	110.53
22	C	505	CLA	C3B-C4B-NB	-2.34	108.44	110.53
29	f	102	SQD	O47-C7-C8	2.34	119.54	110.93
22	b	601	CLA	CHD-C1D-ND	-2.34	121.51	124.80
22	A	402	CLA	CED-O2D-CGD	2.34	121.23	115.92
24	C	515	BCR	C33-C5-C6	-2.34	121.93	124.48
22	d	404	CLA	C2B-C1B-NB	-2.34	107.90	110.33
24	b	618	BCR	C35-C13-C14	-2.34	119.03	122.82
22	C	512	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
30	c	518	DGD	O4E-C4E-C3E	-2.34	104.86	110.38
22	b	602	CLA	C4-C3-C5	2.34	119.28	115.23
22	c	508	CLA	C7-C6-C5	-2.34	107.03	113.26
22	B	606	CLA	C4D-CHA-C1A	2.34	124.03	121.24
22	D	403	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
22	A	403	CLA	C1-O2A-CGA	2.34	122.30	116.65
22	B	606	CLA	CHB-C1B-NB	2.33	127.55	124.05
24	B	617	BCR	C33-C5-C6	-2.33	121.94	124.48
33	t	103	STE	C3-C2-C1	-2.33	108.42	114.51
22	b	604	CLA	O1D-CGD-CBD	2.33	129.12	124.52
22	C	509	CLA	CMB-C2B-C3B	2.33	132.03	126.55
27	c	520	LMG	C9-C8-C7	-2.33	106.36	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	507	CLA	CHD-C1D-C2D	2.33	130.33	125.49
30	c	517	DGD	O1G-C1A-O1A	-2.33	117.81	123.63
22	c	510	CLA	O1D-CGD-CBD	2.33	129.11	124.52
30	c	517	DGD	O2D-C2D-C3D	-2.33	104.89	110.38
22	b	605	CLA	C1-C2-C3	-2.32	122.39	126.20
22	C	501	CLA	CHB-C1B-NB	2.32	127.54	124.05
30	c	517	DGD	O3D-C3D-C4D	-2.32	104.90	110.38
24	C	514	BCR	C8-C7-C6	-2.32	120.79	127.00
27	m	101	LMG	C9-C8-C7	-2.32	106.37	111.78
22	C	507	CLA	CHC-C4B-NB	2.32	127.53	124.05
22	B	610	CLA	C3B-C4B-NB	-2.32	108.46	110.53
27	c	522	LMG	O2-C2-C1	-2.32	104.54	110.08
22	B	601	CLA	C4-C3-C5	2.32	119.26	115.23
22	b	614	CLA	CHD-C1D-ND	-2.32	121.54	124.80
22	C	512	CLA	CMA-C3A-C2A	-2.32	105.01	113.98
22	B	615	CLA	CHB-C4A-NA	2.32	127.75	124.40
24	B	619	BCR	C33-C5-C6	-2.32	121.95	124.48
22	c	510	CLA	C1-C2-C3	-2.32	122.40	126.20
24	C	515	BCR	C2-C1-C6	2.32	113.81	110.44
22	a	404	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
22	B	609	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
22	c	509	CLA	CHC-C1C-NC	2.31	127.79	124.31
22	c	503	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
22	a	404	CLA	CHC-C4B-NB	2.31	127.51	124.05
22	B	608	CLA	O2D-CGD-CBD	2.31	115.27	111.23
22	a	402	CLA	CHB-C1B-NB	2.31	127.51	124.05
23	a	403	PHO	O2D-CGD-O1D	-2.30	119.36	123.85
22	c	502	CLA	CHB-C4A-NA	2.30	127.72	124.40
29	f	102	SQD	O5-C1-C2	-2.30	105.64	110.37
28	d	408	LHG	C20-C19-C18	-2.30	102.74	114.37
22	b	602	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
23	a	403	PHO	C3B-C4B-NB	-2.30	105.97	107.46
24	H	101	BCR	C1-C6-C5	-2.30	119.50	122.64
24	t	101	BCR	C1-C6-C5	-2.30	119.50	122.64
27	D	407	LMG	O3-C3-C2	-2.30	104.97	110.38
22	b	601	CLA	C3B-C4B-NB	-2.30	108.48	110.53
24	C	514	BCR	C32-C1-C6	-2.30	106.64	110.24
29	f	102	SQD	O48-C23-C24	2.29	118.83	111.83
22	B	605	CLA	CHD-C1D-C2D	2.29	130.26	125.49
22	d	403	CLA	C6-C5-C3	2.29	119.06	113.47
22	B	602	CLA	CHA-C4D-ND	2.29	137.28	132.55
27	d	410	LMG	O7-C10-O9	-2.29	118.34	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	411	SQD	C3-C4-C5	2.29	114.39	110.23
22	A	403	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
29	b	620	SQD	O10-C23-C24	-2.29	114.82	123.78
22	C	511	CLA	C3B-C4B-NB	-2.29	108.48	110.53
28	d	408	LHG	C18-C17-C16	-2.29	102.79	114.37
27	D	410	LMG	O1-C7-C8	-2.29	105.89	111.77
22	c	508	CLA	CHD-C1D-ND	-2.29	121.58	124.80
28	B	622	LHG	C11-C10-C9	-2.29	102.81	114.37
22	b	606	CLA	O1D-CGD-CBD	2.28	129.02	124.52
22	c	505	CLA	C1-C2-C3	-2.28	122.46	126.20
24	Y	101	BCR	C1-C6-C5	-2.28	119.52	122.64
22	B	607	CLA	CHB-C1B-NB	2.28	127.47	124.05
22	b	607	CLA	CHB-C1B-NB	2.28	127.47	124.05
28	E	101	LHG	C18-C17-C16	-2.28	102.84	114.37
30	h	101	DGD	O6D-C1D-O3G	-2.28	104.66	110.04
24	A	407	BCR	C15-C16-C17	-2.28	118.86	123.52
22	A	402	CLA	O1D-CGD-CBD	2.28	129.01	124.52
22	C	512	CLA	CHD-C1D-ND	-2.28	121.60	124.80
22	c	504	CLA	CMB-C2B-C3B	2.27	131.90	126.55
22	b	603	CLA	CHD-C1D-ND	-2.27	121.60	124.80
27	c	520	LMG	C40-C39-C38	-2.27	102.87	114.37
22	b	615	CLA	CHA-C4D-ND	2.27	137.24	132.55
30	c	518	DGD	O2E-C2E-C1E	-2.27	104.66	110.08
22	d	401	CLA	C3B-C4B-NB	-2.27	108.50	110.53
24	C	516	BCR	C27-C26-C25	2.27	125.77	122.70
26	A	410	PL9	C35-C34-C36	2.27	119.16	115.23
22	c	504	CLA	O2D-CGD-CBD	2.27	115.19	111.23
28	a	410	LHG	O3-P-O5	-2.27	99.95	108.94
26	d	407	PL9	C30-C29-C31	-2.27	111.29	115.23
24	H	101	BCR	C38-C26-C25	-2.27	122.01	124.48
22	b	609	CLA	C4D-CHA-C1A	2.27	123.95	121.24
23	d	402	PHO	C4D-ND-C1D	-2.27	106.16	108.87
24	C	514	BCR	C15-C14-C13	-2.26	124.10	127.28
22	c	504	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
22	B	612	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
22	a	402	CLA	C16-C17-C18	-2.26	105.85	115.94
24	b	618	BCR	C37-C22-C21	-2.26	119.15	122.82
22	B	611	CLA	C3B-C4B-NB	-2.26	108.51	110.53
30	c	517	DGD	O2G-C2G-C1G	-2.26	100.23	108.34
22	c	512	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
24	C	515	BCR	C36-C18-C17	-2.26	119.16	122.82
26	a	409	PL9	O2-C1-C2	-2.26	116.69	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	619	BCR	C16-C15-C14	-2.26	118.90	123.52
30	C	517	DGD	C8B-C7B-C6B	-2.26	102.95	114.37
27	b	623	LMG	O8-C28-O10	-2.26	117.98	123.63
22	b	616	CLA	O1D-CGD-CBD	2.26	128.97	124.52
22	b	608	CLA	C4A-NA-C1A	2.26	107.71	106.68
22	b	616	CLA	CMB-C2B-C1B	-2.26	121.98	125.42
23	A	405	PHO	C3D-C4D-ND	2.26	110.60	107.71
24	t	101	BCR	C36-C18-C19	2.25	121.53	118.09
22	B	603	CLA	CHB-C4A-NA	2.25	127.65	124.40
24	T	101	BCR	C30-C25-C26	-2.25	119.56	122.64
22	C	511	CLA	C1-C2-C3	-2.25	122.51	126.20
24	c	516	BCR	C2-C1-C6	2.25	113.71	110.44
22	b	607	CLA	CMB-C2B-C3B	2.25	131.84	126.55
22	C	502	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
22	B	607	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
22	C	503	CLA	O2A-C1-C2	-2.25	99.46	108.11
29	B	623	SQD	C1-C2-C3	-2.25	105.28	110.01
22	c	506	CLA	C4-C3-C2	-2.25	117.86	123.63
22	a	402	CLA	CHA-C4D-ND	2.24	137.18	132.55
22	C	506	CLA	CAA-CBA-CGA	-2.24	106.84	113.21
30	A	415	DGD	C3E-C4E-C5E	-2.24	106.16	110.23
27	D	407	LMG	C3-C4-C5	-2.24	106.17	110.23
35	V	201	HEC	CHA-C4D-ND	2.24	126.84	124.42
22	b	604	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
22	c	513	CLA	CHD-C1D-ND	-2.24	121.65	124.80
22	A	402	CLA	O2D-CGD-CBD	-2.24	107.31	111.23
22	B	614	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	B	612	CLA	C1-C2-C3	-2.24	122.53	126.20
22	c	508	CLA	C11-C10-C8	-2.24	108.52	115.97
22	d	401	CLA	O2D-CGD-CBD	2.24	115.14	111.23
22	C	510	CLA	CHB-C4A-NA	2.24	127.63	124.40
22	D	403	CLA	CHB-C4A-NA	2.24	127.63	124.40
24	H	101	BCR	C37-C22-C21	-2.24	119.19	122.82
24	B	618	BCR	C15-C16-C17	-2.24	118.94	123.52
22	b	604	CLA	CHB-C1B-NB	2.24	127.41	124.05
33	C	523	STE	C4-C3-C2	-2.24	104.91	113.13
27	A	411	LMG	O1-C7-C8	-2.23	105.39	110.82
22	C	509	CLA	CHD-C1D-ND	-2.23	121.66	124.80
24	t	101	BCR	C27-C26-C25	2.23	125.72	122.70
22	B	608	CLA	CHD-C1D-ND	-2.23	121.67	124.80
22	B	611	CLA	C7-C6-C5	-2.23	107.32	113.26
27	c	520	LMG	O2-C2-C1	-2.23	104.76	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	502	CLA	CHA-C1A-NA	-2.23	121.35	126.39
23	A	404	PHO	OBD-CAD-C3D	2.23	131.37	127.89
22	B	609	CLA	CHA-C1A-NA	-2.23	121.35	126.39
24	B	617	BCR	C15-C16-C17	-2.23	118.96	123.52
22	B	613	CLA	O1D-CGD-CBD	2.23	128.91	124.52
22	B	605	CLA	C1-O2A-CGA	-2.23	111.26	116.65
24	D	405	BCR	C2-C3-C4	-2.23	106.38	111.28
33	D	412	STE	C12-C11-C10	-2.22	103.13	114.37
33	d	411	STE	O2-C1-O1	-2.22	117.62	123.33
22	b	608	CLA	CHB-C1B-NB	2.22	127.38	124.05
22	b	611	CLA	CHB-C4A-NA	2.22	127.60	124.40
24	B	617	BCR	C8-C7-C6	-2.22	121.07	127.00
22	d	403	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
30	C	517	DGD	O3E-C3E-C2E	-2.22	105.14	110.38
24	c	514	BCR	C2-C1-C6	2.22	113.66	110.44
27	D	411	LMG	O7-C10-O9	-2.22	117.63	123.33
22	C	512	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
24	B	617	BCR	C11-C10-C9	-2.22	124.17	127.28
22	c	506	CLA	CHC-C1C-NC	2.22	127.65	124.31
27	A	411	LMG	C12-C11-C10	-2.22	105.57	113.69
22	b	604	CLA	C3B-C4B-NB	-2.22	108.55	110.53
22	a	404	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
22	B	610	CLA	C2C-C1C-NC	2.22	112.31	109.98
22	C	511	CLA	CHB-C4A-NA	2.21	127.60	124.40
22	B	605	CLA	C16-C15-C13	-2.21	108.61	115.97
26	d	407	PL9	C15-C14-C13	-2.21	117.94	123.63
22	b	609	CLA	CHA-C1A-NA	-2.21	121.38	126.39
22	c	510	CLA	O1A-CGA-CBA	2.21	132.44	123.78
28	e	101	LHG	C11-C10-C9	-2.21	103.18	114.37
22	B	601	CLA	CHB-C4A-NA	2.21	127.59	124.40
35	f	101	HEC	CHC-C4B-C3B	2.21	129.30	125.23
30	c	517	DGD	CBB-CAB-C9B	-2.21	103.20	114.37
22	c	505	CLA	C4D-C3D-CAD	-2.21	105.71	108.11
22	a	404	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
22	b	605	CLA	CHA-C1A-NA	-2.21	121.39	126.39
22	B	613	CLA	CHB-C4A-NA	2.21	127.59	124.40
24	D	405	BCR	C16-C15-C14	-2.21	119.00	123.52
28	A	412	LHG	O8-C23-C24	2.21	118.56	111.83
22	b	614	CLA	CHB-C4A-NA	2.21	127.58	124.40
24	B	618	BCR	C3-C4-C5	-2.20	110.12	114.06
24	t	101	BCR	C4-C5-C6	2.20	125.68	122.70
24	t	101	BCR	C39-C30-C25	2.20	113.70	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	101	BCR	C35-C13-C14	-2.20	119.25	122.82
22	b	616	CLA	CMB-C2B-C3B	2.20	131.73	126.55
30	A	415	DGD	CAB-C9B-C8B	-2.20	103.24	114.37
22	C	507	CLA	C2A-C1A-CHA	2.20	127.69	123.87
28	l	101	LHG	C27-C26-C25	-2.20	103.25	114.37
28	a	410	LHG	C18-C17-C16	-2.20	103.25	114.37
22	C	502	CLA	C1D-ND-C4D	2.20	107.86	106.31
22	c	505	CLA	CMB-C2B-C1B	-2.20	122.07	125.42
30	C	519	DGD	O3D-C3D-C4D	-2.20	105.19	110.38
30	c	517	DGD	CAB-C9B-C8B	-2.20	103.26	114.37
24	a	405	BCR	C16-C15-C14	-2.20	119.02	123.52
29	a	411	SQD	O7-S-C6	2.20	110.04	106.76
22	B	610	CLA	CHB-C4A-NA	2.20	127.57	124.40
26	A	410	PL9	C7-C3-C2	-2.19	120.80	123.39
27	C	520	LMG	O2-C2-C1	-2.19	104.85	110.08
22	C	505	CLA	CMB-C2B-C3B	2.19	131.71	126.55
30	C	518	DGD	C1D-O6D-C5D	-2.19	109.44	113.72
22	b	609	CLA	CHD-C1D-ND	-2.19	121.72	124.80
22	C	504	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
28	D	409	LHG	C27-C26-C25	-2.19	103.32	114.37
22	b	603	CLA	O1A-CGA-CBA	2.19	132.33	123.78
22	B	609	CLA	C1C-C2C-C3C	-2.18	104.68	106.98
24	B	618	BCR	C2-C1-C6	2.18	113.61	110.44
30	c	517	DGD	C5B-C4B-C3B	-2.18	103.34	114.37
22	b	605	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
22	c	502	CLA	CMB-C2B-C1B	-2.18	122.10	125.42
22	b	609	CLA	CHC-C4B-NB	2.18	127.32	124.05
28	E	101	LHG	O8-C23-O10	-2.18	118.18	123.63
22	c	503	CLA	C4D-C3D-CAD	-2.18	105.74	108.11
22	d	405	CLA	C3B-C4B-NB	-2.18	108.59	110.53
22	c	511	CLA	CHB-C4A-NA	2.18	127.54	124.40
22	c	511	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
28	a	410	LHG	C25-C24-C23	2.18	121.67	113.69
30	C	517	DGD	O3G-C1D-C2D	-2.18	104.97	108.27
24	b	617	BCR	C33-C5-C6	-2.17	122.11	124.48
22	C	504	CLA	CHC-C1C-NC	2.17	127.58	124.31
23	a	403	PHO	O1D-CGD-CBD	2.17	128.02	124.72
22	c	502	CLA	CHD-C1D-ND	-2.17	121.74	124.80
24	b	618	BCR	C33-C5-C6	-2.17	122.11	124.48
22	C	508	CLA	CMB-C2B-C3B	2.17	131.66	126.55
30	C	519	DGD	O4D-C4D-C5D	-2.17	103.98	109.32
24	A	407	BCR	C19-C18-C17	-2.17	115.59	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	413	SQD	O5-C1-O6	2.17	115.17	110.04
30	c	518	DGD	C8B-C7B-C6B	-2.17	103.40	114.37
26	A	410	PL9	C27-C28-C29	-2.17	122.66	127.62
27	M	101	LMG	C6-C5-C4	-2.17	107.70	113.02
28	d	409	LHG	O8-C23-C24	2.17	118.44	111.83
24	Y	101	BCR	C33-C5-C6	-2.17	122.12	124.48
24	B	617	BCR	C24-C23-C22	-2.17	123.03	126.23
33	t	102	STE	O2-C1-C2	2.17	120.84	114.00
22	C	502	CLA	CAC-C3C-C4C	2.16	127.61	124.79
22	c	504	CLA	CHD-C4C-NC	2.16	127.59	124.23
30	H	102	DGD	O2D-C2D-C1D	-2.16	104.92	110.08
22	c	502	CLA	C4D-CHA-C1A	2.16	123.82	121.24
34	D	401	BCT	O3-C-O1	-2.16	114.14	119.68
27	M	101	LMG	C18-C17-C16	-2.16	103.44	114.37
30	C	518	DGD	O2D-C2D-C1D	-2.16	104.92	110.08
22	b	604	CLA	C2C-C1C-NC	2.16	112.25	109.98
26	a	409	PL9	C22-C23-C24	-2.16	122.68	127.62
28	a	410	LHG	C20-C19-C18	-2.16	103.45	114.37
22	c	506	CLA	OBD-CAD-C3D	2.16	133.47	128.42
22	B	604	CLA	C6-C7-C8	-2.16	108.79	115.97
22	B	615	CLA	C6-C7-C8	-2.16	108.79	115.97
22	D	402	CLA	CBA-CAA-C2A	-2.16	107.37	113.79
22	B	603	CLA	O2D-CGD-CBD	2.16	115.00	111.23
27	M	101	LMG	O1-C7-C8	-2.16	105.57	110.82
27	c	522	LMG	C1-O6-C5	-2.16	109.51	113.72
30	c	519	DGD	O1G-C1G-C2G	-2.16	102.18	108.40
24	C	515	BCR	C1-C6-C5	-2.16	119.69	122.64
22	D	402	CLA	CHB-C4A-NA	2.15	127.51	124.40
30	H	102	DGD	O1G-C1A-O1A	-2.15	118.25	123.63
22	b	602	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	b	603	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
22	d	405	CLA	O2D-CGD-O1D	-2.15	119.67	123.85
22	B	614	CLA	CAC-C3C-C4C	2.15	127.58	124.79
30	c	518	DGD	O6D-C1D-O3G	-2.15	104.97	110.04
29	a	412	SQD	O48-C23-C24	2.15	118.38	111.83
24	d	406	BCR	C11-C10-C9	-2.15	124.27	127.28
22	B	604	CLA	CGD-CBD-CAD	-2.15	103.90	110.85
28	B	622	LHG	O3-P-O5	-2.15	100.43	108.94
27	M	101	LMG	C40-C39-C38	-2.15	103.52	114.37
22	d	405	CLA	C3D-C4D-ND	2.15	113.47	109.99
27	c	523	LMG	C9-C8-C7	-2.14	106.78	111.78
24	b	617	BCR	C3-C4-C5	-2.14	110.23	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	c	518	DGD	O3E-C3E-C4E	-2.14	105.32	110.38
22	c	505	CLA	C11-C10-C8	-2.14	108.84	115.97
22	B	602	CLA	C4-C3-C5	2.14	118.94	115.23
22	B	606	CLA	O1A-CGA-CBA	2.14	132.16	123.78
24	b	617	BCR	C15-C14-C13	-2.14	124.28	127.28
24	c	515	BCR	C1-C6-C5	-2.14	119.71	122.64
22	c	506	CLA	CHD-C1D-ND	-2.14	121.79	124.80
22	A	402	CLA	C3B-C2B-C1B	-2.14	104.65	107.17
33	J	101	STE	O2-C1-C2	2.14	120.76	114.00
22	c	505	CLA	CHD-C1D-ND	-2.14	121.79	124.80
28	D	409	LHG	O4-P-O3	-2.14	97.87	107.57
22	B	614	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
22	B	607	CLA	CHD-C4C-NC	2.14	127.55	124.23
22	c	510	CLA	C7-C6-C5	-2.14	107.56	113.26
35	F	101	HEC	CMD-C2D-C1D	2.14	128.37	125.03
22	B	602	CLA	CHB-C4A-NA	2.14	127.48	124.40
22	b	605	CLA	C1-O2A-CGA	-2.14	111.48	116.65
22	B	608	CLA	CHB-C4A-NA	2.13	127.48	124.40
24	a	405	BCR	C7-C8-C9	-2.13	123.08	126.23
27	c	523	LMG	C40-C39-C38	-2.13	103.59	114.37
24	c	515	BCR	C34-C9-C10	-2.13	119.36	122.82
27	d	410	LMG	C40-C39-C38	-2.13	103.60	114.37
22	C	511	CLA	C4-C3-C5	2.13	118.92	115.23
24	C	516	BCR	C20-C21-C22	-2.13	124.30	127.28
24	A	407	BCR	C24-C23-C22	-2.13	123.09	126.23
22	b	604	CLA	C3A-C2A-C1A	2.13	104.52	101.34
22	b	607	CLA	C2A-C1A-CHA	2.13	127.56	123.87
30	A	415	DGD	O3G-C3G-C2G	-2.12	105.65	110.82
24	A	407	BCR	C40-C30-C39	-2.12	102.55	108.63
24	t	101	BCR	C28-C27-C26	-2.12	110.27	114.06
24	Y	101	BCR	C15-C16-C17	-2.12	119.18	123.52
24	C	515	BCR	C34-C9-C10	-2.12	119.38	122.82
24	b	618	BCR	C30-C25-C26	-2.12	119.74	122.64
22	C	503	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
26	D	406	PL9	C31-C29-C28	2.12	125.92	121.17
22	b	612	CLA	CHC-C1C-NC	2.12	127.50	124.31
24	C	515	BCR	C34-C9-C8	2.12	121.32	118.09
30	c	517	DGD	C6D-O5D-C1E	2.12	118.33	113.80
27	d	410	LMG	O3-C3-C2	-2.12	105.39	110.38
24	A	407	BCR	C8-C7-C6	-2.12	121.35	127.00
22	B	612	CLA	CHB-C4A-NA	2.11	127.45	124.40
22	B	603	CLA	C6-C5-C3	2.11	118.62	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	412	LHG	O4-P-O3	2.11	117.15	107.57
24	k	101	BCR	C4-C5-C6	2.11	125.56	122.70
22	C	504	CLA	CED-O2D-CGD	2.11	120.71	115.92
22	c	501	CLA	CMB-C2B-C3B	2.11	131.51	126.55
22	b	608	CLA	C6-C7-C8	-2.11	108.95	115.97
22	b	610	CLA	CAA-CBA-CGA	-2.11	107.22	113.21
22	a	404	CLA	CHA-C1A-NA	-2.11	121.62	126.39
22	C	503	CLA	CHD-C1D-ND	-2.11	121.84	124.80
24	B	617	BCR	C36-C18-C17	-2.11	119.40	122.82
22	C	503	CLA	C6-C5-C3	2.11	118.60	113.47
22	b	611	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
27	c	520	LMG	O7-C10-O9	-2.10	118.93	122.99
24	Y	101	BCR	C38-C26-C25	-2.10	122.19	124.48
22	a	404	CLA	C3D-C4D-ND	2.10	113.41	109.99
27	A	411	LMG	O8-C28-O10	-2.10	118.37	123.63
27	c	523	LMG	C3-C4-C5	-2.10	106.43	110.23
24	a	405	BCR	C30-C25-C26	-2.10	119.77	122.64
30	c	517	DGD	C4A-C3A-C2A	-2.10	105.42	113.13
22	C	507	CLA	CBC-CAC-C3C	-2.10	106.73	112.42
23	a	403	PHO	CMB-C2B-C3B	2.10	128.87	124.68
30	H	102	DGD	O3E-C3E-C2E	-2.10	105.43	110.38
24	C	514	BCR	C38-C26-C25	-2.10	122.20	124.48
22	b	616	CLA	C2A-C3A-C4A	2.10	105.25	101.87
33	j	101	STE	O2-C1-C2	2.10	120.62	114.00
26	d	407	PL9	C40-C39-C38	-2.09	118.25	123.63
24	D	405	BCR	C35-C13-C14	-2.09	119.43	122.82
22	A	403	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
22	d	404	CLA	C17-C16-C15	-2.09	103.91	113.28
22	b	610	CLA	CHC-C4B-NB	2.09	127.19	124.05
22	C	512	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
27	M	101	LMG	C38-C37-C36	-2.09	103.80	114.37
22	b	604	CLA	C2A-C1A-CHA	2.09	127.49	123.87
22	C	509	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
22	c	504	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
35	v	201	HEC	O1D-CGD-CBD	-2.09	116.47	123.09
24	c	515	BCR	C35-C13-C12	2.09	121.28	118.09
24	T	101	BCR	C2-C1-C6	2.08	113.47	110.44
30	c	519	DGD	O5D-C1E-C2E	2.08	111.44	108.27
29	a	411	SQD	O4-C4-C3	-2.08	105.47	110.38
22	b	603	CLA	CHD-C4C-NC	2.08	127.46	124.23
35	V	201	HEC	CHD-C4C-NC	2.08	127.64	123.86
22	B	616	CLA	C4D-CHA-C1A	2.08	123.72	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	c	509	CLA	C3A-C2A-C1A	2.08	104.45	101.34
24	D	405	BCR	C33-C5-C6	-2.08	122.22	124.48
33	d	411	STE	C6-C5-C4	-2.08	103.86	114.37
22	b	606	CLA	C1-O2A-CGA	2.08	121.68	116.65
22	b	604	CLA	CGD-CBD-CAD	-2.08	104.12	110.85
24	b	618	BCR	C7-C8-C9	-2.08	123.16	126.23
30	c	519	DGD	O2D-C2D-C1D	-2.08	105.13	110.08
22	C	508	CLA	C1-C2-C3	-2.07	122.80	126.20
22	b	606	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	A	410	PL9	C7-C8-C9	-2.07	123.26	126.83
28	e	101	LHG	C20-C19-C18	-2.07	103.89	114.37
24	b	618	BCR	C15-C16-C17	-2.07	119.28	123.52
22	C	502	CLA	O1D-CGD-CBD	2.07	128.60	124.52
24	C	516	BCR	C29-C30-C25	2.07	113.45	110.44
24	B	618	BCR	C40-C30-C29	-2.07	101.00	108.95
24	b	619	BCR	C15-C16-C17	-2.07	119.28	123.52
22	b	605	CLA	CMB-C2B-C3B	2.07	131.42	126.55
22	B	615	CLA	C1-C2-C3	2.07	129.59	126.20
22	C	504	CLA	CHD-C4C-NC	2.07	127.44	124.23
24	C	516	BCR	C24-C23-C22	-2.07	123.18	126.23
22	d	405	CLA	CHB-C1B-C2B	-2.07	121.43	127.43
24	C	515	BCR	C38-C26-C27	-2.06	109.19	113.60
26	a	409	PL9	C12-C13-C14	-2.06	122.91	127.62
27	C	520	LMG	C38-C37-C36	-2.06	103.95	114.37
27	b	623	LMG	C38-C37-C36	-2.06	103.96	114.37
27	D	410	LMG	O8-C28-O10	-2.06	118.48	123.63
22	B	609	CLA	C7-C6-C5	-2.06	107.78	113.26
22	b	611	CLA	CMB-C2B-C3B	2.06	131.39	126.55
29	b	620	SQD	O48-C23-O10	-2.06	118.48	123.63
22	B	602	CLA	CHC-C4B-NB	2.06	127.13	124.05
24	t	101	BCR	C21-C20-C19	-2.06	117.24	123.20
22	b	603	CLA	CHC-C4B-NB	2.06	127.13	124.05
22	B	609	CLA	CHD-C1D-ND	-2.05	121.92	124.80
28	A	412	LHG	O8-C23-O10	-2.05	118.50	123.63
35	v	201	HEC	C1B-C2B-C3B	2.05	109.14	106.98
22	d	404	CLA	C1-O2A-CGA	2.05	121.61	116.65
22	A	406	CLA	C4A-NA-C1A	2.05	107.61	106.68
29	B	623	SQD	C27-C26-C25	-2.05	104.02	114.37
22	B	606	CLA	CHC-C4B-NB	2.05	127.12	124.05
26	a	409	PL9	C7-C8-C9	-2.05	123.31	126.83
22	C	502	CLA	CHB-C1B-NB	2.05	127.12	124.05
27	A	411	LMG	C9-C8-C7	-2.05	107.01	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	415	DGD	C5B-C4B-C3B	-2.05	104.03	114.37
22	B	615	CLA	C2C-C1C-NC	2.05	112.13	109.98
22	c	507	CLA	CHC-C1C-C2C	-2.05	121.14	126.95
22	c	506	CLA	C4-C3-C5	2.04	118.78	115.23
22	B	606	CLA	CHD-C1D-ND	-2.04	121.93	124.80
29	B	623	SQD	O5-C1-C2	-2.04	106.17	110.37
24	b	618	BCR	C29-C30-C25	2.04	113.40	110.44
22	c	503	CLA	C11-C12-C13	-2.04	109.18	115.97
22	b	608	CLA	CHB-C4A-NA	2.04	127.34	124.40
22	A	406	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
27	C	520	LMG	C20-C19-C18	-2.04	104.06	114.37
24	D	405	BCR	C35-C13-C12	2.04	121.20	118.09
22	c	502	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
22	d	403	CLA	CHA-C1A-NA	-2.04	121.78	126.39
22	c	508	CLA	CHD-C1D-C2D	2.04	129.72	125.49
22	B	616	CLA	C5-C3-C2	2.04	125.74	121.17
22	C	502	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
22	b	602	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
28	A	412	LHG	O3-P-O5	-2.03	100.87	108.94
22	B	608	CLA	CMB-C2B-C3B	2.03	131.33	126.55
27	a	416	LMG	C32-C31-C30	-2.03	104.09	114.37
29	B	623	SQD	C25-C24-C23	-2.03	106.25	113.69
23	d	402	PHO	C4B-NB-C1B	2.03	111.78	108.82
30	c	519	DGD	O6E-C1E-O5D	-2.03	105.24	110.04
30	c	519	DGD	CDB-CCB-CBB	-2.03	104.10	114.37
22	c	508	CLA	C3B-C4B-NB	-2.03	108.72	110.53
27	d	410	LMG	C3-C4-C5	-2.03	106.55	110.23
24	x	101	BCR	C33-C5-C6	-2.03	122.27	124.48
26	A	410	PL9	O2-C1-C2	-2.03	117.21	121.83
27	b	623	LMG	C40-C39-C38	-2.03	104.12	114.37
22	d	405	CLA	CHB-C1B-NB	2.03	127.09	124.05
28	B	621	LHG	C20-C19-C18	-2.03	104.12	114.37
22	b	608	CLA	C2A-C1A-CHA	2.03	127.39	123.87
22	c	507	CLA	C3B-C4B-NB	-2.03	108.72	110.53
29	f	102	SQD	O48-C23-O10	-2.03	118.56	123.63
24	b	617	BCR	C29-C28-C27	2.03	115.73	111.28
28	l	101	LHG	C13-C12-C11	-2.03	104.13	114.37
22	b	611	CLA	CAC-C3C-C4C	2.03	127.42	124.79
22	c	507	CLA	C2C-C1C-NC	2.03	112.11	109.98
22	A	402	CLA	C1C-C2C-C3C	-2.02	104.85	106.98
22	A	406	CLA	CHC-C4B-NB	2.02	127.08	124.05
23	d	402	PHO	CMA-C3A-C4A	-2.02	110.25	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	t	101	BCR	C15-C14-C13	-2.02	124.45	127.28
23	A	404	PHO	CED-O2D-CGD	2.02	120.49	115.92
22	b	603	CLA	C4-C3-C5	2.02	118.73	115.23
24	b	618	BCR	C27-C26-C25	2.02	125.43	122.70
22	C	509	CLA	C2A-C3A-C4A	2.02	105.12	101.87
22	d	405	CLA	CHD-C1D-ND	-2.01	121.97	124.80
35	f	101	HEC	C1D-C2D-C3D	-2.01	104.86	106.98
27	C	520	LMG	C40-C39-C38	-2.01	104.19	114.37
22	d	404	CLA	CMD-C2D-C3D	2.01	132.31	127.69
27	a	416	LMG	C4-C3-C2	-2.01	107.30	110.83
26	d	407	PL9	C32-C33-C34	-2.01	123.02	127.62
22	d	403	CLA	C2A-C1A-CHA	2.01	127.36	123.87
30	C	518	DGD	CDB-CCB-CBB	-2.01	104.20	114.37
22	c	501	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
22	C	503	CLA	CHB-C4A-NA	2.01	127.30	124.40
35	F	101	HEC	O2D-CGD-CBD	2.01	120.35	114.00
24	c	515	BCR	C28-C27-C26	-2.01	110.47	114.06
23	A	405	PHO	CAC-C3C-C2C	2.01	131.25	127.56
22	B	608	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
22	C	504	CLA	CHB-C4A-NA	2.01	127.30	124.40
22	B	613	CLA	CAC-C3C-C4C	2.01	127.40	124.79
22	b	608	CLA	O2D-CGD-CBD	2.01	114.74	111.23
22	C	510	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
22	b	606	CLA	C2C-C1C-NC	2.01	112.09	109.98
27	C	520	LMG	O3-C3-C2	-2.00	105.65	110.38
22	D	404	CLA	C2C-C1C-NC	2.00	112.09	109.98
22	C	507	CLA	C4-C3-C5	2.00	118.71	115.23
30	h	101	DGD	O3G-C1D-C2D	-2.00	105.23	108.27
22	B	608	CLA	CHA-C1A-NA	-2.00	121.86	126.39
30	C	519	DGD	O3E-C3E-C2E	-2.00	105.66	110.38
30	C	519	DGD	O6E-C5E-C4E	2.00	113.30	109.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	F	101	HEC	NA
35	V	201	HEC	NA
35	f	101	HEC	NA
35	v	201	HEC	NA

All (1711) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	B	601	CLA	C1A-C2A-CAA-CBA
22	B	606	CLA	C2B-C3B-CAB-CBB
22	B	606	CLA	C4B-C3B-CAB-CBB
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	512	CLA	C11-C10-C8-C9
22	C	513	CLA	O2A-C1-C2-C3
22	b	605	CLA	C4B-C3B-CAB-CBB
22	b	614	CLA	CAD-CBD-CGD-O1D
22	b	614	CLA	CAD-CBD-CGD-O2D
22	b	616	CLA	CBD-CGD-O2D-CED
22	c	507	CLA	CHA-CBD-CGD-O1D
22	c	507	CLA	CHA-CBD-CGD-O2D
22	c	510	CLA	C11-C12-C13-C14
22	c	513	CLA	CBD-CGD-O2D-CED
24	B	617	BCR	C35-C13-C14-C15
24	C	514	BCR	C11-C12-C13-C14
24	C	514	BCR	C11-C12-C13-C35
24	C	515	BCR	C11-C12-C13-C14
24	C	516	BCR	C17-C18-C19-C20
24	C	516	BCR	C36-C18-C19-C20
24	C	516	BCR	C37-C22-C23-C24
24	D	405	BCR	C23-C24-C25-C26
24	D	405	BCR	C23-C24-C25-C30
24	H	101	BCR	C11-C12-C13-C35
24	T	101	BCR	C11-C12-C13-C35
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	b	617	BCR	C20-C21-C22-C37
24	b	618	BCR	C16-C17-C18-C36
24	c	514	BCR	C35-C13-C14-C15
24	c	514	BCR	C16-C17-C18-C19
24	c	514	BCR	C16-C17-C18-C36
24	c	514	BCR	C20-C21-C22-C23
24	c	514	BCR	C20-C21-C22-C37
24	d	406	BCR	C37-C22-C23-C24
24	k	101	BCR	C5-C6-C7-C8
26	A	410	PL9	C12-C13-C14-C15
26	A	410	PL9	C12-C13-C14-C16
26	A	410	PL9	C22-C23-C24-C26
26	A	410	PL9	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
26	A	410	PL9	C37-C38-C39-C41
26	D	406	PL9	C32-C33-C34-C36
26	a	409	PL9	C12-C13-C14-C15
26	a	409	PL9	C17-C18-C19-C21
26	a	409	PL9	C19-C21-C22-C23
26	a	409	PL9	C22-C23-C24-C25
26	a	409	PL9	C22-C23-C24-C26
26	a	409	PL9	C32-C33-C34-C36
26	a	409	PL9	C37-C38-C39-C41
26	a	409	PL9	C42-C43-C44-C46
26	d	407	PL9	C32-C33-C34-C36
26	d	407	PL9	C42-C43-C44-C45
27	A	411	LMG	O9-C10-O7-C8
27	D	410	LMG	O1-C7-C8-C9
27	D	410	LMG	O1-C7-C8-O7
27	b	623	LMG	C11-C10-O7-C8
27	c	523	LMG	O6-C1-O1-C7
28	A	412	LHG	C3-O3-P-O5
28	A	412	LHG	C3-O3-P-O6
28	B	621	LHG	C4-O6-P-O3
28	B	622	LHG	O1-C1-C2-C3
28	D	409	LHG	O1-C1-C2-C3
28	D	409	LHG	C3-O3-P-O5
28	D	409	LHG	C4-O6-P-O3
28	D	409	LHG	C4-O6-P-O4
28	E	101	LHG	O1-C1-C2-C3
28	E	101	LHG	O10-C23-O8-C6
28	a	410	LHG	C3-O3-P-O4
28	a	410	LHG	C3-O3-P-O6
28	d	408	LHG	C3-O3-P-O4
28	d	408	LHG	C3-O3-P-O6
28	d	408	LHG	C4-O6-P-O3
28	d	408	LHG	C4-O6-P-O4
28	d	408	LHG	C4-O6-P-O5
28	e	101	LHG	C1-C2-C3-O3
28	e	101	LHG	O2-C2-C3-O3
28	e	101	LHG	C3-O3-P-O5
28	e	101	LHG	C3-O3-P-O6
28	e	101	LHG	C4-O6-P-O3
28	e	101	LHG	C4-O6-P-O5
28	e	101	LHG	O6-C4-C5-O7
28	e	101	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
28	l	101	LHG	C4-O6-P-O3
29	A	414	SQD	C46-C45-O47-C7
29	B	623	SQD	O5-C1-O6-C44
29	B	623	SQD	O6-C44-C45-O47
29	B	623	SQD	O49-C7-O47-C45
29	D	408	SQD	O5-C1-O6-C44
29	a	412	SQD	O6-C44-C45-O47
29	b	620	SQD	O10-C23-O48-C46
29	f	102	SQD	C2-C1-O6-C44
29	f	102	SQD	O5-C1-O6-C44
30	A	415	DGD	C2B-C1B-O2G-C2G
30	A	415	DGD	O1B-C1B-O2G-C2G
35	V	201	HEC	C2C-C3C-CAC-CBC
35	f	101	HEC	C2B-C3B-CAB-CBB
35	f	101	HEC	C4B-C3B-CAB-CBB
35	F	101	HEC	C4B-C3B-CAB-CBB
27	c	523	LMG	O10-C28-O8-C9
29	D	408	SQD	O10-C23-O48-C46
35	F	101	HEC	C2B-C3B-CAB-CBB
35	V	201	HEC	C4C-C3C-CAC-CBC
22	b	616	CLA	O1D-CGD-O2D-CED
28	E	101	LHG	C24-C23-O8-C6
28	e	101	LHG	C24-C23-O8-C6
29	D	408	SQD	C24-C23-O48-C46
29	b	620	SQD	C24-C23-O48-C46
27	M	101	LMG	O10-C28-O8-C9
27	c	522	LMG	O10-C28-O8-C9
29	a	412	SQD	O10-C23-O48-C46
29	f	102	SQD	O10-C23-O48-C46
22	c	513	CLA	O1D-CGD-O2D-CED
27	D	410	LMG	O9-C10-O7-C8
27	b	623	LMG	O9-C10-O7-C8
29	a	412	SQD	O49-C7-O47-C45
26	A	410	PL9	C47-C48-C49-C50
22	b	601	CLA	C3-C5-C6-C7
22	d	405	CLA	C3-C5-C6-C7
29	B	623	SQD	C45-C46-O48-C23
27	M	101	LMG	C29-C28-O8-C9
27	c	522	LMG	C29-C28-O8-C9
27	c	523	LMG	C29-C28-O8-C9
29	f	102	SQD	C24-C23-O48-C46
27	A	411	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
29	B	623	SQD	C8-C7-O47-C45
29	a	412	SQD	C8-C7-O47-C45
22	A	406	CLA	C4-C3-C5-C6
22	B	614	CLA	C4-C3-C5-C6
22	b	603	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
22	A	406	CLA	C2-C3-C5-C6
22	B	614	CLA	C2-C3-C5-C6
26	A	410	PL9	C23-C24-C26-C27
26	A	410	PL9	C43-C44-C46-C47
26	D	406	PL9	C33-C34-C36-C37
26	d	407	PL9	C38-C39-C41-C42
22	b	602	CLA	C3-C5-C6-C7
27	c	520	LMG	C11-C10-O7-C8
26	A	410	PL9	C22-C23-C24-C25
22	B	601	CLA	O1A-CGA-O2A-C1
29	A	414	SQD	O49-C7-O47-C45
22	B	601	CLA	CBA-CGA-O2A-C1
29	a	412	SQD	C24-C23-O48-C46
27	a	416	LMG	O6-C5-C6-O5
27	C	520	LMG	C11-C10-O7-C8
29	b	620	SQD	C8-C7-O47-C45
26	A	410	PL9	C47-C48-C49-C51
26	d	407	PL9	C47-C48-C49-C51
22	C	501	CLA	CBD-CGD-O2D-CED
27	a	416	LMG	C4-C5-C6-O5
22	B	603	CLA	C4-C3-C5-C6
22	b	605	CLA	C4-C3-C5-C6
22	B	603	CLA	C2-C3-C5-C6
22	C	504	CLA	C2-C3-C5-C6
22	b	603	CLA	C2-C3-C5-C6
22	b	605	CLA	C2-C3-C5-C6
26	a	409	PL9	C33-C34-C36-C37
26	A	410	PL9	C9-C11-C12-C13
26	A	410	PL9	C34-C36-C37-C38
26	A	410	PL9	C44-C46-C47-C48
26	a	409	PL9	C24-C26-C27-C28
26	a	409	PL9	C34-C36-C37-C38
26	d	407	PL9	C34-C36-C37-C38
35	v	201	HEC	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	CBA-CGA-O2A-C1
22	C	510	CLA	CBD-CGD-O2D-CED
22	C	511	CLA	CBD-CGD-O2D-CED
27	d	410	LMG	C10-C11-C12-C13
26	D	406	PL9	C37-C38-C39-C40
26	d	407	PL9	C32-C33-C34-C35
33	D	412	STE	C13-C14-C15-C16
22	b	609	CLA	CBD-CGD-O2D-CED
22	c	508	CLA	CBD-CGD-O2D-CED
22	c	511	CLA	CBD-CGD-O2D-CED
27	D	410	LMG	C11-C10-O7-C8
30	C	517	DGD	C1B-C2B-C3B-C4B
33	C	523	STE	C4-C5-C6-C7
35	v	201	HEC	C4C-C3C-CAC-CBC
28	E	101	LHG	C1-C2-C3-O3
22	B	616	CLA	CBA-CGA-O2A-C1
27	a	416	LMG	C29-C28-O8-C9
29	B	623	SQD	C24-C23-O48-C46
22	C	509	CLA	CBD-CGD-O2D-CED
22	C	504	CLA	C4-C3-C5-C6
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	409	PL9	C23-C24-C26-C27
22	B	613	CLA	C11-C12-C13-C14
22	C	507	CLA	C11-C10-C8-C9
22	D	403	CLA	C14-C13-C15-C16
22	D	404	CLA	C11-C12-C13-C14
22	b	601	CLA	C14-C13-C15-C16
22	b	602	CLA	C11-C10-C8-C9
22	b	613	CLA	C11-C12-C13-C14
22	c	509	CLA	C6-C7-C8-C9
22	c	511	CLA	C14-C13-C15-C16
23	A	405	PHO	C6-C7-C8-C9
29	B	623	SQD	C2-C1-O6-C44
28	E	101	LHG	O2-C2-C3-O3
27	A	411	LMG	O6-C5-C6-O5
24	A	407	BCR	C36-C18-C19-C20
24	C	515	BCR	C37-C22-C23-C24
24	C	516	BCR	C7-C8-C9-C34
24	D	405	BCR	C36-C18-C19-C20
24	T	101	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
24	Y	101	BCR	C37-C22-C23-C24
24	c	514	BCR	C7-C8-C9-C34
24	c	514	BCR	C11-C12-C13-C35
24	k	101	BCR	C7-C8-C9-C34
24	t	101	BCR	C7-C8-C9-C34
27	b	623	LMG	C28-C29-C30-C31
22	B	616	CLA	O1A-CGA-O2A-C1
27	a	416	LMG	C11-C10-O7-C8
22	c	506	CLA	CBA-CGA-O2A-C1
22	a	404	CLA	C10-C11-C12-C13
22	B	616	CLA	C2-C1-O2A-CGA
26	A	410	PL9	C7-C8-C9-C10
24	C	514	BCR	C14-C15-C16-C17
22	b	611	CLA	C15-C16-C17-C18
26	a	409	PL9	C47-C48-C49-C50
22	c	506	CLA	C15-C16-C17-C18
22	B	612	CLA	CBD-CGD-O2D-CED
22	B	611	CLA	C12-C13-C15-C16
22	b	613	CLA	C11-C10-C8-C7
26	a	409	PL9	C20-C19-C21-C22
22	D	404	CLA	C10-C11-C12-C13
22	a	404	CLA	C15-C16-C17-C18
28	a	410	LHG	C7-C8-C9-C10
26	A	410	PL9	C39-C41-C42-C43
33	d	412	STE	C2-C3-C4-C5
22	C	505	CLA	C5-C6-C7-C8
22	b	611	CLA	C13-C15-C16-C17
22	d	401	CLA	C8-C10-C11-C12
30	h	101	DGD	O6E-C5E-C6E-O5E
27	D	410	LMG	C28-C29-C30-C31
27	D	411	LMG	C28-C29-C30-C31
27	d	410	LMG	C28-C29-C30-C31
28	B	622	LHG	C23-C24-C25-C26
28	E	101	LHG	C23-C24-C25-C26
33	R	101	STE	C1-C2-C3-C4
33	b	624	STE	C1-C2-C3-C4
22	c	506	CLA	O1A-CGA-O2A-C1
22	B	602	CLA	C13-C15-C16-C17
22	B	612	CLA	C13-C15-C16-C17
22	B	614	CLA	C13-C15-C16-C17
22	C	505	CLA	C10-C11-C12-C13
22	C	509	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	C	513	CLA	C15-C16-C17-C18
22	c	505	CLA	C5-C6-C7-C8
22	c	510	CLA	C10-C11-C12-C13
22	c	510	CLA	C15-C16-C17-C18
22	c	512	CLA	C13-C15-C16-C17
22	b	606	CLA	C2A-CAA-CBA-CGA
24	c	514	BCR	C18-C19-C20-C21
22	C	503	CLA	C5-C6-C7-C8
22	C	512	CLA	C10-C11-C12-C13
22	b	611	CLA	C8-C10-C11-C12
22	b	615	CLA	C10-C11-C12-C13
27	D	407	LMG	C10-C11-C12-C13
27	c	520	LMG	C28-C29-C30-C31
28	B	622	LHG	C7-C8-C9-C10
28	a	410	LHG	C23-C24-C25-C26
30	c	517	DGD	C1B-C2B-C3B-C4B
30	c	519	DGD	C1A-C2A-C3A-C4A
33	B	626	STE	C1-C2-C3-C4
33	C	521	STE	C1-C2-C3-C4
22	B	614	CLA	C3-C5-C6-C7
29	b	620	SQD	O5-C1-O6-C44
22	B	605	CLA	C15-C16-C17-C18
22	B	606	CLA	C15-C16-C17-C18
22	B	609	CLA	C13-C15-C16-C17
22	B	613	CLA	C8-C10-C11-C12
22	C	508	CLA	C15-C16-C17-C18
22	b	607	CLA	C10-C11-C12-C13
28	a	410	LHG	O2-C2-C3-O3
22	C	513	CLA	O1A-CGA-O2A-C1
22	B	601	CLA	C5-C6-C7-C8
22	C	506	CLA	C8-C10-C11-C12
28	e	101	LHG	O9-C7-O7-C5
22	B	608	CLA	C15-C16-C17-C18
30	C	519	DGD	C8A-C9A-CAA-CBA
22	C	506	CLA	C15-C16-C17-C18
22	c	509	CLA	C10-C11-C12-C13
22	c	509	CLA	C13-C15-C16-C17
26	A	410	PL9	C32-C33-C34-C36
33	b	625	STE	C1-C2-C3-C4
22	c	512	CLA	C8-C10-C11-C12
28	d	409	LHG	C24-C25-C26-C27
24	c	514	BCR	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
22	b	603	CLA	C13-C15-C16-C17
22	c	506	CLA	C13-C15-C16-C17
27	m	101	LMG	C10-C11-C12-C13
27	c	522	LMG	O9-C10-O7-C8
28	a	410	LHG	C1-C2-C3-O3
22	B	601	CLA	C13-C15-C16-C17
22	D	404	CLA	C13-C15-C16-C17
22	b	601	CLA	C8-C10-C11-C12
22	c	507	CLA	C5-C6-C7-C8
22	c	511	CLA	C13-C15-C16-C17
22	C	505	CLA	C15-C16-C17-C18
22	c	510	CLA	C8-C10-C11-C12
22	c	511	CLA	C15-C16-C17-C18
22	B	611	CLA	C13-C15-C16-C17
22	c	503	CLA	C8-C10-C11-C12
22	c	512	CLA	CBA-CGA-O2A-C1
26	A	410	PL9	C40-C39-C41-C42
27	c	522	LMG	C11-C10-O7-C8
22	A	403	CLA	C14-C13-C15-C16
26	D	406	PL9	C27-C28-C29-C30
30	C	518	DGD	C2E-C1E-O5D-C6D
30	c	518	DGD	C2E-C1E-O5D-C6D
27	A	411	LMG	C4-C5-C6-O5
28	A	412	LHG	O2-C2-C3-O3
24	A	407	BCR	C35-C13-C14-C15
24	A	407	BCR	C20-C21-C22-C37
24	B	617	BCR	C16-C17-C18-C36
24	B	617	BCR	C20-C21-C22-C37
24	C	514	BCR	C16-C17-C18-C36
24	C	516	BCR	C11-C10-C9-C34
24	D	405	BCR	C20-C21-C22-C37
24	c	515	BCR	C16-C17-C18-C36
24	k	101	BCR	C35-C13-C14-C15
24	t	101	BCR	C35-C13-C14-C15
24	t	101	BCR	C16-C17-C18-C36
24	x	101	BCR	C16-C17-C18-C36
22	c	512	CLA	C3-C5-C6-C7
22	d	403	CLA	C3-C5-C6-C7
22	b	614	CLA	C5-C6-C7-C8
24	A	407	BCR	C11-C12-C13-C35
24	C	515	BCR	C11-C12-C13-C35
24	C	515	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	H	101	BCR	C37-C22-C23-C24
24	k	101	BCR	C36-C18-C19-C20
24	D	405	BCR	C21-C22-C23-C24
24	d	406	BCR	C21-C22-C23-C24
28	a	410	LHG	O1-C1-C2-C3
28	d	408	LHG	O1-C1-C2-C3
28	d	409	LHG	O1-C1-C2-C3
22	b	607	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C19
30	c	519	DGD	O1A-C1A-O1G-C1G
22	C	512	CLA	C3-C5-C6-C7
24	C	514	BCR	C11-C10-C9-C8
24	C	516	BCR	C20-C21-C22-C23
24	T	101	BCR	C12-C13-C14-C15
24	b	617	BCR	C20-C21-C22-C23
24	b	618	BCR	C20-C21-C22-C23
24	k	101	BCR	C11-C10-C9-C8
24	x	101	BCR	C11-C10-C9-C8
24	x	101	BCR	C16-C17-C18-C19
30	C	518	DGD	O6E-C1E-O5D-C6D
29	a	411	SQD	O6-C44-C45-O47
22	B	605	CLA	C8-C10-C11-C12
22	B	616	CLA	C11-C12-C13-C15
22	a	402	CLA	C16-C17-C18-C19
22	a	402	CLA	C16-C17-C18-C20
22	b	607	CLA	C16-C17-C18-C19
22	c	511	CLA	C16-C17-C18-C19
27	a	416	LMG	O10-C28-O8-C9
22	b	610	CLA	C15-C16-C17-C18
22	b	615	CLA	C5-C6-C7-C8
28	l	101	LHG	C29-C30-C31-C32
33	J	101	STE	C5-C6-C7-C8
33	d	412	STE	C11-C12-C13-C14
27	D	407	LMG	C34-C35-C36-C37
27	b	623	LMG	C23-C24-C25-C26
27	c	522	LMG	C16-C17-C18-C19
28	B	621	LHG	C17-C18-C19-C20
28	a	410	LHG	C10-C11-C12-C13
29	B	623	SQD	C11-C12-C13-C14
30	H	102	DGD	C7A-C8A-C9A-CAA
33	D	412	STE	C9-C10-C11-C12
33	b	625	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	t	103	STE	C5-C6-C7-C8
22	b	615	CLA	C15-C16-C17-C18
27	c	523	LMG	C15-C16-C17-C18
28	A	412	LHG	C29-C30-C31-C32
29	A	414	SQD	C12-C13-C14-C15
30	C	517	DGD	C5B-C6B-C7B-C8B
30	c	518	DGD	CAB-CBB-CCB-CDB
33	B	620	STE	C9-C10-C11-C12
33	m	102	STE	C3-C4-C5-C6
22	C	501	CLA	O1D-CGD-O2D-CED
27	A	411	LMG	C35-C36-C37-C38
27	A	411	LMG	C38-C39-C40-C41
27	D	411	LMG	C14-C15-C16-C17
27	d	410	LMG	C33-C34-C35-C36
28	B	621	LHG	C31-C32-C33-C34
29	a	411	SQD	C17-C18-C19-C20
29	a	411	SQD	C25-C26-C27-C28
29	a	412	SQD	C10-C11-C12-C13
29	b	620	SQD	C25-C26-C27-C28
30	C	518	DGD	C5A-C6A-C7A-C8A
30	C	519	DGD	CBA-CCA-CDA-CEA
30	h	101	DGD	C7A-C8A-C9A-CAA
33	b	621	STE	C4-C5-C6-C7
28	D	409	LHG	O1-C1-C2-O2
28	E	101	LHG	O1-C1-C2-O2
27	D	411	LMG	C16-C17-C18-C19
27	a	416	LMG	C41-C42-C43-C44
27	b	623	LMG	C11-C12-C13-C14
28	d	408	LHG	C32-C33-C34-C35
28	d	409	LHG	C32-C33-C34-C35
30	C	518	DGD	C9A-CAA-CBA-CCA
33	D	412	STE	C2-C3-C4-C5
33	d	413	STE	C6-C7-C8-C9
33	k	102	STE	C6-C7-C8-C9
22	C	506	CLA	C13-C15-C16-C17
27	A	411	LMG	C14-C15-C16-C17
27	C	520	LMG	C18-C19-C20-C21
27	a	416	LMG	C15-C16-C17-C18
30	c	518	DGD	CCA-CDA-CEA-CFA
30	c	518	DGD	CBB-CCB-CDB-CEB
22	B	606	CLA	C16-C17-C18-C19
22	B	615	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
22	c	511	CLA	C16-C17-C18-C20
22	d	403	CLA	C16-C17-C18-C20
22	d	405	CLA	C16-C17-C18-C20
22	c	512	CLA	O1A-CGA-O2A-C1
22	B	606	CLA	C2A-CAA-CBA-CGA
33	t	103	STE	C11-C12-C13-C14
27	c	523	LMG	C11-C10-O7-C8
27	M	101	LMG	C17-C18-C19-C20
28	B	622	LHG	C14-C15-C16-C17
30	A	415	DGD	C2A-C3A-C4A-C5A
30	C	517	DGD	C8A-C9A-CAA-CBA
33	B	620	STE	C4-C5-C6-C7
35	V	201	HEC	C2B-C3B-CAB-CBB
22	c	504	CLA	C11-C10-C8-C7
27	c	520	LMG	C36-C37-C38-C39
30	h	101	DGD	C5B-C6B-C7B-C8B
28	D	409	LHG	O2-C2-C3-O3
22	c	505	CLA	C15-C16-C17-C18
22	d	405	CLA	C10-C11-C12-C13
27	A	411	LMG	C11-C12-C13-C14
27	D	407	LMG	C32-C33-C34-C35
27	D	410	LMG	C14-C15-C16-C17
27	d	410	LMG	C36-C37-C38-C39
30	C	518	DGD	C7B-C8B-C9B-CAB
33	a	415	STE	C5-C6-C7-C8
22	B	601	CLA	C3A-C2A-CAA-CBA
22	C	510	CLA	O1D-CGD-O2D-CED
22	b	609	CLA	O1D-CGD-O2D-CED
27	c	523	LMG	C12-C13-C14-C15
28	E	101	LHG	C9-C10-C11-C12
27	c	522	LMG	C34-C35-C36-C37
22	C	512	CLA	C13-C15-C16-C17
22	b	601	CLA	C10-C11-C12-C13
22	c	508	CLA	O1D-CGD-O2D-CED
27	m	101	LMG	C14-C15-C16-C17
22	B	606	CLA	C16-C17-C18-C20
29	B	623	SQD	O10-C23-O48-C46
28	A	412	LHG	C32-C33-C34-C35
22	C	505	CLA	CBD-CGD-O2D-CED
22	C	513	CLA	CBD-CGD-O2D-CED
27	m	101	LMG	C32-C33-C34-C35
29	a	411	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	a	416	LMG	O1-C7-C8-C9
29	a	411	SQD	O6-C44-C45-C46
28	A	412	LHG	C11-C12-C13-C14
28	B	622	LHG	C27-C28-C29-C30
29	a	411	SQD	C34-C35-C36-C37
30	c	517	DGD	C7A-C8A-C9A-CAA
33	l	102	STE	C14-C15-C16-C17
22	B	605	CLA	C3-C5-C6-C7
28	d	409	LHG	C23-C24-C25-C26
22	B	606	CLA	C8-C10-C11-C12
27	A	411	LMG	C33-C34-C35-C36
27	b	623	LMG	C16-C17-C18-C19
27	m	101	LMG	C33-C34-C35-C36
28	B	621	LHG	C14-C15-C16-C17
28	D	409	LHG	C33-C34-C35-C36
28	d	408	LHG	C29-C30-C31-C32
28	d	409	LHG	C34-C35-C36-C37
28	e	101	LHG	C26-C27-C28-C29
29	A	414	SQD	C10-C11-C12-C13
30	A	415	DGD	C5B-C6B-C7B-C8B
30	C	518	DGD	CAB-CBB-CCB-CDB
33	b	627	STE	C11-C12-C13-C14
33	d	413	STE	C13-C14-C15-C16
27	a	416	LMG	C12-C13-C14-C15
28	e	101	LHG	C11-C10-C9-C8
33	D	412	STE	C11-C12-C13-C14
33	t	102	STE	C6-C7-C8-C9
33	t	103	STE	C2-C3-C4-C5
27	C	520	LMG	C32-C33-C34-C35
27	D	407	LMG	C17-C18-C19-C20
27	D	411	LMG	C29-C30-C31-C32
27	a	416	LMG	C33-C34-C35-C36
28	A	412	LHG	C14-C15-C16-C17
28	E	101	LHG	C27-C28-C29-C30
28	e	101	LHG	C13-C14-C15-C16
29	B	623	SQD	C33-C34-C35-C36
29	a	411	SQD	C24-C25-C26-C27
29	f	102	SQD	C29-C30-C31-C32
30	h	101	DGD	C2B-C3B-C4B-C5B
33	T	102	STE	C11-C12-C13-C14
22	B	616	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
22	b	605	CLA	C2B-C3B-CAB-CBB
24	d	406	BCR	C23-C24-C25-C26
24	d	406	BCR	C23-C24-C25-C30
24	k	101	BCR	C1-C6-C7-C8
27	c	522	LMG	C30-C31-C32-C33
28	e	101	LHG	C8-C7-O7-C5
29	D	408	SQD	C44-C45-C46-O48
22	A	402	CLA	C15-C16-C17-C18
28	D	409	LHG	C11-C12-C13-C14
28	l	101	LHG	C14-C15-C16-C17
33	C	522	STE	C5-C6-C7-C8
33	a	415	STE	C3-C4-C5-C6
28	d	409	LHG	C26-C27-C28-C29
33	D	412	STE	C7-C8-C9-C10
22	B	614	CLA	C8-C10-C11-C12
27	A	411	LMG	C31-C32-C33-C34
28	D	409	LHG	C25-C26-C27-C28
30	A	415	DGD	CBB-CCB-CDB-CEB
30	C	518	DGD	CBA-CCA-CDA-CEA
30	h	101	DGD	C9A-CAA-CBA-CCA
33	B	625	STE	C2-C3-C4-C5
33	a	415	STE	C9-C10-C11-C12
27	M	101	LMG	C36-C37-C38-C39
28	a	410	LHG	C30-C31-C32-C33
29	A	413	SQD	C30-C31-C32-C33
30	A	415	DGD	CAA-CBA-CCA-CDA
33	B	625	STE	C12-C13-C14-C15
27	M	101	LMG	O9-C10-O7-C8
27	d	410	LMG	C30-C31-C32-C33
26	d	407	PL9	C42-C43-C44-C46
24	B	619	BCR	C10-C11-C12-C13
24	C	514	BCR	C18-C19-C20-C21
24	d	406	BCR	C18-C19-C20-C21
27	c	520	LMG	C33-C34-C35-C36
29	A	413	SQD	C9-C10-C11-C12
33	D	412	STE	C6-C7-C8-C9
27	m	101	LMG	C29-C28-O8-C9
29	a	411	SQD	C24-C23-O48-C46
22	d	405	CLA	C6-C7-C8-C9
28	B	622	LHG	C29-C30-C31-C32
30	C	519	DGD	CAB-CBB-CCB-CDB
33	B	626	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
33	b	626	STE	C2-C3-C4-C5
33	c	521	STE	C9-C10-C11-C12
27	c	522	LMG	C11-C12-C13-C14
29	A	413	SQD	C24-C25-C26-C27
33	R	101	STE	C4-C5-C6-C7
33	T	102	STE	C10-C11-C12-C13
33	b	625	STE	C5-C6-C7-C8
30	c	518	DGD	O6E-C1E-O5D-C6D
30	A	415	DGD	C4B-C5B-C6B-C7B
30	H	102	DGD	C5B-C6B-C7B-C8B
33	B	625	STE	C3-C4-C5-C6
33	M	102	STE	C11-C10-C9-C8
27	c	523	LMG	C2-C1-O1-C7
22	C	510	CLA	C15-C16-C17-C18
33	b	622	STE	C13-C14-C15-C16
29	A	413	SQD	C11-C12-C13-C14
33	d	411	STE	C7-C8-C9-C10
29	D	408	SQD	C32-C33-C34-C35
29	a	412	SQD	C11-C12-C13-C14
29	a	412	SQD	C15-C16-C17-C18
33	B	625	STE	C5-C6-C7-C8
33	T	102	STE	C3-C4-C5-C6
33	b	621	STE	C7-C8-C9-C10
33	b	627	STE	C7-C8-C9-C10
33	c	521	STE	C2-C3-C4-C5
27	D	410	LMG	C29-C28-O8-C9
22	C	507	CLA	C16-C17-C18-C19
22	D	403	CLA	C16-C17-C18-C20
22	b	601	CLA	C16-C17-C18-C20
22	c	505	CLA	C16-C17-C18-C19
27	M	101	LMG	C11-C10-O7-C8
28	E	101	LHG	C11-C12-C13-C14
27	m	101	LMG	O9-C10-O7-C8
27	a	416	LMG	C13-C14-C15-C16
28	D	409	LHG	C28-C29-C30-C31
28	E	101	LHG	C32-C33-C34-C35
29	b	620	SQD	C27-C28-C29-C30
29	f	102	SQD	C32-C33-C34-C35
30	A	415	DGD	CCB-CDB-CEB-CFB
33	b	627	STE	C10-C11-C12-C13
33	d	412	STE	C6-C7-C8-C9
33	M	102	STE	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	Y	101	BCR	C11-C12-C13-C35
29	B	623	SQD	C34-C35-C36-C37
33	H	103	STE	C11-C12-C13-C14
26	a	409	PL9	C37-C38-C39-C40
28	d	409	LHG	C29-C30-C31-C32
29	a	412	SQD	C12-C13-C14-C15
27	a	416	LMG	C8-C7-O1-C1
27	m	101	LMG	C16-C17-C18-C19
22	C	507	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C20
22	c	512	CLA	C16-C17-C18-C19
22	c	512	CLA	C16-C17-C18-C20
27	A	411	LMG	C36-C37-C38-C39
27	D	411	LMG	C30-C31-C32-C33
27	c	520	LMG	C39-C40-C41-C42
28	A	412	LHG	C30-C31-C32-C33
33	b	625	STE	C3-C4-C5-C6
26	D	406	PL9	C35-C34-C36-C37
26	D	406	PL9	C45-C44-C46-C47
27	d	410	LMG	C32-C33-C34-C35
29	B	623	SQD	C28-C29-C30-C31
30	c	519	DGD	C8B-C9B-CAB-CBB
33	B	620	STE	C2-C3-C4-C5
33	T	102	STE	C2-C3-C4-C5
33	d	411	STE	C11-C12-C13-C14
22	C	511	CLA	O1D-CGD-O2D-CED
27	A	411	LMG	C16-C17-C18-C19
27	c	523	LMG	C37-C38-C39-C40
33	a	415	STE	C4-C5-C6-C7
33	b	627	STE	C9-C10-C11-C12
22	B	616	CLA	C3-C5-C6-C7
27	b	623	LMG	O6-C5-C6-O5
22	C	509	CLA	C5-C6-C7-C8
22	C	509	CLA	C13-C15-C16-C17
28	B	621	LHG	C27-C28-C29-C30
30	C	517	DGD	C2A-C3A-C4A-C5A
30	C	518	DGD	CBB-CCB-CDB-CEB
33	B	625	STE	C9-C10-C11-C12
33	a	415	STE	C2-C3-C4-C5
27	c	522	LMG	C10-C11-C12-C13
27	D	407	LMG	C21-C22-C23-C24
33	H	103	STE	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
27	D	407	LMG	O6-C5-C6-O5
27	A	411	LMG	C17-C18-C19-C20
28	A	412	LHG	C34-C35-C36-C37
28	B	622	LHG	C18-C19-C20-C21
28	E	101	LHG	C28-C29-C30-C31
28	E	101	LHG	C29-C30-C31-C32
28	a	410	LHG	C25-C26-C27-C28
28	d	408	LHG	C33-C34-C35-C36
33	I	101	STE	C4-C5-C6-C7
22	D	404	CLA	C5-C6-C7-C8
22	B	613	CLA	C16-C17-C18-C20
22	C	509	CLA	C16-C17-C18-C19
27	m	101	LMG	C39-C40-C41-C42
22	B	612	CLA	C10-C11-C12-C13
27	c	522	LMG	C40-C41-C42-C43
27	c	523	LMG	C33-C34-C35-C36
29	D	408	SQD	C31-C32-C33-C34
33	R	101	STE	C6-C7-C8-C9
33	T	102	STE	C11-C10-C9-C8
29	a	411	SQD	O47-C45-C46-O48
30	A	415	DGD	O2G-C2G-C3G-O3G
28	A	412	LHG	C27-C28-C29-C30
28	E	101	LHG	C33-C34-C35-C36
28	B	621	LHG	C29-C30-C31-C32
28	a	410	LHG	C14-C15-C16-C17
33	B	625	STE	C7-C8-C9-C10
27	M	101	LMG	C14-C15-C16-C17
27	b	623	LMG	C18-C19-C20-C21
29	B	623	SQD	C13-C14-C15-C16
30	c	517	DGD	C2A-C3A-C4A-C5A
33	B	624	STE	C3-C4-C5-C6
33	H	103	STE	C13-C14-C15-C16
33	b	624	STE	C10-C11-C12-C13
27	c	522	LMG	C41-C42-C43-C44
27	m	101	LMG	C18-C19-C20-C21
22	c	505	CLA	C2-C3-C5-C6
33	T	102	STE	C9-C10-C11-C12
33	d	413	STE	C9-C10-C11-C12
27	D	410	LMG	C34-C35-C36-C37
30	C	518	DGD	C6B-C7B-C8B-C9B
22	C	509	CLA	O1D-CGD-O2D-CED
27	A	411	LMG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
27	b	623	LMG	C41-C42-C43-C44
30	C	517	DGD	CBA-CCA-CDA-CEA
22	B	602	CLA	C8-C10-C11-C12
22	c	503	CLA	C5-C6-C7-C8
28	a	410	LHG	C15-C16-C17-C18
33	H	103	STE	C10-C11-C12-C13
33	t	103	STE	C4-C5-C6-C7
22	c	511	CLA	O1D-CGD-O2D-CED
30	c	519	DGD	C3A-C4A-C5A-C6A
33	b	621	STE	C5-C6-C7-C8
28	B	622	LHG	O1-C1-C2-O2
33	m	102	STE	C4-C5-C6-C7
22	c	511	CLA	C1A-C2A-CAA-CBA
22	c	513	CLA	C1A-C2A-CAA-CBA
27	M	101	LMG	C38-C39-C40-C41
30	H	102	DGD	C6B-C7B-C8B-C9B
33	C	521	STE	C6-C7-C8-C9
28	E	101	LHG	C15-C16-C17-C18
28	l	101	LHG	O6-C4-C5-C6
27	C	520	LMG	O9-C10-O7-C8
30	C	517	DGD	CCB-CDB-CEB-CFB
30	c	518	DGD	C1B-C2B-C3B-C4B
22	A	403	CLA	C11-C12-C13-C15
22	B	603	CLA	C11-C12-C13-C15
22	B	615	CLA	C11-C12-C13-C15
22	C	512	CLA	C11-C12-C13-C15
22	a	402	CLA	C12-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C10
22	c	506	CLA	C6-C7-C8-C10
22	c	506	CLA	C11-C12-C13-C15
22	c	508	CLA	C12-C13-C15-C16
22	c	509	CLA	C6-C7-C8-C10
22	c	513	CLA	C11-C12-C13-C15
22	d	401	CLA	C6-C7-C8-C10
22	d	405	CLA	C11-C12-C13-C15
27	a	416	LMG	C36-C37-C38-C39
33	b	625	STE	C7-C8-C9-C10
22	C	509	CLA	C10-C11-C12-C13
22	b	613	CLA	C13-C15-C16-C17
22	c	512	CLA	C5-C6-C7-C8
27	A	411	LMG	C34-C35-C36-C37
27	b	623	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
27	D	410	LMG	C33-C34-C35-C36
27	c	523	LMG	C30-C31-C32-C33
27	m	101	LMG	C12-C13-C14-C15
27	D	407	LMG	C38-C39-C40-C41
22	C	512	CLA	C15-C16-C17-C18
22	B	604	CLA	C14-C13-C15-C16
22	B	610	CLA	C14-C13-C15-C16
22	B	615	CLA	C11-C12-C13-C14
22	c	504	CLA	C11-C10-C8-C9
22	d	405	CLA	C11-C12-C13-C14
22	d	405	CLA	C14-C13-C15-C16
28	B	621	LHG	C12-C13-C14-C15
28	e	101	LHG	C10-C11-C12-C13
29	B	623	SQD	C9-C10-C11-C12
22	B	611	CLA	C8-C10-C11-C12
22	b	613	CLA	CBD-CGD-O2D-CED
35	F	101	HEC	C4C-C3C-CAC-CBC
22	C	510	CLA	C10-C11-C12-C13
30	C	517	DGD	C3A-C4A-C5A-C6A
28	e	101	LHG	C7-C8-C9-C10
26	A	410	PL9	C19-C21-C22-C23
27	M	101	LMG	C7-C8-C9-O8
27	c	522	LMG	C7-C8-C9-O8
27	c	523	LMG	O1-C7-C8-C9
28	E	101	LHG	C4-C5-C6-O8
29	B	623	SQD	O6-C44-C45-C46
29	a	411	SQD	C44-C45-C46-O48
30	A	415	DGD	C1G-C2G-C3G-O3G
30	C	518	DGD	O1A-C1A-O1G-C1G
27	c	523	LMG	C13-C14-C15-C16
27	M	101	LMG	C29-C30-C31-C32
27	m	101	LMG	C37-C38-C39-C40
33	b	622	STE	C10-C11-C12-C13
22	C	513	CLA	O1D-CGD-O2D-CED
22	b	611	CLA	C16-C17-C18-C19
27	D	407	LMG	C15-C16-C17-C18
27	b	623	LMG	C32-C33-C34-C35
28	l	101	LHG	C27-C28-C29-C30
29	A	414	SQD	C31-C32-C33-C34
30	c	519	DGD	CCB-CDB-CEB-CFB
30	h	101	DGD	CCA-CDA-CEA-CFA
30	h	101	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
33	b	622	STE	C14-C15-C16-C17
27	D	407	LMG	C30-C31-C32-C33
33	b	625	STE	C2-C3-C4-C5
24	A	407	BCR	C11-C10-C9-C34
24	d	406	BCR	C16-C17-C18-C36
22	a	404	CLA	C5-C6-C7-C8
33	j	101	STE	C1-C2-C3-C4
30	C	517	DGD	O6E-C5E-C6E-O5E
29	A	413	SQD	C16-C17-C18-C19
33	b	625	STE	C11-C10-C9-C8
28	B	622	LHG	C28-C29-C30-C31
33	C	522	STE	C2-C3-C4-C5
27	d	410	LMG	O6-C5-C6-O5
24	c	514	BCR	C21-C22-C23-C24
27	a	416	LMG	C30-C31-C32-C33
33	R	101	STE	C3-C4-C5-C6
30	c	517	DGD	O6E-C5E-C6E-O5E
33	t	103	STE	C10-C11-C12-C13
22	b	614	CLA	C8-C10-C11-C12
22	c	506	CLA	C8-C10-C11-C12
30	C	518	DGD	C6A-C7A-C8A-C9A
28	e	101	LHG	C25-C26-C27-C28
29	D	408	SQD	C30-C31-C32-C33
22	C	512	CLA	O2A-C1-C2-C3
29	b	620	SQD	C46-C45-O47-C7
27	c	522	LMG	C14-C15-C16-C17
28	D	409	LHG	C29-C30-C31-C32
28	d	409	LHG	C25-C26-C27-C28
28	l	101	LHG	C17-C18-C19-C20
30	C	519	DGD	C5A-C6A-C7A-C8A
27	M	101	LMG	C11-C12-C13-C14
33	b	621	STE	C10-C11-C12-C13
33	b	624	STE	C3-C4-C5-C6
27	c	523	LMG	C31-C32-C33-C34
27	d	410	LMG	C12-C13-C14-C15
29	A	413	SQD	C14-C15-C16-C17
27	D	410	LMG	C10-C11-C12-C13
28	B	621	LHG	C7-C8-C9-C10
22	B	612	CLA	O1D-CGD-O2D-CED
27	a	416	LMG	C23-C24-C25-C26
29	b	620	SQD	C10-C11-C12-C13
24	B	619	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	C	514	BCR	C12-C13-C14-C15
27	C	520	LMG	C29-C28-O8-C9
27	A	411	LMG	C40-C41-C42-C43
29	a	412	SQD	C31-C32-C33-C34
30	C	517	DGD	C8B-C9B-CAB-CBB
27	b	623	LMG	C24-C25-C26-C27
29	A	414	SQD	C14-C15-C16-C17
29	B	623	SQD	C29-C30-C31-C32
29	f	102	SQD	C24-C25-C26-C27
22	c	505	CLA	C4-C3-C5-C6
26	a	409	PL9	C25-C24-C26-C27
22	c	510	CLA	C2-C3-C5-C6
27	M	101	LMG	C20-C21-C22-C23
28	A	412	LHG	C9-C10-C11-C12
30	A	415	DGD	C5A-C6A-C7A-C8A
22	b	615	CLA	C16-C17-C18-C19
27	D	407	LMG	C20-C21-C22-C23
27	D	407	LMG	C39-C40-C41-C42
27	c	523	LMG	C17-C18-C19-C20
28	D	409	LHG	C34-C35-C36-C37
33	B	620	STE	C11-C12-C13-C14
33	J	101	STE	C6-C7-C8-C9
30	c	517	DGD	O6D-C5D-C6D-O5D
27	C	520	LMG	C15-C16-C17-C18
27	m	101	LMG	C20-C21-C22-C23
28	E	101	LHG	C25-C26-C27-C28
30	c	519	DGD	C4B-C5B-C6B-C7B
30	h	101	DGD	CBA-CCA-CDA-CEA
33	k	102	STE	C2-C3-C4-C5
30	C	518	DGD	CDB-CEB-CFB-CGB
27	a	416	LMG	C17-C18-C19-C20
27	c	520	LMG	C38-C39-C40-C41
30	c	518	DGD	C6A-C7A-C8A-C9A
30	h	101	DGD	CAB-CBB-CCB-CDB
33	d	413	STE	C2-C3-C4-C5
28	A	412	LHG	C17-C18-C19-C20
33	d	413	STE	C15-C16-C17-C18
30	c	518	DGD	C7B-C8B-C9B-CAB
28	E	101	LHG	C19-C20-C21-C22
30	H	102	DGD	O2G-C1B-C2B-C3B
33	t	103	STE	C7-C8-C9-C10
22	D	402	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
22	d	405	CLA	C16-C17-C18-C19
30	C	517	DGD	CDA-CEA-CFA-CGA
33	B	624	STE	C7-C8-C9-C10
33	H	103	STE	C1-C2-C3-C4
33	B	625	STE	C4-C5-C6-C7
30	A	415	DGD	CEA-CFA-CGA-CHA
22	b	607	CLA	CBD-CGD-O2D-CED
26	a	409	PL9	C17-C18-C19-C20
27	D	407	LMG	C35-C36-C37-C38
27	D	410	LMG	C15-C16-C17-C18
33	j	101	STE	C2-C3-C4-C5
24	b	617	BCR	C14-C15-C16-C17
30	c	517	DGD	C8B-C9B-CAB-CBB
33	j	101	STE	C4-C5-C6-C7
27	b	623	LMG	C42-C43-C44-C45
30	C	519	DGD	CDA-CEA-CFA-CGA
29	A	413	SQD	C26-C27-C28-C29
22	D	402	CLA	C16-C17-C18-C20
22	C	505	CLA	C4-C3-C5-C6
22	c	510	CLA	C4-C3-C5-C6
26	a	409	PL9	C40-C39-C41-C42
22	b	609	CLA	C2-C3-C5-C6
33	c	521	STE	C10-C11-C12-C13
28	D	409	LHG	C23-C24-C25-C26
30	c	518	DGD	C1A-C2A-C3A-C4A
28	D	409	LHG	C10-C11-C12-C13
33	H	103	STE	C3-C4-C5-C6
30	C	518	DGD	CDA-CEA-CFA-CGA
27	c	522	LMG	C38-C39-C40-C41
30	A	415	DGD	C6B-C7B-C8B-C9B
28	a	410	LHG	O1-C1-C2-O2
28	d	408	LHG	O1-C1-C2-O2
28	d	409	LHG	O1-C1-C2-O2
22	A	403	CLA	C11-C12-C13-C14
22	C	512	CLA	C11-C12-C13-C14
22	a	402	CLA	C14-C13-C15-C16
22	b	604	CLA	C14-C13-C15-C16
22	b	607	CLA	C6-C7-C8-C9
22	b	607	CLA	C11-C12-C13-C14
22	c	506	CLA	C6-C7-C8-C9
22	c	506	CLA	C11-C12-C13-C14
22	c	508	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	c	512	CLA	C14-C13-C15-C16
22	c	513	CLA	C11-C12-C13-C14
22	d	401	CLA	C6-C7-C8-C9
30	c	518	DGD	C5B-C6B-C7B-C8B
22	B	616	CLA	C5-C6-C7-C8
22	b	610	CLA	C4B-C3B-CAB-CBB
27	M	101	LMG	C31-C32-C33-C34
30	H	102	DGD	CBA-CCA-CDA-CEA
29	b	620	SQD	C19-C20-C21-C22
29	D	408	SQD	C2-C1-O6-C44
27	c	522	LMG	C29-C30-C31-C32
27	m	101	LMG	C31-C32-C33-C34
29	A	413	SQD	C34-C35-C36-C37
29	A	413	SQD	C17-C18-C19-C20
29	a	411	SQD	C18-C19-C20-C21
33	d	411	STE	C10-C11-C12-C13
27	M	101	LMG	C40-C41-C42-C43
27	m	101	LMG	C22-C23-C24-C25
33	m	102	STE	C7-C8-C9-C10
22	B	604	CLA	C11-C12-C13-C15
22	B	604	CLA	C12-C13-C15-C16
22	B	615	CLA	C6-C7-C8-C10
22	C	502	CLA	C12-C13-C15-C16
22	C	507	CLA	C11-C10-C8-C7
22	C	512	CLA	C11-C10-C8-C7
22	b	604	CLA	C12-C13-C15-C16
22	b	607	CLA	C11-C12-C13-C15
22	b	609	CLA	C12-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C7
22	c	512	CLA	C12-C13-C15-C16
22	d	401	CLA	C12-C13-C15-C16
22	d	405	CLA	C12-C13-C15-C16
22	D	403	CLA	C13-C15-C16-C17
30	C	517	DGD	O6D-C5D-C6D-O5D
28	l	101	LHG	C13-C14-C15-C16
30	h	101	DGD	C6B-C7B-C8B-C9B
22	A	403	CLA	C15-C16-C17-C18
22	B	607	CLA	C16-C17-C18-C20
28	B	622	LHG	C19-C20-C21-C22
28	e	101	LHG	C14-C15-C16-C17
22	b	609	CLA	C4-C3-C5-C6
26	d	407	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	C4B-C5B-C6B-C7B
22	b	607	CLA	C8-C10-C11-C12
33	b	621	STE	C13-C14-C15-C16
33	b	624	STE	C5-C6-C7-C8
33	b	627	STE	C6-C7-C8-C9
24	C	514	BCR	C9-C10-C11-C12
24	c	514	BCR	C15-C16-C17-C18
22	C	504	CLA	C5-C6-C7-C8
30	C	519	DGD	O6D-C5D-C6D-O5D
27	M	101	LMG	C39-C40-C41-C42
29	B	623	SQD	C17-C18-C19-C20
30	c	517	DGD	CBB-CCB-CDB-CEB
33	b	624	STE	C11-C12-C13-C14
27	C	520	LMG	C14-C15-C16-C17
27	a	416	LMG	C32-C33-C34-C35
28	D	409	LHG	C17-C18-C19-C20
33	b	625	STE	C6-C7-C8-C9
30	h	101	DGD	CDB-CEB-CFB-CGB
27	m	101	LMG	C11-C12-C13-C14
30	h	101	DGD	C5A-C6A-C7A-C8A
33	a	413	STE	C2-C3-C4-C5
29	a	412	SQD	C44-C45-C46-O48
30	A	415	DGD	O1G-C1G-C2G-C3G
30	A	415	DGD	CDB-CEB-CFB-CGB
30	c	518	DGD	CDA-CEA-CFA-CGA
22	b	616	CLA	C10-C11-C12-C13
33	T	102	STE	C6-C7-C8-C9
33	a	413	STE	C4-C5-C6-C7
28	A	412	LHG	C11-C10-C9-C8
29	A	414	SQD	C16-C17-C18-C19
30	A	415	DGD	C2B-C3B-C4B-C5B
30	c	519	DGD	C5B-C6B-C7B-C8B
33	M	102	STE	C4-C5-C6-C7
33	D	412	STE	C11-C10-C9-C8
33	J	101	STE	C3-C4-C5-C6
33	d	412	STE	C3-C4-C5-C6
33	m	102	STE	C5-C6-C7-C8
28	B	621	LHG	C10-C11-C12-C13
26	D	406	PL9	C43-C44-C46-C47
26	d	407	PL9	C13-C14-C16-C17
29	A	414	SQD	O47-C45-C46-O48
28	A	412	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	a	410	LHG	C16-C17-C18-C19
26	a	409	PL9	C42-C43-C44-C45
22	D	403	CLA	C16-C17-C18-C19
28	d	408	LHG	O9-C7-O7-C5
28	B	621	LHG	O6-C4-C5-O7
28	l	101	LHG	O6-C4-C5-O7
30	H	102	DGD	CCB-CDB-CEB-CFB
24	B	617	BCR	C1-C6-C7-C8
24	H	101	BCR	C23-C24-C25-C30
24	b	617	BCR	C1-C6-C7-C8
24	c	514	BCR	C1-C6-C7-C8
22	a	404	CLA	CBA-CGA-O2A-C1
22	C	502	CLA	C15-C16-C17-C18
27	c	522	LMG	C32-C33-C34-C35
30	H	102	DGD	CAB-CBB-CCB-CDB
33	b	626	STE	C5-C6-C7-C8
22	b	611	CLA	C16-C17-C18-C20
22	c	504	CLA	C11-C12-C13-C15
22	c	505	CLA	C16-C17-C18-C20
22	b	614	CLA	C15-C16-C17-C18
29	A	413	SQD	O6-C44-C45-O47
26	a	409	PL9	C4-C3-C7-C8
28	e	101	LHG	C16-C17-C18-C19
27	b	623	LMG	C37-C38-C39-C40
29	b	620	SQD	O49-C7-O47-C45
33	b	622	STE	C5-C6-C7-C8
24	t	101	BCR	C10-C11-C12-C13
26	d	407	PL9	C43-C44-C46-C47
27	C	520	LMG	C30-C31-C32-C33
30	c	518	DGD	C7A-C8A-C9A-CAA
30	c	517	DGD	C1A-C2A-C3A-C4A
33	k	102	STE	C5-C6-C7-C8
22	B	604	CLA	C11-C12-C13-C14
22	b	613	CLA	C11-C10-C8-C9
28	a	410	LHG	C29-C30-C31-C32
27	a	416	LMG	C35-C36-C37-C38
24	A	407	BCR	C14-C15-C16-C17
29	b	620	SQD	C13-C14-C15-C16
30	c	517	DGD	CDB-CEB-CFB-CGB
22	B	615	CLA	C16-C17-C18-C19
22	D	402	CLA	C16-C17-C18-C19
22	b	601	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	a	411	SQD	C11-C12-C13-C14
30	C	518	DGD	C3A-C4A-C5A-C6A
30	H	102	DGD	C3B-C4B-C5B-C6B
27	D	410	LMG	C16-C17-C18-C19
30	C	519	DGD	C3A-C4A-C5A-C6A
22	B	604	CLA	C2C-C3C-CAC-CBC
22	c	512	CLA	C2A-CAA-CBA-CGA
30	c	519	DGD	O6D-C5D-C6D-O5D
22	c	507	CLA	C15-C16-C17-C18
24	T	101	BCR	C13-C14-C15-C16
30	h	101	DGD	O2G-C1B-C2B-C3B
33	C	522	STE	C1-C2-C3-C4
33	l	102	STE	C1-C2-C3-C4
22	C	505	CLA	C2-C3-C5-C6
22	B	611	CLA	C16-C17-C18-C20
33	H	103	STE	C9-C10-C11-C12
29	A	414	SQD	C8-C7-O47-C45
28	A	412	LHG	C12-C13-C14-C15
30	h	101	DGD	C1A-C2A-C3A-C4A
22	c	510	CLA	C5-C6-C7-C8
29	A	414	SQD	C9-C10-C11-C12
30	A	415	DGD	CBA-CCA-CDA-CEA
33	B	626	STE	C5-C6-C7-C8
33	l	102	STE	C9-C10-C11-C12
24	B	617	BCR	C11-C10-C9-C34
24	C	514	BCR	C20-C21-C22-C37
24	C	515	BCR	C11-C10-C9-C34
24	Y	101	BCR	C35-C13-C14-C15
24	c	514	BCR	C11-C10-C9-C34
24	c	515	BCR	C20-C21-C22-C37
24	k	101	BCR	C11-C10-C9-C34
28	E	101	LHG	C24-C25-C26-C27
28	B	621	LHG	O6-C4-C5-C6
28	e	101	LHG	O6-C4-C5-C6
22	B	613	CLA	C16-C17-C18-C19
27	M	101	LMG	C12-C13-C14-C15
30	c	517	DGD	C2B-C3B-C4B-C5B
35	V	201	HEC	C4B-C3B-CAB-CBB
24	a	405	BCR	C37-C22-C23-C24
28	e	101	LHG	C28-C29-C30-C31
28	B	622	LHG	C12-C13-C14-C15
22	B	605	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C11-C10-C8-C7
22	C	512	CLA	C12-C13-C15-C16
22	D	404	CLA	C11-C10-C8-C7
22	c	512	CLA	C11-C12-C13-C15
22	d	401	CLA	C11-C12-C13-C15
27	C	520	LMG	C12-C13-C14-C15
28	e	101	LHG	C27-C28-C29-C30
30	h	101	DGD	C9B-CAB-CBB-CCB
33	b	621	STE	C6-C7-C8-C9
29	D	408	SQD	O6-C44-C45-C46
24	C	516	BCR	C7-C8-C9-C10
24	c	515	BCR	C21-C22-C23-C24
24	k	101	BCR	C17-C18-C19-C20
24	k	101	BCR	C21-C22-C23-C24
27	d	410	LMG	C14-C15-C16-C17
30	c	517	DGD	O1A-C1A-O1G-C1G
30	C	518	DGD	C2G-C3G-O3G-C1D
30	C	518	DGD	C5D-C6D-O5D-C1E
30	c	518	DGD	C2G-C3G-O3G-C1D
30	c	518	DGD	C5D-C6D-O5D-C1E
22	D	404	CLA	C16-C17-C18-C19
28	B	622	LHG	C25-C26-C27-C28
22	C	506	CLA	C4-C3-C5-C6
27	m	101	LMG	O10-C28-O8-C9
27	M	101	LMG	C19-C20-C21-C22
28	d	408	LHG	C11-C12-C13-C14
28	B	621	LHG	C16-C17-C18-C19
30	H	102	DGD	CCA-CDA-CEA-CFA
30	c	518	DGD	C8B-C9B-CAB-CBB
33	d	411	STE	C4-C5-C6-C7
23	a	403	PHO	O2A-C1-C2-C3
22	d	401	CLA	C16-C17-C18-C20
27	b	623	LMG	O10-C28-O8-C9
30	C	517	DGD	C5A-C6A-C7A-C8A
24	B	617	BCR	C12-C13-C14-C15
24	B	619	BCR	C11-C10-C9-C8
29	A	414	SQD	C32-C33-C34-C35
29	f	102	SQD	O49-C7-O47-C45
33	c	521	STE	C1-C2-C3-C4
22	B	607	CLA	C16-C17-C18-C19
28	a	410	LHG	C28-C29-C30-C31
30	H	102	DGD	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	c	517	DGD	C4B-C5B-C6B-C7B
33	Z	101	STE	C11-C12-C13-C14
35	f	101	HEC	C4C-C3C-CAC-CBC
27	D	407	LMG	C16-C17-C18-C19
26	A	410	PL9	C18-C19-C21-C22
30	H	102	DGD	C9A-CAA-CBA-CCA
33	B	626	STE	C4-C5-C6-C7
22	b	604	CLA	C13-C15-C16-C17
27	c	522	LMG	O7-C8-C9-O8
27	c	523	LMG	O1-C7-C8-O7
29	a	412	SQD	O47-C45-C46-O48
29	b	620	SQD	O47-C45-C46-O48
30	A	415	DGD	O1G-C1G-C2G-O2G
30	c	517	DGD	O1G-C1G-C2G-O2G
22	B	606	CLA	C13-C15-C16-C17
30	C	517	DGD	C4D-C5D-C6D-O5D
22	b	607	CLA	C11-C10-C8-C9
22	b	616	CLA	C11-C10-C8-C9
22	c	509	CLA	C11-C12-C13-C14
22	d	401	CLA	C14-C13-C15-C16
22	B	609	CLA	C16-C17-C18-C19
27	c	520	LMG	C35-C36-C37-C38
28	d	408	LHG	C31-C32-C33-C34
29	D	408	SQD	C29-C30-C31-C32
29	a	411	SQD	C27-C28-C29-C30
27	a	416	LMG	O8-C28-C29-C30
30	c	517	DGD	O1G-C1A-C2A-C3A
27	b	623	LMG	C12-C13-C14-C15
28	a	410	LHG	C32-C33-C34-C35
33	C	523	STE	C5-C6-C7-C8
33	b	626	STE	C4-C5-C6-C7
33	l	102	STE	C7-C8-C9-C10
22	C	513	CLA	C5-C6-C7-C8
27	b	623	LMG	C31-C32-C33-C34
33	C	521	STE	C3-C4-C5-C6
27	m	101	LMG	C19-C20-C21-C22
22	b	609	CLA	C15-C16-C17-C18
33	H	103	STE	C12-C13-C14-C15
33	a	413	STE	C5-C6-C7-C8
22	B	610	CLA	C16-C17-C18-C19
22	b	615	CLA	C16-C17-C18-C20
28	B	621	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
33	I	101	STE	C7-C8-C9-C10
33	T	102	STE	C5-C6-C7-C8
33	D	412	STE	C4-C5-C6-C7
27	m	101	LMG	C38-C39-C40-C41
27	a	416	LMG	C20-C21-C22-C23
29	f	102	SQD	C33-C34-C35-C36
22	c	510	CLA	C16-C17-C18-C19
22	d	401	CLA	C16-C17-C18-C19
27	c	520	LMG	C31-C32-C33-C34
30	c	517	DGD	C4D-C5D-C6D-O5D
28	E	101	LHG	C34-C35-C36-C37
28	d	408	LHG	C12-C13-C14-C15
29	a	412	SQD	C29-C30-C31-C32
30	c	519	DGD	C8A-C9A-CAA-CBA
22	B	610	CLA	C15-C16-C17-C18
30	c	517	DGD	C4A-C5A-C6A-C7A
26	A	410	PL9	C24-C26-C27-C28
27	m	101	LMG	C30-C31-C32-C33
22	B	601	CLA	C4B-C3B-CAB-CBB
22	C	508	CLA	C1A-C2A-CAA-CBA
22	C	513	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	C1A-C2A-CAA-CBA
22	b	601	CLA	C4B-C3B-CAB-CBB
22	c	512	CLA	C1A-C2A-CAA-CBA
22	c	512	CLA	C4B-C3B-CAB-CBB
22	C	507	CLA	C2-C3-C5-C6
29	B	623	SQD	C35-C36-C37-C38
27	C	520	LMG	C37-C38-C39-C40
27	c	522	LMG	C36-C37-C38-C39
30	C	517	DGD	C9B-CAB-CBB-CCB
28	B	621	LHG	C34-C35-C36-C37
30	C	518	DGD	C9B-CAB-CBB-CCB
33	l	102	STE	C2-C3-C4-C5
22	C	507	CLA	C5-C6-C7-C8
22	A	403	CLA	C11-C10-C8-C7
22	B	605	CLA	C12-C13-C15-C16
22	B	613	CLA	C12-C13-C15-C16
22	B	615	CLA	C12-C13-C15-C16
22	C	505	CLA	C6-C7-C8-C10
22	C	508	CLA	C11-C10-C8-C7
22	b	614	CLA	C12-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	c	506	CLA	C11-C10-C8-C7
22	d	403	CLA	C6-C7-C8-C10
29	D	408	SQD	C27-C28-C29-C30
29	a	412	SQD	C14-C15-C16-C17
28	l	101	LHG	C19-C20-C21-C22
30	H	102	DGD	CDA-CEA-CFA-CGA
33	a	415	STE	C10-C11-C12-C13
22	c	509	CLA	CAA-CBA-CGA-O2A
27	A	411	LMG	C30-C31-C32-C33
28	l	101	LHG	C34-C35-C36-C37
33	B	620	STE	C7-C8-C9-C10
22	B	614	CLA	O1D-CGD-O2D-CED
22	d	404	CLA	C2C-C3C-CAC-CBC
33	b	622	STE	C1-C2-C3-C4
27	m	101	LMG	C17-C18-C19-C20
28	e	101	LHG	C12-C13-C14-C15
29	a	411	SQD	C10-C11-C12-C13
30	c	517	DGD	C3B-C4B-C5B-C6B
33	b	622	STE	C11-C12-C13-C14
28	d	408	LHG	C19-C20-C21-C22
30	C	517	DGD	O1G-C1A-C2A-C3A
28	d	408	LHG	C26-C27-C28-C29
22	B	614	CLA	C6-C7-C8-C9
22	C	505	CLA	C6-C7-C8-C9
22	C	506	CLA	C14-C13-C15-C16
22	C	510	CLA	C11-C10-C8-C9
22	b	609	CLA	C14-C13-C15-C16
22	b	615	CLA	C11-C10-C8-C9
22	c	512	CLA	C11-C12-C13-C14
22	d	401	CLA	C11-C10-C8-C9
22	b	607	CLA	C5-C6-C7-C8
22	B	615	CLA	C5-C6-C7-C8
27	c	522	LMG	C31-C32-C33-C34
29	a	411	SQD	C11-C10-C9-C8
28	D	409	LHG	C11-C10-C9-C8
33	l	102	STE	C10-C11-C12-C13
29	B	623	SQD	C27-C28-C29-C30
27	M	101	LMG	O7-C8-C9-O8
27	a	416	LMG	O1-C7-C8-O7
28	E	101	LHG	O7-C5-C6-O8
29	b	620	SQD	O6-C44-C45-O47
33	d	411	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C16-C17-C18-C20
28	B	622	LHG	C24-C25-C26-C27
30	C	518	DGD	C8B-C9B-CAB-CBB
27	c	522	LMG	O1-C7-C8-C9
30	c	517	DGD	O1G-C1G-C2G-C3G
33	b	622	STE	C4-C5-C6-C7
26	a	409	PL9	C43-C44-C46-C47
28	B	621	LHG	C23-C24-C25-C26
22	B	601	CLA	CAD-CBD-CGD-O2D
22	B	607	CLA	CAD-CBD-CGD-O2D
22	C	502	CLA	CAD-CBD-CGD-O2D
22	C	504	CLA	CAD-CBD-CGD-O2D
22	b	609	CLA	CAD-CBD-CGD-O2D
22	c	502	CLA	CAD-CBD-CGD-O2D
22	c	504	CLA	CAD-CBD-CGD-O2D
27	c	523	LMG	C34-C35-C36-C37
35	F	101	HEC	C2C-C3C-CAC-CBC
28	B	621	LHG	C13-C14-C15-C16
28	B	622	LHG	C32-C33-C34-C35
22	b	613	CLA	C16-C17-C18-C20
30	C	519	DGD	C3B-C4B-C5B-C6B
22	C	512	CLA	C8-C10-C11-C12
30	H	102	DGD	C7B-C8B-C9B-CAB
33	t	102	STE	C3-C4-C5-C6
27	c	522	LMG	C39-C40-C41-C42
22	B	601	CLA	CAD-CBD-CGD-O1D
22	B	607	CLA	CAD-CBD-CGD-O1D
22	C	502	CLA	CAD-CBD-CGD-O1D
22	C	504	CLA	CAD-CBD-CGD-O1D
22	C	506	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
22	c	504	CLA	CAD-CBD-CGD-O1D
24	B	619	BCR	C11-C10-C9-C34
24	T	101	BCR	C9-C10-C11-C12
24	d	406	BCR	C11-C10-C9-C34
28	B	621	LHG	C4-O6-P-O5
28	D	409	LHG	C4-O6-P-O5
28	a	410	LHG	C3-O3-P-O5
28	e	101	LHG	C4-O6-P-O4
28	l	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
22	C	509	CLA	C3-C5-C6-C7
22	b	616	CLA	C11-C12-C13-C14
24	b	618	BCR	C14-C15-C16-C17
33	M	103	STE	C1-C2-C3-C4
22	c	512	CLA	C4-C3-C5-C6
33	t	102	STE	C11-C10-C9-C8
22	C	506	CLA	C2-C3-C5-C6
24	B	617	BCR	C11-C12-C13-C35
24	b	618	BCR	C37-C22-C23-C24
30	c	517	DGD	CAA-CBA-CCA-CDA
22	b	606	CLA	C10-C11-C12-C13
28	E	101	LHG	C16-C17-C18-C19
27	m	101	LMG	C28-C29-C30-C31
22	a	404	CLA	O1A-CGA-O2A-C1
22	c	501	CLA	CBD-CGD-O2D-CED
22	b	604	CLA	C3-C5-C6-C7
30	c	517	DGD	C5B-C6B-C7B-C8B
26	A	410	PL9	C4-C3-C7-C8
22	b	608	CLA	C13-C15-C16-C17
33	l	102	STE	C15-C16-C17-C18
22	B	604	CLA	O2A-C1-C2-C3
27	D	410	LMG	C9-C8-O7-C10
27	a	416	LMG	C9-C8-O7-C10
29	B	623	SQD	C46-C45-O47-C7
29	f	102	SQD	C46-C45-O47-C7
33	b	621	STE	C11-C10-C9-C8
29	A	414	SQD	C7-C8-C9-C10
30	A	415	DGD	CFA-CGA-CHA-CIA
22	d	404	CLA	C4C-C3C-CAC-CBC
22	c	510	CLA	C16-C17-C18-C20
22	C	508	CLA	C5-C6-C7-C8
33	d	413	STE	C4-C5-C6-C7
33	B	624	STE	C6-C7-C8-C9
22	B	614	CLA	CBD-CGD-O2D-CED
30	C	519	DGD	C9B-CAB-CBB-CCB
30	c	517	DGD	CBA-CCA-CDA-CEA
22	C	502	CLA	C14-C13-C15-C16
22	C	508	CLA	C11-C10-C8-C9
22	C	512	CLA	C14-C13-C15-C16
22	B	613	CLA	C11-C12-C13-C15
22	C	506	CLA	C12-C13-C15-C16
22	D	402	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
22	D	404	CLA	C11-C12-C13-C15
22	d	401	CLA	C11-C10-C8-C7
27	D	407	LMG	C37-C38-C39-C40
33	b	622	STE	C7-C8-C9-C10
24	A	407	BCR	C16-C17-C18-C19
24	c	515	BCR	C12-C13-C14-C15
27	b	623	LMG	C30-C31-C32-C33
28	B	622	LHG	C9-C10-C11-C12
24	c	516	BCR	C14-C15-C16-C17
30	C	517	DGD	C7A-C8A-C9A-CAA
29	b	620	SQD	C9-C10-C11-C12
22	c	506	CLA	C4-C3-C5-C6
28	B	621	LHG	C30-C31-C32-C33
26	d	407	PL9	C28-C29-C31-C32
28	d	409	LHG	C27-C28-C29-C30
30	h	101	DGD	C7B-C8B-C9B-CAB
33	c	521	STE	C4-C5-C6-C7
27	A	411	LMG	O1-C7-C8-O7
30	C	517	DGD	O1G-C1G-C2G-O2G
22	c	504	CLA	C5-C6-C7-C8
22	A	406	CLA	C5-C6-C7-C8
24	C	514	BCR	C13-C14-C15-C16
30	c	517	DGD	C3A-C4A-C5A-C6A
22	A	403	CLA	C4C-C3C-CAC-CBC
22	B	614	CLA	C16-C17-C18-C20
28	a	410	LHG	C27-C28-C29-C30
29	B	623	SQD	C31-C32-C33-C34
27	a	416	LMG	C22-C23-C24-C25
27	c	523	LMG	C36-C37-C38-C39
28	A	412	LHG	C33-C34-C35-C36
28	B	621	LHG	C24-C25-C26-C27
28	e	101	LHG	C18-C19-C20-C21
22	c	506	CLA	C2-C1-O2A-CGA
22	B	609	CLA	C16-C17-C18-C20
22	B	601	CLA	CAA-CBA-CGA-O2A
30	C	517	DGD	C2B-C3B-C4B-C5B
29	b	620	SQD	C44-C45-C46-O48
27	A	411	LMG	C28-C29-C30-C31
22	B	606	CLA	C3-C5-C6-C7
30	c	519	DGD	C2A-C1A-O1G-C1G
22	c	506	CLA	C16-C17-C18-C20
26	a	409	PL9	C12-C13-C14-C16

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Mol	Chain	Res	Type	Atoms
22	A	403	CLA	C2C-C3C-CAC-CBC
22	a	402	CLA	C2C-C3C-CAC-CBC
33	H	103	STE	C5-C6-C7-C8
27	m	101	LMG	C8-C7-O1-C1
27	D	410	LMG	C11-C12-C13-C14
29	b	620	SQD	C30-C31-C32-C33
28	d	408	LHG	C17-C18-C19-C20
22	B	614	CLA	C2A-CAA-CBA-CGA
22	B	610	CLA	C16-C17-C18-C20
33	C	523	STE	C6-C7-C8-C9
22	B	603	CLA	C11-C12-C13-C14
22	B	605	CLA	C11-C10-C8-C9
22	B	611	CLA	C6-C7-C8-C9
22	B	615	CLA	C6-C7-C8-C9
22	c	505	CLA	C11-C10-C8-C9
22	d	403	CLA	C6-C7-C8-C9
33	T	102	STE	C4-C5-C6-C7
27	D	411	LMG	C13-C14-C15-C16
22	b	605	CLA	C15-C16-C17-C18
33	I	101	STE	C11-C10-C9-C8
22	c	512	CLA	C2-C3-C5-C6
27	a	416	LMG	C16-C17-C18-C19
28	B	621	LHG	C35-C36-C37-C38
22	C	508	CLA	C12-C13-C15-C16
22	c	511	CLA	C12-C13-C15-C16
28	e	101	LHG	C19-C20-C21-C22
29	A	414	SQD	C11-C12-C13-C14
28	B	621	LHG	O9-C7-O7-C5
22	B	611	CLA	C16-C17-C18-C19
28	B	621	LHG	C11-C12-C13-C14
26	a	409	PL9	C21-C22-C23-C24
26	a	409	PL9	C38-C39-C41-C42
33	C	522	STE	C10-C11-C12-C13
22	b	616	CLA	C11-C12-C13-C15
24	D	405	BCR	C11-C10-C9-C34
24	b	617	BCR	C35-C13-C14-C15
29	A	414	SQD	C44-C45-C46-O48
30	A	415	DGD	O6D-C1D-O3G-C3G
22	b	612	CLA	C10-C11-C12-C13
27	D	410	LMG	C31-C32-C33-C34
22	b	613	CLA	O1D-CGD-O2D-CED
28	B	622	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
28	A	412	LHG	C2-C3-O3-P
28	d	409	LHG	C2-C3-O3-P
29	f	102	SQD	C25-C26-C27-C28
35	v	201	HEC	CAD-CBD-CGD-O1D
22	c	509	CLA	C15-C16-C17-C18
22	C	507	CLA	C4-C3-C5-C6
22	C	510	CLA	C4-C3-C5-C6
22	B	614	CLA	C16-C17-C18-C19
22	b	614	CLA	C13-C15-C16-C17
29	B	623	SQD	C32-C33-C34-C35
29	A	413	SQD	O6-C44-C45-C46
33	Z	101	STE	C12-C13-C14-C15
28	B	621	LHG	C18-C19-C20-C21
22	B	602	CLA	C6-C7-C8-C9
22	B	605	CLA	C6-C7-C8-C9
22	B	614	CLA	C14-C13-C15-C16
22	C	503	CLA	C11-C10-C8-C9
22	C	505	CLA	C14-C13-C15-C16
22	D	404	CLA	C11-C10-C8-C9
22	a	404	CLA	C11-C10-C8-C9
22	b	603	CLA	C11-C12-C13-C14
22	c	512	CLA	C6-C7-C8-C9
27	m	101	LMG	C35-C36-C37-C38
22	b	606	CLA	C15-C16-C17-C18
30	C	518	DGD	C4A-C5A-C6A-C7A
33	T	102	STE	C7-C8-C9-C10
33	b	621	STE	C2-C3-C4-C5
27	c	523	LMG	C9-C8-O7-C10
27	c	523	LMG	O9-C10-O7-C8
22	C	505	CLA	O1D-CGD-O2D-CED
29	a	412	SQD	O6-C44-C45-C46
26	A	410	PL9	C20-C19-C21-C22
30	C	518	DGD	C1B-C2B-C3B-C4B
33	k	102	STE	C1-C2-C3-C4
33	d	413	STE	C7-C8-C9-C10
26	A	410	PL9	C12-C11-C9-C8
35	f	101	HEC	CAD-CBD-CGD-O1D
27	a	416	LMG	C37-C38-C39-C40
22	c	508	CLA	C1A-C2A-CAA-CBA
24	H	101	BCR	C12-C13-C14-C15
30	c	519	DGD	CAA-CBA-CCA-CDA
29	a	411	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
28	D	409	LHG	C30-C31-C32-C33
22	B	601	CLA	C2B-C3B-CAB-CBB
22	b	601	CLA	C2B-C3B-CAB-CBB
22	c	512	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C5-C6-C7-C8
24	C	516	BCR	C23-C24-C25-C30
24	H	101	BCR	C23-C24-C25-C26
24	b	617	BCR	C5-C6-C7-C8
24	c	514	BCR	C5-C6-C7-C8
24	t	101	BCR	C5-C6-C7-C8
24	x	101	BCR	C23-C24-C25-C30
28	e	101	LHG	C2-C3-O3-P
28	l	101	LHG	C16-C17-C18-C19
35	V	201	HEC	CAD-CBD-CGD-O2D
22	a	404	CLA	C4-C3-C5-C6
28	D	409	LHG	O6-C4-C5-C6
29	a	412	SQD	C19-C20-C21-C22
35	v	201	HEC	CAD-CBD-CGD-O2D
28	d	409	LHG	C9-C10-C11-C12
22	D	403	CLA	C12-C13-C15-C16
22	a	404	CLA	C11-C10-C8-C7
22	b	601	CLA	C12-C13-C15-C16
22	b	604	CLA	C11-C12-C13-C15
22	c	510	CLA	C11-C12-C13-C15
22	c	506	CLA	C16-C17-C18-C19
22	b	610	CLA	C2A-CAA-CBA-CGA
27	C	520	LMG	C39-C40-C41-C42
28	E	101	LHG	C10-C11-C12-C13
27	c	522	LMG	O1-C7-C8-O7
33	M	102	STE	O1-C1-C2-C3
30	C	517	DGD	C7B-C8B-C9B-CAB
29	a	412	SQD	C13-C14-C15-C16
33	a	414	STE	C5-C6-C7-C8
35	F	101	HEC	CAD-CBD-CGD-O1D
33	a	414	STE	C4-C5-C6-C7
27	M	101	LMG	C13-C14-C15-C16
28	e	101	LHG	C15-C16-C17-C18
29	D	408	SQD	C34-C35-C36-C37
28	a	410	LHG	C18-C19-C20-C21
27	D	411	LMG	O9-C10-C11-C12
22	c	508	CLA	C4-C3-C5-C6
22	b	606	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
22	C	510	CLA	C2-C3-C5-C6
33	c	521	STE	O2-C1-C2-C3
30	H	102	DGD	O6E-C5E-C6E-O5E
29	a	411	SQD	O10-C23-O48-C46
27	a	416	LMG	O9-C10-O7-C8
28	l	101	LHG	C31-C32-C33-C34
24	A	407	BCR	C9-C10-C11-C12
28	B	621	LHG	C9-C10-C11-C12
24	b	618	BCR	C6-C7-C8-C9
24	b	618	BCR	C22-C23-C24-C25
30	h	101	DGD	C3A-C4A-C5A-C6A
22	B	604	CLA	C4-C3-C5-C6
22	d	405	CLA	C4-C3-C5-C6
33	d	412	STE	C1-C2-C3-C4
22	C	503	CLA	C8-C10-C11-C12
33	J	101	STE	O1-C1-C2-C3
33	M	102	STE	O2-C1-C2-C3
33	a	414	STE	C6-C7-C8-C9
27	M	101	LMG	C10-C11-C12-C13
35	f	101	HEC	C2A-CAA-CBA-CGA
28	e	101	LHG	C11-C12-C13-C14
30	C	517	DGD	O1G-C1G-C2G-C3G
30	c	517	DGD	C1G-C2G-C3G-O3G
35	F	101	HEC	CAD-CBD-CGD-O2D
28	A	412	LHG	C23-C24-C25-C26
22	B	610	CLA	C2A-CAA-CBA-CGA
22	b	607	CLA	O1D-CGD-O2D-CED
22	b	601	CLA	C4-C3-C5-C6
22	b	604	CLA	C4-C3-C5-C6
26	D	406	PL9	C40-C39-C41-C42
29	A	414	SQD	C30-C31-C32-C33
30	c	519	DGD	C7B-C8B-C9B-CAB
22	C	504	CLA	C4B-C3B-CAB-CBB
22	b	604	CLA	C5-C6-C7-C8
33	d	412	STE	O2-C1-C2-C3
29	B	623	SQD	C11-C10-C9-C8
30	c	518	DGD	C8A-C9A-CAA-CBA
24	d	406	BCR	C20-C21-C22-C37
35	f	101	HEC	CAD-CBD-CGD-O2D
22	c	502	CLA	O1A-CGA-O2A-C1
22	C	508	CLA	C16-C17-C18-C19
30	C	518	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
27	b	623	LMG	C13-C14-C15-C16
33	b	625	STE	C12-C13-C14-C15
22	c	505	CLA	C11-C10-C8-C7
35	V	201	HEC	CAD-CBD-CGD-O1D
33	b	624	STE	C6-C7-C8-C9
22	B	605	CLA	C14-C13-C15-C16
22	B	613	CLA	C14-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C9
22	b	601	CLA	C11-C12-C13-C14
30	c	519	DGD	C2A-C3A-C4A-C5A
22	c	508	CLA	C16-C17-C18-C19
27	M	101	LMG	C8-C7-O1-C1
29	a	411	SQD	C5-C6-S-O8
29	b	620	SQD	C45-C44-O6-C1
30	c	517	DGD	C5D-C6D-O5D-C1E
33	c	521	STE	O1-C1-C2-C3
22	c	501	CLA	C2A-CAA-CBA-CGA
22	D	402	CLA	C2-C1-O2A-CGA
22	d	403	CLA	C2-C1-O2A-CGA
22	B	602	CLA	C3A-C2A-CAA-CBA
22	c	512	CLA	C3A-C2A-CAA-CBA
30	h	101	DGD	O1B-C1B-C2B-C3B
30	C	517	DGD	O1A-C1A-O1G-C1G
33	b	626	STE	C3-C4-C5-C6
27	c	522	LMG	C15-C16-C17-C18
33	C	522	STE	C7-C8-C9-C10
33	t	103	STE	O2-C1-C2-C3
28	l	101	LHG	C23-C24-C25-C26
22	D	402	CLA	C10-C11-C12-C13
30	H	102	DGD	CDB-CEB-CFB-CGB
22	b	613	CLA	C16-C17-C18-C19
27	c	522	LMG	C35-C36-C37-C38
28	D	409	LHG	C1-C2-C3-O3
33	d	412	STE	C4-C5-C6-C7
27	A	411	LMG	O6-C1-O1-C7
29	b	620	SQD	C18-C19-C20-C21
22	c	502	CLA	CBA-CGA-O2A-C1
27	C	520	LMG	O1-C7-C8-C9
29	A	414	SQD	C17-C18-C19-C20
29	A	414	SQD	C24-C25-C26-C27
30	C	519	DGD	C2A-C3A-C4A-C5A
29	A	414	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
28	a	410	LHG	C17-C18-C19-C20
26	a	409	PL9	C47-C48-C49-C51
30	c	518	DGD	C3B-C4B-C5B-C6B
27	b	623	LMG	C36-C37-C38-C39
29	b	620	SQD	C11-C12-C13-C14
27	d	410	LMG	O7-C10-C11-C12
28	a	410	LHG	C33-C34-C35-C36
29	A	413	SQD	C29-C30-C31-C32
27	a	416	LMG	O7-C8-C9-O8
33	t	103	STE	O1-C1-C2-C3
22	b	602	CLA	C8-C10-C11-C12
22	A	402	CLA	C14-C13-C15-C16
22	B	615	CLA	C14-C13-C15-C16
22	b	614	CLA	C14-C13-C15-C16
22	c	506	CLA	C11-C10-C8-C9
22	c	508	CLA	C11-C12-C13-C14
22	c	511	CLA	C11-C10-C8-C9
22	d	401	CLA	C11-C12-C13-C14
29	A	414	SQD	O48-C23-C24-C25
22	c	503	CLA	O1A-CGA-O2A-C1
33	d	412	STE	O1-C1-C2-C3
22	B	609	CLA	C4-C3-C5-C6
26	A	410	PL9	C33-C34-C36-C37
27	D	407	LMG	C12-C13-C14-C15
22	C	512	CLA	C2A-CAA-CBA-CGA
22	A	402	CLA	C12-C13-C15-C16
22	A	403	CLA	C12-C13-C15-C16
22	B	611	CLA	C6-C7-C8-C10
22	B	613	CLA	C6-C7-C8-C10
22	C	505	CLA	C12-C13-C15-C16
22	C	511	CLA	C6-C7-C8-C10
22	b	601	CLA	C11-C12-C13-C15
22	b	603	CLA	C11-C12-C13-C15
29	b	620	SQD	C11-C10-C9-C8
29	A	414	SQD	C44-C45-O47-C7
22	A	402	CLA	C2C-C3C-CAC-CBC
22	b	610	CLA	C2B-C3B-CAB-CBB
24	B	618	BCR	C23-C24-C25-C30
24	C	516	BCR	C23-C24-C25-C26
24	T	101	BCR	C5-C6-C7-C8
24	t	101	BCR	C1-C6-C7-C8
24	x	101	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	A	402	CLA	C4C-C3C-CAC-CBC
29	a	411	SQD	O47-C7-C8-C9
30	C	518	DGD	O1B-C1B-O2G-C2G
33	d	413	STE	C12-C13-C14-C15
27	c	523	LMG	C32-C33-C34-C35
33	k	102	STE	C3-C4-C5-C6
33	l	102	STE	C12-C13-C14-C15
27	M	101	LMG	C30-C31-C32-C33
33	M	103	STE	C4-C5-C6-C7
22	B	609	CLA	C2-C3-C5-C6
30	h	101	DGD	C4E-C5E-C6E-O5E
29	a	411	SQD	C28-C29-C30-C31
22	b	611	CLA	C10-C11-C12-C13
22	B	611	CLA	C10-C11-C12-C13
22	B	614	CLA	C15-C16-C17-C18
27	c	520	LMG	C30-C31-C32-C33
27	a	416	LMG	O7-C10-C11-C12
30	c	517	DGD	O2G-C1B-C2B-C3B
24	c	515	BCR	C13-C14-C15-C16
27	M	101	LMG	C22-C23-C24-C25
28	a	410	LHG	O10-C23-O8-C6
33	J	101	STE	O2-C1-C2-C3
24	c	514	BCR	C10-C11-C12-C13
28	B	621	LHG	O7-C7-C8-C9
22	c	506	CLA	C2-C3-C5-C6
22	C	501	CLA	C2A-CAA-CBA-CGA
22	A	403	CLA	C11-C10-C8-C9
22	c	503	CLA	C11-C10-C8-C9
22	d	405	CLA	C11-C10-C8-C9
22	C	507	CLA	C10-C11-C12-C13
24	c	516	BCR	C37-C22-C23-C24
27	A	411	LMG	C7-C8-C9-O8
22	B	602	CLA	C1A-C2A-CAA-CBA
22	B	605	CLA	C4B-C3B-CAB-CBB
22	d	401	CLA	C4B-C3B-CAB-CBB
30	H	102	DGD	C4E-C5E-C6E-O5E
26	a	409	PL9	C45-C44-C46-C47
30	c	517	DGD	O6E-C1E-O5D-C6D
29	A	413	SQD	O47-C7-C8-C9
29	b	620	SQD	O47-C7-C8-C9
29	B	623	SQD	C10-C11-C12-C13
27	a	416	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	H	101	BCR	C11-C12-C13-C14
24	b	617	BCR	C21-C22-C23-C24
24	k	101	BCR	C7-C8-C9-C10
22	b	606	CLA	C8-C10-C11-C12
22	c	503	CLA	CBA-CGA-O2A-C1
28	B	622	LHG	C30-C31-C32-C33
22	B	613	CLA	CAA-CBA-CGA-O2A
29	a	411	SQD	C19-C20-C21-C22
33	B	625	STE	C13-C14-C15-C16
22	a	402	CLA	C4C-C3C-CAC-CBC
33	T	102	STE	C12-C13-C14-C15
29	a	411	SQD	C5-C6-S-O7
22	B	601	CLA	C2-C1-O2A-CGA
22	B	613	CLA	C2-C1-O2A-CGA
27	c	520	LMG	C34-C35-C36-C37
22	b	614	CLA	C11-C10-C8-C7
22	c	503	CLA	C11-C10-C8-C7
22	c	508	CLA	C11-C10-C8-C7
30	c	517	DGD	C6A-C7A-C8A-C9A
33	C	521	STE	C5-C6-C7-C8
27	a	416	LMG	C34-C35-C36-C37
28	B	622	LHG	C31-C32-C33-C34
30	C	517	DGD	O1B-C1B-O2G-C2G
26	D	406	PL9	C47-C48-C49-C51
33	l	102	STE	C4-C5-C6-C7
30	C	519	DGD	O1A-C1A-O1G-C1G
22	c	509	CLA	CAA-CBA-CGA-O1A
24	B	618	BCR	C20-C21-C22-C23
24	c	516	BCR	C11-C10-C9-C8
33	C	521	STE	O2-C1-C2-C3
23	A	405	PHO	C8-C10-C11-C12
33	J	101	STE	C7-C8-C9-C10
27	m	101	LMG	O8-C28-C29-C30
22	b	610	CLA	C8-C10-C11-C12
22	B	603	CLA	C2A-CAA-CBA-CGA
22	B	611	CLA	C14-C13-C15-C16
22	c	505	CLA	C6-C7-C8-C9
33	H	103	STE	C14-C15-C16-C17
22	c	511	CLA	C8-C10-C11-C12
22	b	601	CLA	C2-C3-C5-C6
22	C	508	CLA	O1A-CGA-O2A-C1
28	d	409	LHG	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
33	C	521	STE	C2-C3-C4-C5
22	b	612	CLA	CAA-CBA-CGA-O2A
24	T	101	BCR	C7-C8-C9-C10
24	Y	101	BCR	C21-C22-C23-C24
29	a	411	SQD	O49-C7-C8-C9
30	C	517	DGD	O1B-C1B-C2B-C3B
22	b	613	CLA	CAA-CBA-CGA-O2A
30	c	518	DGD	C4A-C5A-C6A-C7A
22	B	601	CLA	O1D-CGD-O2D-CED
27	c	520	LMG	O1-C7-C8-C9
26	A	410	PL9	C30-C29-C31-C32
29	A	413	SQD	C31-C32-C33-C34
22	c	513	CLA	C13-C15-C16-C17
28	d	408	LHG	C30-C31-C32-C33
22	b	607	CLA	CAD-CBD-CGD-O2D
22	c	509	CLA	CAD-CBD-CGD-O2D
22	B	612	CLA	C8-C10-C11-C12
28	l	101	LHG	O10-C23-O8-C6
33	B	625	STE	C10-C11-C12-C13
33	C	521	STE	O1-C1-C2-C3
22	b	612	CLA	CAA-CBA-CGA-O1A
27	b	623	LMG	O10-C28-C29-C30
22	b	616	CLA	C8-C10-C11-C12
33	B	626	STE	O2-C1-C2-C3
29	A	414	SQD	O10-C23-C24-C25
30	c	517	DGD	O1B-C1B-C2B-C3B
33	D	412	STE	C1-C2-C3-C4
22	B	612	CLA	CAA-CBA-CGA-O2A
33	b	624	STE	O2-C1-C2-C3
33	k	102	STE	O2-C1-C2-C3

There are no ring outliers.

99 monomers are involved in 179 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	m	101	LMG	2	0
22	D	404	CLA	2	0
22	b	615	CLA	3	0
28	B	622	LHG	1	0
22	B	607	CLA	2	0
24	H	101	BCR	4	0
33	D	412	STE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	t	103	STE	1	0
26	A	410	PL9	8	0
24	D	405	BCR	2	0
27	c	523	LMG	1	0
22	B	610	CLA	3	0
32	A	417[B]	OEY	1	0
22	c	501	CLA	2	0
24	a	405	BCR	1	0
22	b	616	CLA	1	0
22	c	512	CLA	2	0
22	B	612	CLA	1	0
22	B	601	CLA	1	0
24	d	406	BCR	7	0
22	C	506	CLA	1	0
33	b	621	STE	2	0
22	C	503	CLA	1	0
24	B	619	BCR	4	0
29	a	412	SQD	3	0
24	A	407	BCR	1	0
22	A	402	CLA	1	0
30	h	101	DGD	1	0
33	T	102	STE	1	0
33	d	412	STE	1	0
22	C	505	CLA	2	0
24	c	514	BCR	1	0
24	C	514	BCR	2	0
22	b	614	CLA	1	0
26	a	409	PL9	4	0
22	B	616	CLA	1	0
22	b	604	CLA	4	0
24	b	618	BCR	4	0
22	C	501	CLA	1	0
22	c	507	CLA	2	0
22	c	513	CLA	2	0
22	b	611	CLA	1	0
24	b	619	BCR	1	0
33	M	102	STE	1	0
22	C	509	CLA	5	0
22	B	602	CLA	1	0
24	T	101	BCR	4	0
22	b	608	CLA	1	0
33	d	411	STE	1	0

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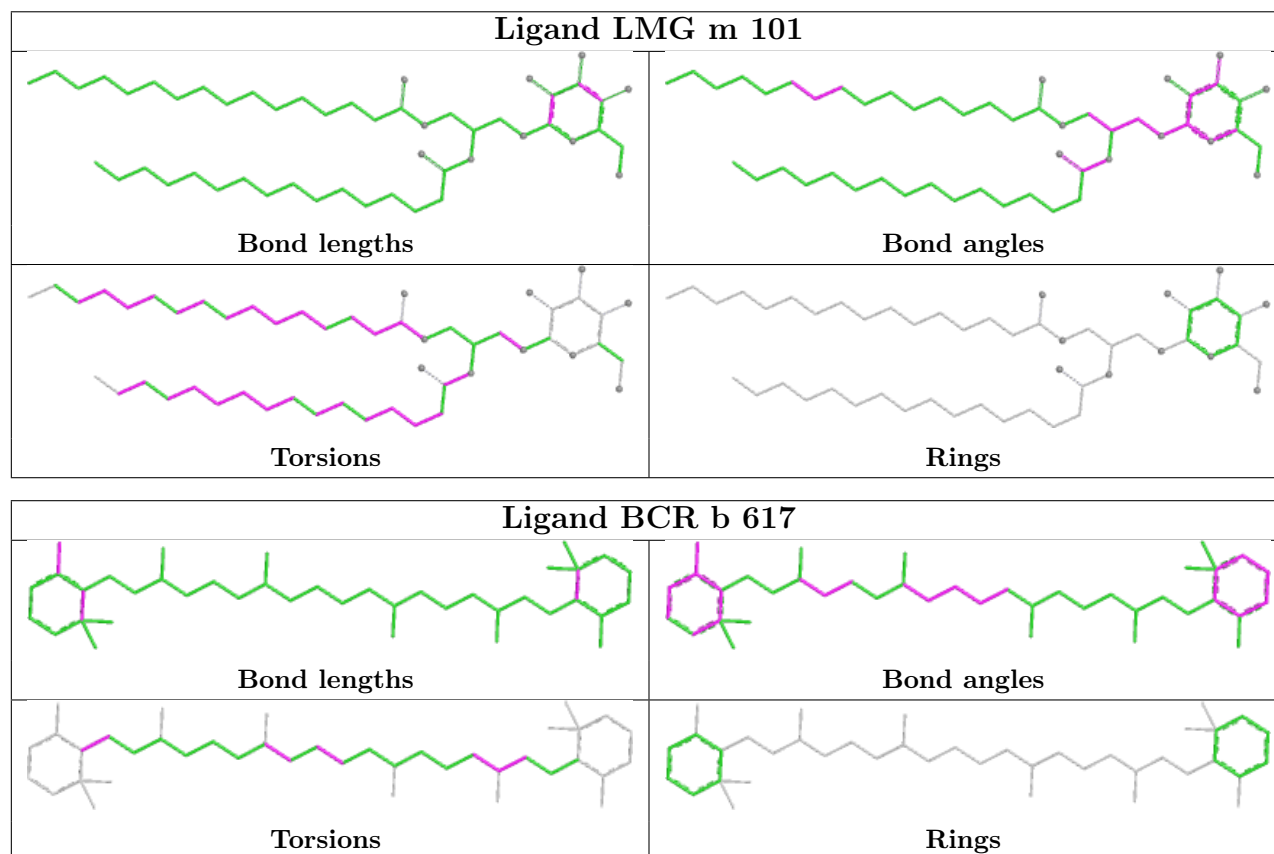
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	402	PHO	2	0
35	v	201	HEC	3	0
22	c	506	CLA	1	0
22	B	605	CLA	3	0
29	f	102	SQD	1	0
35	V	201	HEC	2	0
27	b	623	LMG	2	0
35	f	101	HEC	5	0
33	B	620	STE	1	0
29	A	414	SQD	1	0
28	a	410	LHG	1	0
29	B	623	SQD	2	0
33	B	624	STE	2	0
27	c	522	LMG	2	0
22	c	509	CLA	1	0
32	a	418[B]	OEY	1	0
22	b	605	CLA	2	0
22	B	606	CLA	2	0
22	b	609	CLA	2	0
35	F	101	HEC	5	0
23	a	403	PHO	1	0
24	C	515	BCR	2	0
22	b	602	CLA	1	0
24	t	101	BCR	4	0
30	A	415	DGD	1	0
22	D	403	CLA	3	0
22	b	612	CLA	1	0
29	b	620	SQD	1	0
22	c	508	CLA	3	0
22	b	610	CLA	1	0
22	B	613	CLA	1	0
33	b	627	STE	2	0
22	c	504	CLA	4	0
22	d	404	CLA	1	0
22	B	604	CLA	5	0
24	Y	101	BCR	2	0
30	C	518	DGD	1	0
22	c	511	CLA	2	0
30	c	517	DGD	1	0
22	d	403	CLA	2	0
24	c	516	BCR	1	0
33	b	622	STE	2	0

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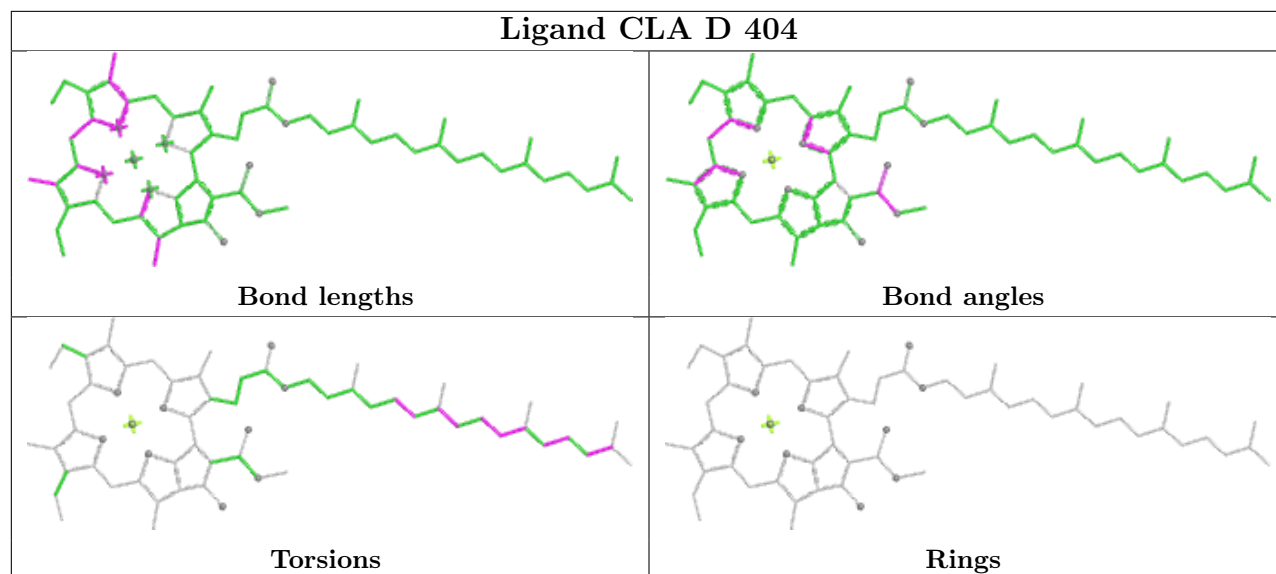
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	d	413	STE	2	0
22	b	606	CLA	4	0
23	A	405	PHO	1	0
24	B	618	BCR	5	0
22	C	513	CLA	4	0
33	t	102	STE	1	0
28	E	101	LHG	3	0
22	a	404	CLA	1	0

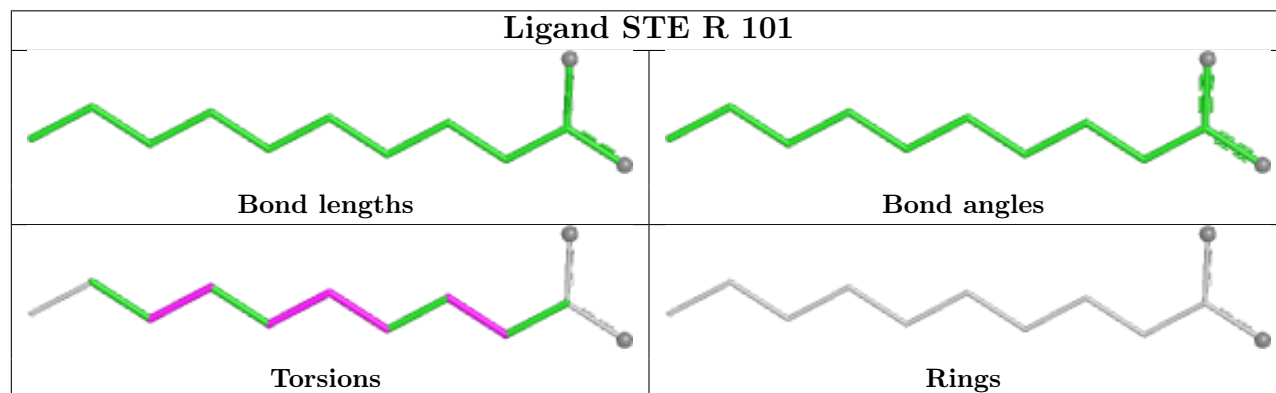
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



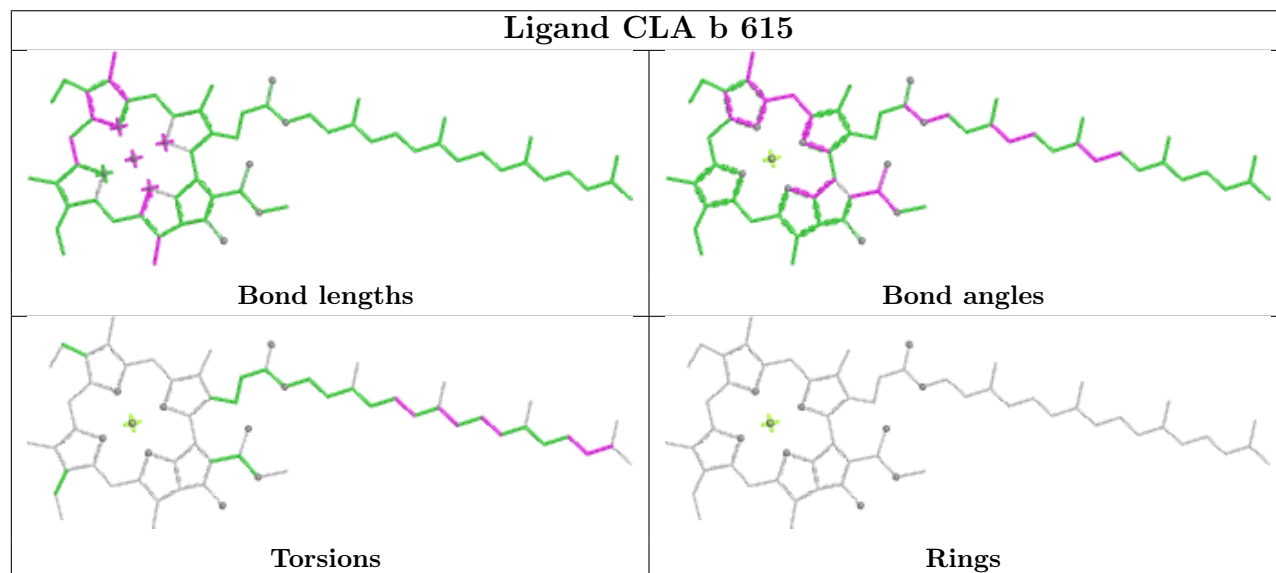
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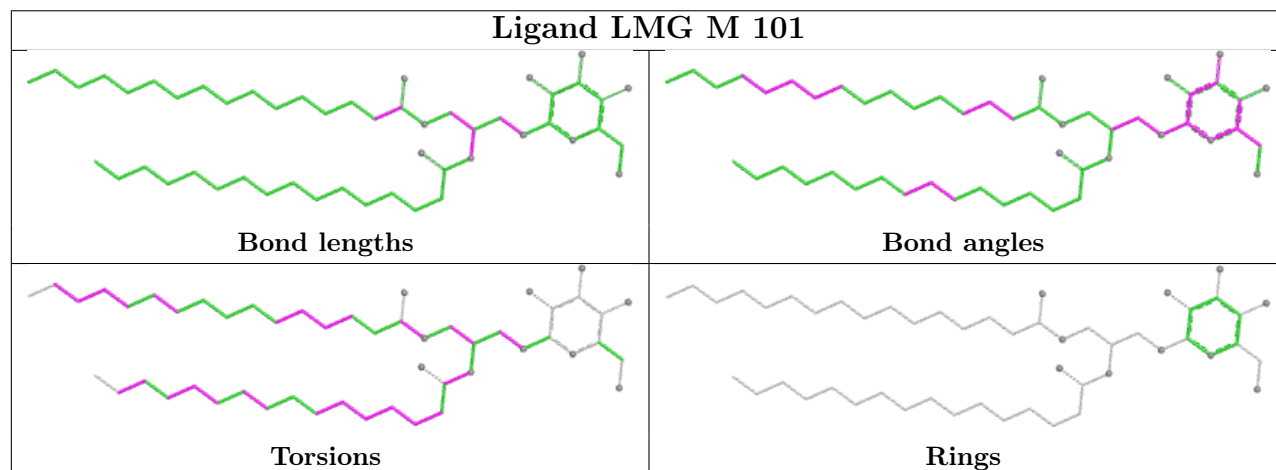
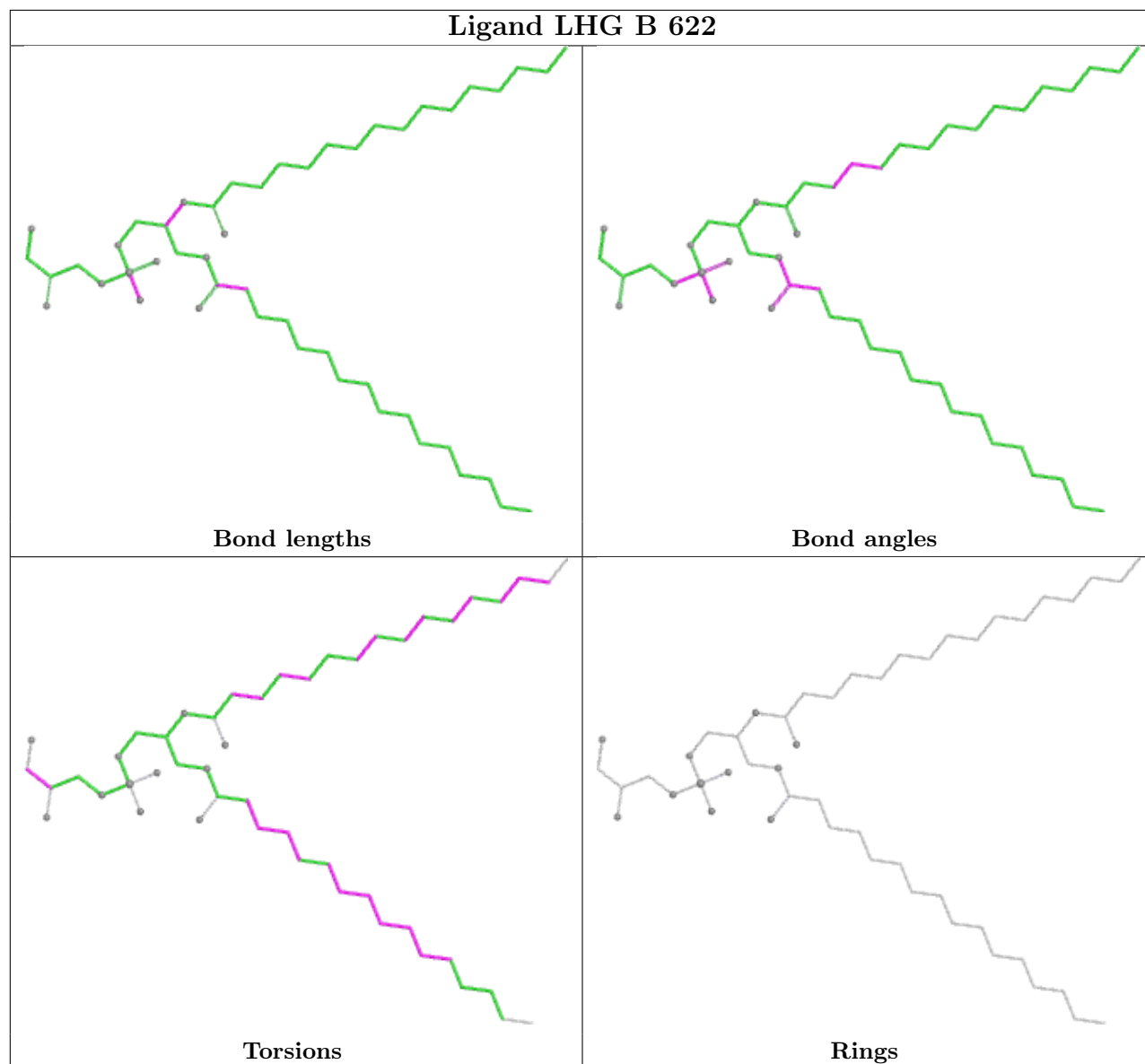


Ligand STE R 101

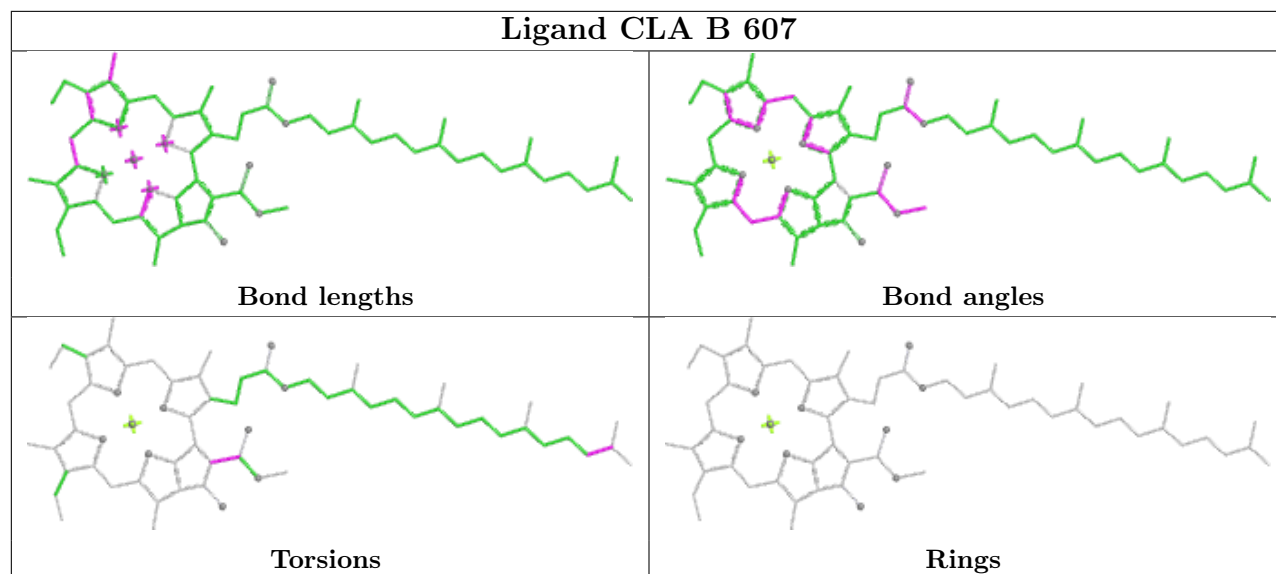


Ligand CLA b 615

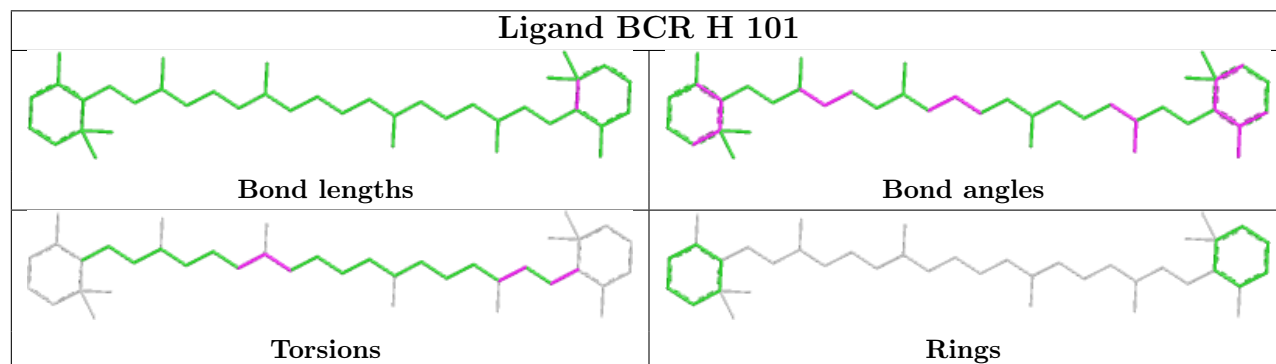




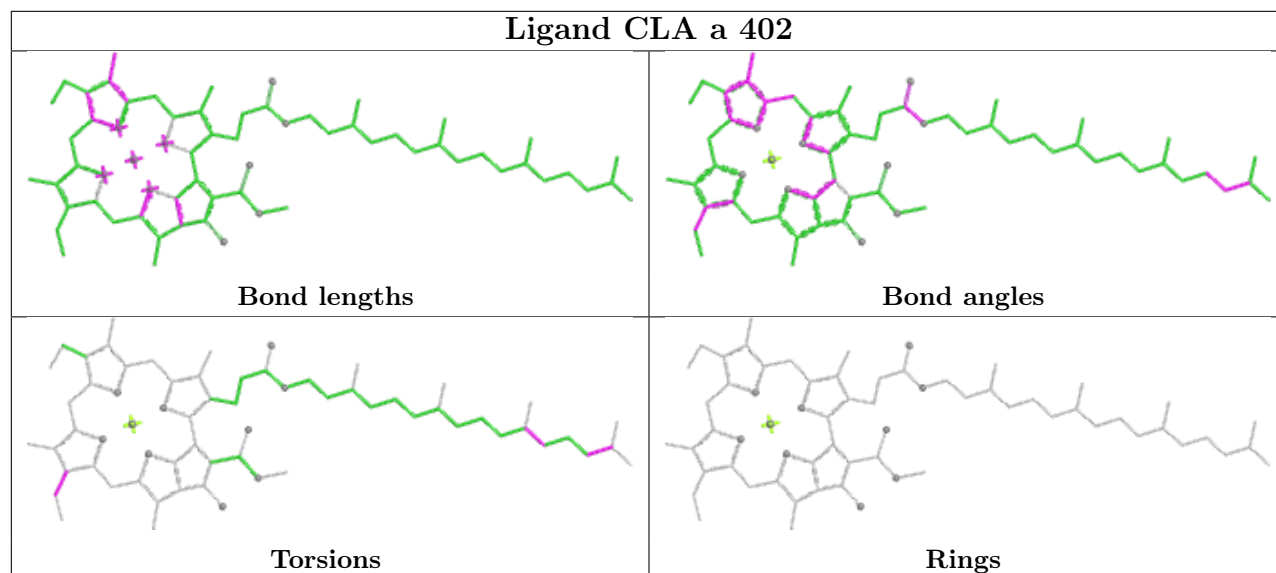
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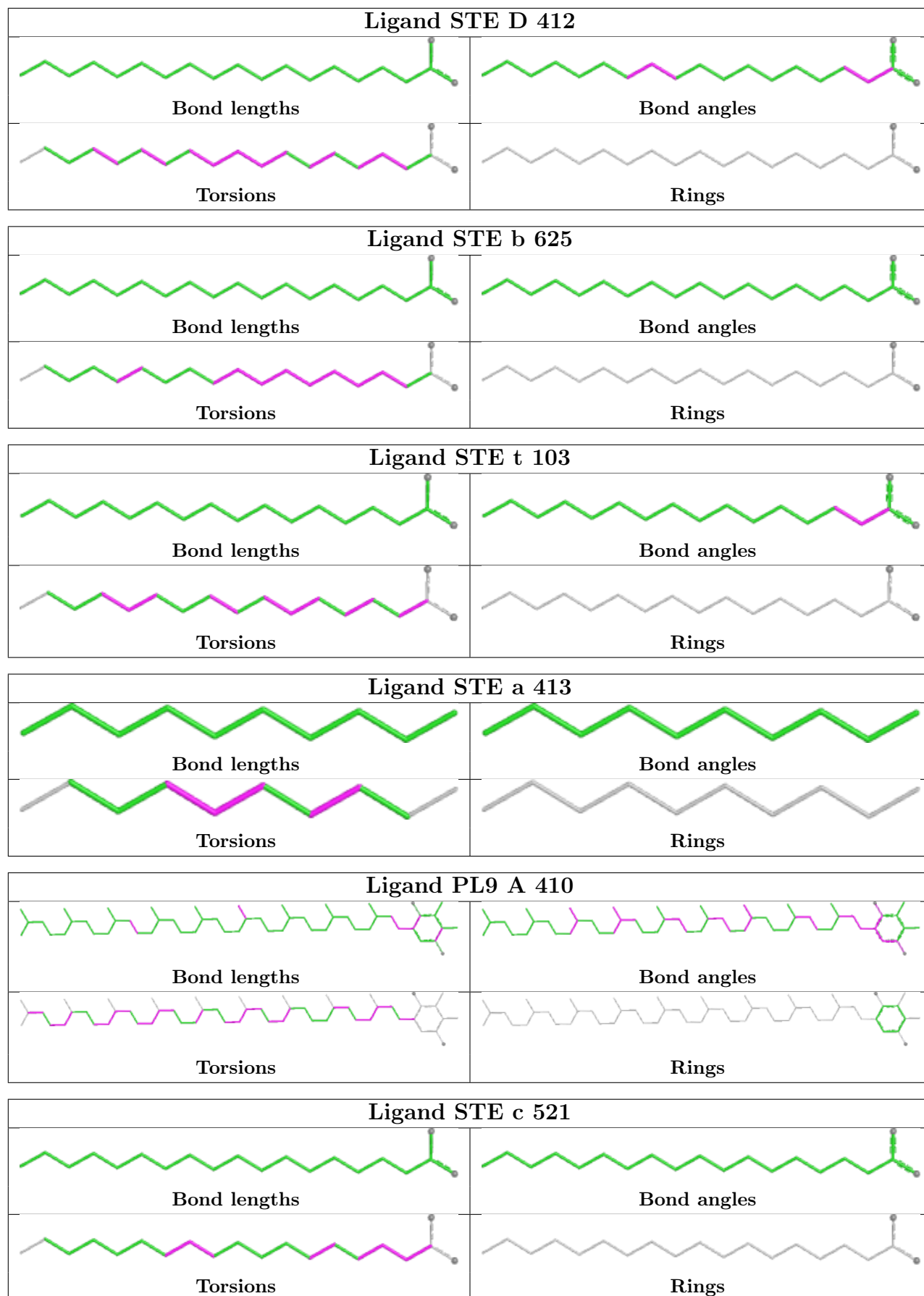


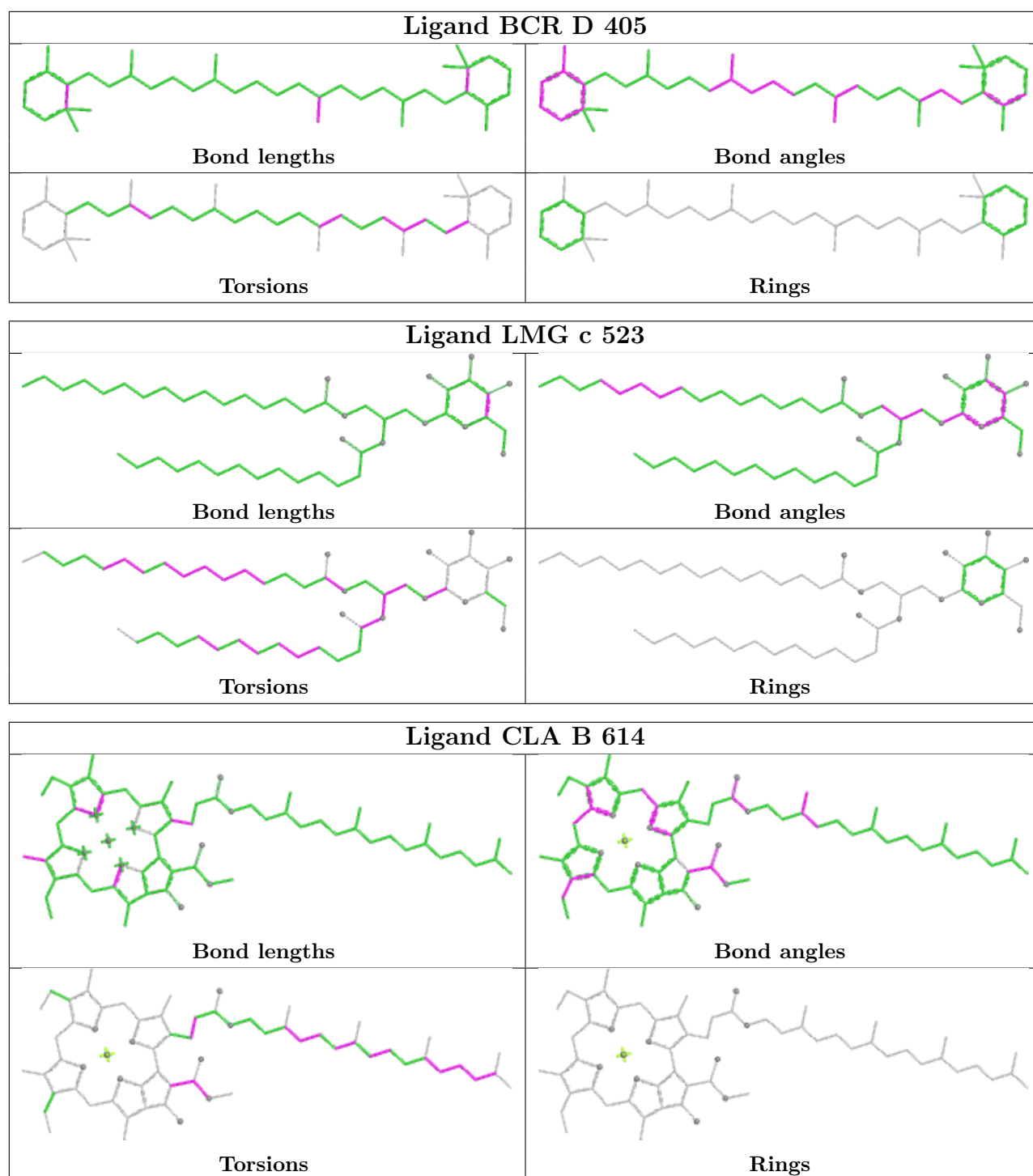
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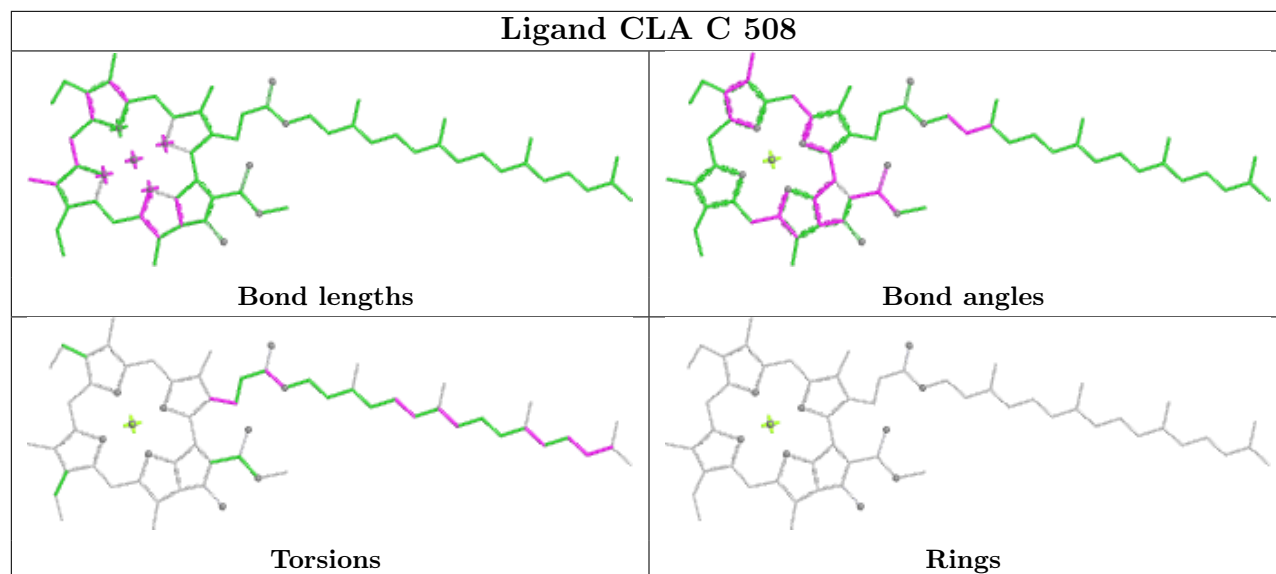
Ligand CLA a 402



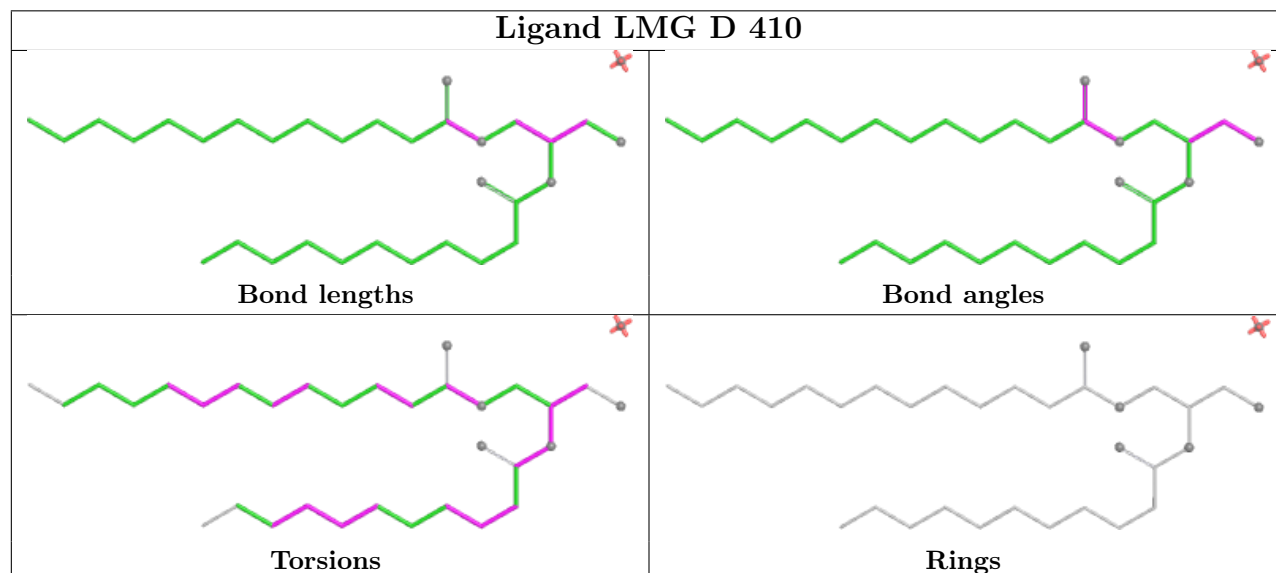




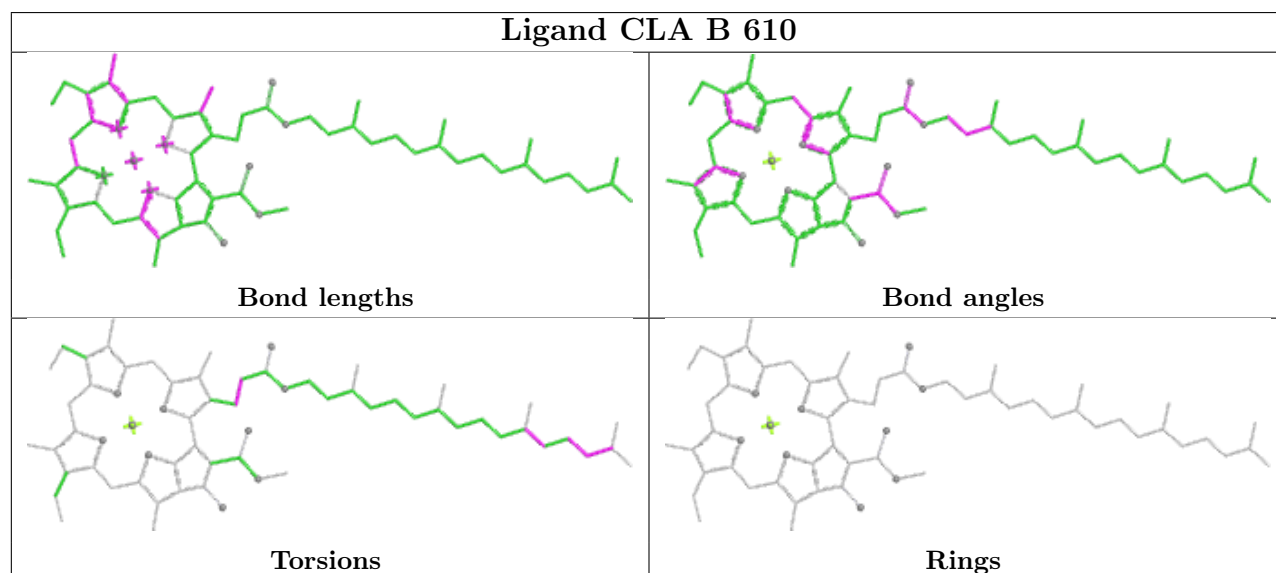
Ligand CLA C 508



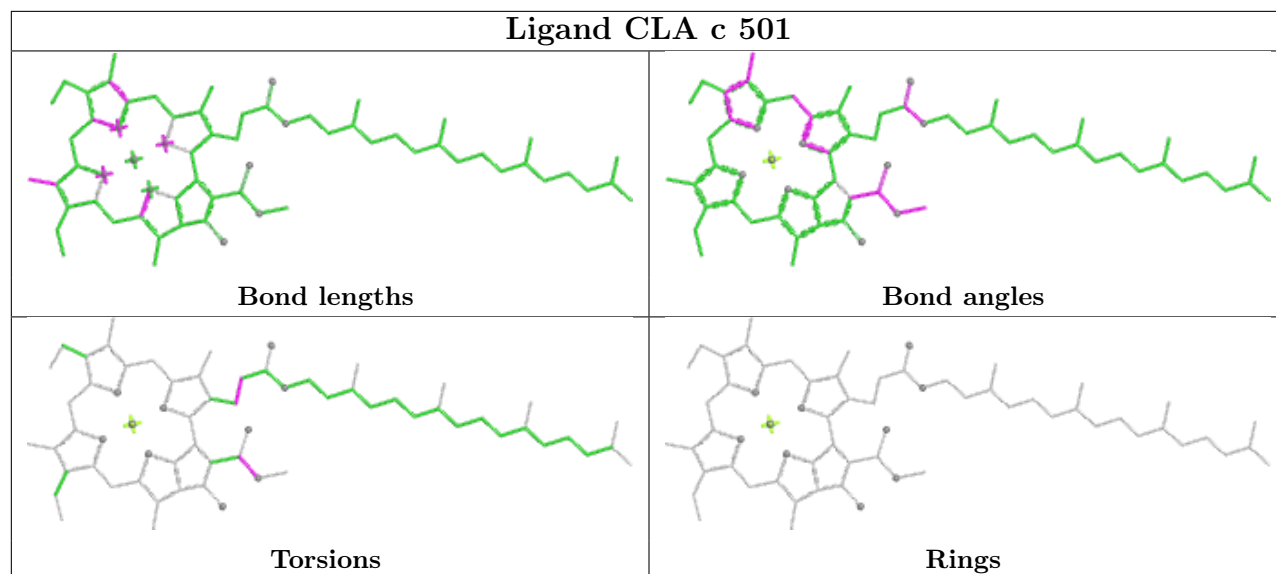
Ligand LMG D 410



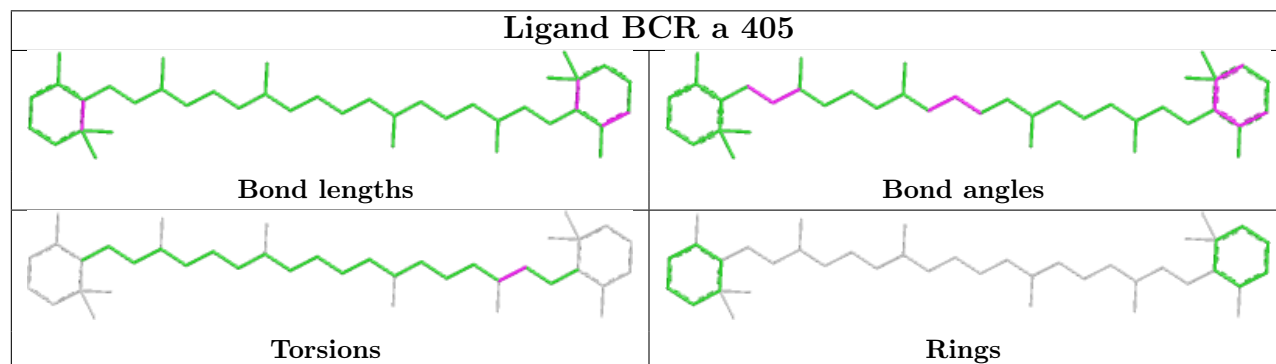
Ligand CLA B 610



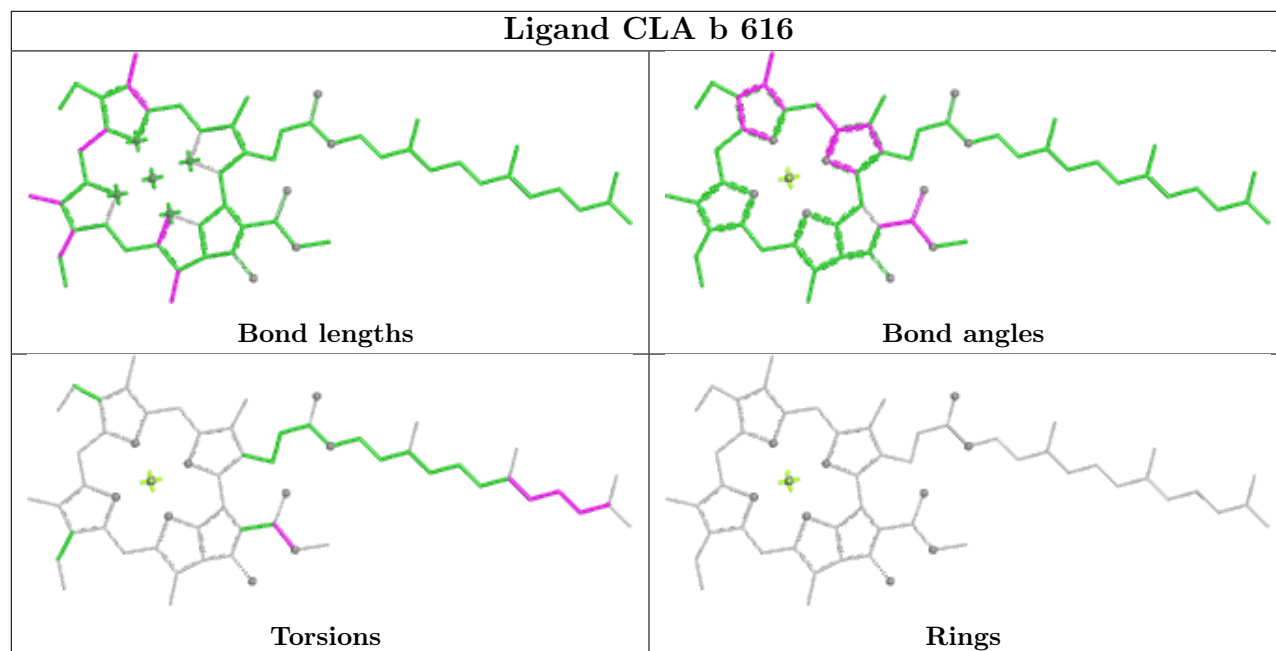
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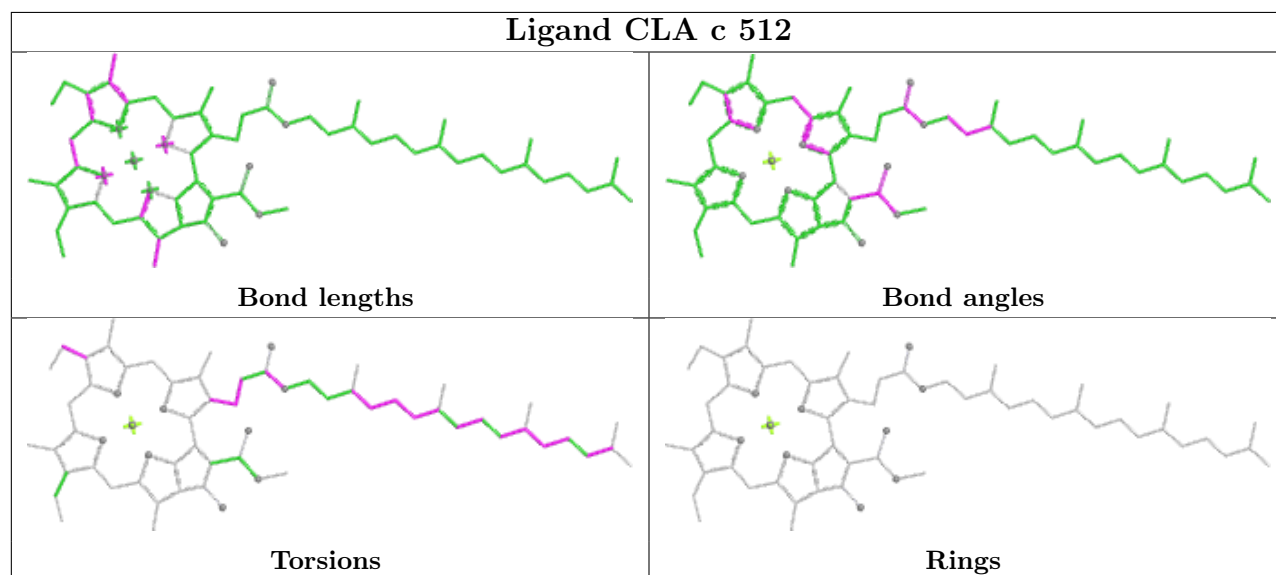
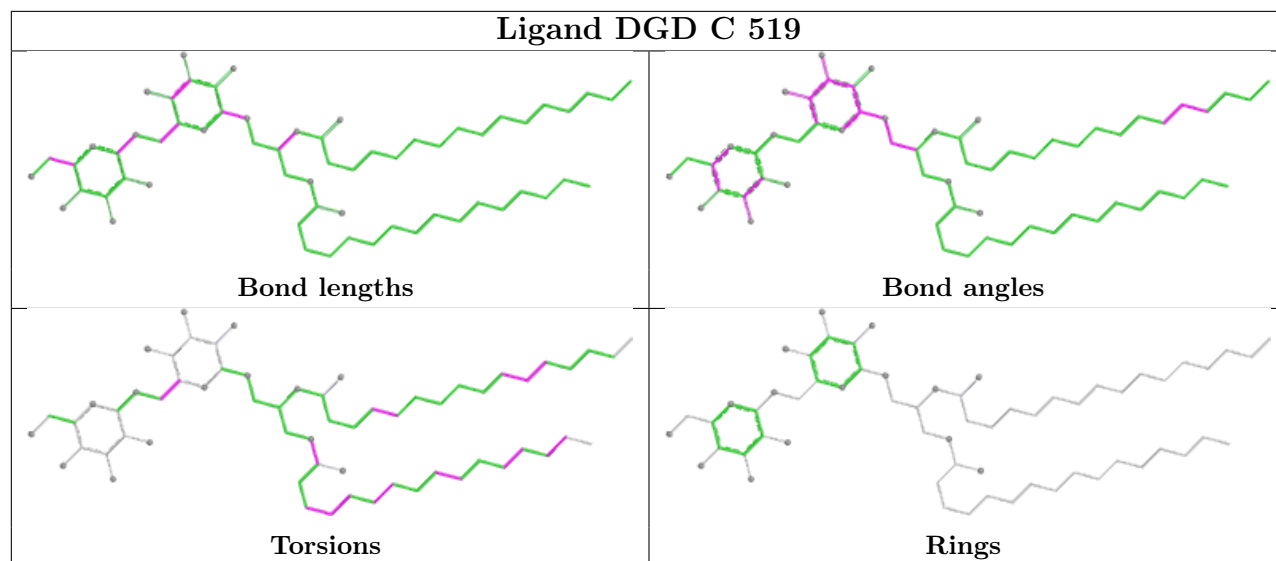


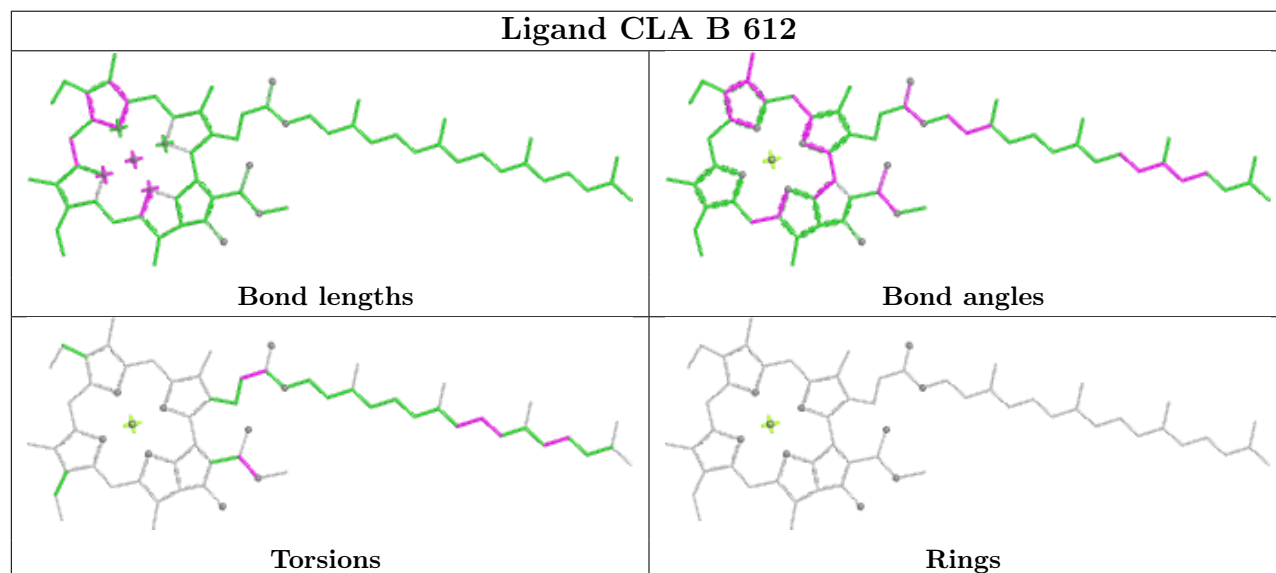
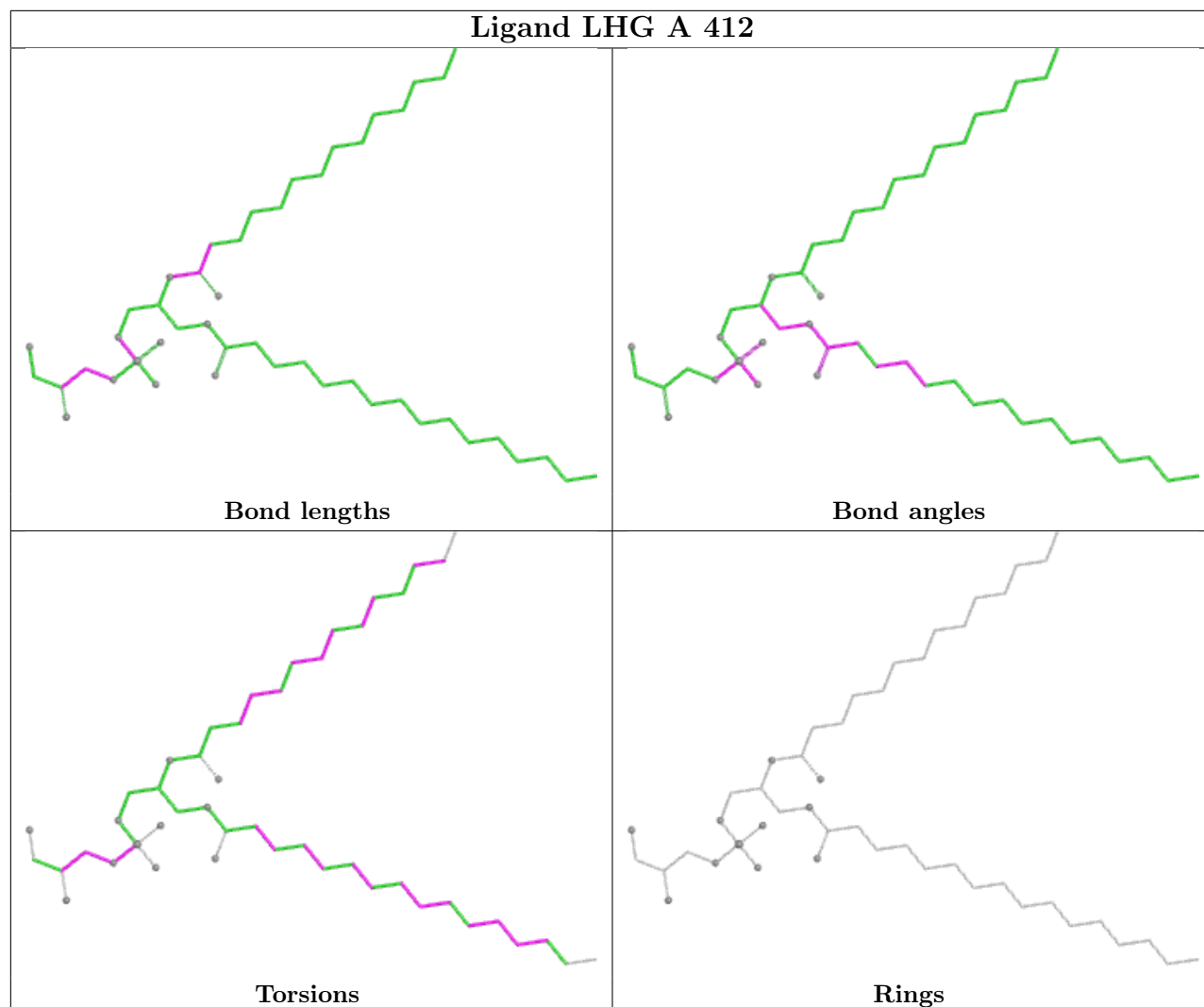
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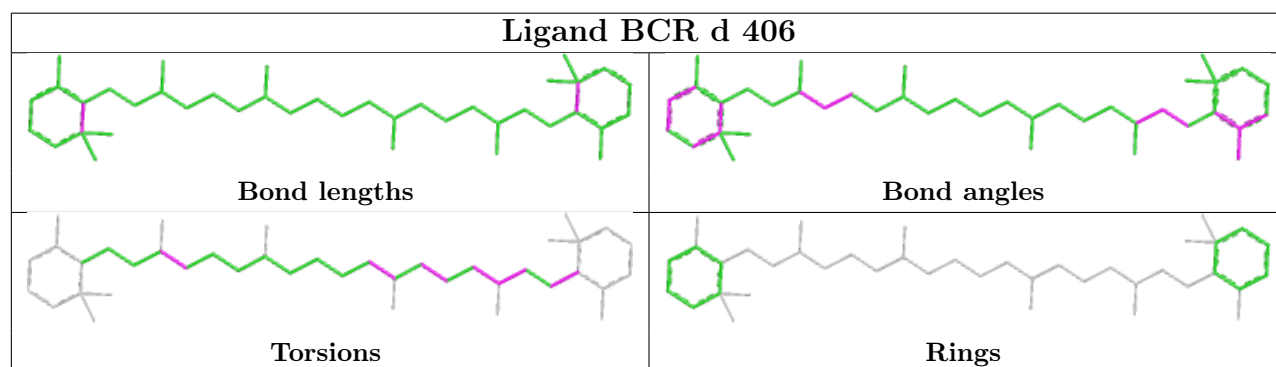
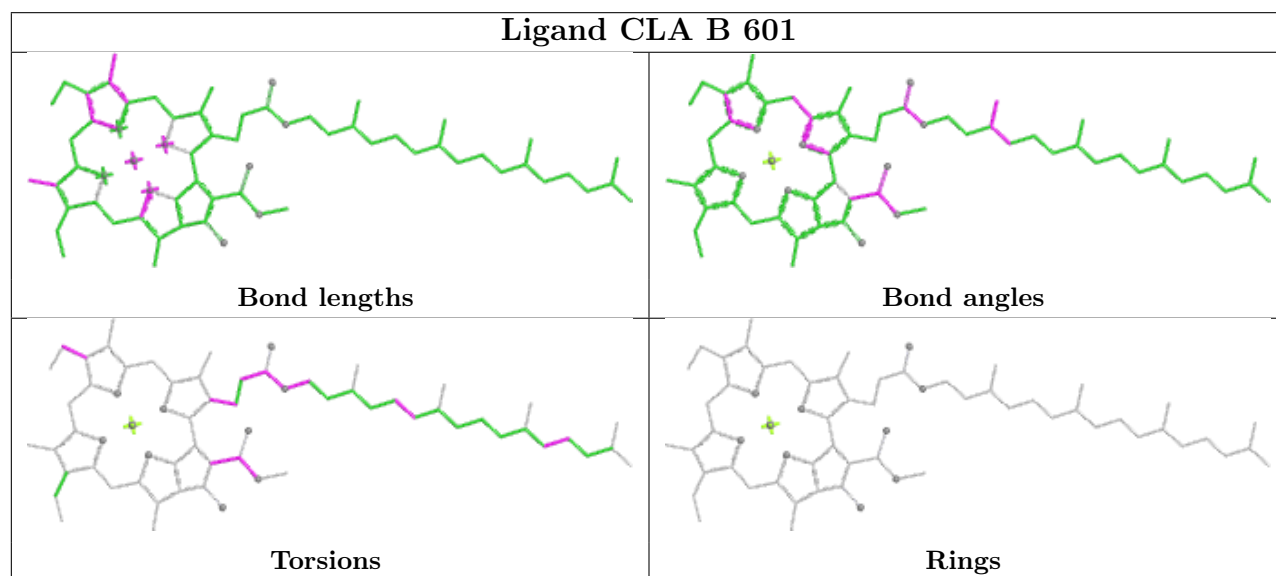
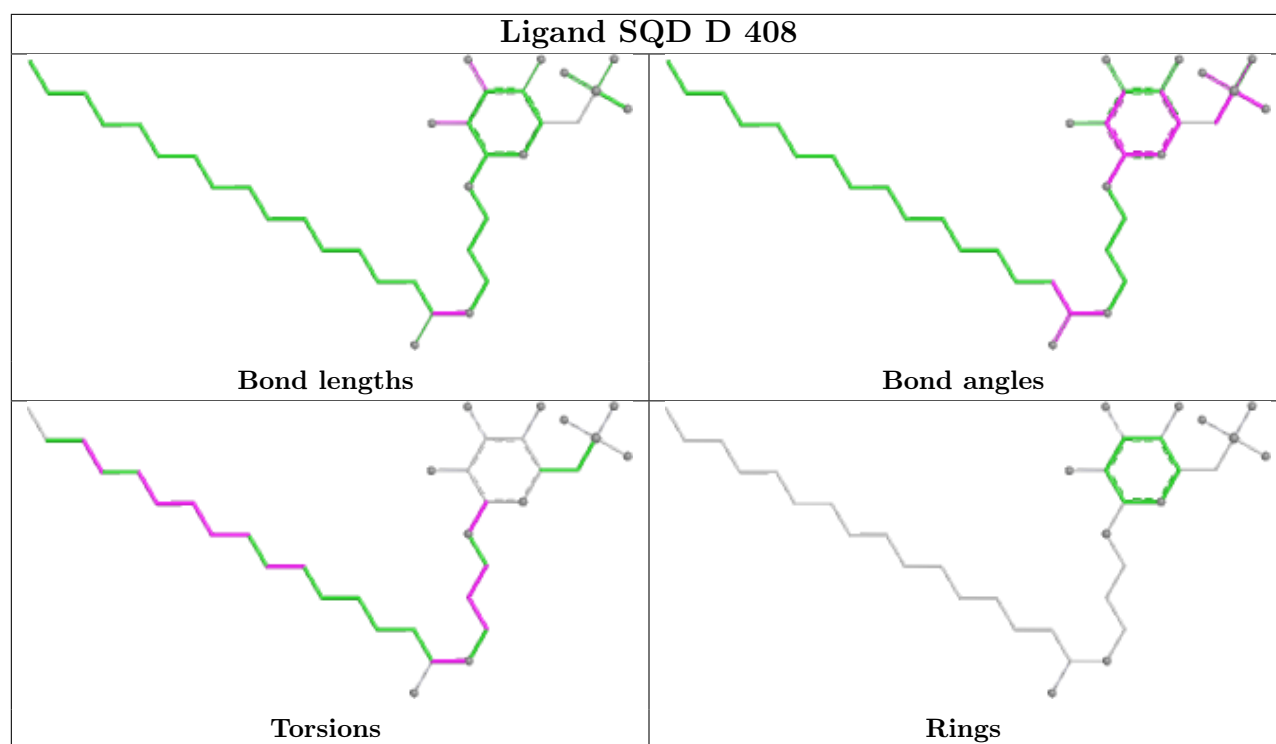


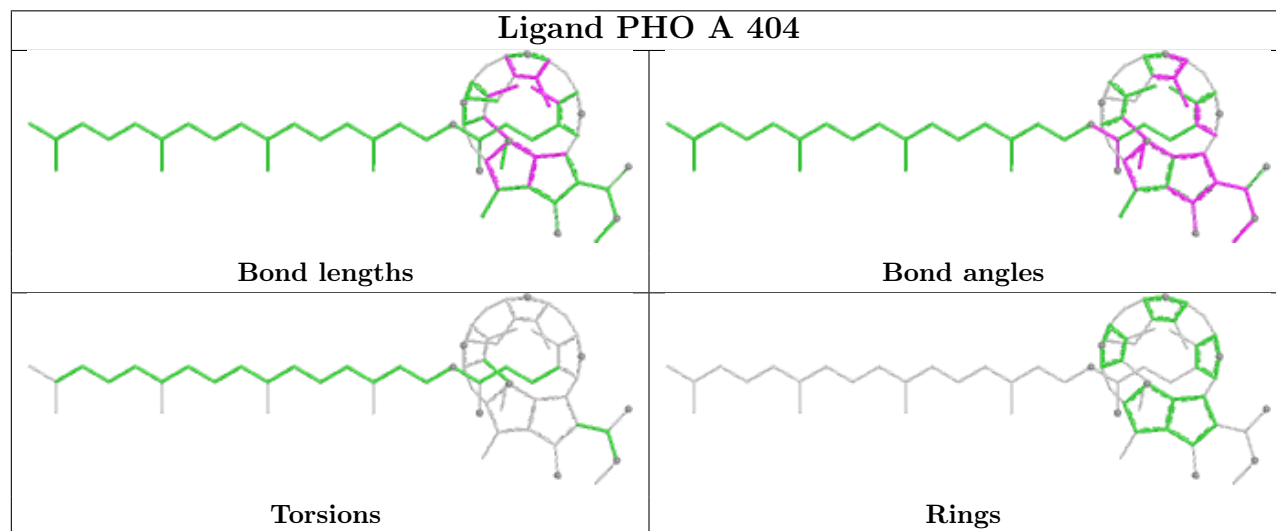
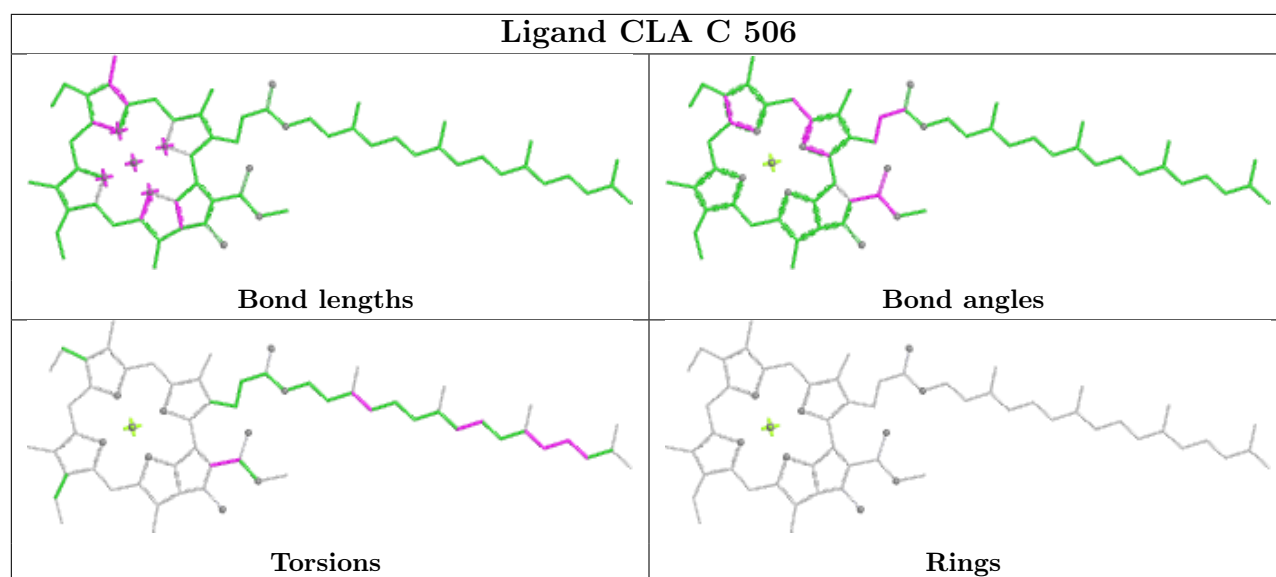
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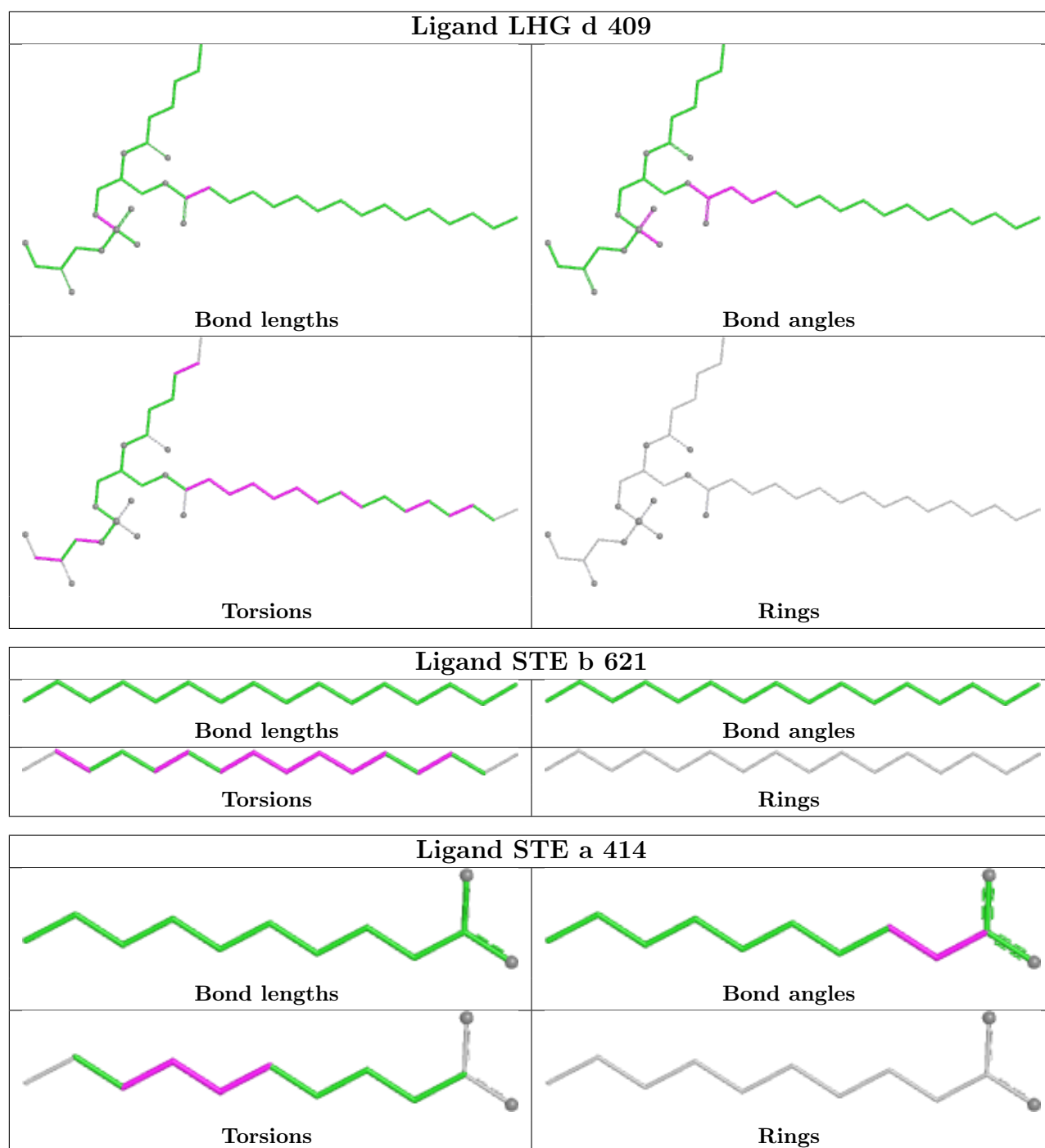


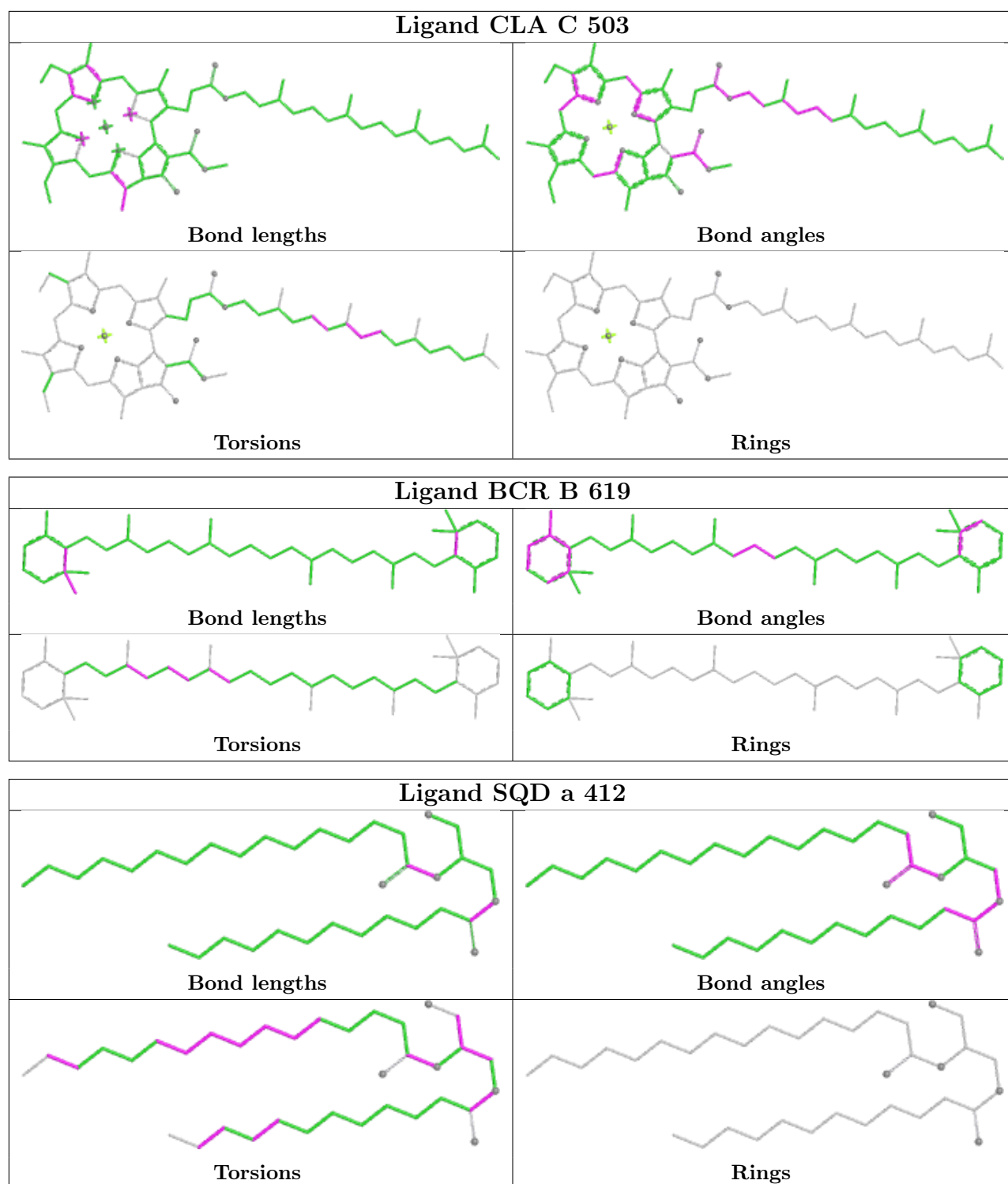


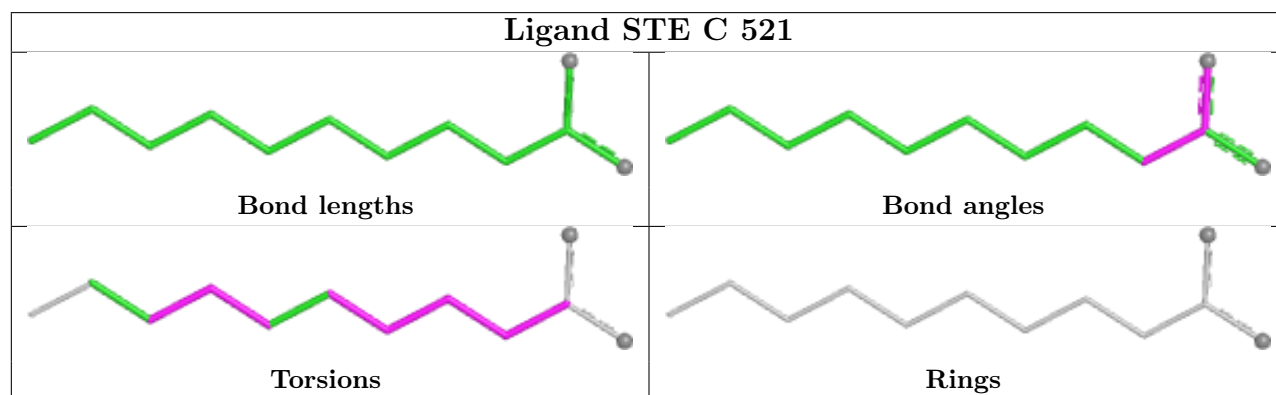
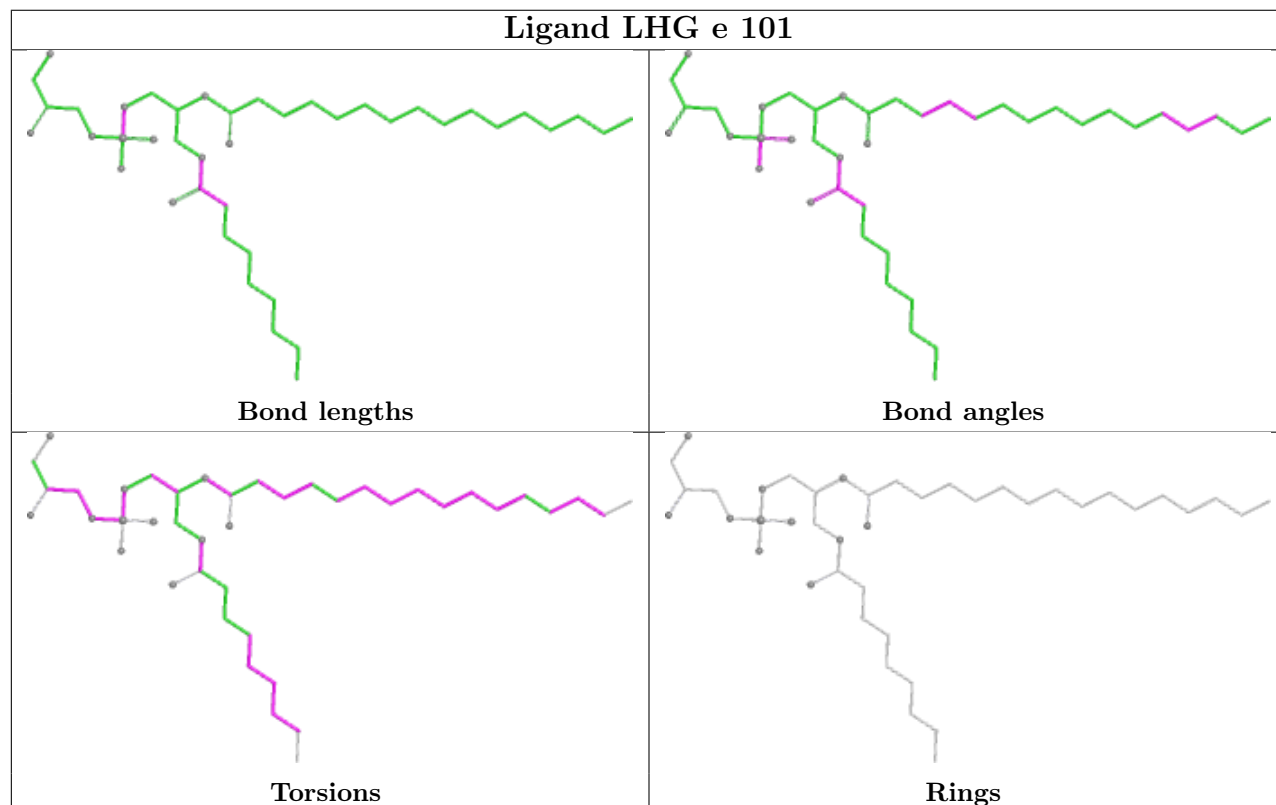
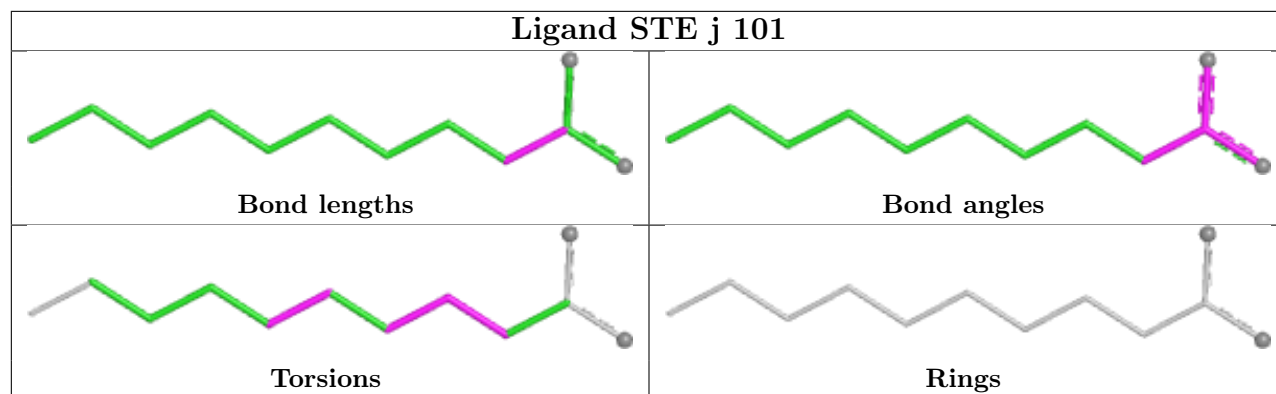


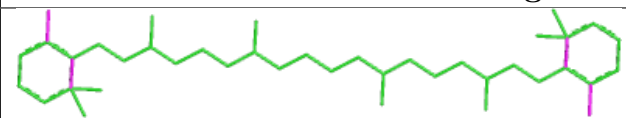
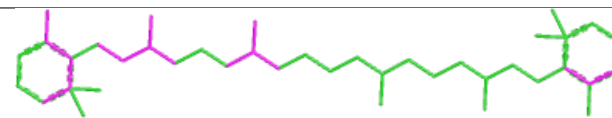
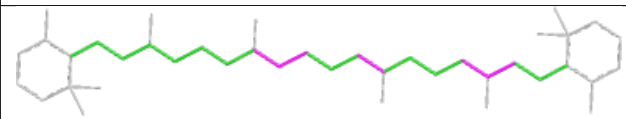
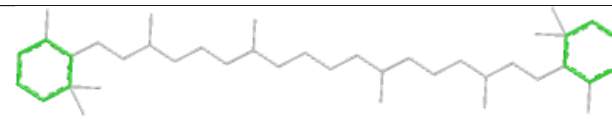


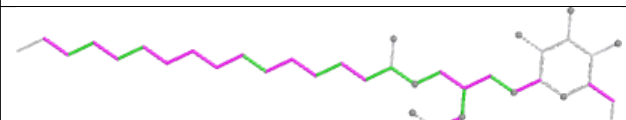
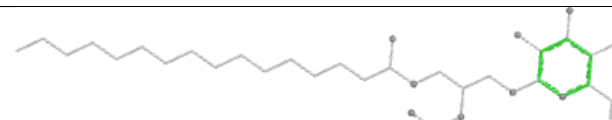


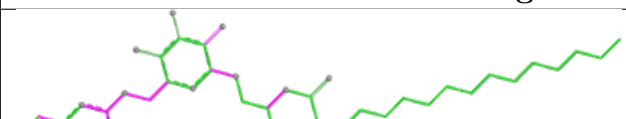
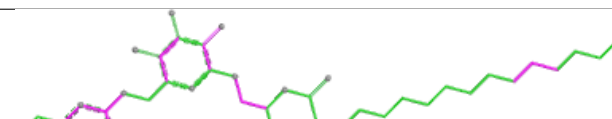
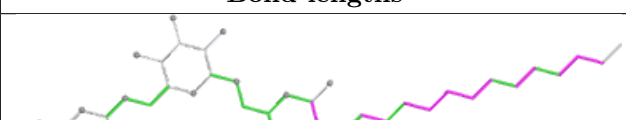
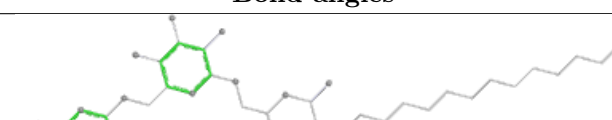


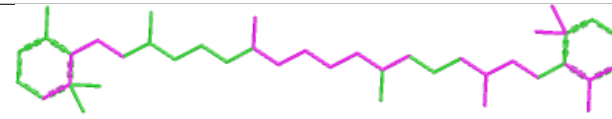
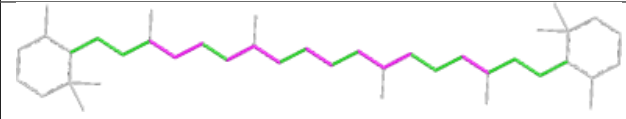
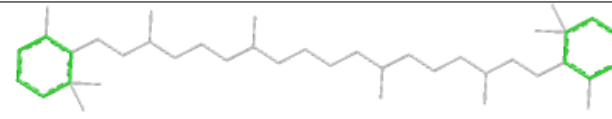


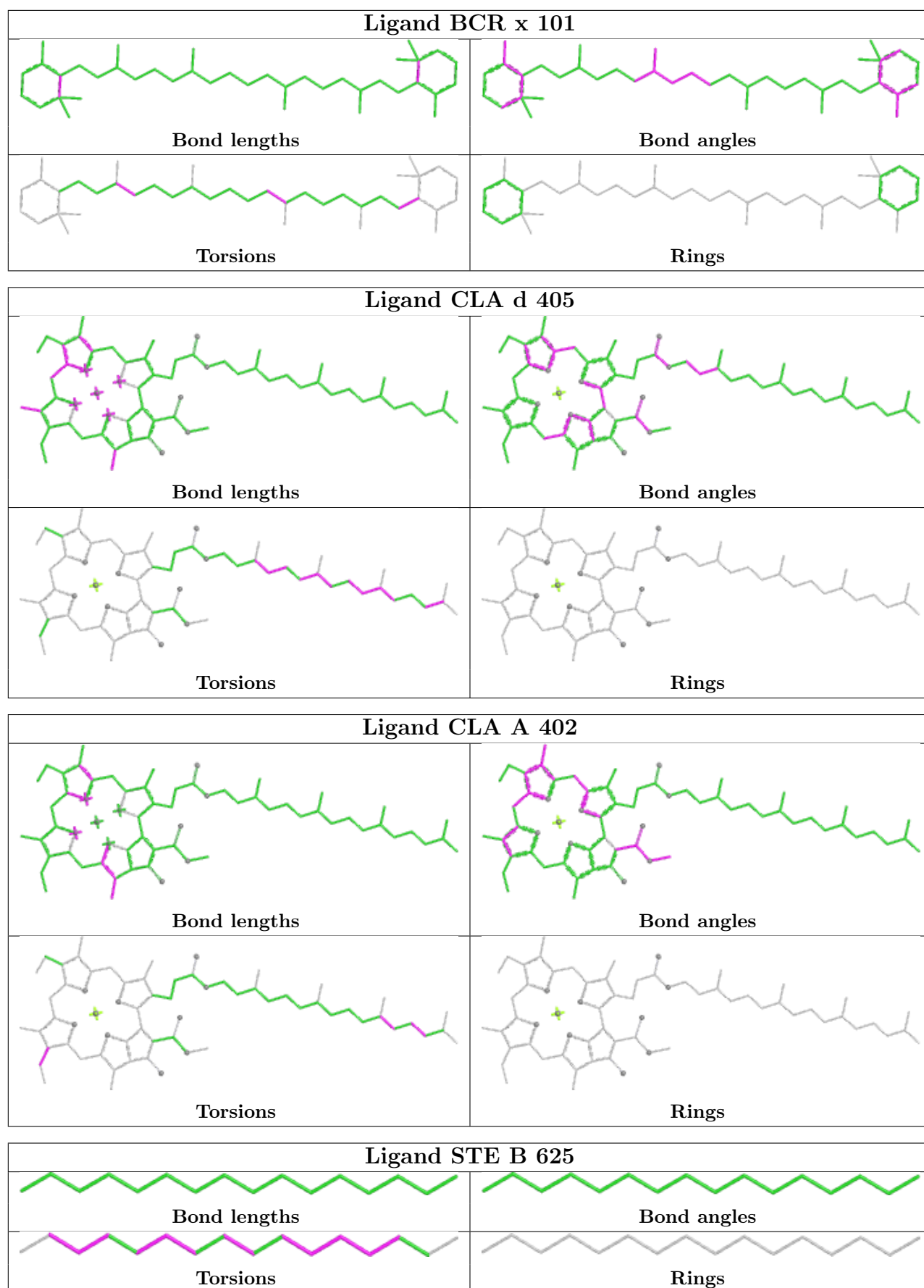


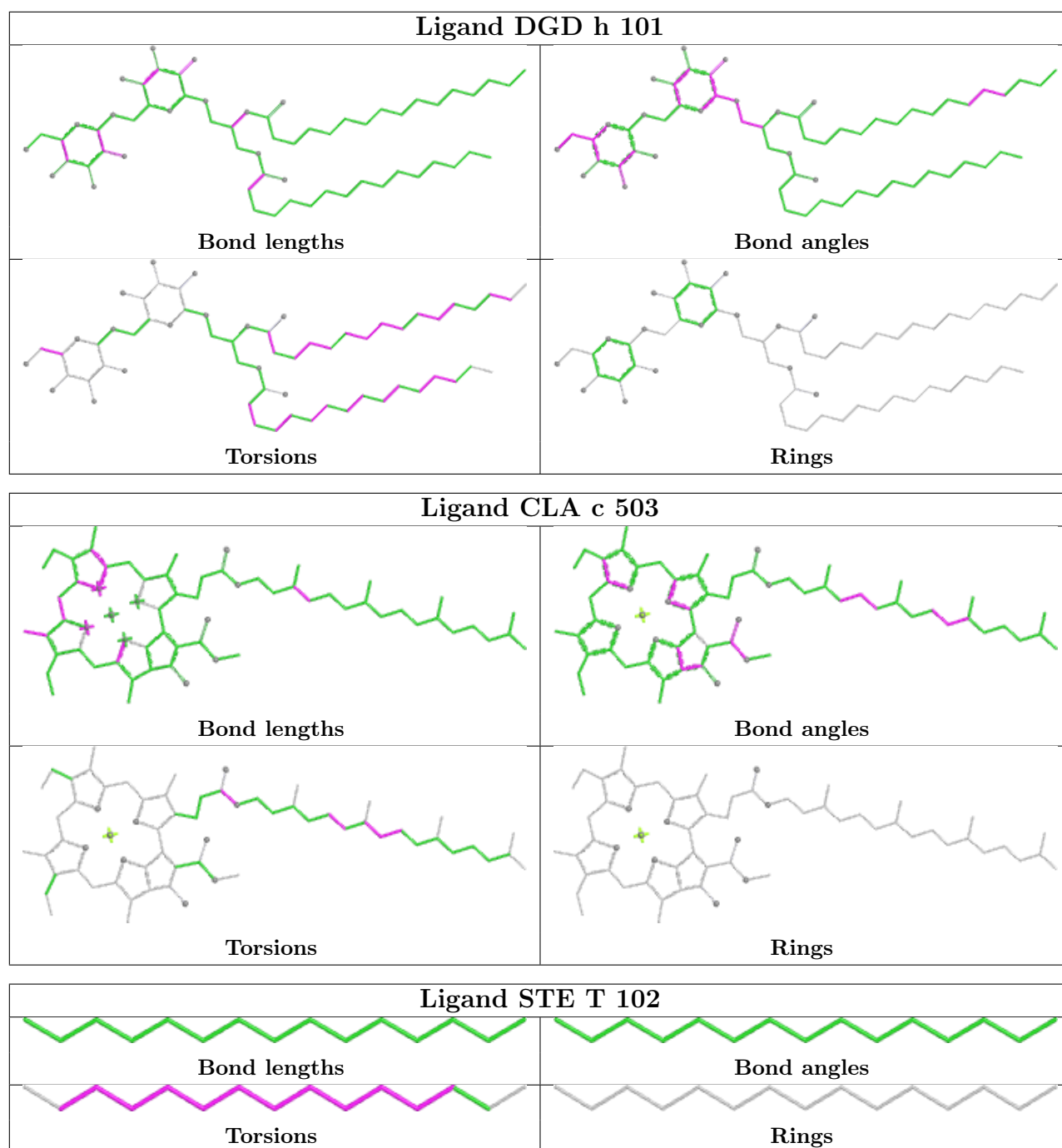
Ligand BCR c 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

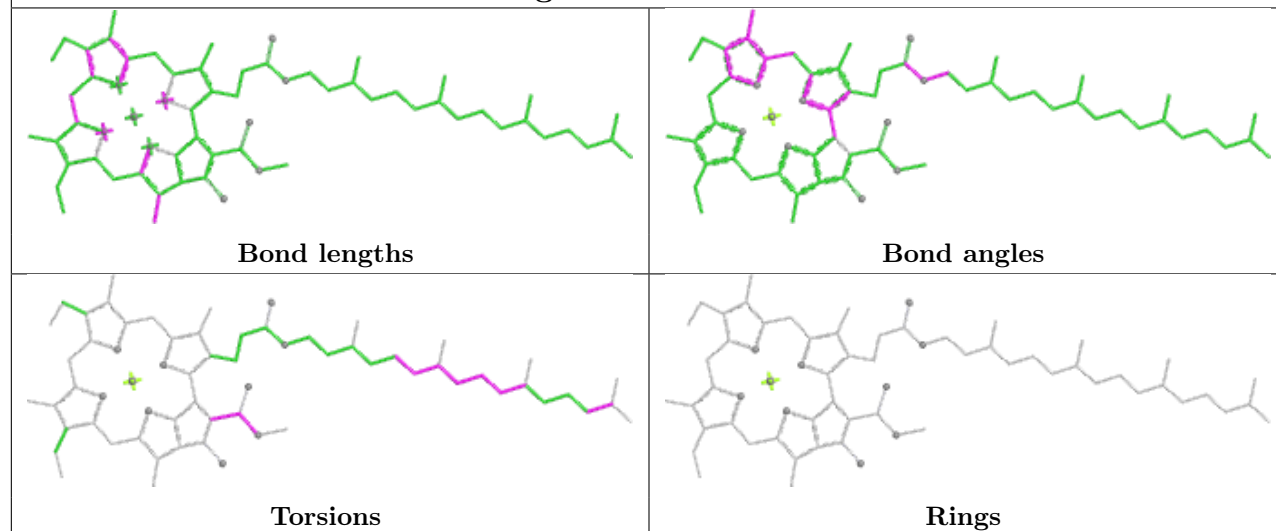
Ligand DGD H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

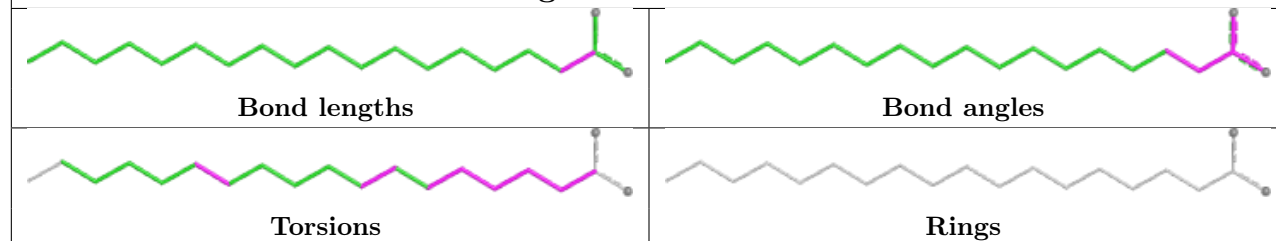




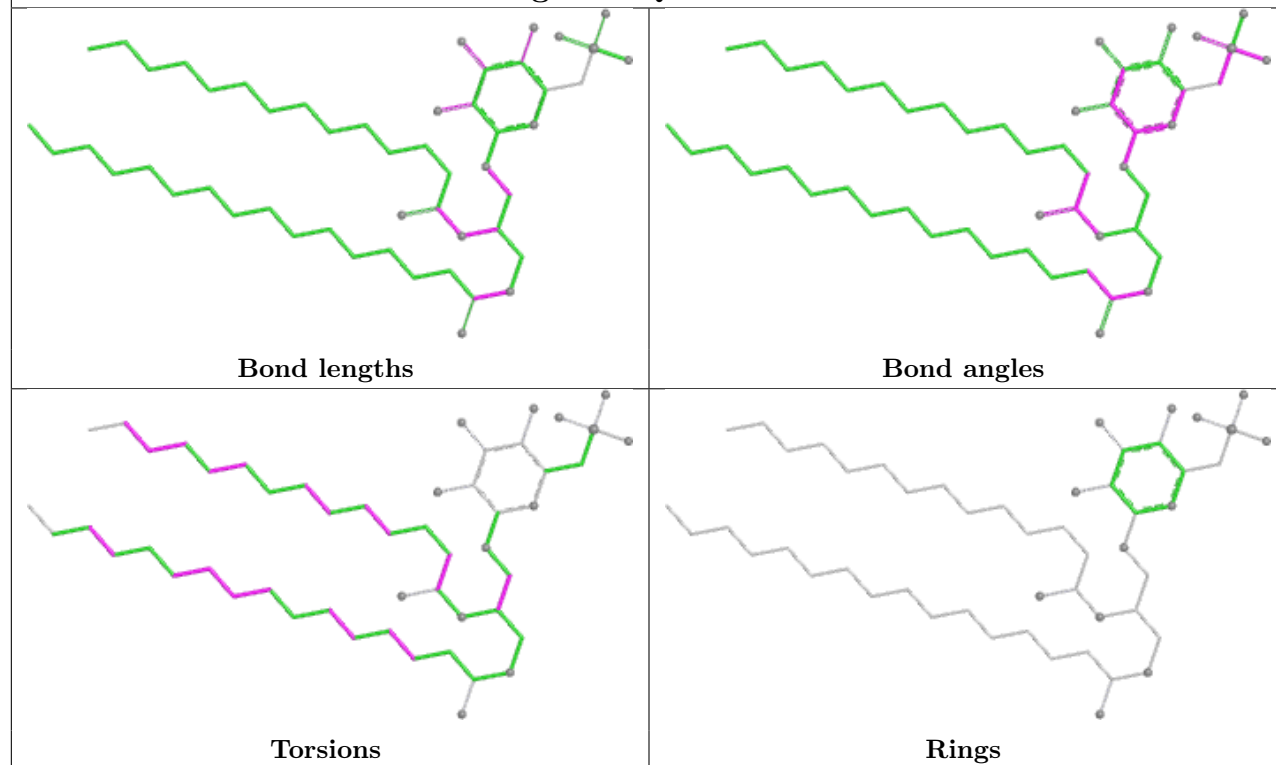
Ligand CLA b 607

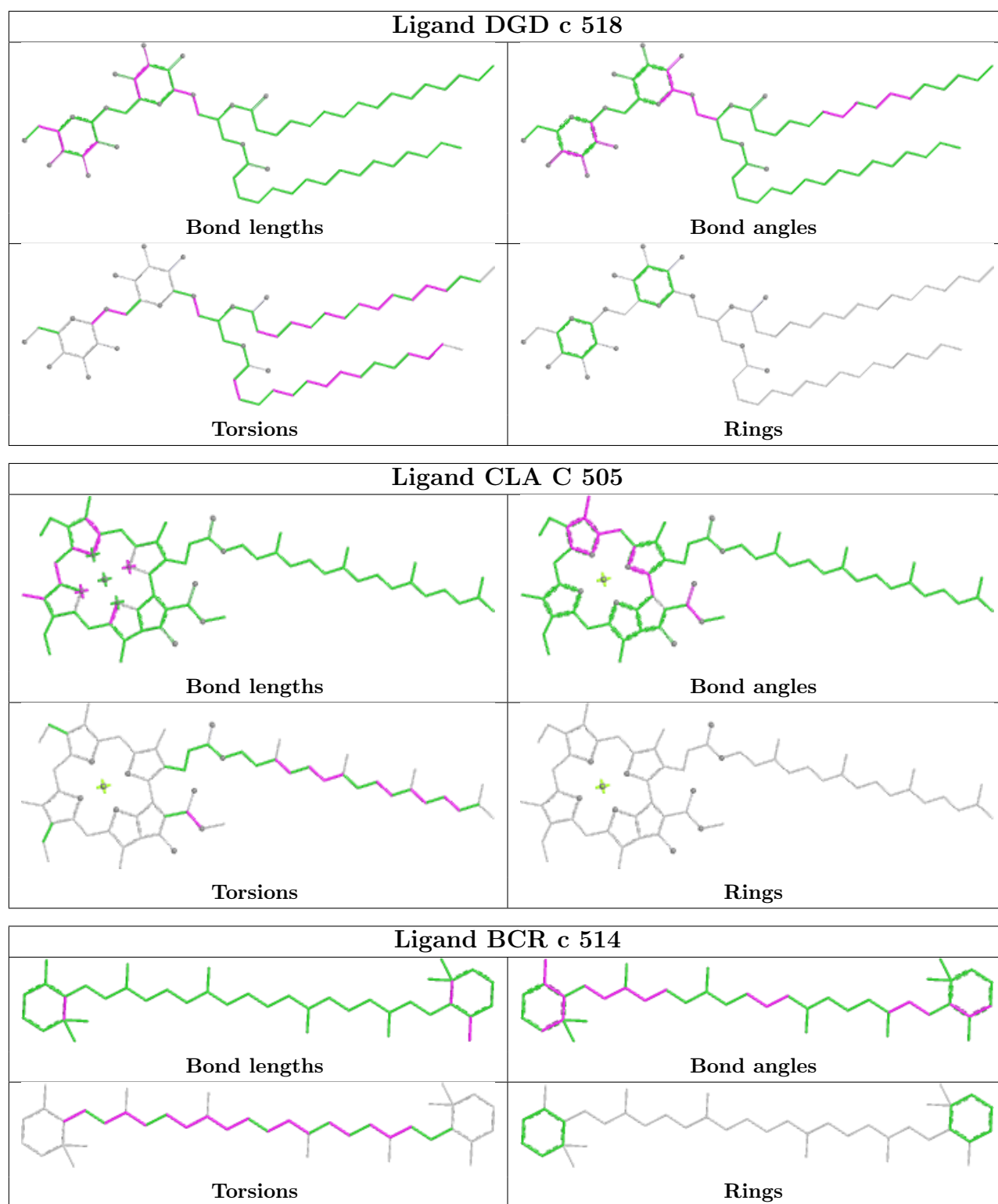


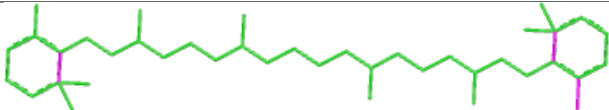
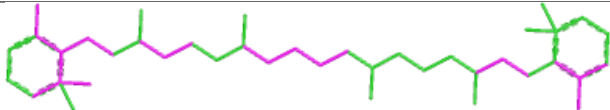
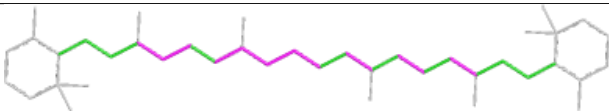
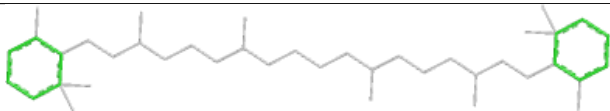
Ligand STE d 412

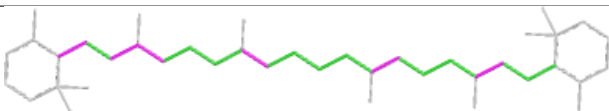
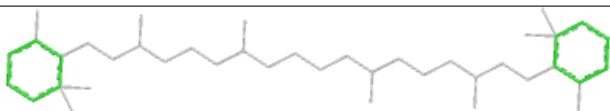


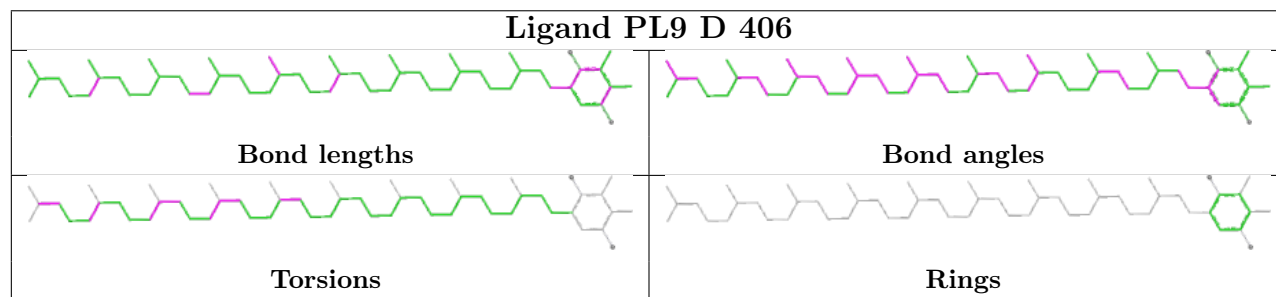
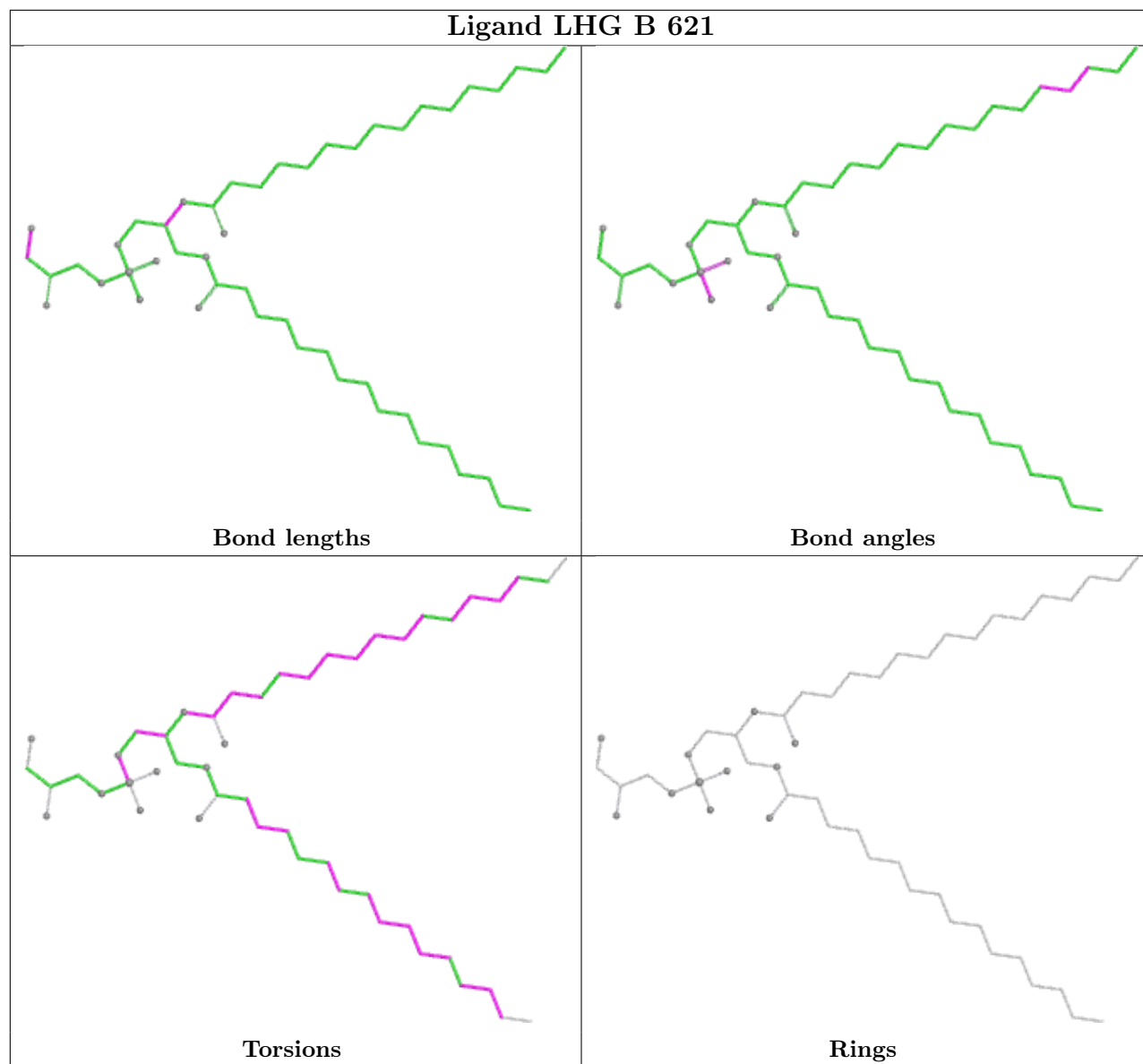
Ligand SQD A 413



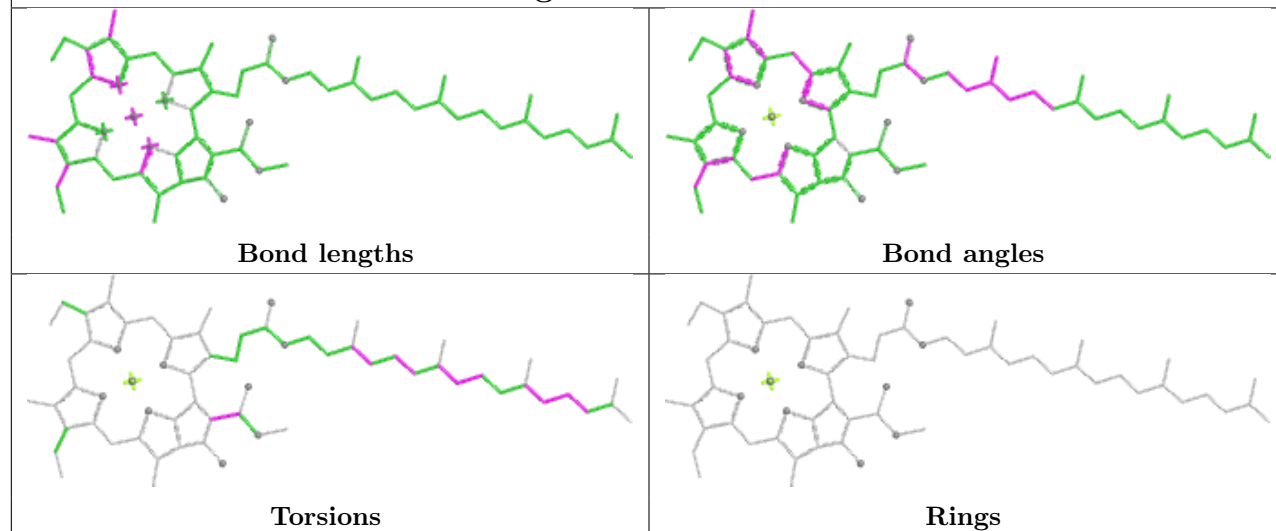


Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

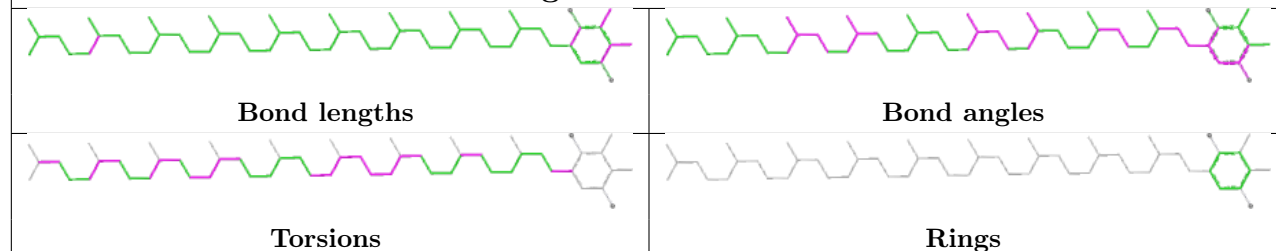
Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



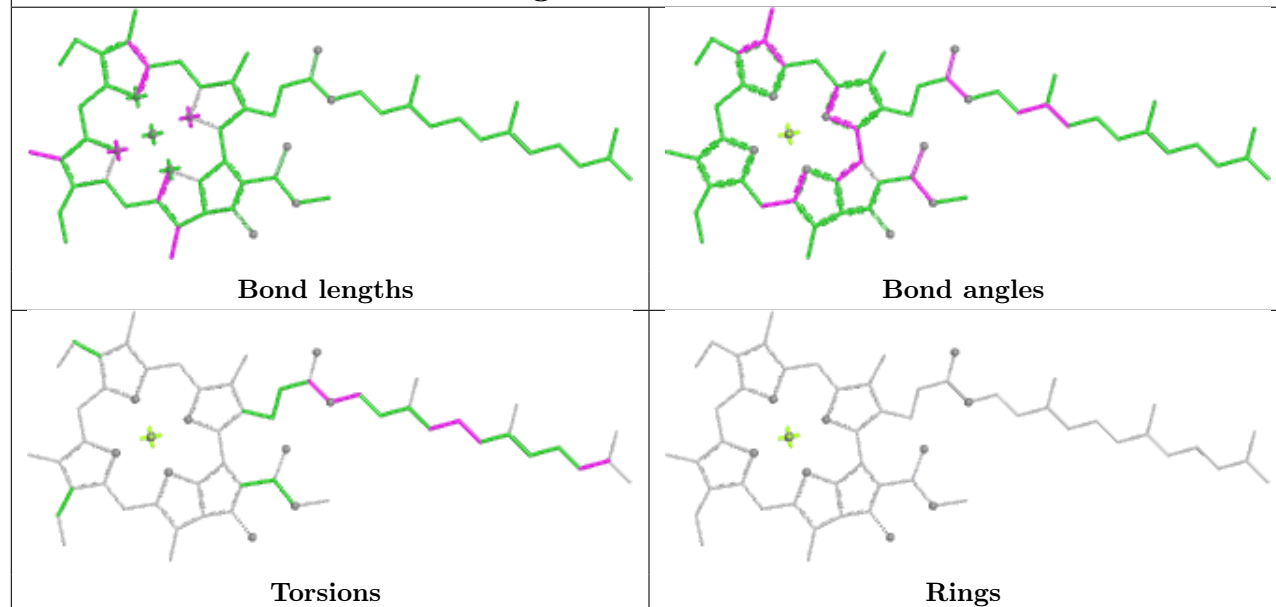
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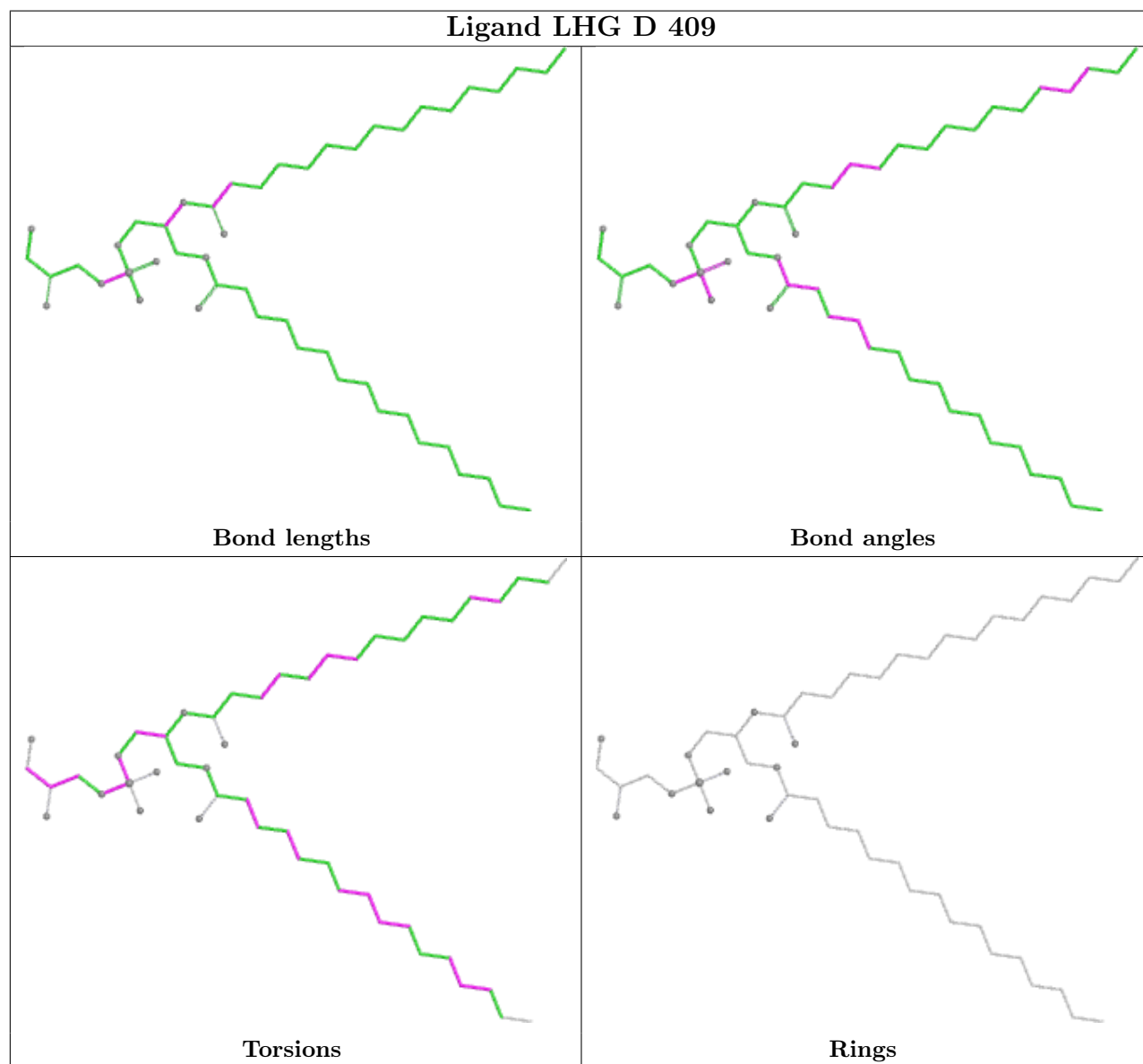
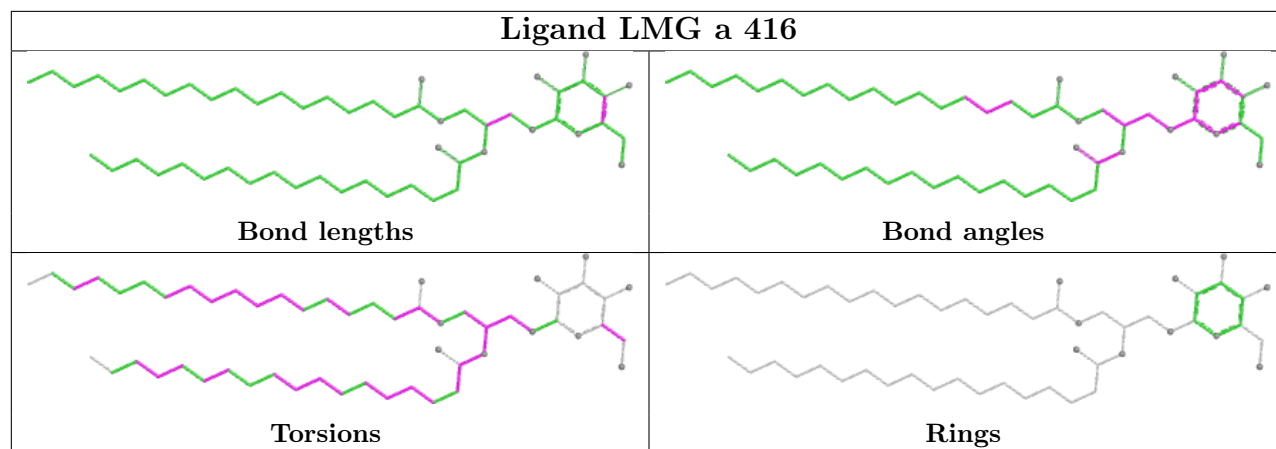


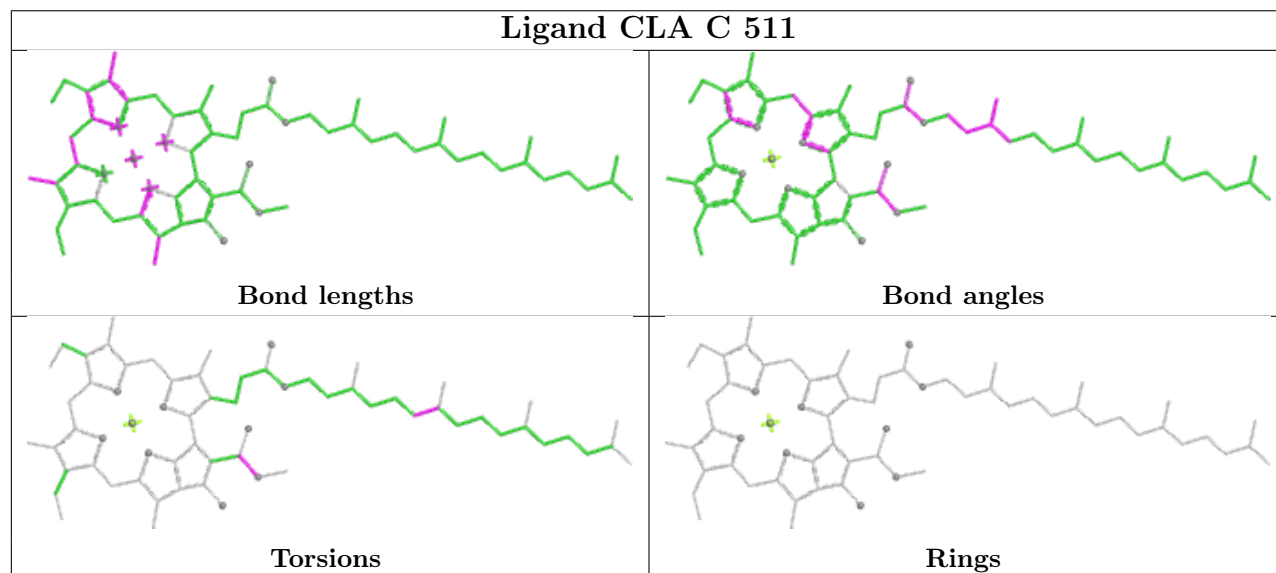
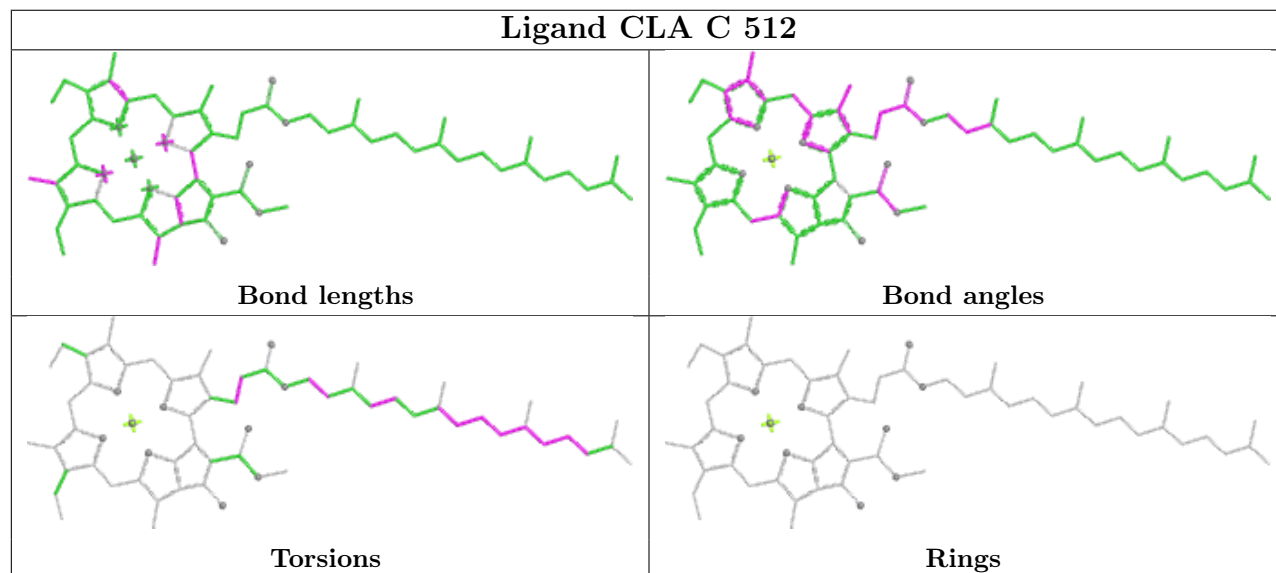
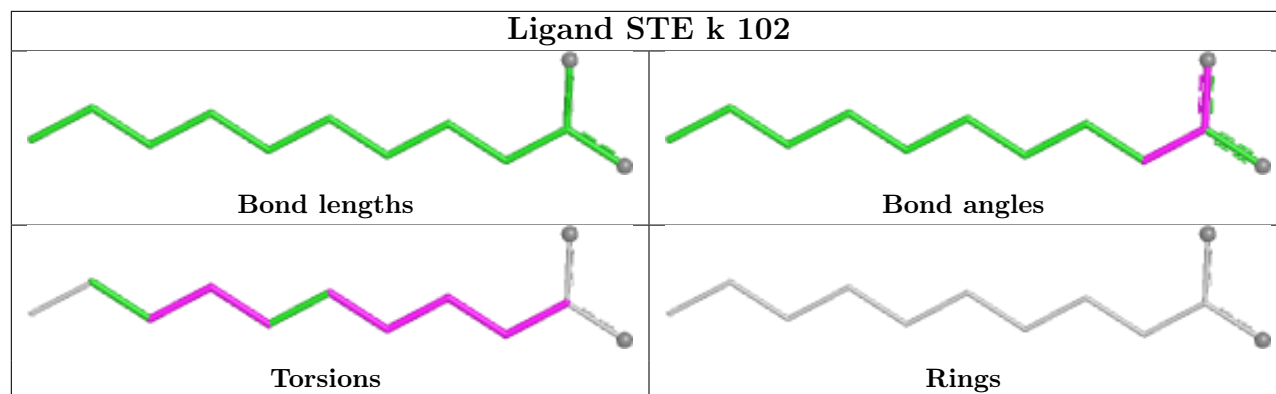
Ligand PL9 a 409

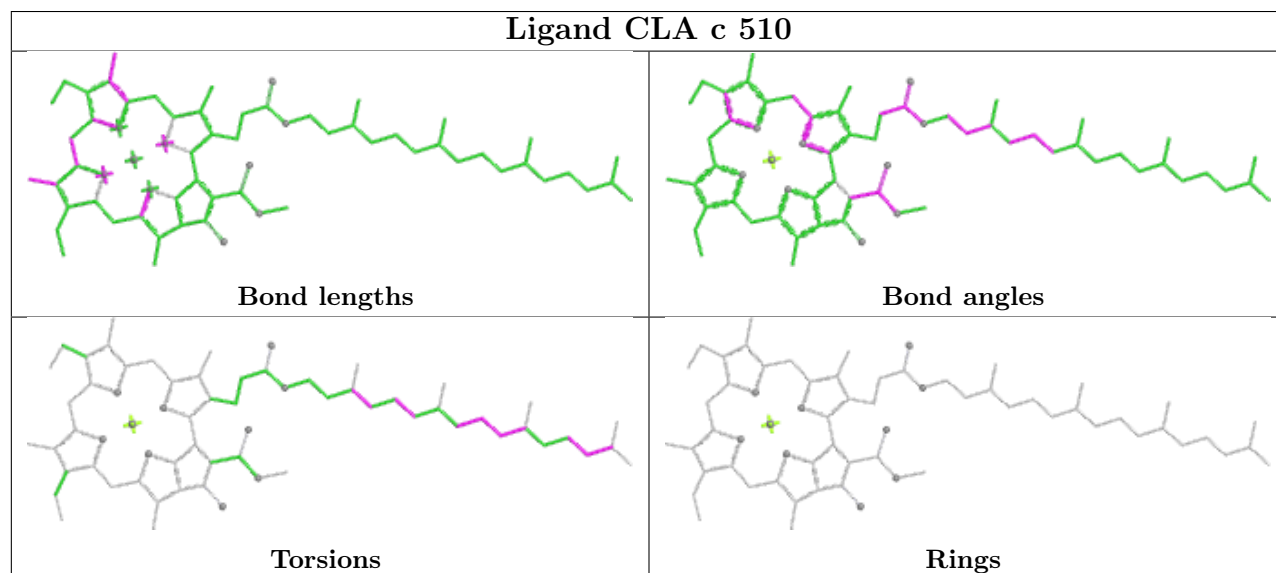
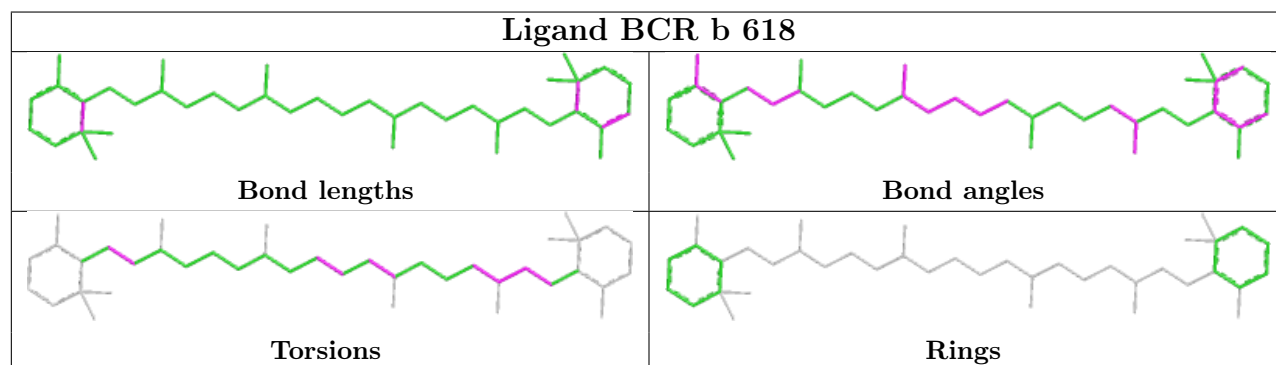
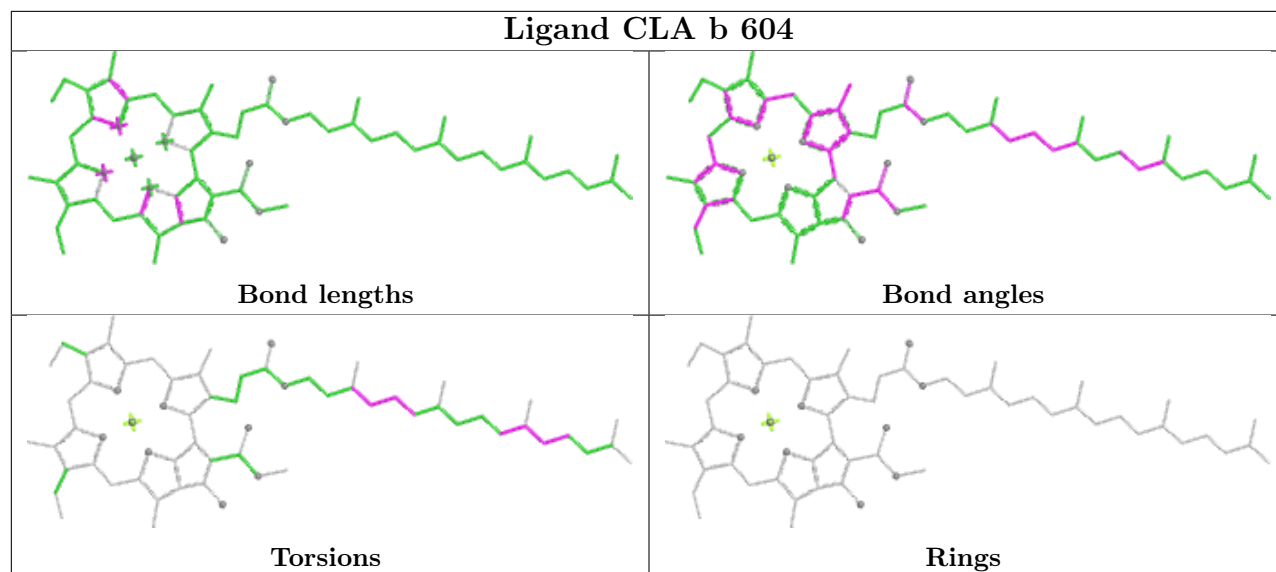


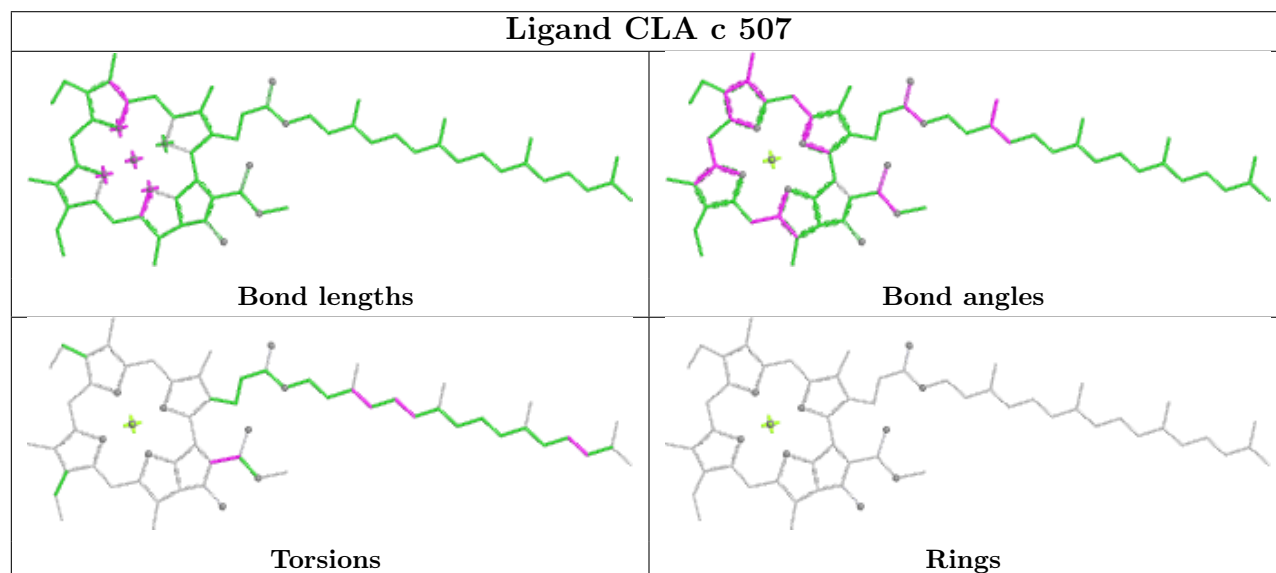
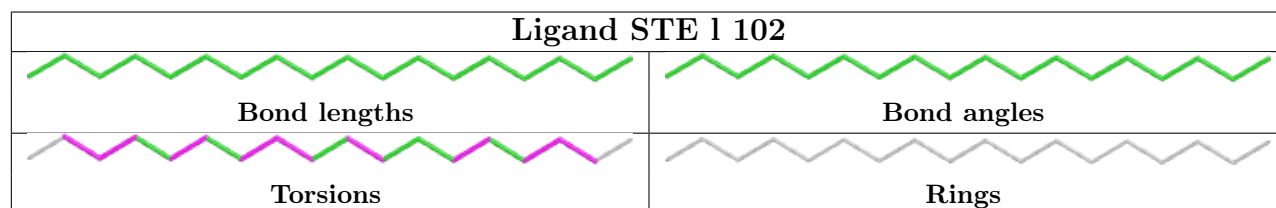
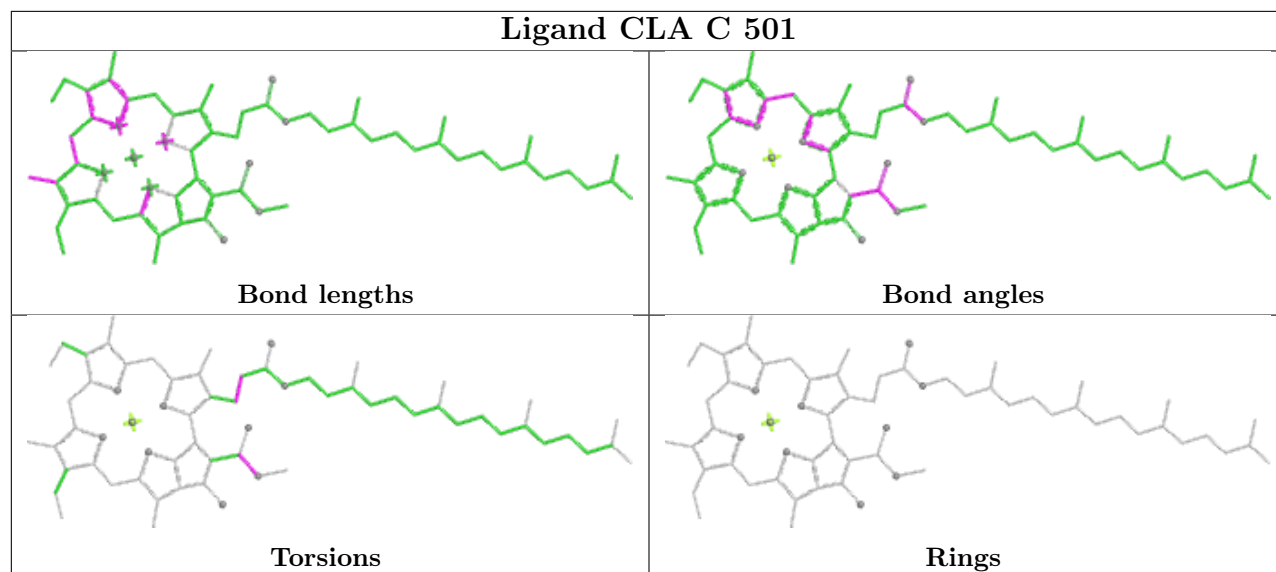
Ligand CLA B 616



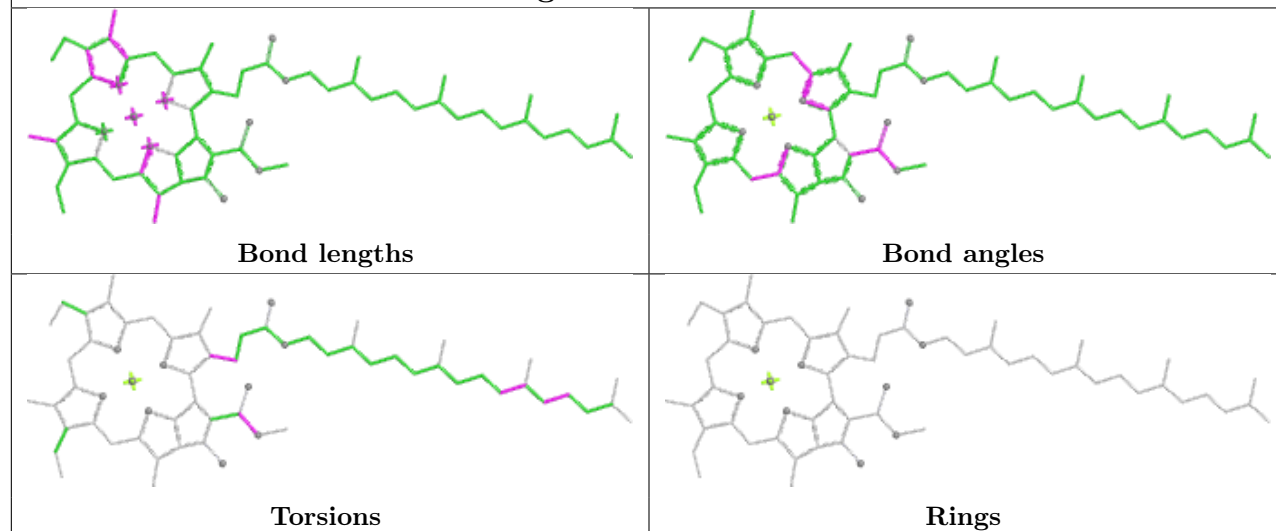




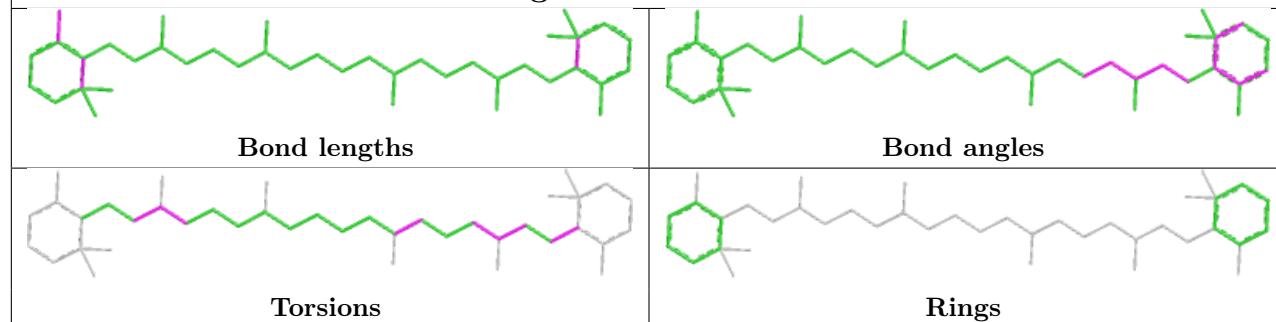




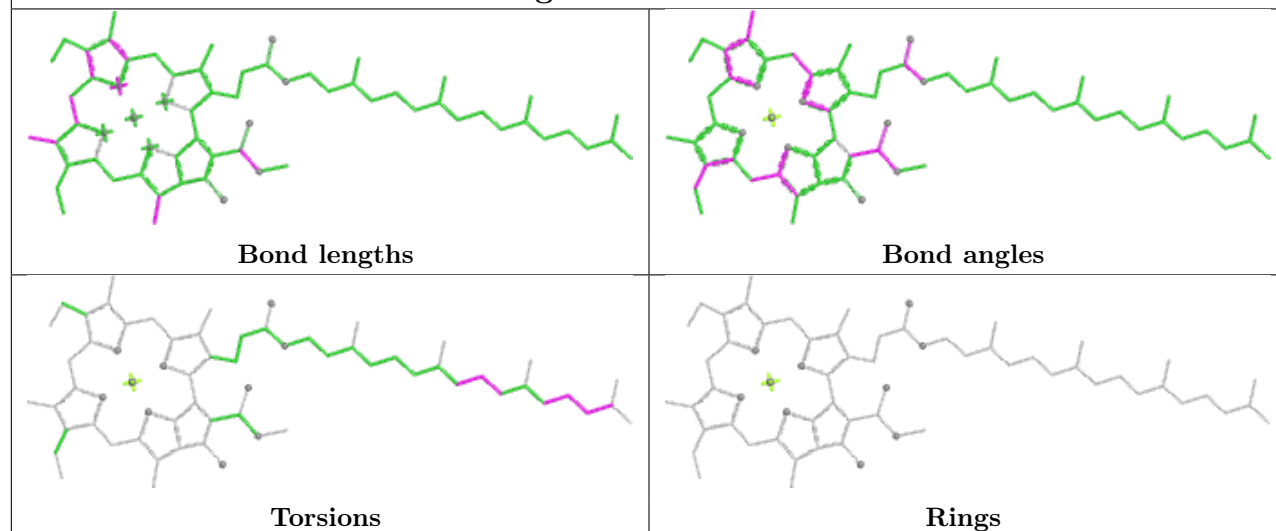
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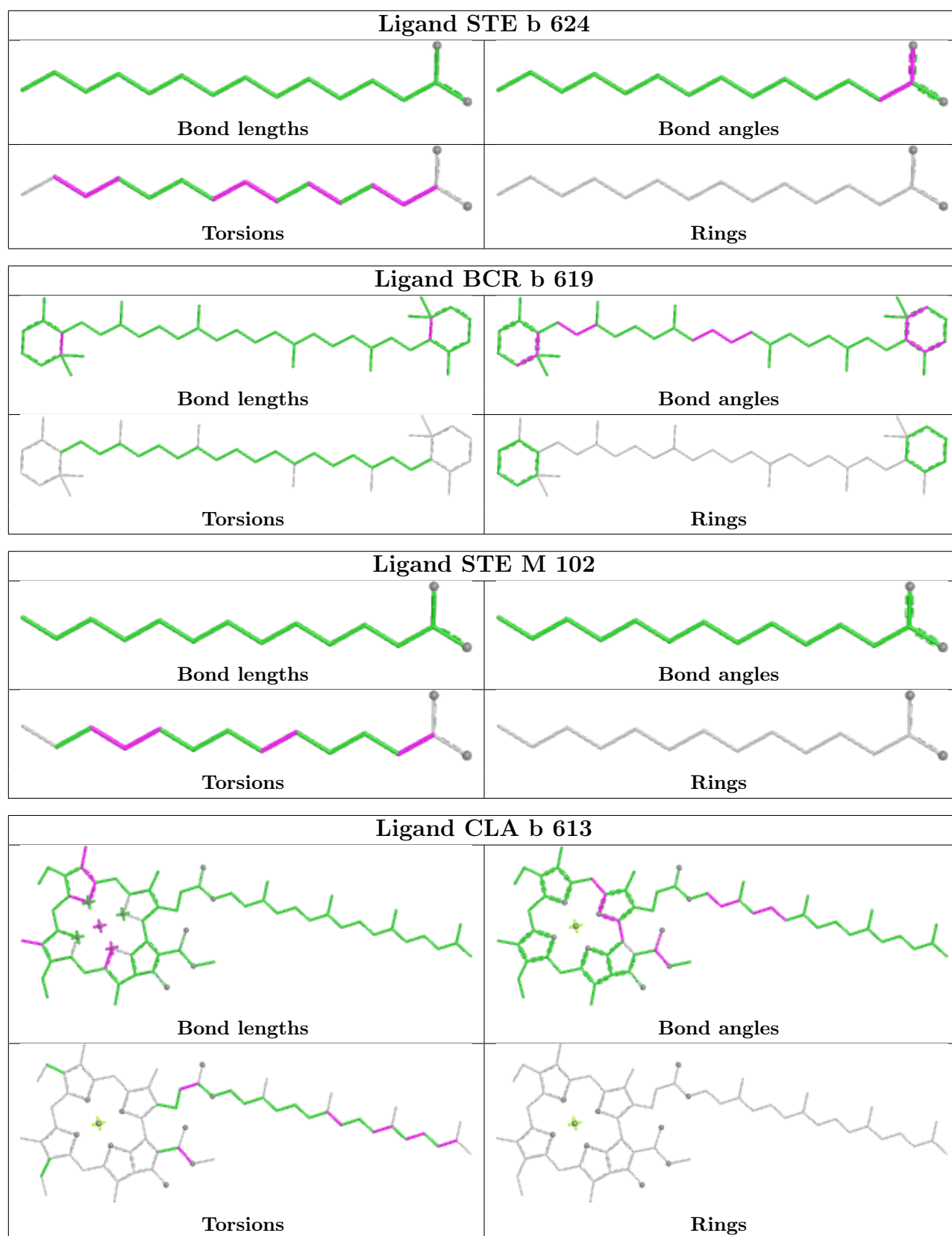


Ligand BCR C 516

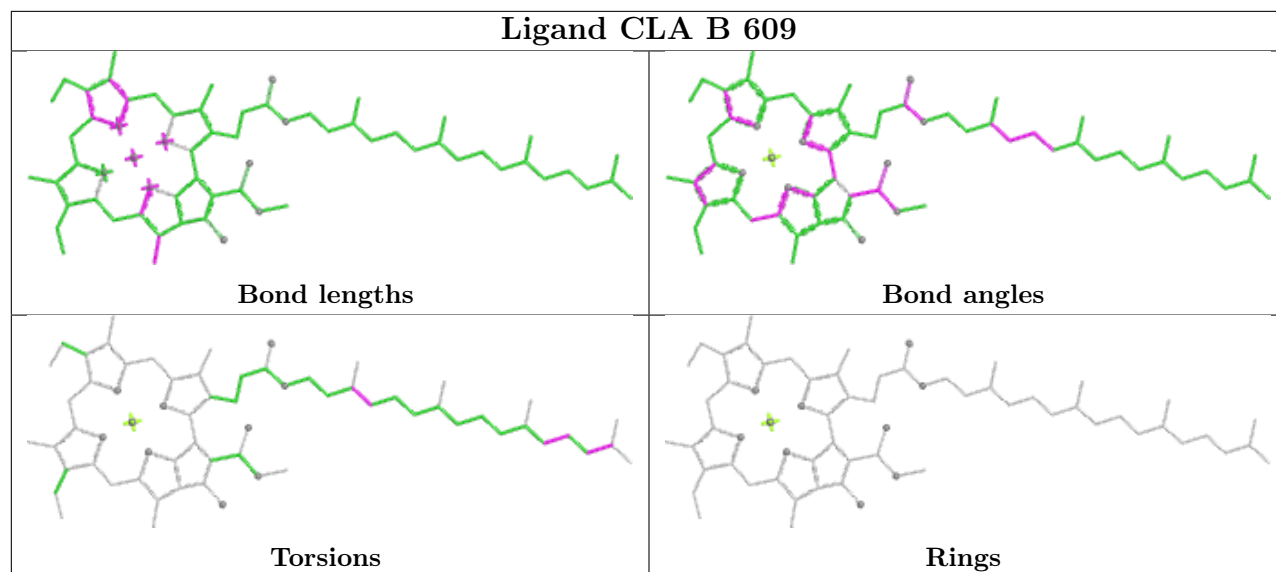


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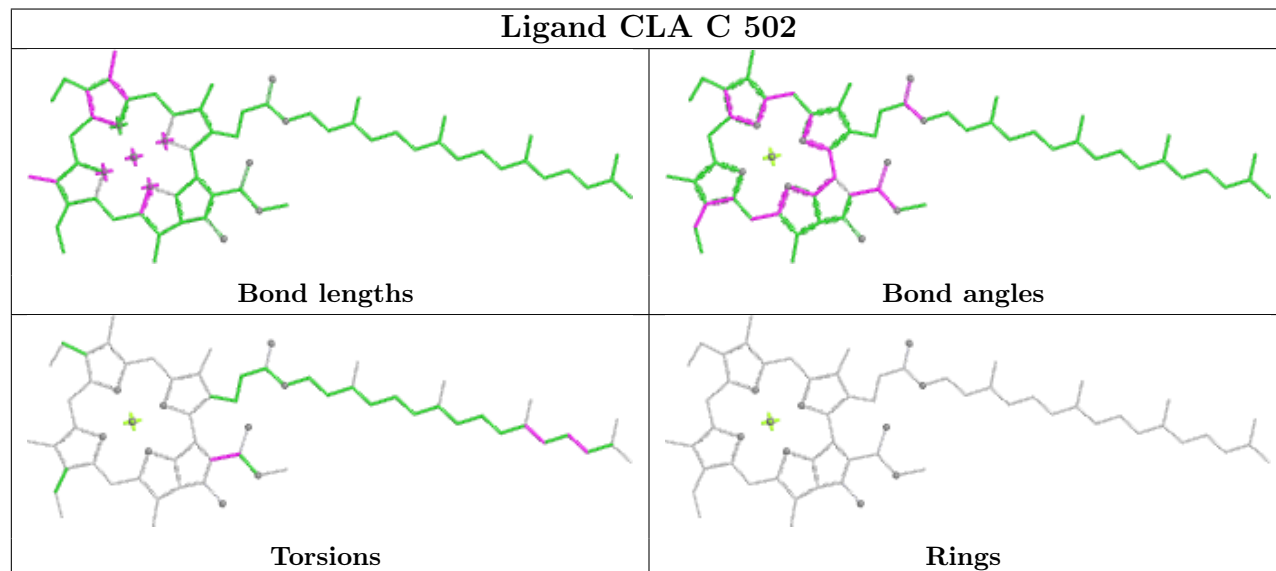




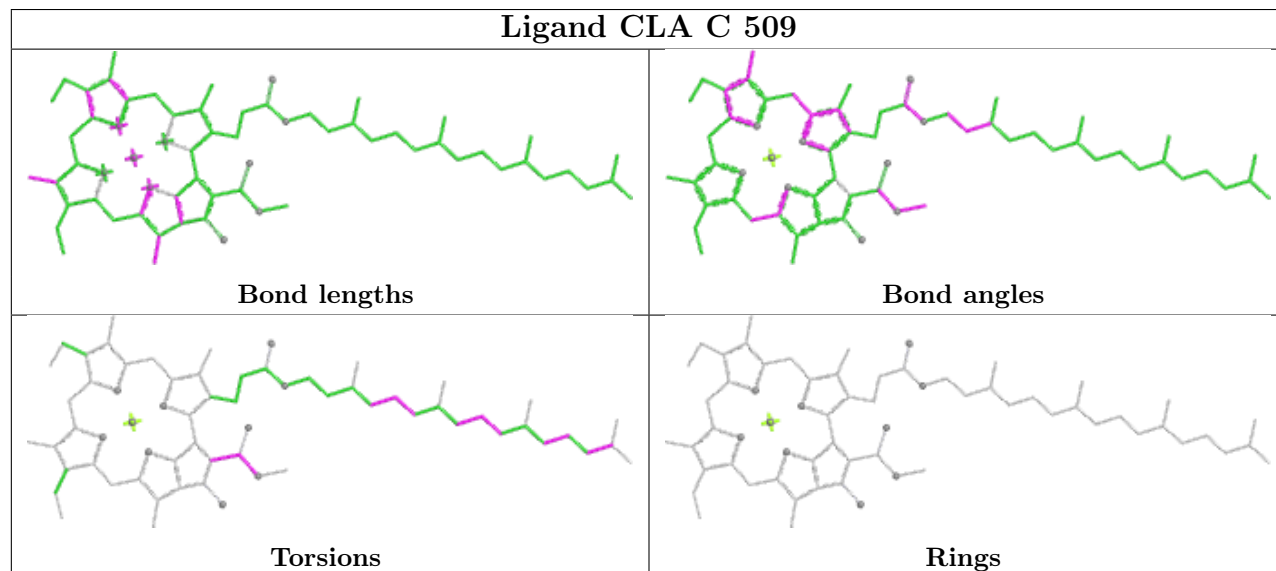
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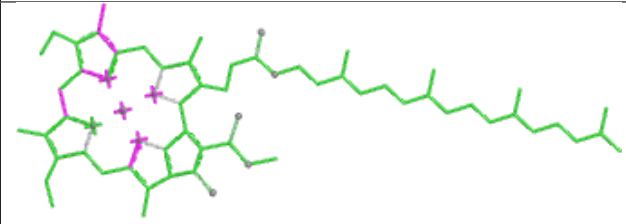
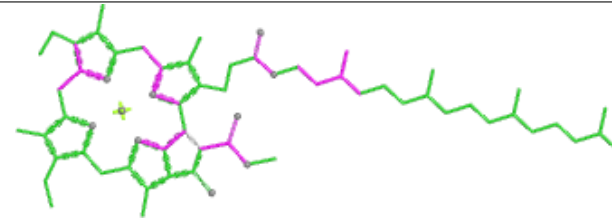
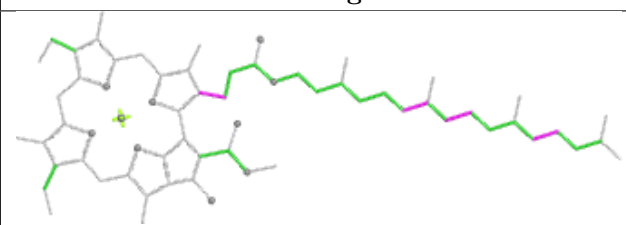
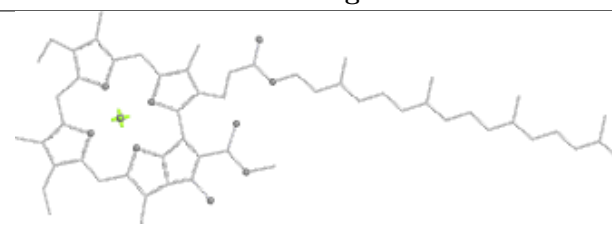


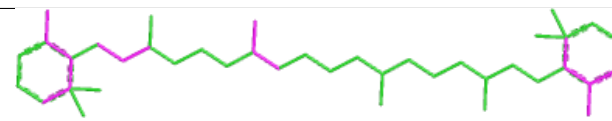
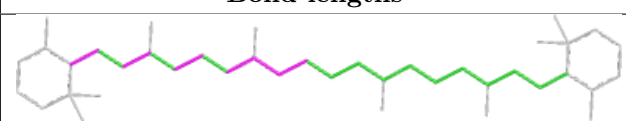
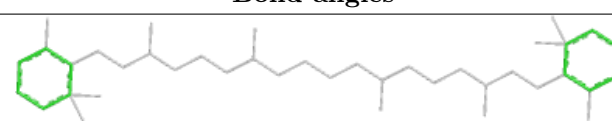
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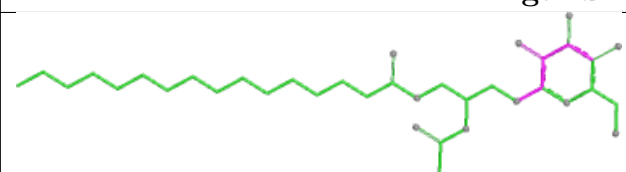
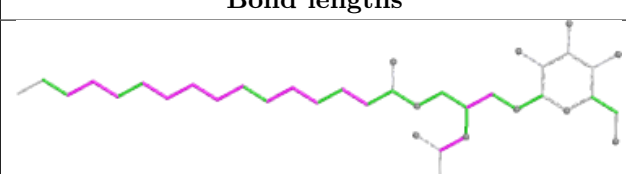
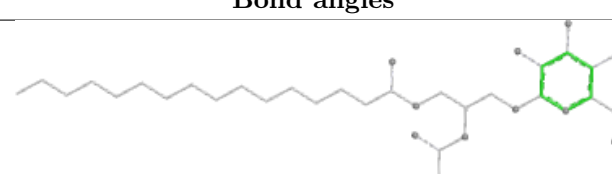
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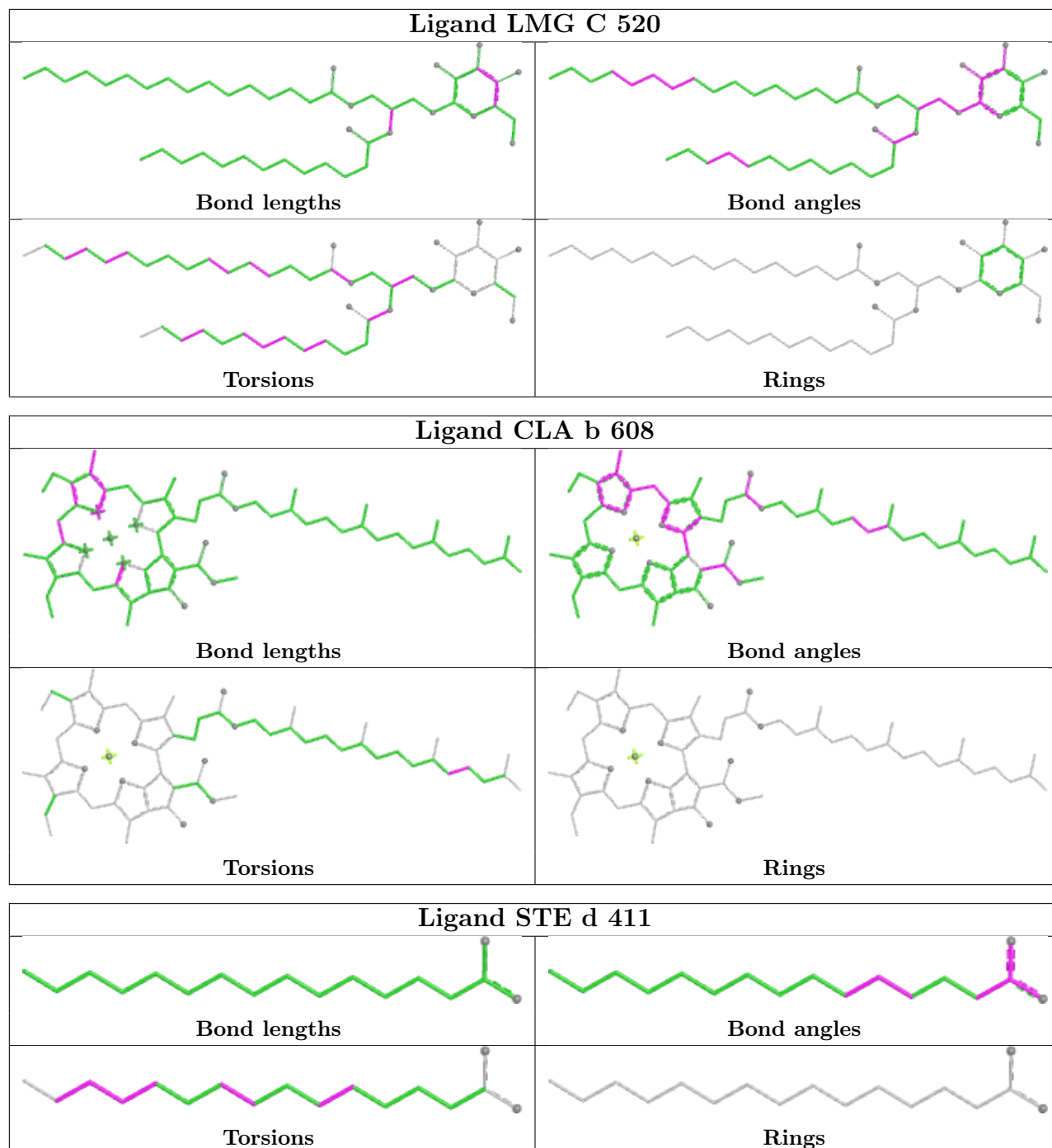


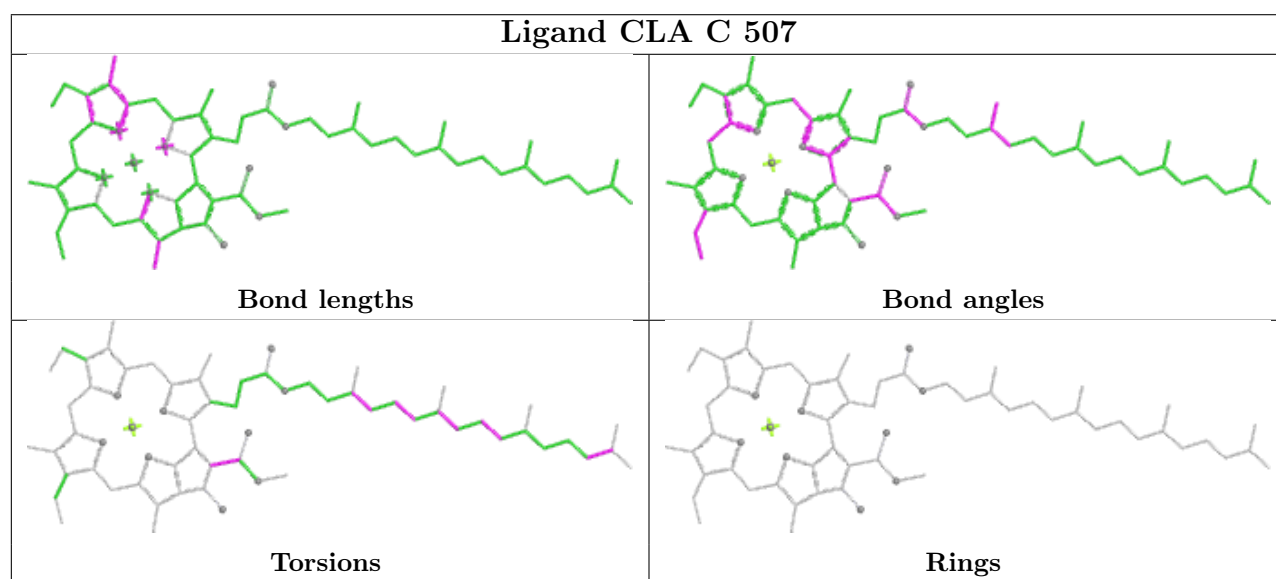
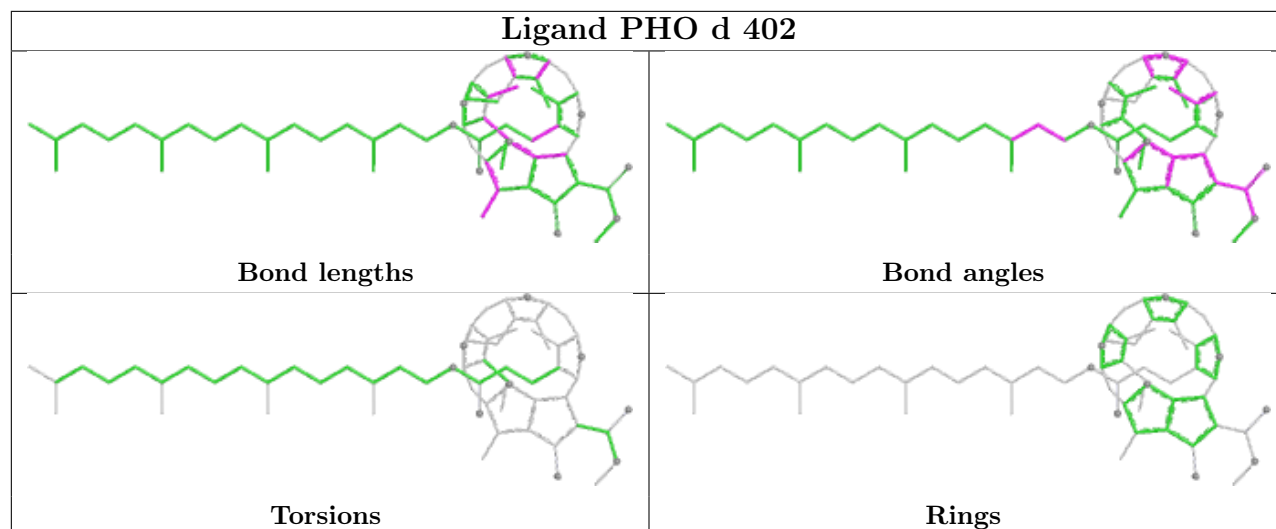
Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

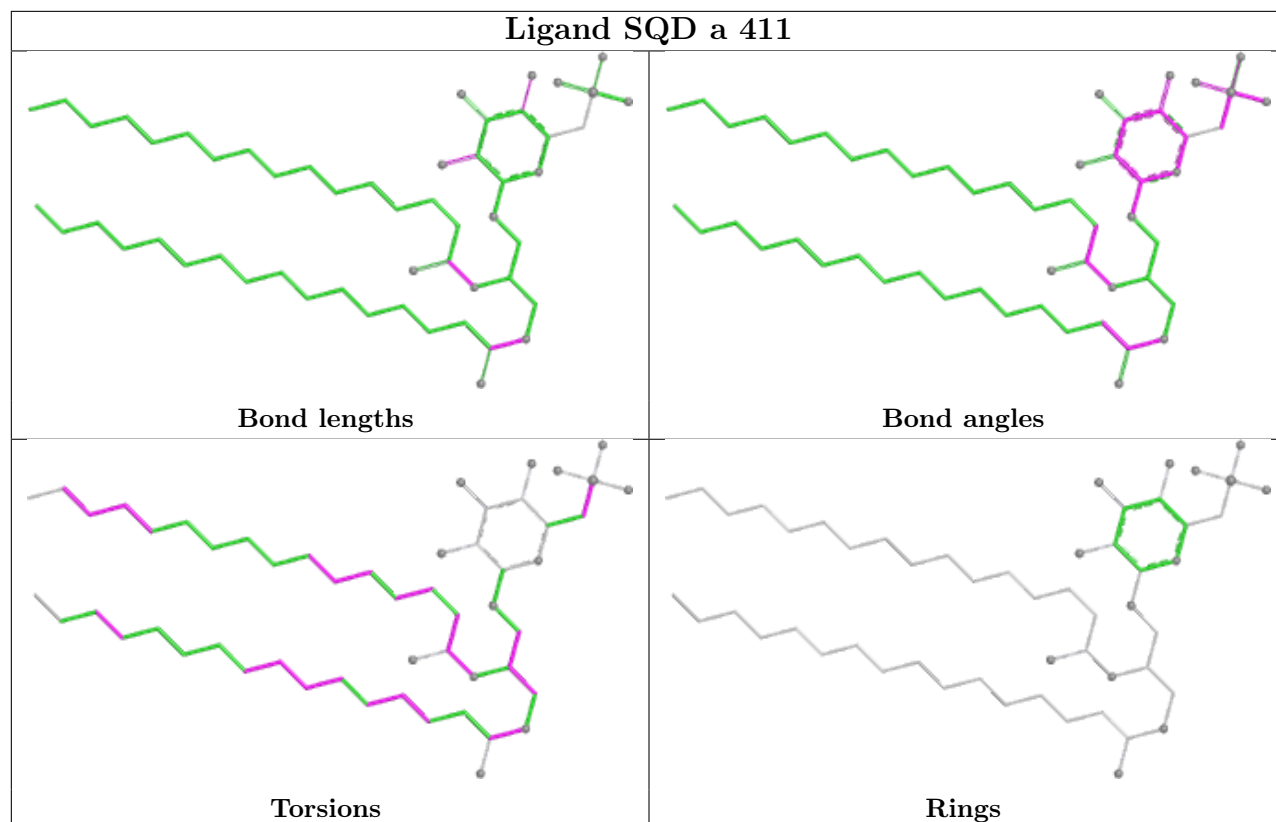
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE M 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

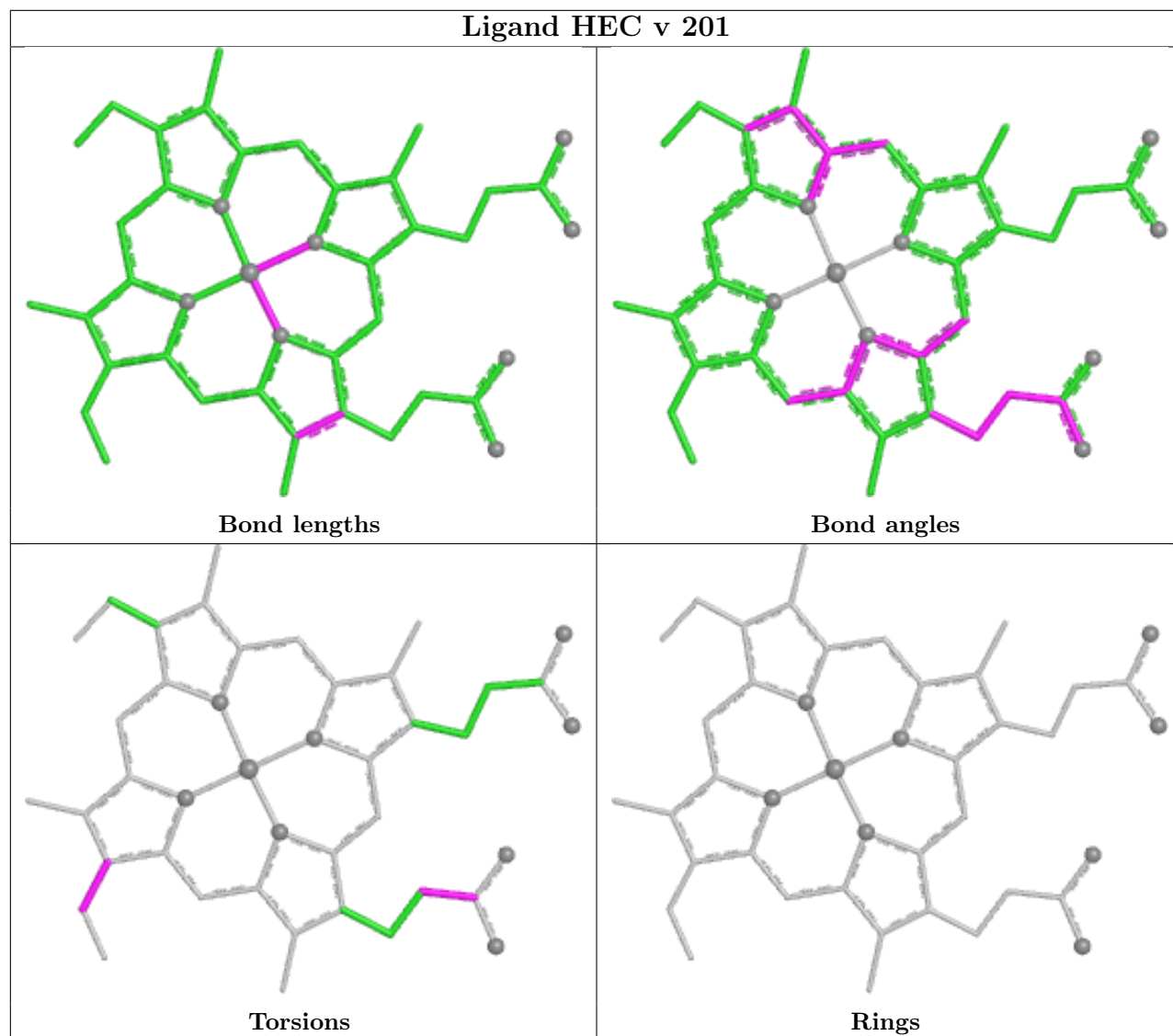
Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings



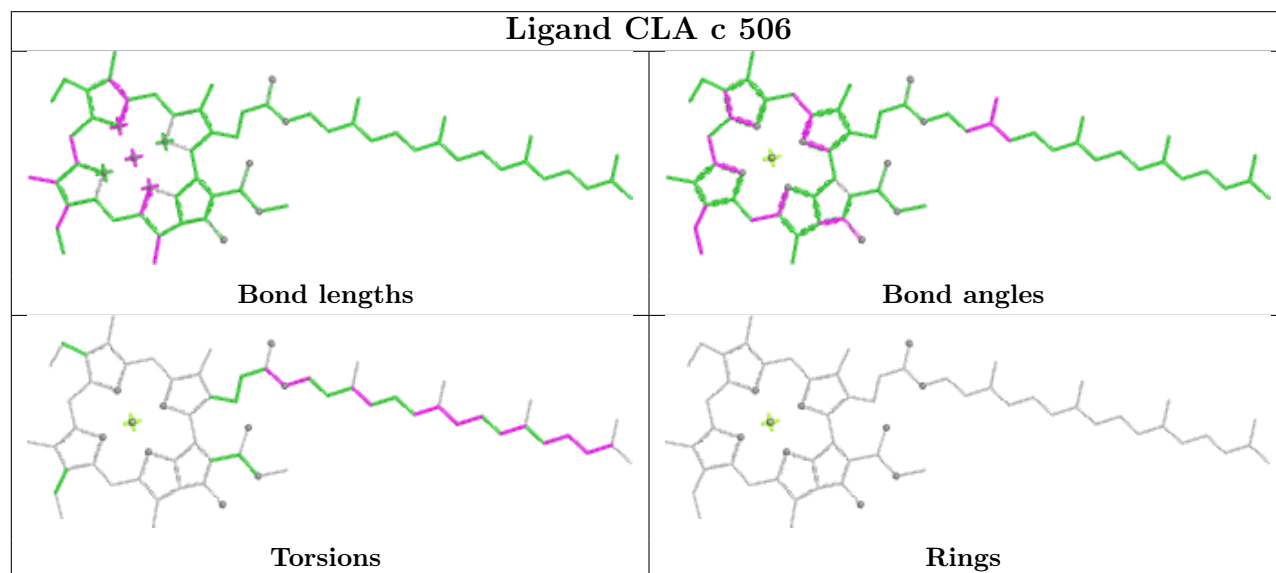


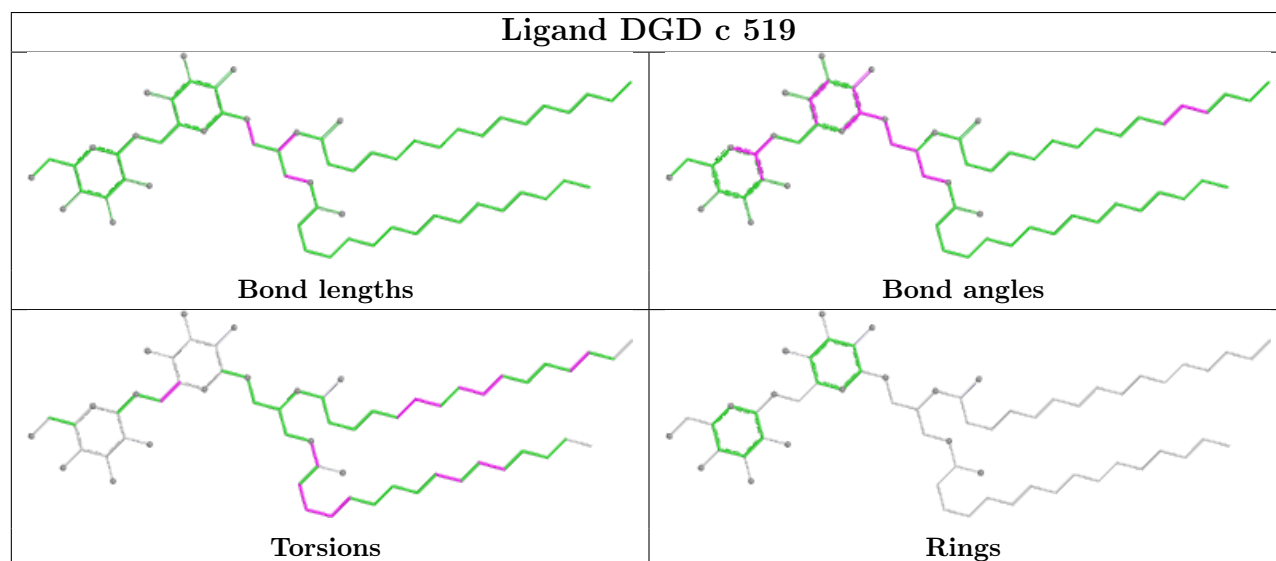
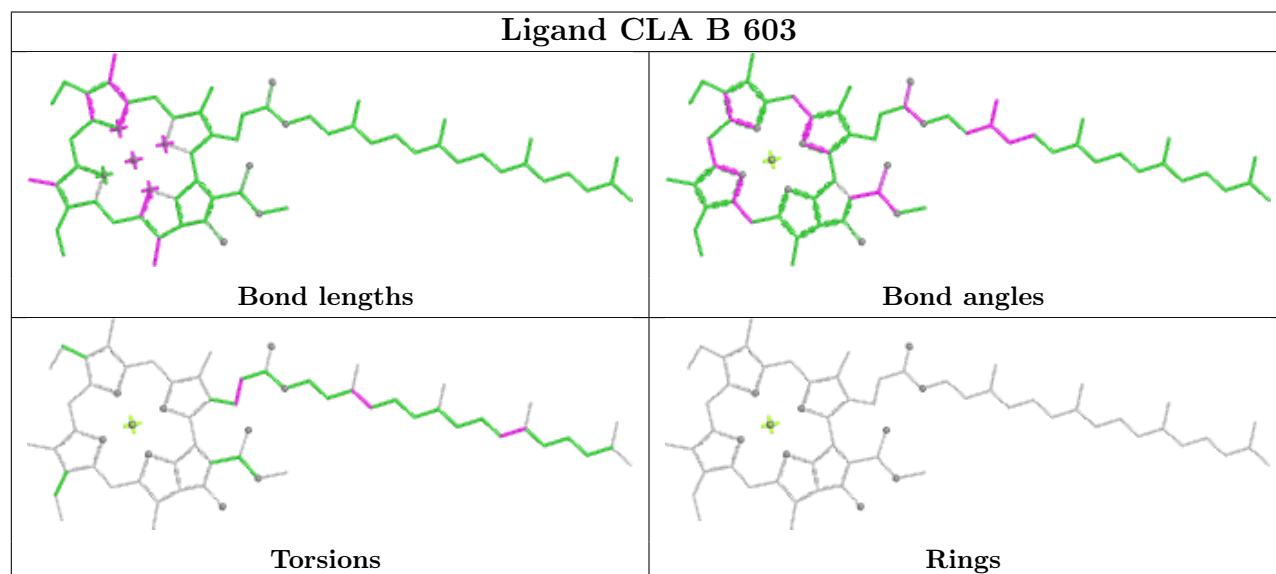
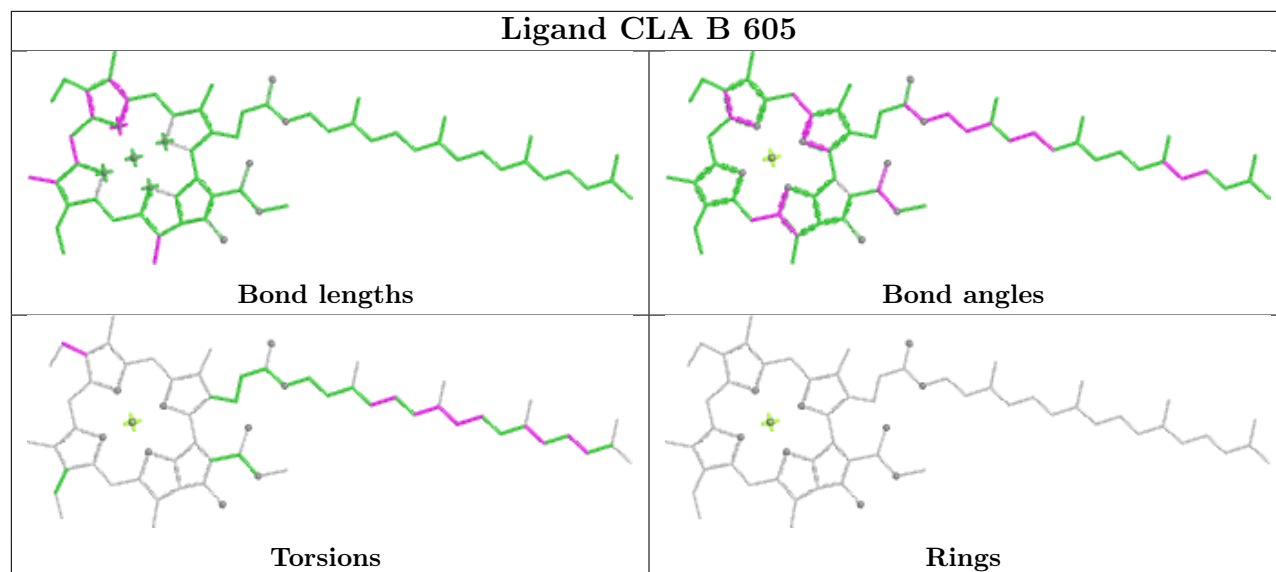


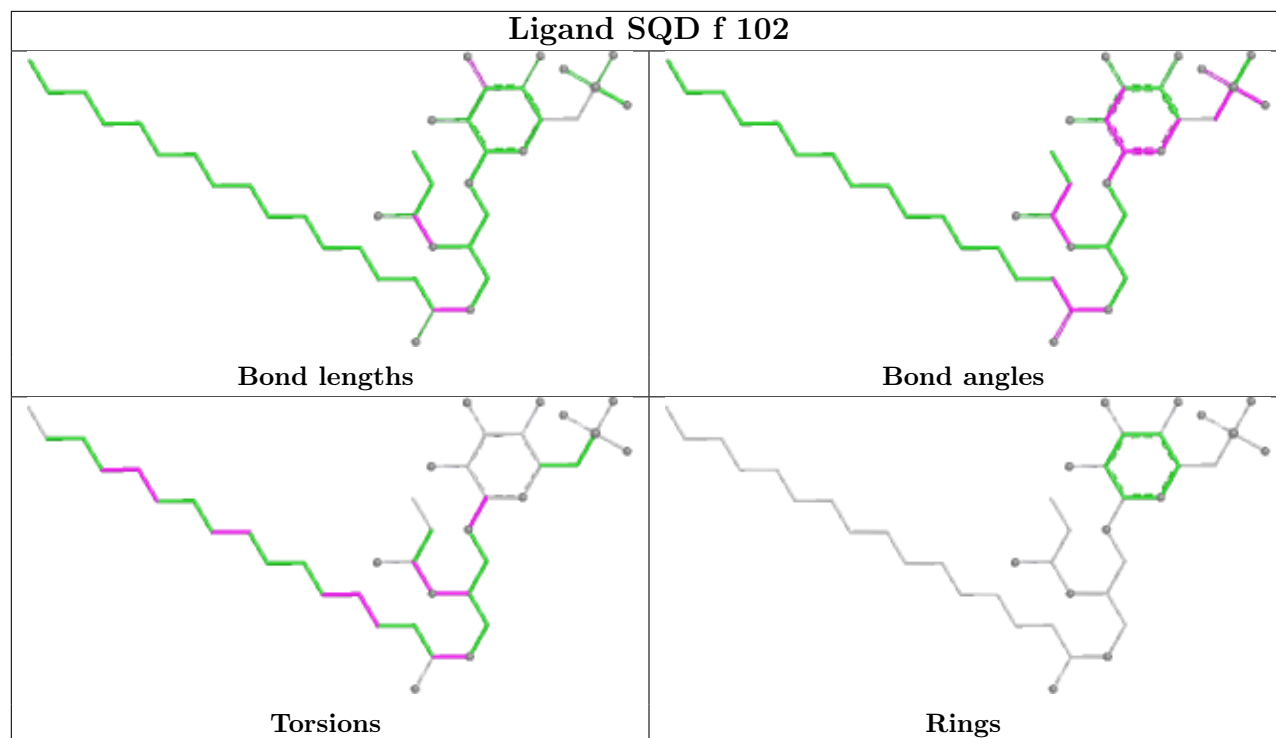
Ligand HEC v 201



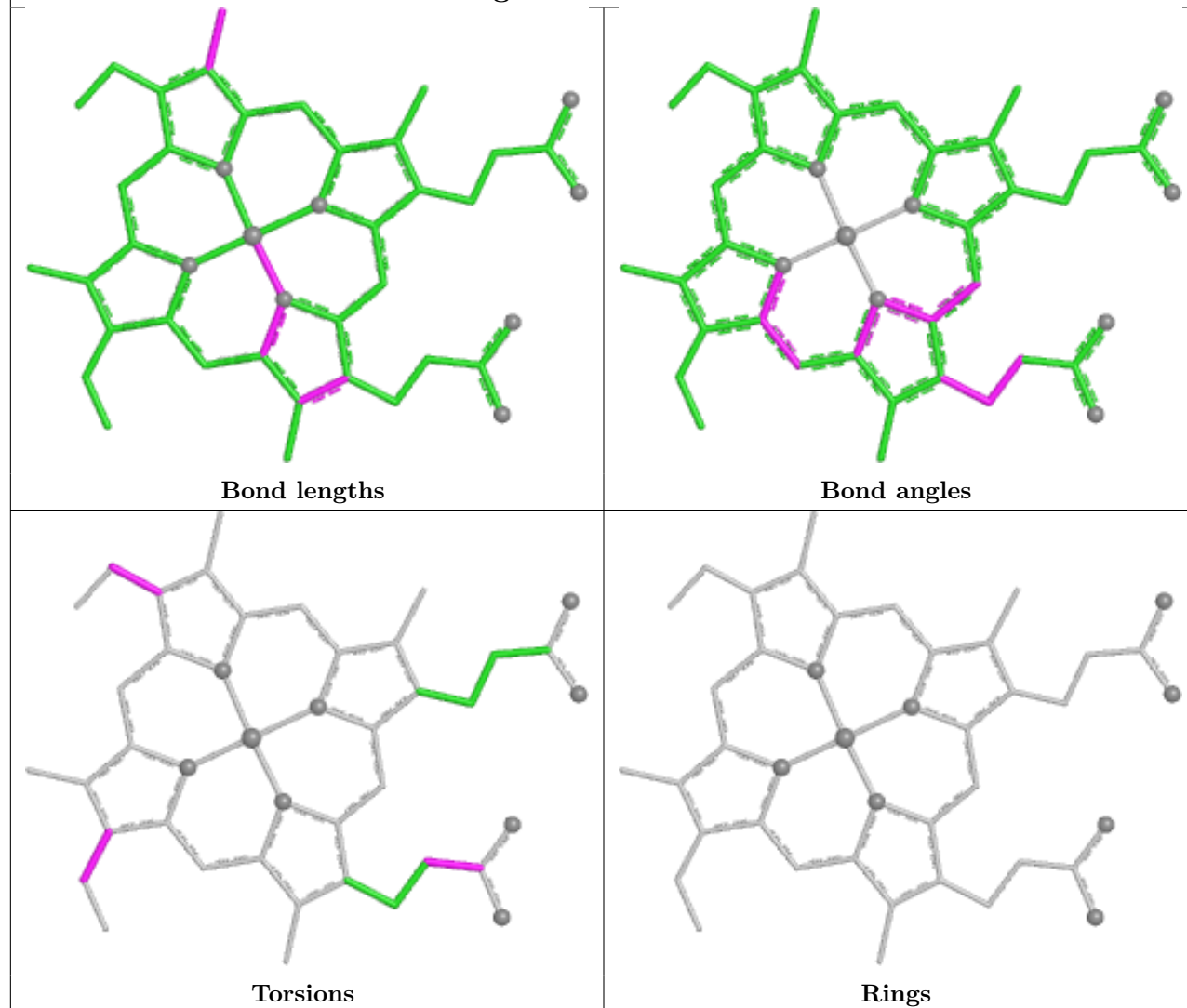
Ligand CLA c 506



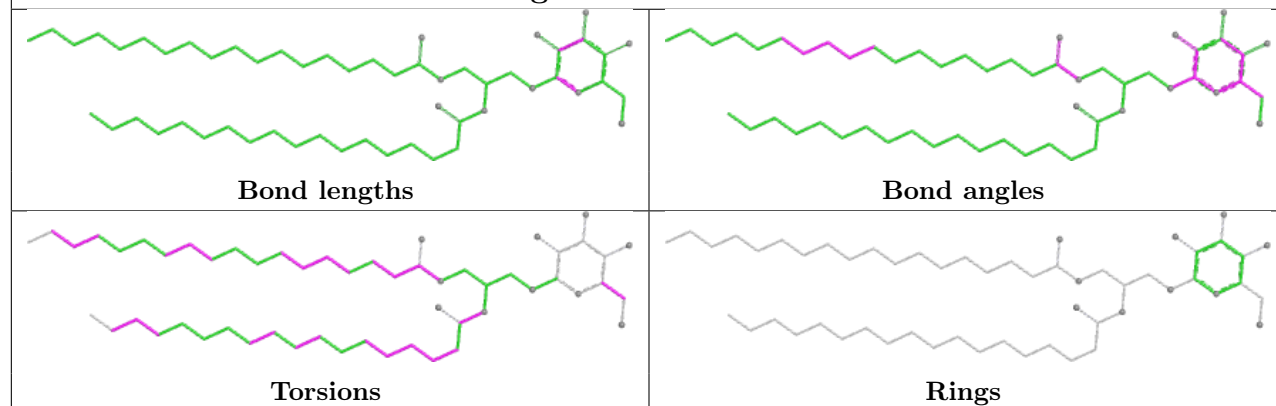


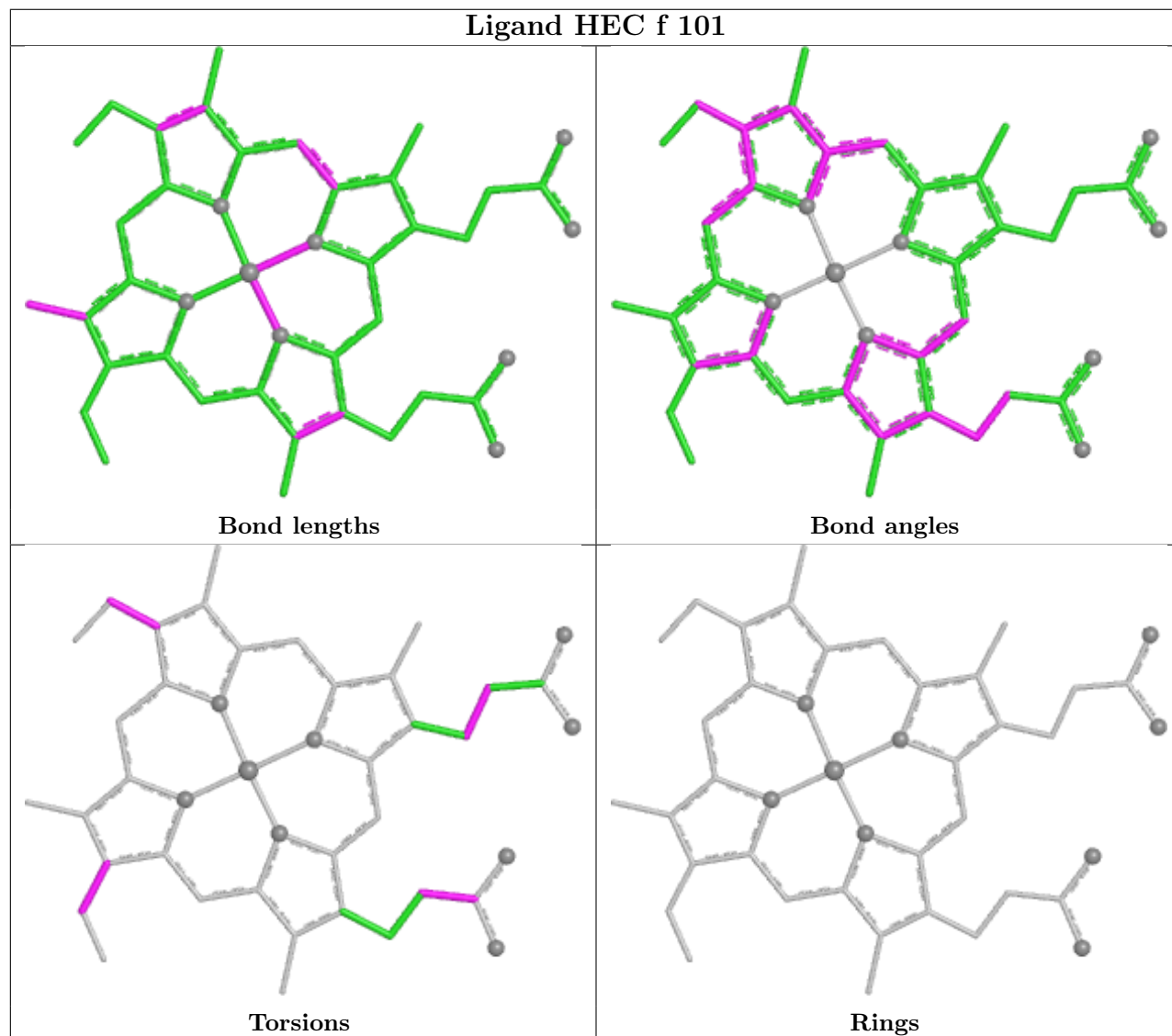
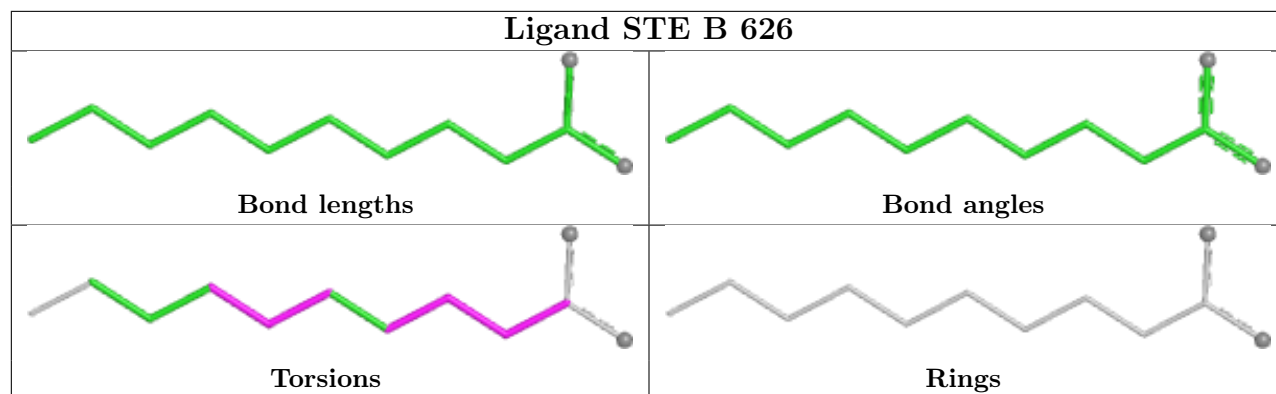


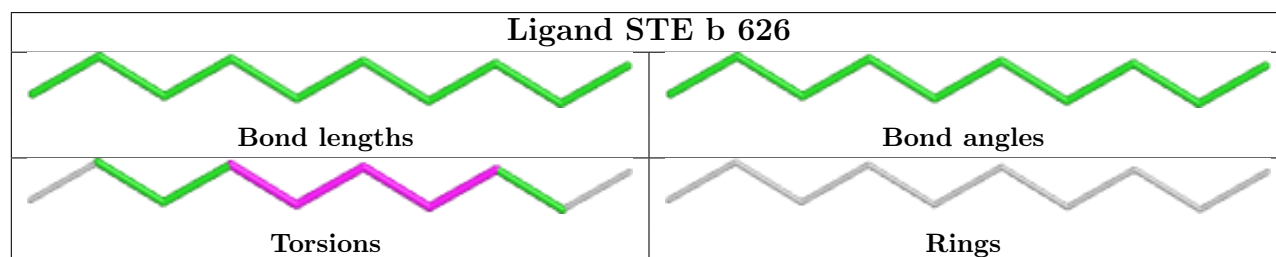
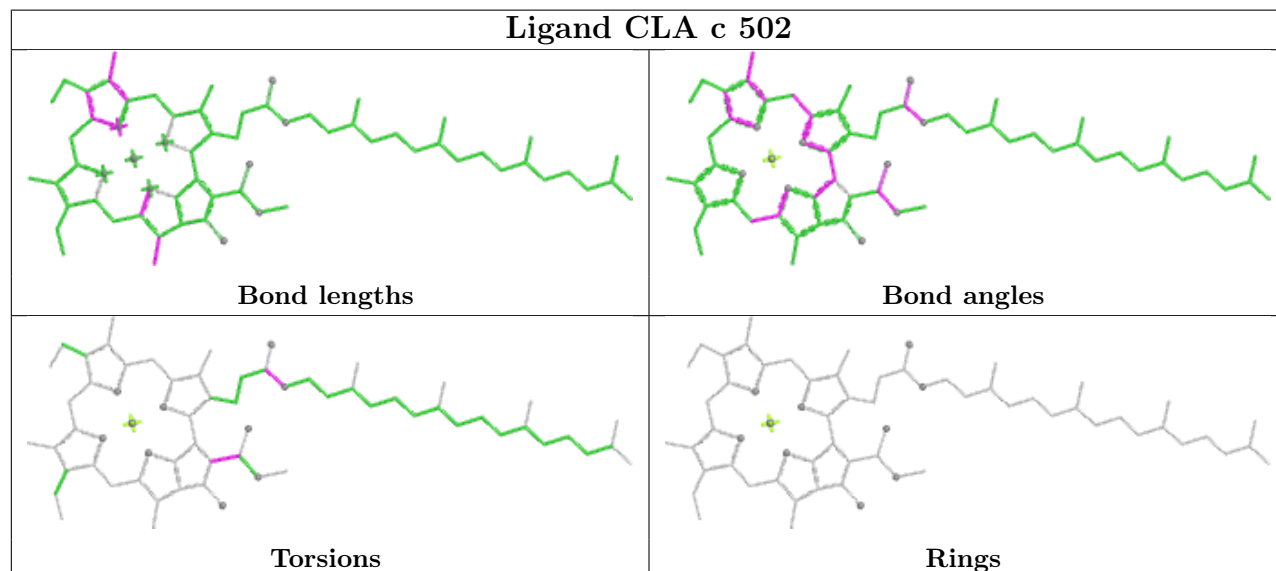
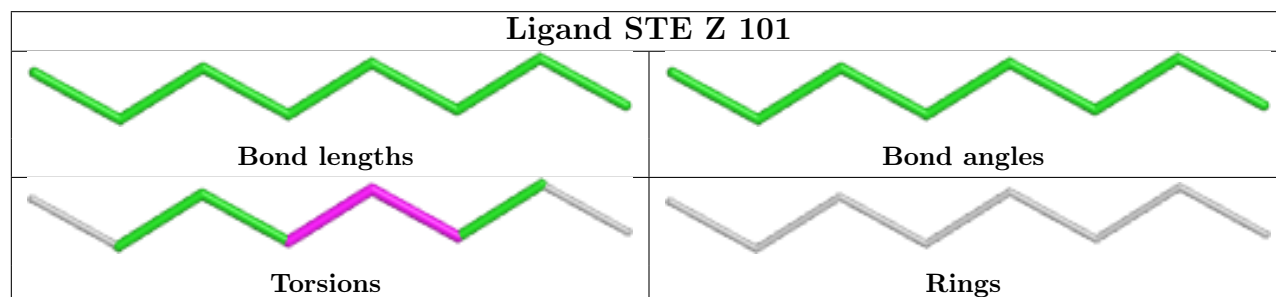
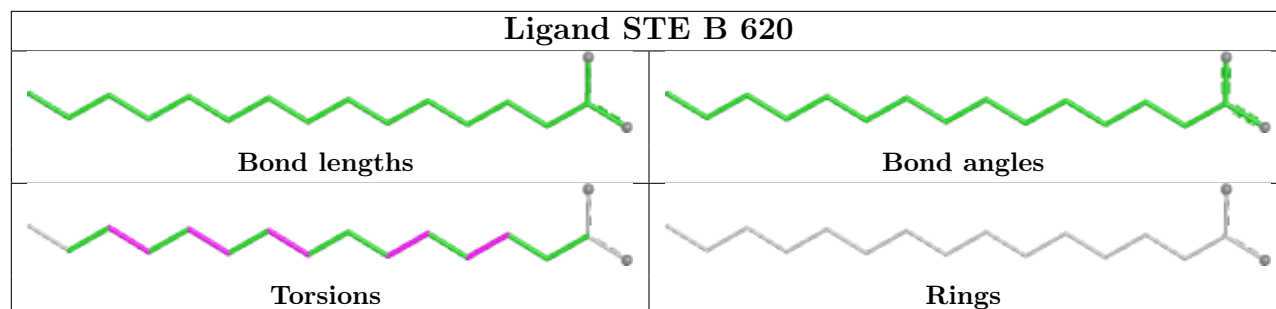
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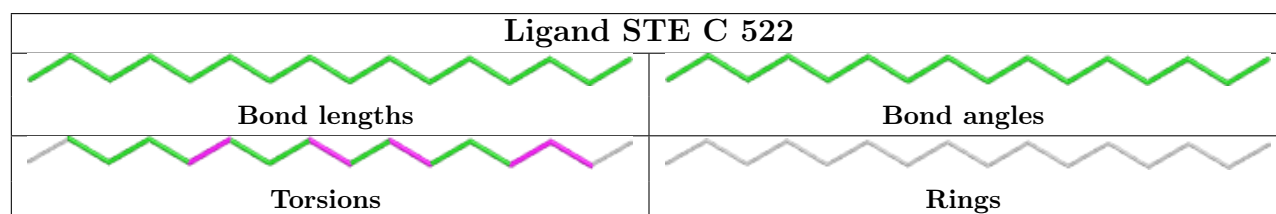
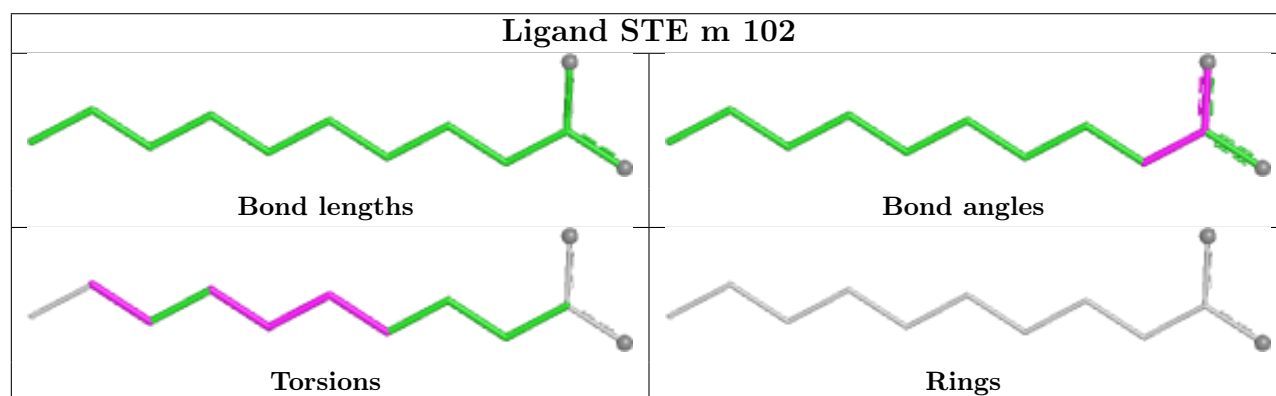
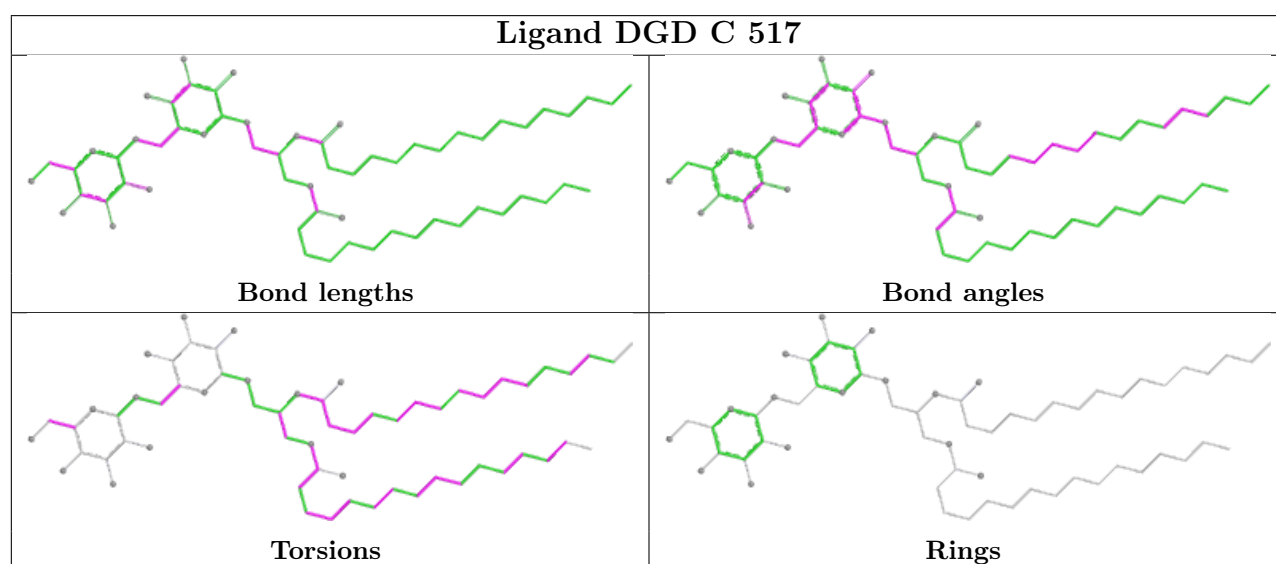
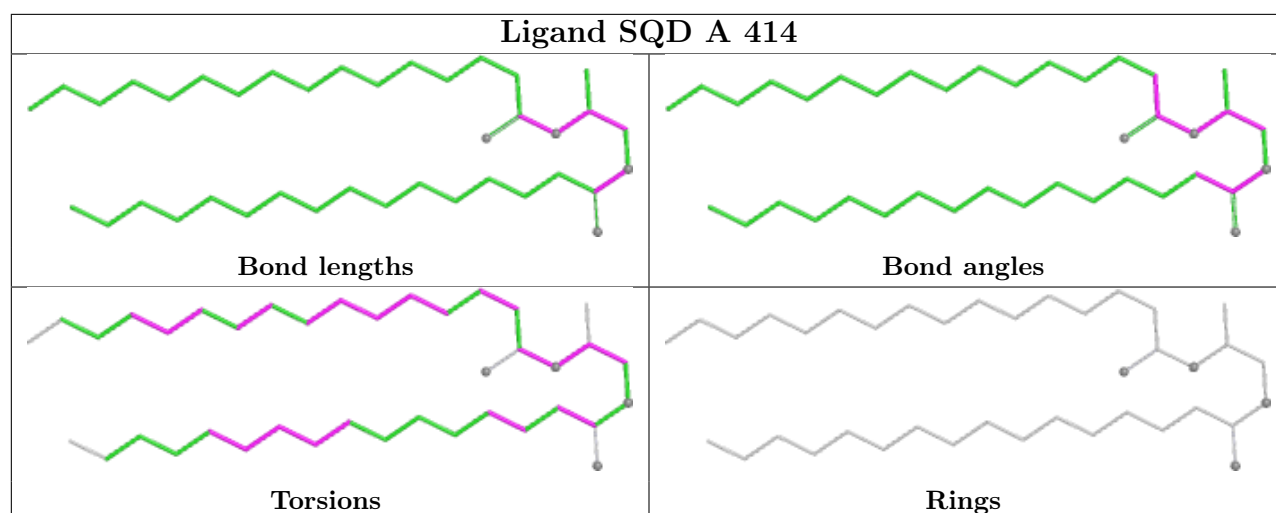


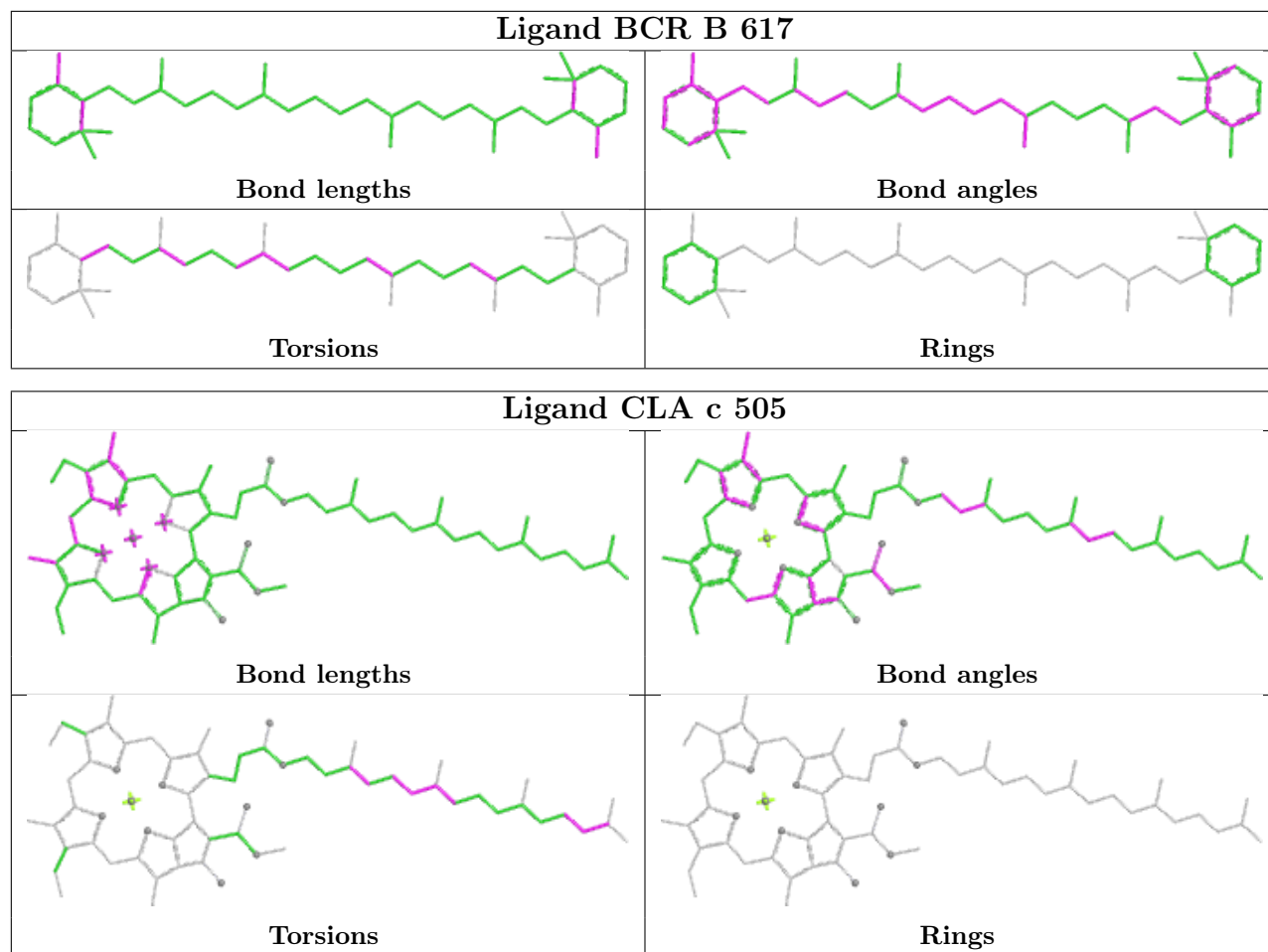
Ligand LMG b 623

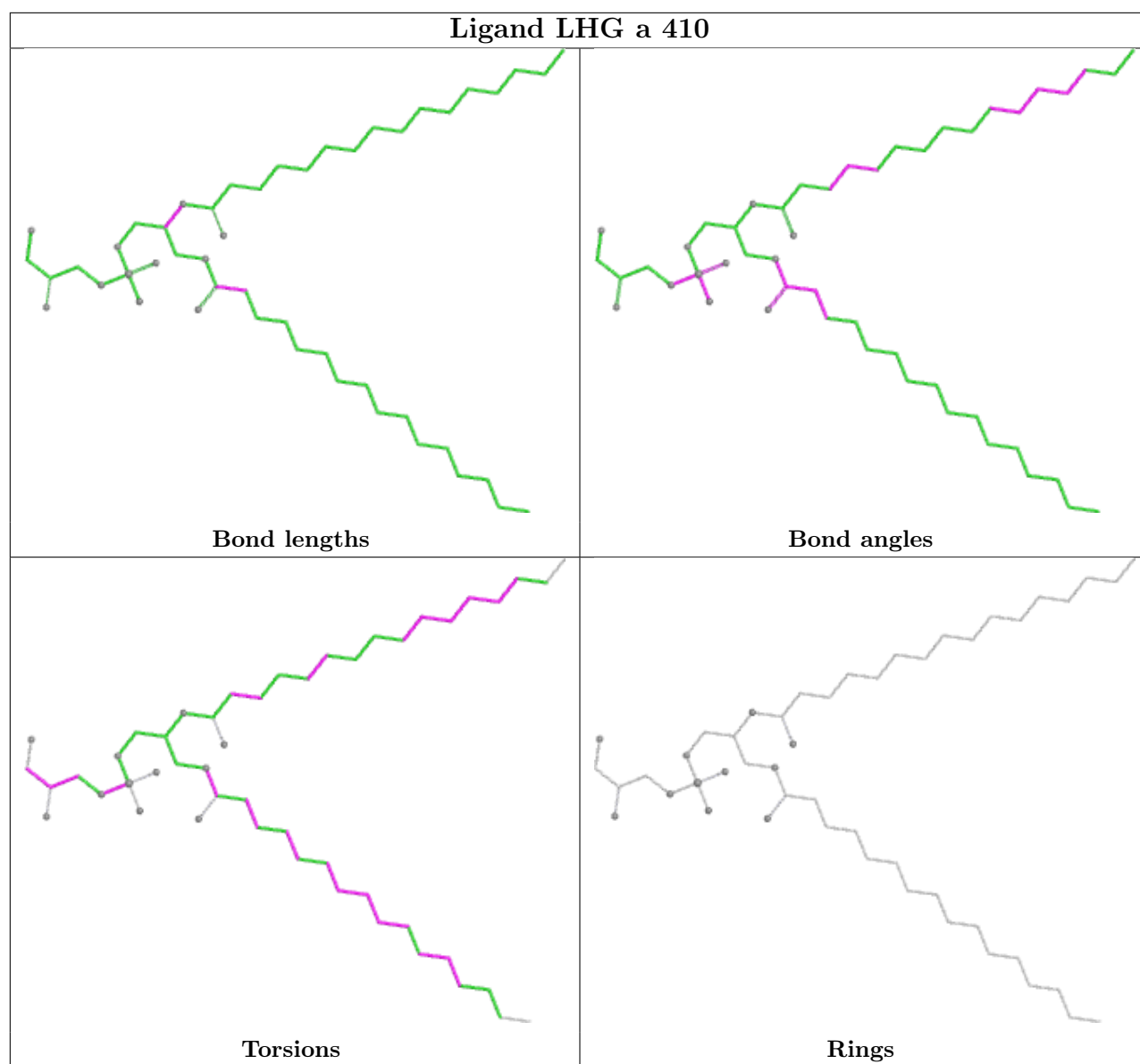


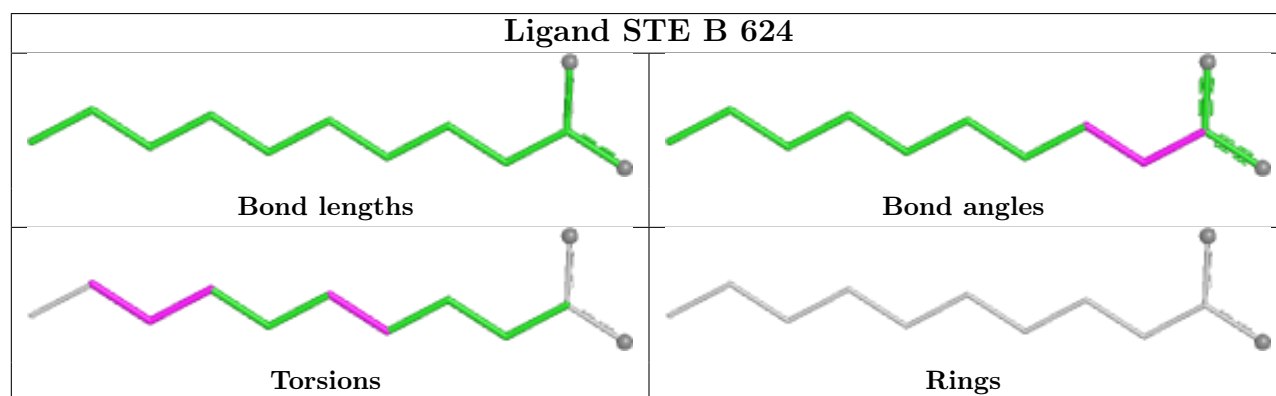
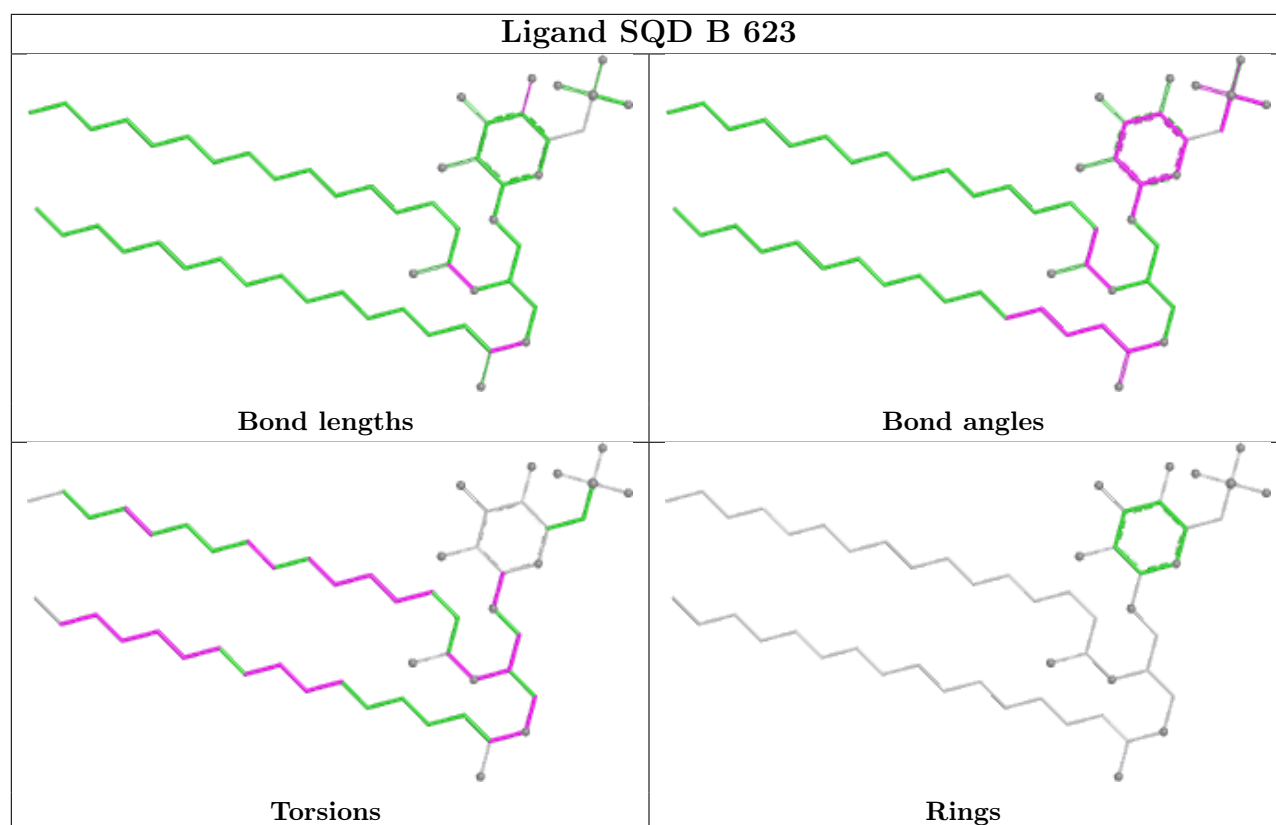


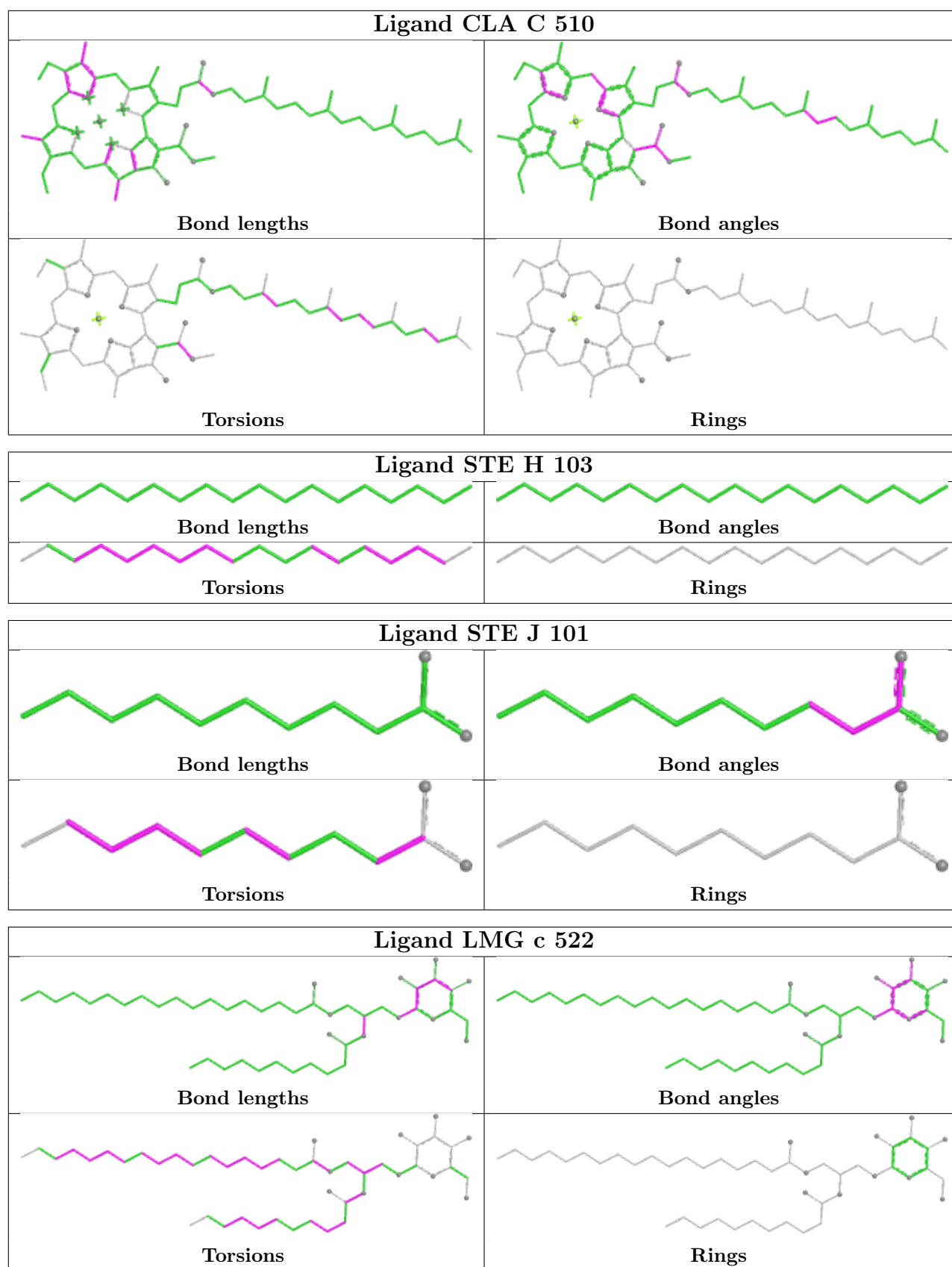




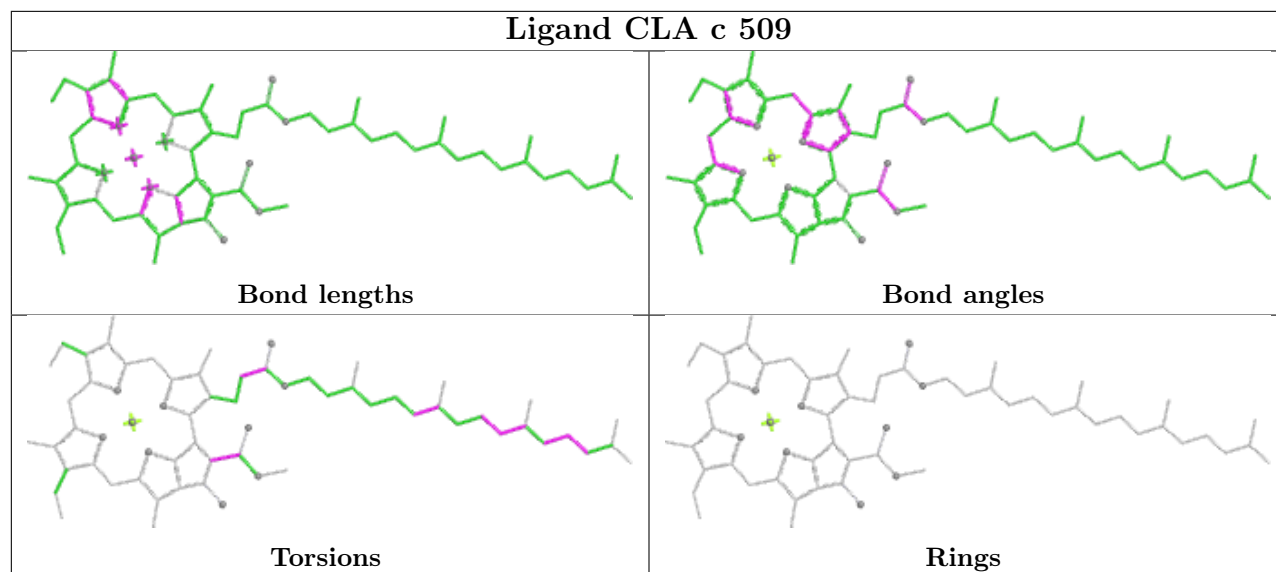




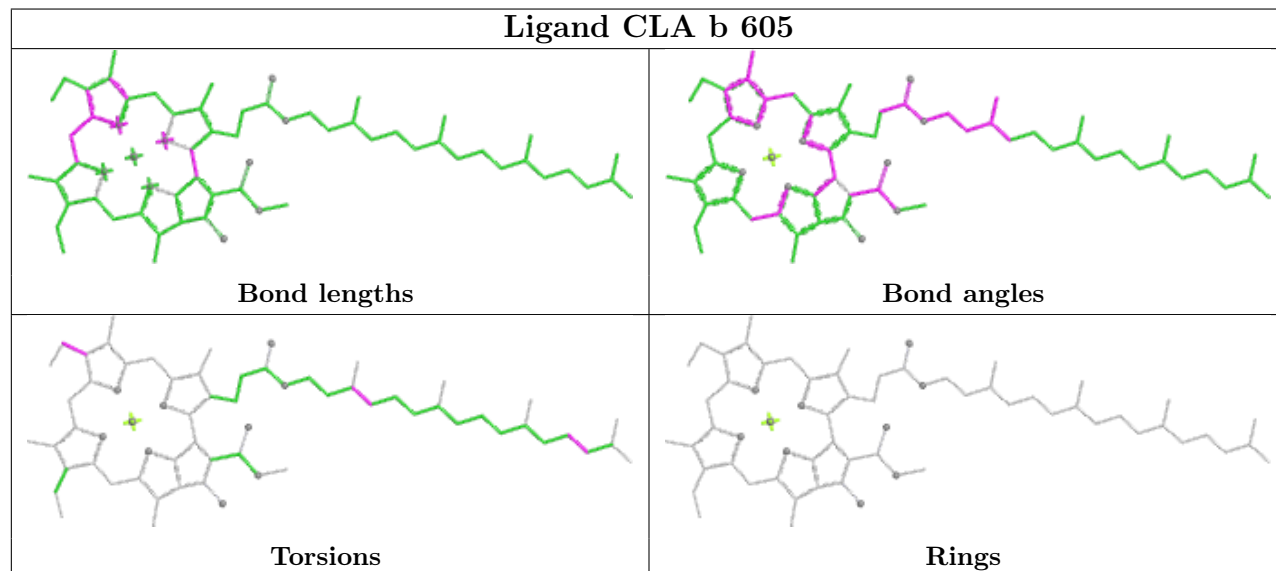




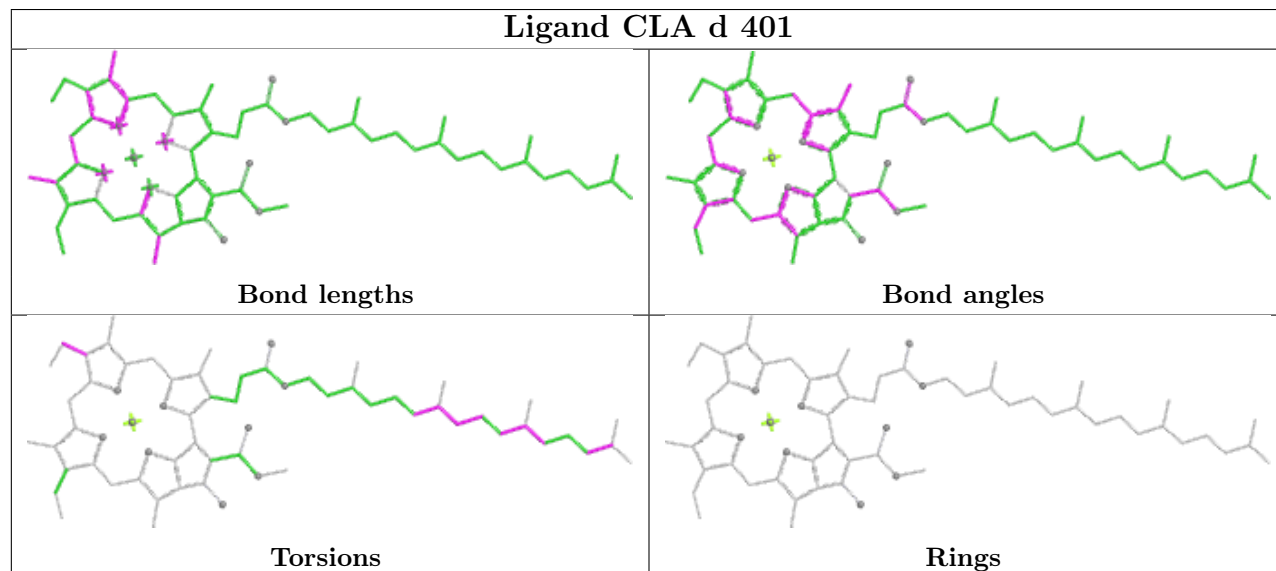
Ligand CLA c 509

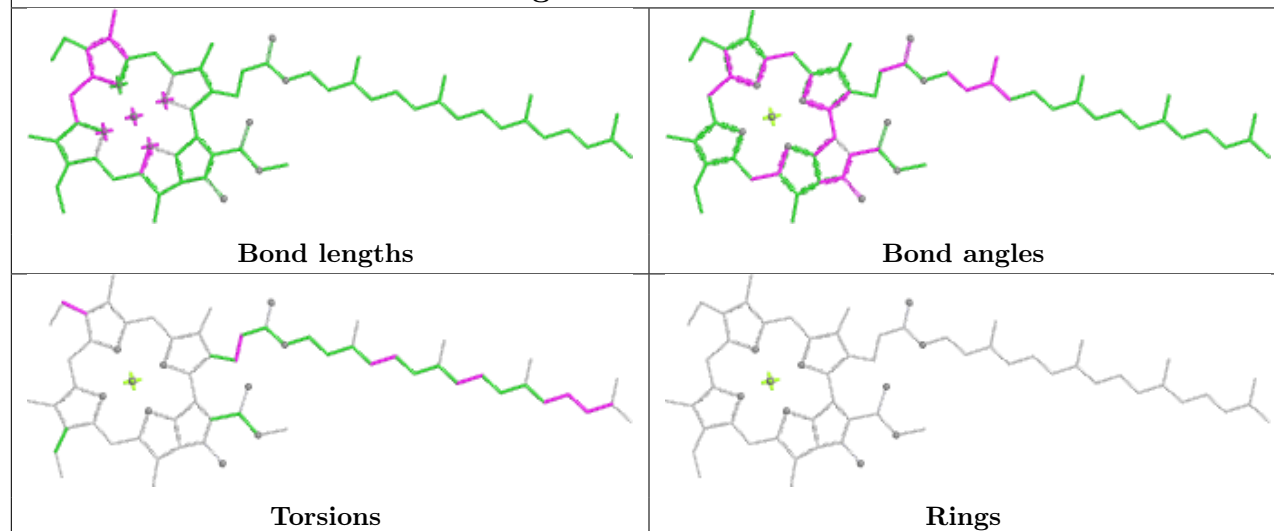
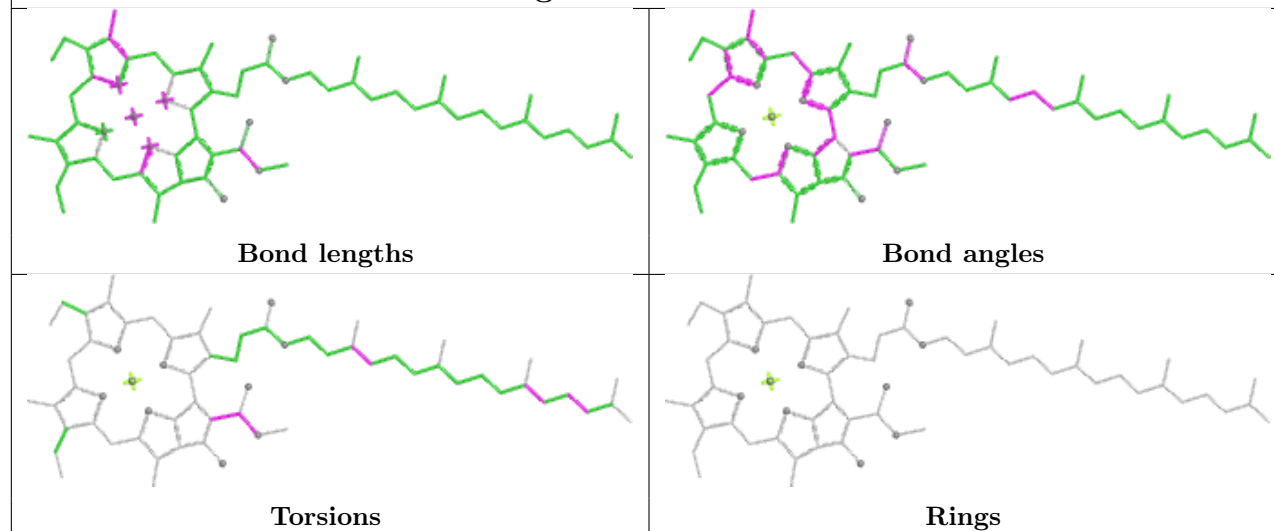


Ligand CLA b 605

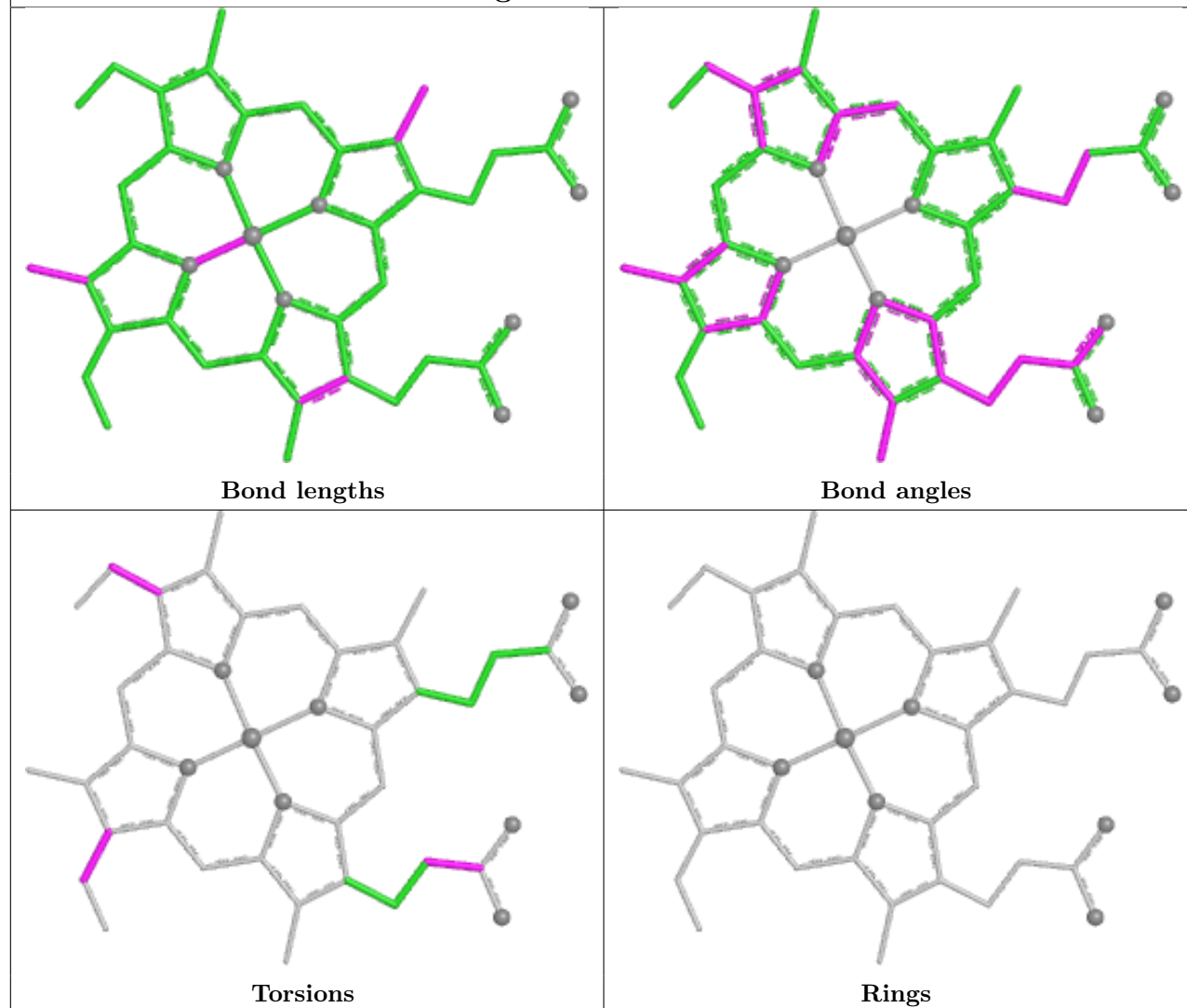


Ligand CLA d 401

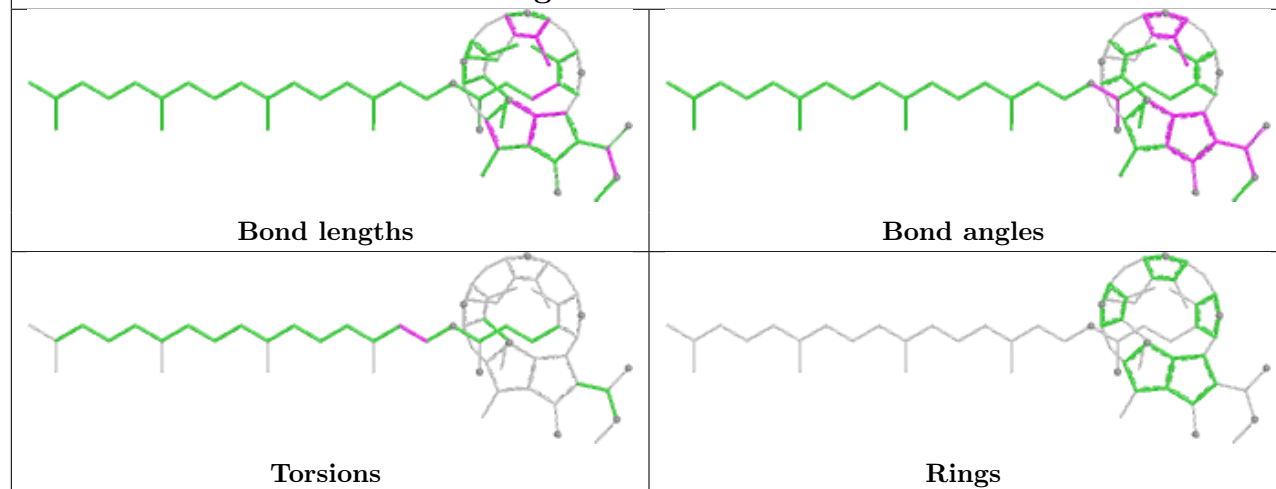


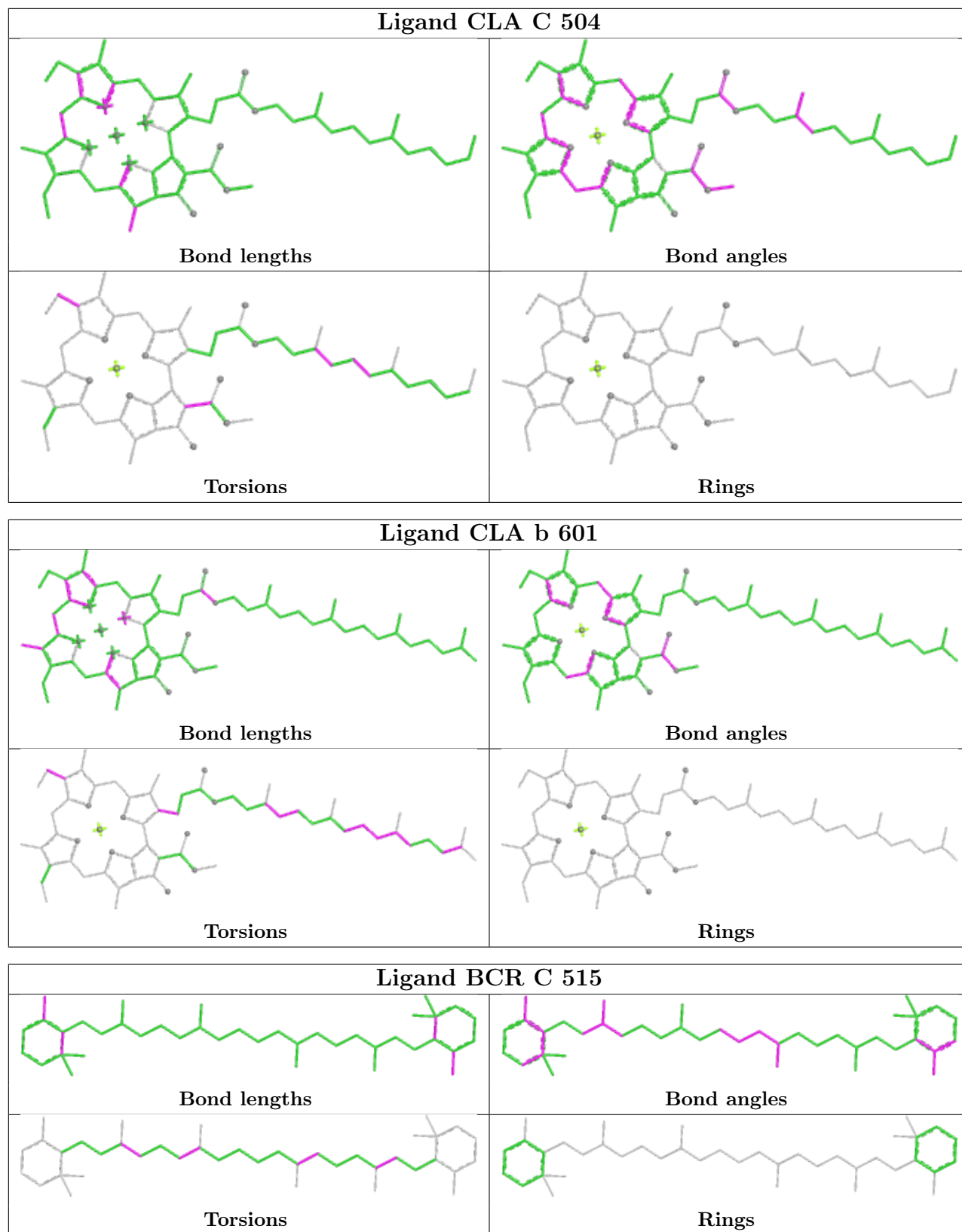
Ligand CLA B 606**Ligand CLA b 609**

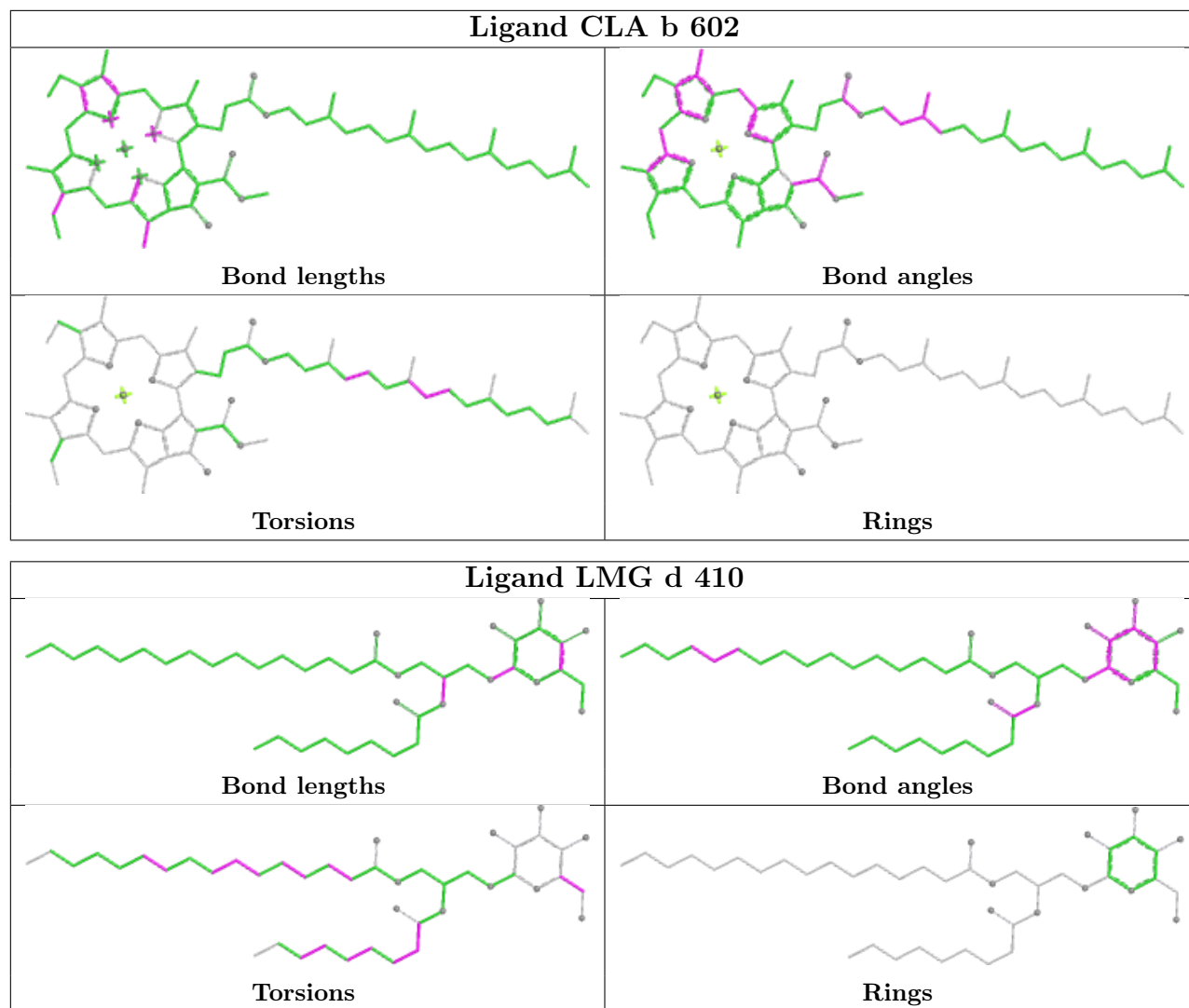
Ligand HEC F 101

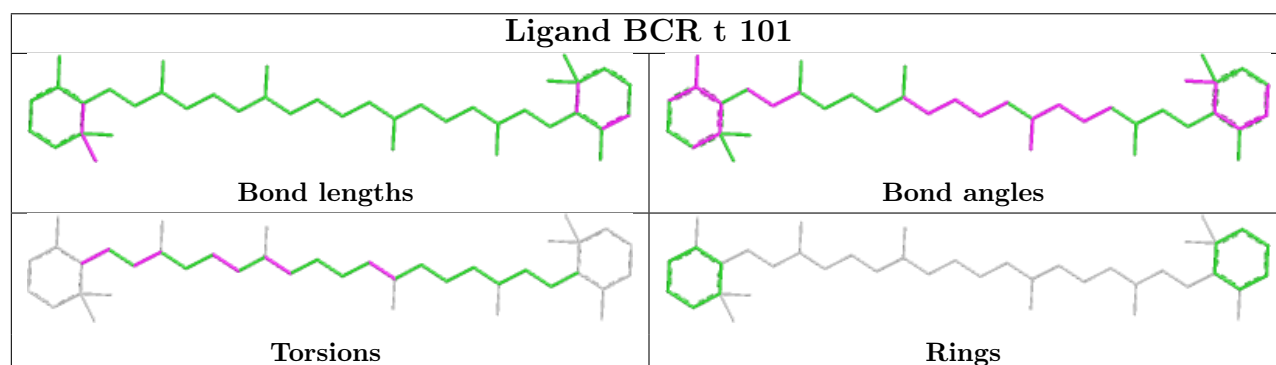
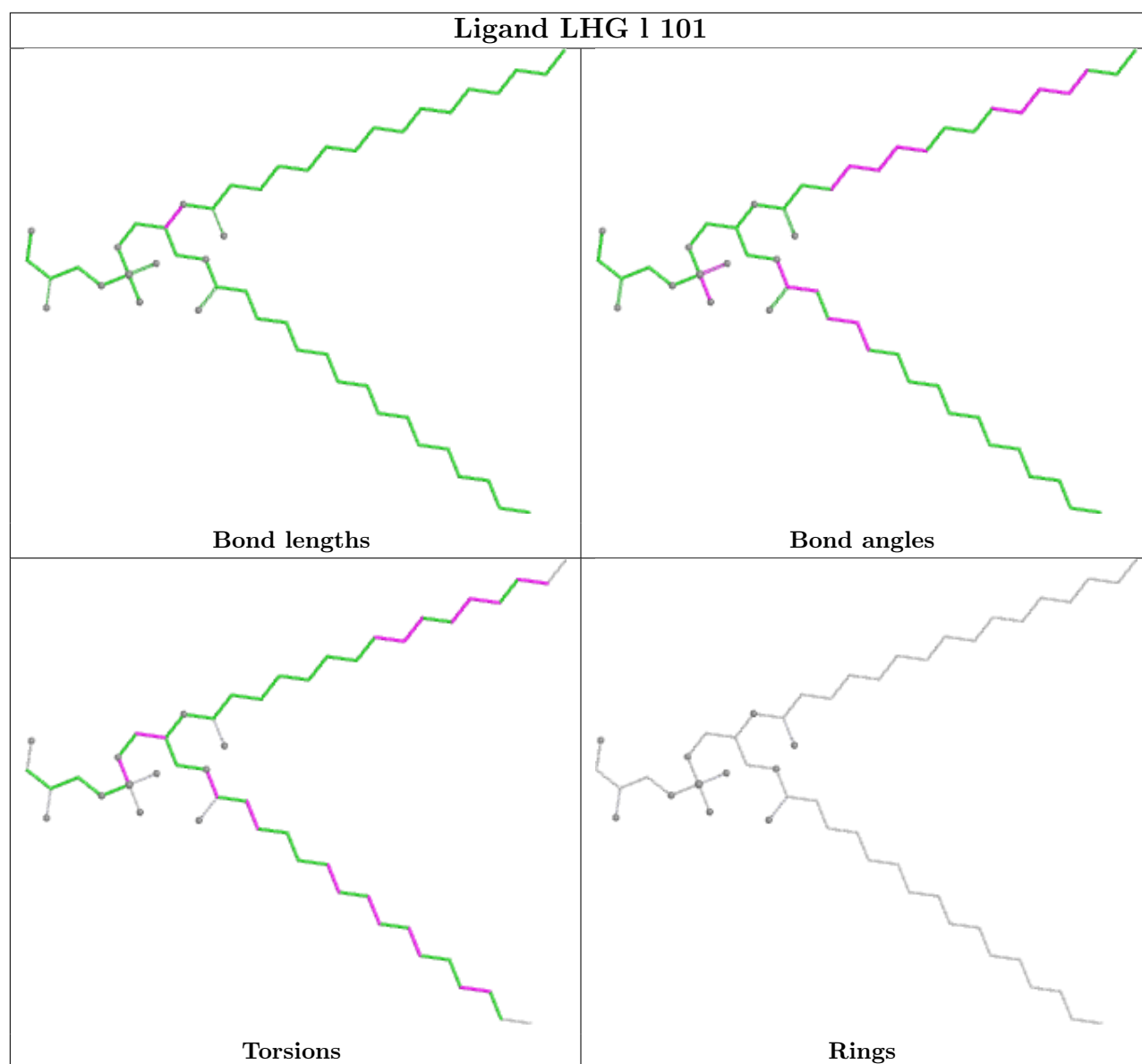


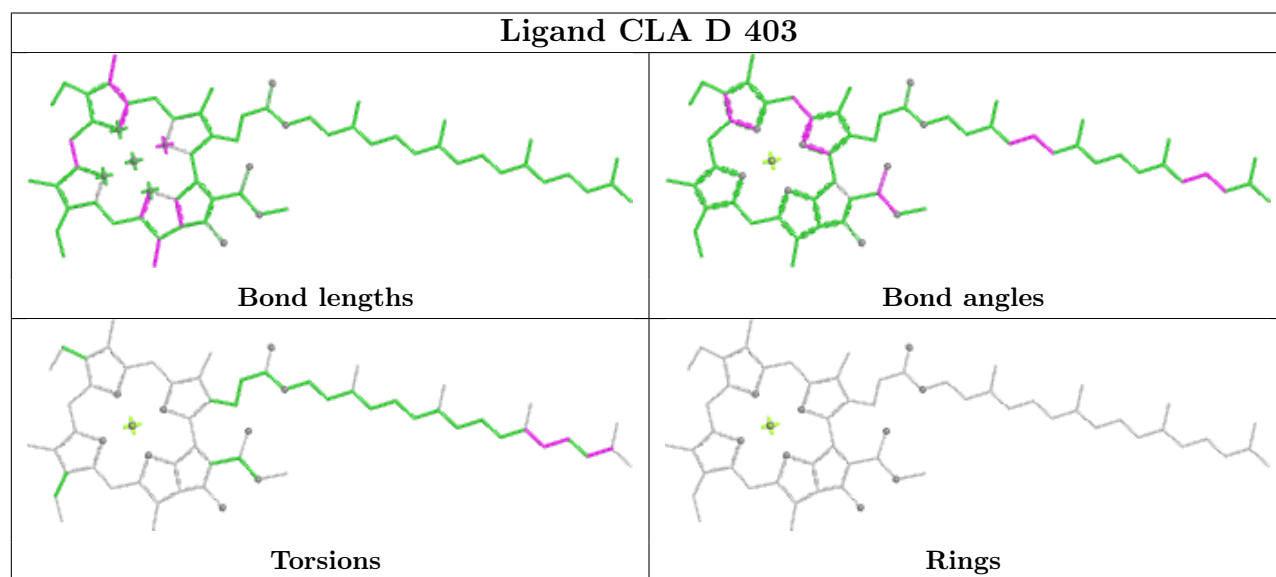
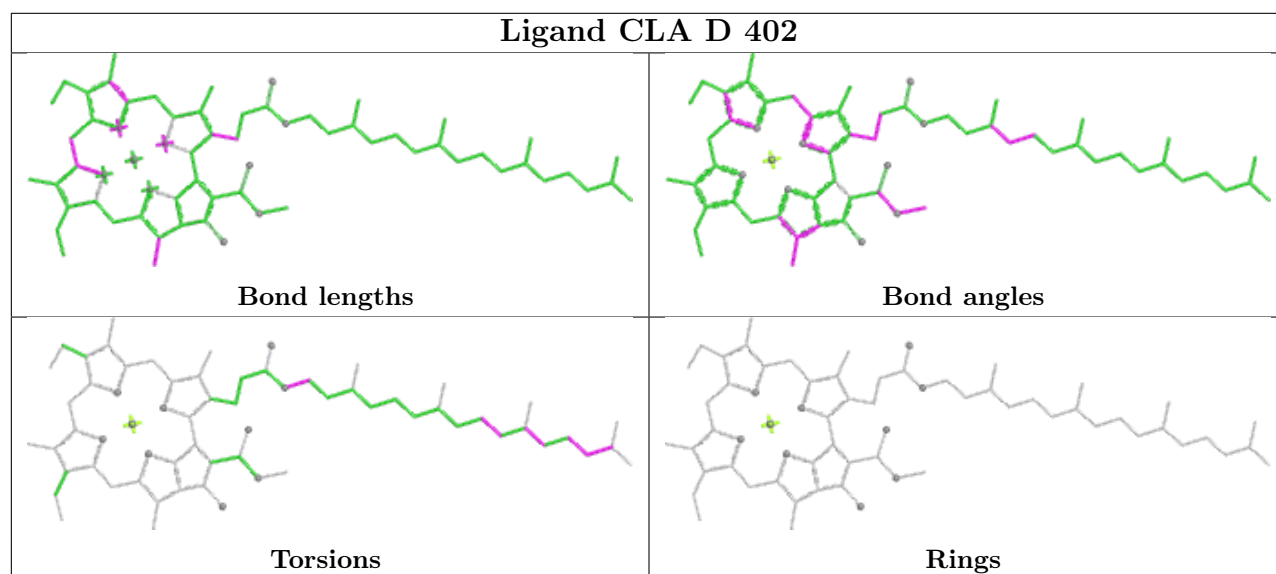
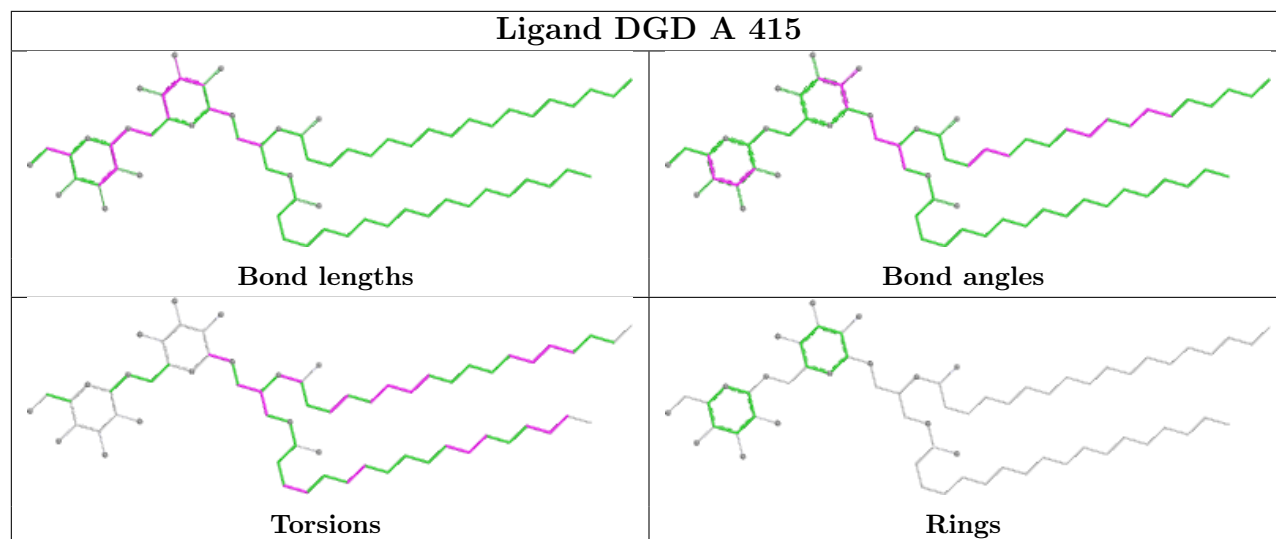
Ligand PHO a 403

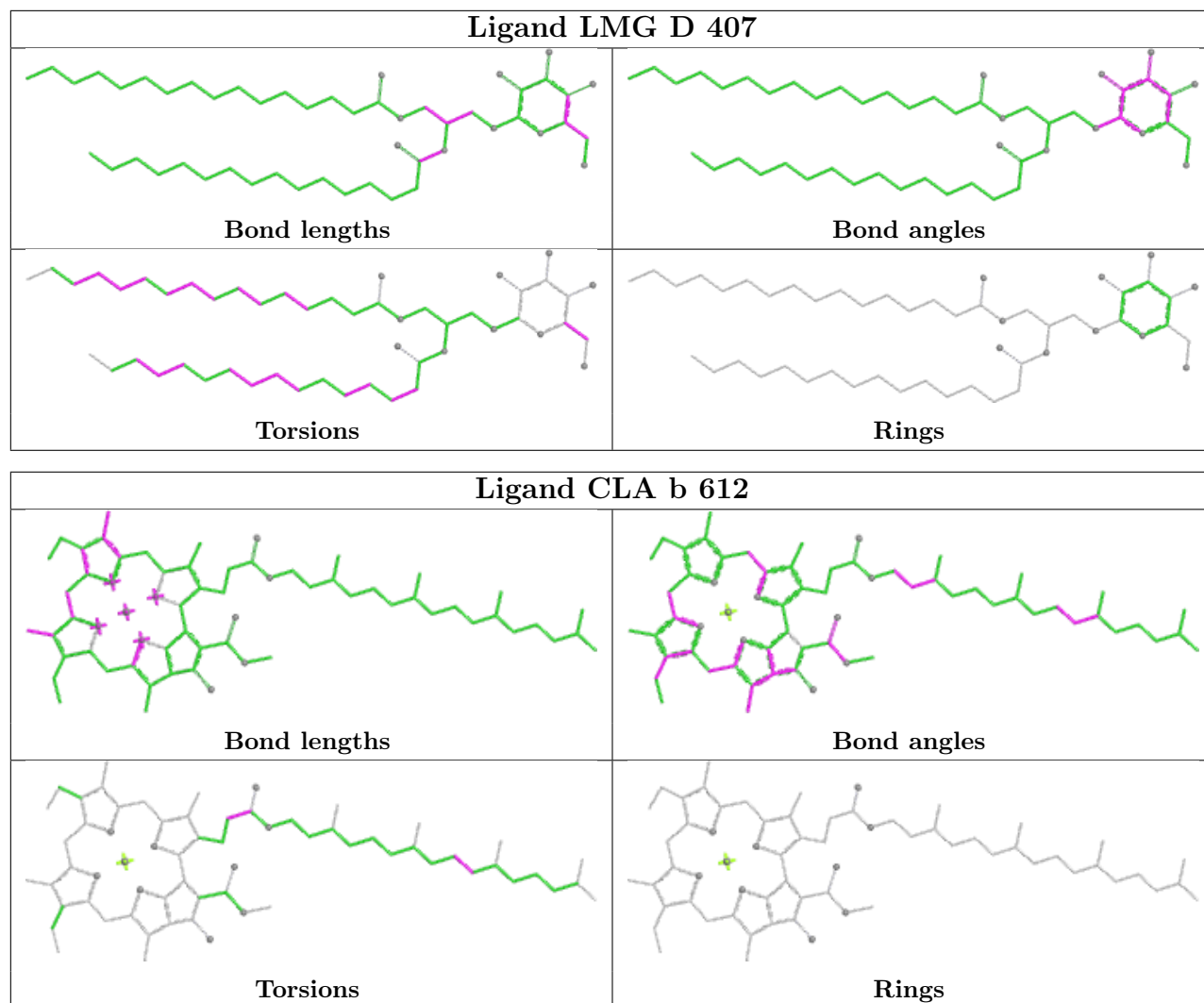


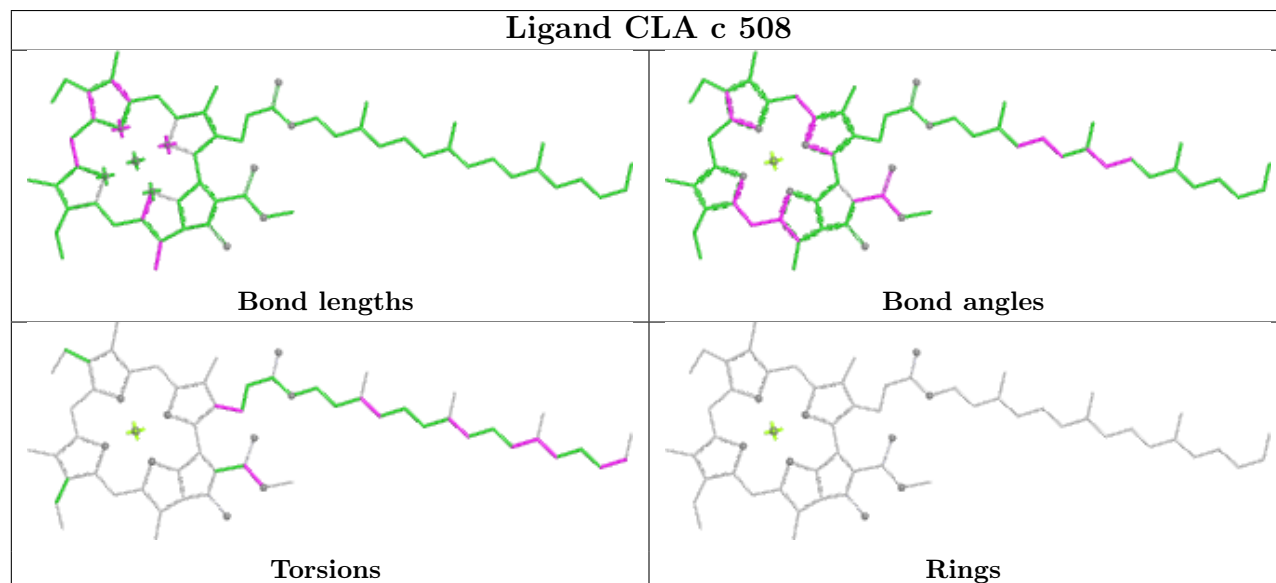
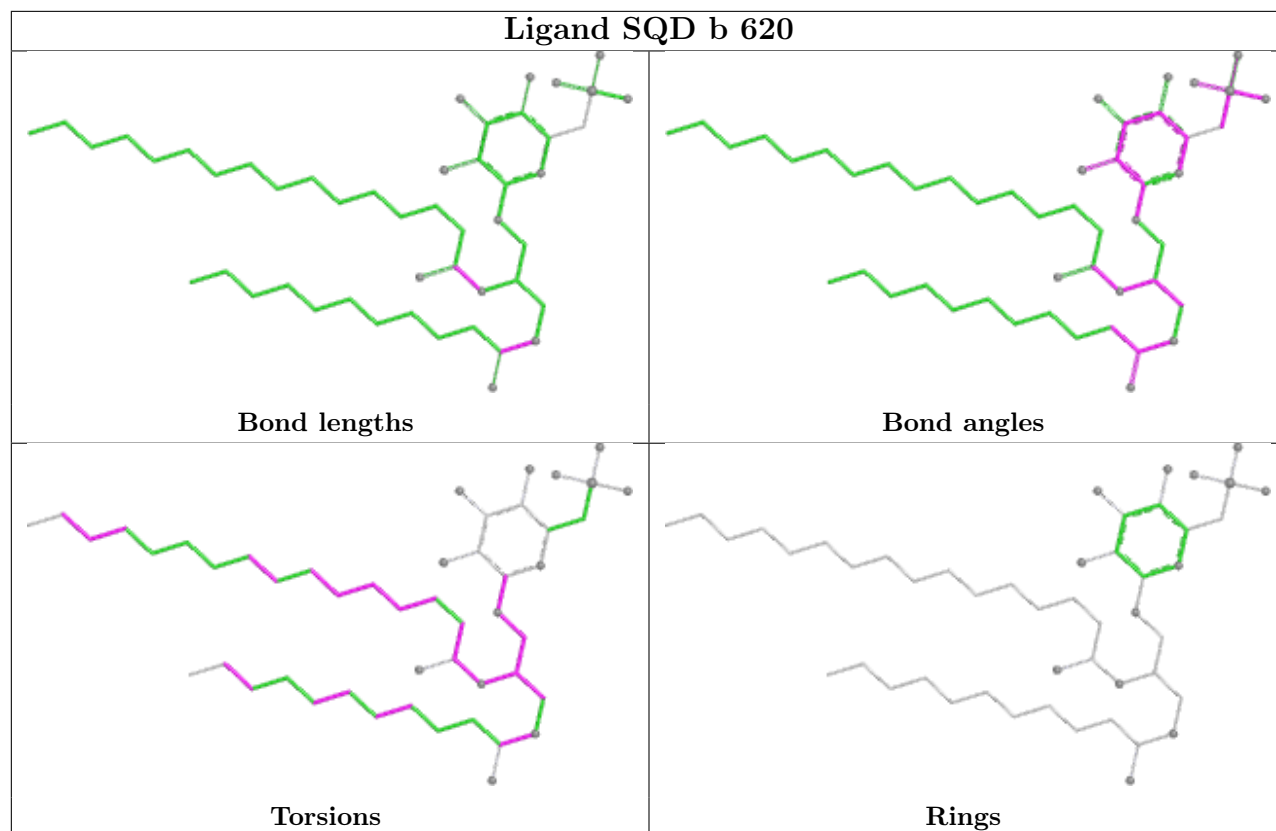


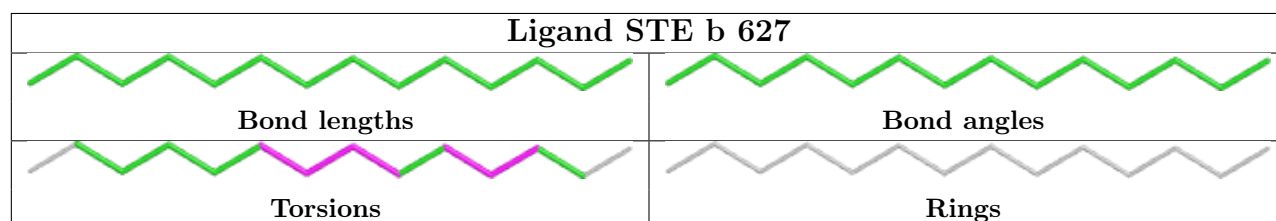
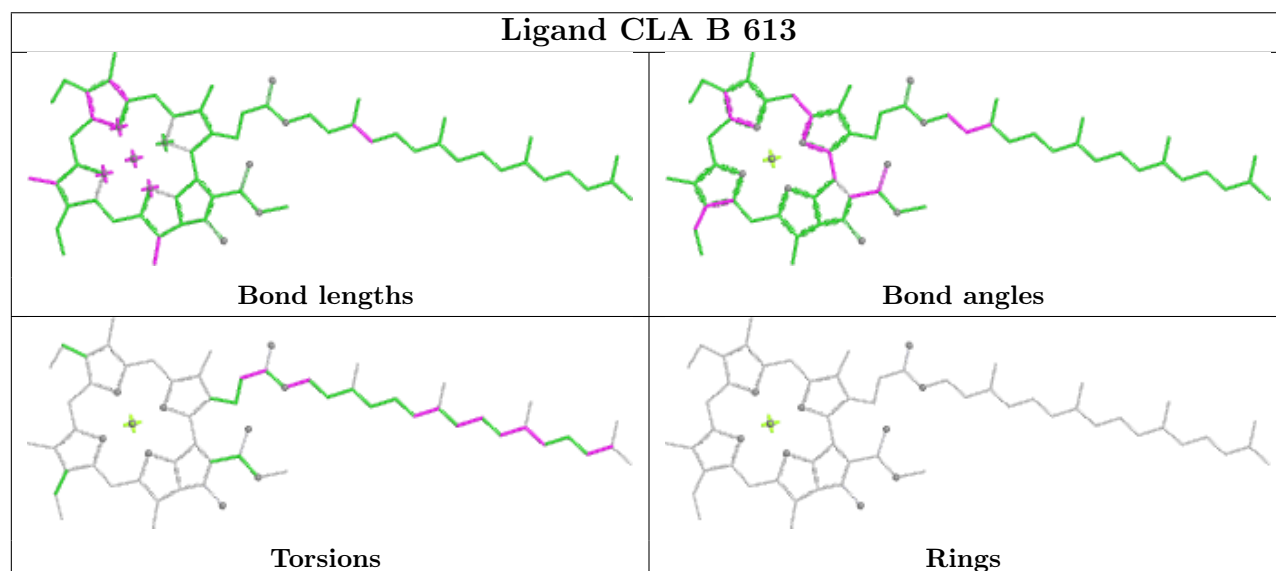
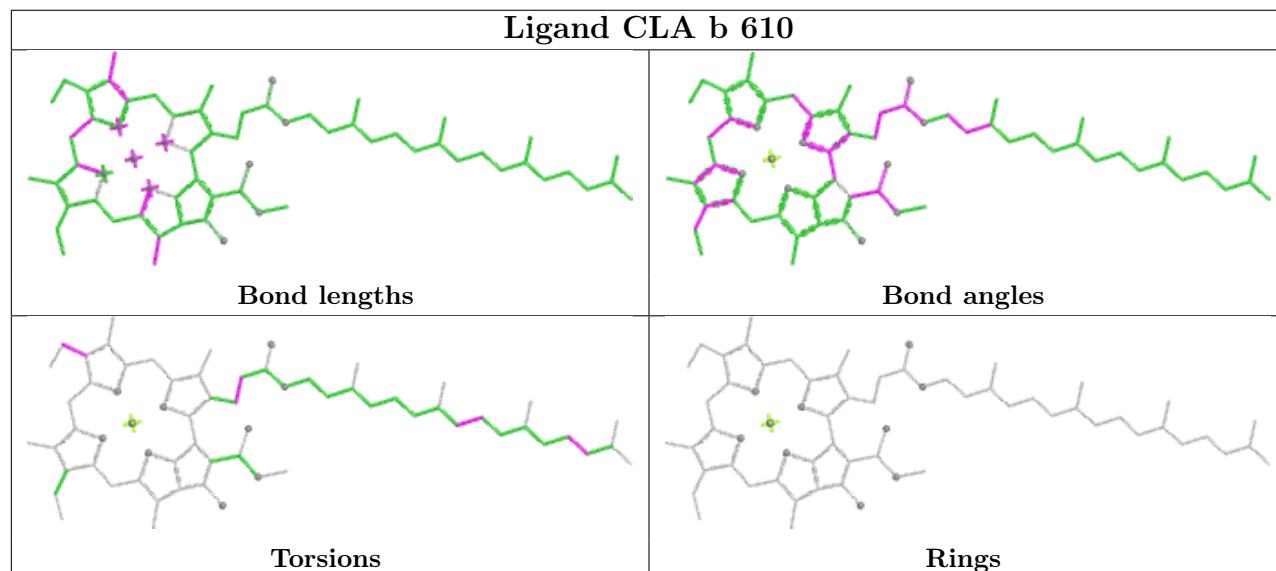
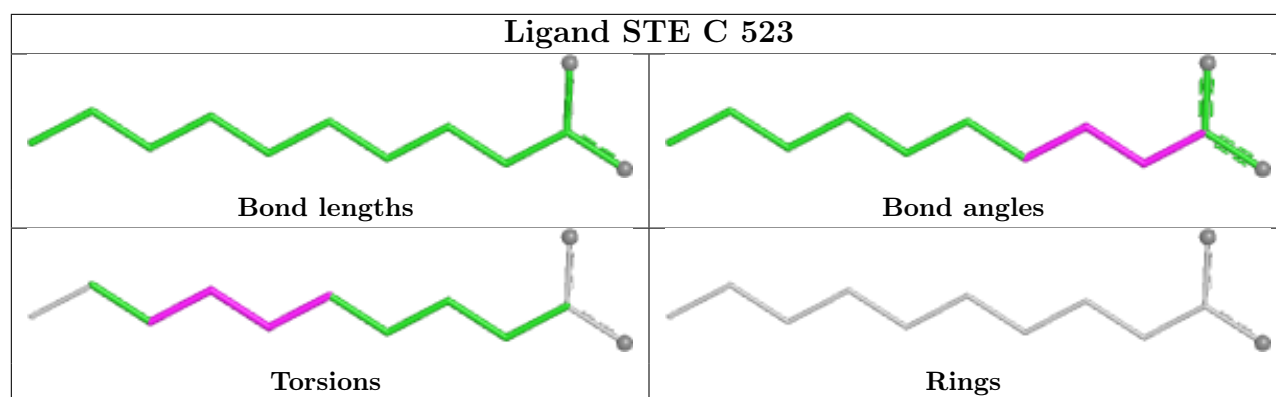




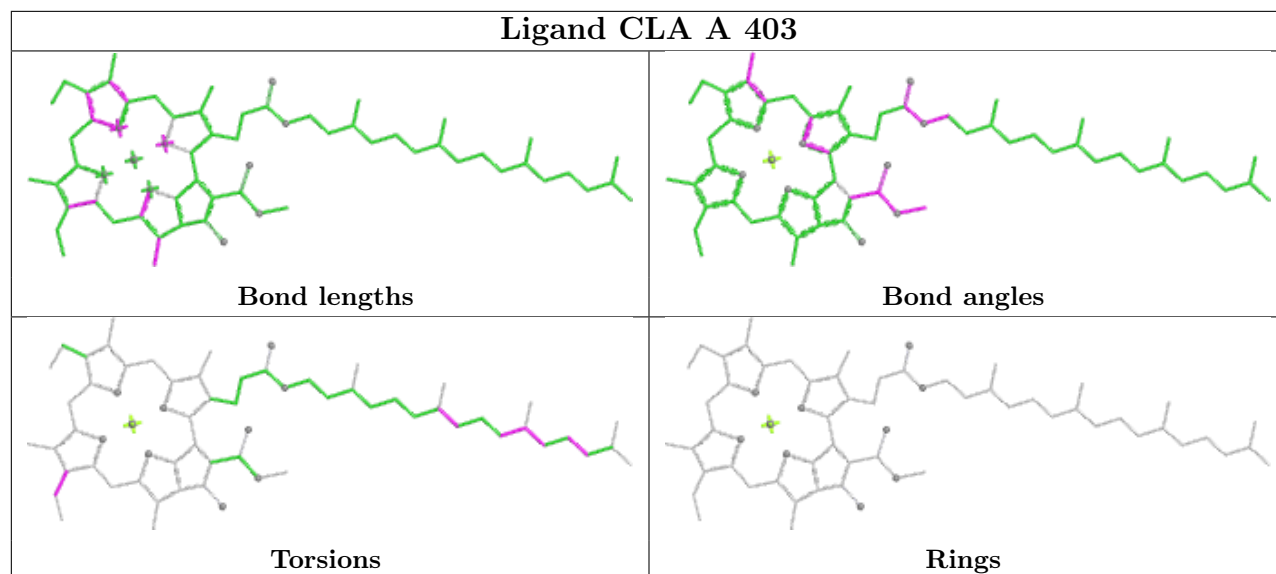




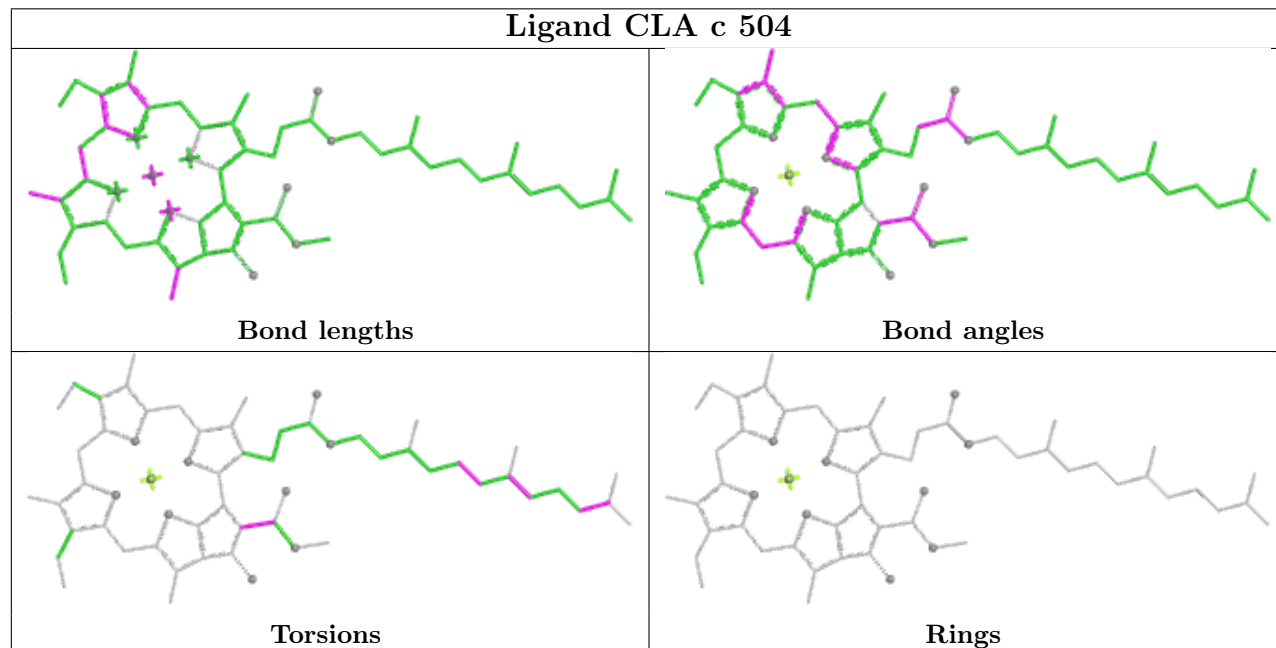


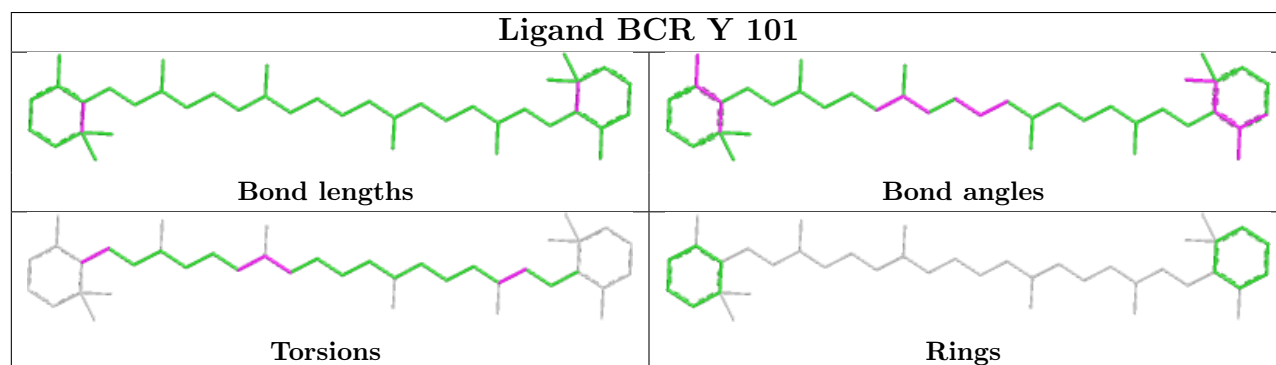
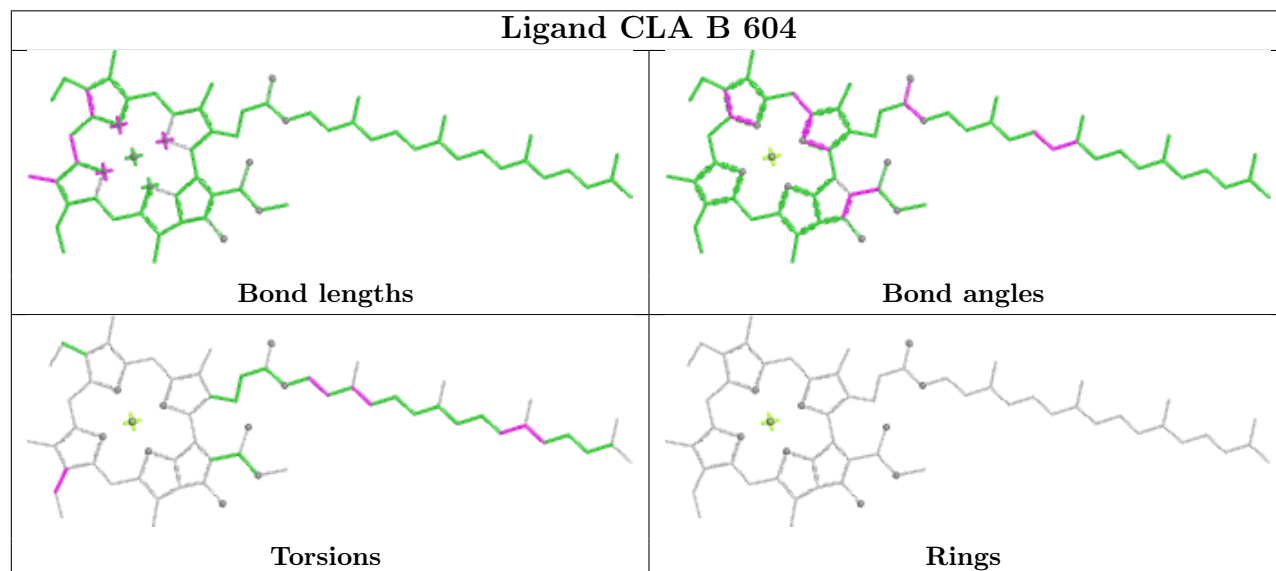
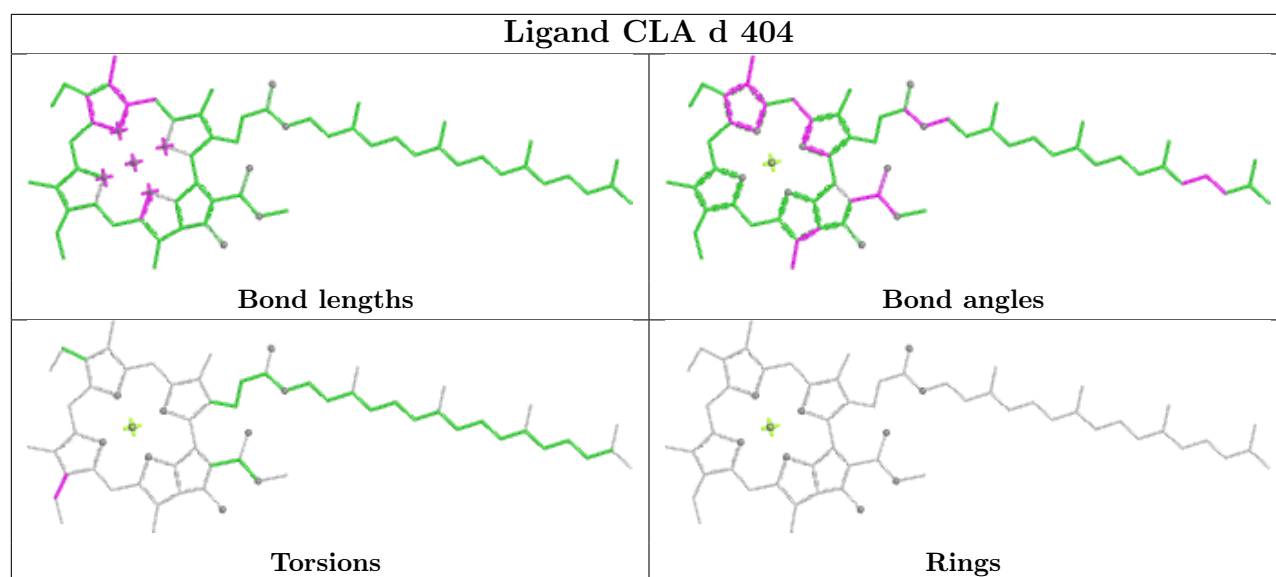


Ligand CLA A 403

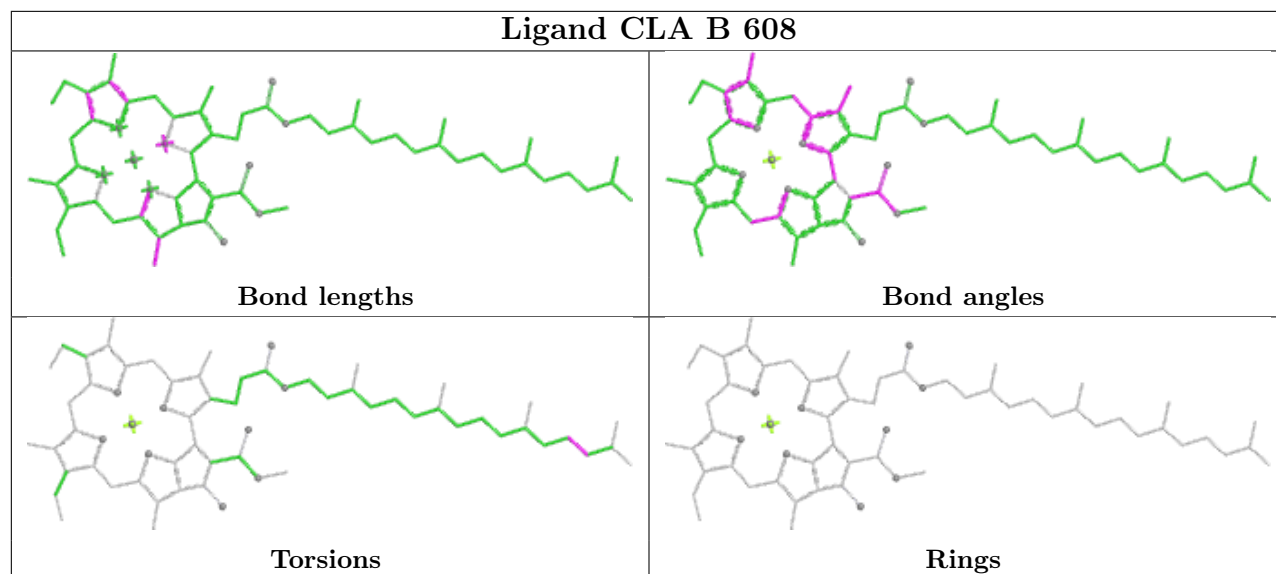


Ligand CLA c 504

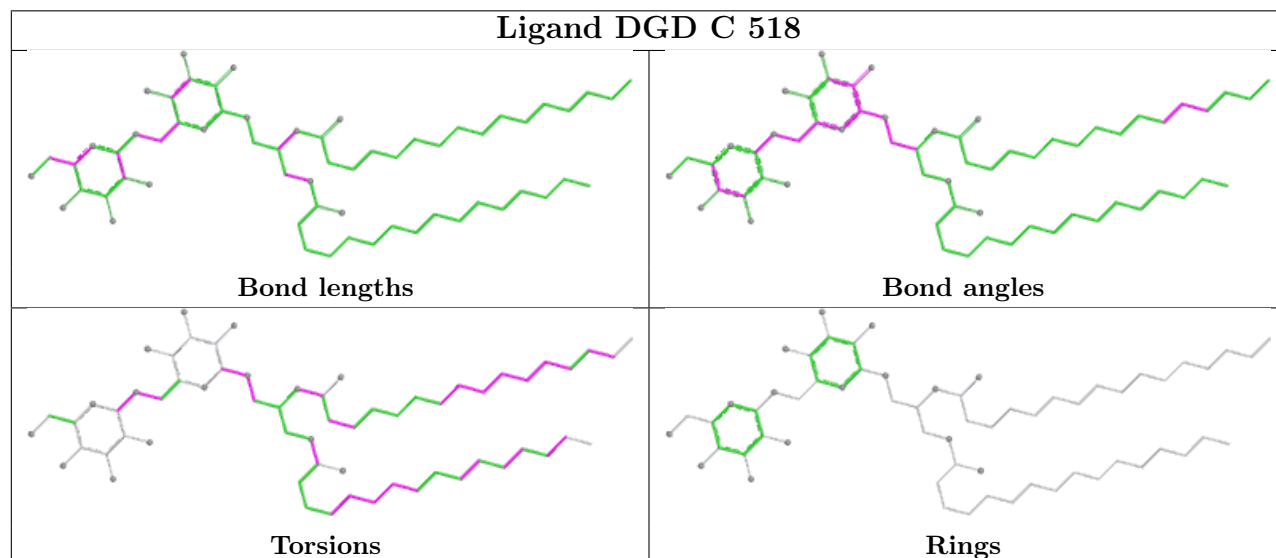




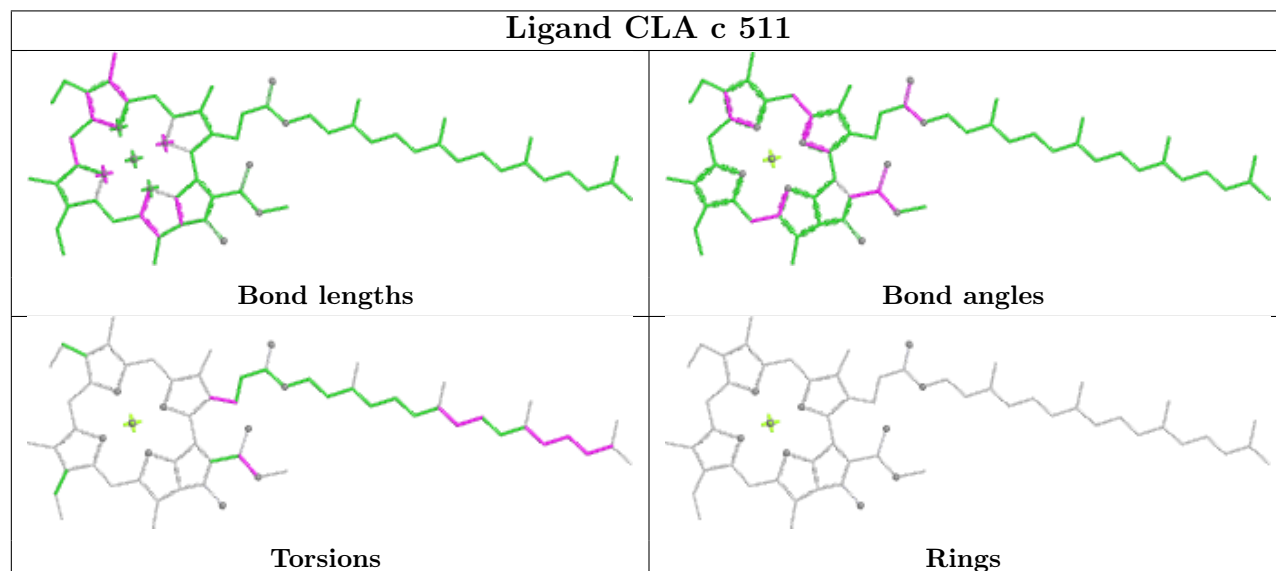
Ligand CLA B 608

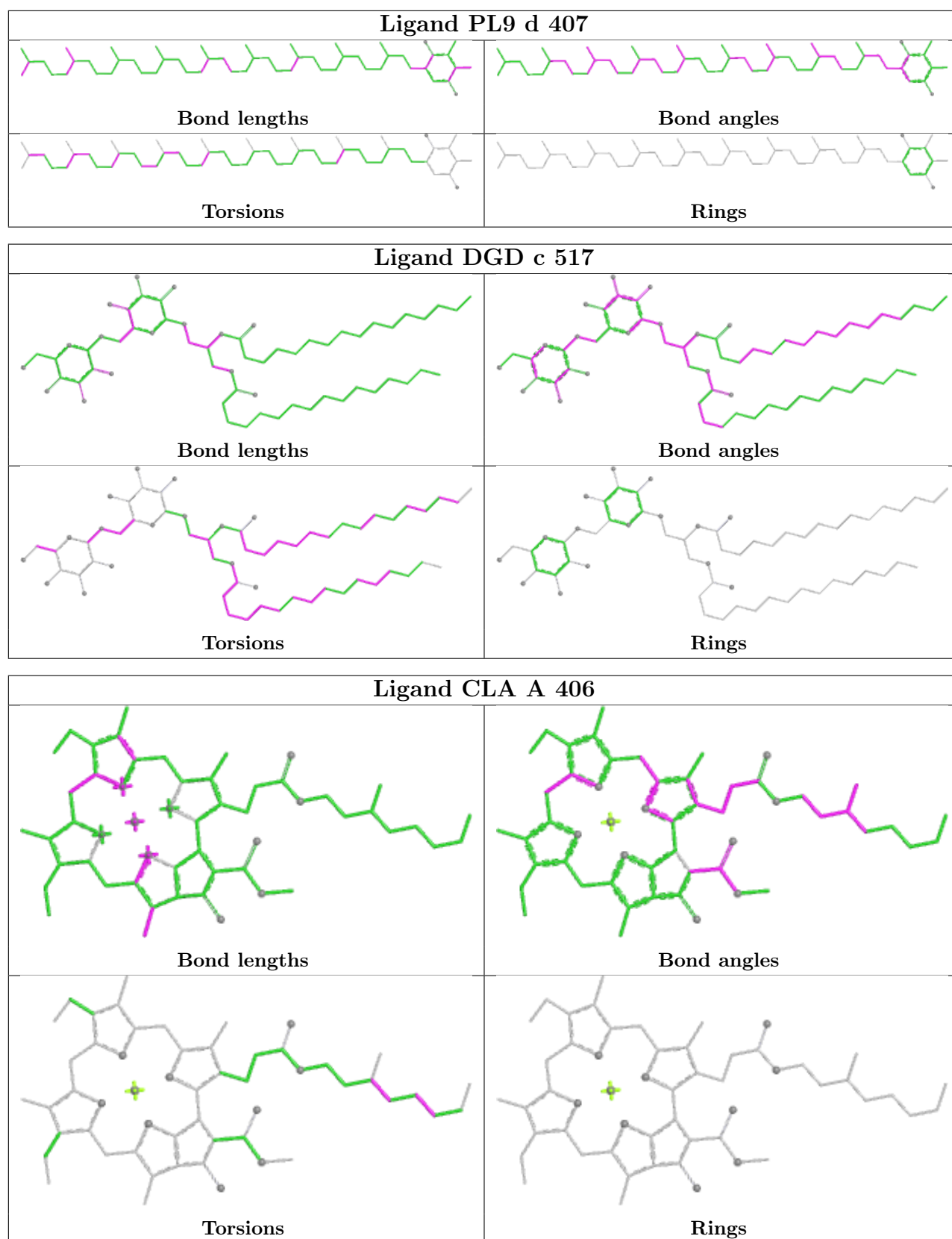


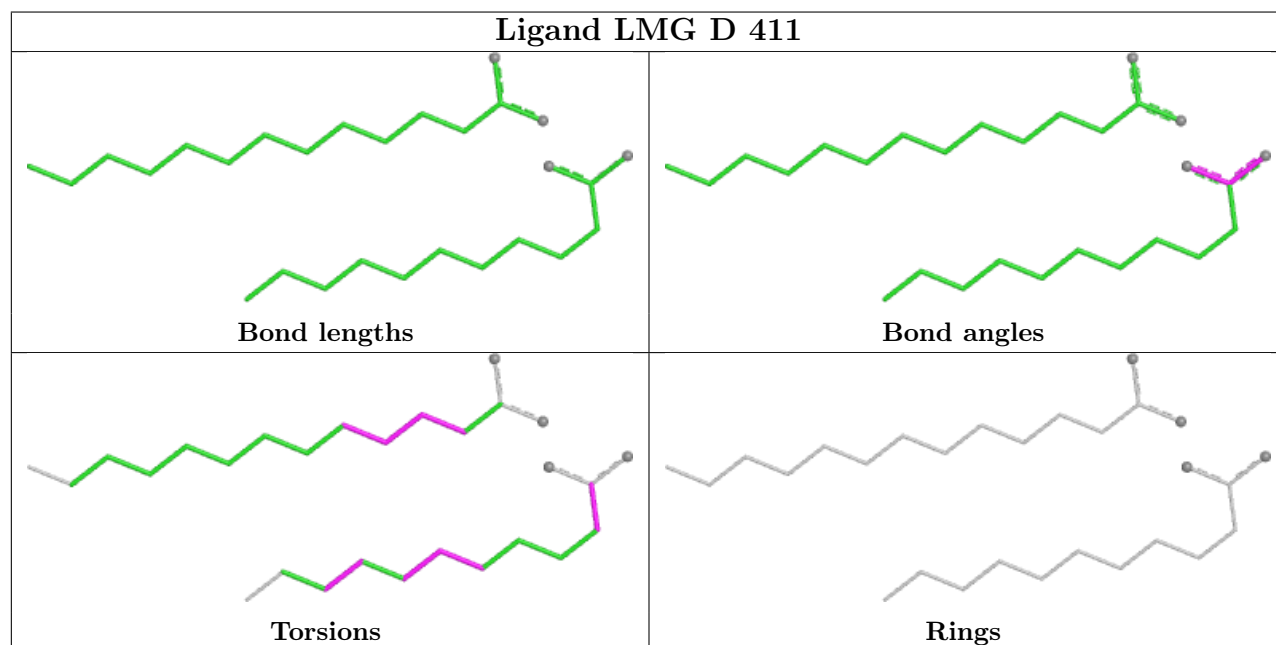
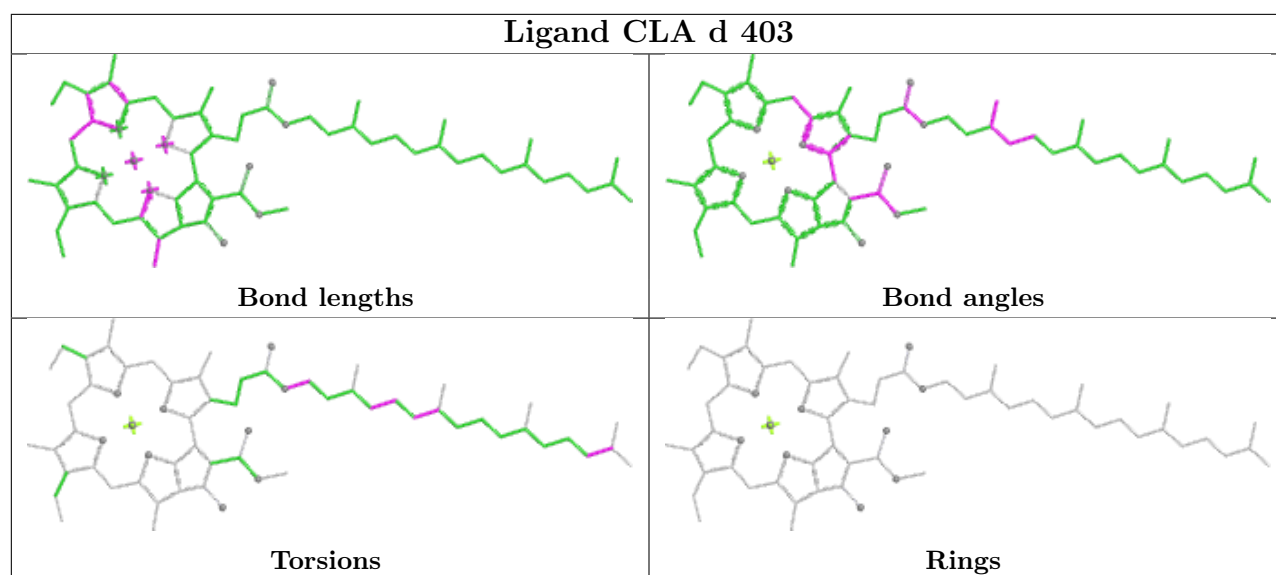
Ligand DGD C 518

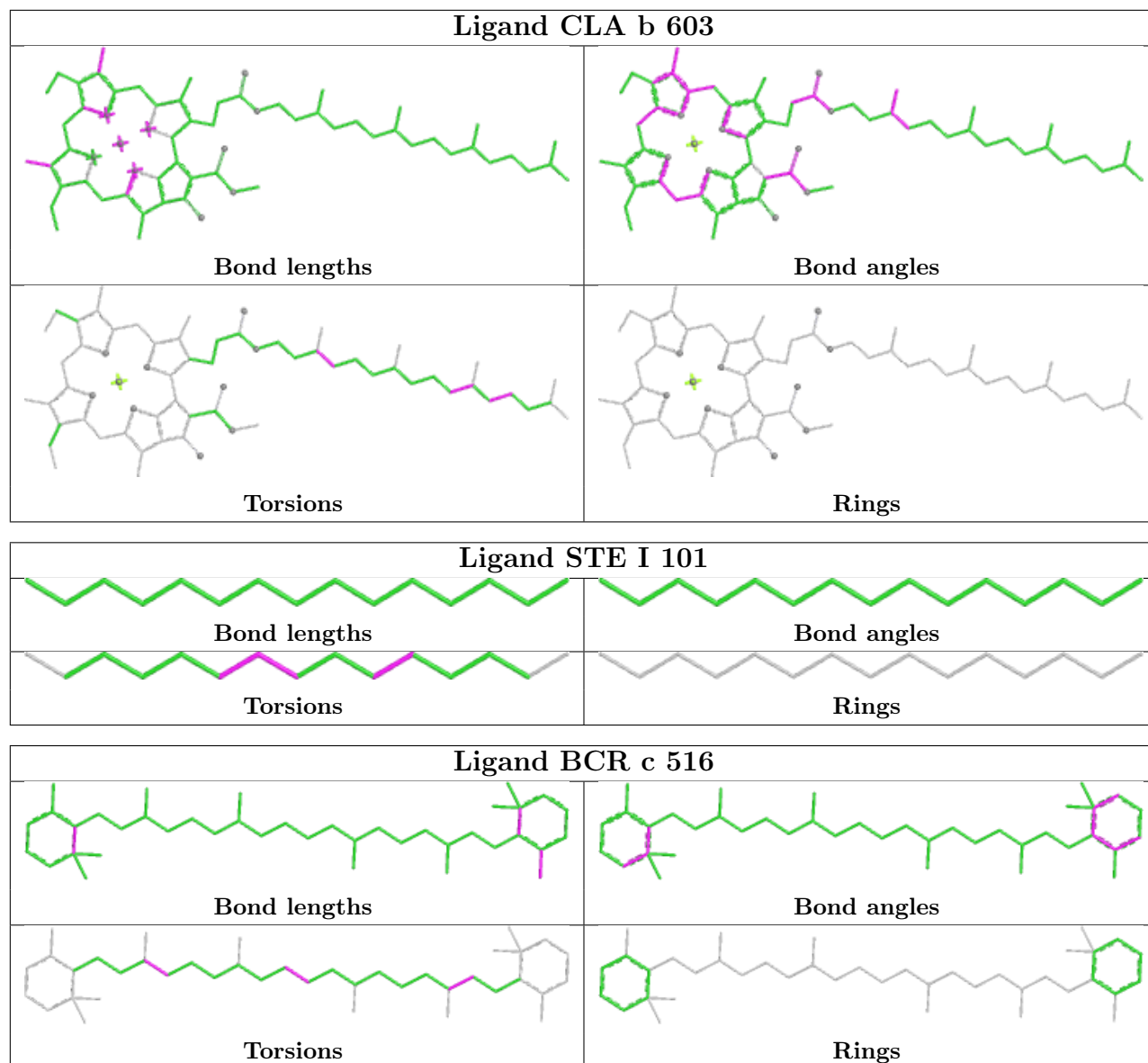


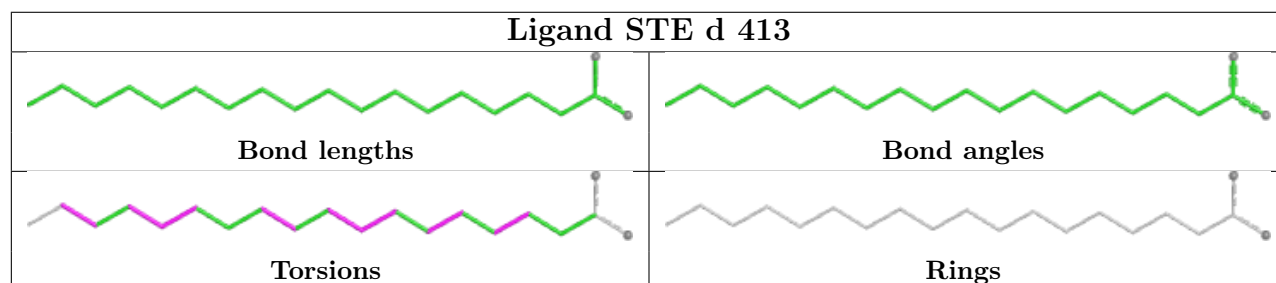
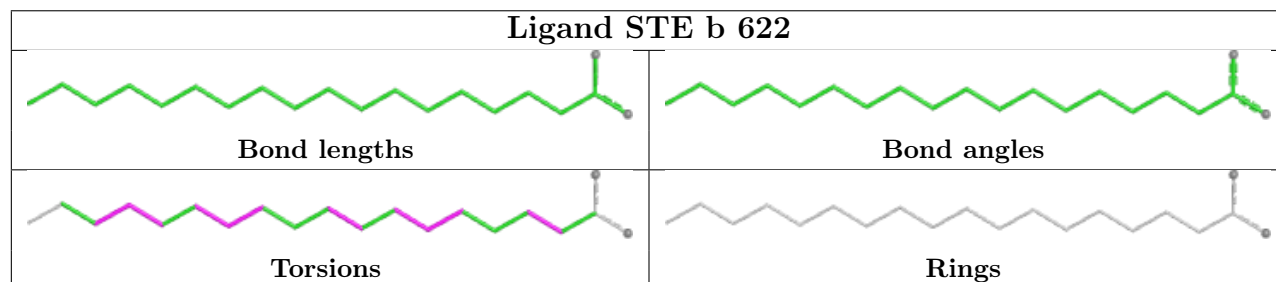
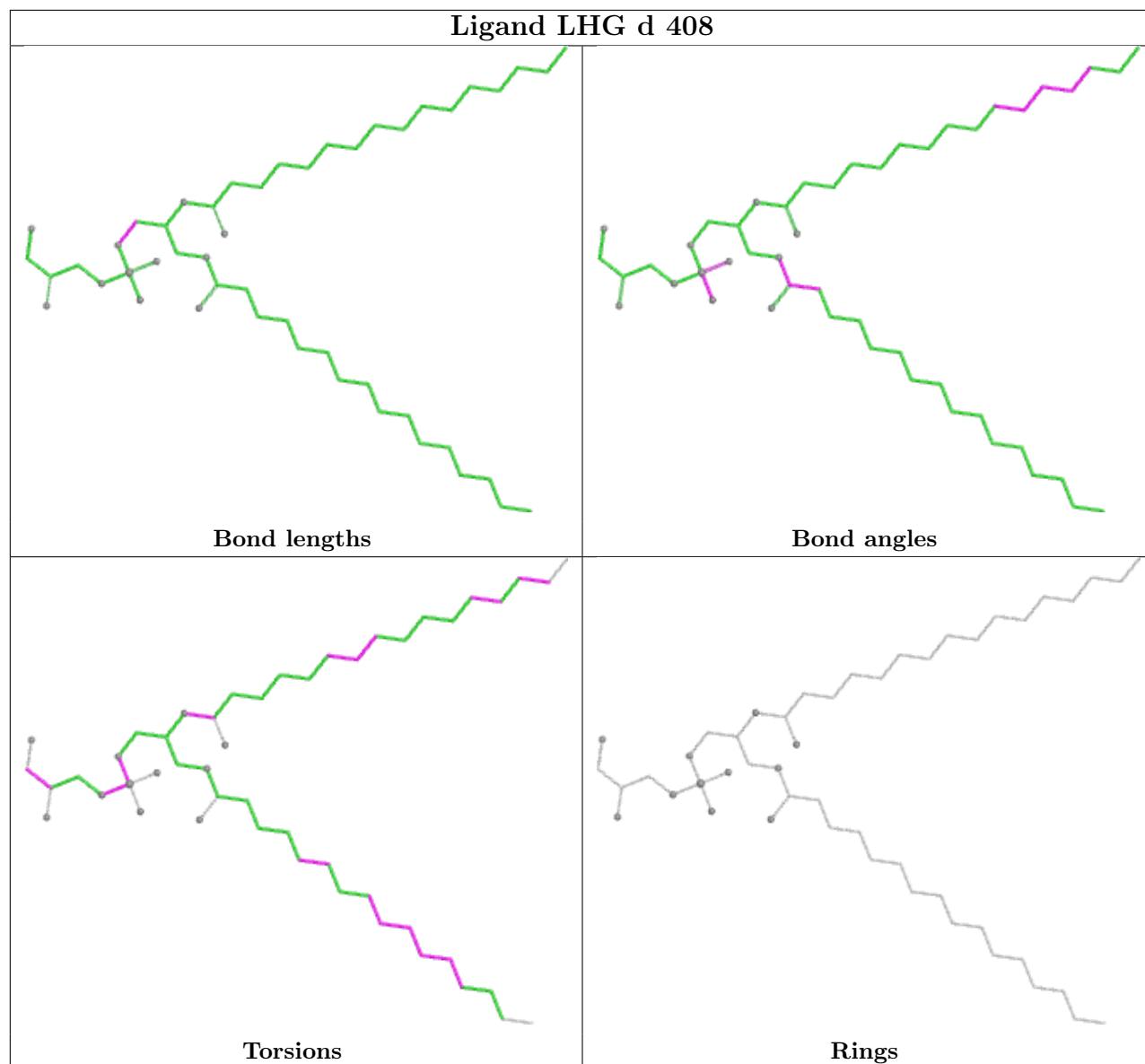
Ligand CLA c 511



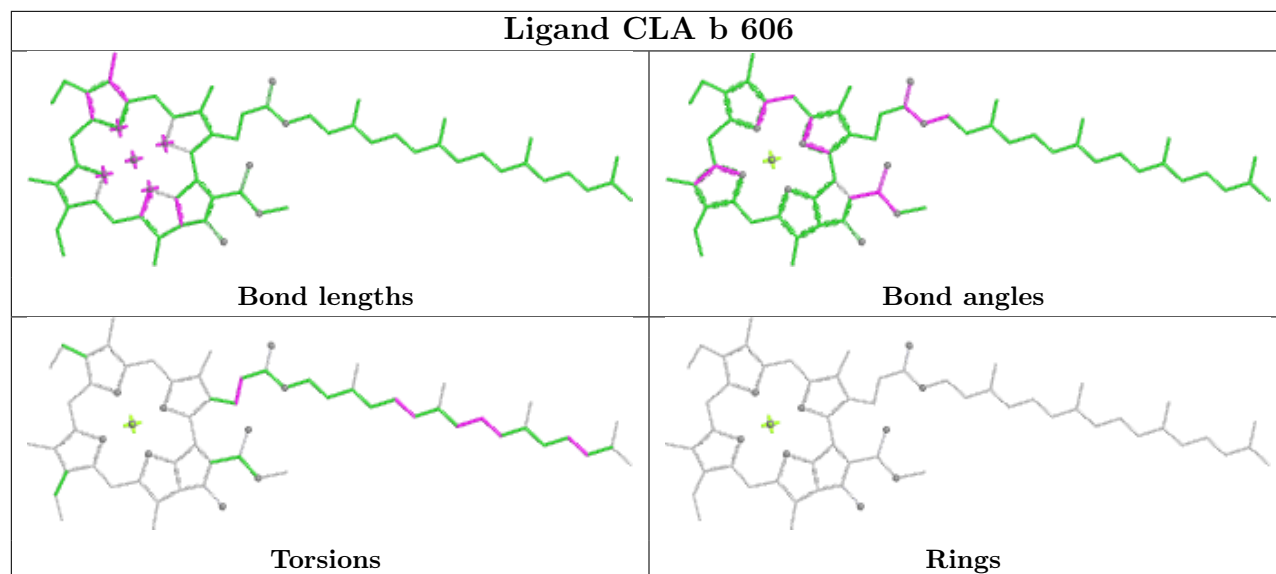




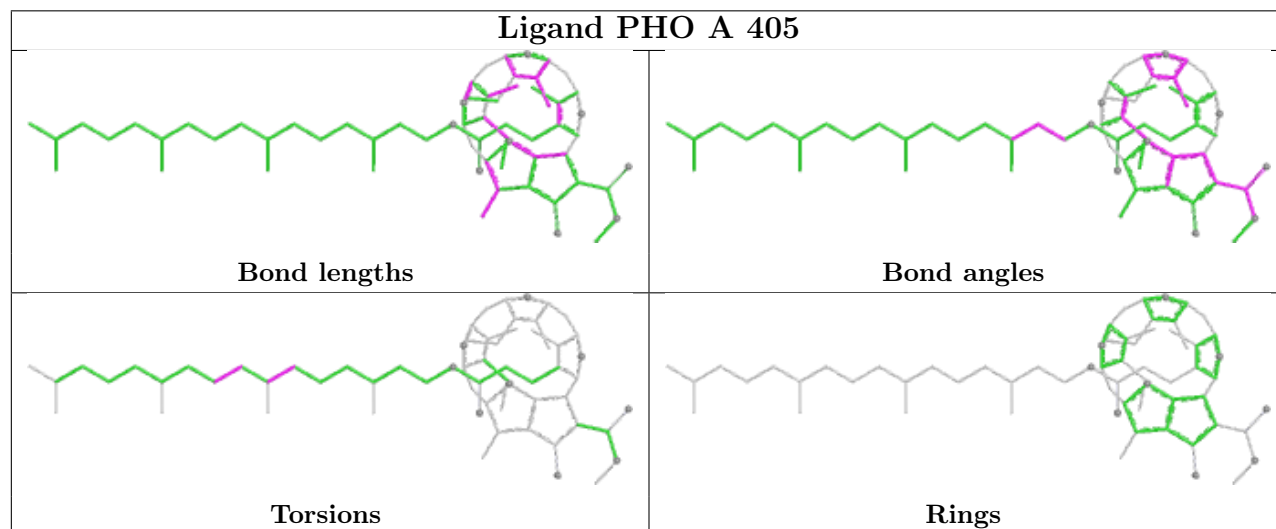




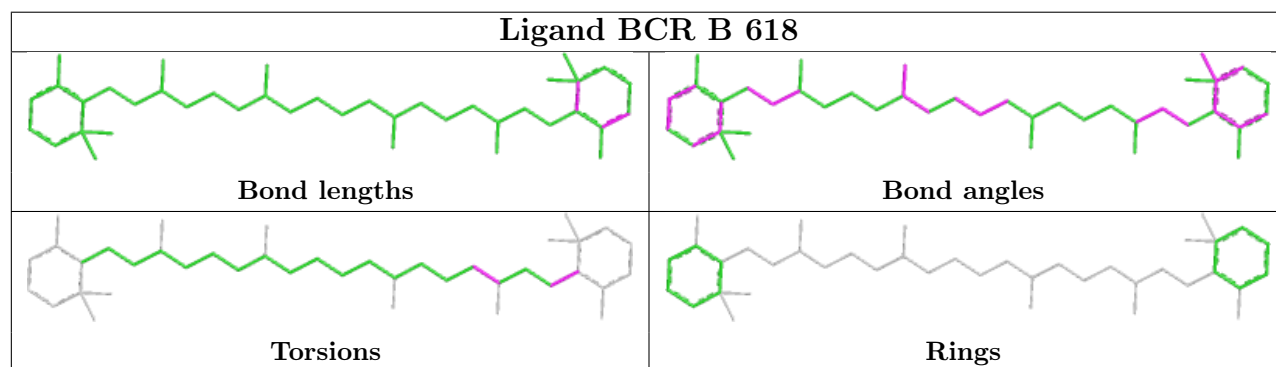
Ligand CLA b 606

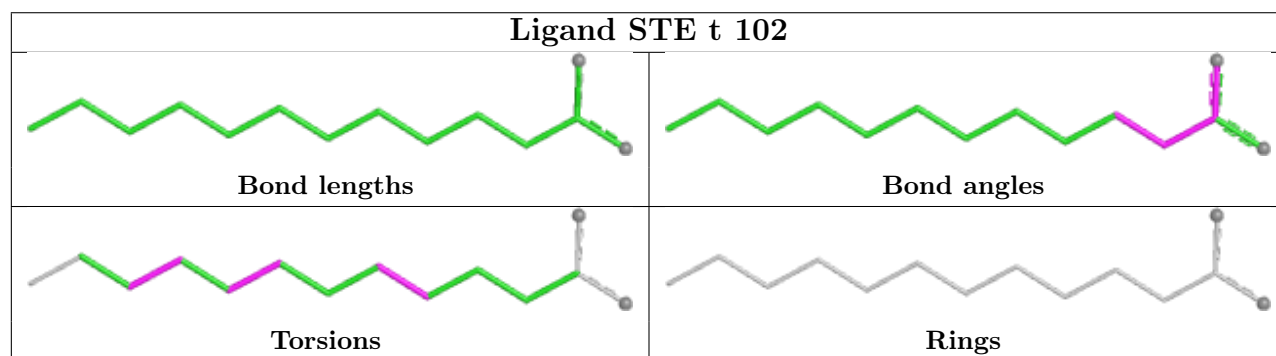
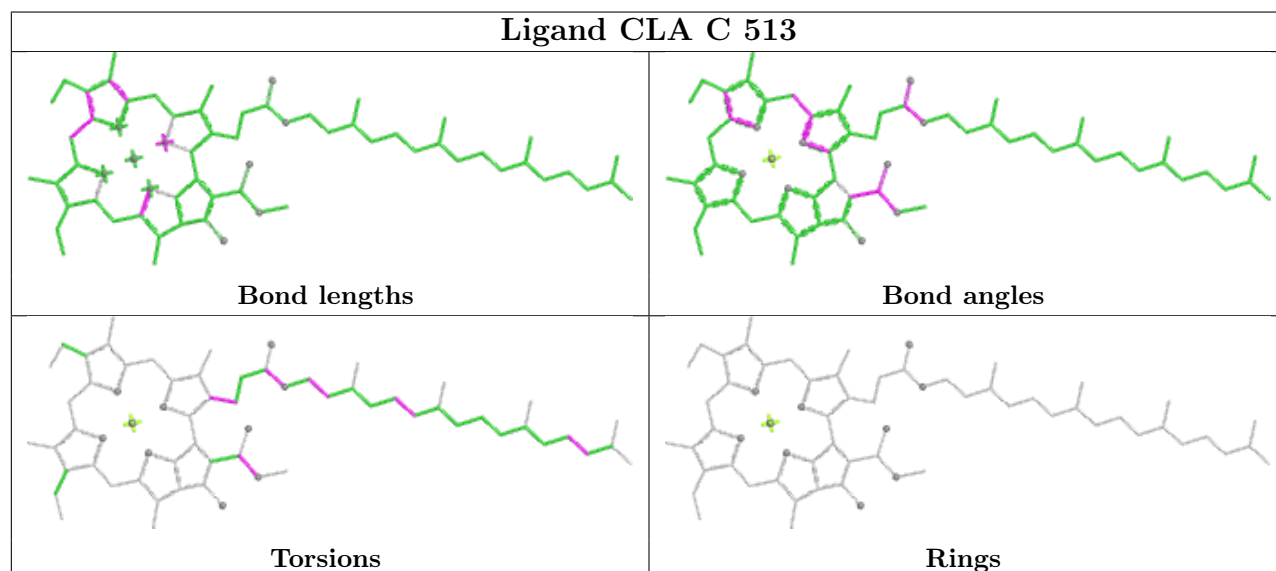
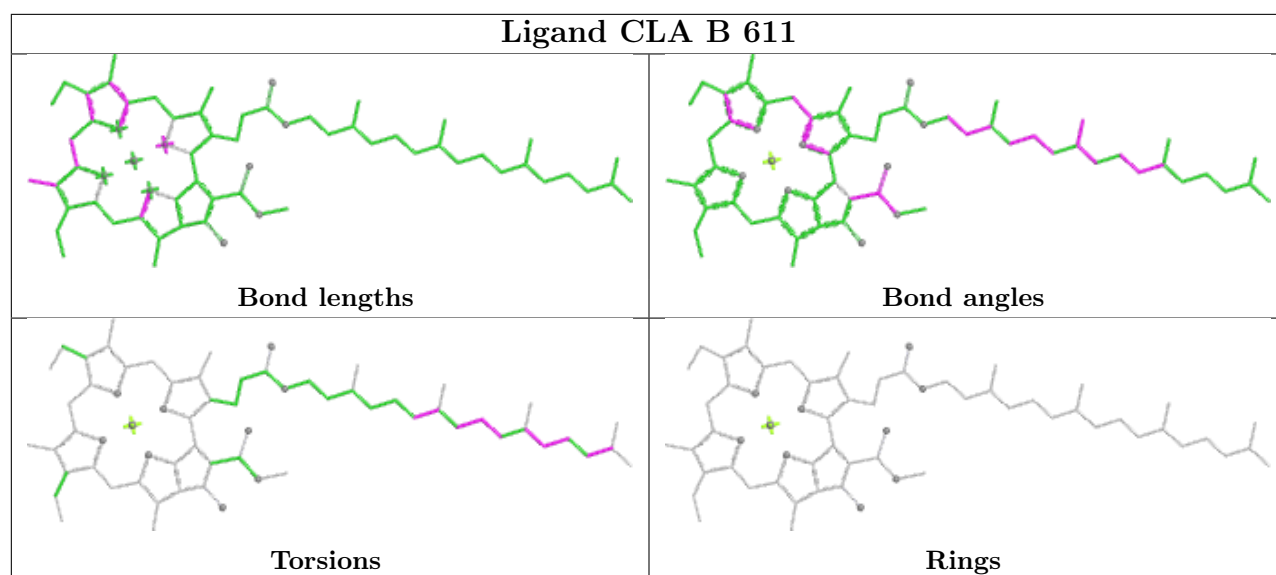


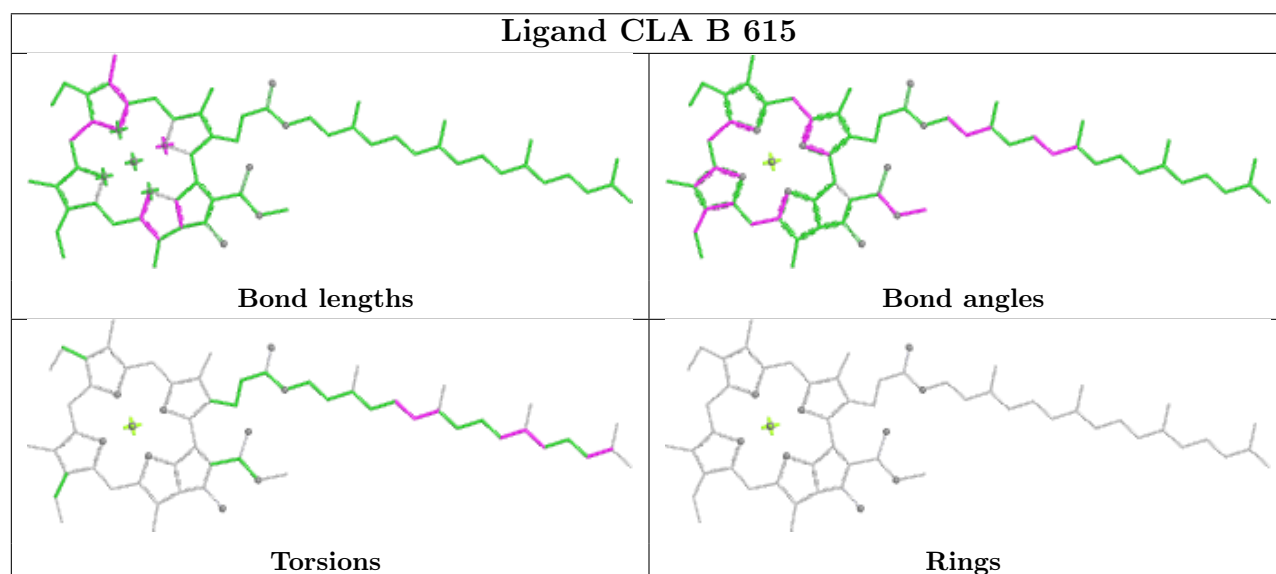
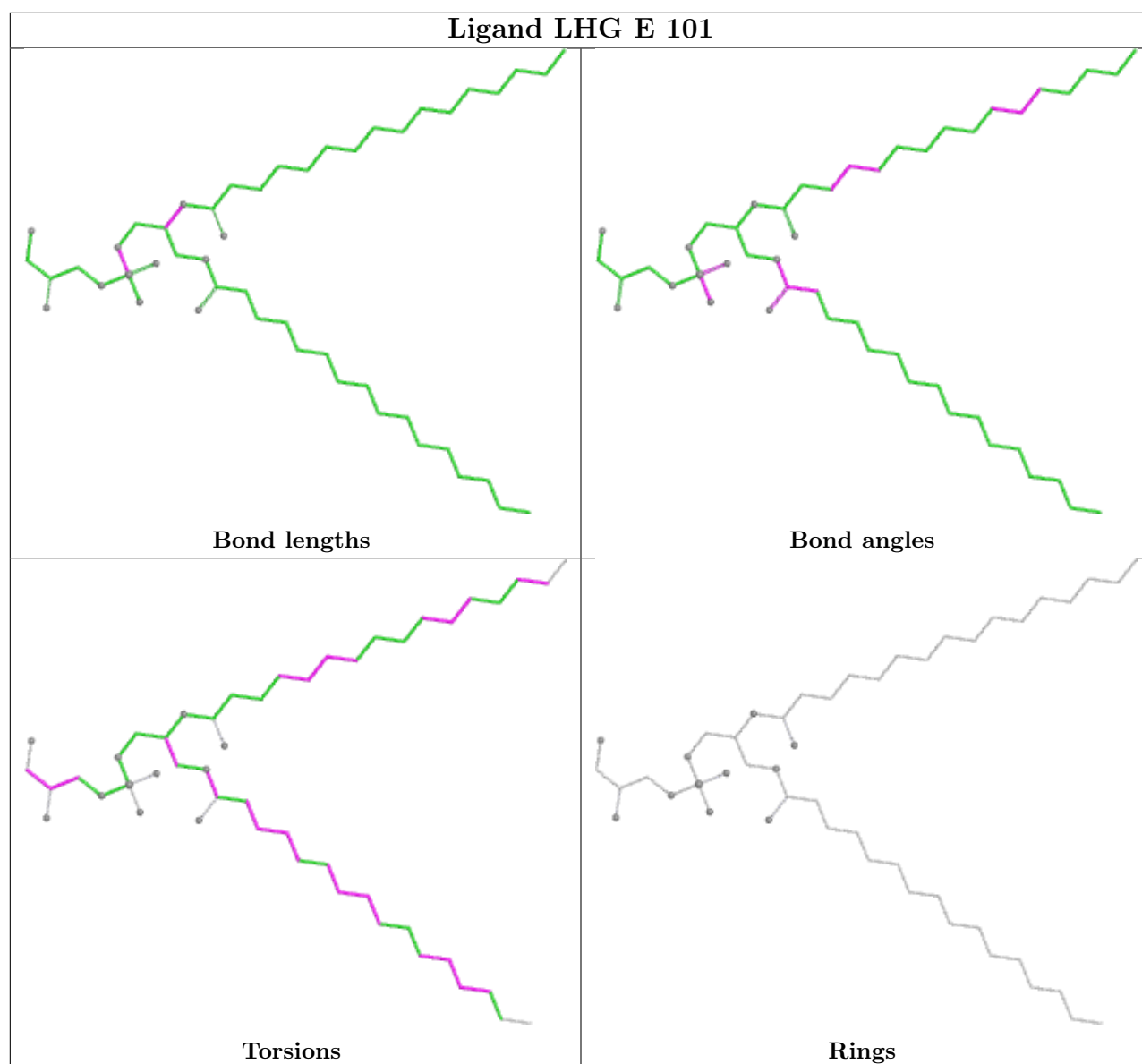
Ligand PHO A 405

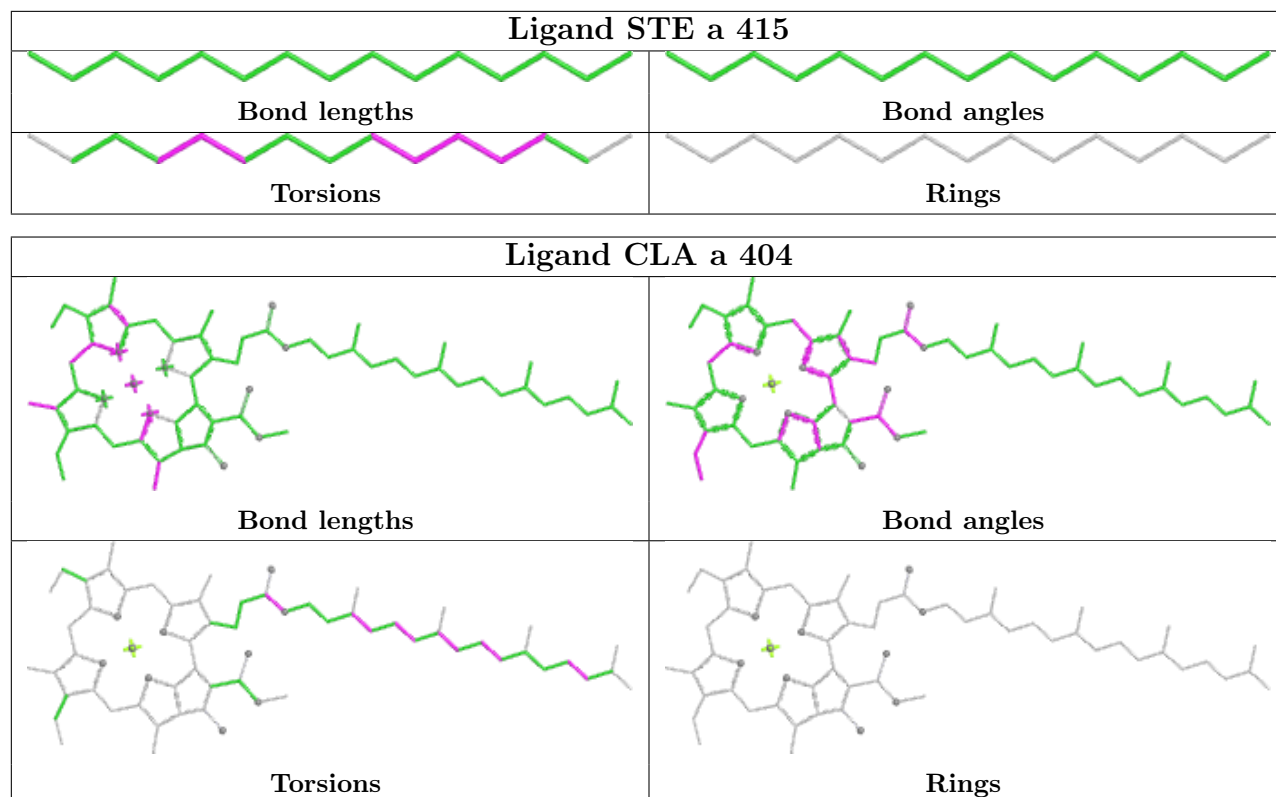


Ligand BCR B 618









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.63	1 (0%) 90 89	13, 29, 48, 84	60 (17%)
1	a	334/344 (97%)	-0.50	3 (0%) 81 80	12, 31, 57, 89	60 (17%)
2	B	505/506 (99%)	-0.50	2 (0%) 88 88	17, 34, 63, 91	4 (0%)
2	b	505/506 (99%)	-0.35	3 (0%) 85 85	24, 38, 72, 105	0
3	C	442/461 (95%)	-0.49	0 100 100	14, 37, 54, 80	7 (1%)
3	c	451/461 (97%)	-0.35	2 (0%) 88 88	14, 41, 65, 109	8 (1%)
4	D	341/352 (96%)	-0.69	0 100 100	15, 31, 48, 87	1 (0%)
4	d	341/352 (96%)	-0.50	0 100 100	16, 35, 57, 84	2 (0%)
5	E	82/84 (97%)	0.14	1 (1%) 76 76	28, 51, 74, 86	1 (1%)
5	e	82/84 (97%)	0.26	1 (1%) 76 76	39, 60, 79, 92	0
6	F	34/45 (75%)	-0.20	0 100 100	36, 43, 64, 85	0
6	f	34/45 (75%)	-0.03	0 100 100	40, 48, 78, 92	0
7	H	65/66 (98%)	-0.33	2 (3%) 51 50	32, 42, 62, 74	0
7	h	63/66 (95%)	0.00	1 (1%) 70 70	40, 52, 67, 76	0
8	I	35/38 (92%)	-0.46	0 100 100	33, 40, 75, 90	0
8	i	35/38 (92%)	-0.25	0 100 100	31, 42, 77, 93	0
9	J	36/40 (90%)	-0.18	0 100 100	34, 51, 71, 98	0
9	j	36/40 (90%)	0.01	1 (2%) 55 54	38, 53, 93, 112	0
10	K	37/46 (80%)	-0.11	0 100 100	42, 52, 74, 80	0
10	k	37/46 (80%)	0.06	0 100 100	46, 55, 72, 80	0
11	L	37/37 (100%)	-0.60	0 100 100	25, 31, 66, 71	0
11	l	36/37 (97%)	-0.52	0 100 100	25, 32, 80, 89	0
12	M	32/36 (88%)	-0.52	1 (3%) 51 50	25, 36, 61, 77	0
12	m	31/36 (86%)	-0.51	0 100 100	26, 36, 51, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.20	3 (1%) 76 76	26, 43, 83, 137	1 (0%)
13	o	244/272 (89%)	-0.24	1 (0%) 88 88	26, 42, 82, 138	0
14	R	34/40 (85%)	0.71	1 (2%) 53 52	58, 72, 93, 105	0
14	r	31/40 (77%)	1.07	4 (12%) 7 6	69, 92, 108, 120	0
15	T	29/30 (96%)	-0.57	0 100 100	27, 33, 66, 79	0
15	t	29/30 (96%)	-0.45	2 (6%) 23 21	28, 33, 85, 86	0
16	U	97/134 (72%)	-0.25	0 100 100	33, 46, 70, 91	0
16	u	97/134 (72%)	-0.33	0 100 100	32, 41, 58, 87	0
17	V	137/163 (84%)	-0.41	0 100 100	30, 41, 59, 83	0
17	v	137/163 (84%)	-0.18	0 100 100	33, 48, 70, 86	0
18	X	38/41 (92%)	-0.09	0 100 100	38, 51, 73, 82	0
18	x	39/41 (95%)	0.18	1 (2%) 57 56	48, 58, 84, 102	0
19	Y	27/46 (58%)	0.94	4 (14%) 5 5	51, 72, 96, 97	0
19	y	30/46 (65%)	0.68	0 100 100	60, 70, 92, 103	0
20	Z	62/62 (100%)	0.64	1 (1%) 70 70	51, 66, 117, 129	0
20	z	62/62 (100%)	0.65	2 (3%) 50 49	57, 72, 111, 122	0
All	All	5302/5686 (93%)	-0.33	37 (0%) 84 84	12, 39, 76, 138	144 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	4.2
13	O	59	LYS	4.1
14	R	35	LEU	3.8
7	H	41	PHE	3.8
5	e	79	PHE	3.4
14	r	32	GLN	3.4
20	Z	62	VAL	3.2
15	t	30	THR	2.9
13	O	58	ASN	2.8
2	B	495	PHE	2.7
2	b	495	PHE	2.7
20	z	33	TRP	2.7
1	a	250	ALA	2.6
18	x	40	SER	2.6
2	B	490	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
19	Y	22	LEU	2.5
1	a	249	VAL	2.4
1	a	11	ALA	2.4
19	Y	25	ILE	2.4
20	z	30	PRO	2.4
5	E	3	GLY	2.4
14	r	20	VAL	2.3
9	j	6	GLY	2.3
7	h	41	PHE	2.3
3	c	23	ALA	2.2
1	A	13	LEU	2.2
19	Y	20	ALA	2.2
15	t	29	ILE	2.1
2	b	499	VAL	2.1
7	H	65	LEU	2.1
3	c	24	THR	2.1
14	r	31	VAL	2.1
12	M	33	GLN	2.1
2	b	487	SER	2.1
13	O	56	PRO	2.0
19	Y	27	MET	2.0
14	r	3	TRP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	M	1	10/11	0.94	0.09	40,51,73,84	0
15	FME	t	1	10/11	0.94	0.08	32,45,72,72	0
8	FME	I	1	10/11	0.95	0.08	33,44,65,71	0
12	FME	m	1	10/11	0.96	0.09	34,45,71,80	0
15	FME	T	1	10/11	0.96	0.06	27,46,65,65	0
8	FME	i	1	10/11	0.96	0.08	36,50,62,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	STE	H	103	18/20	0.75	0.18	51,74,87,90	0
33	STE	a	414	12/20	0.78	0.14	35,62,69,75	0
33	STE	d	413	20/20	0.78	0.16	38,68,92,97	0
33	STE	b	625	20/20	0.79	0.17	49,66,82,85	0
33	STE	a	413	10/20	0.80	0.15	40,62,75,75	0
33	STE	b	627	14/20	0.81	0.16	52,65,84,93	0
33	STE	b	626	10/20	0.81	0.16	39,53,59,69	0
27	LMG	b	623	55/55	0.82	0.15	49,71,96,103	0
27	LMG	a	416	55/55	0.82	0.16	37,63,101,136	0
33	STE	R	101	12/20	0.82	0.16	55,77,85,87	0
33	STE	I	101	15/20	0.83	0.14	38,55,77,81	0
28	LHG	E	101	49/49	0.83	0.14	43,76,103,113	0
28	LHG	e	101	42/49	0.83	0.14	51,78,103,123	0
27	LMG	c	522	48/55	0.83	0.14	43,75,106,112	0
33	STE	m	102	12/20	0.83	0.17	49,62,82,84	0
33	STE	T	102	15/20	0.84	0.14	42,58,79,80	0
33	STE	k	102	12/20	0.84	0.11	43,65,78,83	0
33	STE	C	521	12/20	0.84	0.13	41,58,69,70	0
33	STE	a	415	15/20	0.85	0.18	39,68,86,93	0
33	STE	b	621	16/20	0.85	0.13	29,47,69,70	0
33	STE	B	626	12/20	0.85	0.15	49,62,79,84	0
33	STE	B	625	16/20	0.85	0.14	43,62,82,84	0
27	LMG	D	410	33/55	0.86	0.13	35,55,80,90	0
22	CLA	b	601	65/65	0.86	0.11	46,65,86,102	0
33	STE	d	412	20/20	0.86	0.11	36,54,71,77	0
29	SQD	a	412	36/54	0.86	0.12	31,63,87,91	0
33	STE	b	622	20/20	0.86	0.12	34,60,72,74	0
33	STE	B	620	17/20	0.86	0.12	33,52,69,70	0
33	STE	t	103	18/20	0.86	0.12	44,57,78,85	0
27	LMG	c	520	37/55	0.87	0.13	43,67,84,90	0
33	STE	c	521	20/20	0.87	0.10	37,59,72,75	0
27	LMG	A	411	48/55	0.87	0.11	35,56,78,89	0
30	DGD	A	415	66/66	0.87	0.11	42,64,85,88	0
33	STE	j	101	12/20	0.87	0.12	45,57,71,73	0
33	STE	b	624	16/20	0.87	0.12	42,62,79,80	0
33	STE	C	523	12/20	0.87	0.11	36,48,55,59	0
33	STE	t	102	14/20	0.87	0.11	34,50,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	PL9	A	410	55/55	0.87	0.13	32,65,86,92	0
26	PL9	a	409	55/55	0.88	0.13	34,68,87,99	0
27	LMG	c	523	49/55	0.88	0.11	36,57,92,106	0
33	STE	Z	101	8/20	0.88	0.14	37,55,66,66	0
29	SQD	A	414	39/54	0.88	0.13	40,64,96,106	0
33	STE	J	101	12/20	0.88	0.12	46,57,67,69	0
29	SQD	B	623	54/54	0.89	0.10	37,61,86,98	0
33	STE	C	522	16/20	0.89	0.12	34,51,75,83	0
27	LMG	C	520	48/55	0.89	0.11	41,67,88,95	0
33	STE	M	103	10/20	0.89	0.13	32,43,56,63	0
29	SQD	b	620	49/54	0.90	0.09	40,58,92,111	0
33	STE	D	412	20/20	0.90	0.10	34,52,73,77	0
29	SQD	f	102	41/54	0.90	0.13	52,83,112,115	0
33	STE	l	102	18/20	0.90	0.11	36,48,82,86	0
27	LMG	m	101	51/55	0.90	0.10	34,50,80,88	0
33	STE	d	411	17/20	0.90	0.12	39,56,68,71	0
24	BCR	C	514	40/40	0.90	0.10	39,54,67,68	0
33	STE	B	624	12/20	0.91	0.10	31,47,59,67	0
27	LMG	D	411	28/55	0.91	0.11	34,48,64,74	0
22	CLA	B	601	65/65	0.91	0.10	27,57,88,102	0
29	SQD	D	408	36/54	0.92	0.11	42,67,91,95	0
29	SQD	a	411	54/54	0.92	0.10	39,62,89,99	0
22	CLA	C	513	65/65	0.92	0.09	38,62,94,108	0
27	LMG	M	101	51/55	0.92	0.08	30,46,67,80	0
24	BCR	D	405	40/40	0.92	0.09	26,42,77,91	0
24	BCR	Y	101	40/40	0.92	0.09	32,48,64,68	0
24	BCR	d	406	40/40	0.92	0.10	35,52,96,100	0
24	BCR	x	101	40/40	0.92	0.09	34,49,67,71	0
30	DGD	h	101	62/66	0.93	0.09	32,46,57,68	0
24	BCR	c	514	40/40	0.93	0.09	44,57,70,72	0
24	BCR	H	101	40/40	0.93	0.08	28,44,58,65	0
24	BCR	k	101	40/40	0.93	0.09	34,57,72,73	0
30	DGD	H	102	62/66	0.93	0.08	26,43,57,60	0
24	BCR	c	516	40/40	0.94	0.09	35,48,63,67	0
24	BCR	C	515	40/40	0.94	0.08	26,39,52,64	0
22	CLA	c	512	65/65	0.94	0.09	37,54,91,108	0
22	CLA	c	513	65/65	0.94	0.10	41,66,110,114	0
24	BCR	B	618	40/40	0.94	0.07	24,36,49,50	0
24	BCR	b	617	40/40	0.94	0.07	28,40,50,53	0
24	BCR	b	618	40/40	0.94	0.06	27,38,52,52	0
27	LMG	d	410	44/55	0.94	0.09	30,49,84,89	0
33	STE	M	102	15/20	0.94	0.08	35,45,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	DGD	C	518	62/66	0.94	0.09	27,49,99,122	0
24	BCR	b	619	40/40	0.94	0.08	27,47,63,72	0
30	DGD	c	518	62/66	0.94	0.08	29,51,95,99	0
27	LMG	D	407	51/55	0.94	0.10	26,54,85,89	0
28	LHG	a	410	49/49	0.94	0.10	28,48,77,84	0
22	CLA	C	512	65/65	0.94	0.09	32,52,84,94	0
29	SQD	A	413	52/54	0.94	0.10	34,58,103,107	0
28	LHG	A	412	47/49	0.95	0.10	26,49,84,100	0
24	BCR	C	516	40/40	0.95	0.08	33,48,64,65	0
22	CLA	c	511	65/65	0.95	0.09	30,50,70,75	0
28	LHG	d	409	39/49	0.95	0.09	30,45,75,83	0
22	CLA	C	511	65/65	0.95	0.08	27,48,66,69	0
24	BCR	T	101	40/40	0.95	0.06	23,36,52,54	0
22	CLA	C	506	65/65	0.95	0.09	26,41,85,102	0
24	BCR	a	405	40/40	0.95	0.06	23,33,43,46	0
22	CLA	d	405	65/65	0.95	0.08	26,48,89,100	0
23	PHO	d	402	64/64	0.95	0.06	25,35,45,52	0
24	BCR	A	407	40/40	0.95	0.06	19,33,41,42	0
24	BCR	B	617	40/40	0.95	0.07	25,38,57,65	0
24	BCR	c	515	40/40	0.95	0.07	28,41,58,63	0
22	CLA	b	606	65/65	0.95	0.08	26,39,76,82	0
30	DGD	C	517	62/66	0.95	0.09	22,42,80,92	0
24	BCR	B	619	40/40	0.95	0.06	24,41,59,71	0
22	CLA	b	609	65/65	0.95	0.07	28,42,65,68	0
22	CLA	c	509	65/65	0.95	0.08	32,45,61,69	0
22	CLA	B	616	60/65	0.96	0.08	23,36,91,109	0
22	CLA	b	610	65/65	0.96	0.07	22,35,51,53	0
22	CLA	b	612	65/65	0.96	0.07	20,33,47,54	0
30	DGD	C	519	62/66	0.96	0.08	24,47,77,91	0
22	CLA	b	614	65/65	0.96	0.07	23,37,75,82	0
30	DGD	c	517	62/66	0.96	0.07	20,42,74,76	0
22	CLA	b	615	65/65	0.96	0.07	26,38,61,66	0
30	DGD	c	519	62/66	0.96	0.09	26,52,87,92	0
22	CLA	b	616	60/65	0.96	0.07	26,40,82,91	0
22	CLA	c	501	65/65	0.96	0.07	28,38,50,55	0
22	CLA	c	502	65/65	0.96	0.06	28,39,58,65	0
24	BCR	t	101	40/40	0.96	0.06	24,36,51,57	0
22	CLA	c	503	65/65	0.96	0.06	27,42,53,57	0
22	CLA	c	504	60/65	0.96	0.08	29,44,81,89	0
26	PL9	D	406	55/55	0.96	0.06	18,33,46,50	0
22	CLA	c	505	65/65	0.96	0.07	23,40,71,74	0
26	PL9	d	407	55/55	0.96	0.06	18,34,43,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	c	506	65/65	0.96	0.08	29,45,94,103	0
22	CLA	c	507	65/65	0.96	0.07	26,42,60,70	0
22	CLA	c	508	64/65	0.96	0.08	28,42,82,101	0
22	CLA	C	501	65/65	0.96	0.06	21,35,47,53	0
22	CLA	c	510	65/65	0.96	0.07	26,45,59,77	0
22	CLA	C	502	65/65	0.96	0.06	25,39,52,58	0
22	CLA	C	503	65/65	0.96	0.06	26,39,47,50	0
22	CLA	C	504	59/65	0.96	0.07	27,40,82,87	0
22	CLA	d	401	65/65	0.96	0.08	24,37,86,97	0
22	CLA	d	404	65/65	0.96	0.06	19,28,45,54	0
22	CLA	C	505	65/65	0.96	0.08	23,38,71,87	0
23	PHO	A	405	64/64	0.96	0.05	21,30,38,40	0
23	PHO	a	403	64/64	0.96	0.05	19,29,37,48	0
22	CLA	B	605	65/65	0.96	0.06	20,31,46,48	0
28	LHG	B	622	49/49	0.96	0.07	29,43,69,78	0
22	CLA	C	507	65/65	0.96	0.07	24,39,57,59	0
22	CLA	C	508	65/65	0.96	0.07	24,38,99,119	0
22	CLA	C	509	65/65	0.96	0.07	25,42,62,65	0
22	CLA	C	510	65/65	0.96	0.07	26,42,63,69	0
22	CLA	B	606	65/65	0.96	0.07	20,34,67,72	0
22	CLA	B	609	65/65	0.96	0.07	24,36,56,65	0
22	CLA	B	610	65/65	0.96	0.07	20,32,40,47	0
22	CLA	a	404	65/65	0.96	0.08	19,35,84,101	0
22	CLA	B	614	65/65	0.96	0.08	19,37,81,90	0
22	CLA	b	605	65/65	0.96	0.06	20,34,50,55	0
22	CLA	B	615	65/65	0.96	0.07	24,35,63,75	0
22	CLA	b	608	65/65	0.96	0.07	23,41,63,71	0
34	BCT	a	408	4/4	0.96	0.09	27,33,39,46	0
22	CLA	D	404	65/65	0.97	0.07	22,43,109,119	0
22	CLA	a	402	65/65	0.97	0.05	17,28,49,59	0
22	CLA	B	603	65/65	0.97	0.06	18,31,65,69	0
22	CLA	B	611	65/65	0.97	0.05	19,30,46,51	0
22	CLA	b	602	65/65	0.97	0.07	25,40,64,71	0
22	CLA	b	603	65/65	0.97	0.06	21,35,71,79	0
22	CLA	b	604	65/65	0.97	0.07	17,37,86,98	0
22	CLA	B	612	65/65	0.97	0.06	17,31,49,54	0
22	CLA	B	613	65/65	0.97	0.06	17,31,70,80	0
22	CLA	b	607	65/65	0.97	0.07	19,35,69,74	0
22	CLA	B	604	65/65	0.97	0.07	20,32,74,85	0
22	CLA	A	403	65/65	0.97	0.07	22,33,88,98	0
22	CLA	A	402	65/65	0.97	0.06	16,26,45,55	0
22	CLA	d	403	65/65	0.97	0.06	18,31,53,65	0

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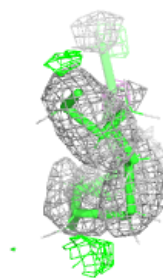
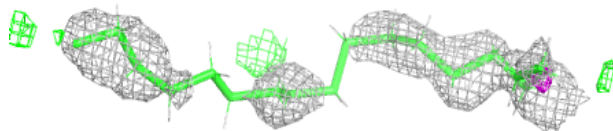
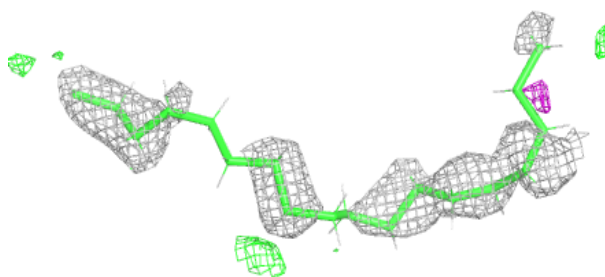
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	CLA	b	611	65/65	0.97	0.06	21,32,55,60	0
22	CLA	B	607	65/65	0.97	0.07	16,31,62,74	0
28	LHG	B	621	49/49	0.97	0.07	25,39,58,66	0
23	PHO	A	404	64/64	0.97	0.05	17,27,36,43	0
28	LHG	D	409	49/49	0.97	0.06	22,39,51,55	0
22	CLA	b	613	65/65	0.97	0.06	16,33,71,82	0
22	CLA	B	608	65/65	0.97	0.06	17,32,54,58	0
28	LHG	d	408	49/49	0.97	0.06	25,40,51,57	0
22	CLA	B	602	65/65	0.97	0.06	22,35,55,61	0
22	CLA	D	402	65/65	0.97	0.06	15,28,52,62	0
28	LHG	l	101	49/49	0.97	0.06	27,42,52,59	0
34	BCT	D	401	4/4	0.97	0.06	29,31,31,37	0
22	CLA	D	403	65/65	0.97	0.05	18,27,44,55	0
35	HEC	F	101	43/43	0.97	0.08	31,45,59,61	0
35	HEC	f	101	43/43	0.97	0.08	36,52,70,71	0
22	CLA	A	406	54/65	0.98	0.05	17,32,63,66	0
35	HEC	v	201	43/43	0.98	0.06	25,36,44,46	0
21	FE2	a	401	1/1	0.99	0.02	29,29,29,29	0
25	CL	A	408	1/1	0.99	0.03	28,28,28,28	0
25	CL	A	409	1/1	0.99	0.04	27,27,27,27	0
25	CL	a	406	1/1	0.99	0.03	26,26,26,26	0
31	OEX	A	416[A]	10/10	0.99	0.03	28,31,34,36	10
31	OEX	a	417[A]	10/10	0.99	0.03	25,31,35,35	10
35	HEC	V	201	43/43	0.99	0.05	22,31,40,41	0
32	OEY	A	417[B]	11/11	0.99	0.03	18,21,25,25	11
32	OEY	a	418[B]	11/11	0.99	0.03	16,21,24,25	11
25	CL	a	407	1/1	1.00	0.04	26,26,26,26	0
21	FE2	A	401	1/1	1.00	0.04	29,29,29,29	0

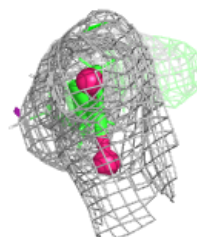
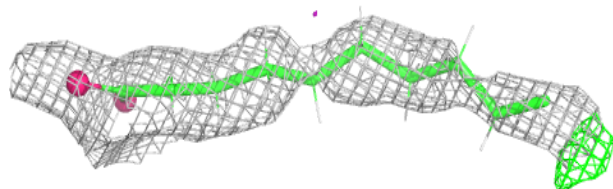
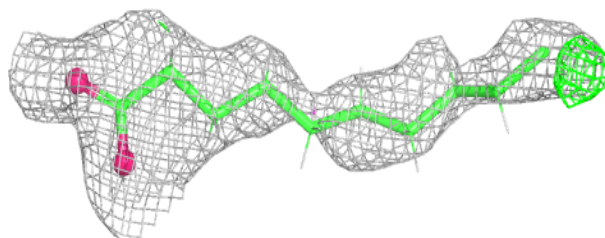
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE H 103:

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

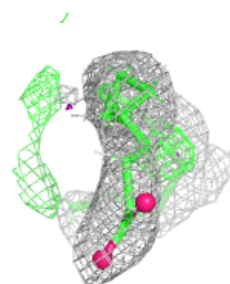
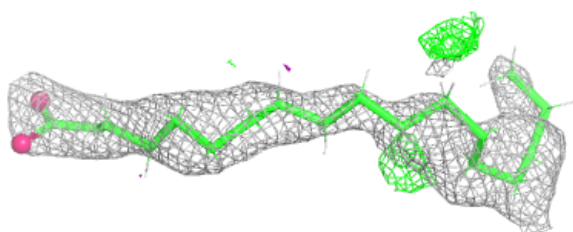
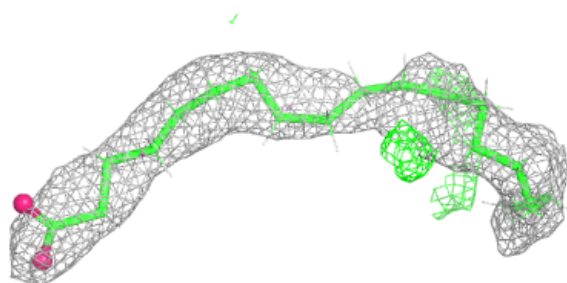
**Electron density around STE a 414:**

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

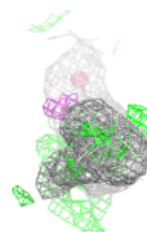
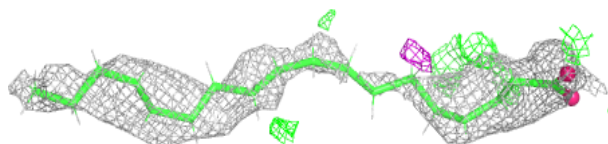
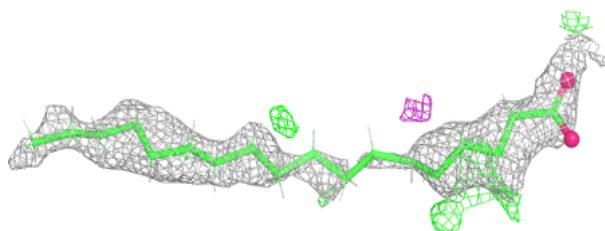


Electron density around STE d 413:

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

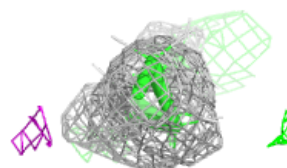
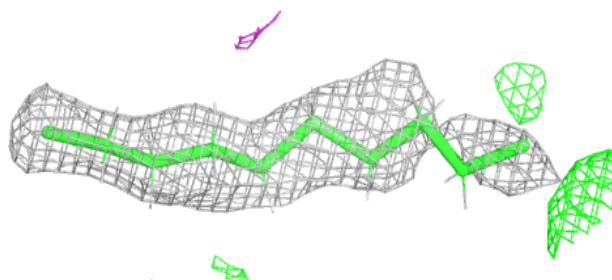
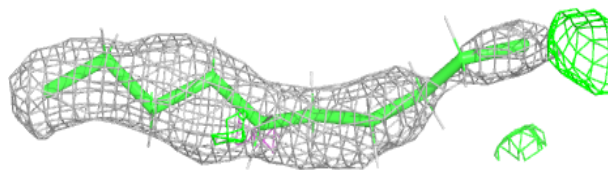
**Electron density around STE b 625:**

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

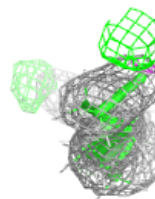
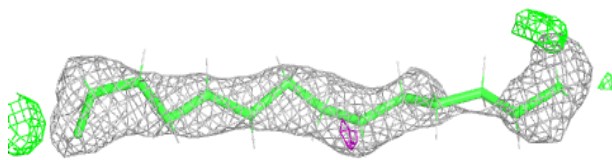
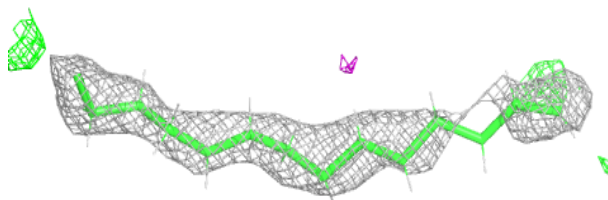


Electron density around STE a 413:

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

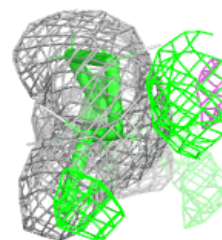
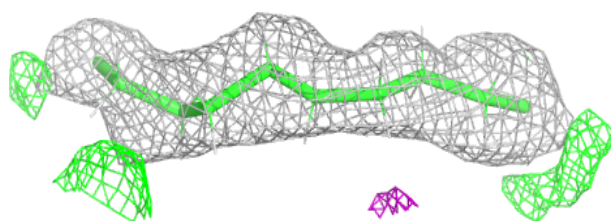
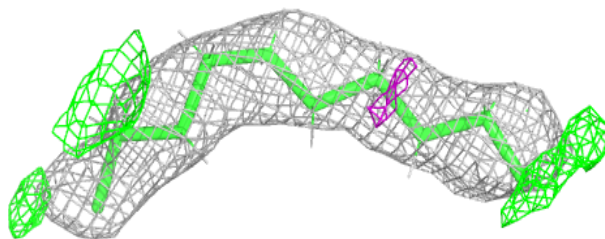
**Electron density around STE b 627:**

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

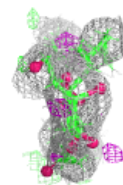
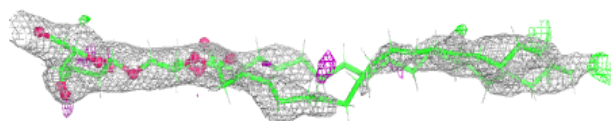
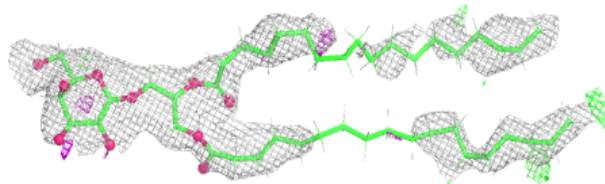


Electron density around STE b 626:

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

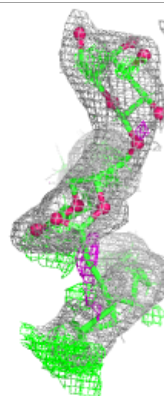
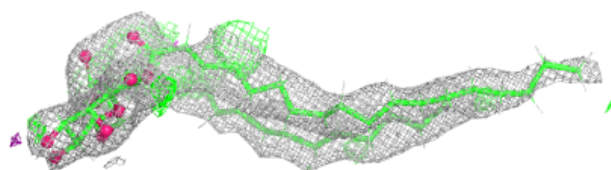
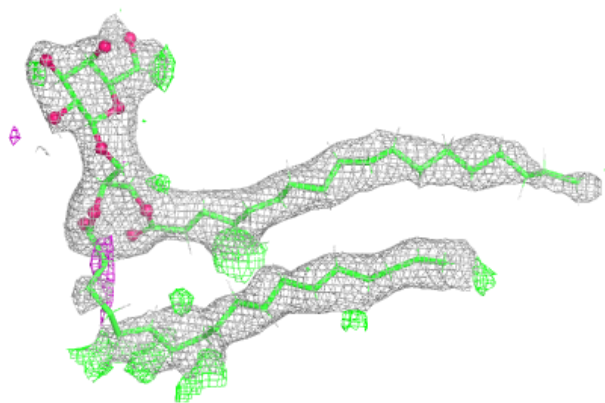
**Electron density around LMG b 623:**

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

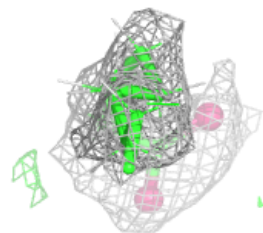
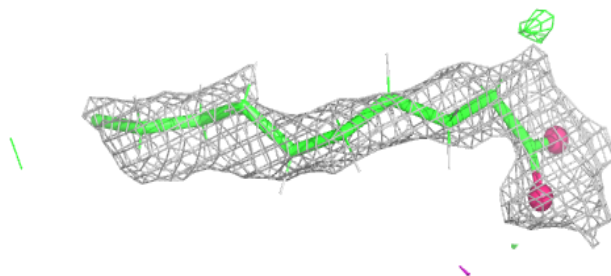
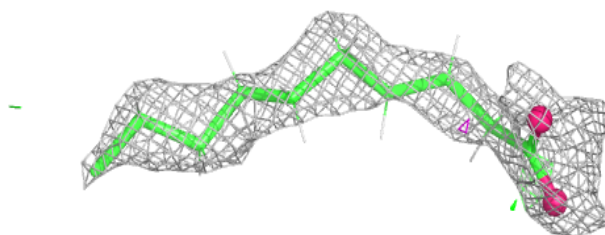


Electron density around LMG a 416:

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

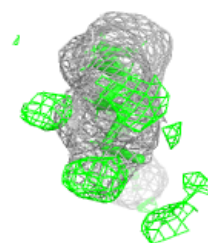
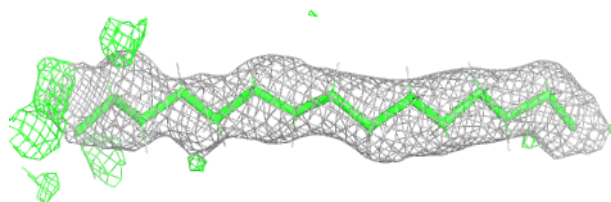
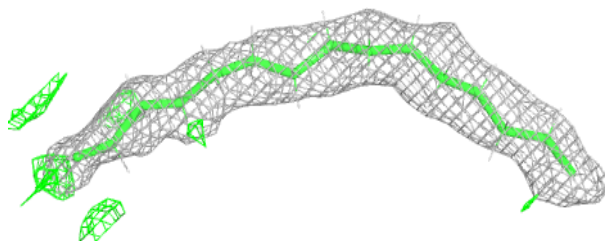
**Electron density around STE R 101:**

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



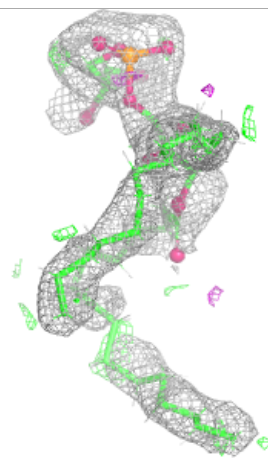
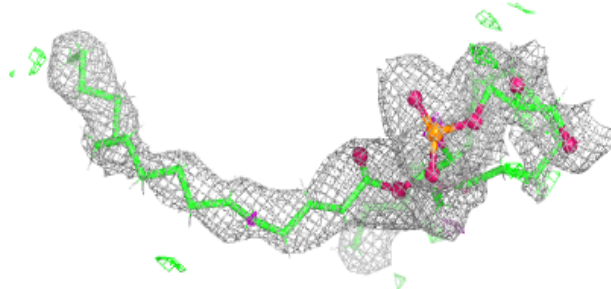
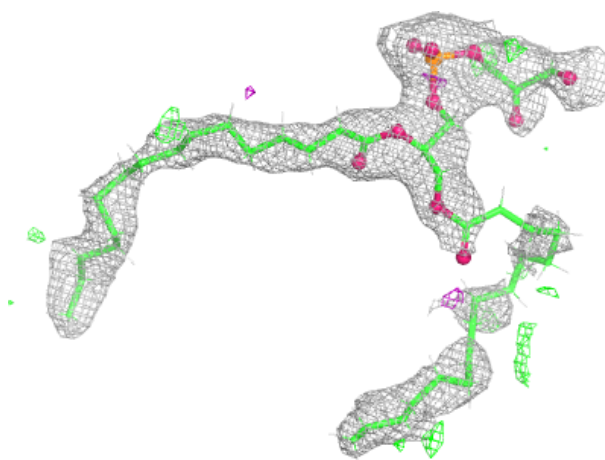
Electron density around STE I 101:

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



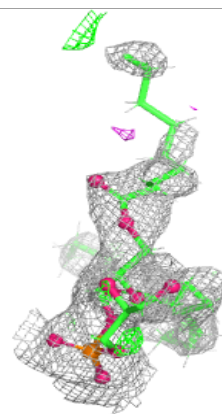
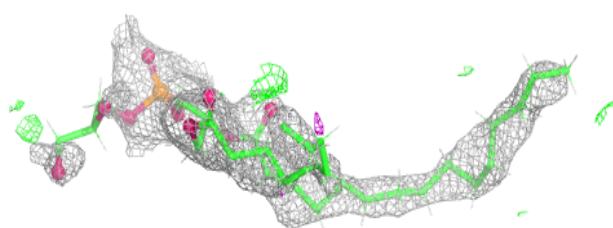
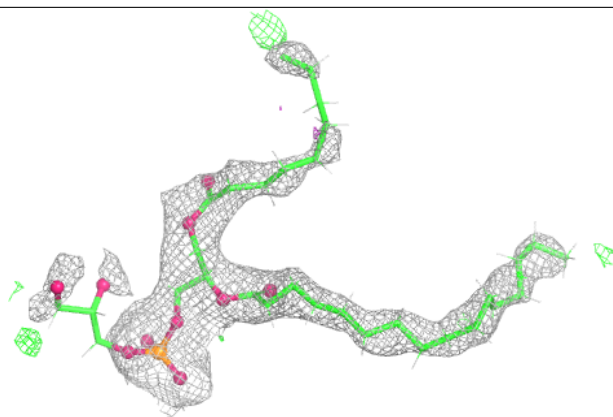
Electron density around LHG E 101:

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

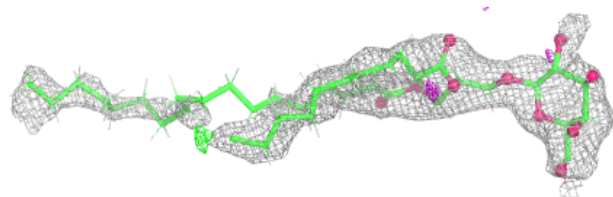
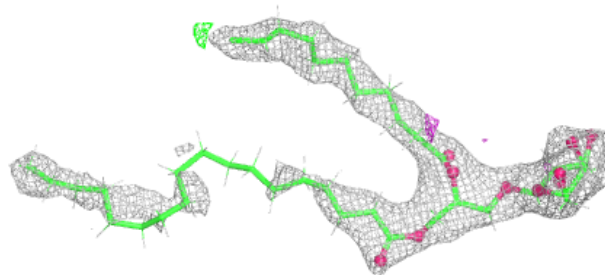


Electron density around LHG e 101:

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

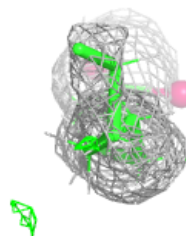
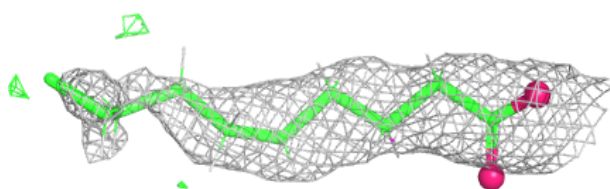
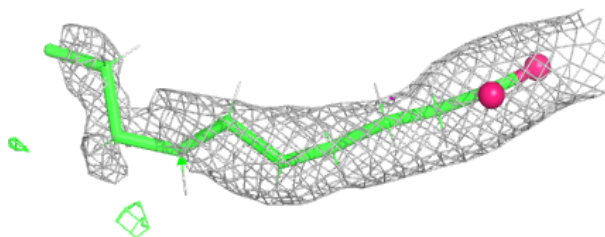
**Electron density around LMG c 522:**

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

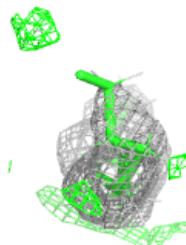
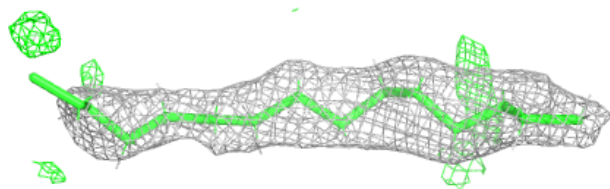
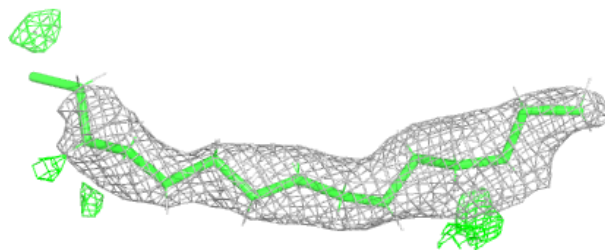


Electron density around STE m 102:

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

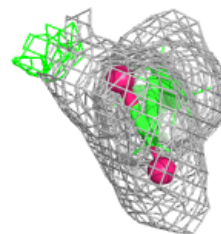
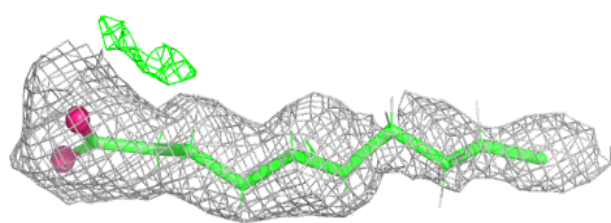
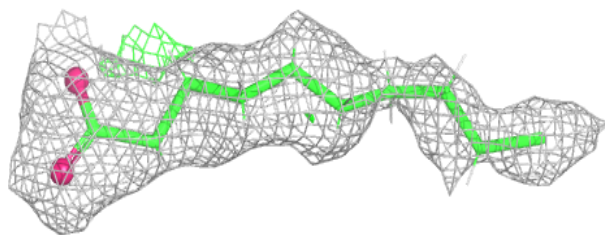
**Electron density around STE T 102:**

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

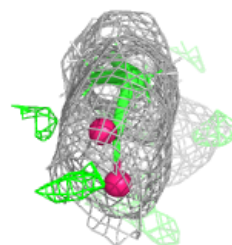
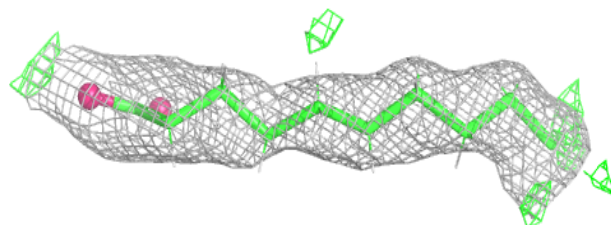
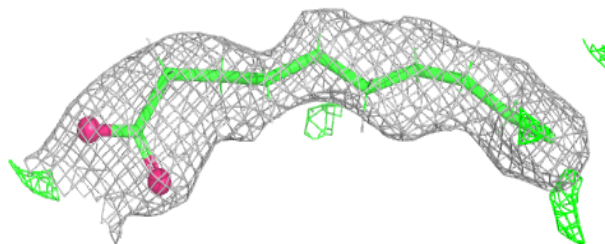


Electron density around STE k 102:

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and green (positive)

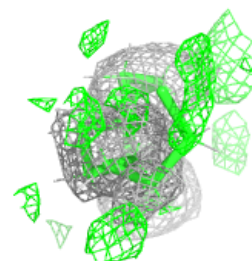
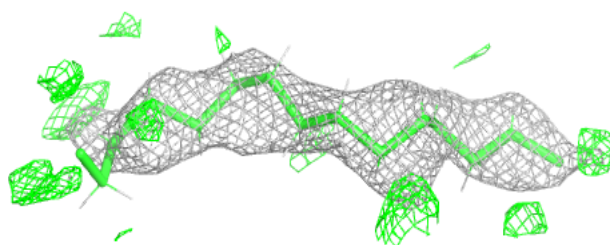
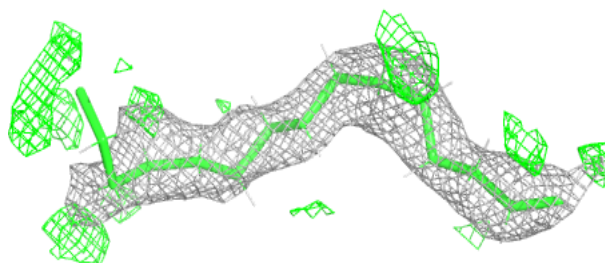
**Electron density around STE C 521:**

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

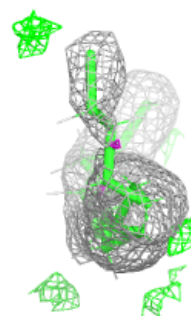
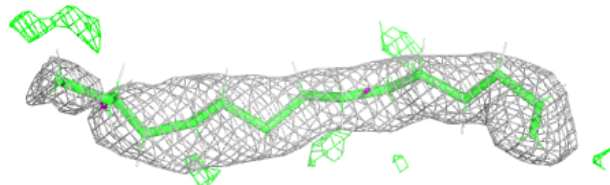
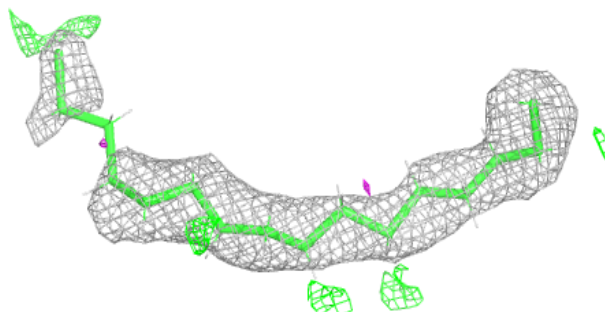


Electron density around STE a 415:

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and green (positive)

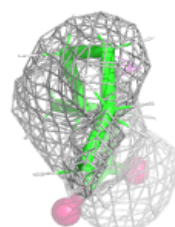
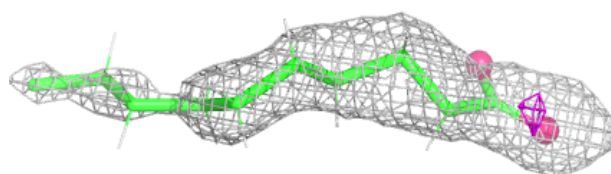
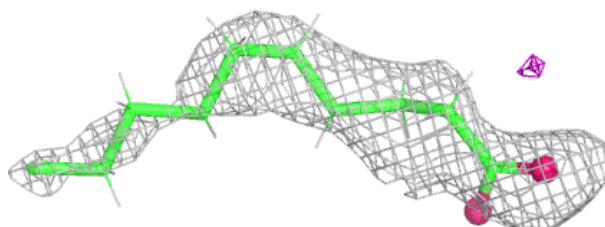
**Electron density around STE b 621:**

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and green (positive)

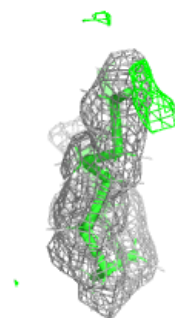
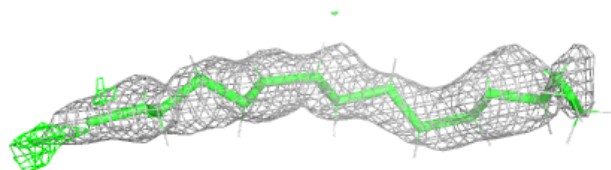
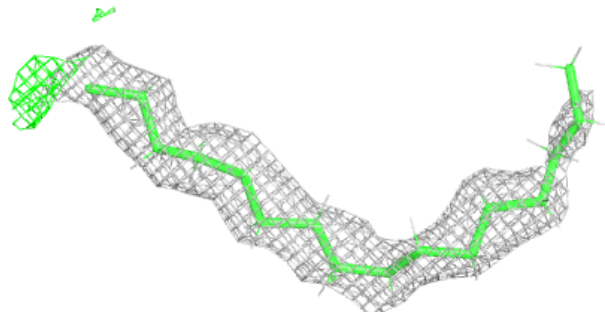


Electron density around STE B 626:

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and green (positive)

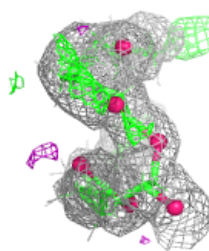
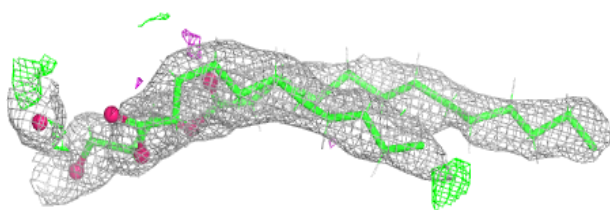
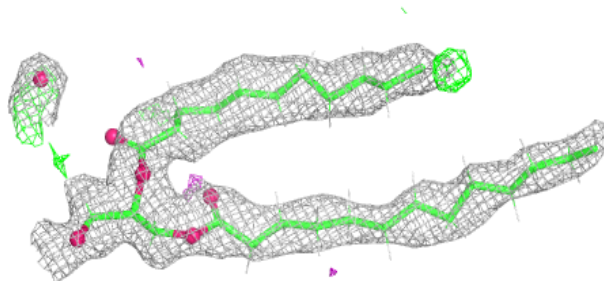
**Electron density around STE B 625:**

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and green (positive)

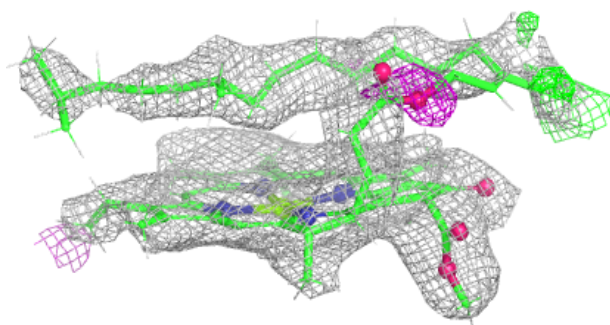
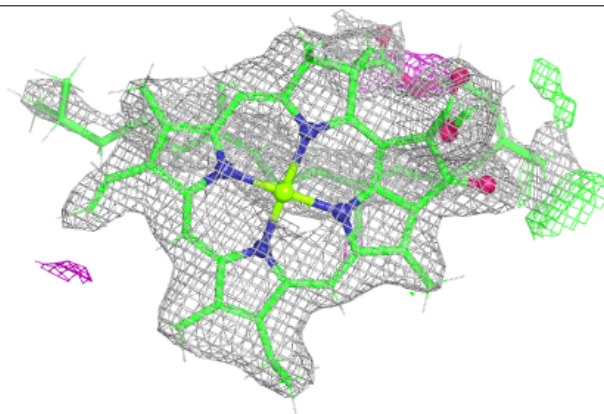


Electron density around LMG D 410:

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

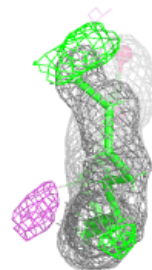
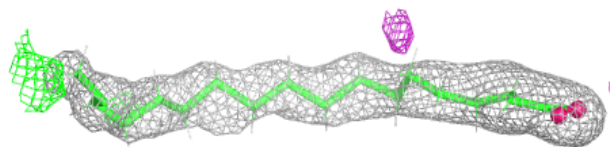
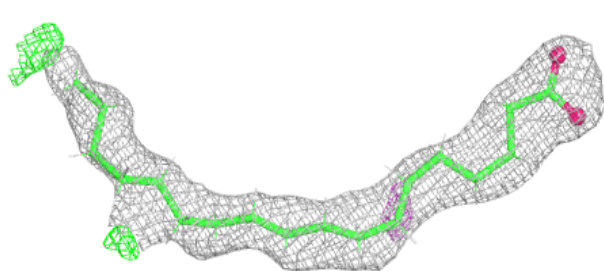
**Electron density around CLA b 601:**

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



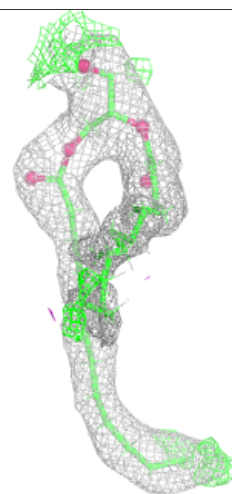
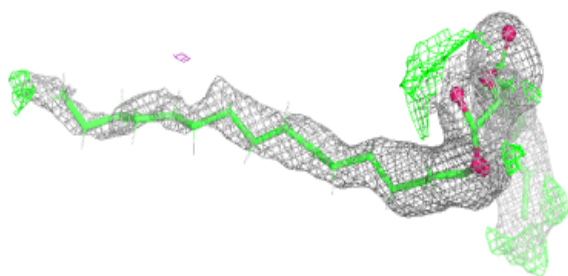
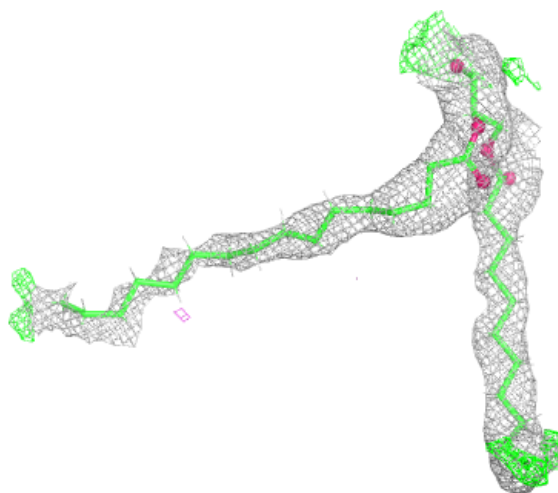
Electron density around STE d 412:

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



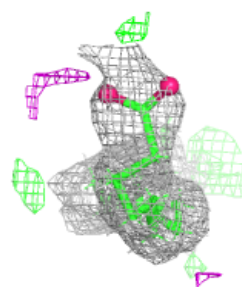
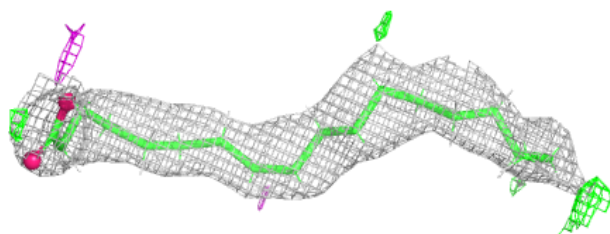
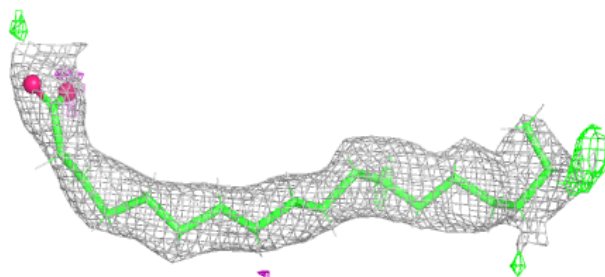
Electron density around SQD a 412:

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

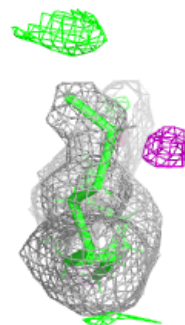
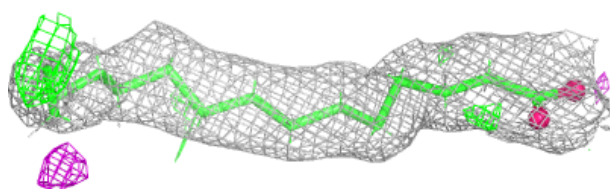
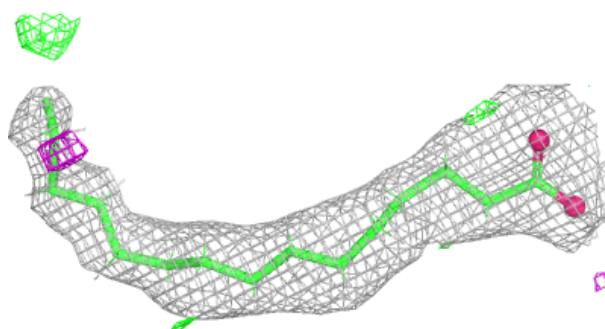


Electron density around STE b 622:

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

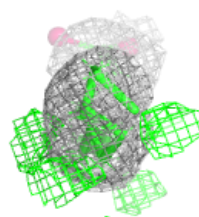
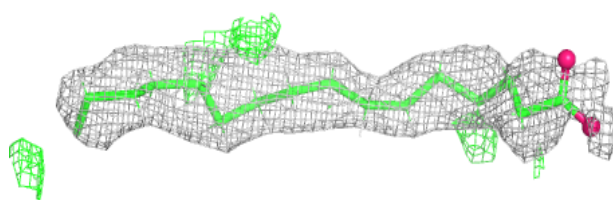
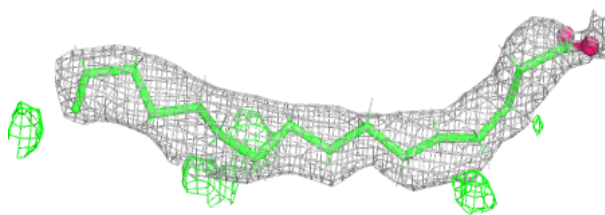
**Electron density around STE B 620:**

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

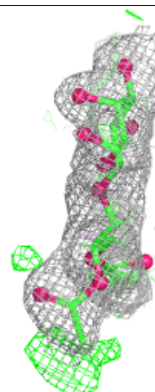
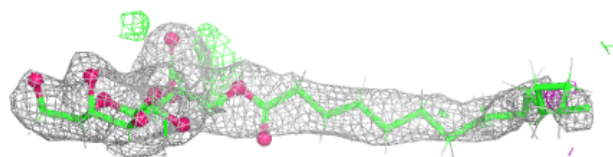
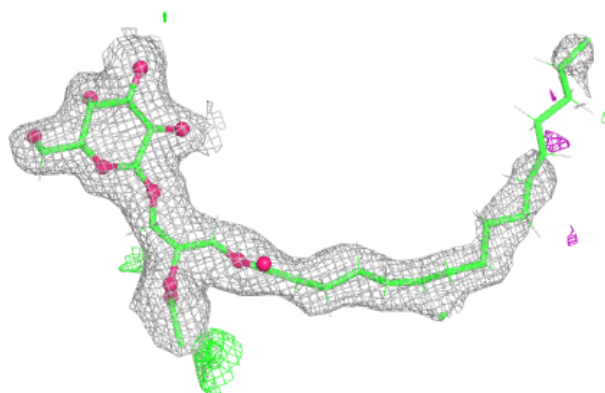


Electron density around STE t 103:

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

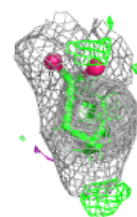
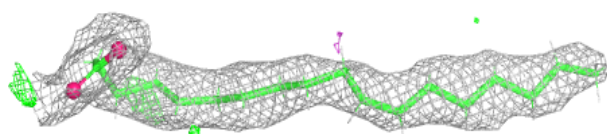
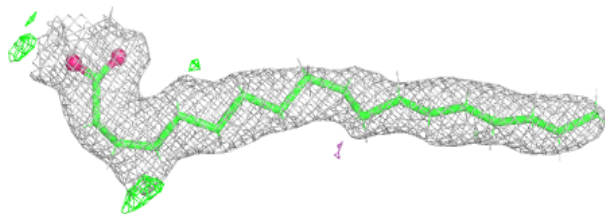
**Electron density around LMG c 520:**

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

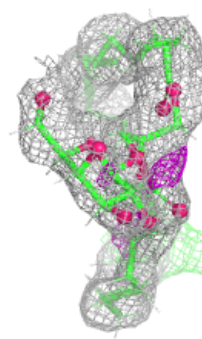
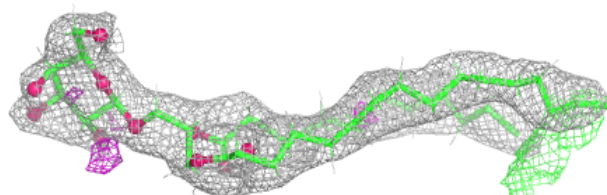
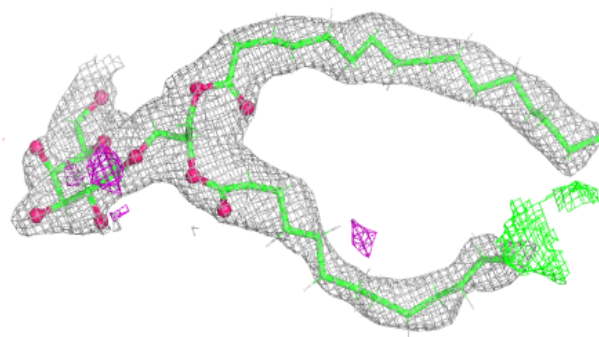


Electron density around STE c 521:

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

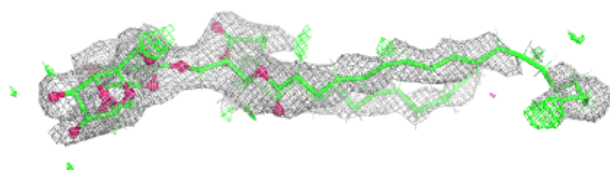
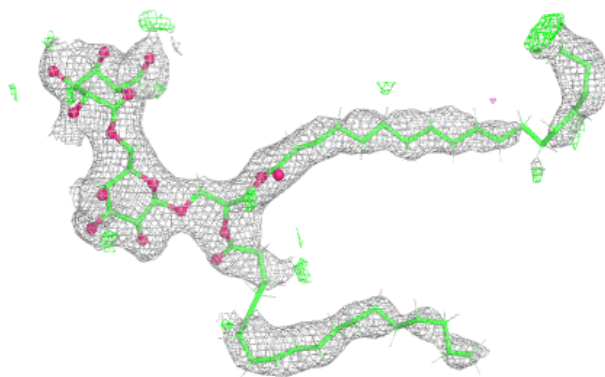
**Electron density around LMG A 411:**

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

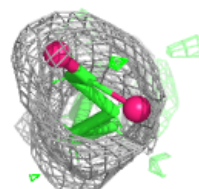
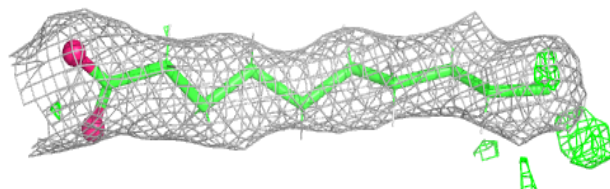
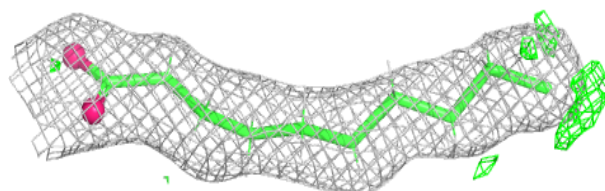


Electron density around DGD A 415:

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

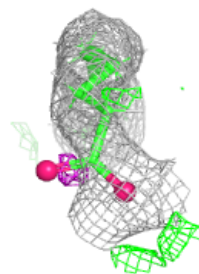
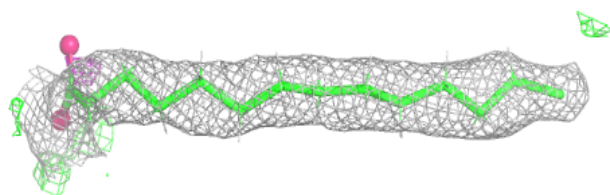
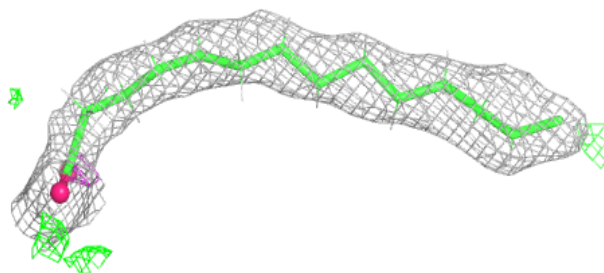
**Electron density around STE j 101:**

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

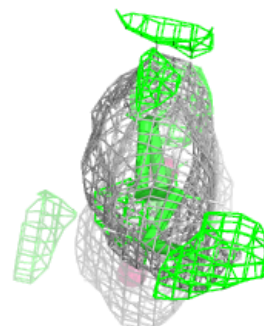
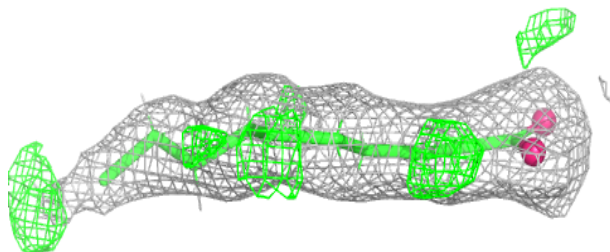
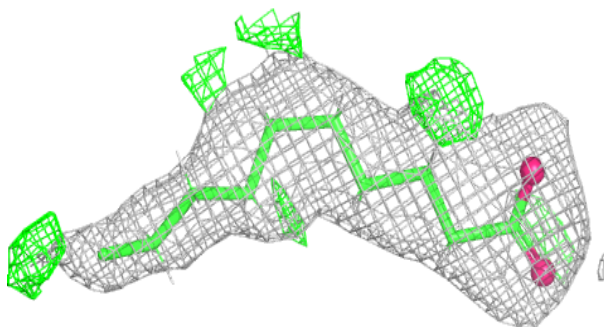


Electron density around STE b 624:

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

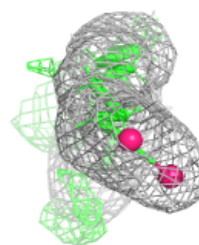
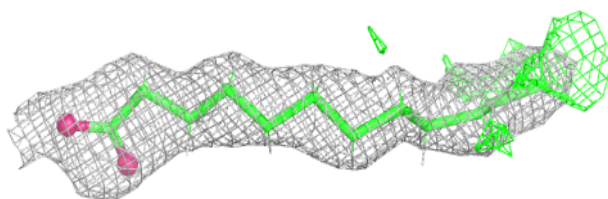
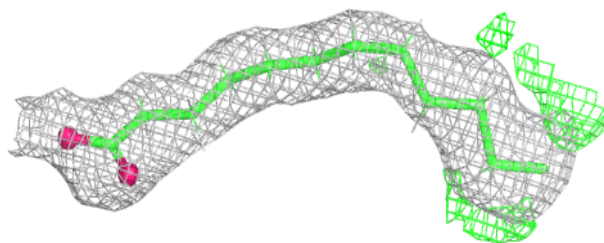
**Electron density around STE C 523:**

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

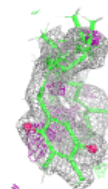
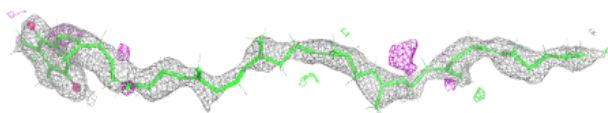
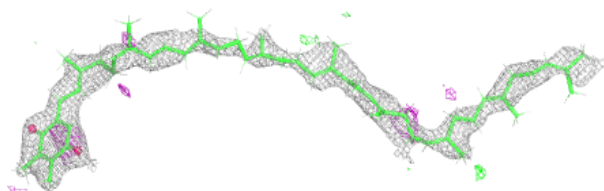


Electron density around STE t 102:

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

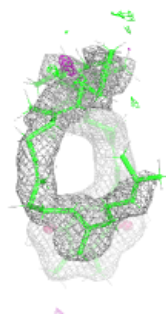
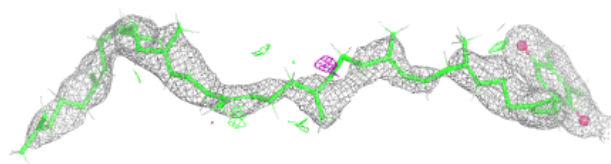
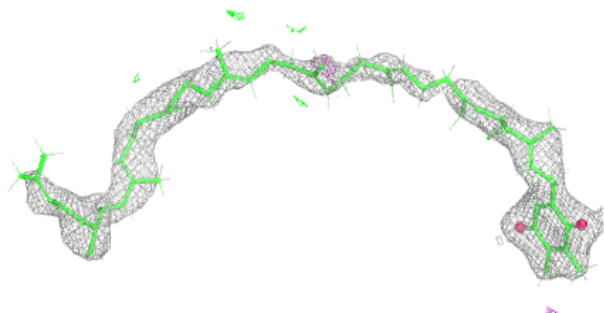
**Electron density around PL9 A 410:**

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

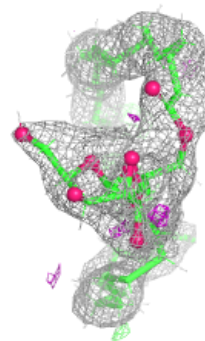
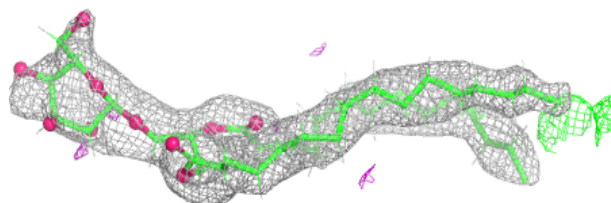
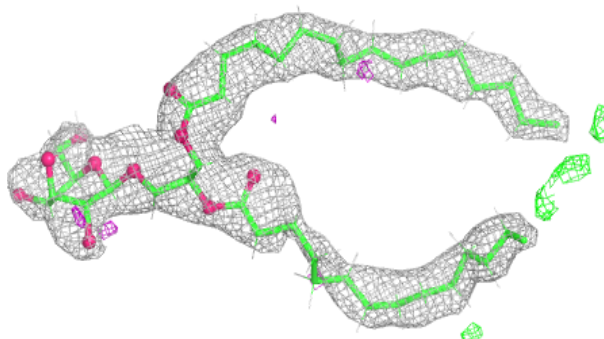


Electron density around PL9 a 409:

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

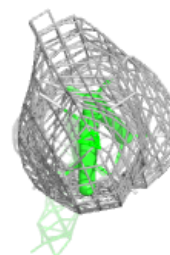
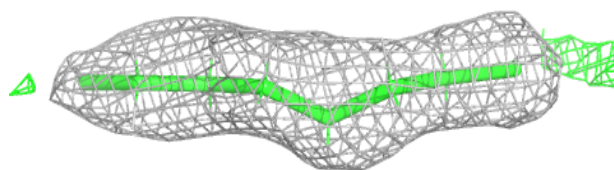
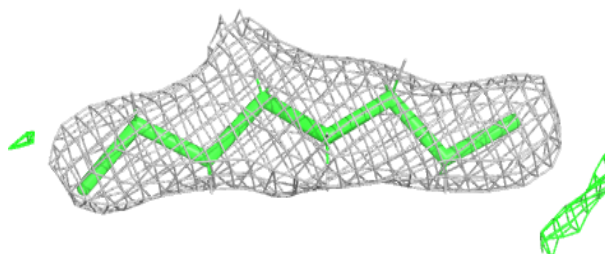
**Electron density around LMG c 523:**

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

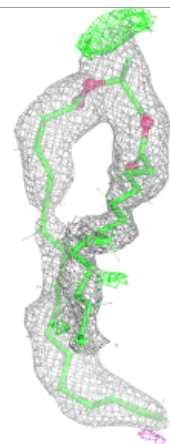
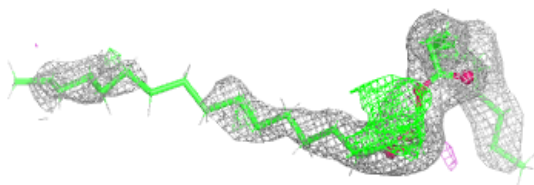
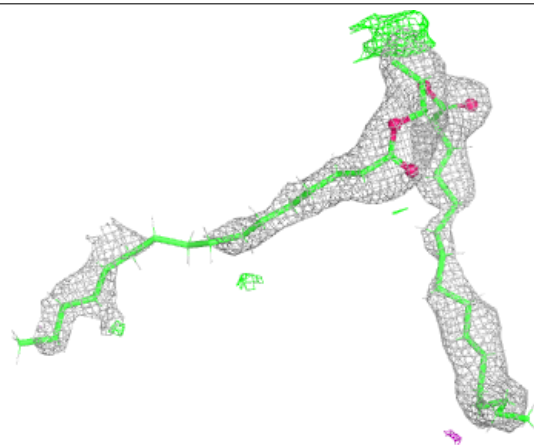


Electron density around STE Z 101:

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

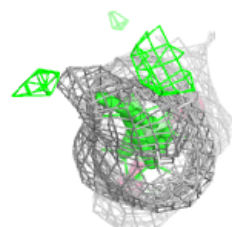
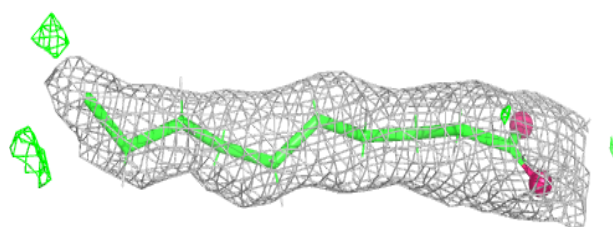
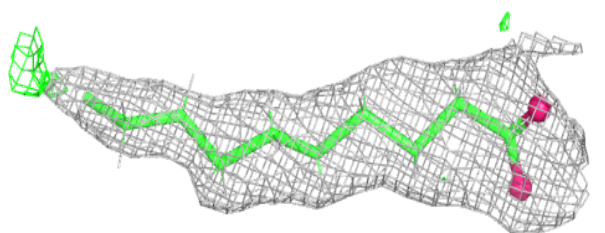
**Electron density around SQD A 414:**

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

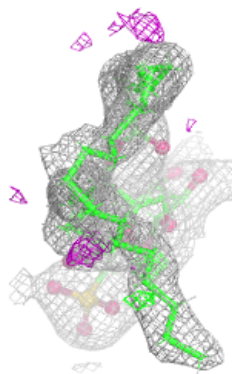
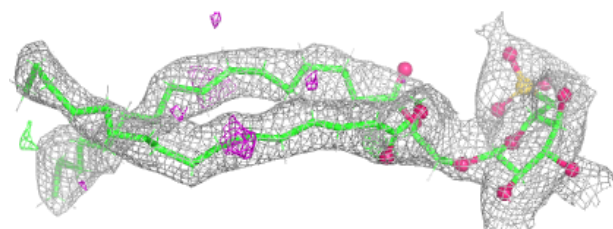
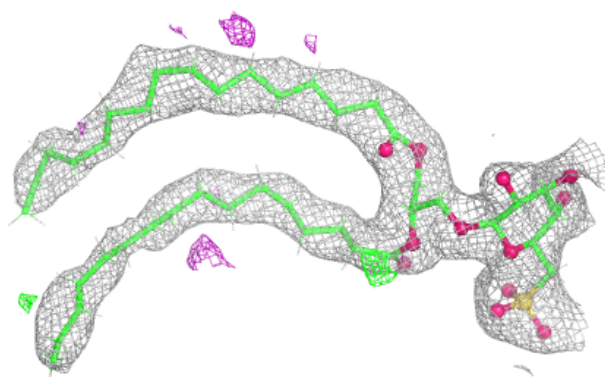


Electron density around STE J 101:

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

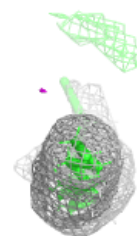
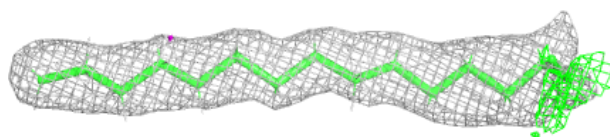
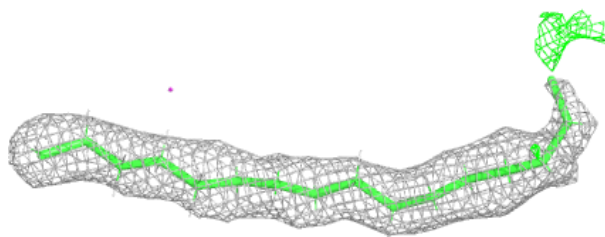
**Electron density around SQD B 623:**

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

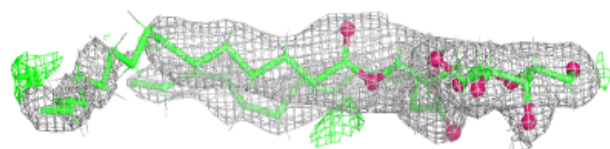
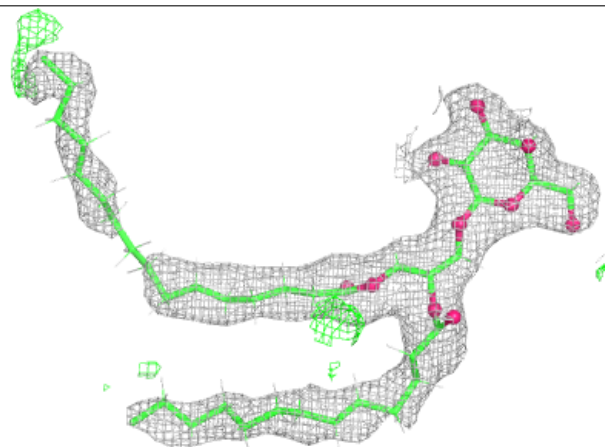


Electron density around STE C 522:

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

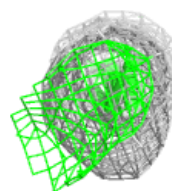
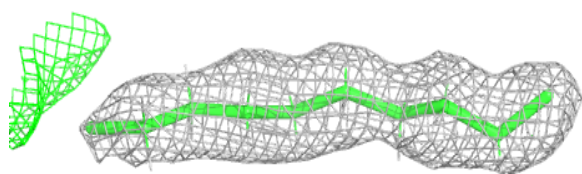
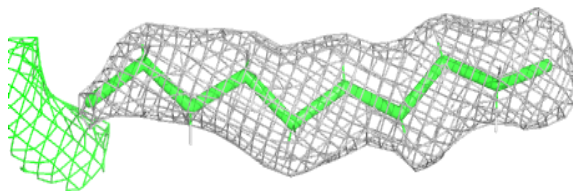
**Electron density around LMG C 520:**

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

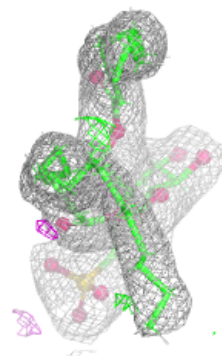
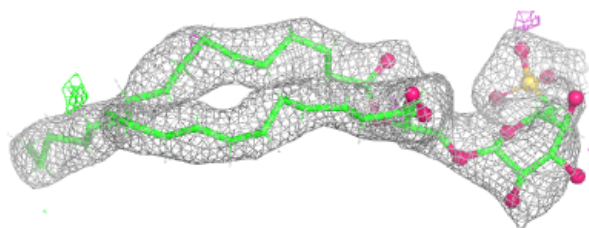
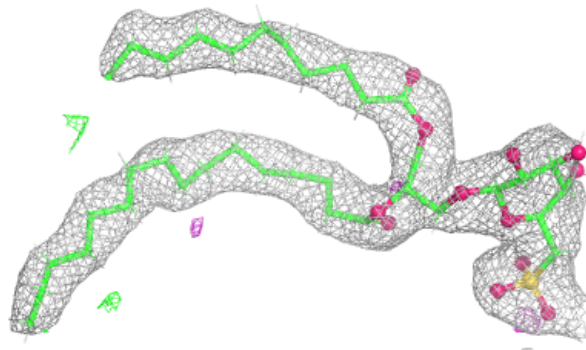


Electron density around STE M 103:

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

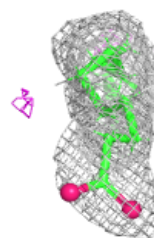
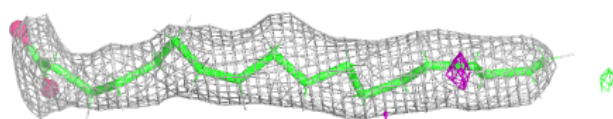
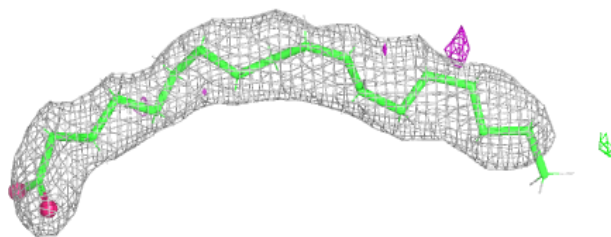
**Electron density around SQD b 620:**

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

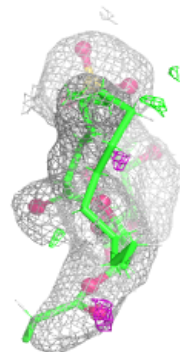
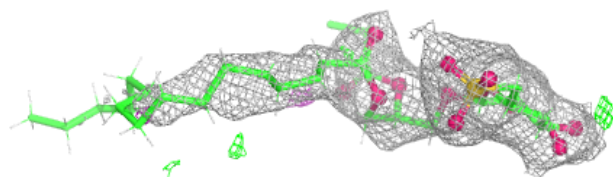
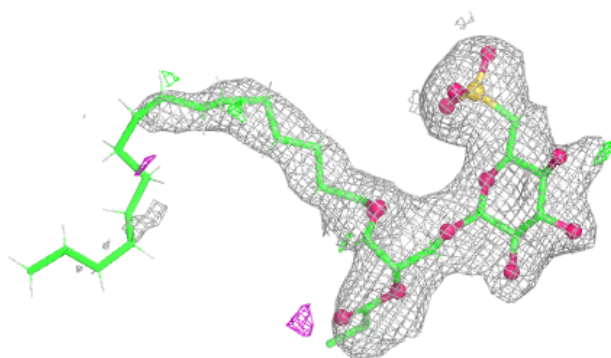


Electron density around STE D 412:

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

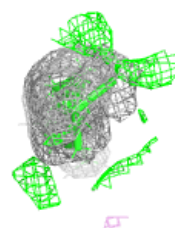
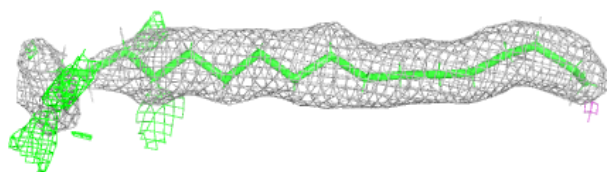
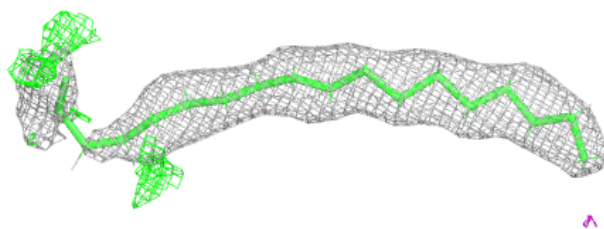
**Electron density around SQD f 102:**

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

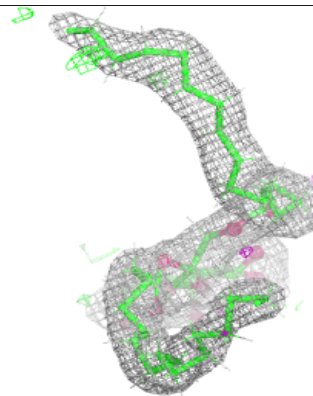
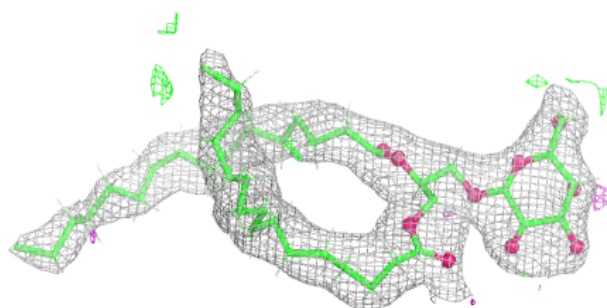
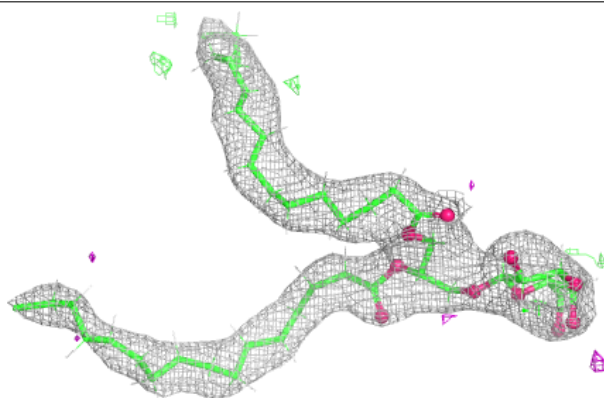


Electron density around STE 1 102:

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

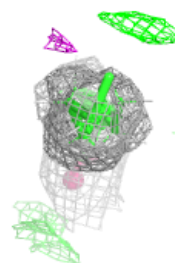
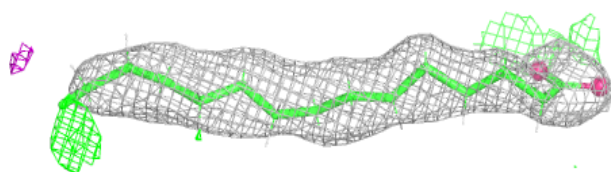
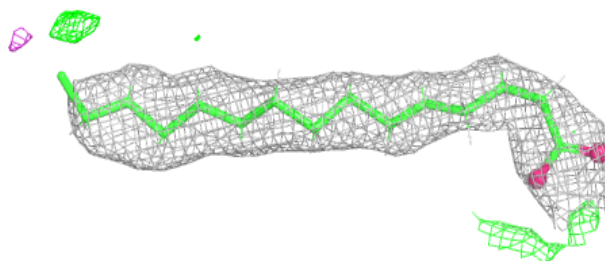
**Electron density around LMG m 101:**

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

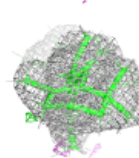
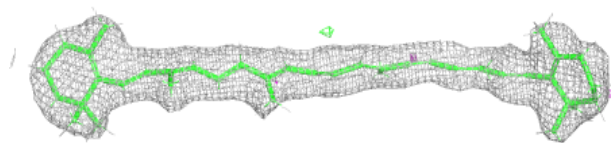
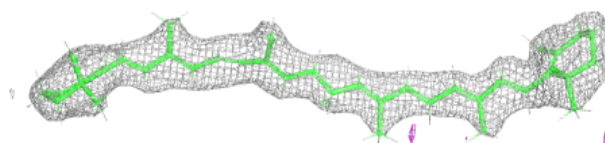


Electron density around STE d 411:

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

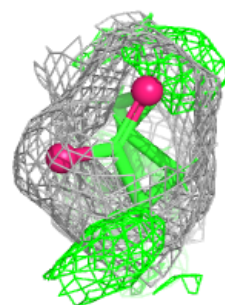
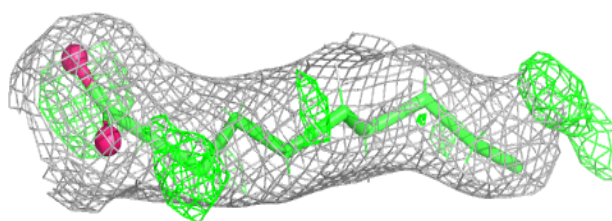
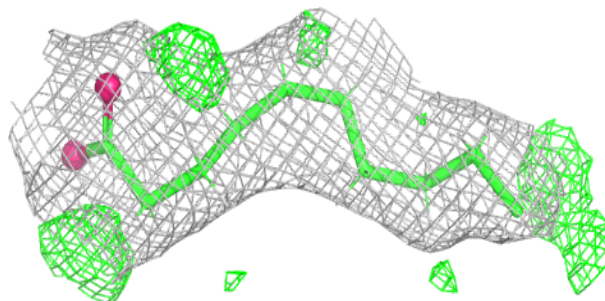
**Electron density around BCR C 514:**

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

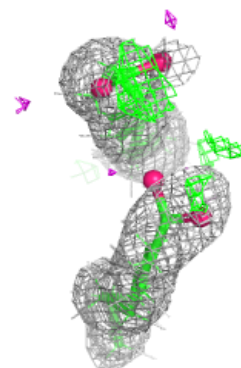
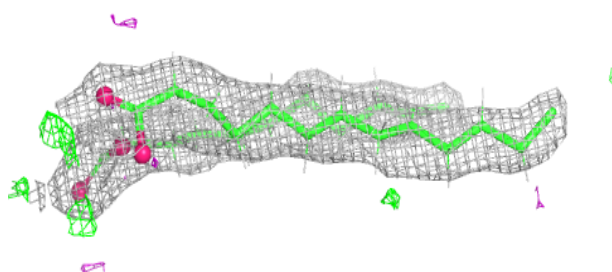
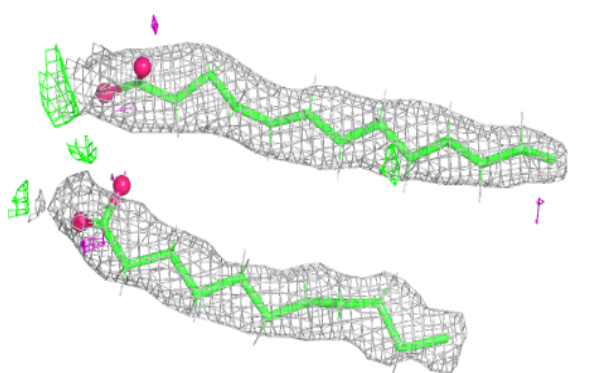


Electron density around STE B 624:

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

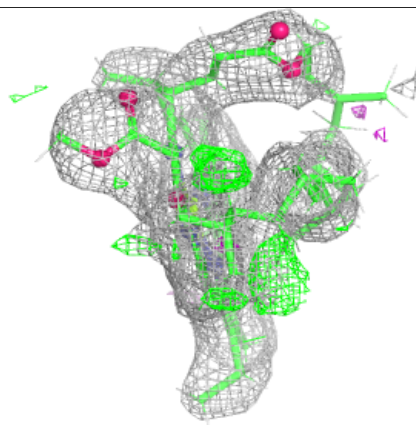
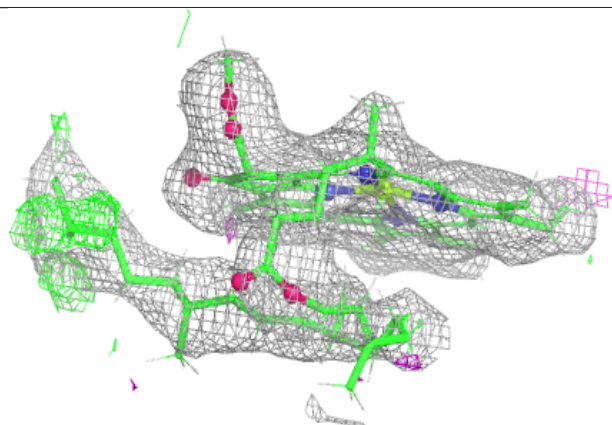
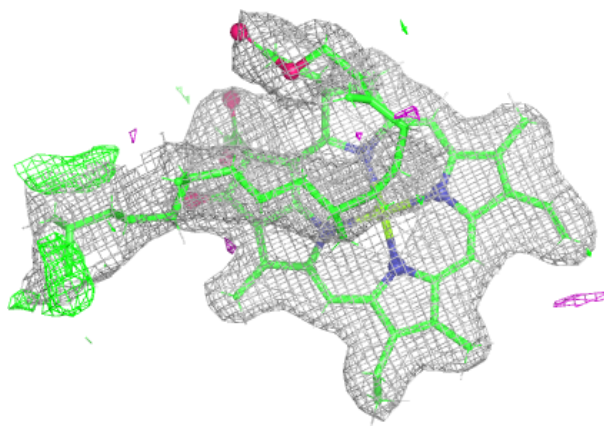
**Electron density around LMG D 411:**

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

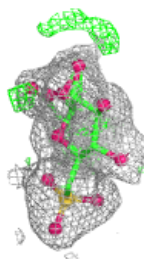
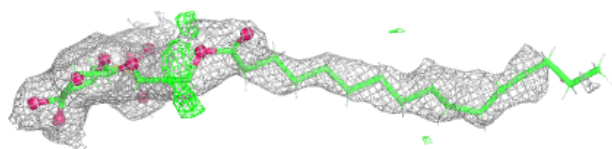
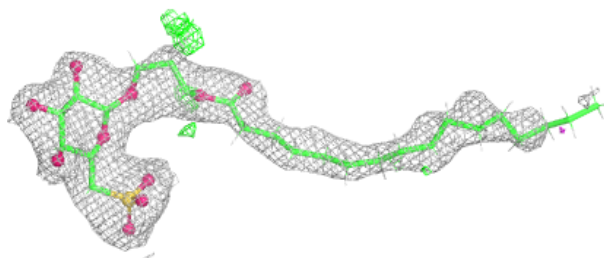


Electron density around CLA B 601:

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

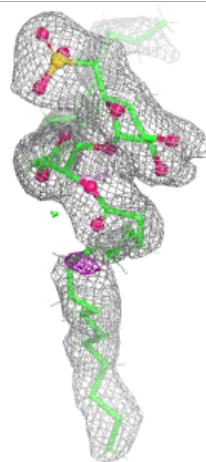
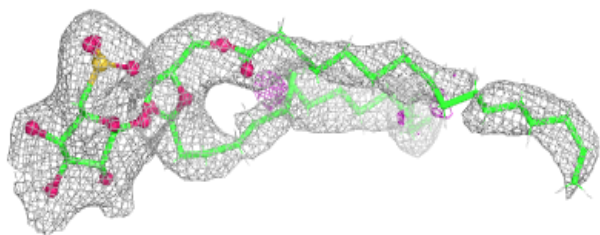
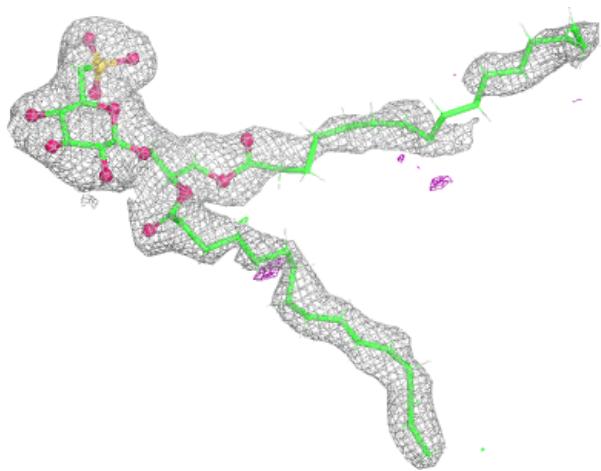
**Electron density around SQD D 408:**

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



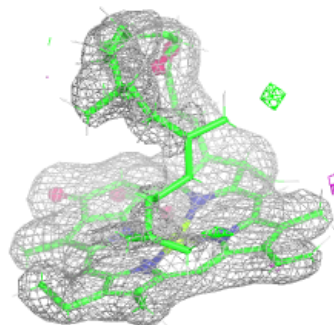
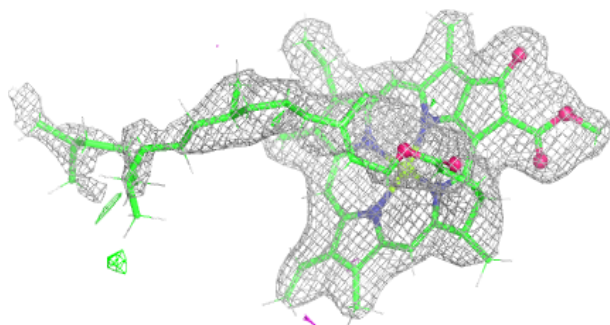
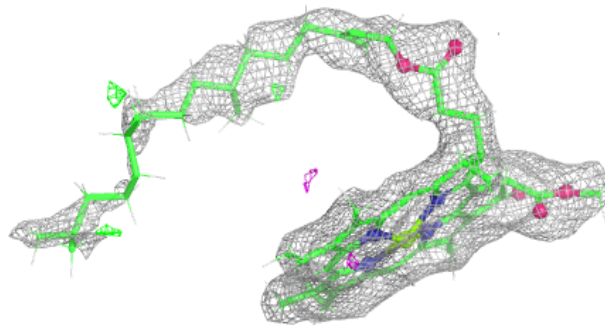
Electron density around SQD a 411:

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

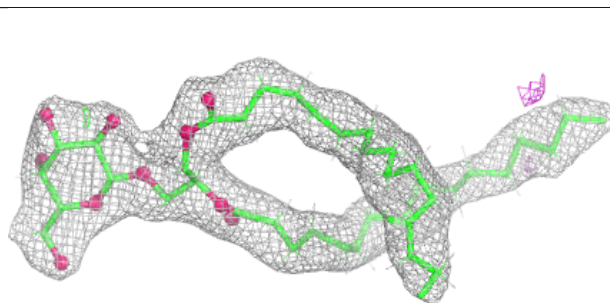
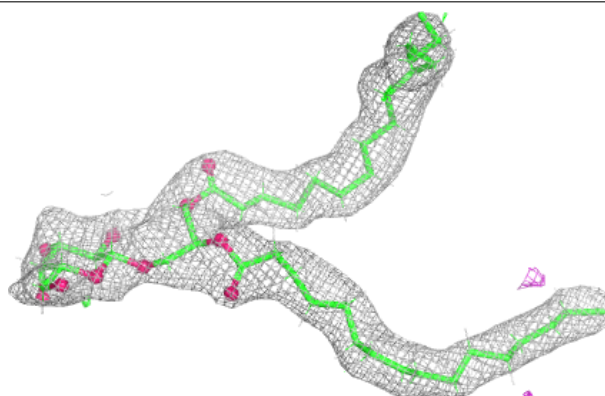


Electron density around CLA C 513:

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

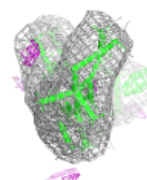
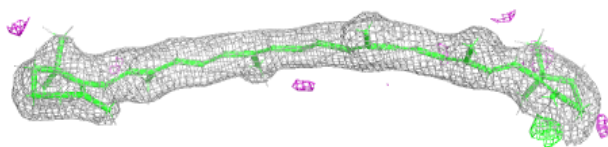
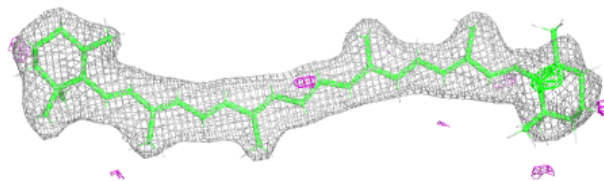
**Electron density around LMG M 101:**

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

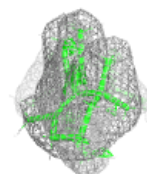
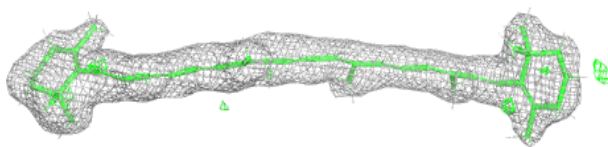


Electron density around BCR D 405:

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

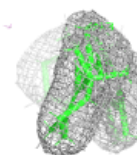
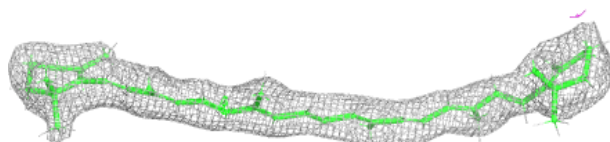
**Electron density around BCR Y 101:**

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

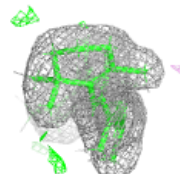
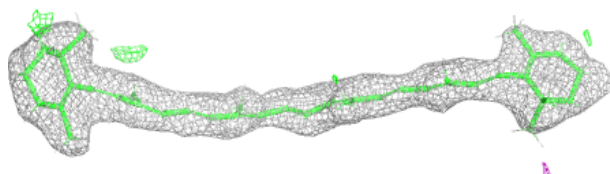
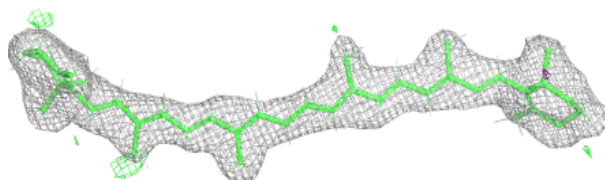


Electron density around BCR d 406:

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

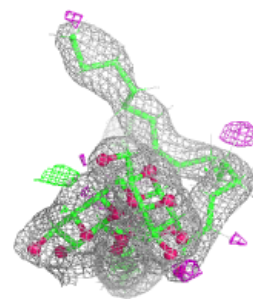
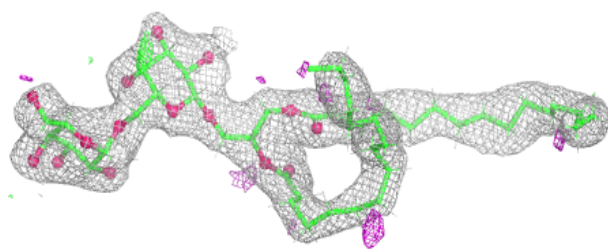
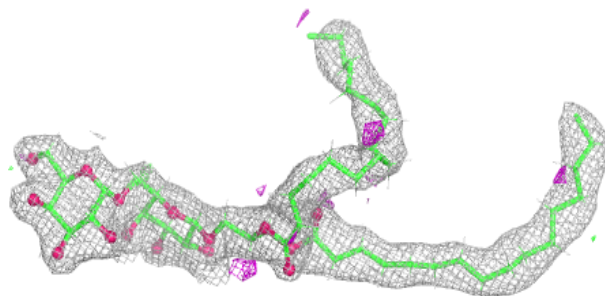
**Electron density around BCR x 101:**

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

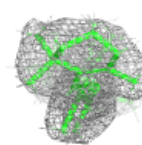
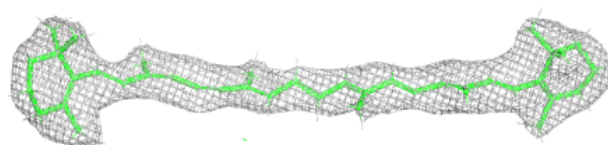
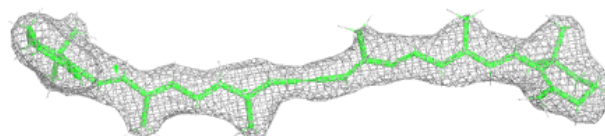


Electron density around DGD h 101:

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

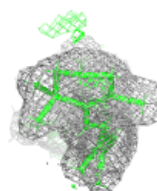
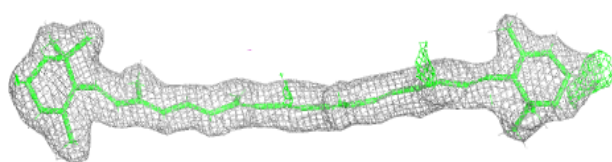
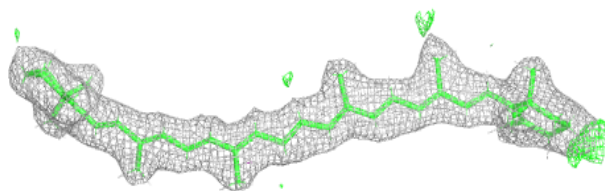
**Electron density around BCR c 514:**

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

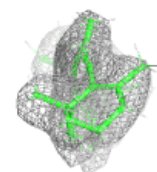
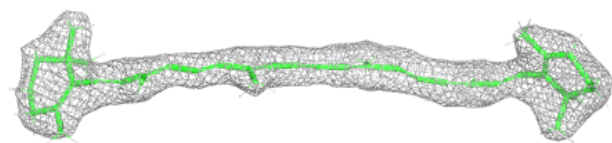
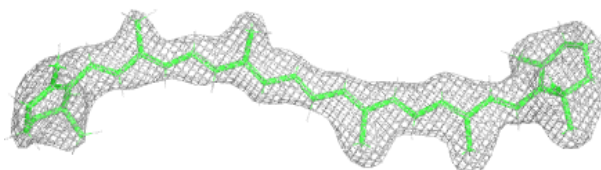


Electron density around BCR H 101:

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

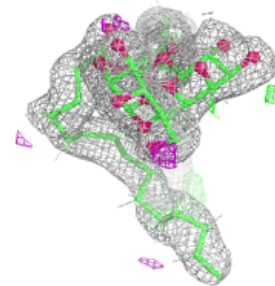
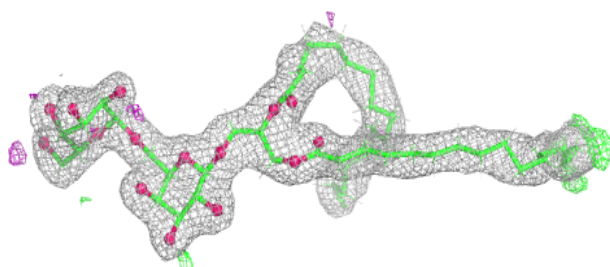
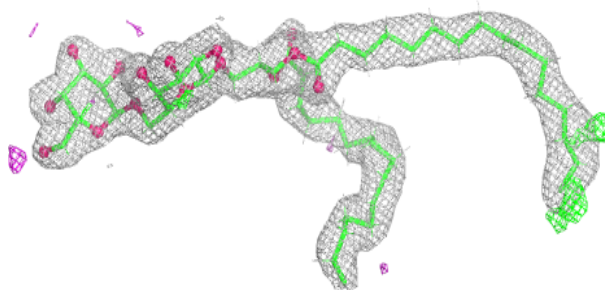
**Electron density around BCR k 101:**

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

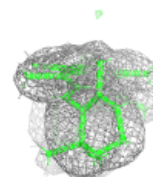
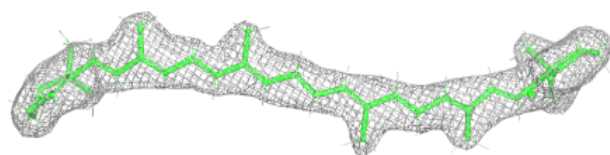
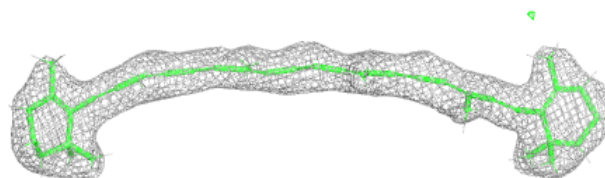


Electron density around DGD H 102:

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

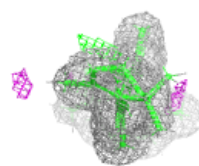
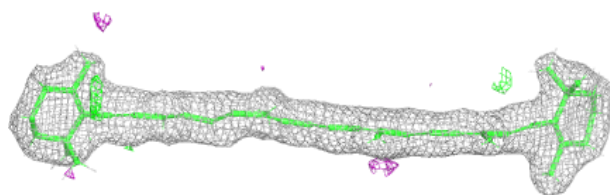
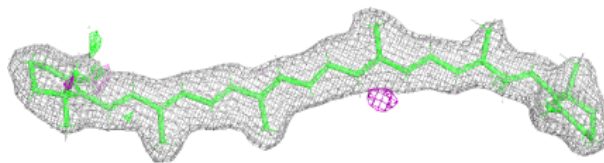
**Electron density around BCR c 516:**

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



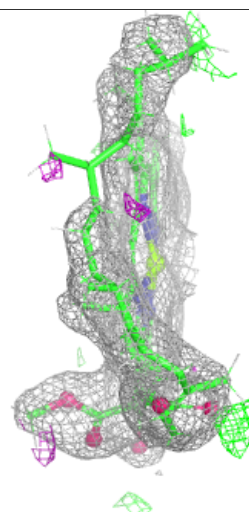
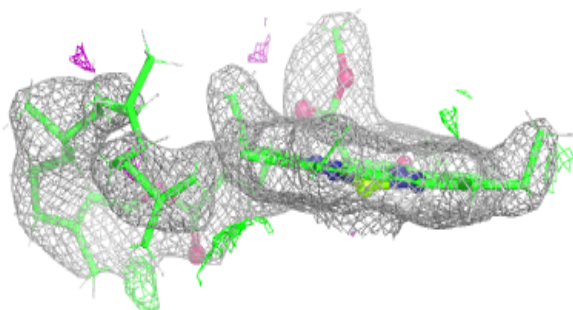
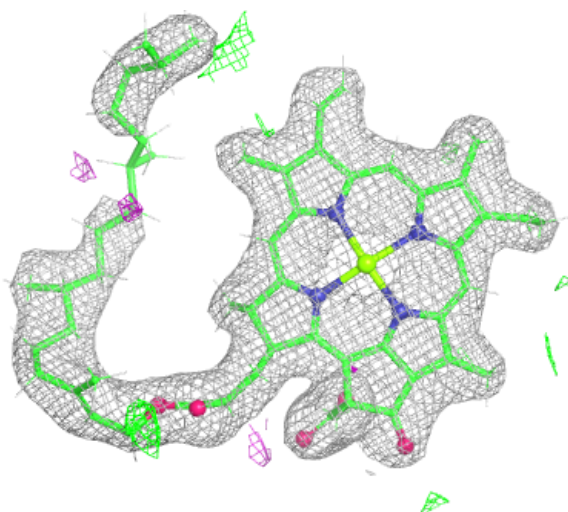
Electron density around BCR C 515:

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



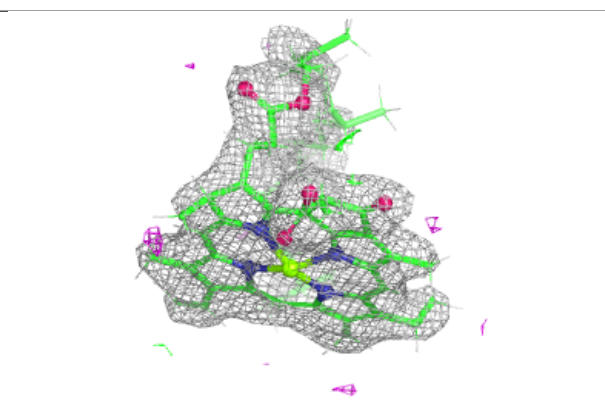
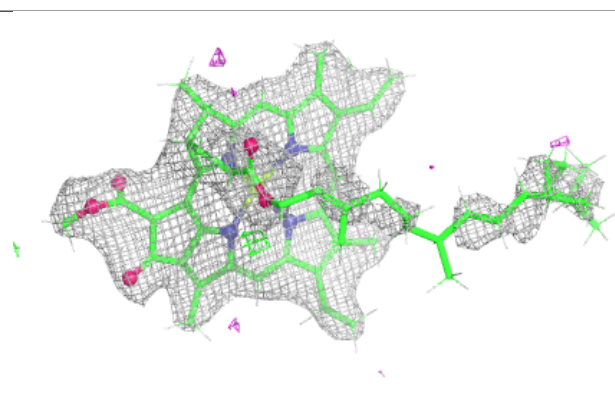
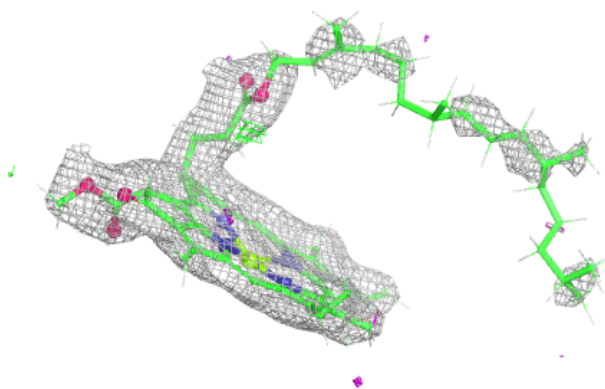
Electron density around CLA c 512:

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

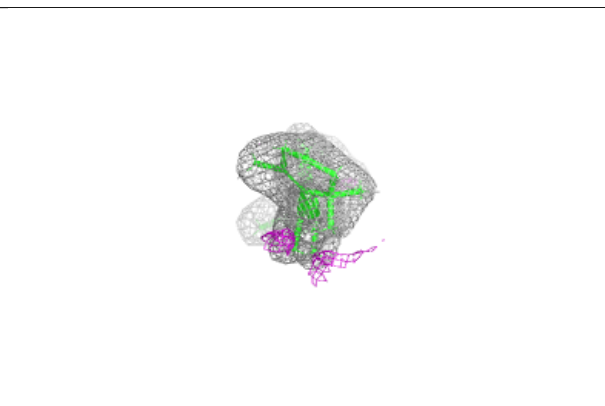
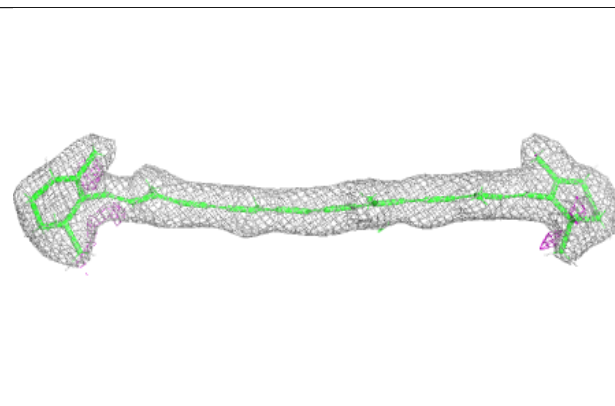
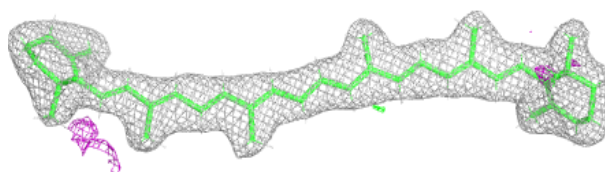


Electron density around CLA c 513:

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

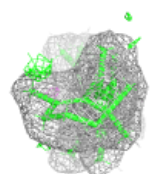
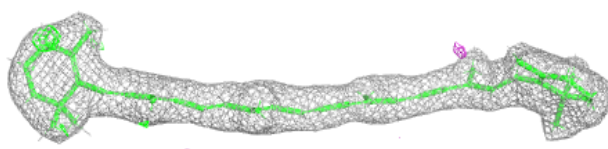
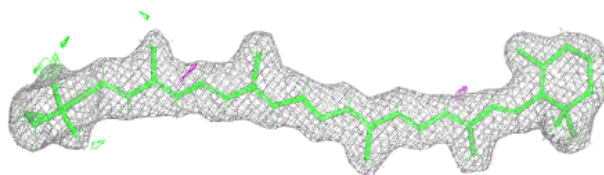
**Electron density around BCR B 618:**

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

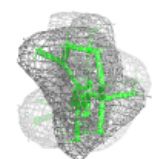
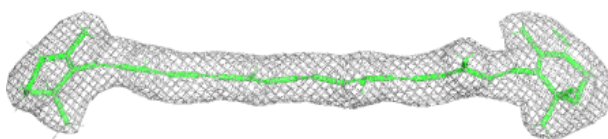
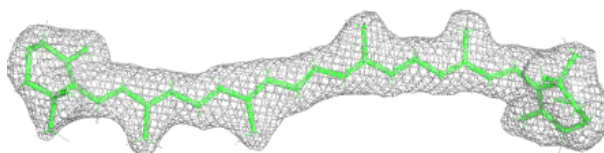


Electron density around BCR b 617:

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

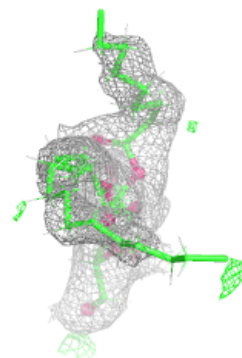
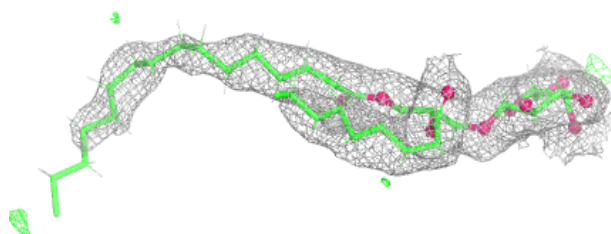
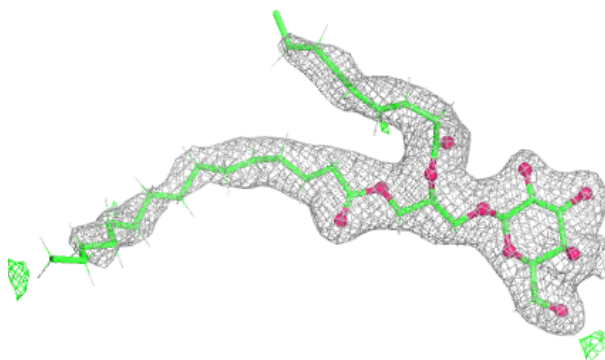
**Electron density around BCR b 618:**

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

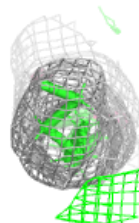
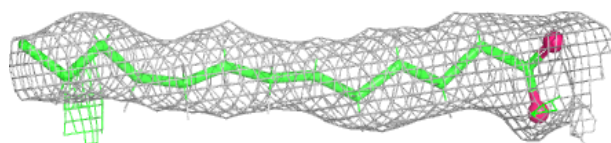
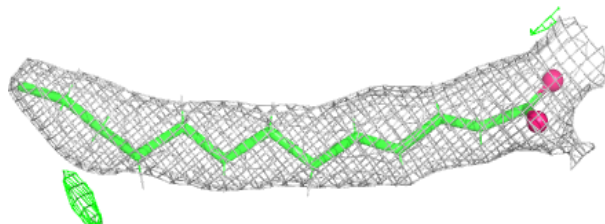


Electron density around LMG d 410:

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

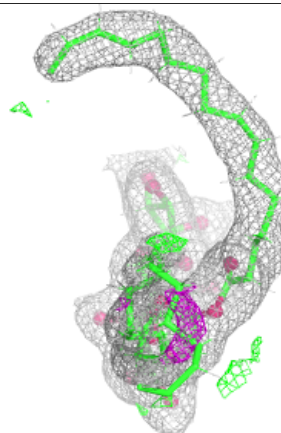
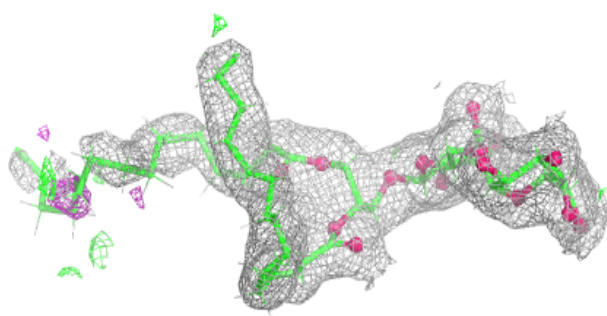
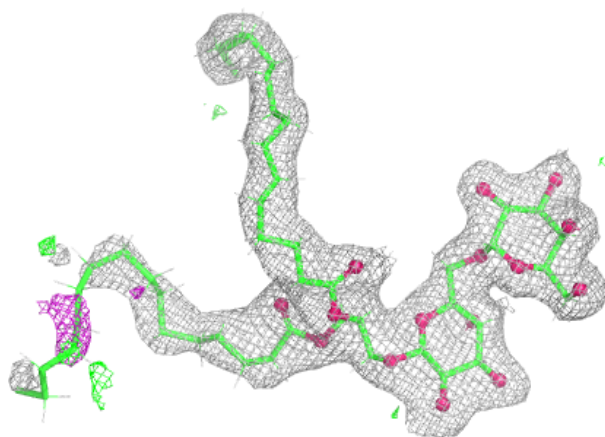
**Electron density around STE M 102:**

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

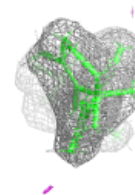
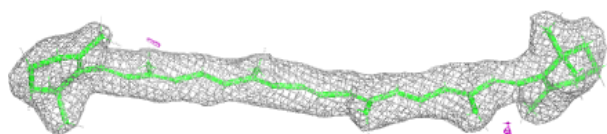
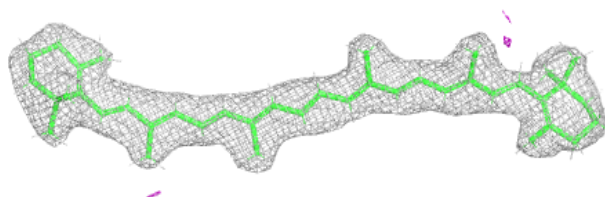


Electron density around DGD C 518:

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

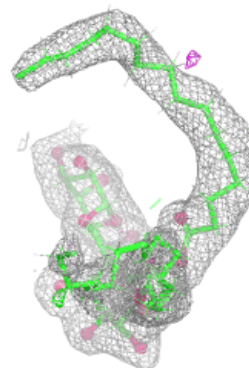
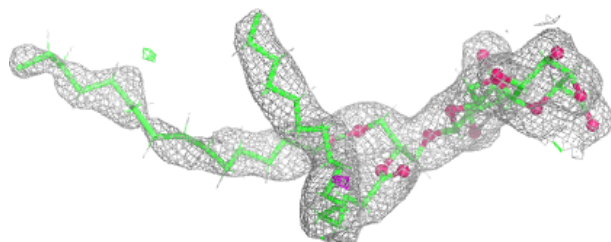
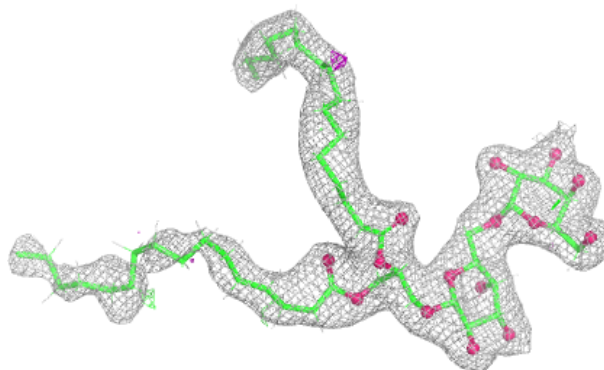
**Electron density around BCR b 619:**

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

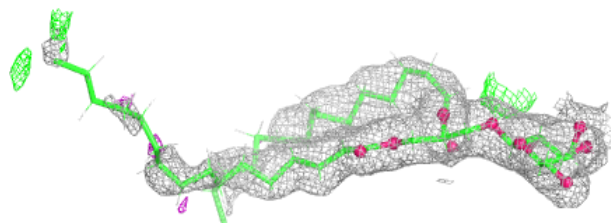
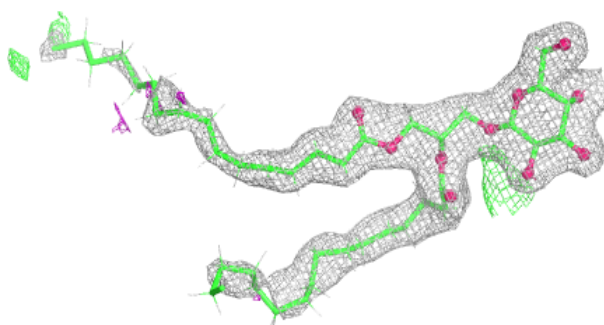


Electron density around DGD c 518:

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

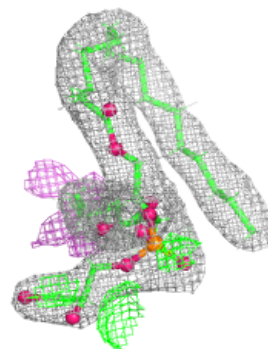
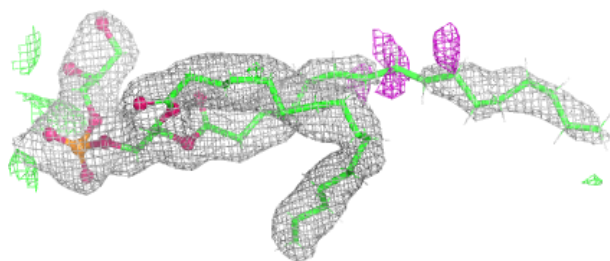
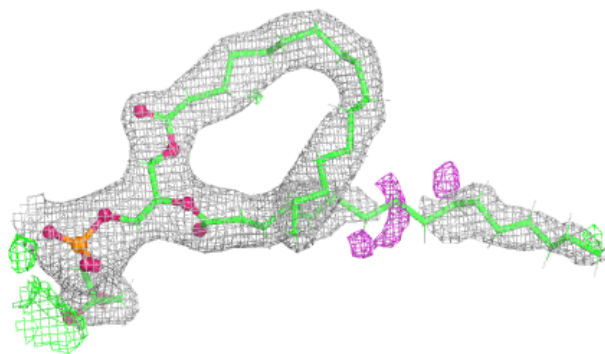
**Electron density around LMG D 407:**

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



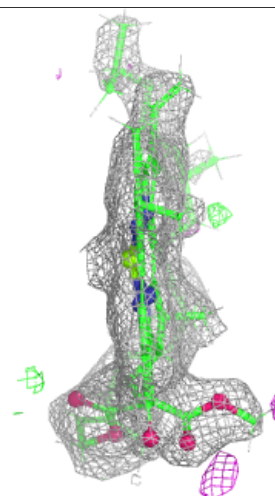
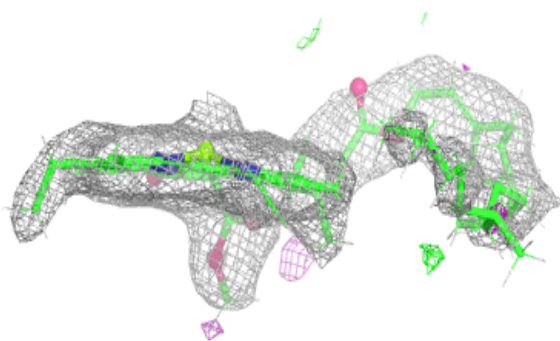
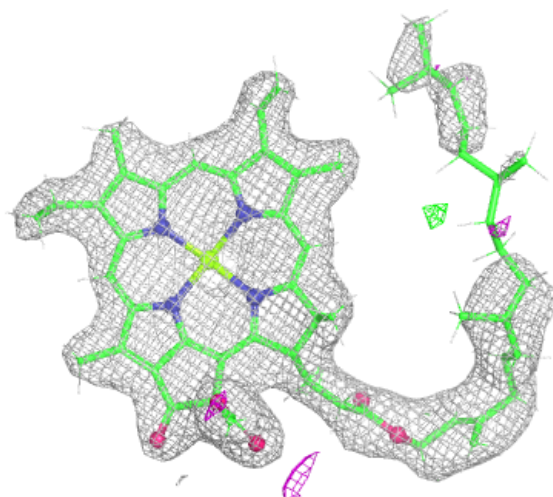
Electron density around LHG a 410:

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



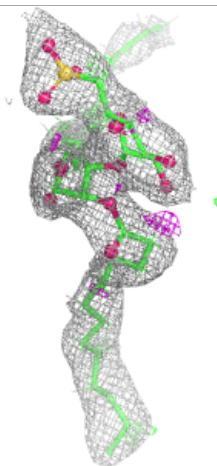
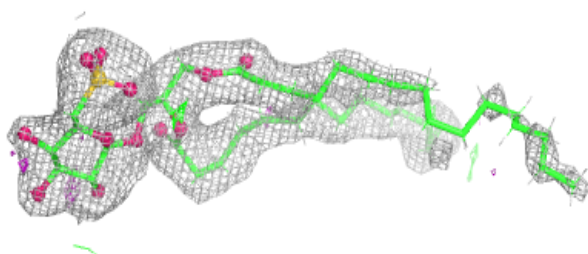
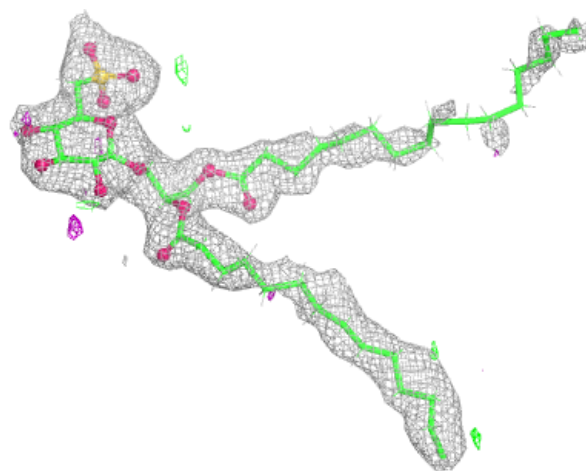
Electron density around CLA C 512:

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



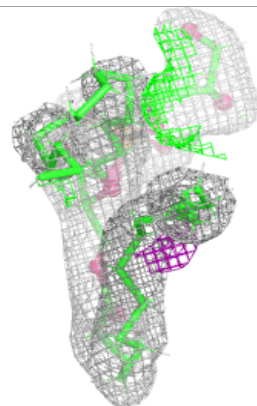
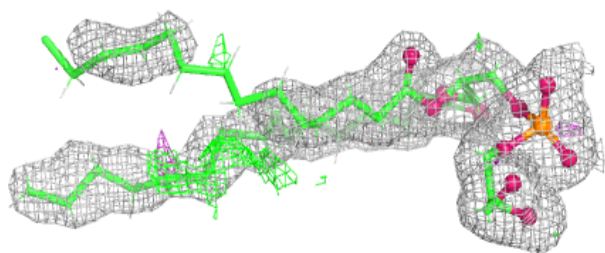
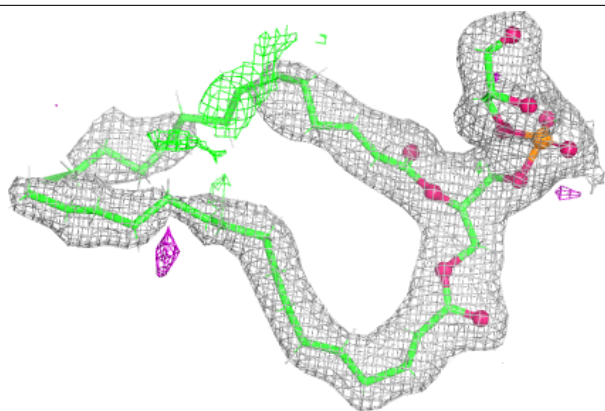
Electron density around SQD A 413:

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

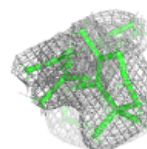
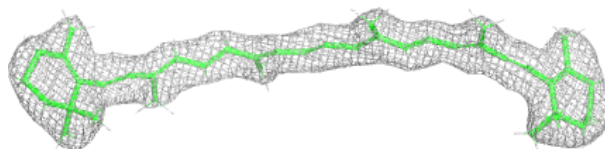


Electron density around LHG A 412:

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

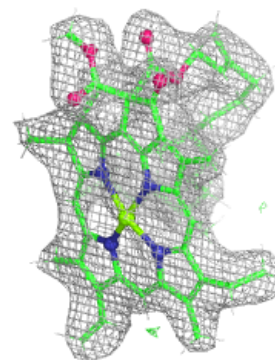
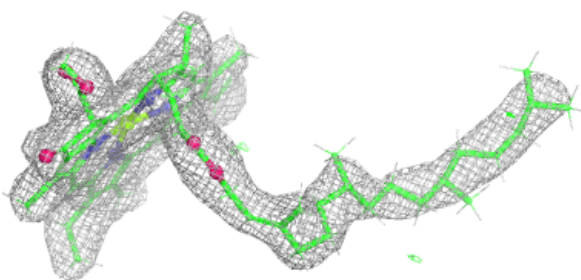
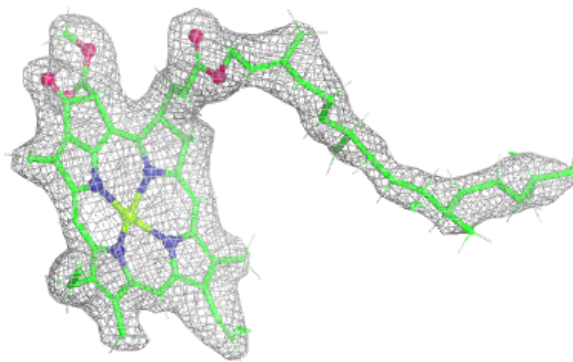
**Electron density around BCR C 516:**

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

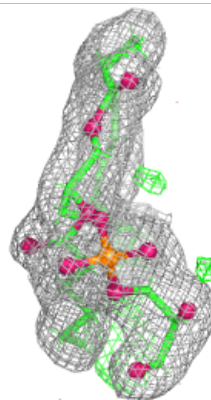
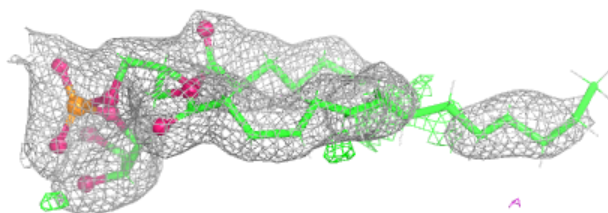
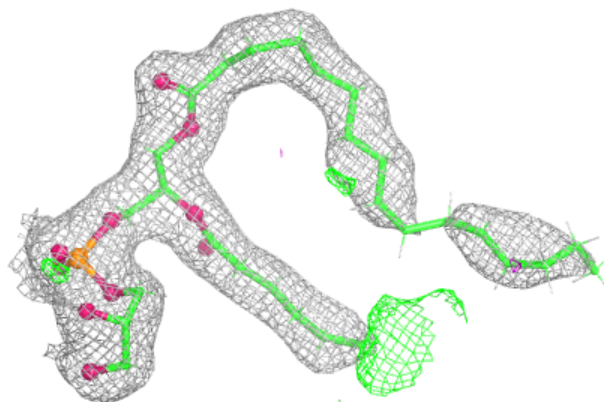


Electron density around CLA c 511:

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

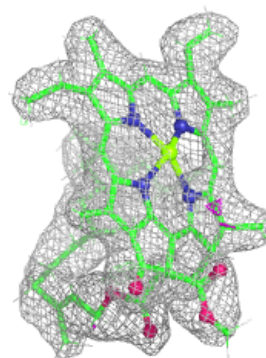
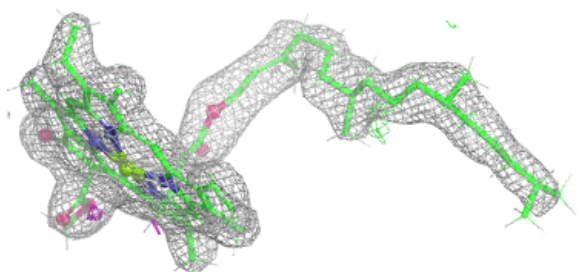
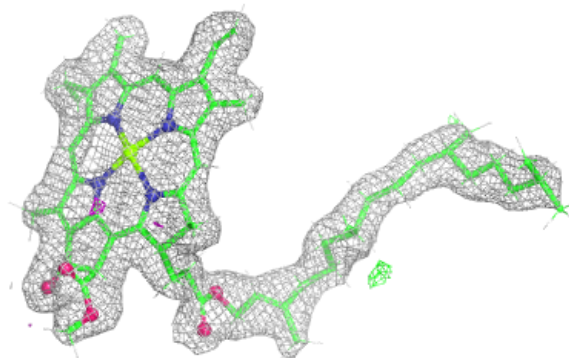
**Electron density around LHG d 409:**

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

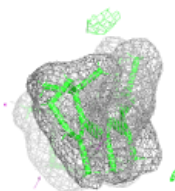
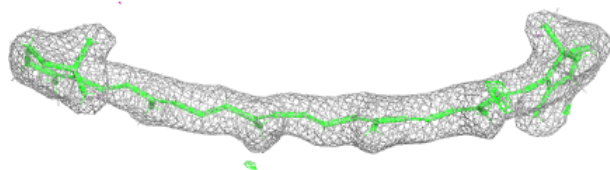
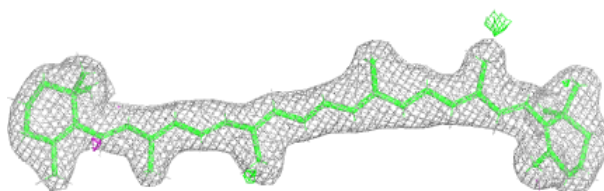


Electron density around CLA C 511:

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

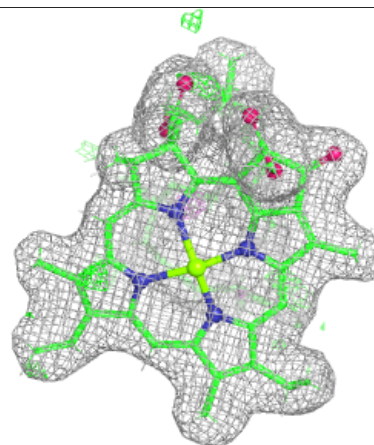
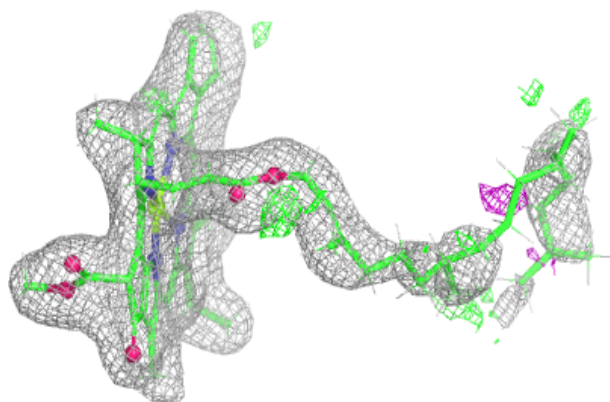
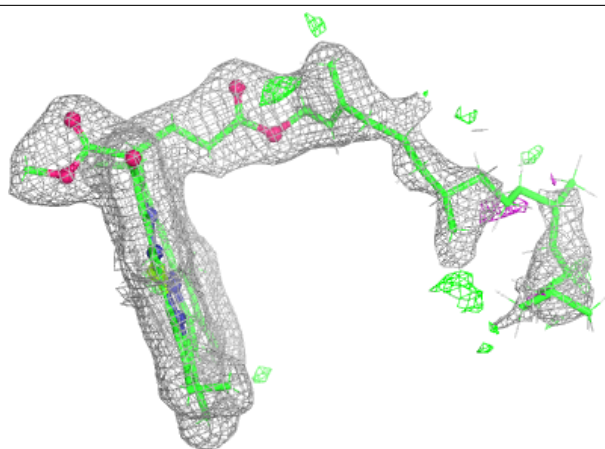
**Electron density around BCR T 101:**

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

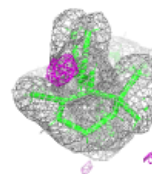
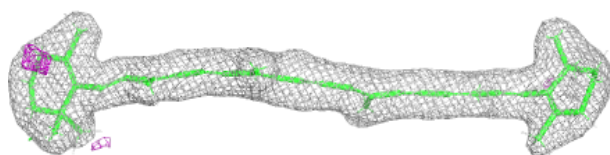
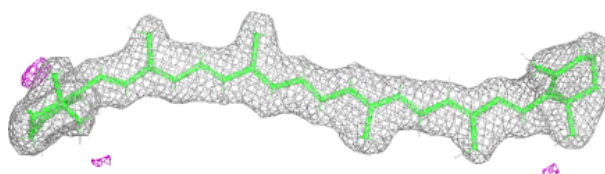


Electron density around CLA C 506:

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

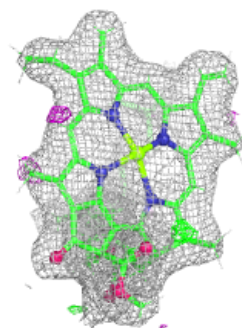
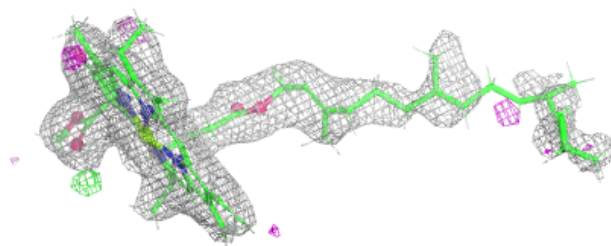
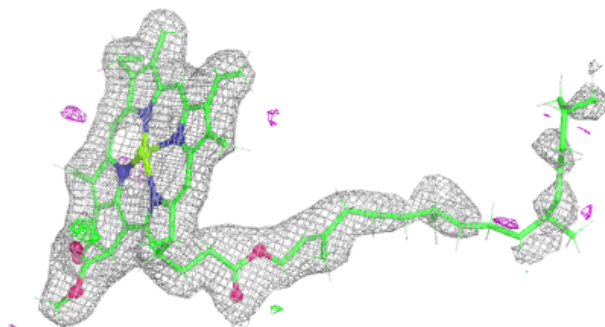
**Electron density around BCR a 405:**

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

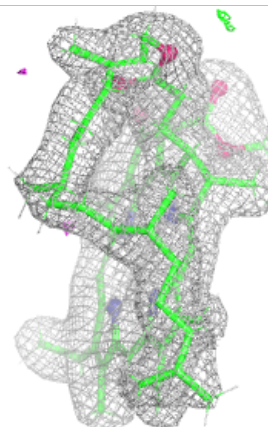
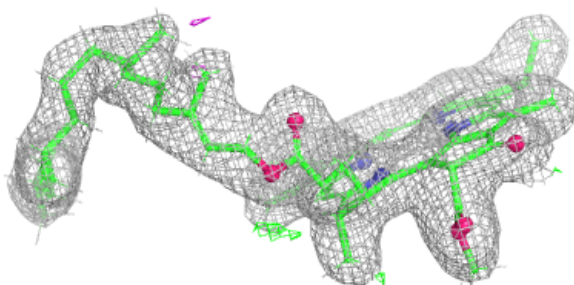
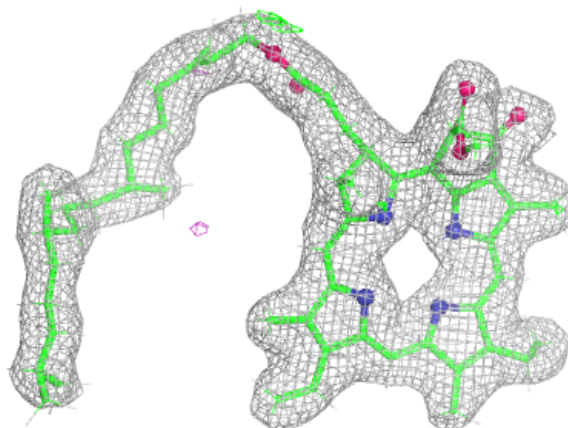


Electron density around CLA d 405:

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

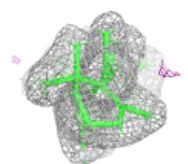
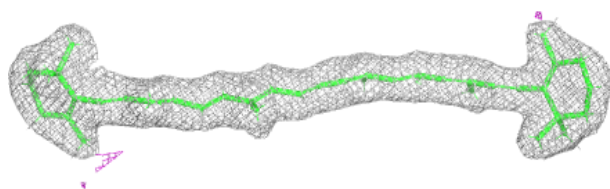
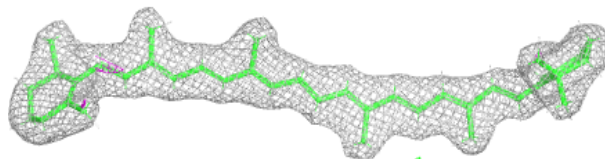
**Electron density around PHO d 402:**

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

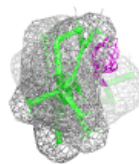
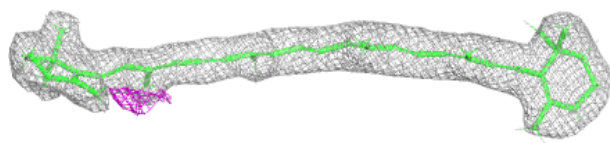
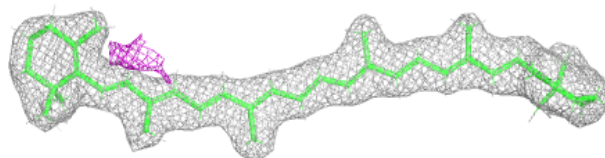


Electron density around BCR A 407:

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

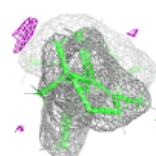
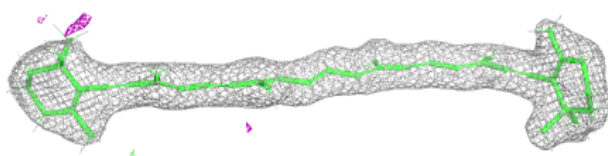
**Electron density around BCR B 617:**

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

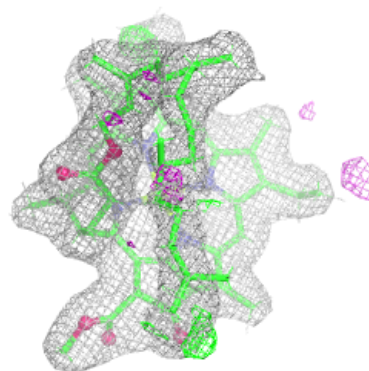
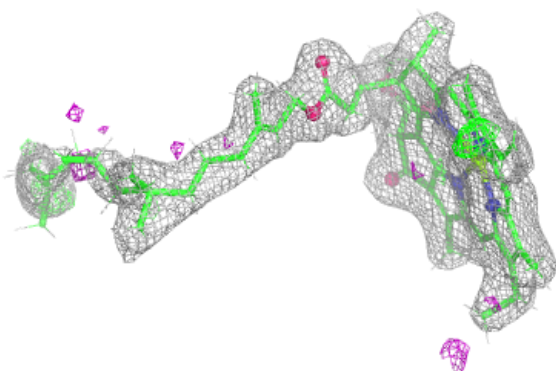
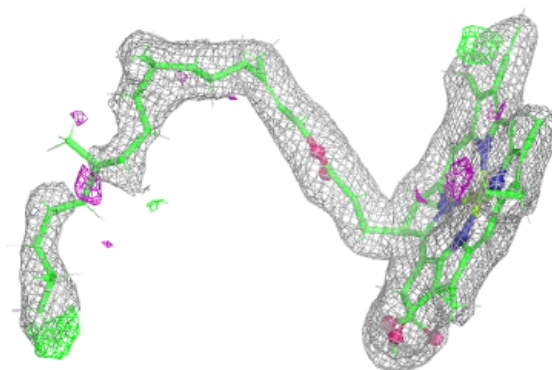


Electron density around BCR c 515:

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

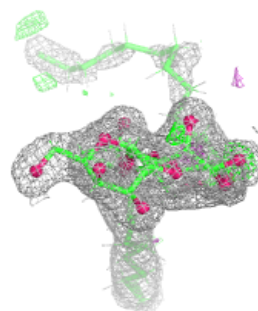
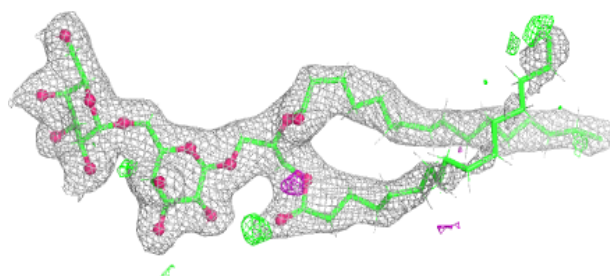
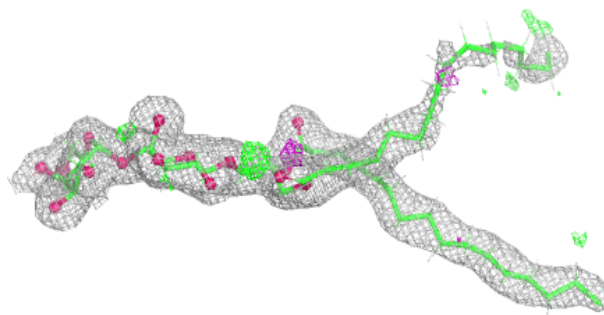
**Electron density around CLA b 606:**

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

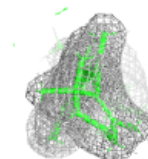
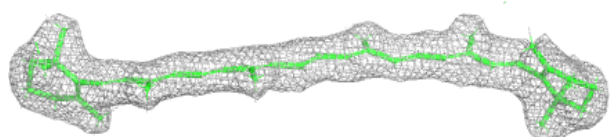
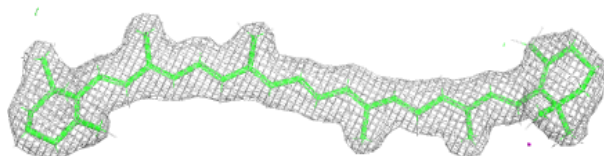


Electron density around DGD C 517:

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

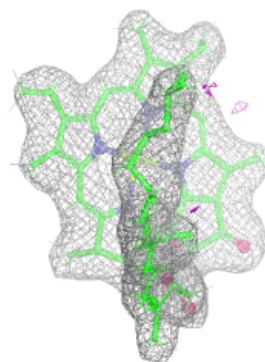
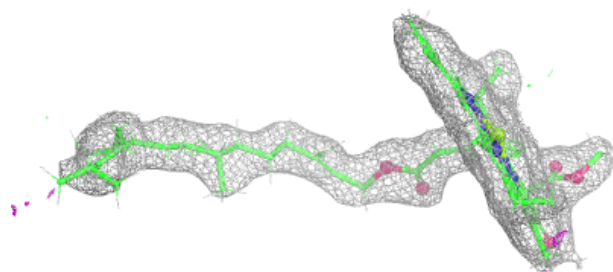
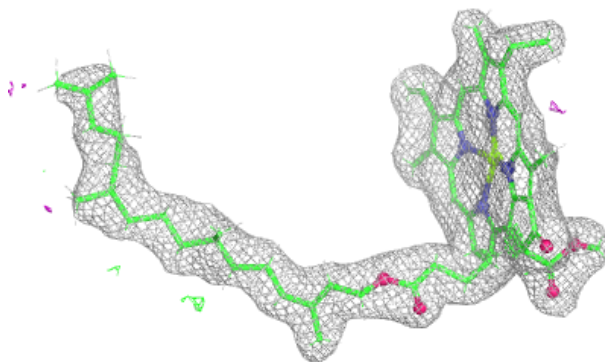
**Electron density around BCR B 619:**

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



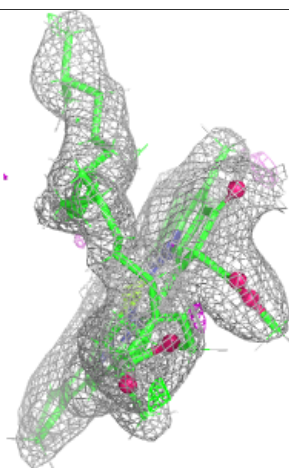
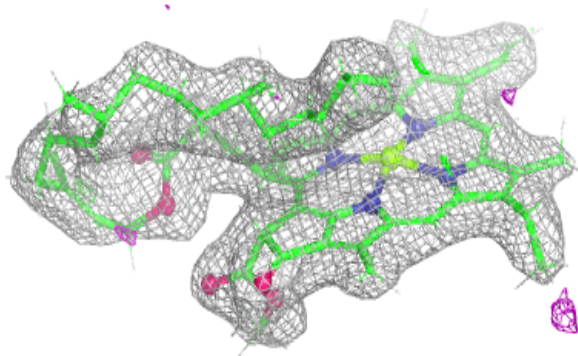
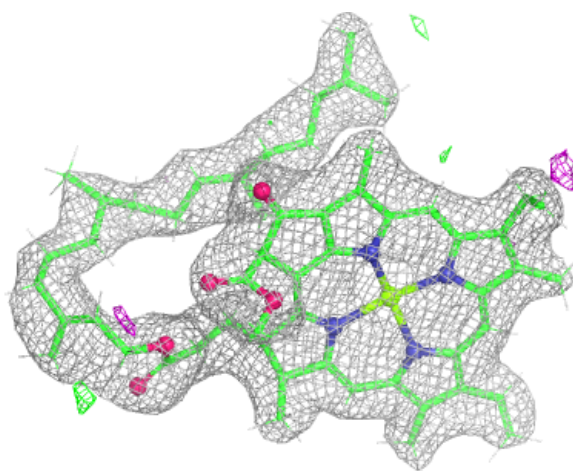
Electron density around CLA b 609:

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



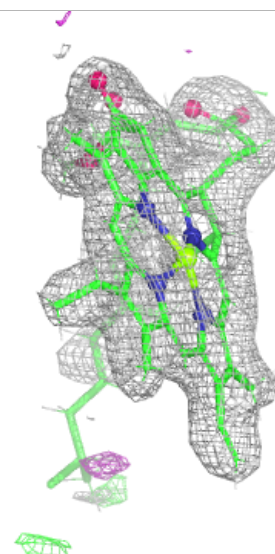
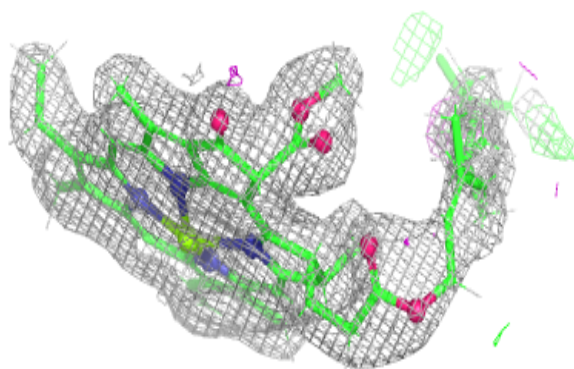
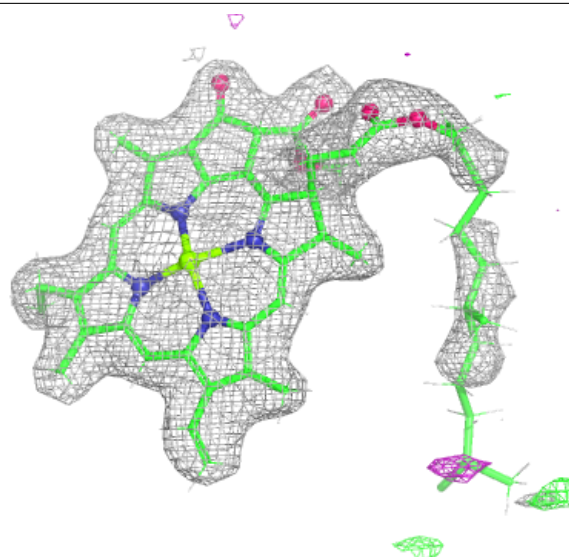
Electron density around CLA c 509:

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



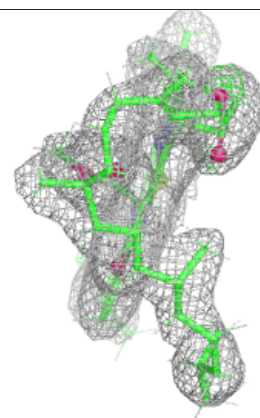
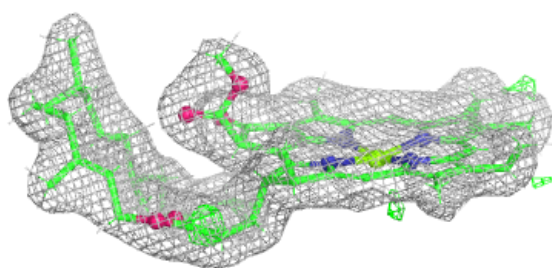
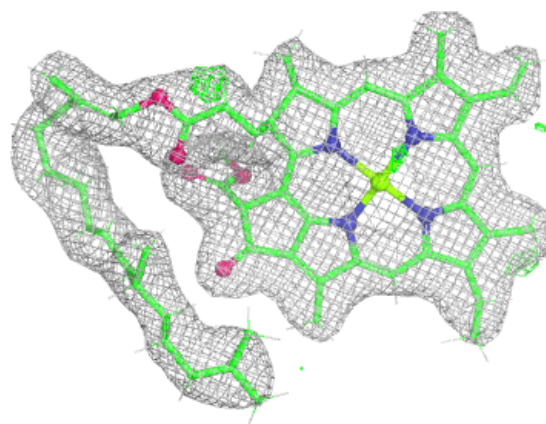
Electron density around CLA B 616:

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

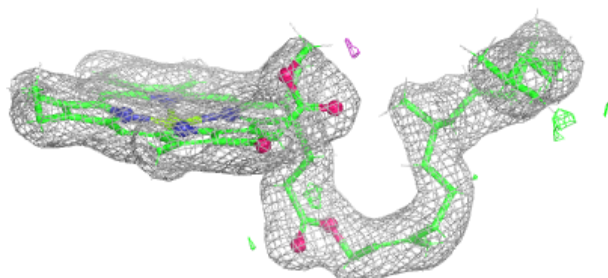
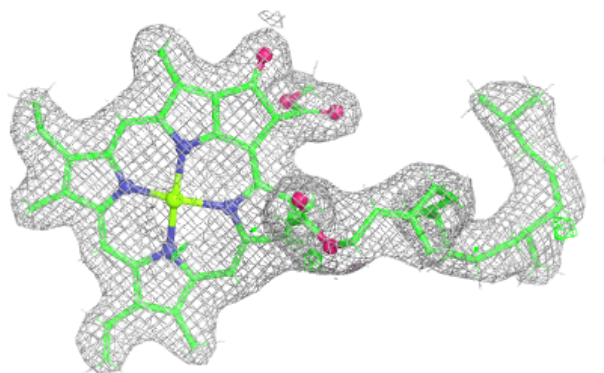


Electron density around CLA b 610:

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

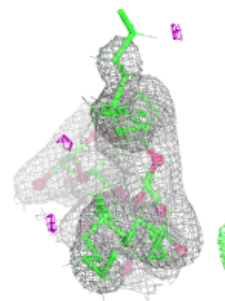
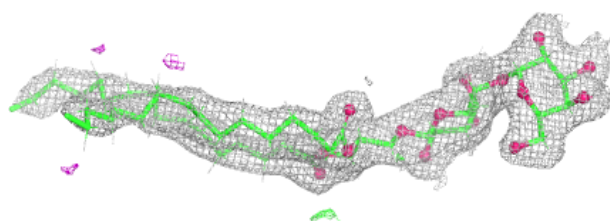
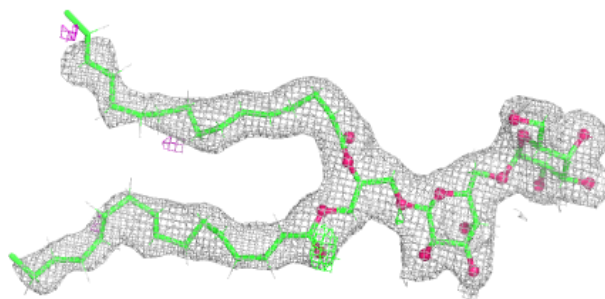
**Electron density around CLA b 612:**

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

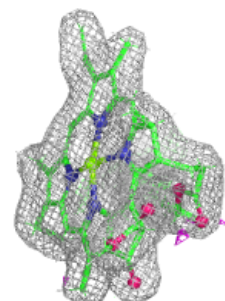
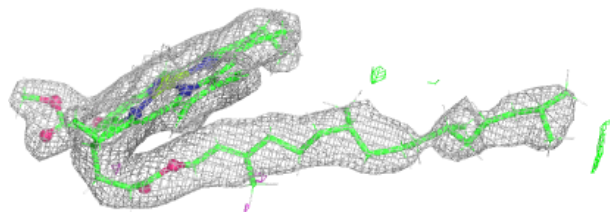
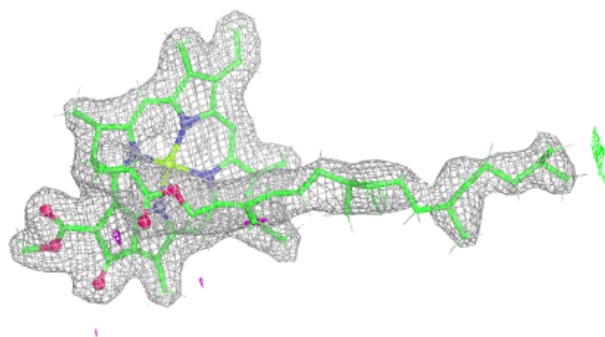


Electron density around DGD C 519:

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

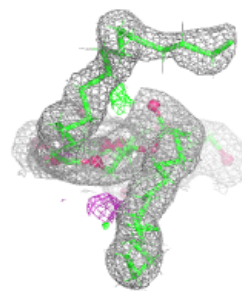
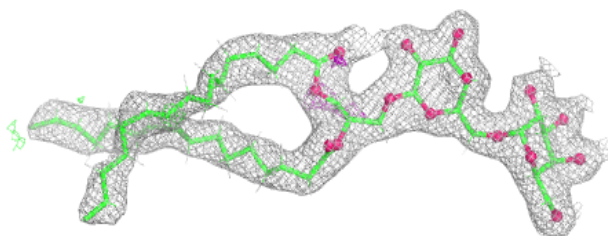
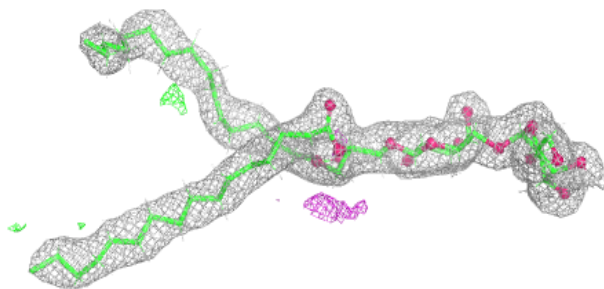
**Electron density around CLA b 614:**

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



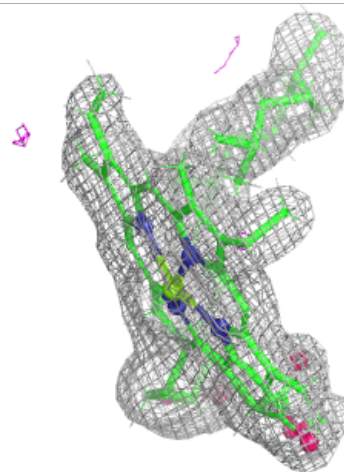
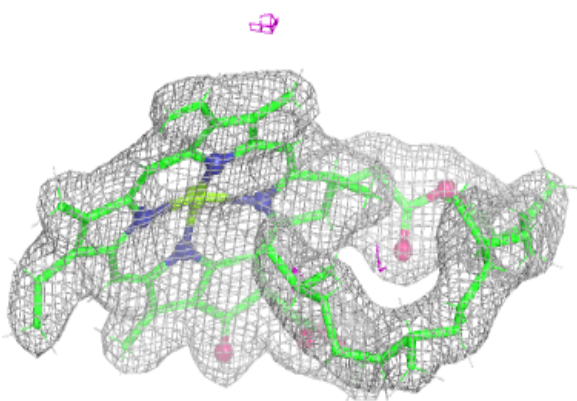
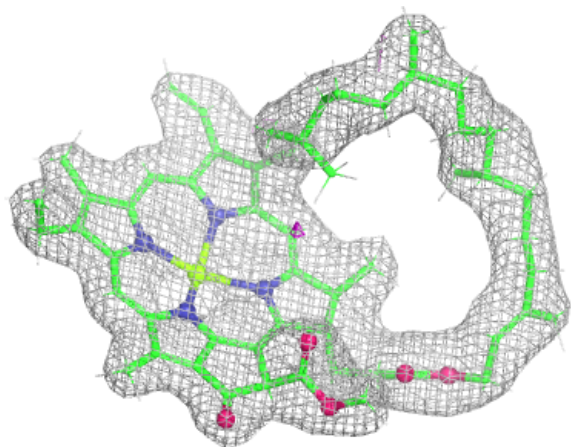
Electron density around DGD c 517:

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



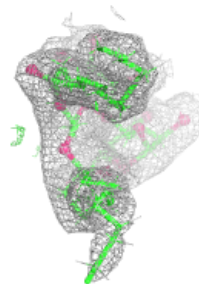
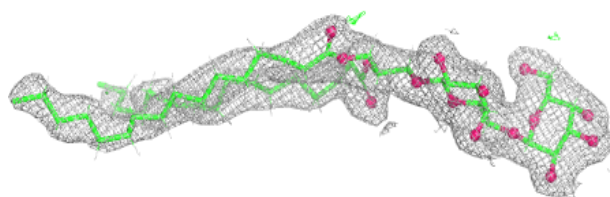
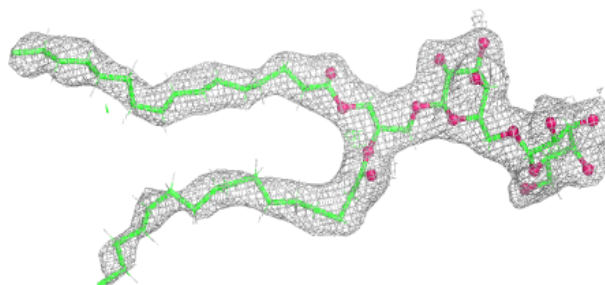
Electron density around CLA b 615:

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



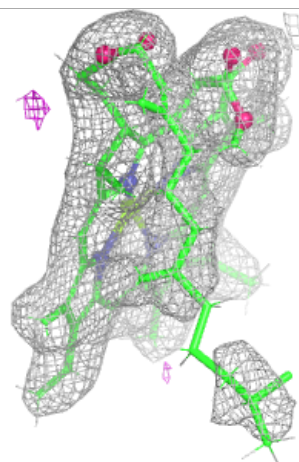
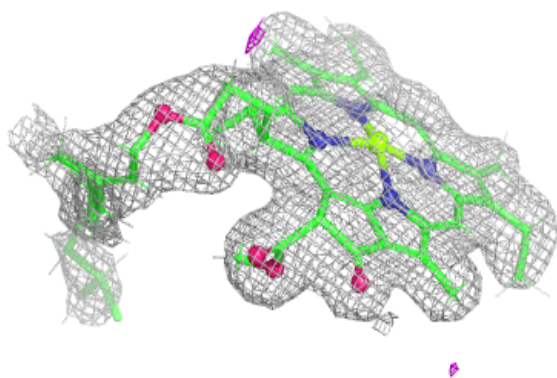
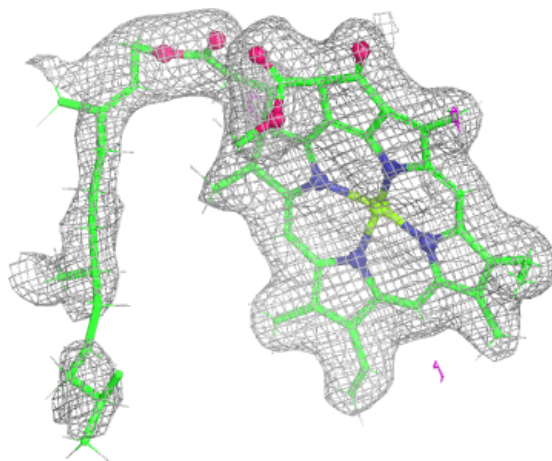
Electron density around DGD c 519:

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



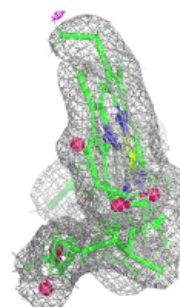
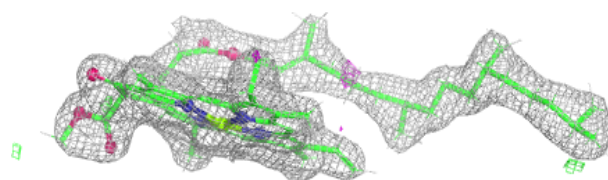
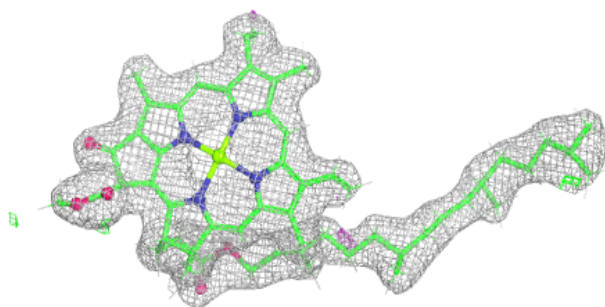
Electron density around CLA b 616:

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

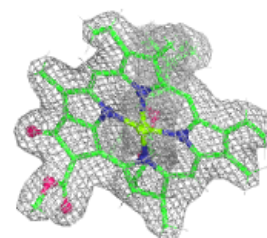
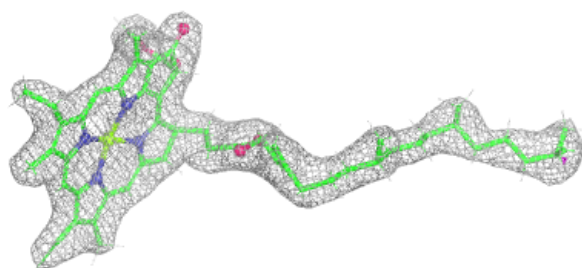
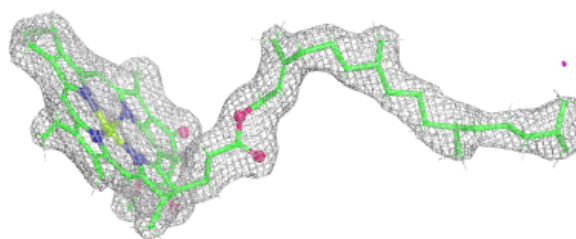


Electron density around CLA c 501:

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

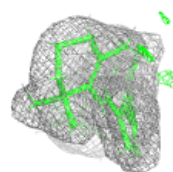
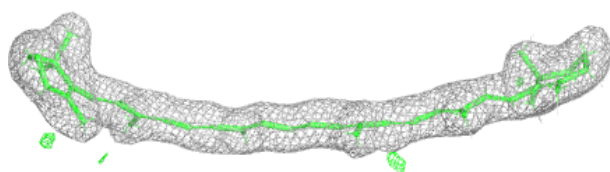
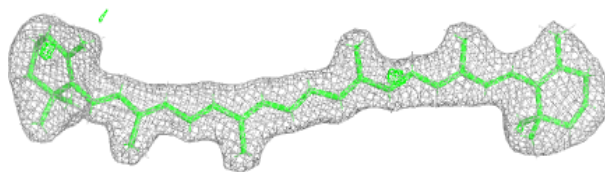
**Electron density around CLA c 502:**

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



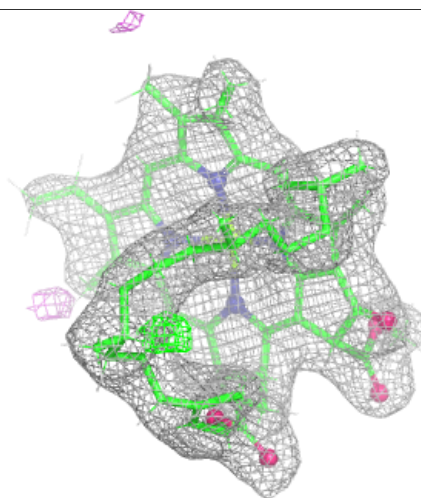
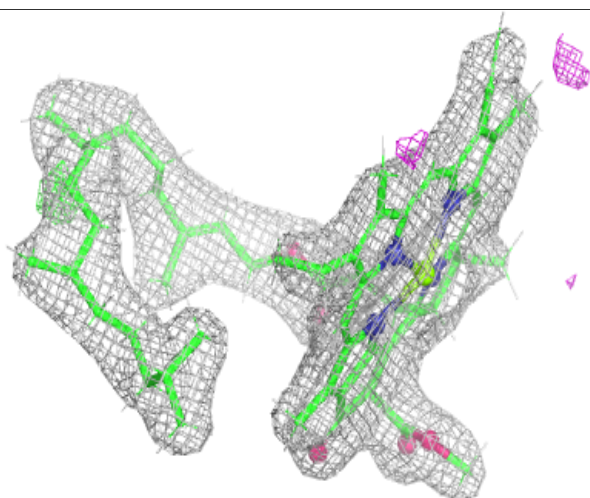
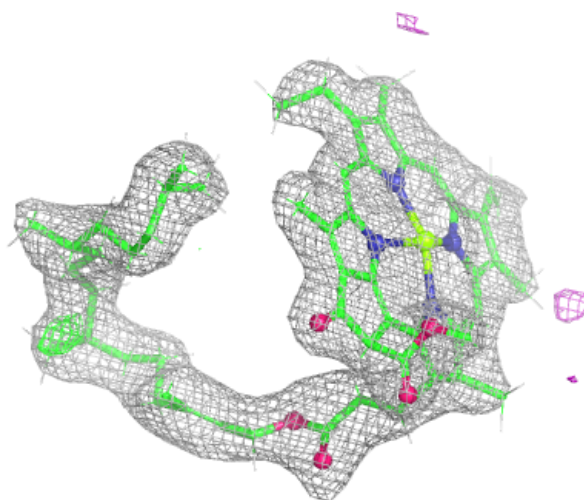
Electron density around BCR t 101:

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



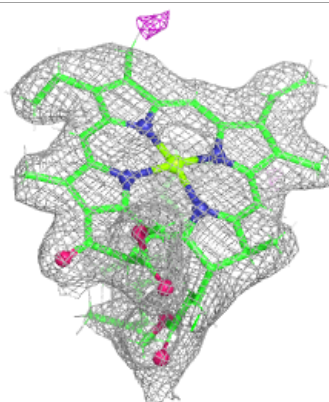
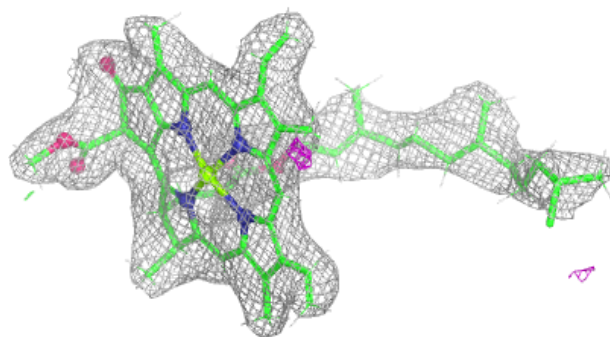
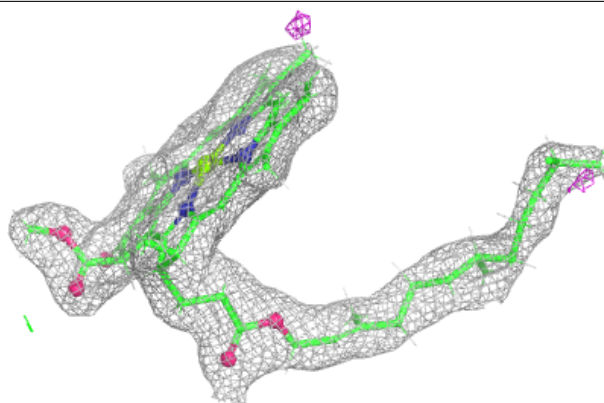
Electron density around CLA c 503:

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

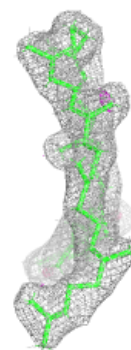
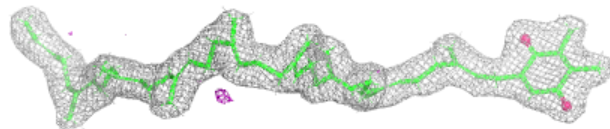
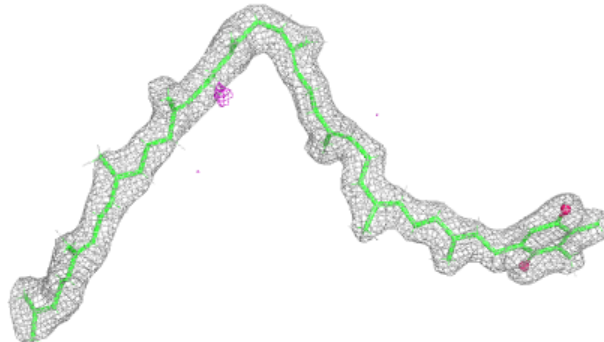


Electron density around CLA c 504:

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

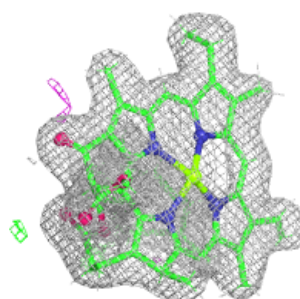
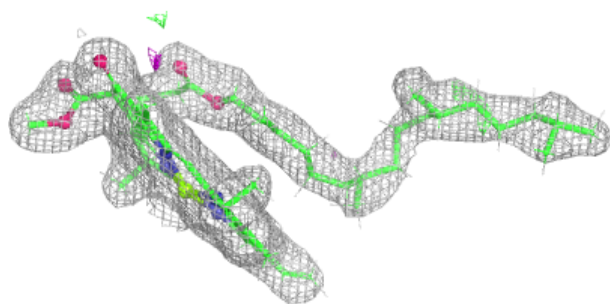
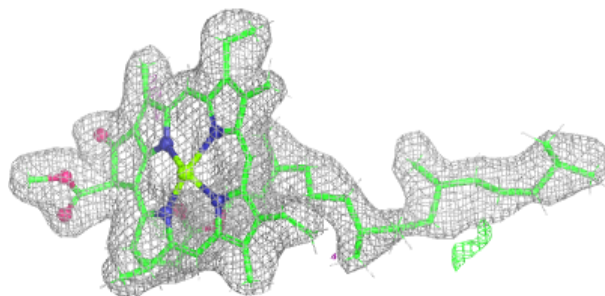
**Electron density around PL9 D 406:**

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

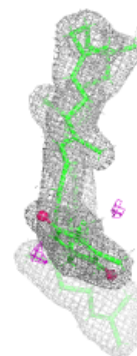
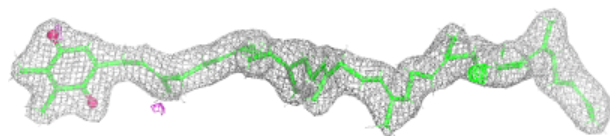
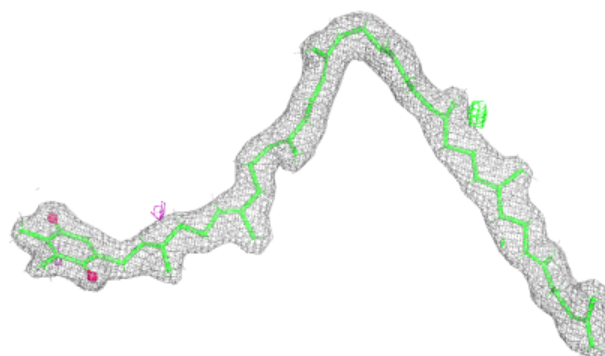


Electron density around CLA c 505:

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

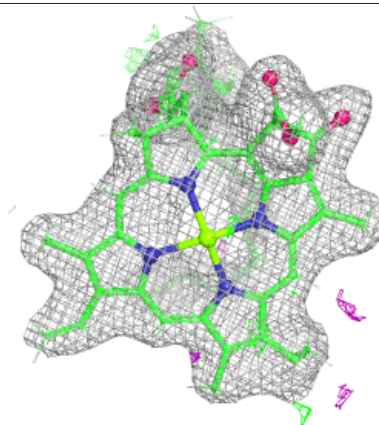
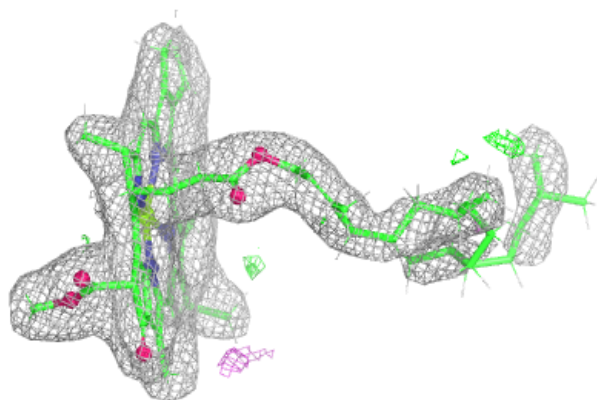
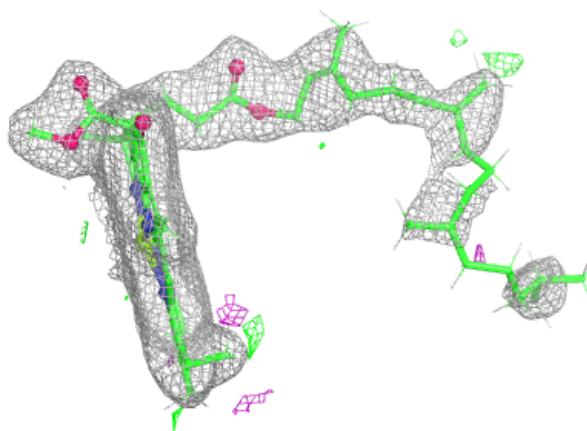
**Electron density around PL9 d 407:**

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



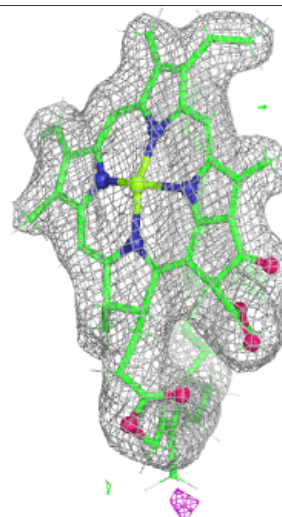
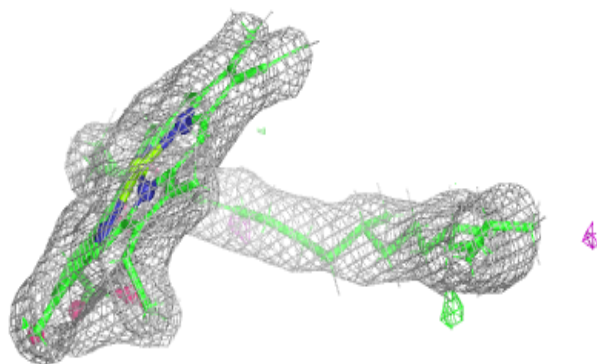
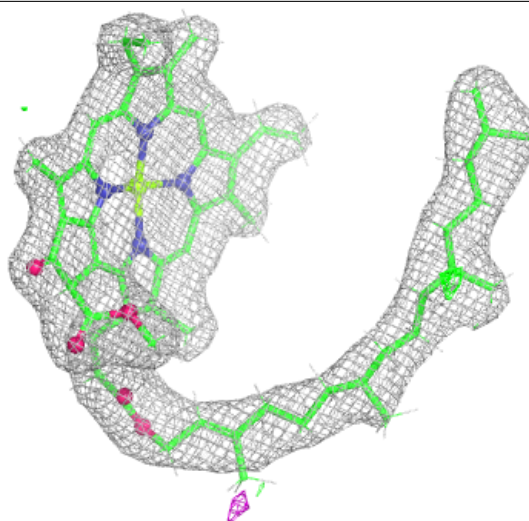
Electron density around CLA c 506:

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



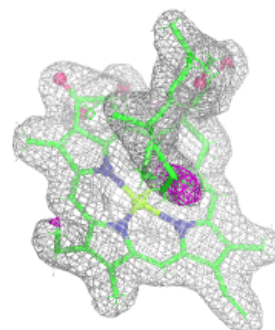
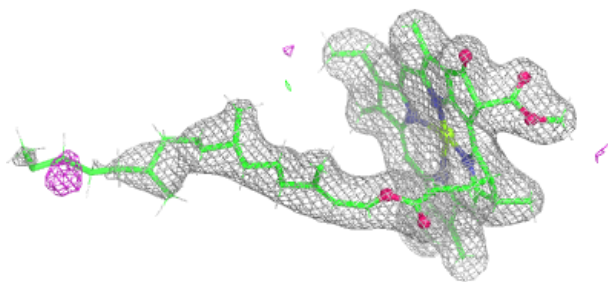
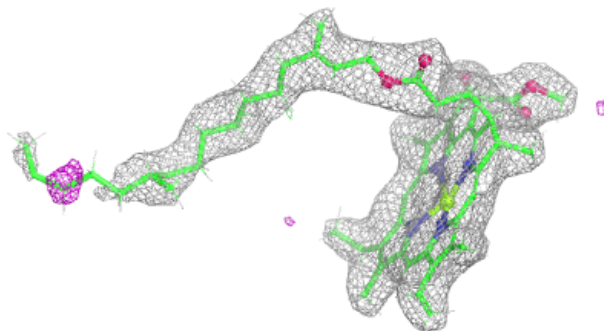
Electron density around CLA c 507:

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

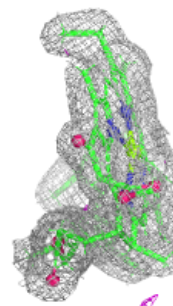
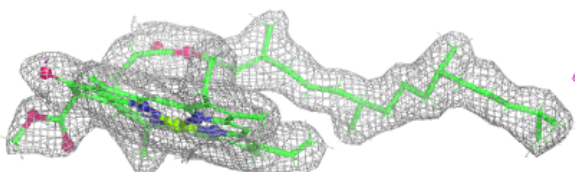
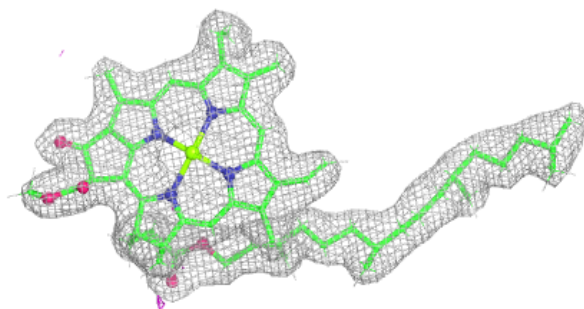


Electron density around CLA c 508:

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

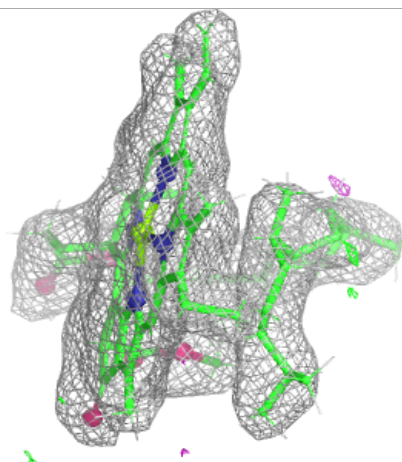
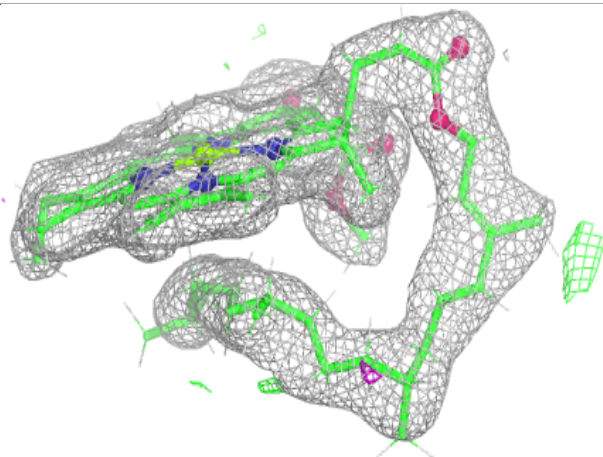
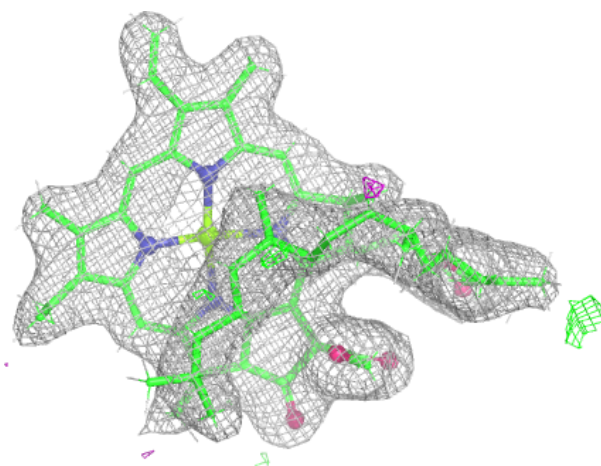
**Electron density around CLA C 501:**

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



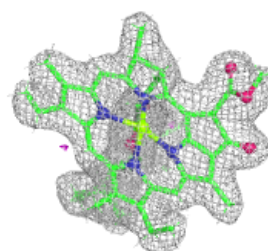
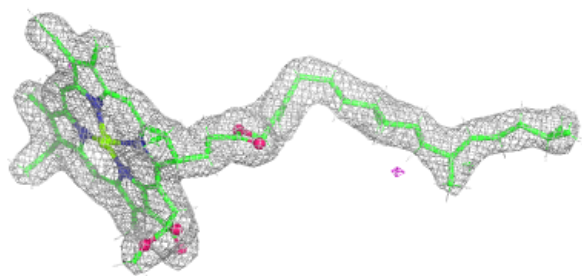
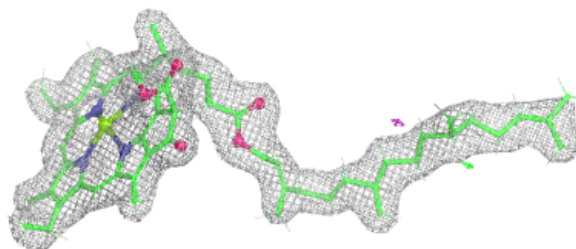
Electron density around CLA c 510:

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



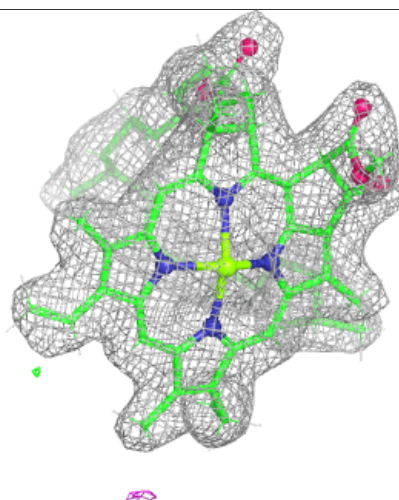
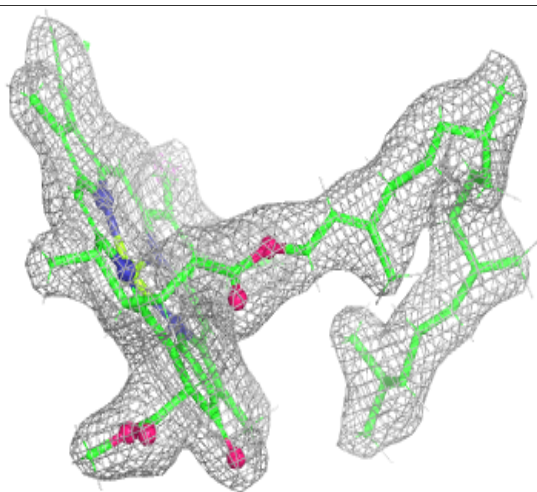
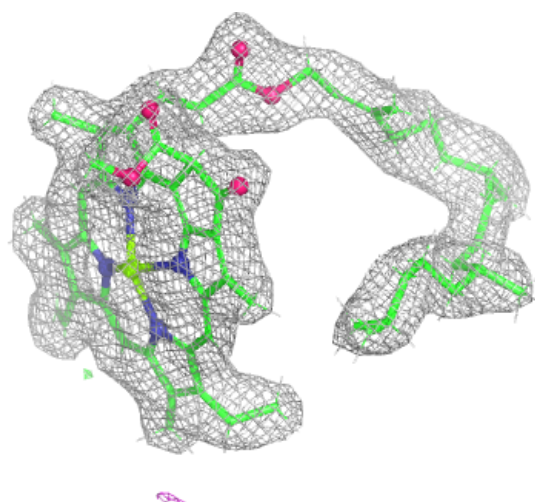
Electron density around CLA C 502:

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



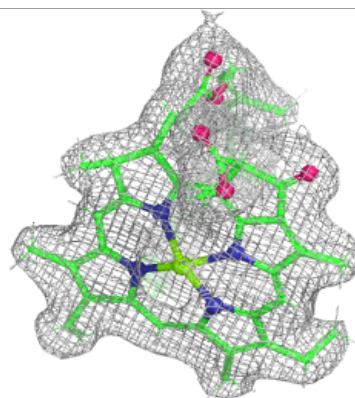
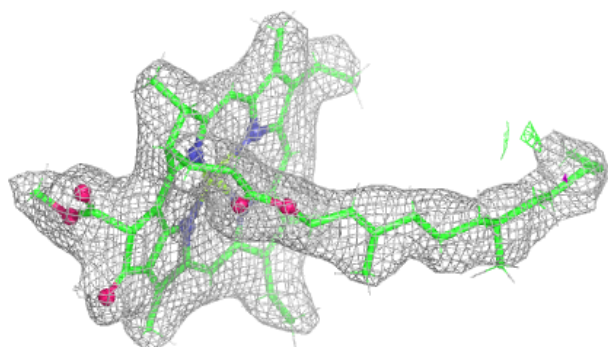
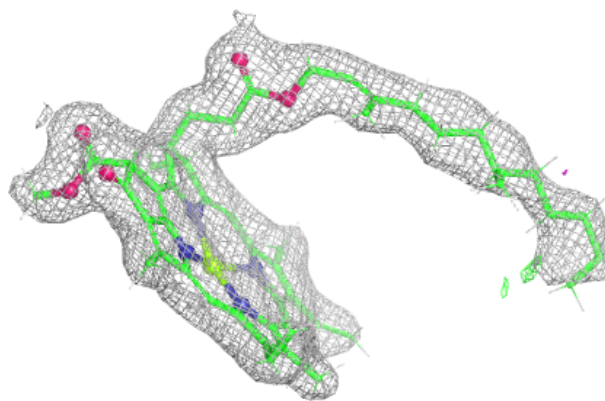
Electron density around CLA C 503:

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

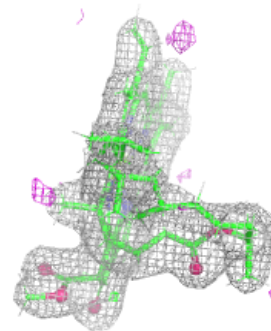
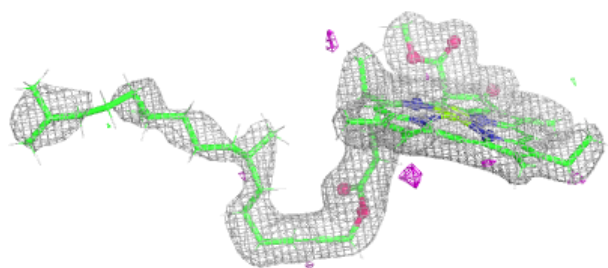
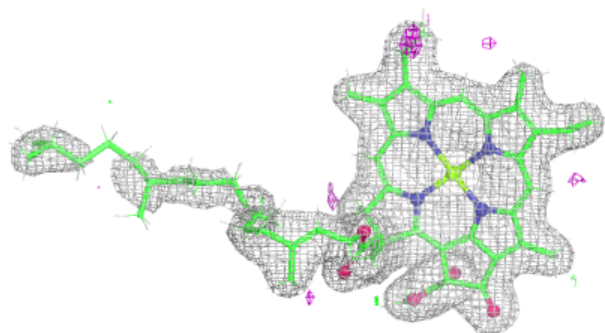


Electron density around CLA C 504:

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

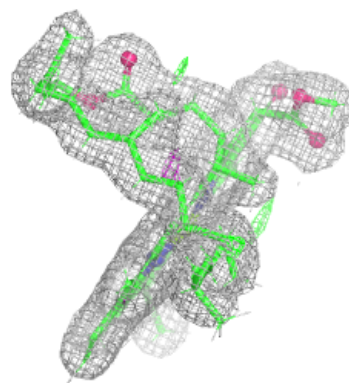
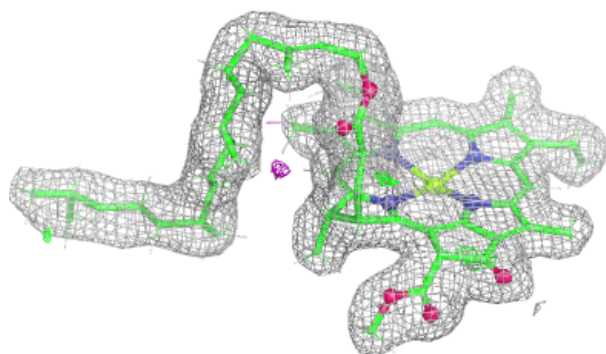
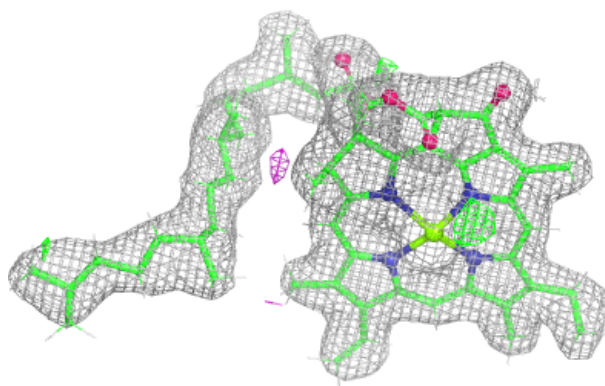
**Electron density around CLA d 401:**

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

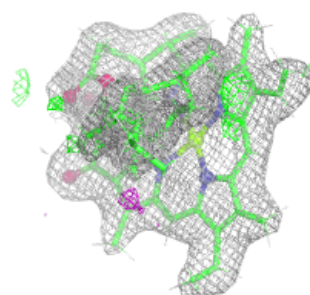
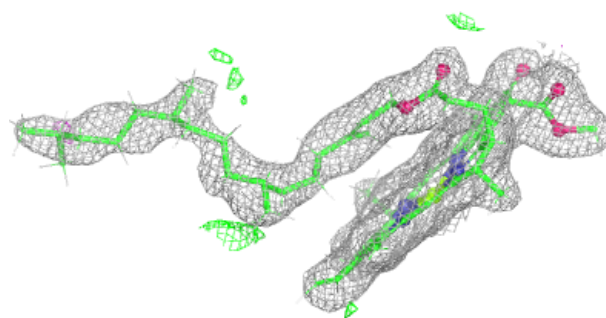
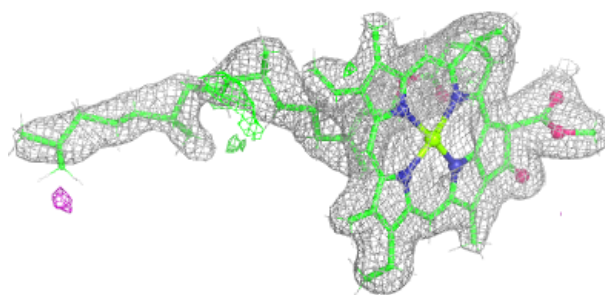


Electron density around CLA d 404:

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

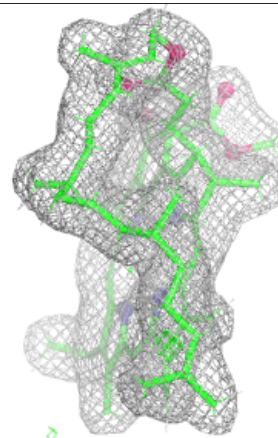
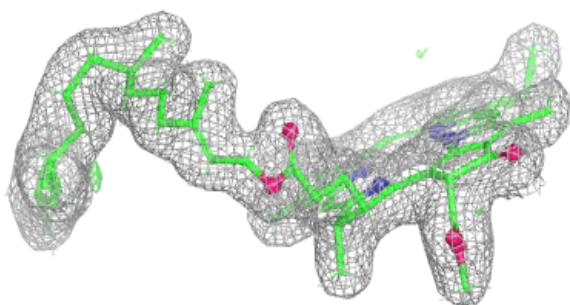
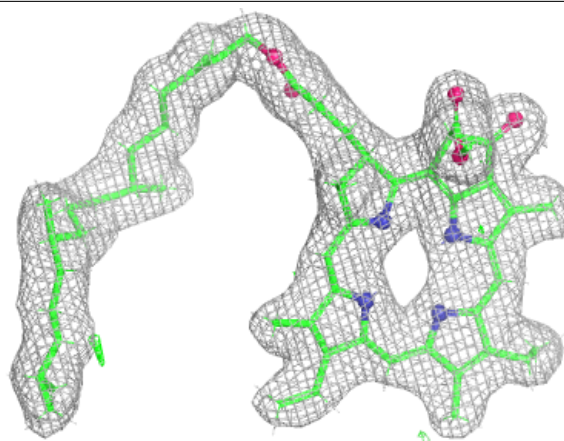
**Electron density around CLA C 505:**

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



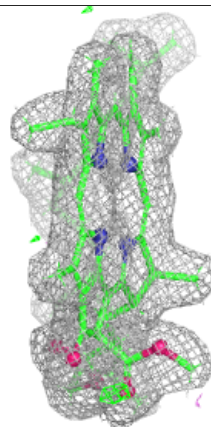
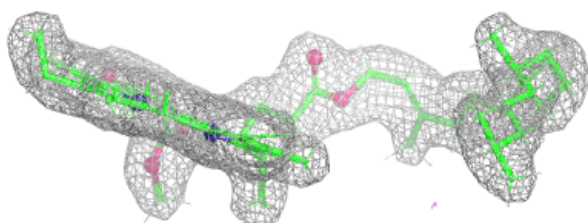
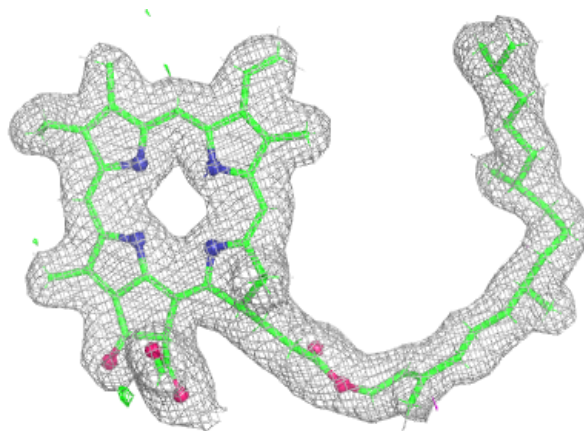
Electron density around PHO A 405:

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

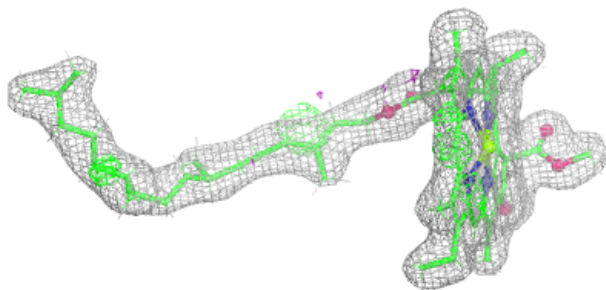
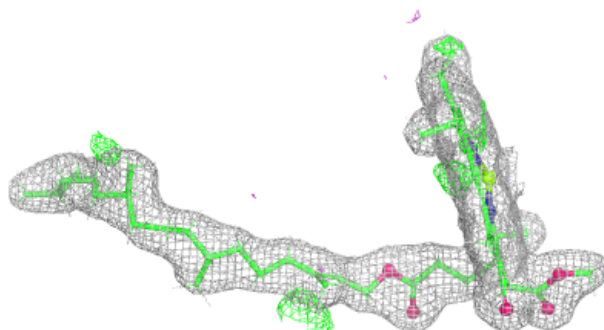


Electron density around PHO a 403:

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

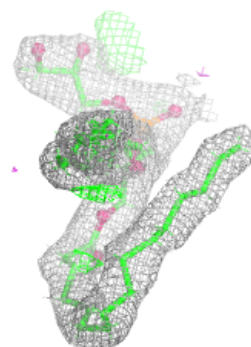
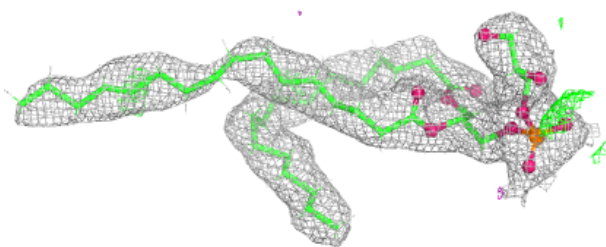
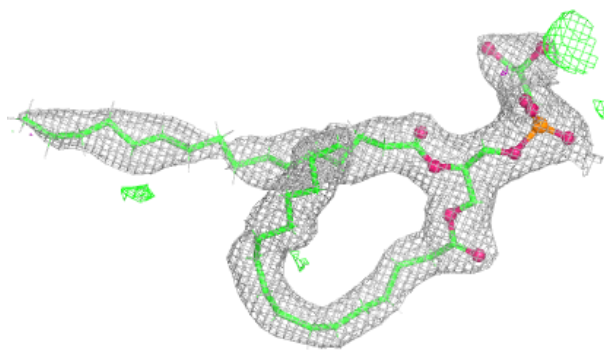
**Electron density around CLA B 605:**

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



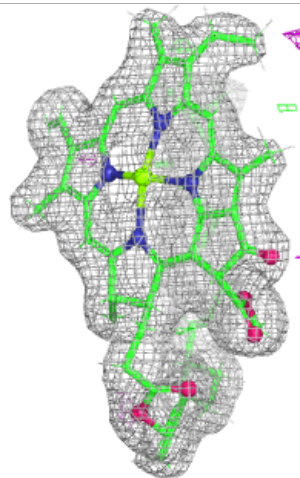
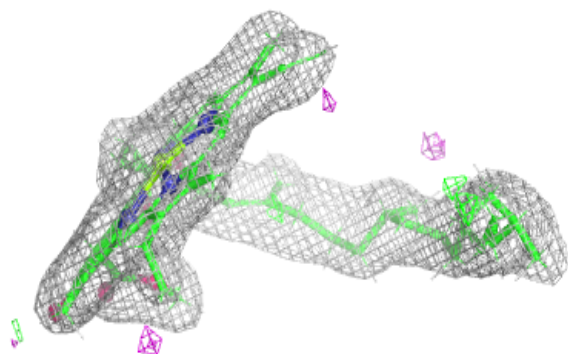
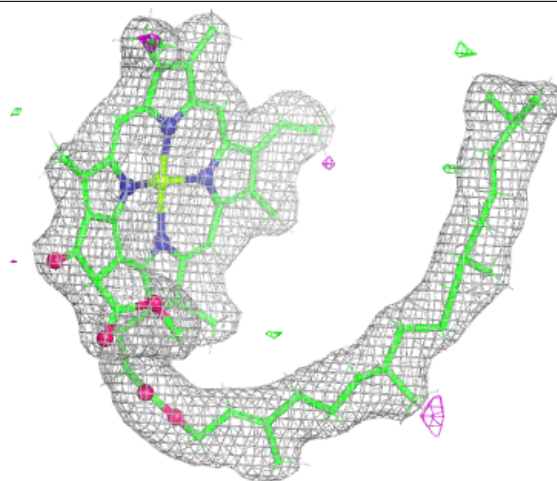
Electron density around LHG B 622:

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



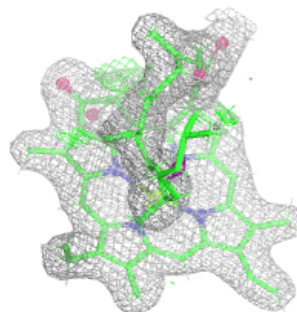
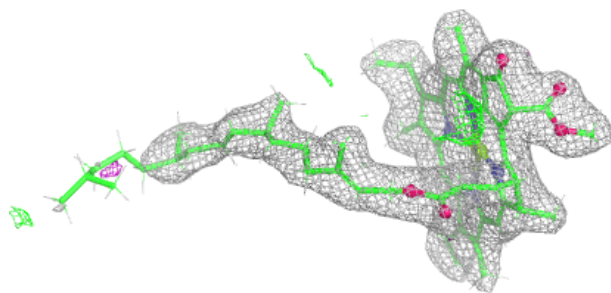
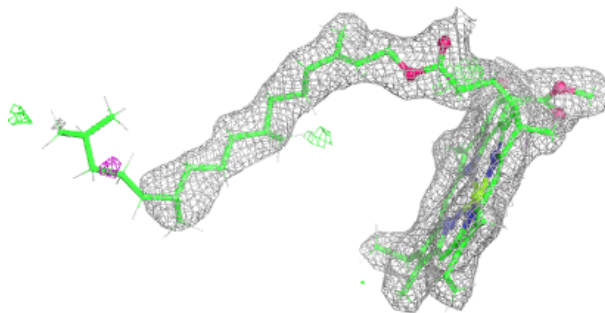
Electron density around CLA C 507:

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



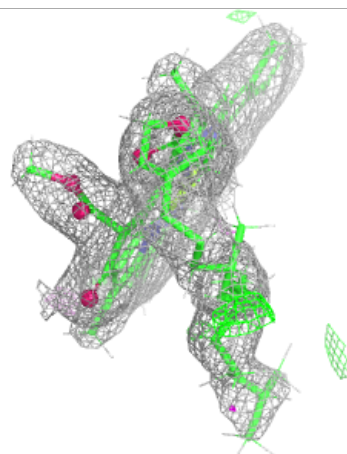
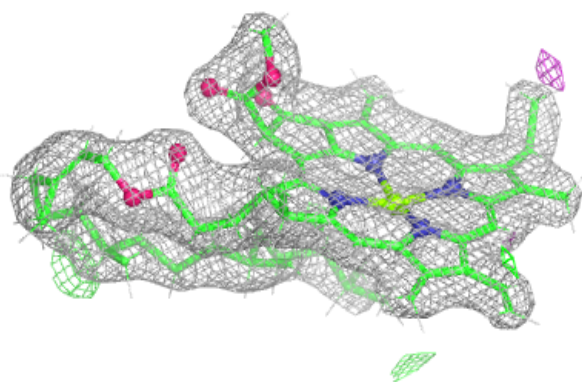
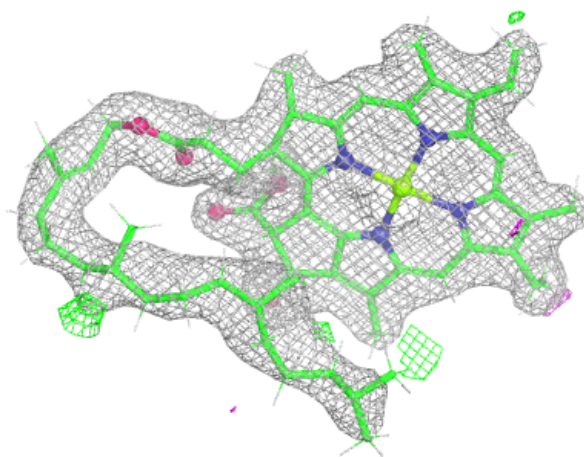
Electron density around CLA C 508:

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



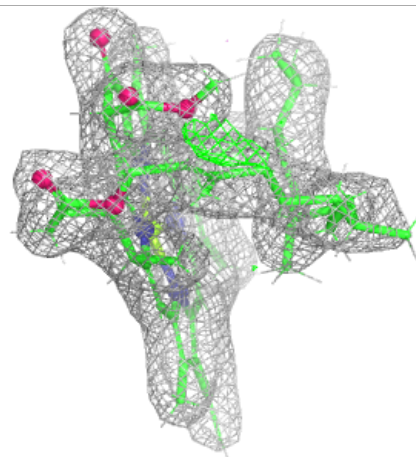
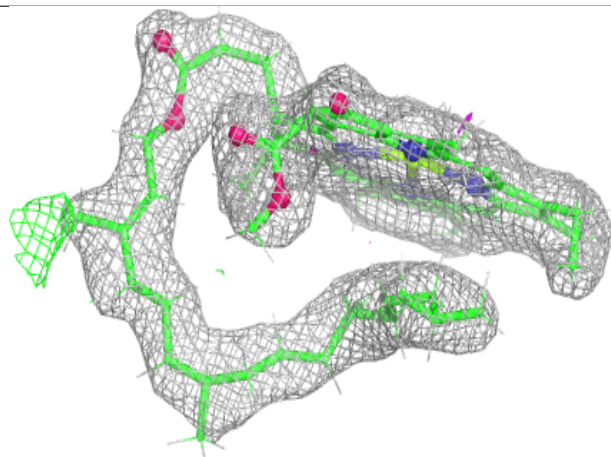
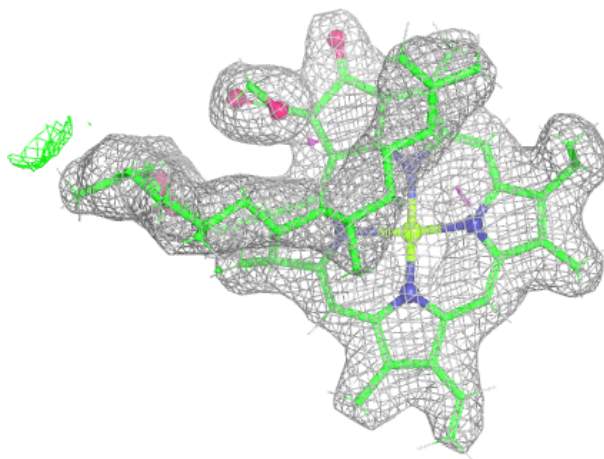
Electron density around CLA C 509:

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



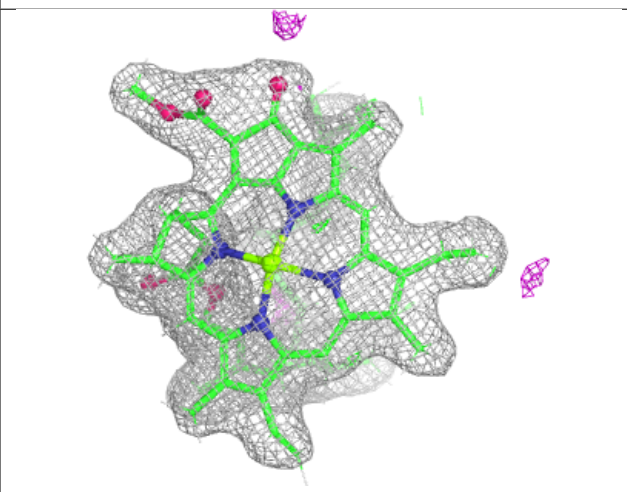
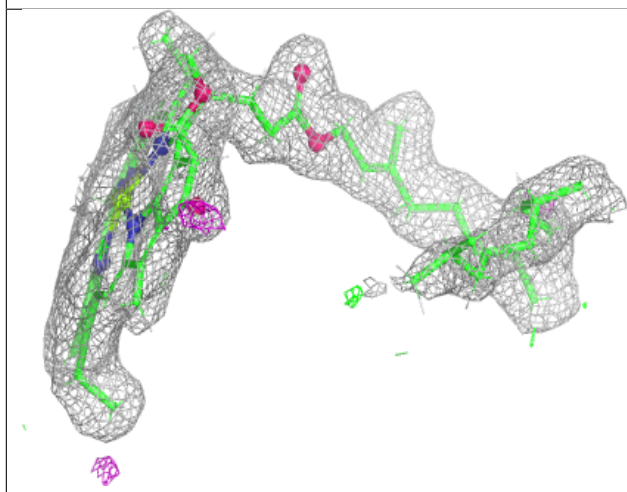
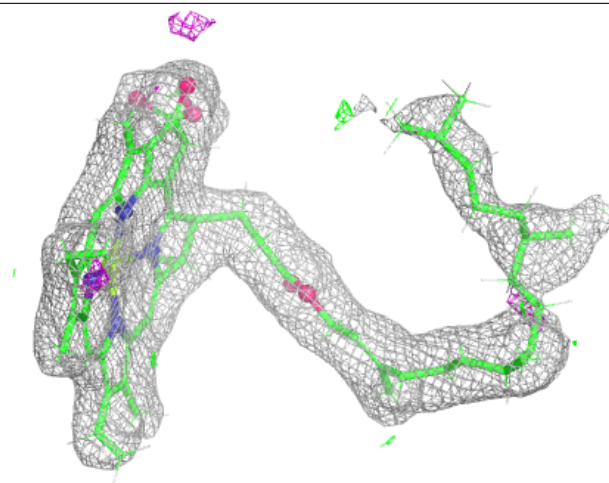
Electron density around CLA C 510:

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



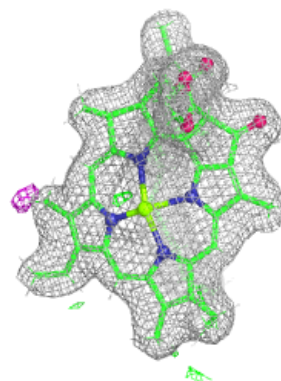
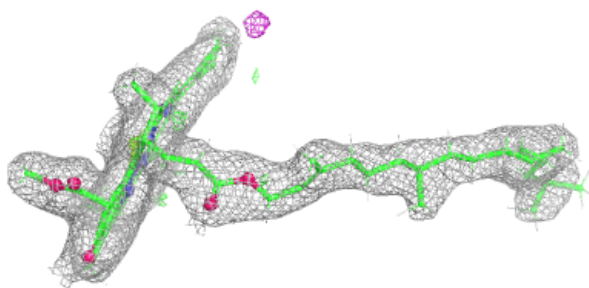
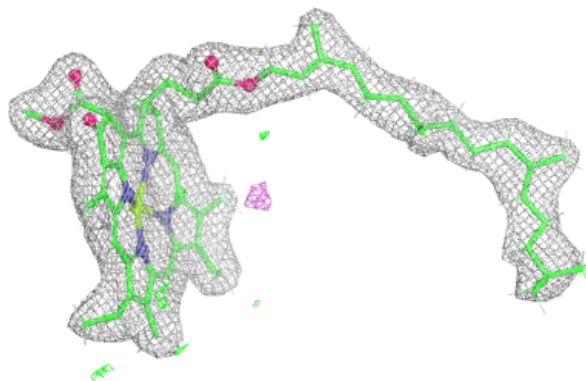
Electron density around CLA B 606:

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



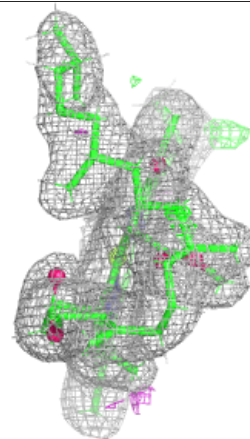
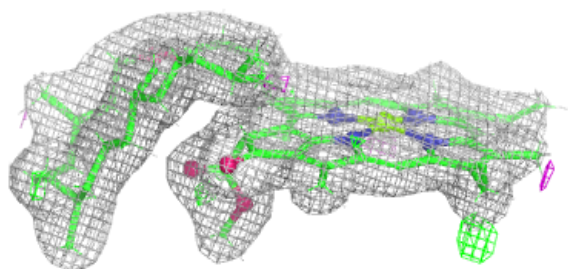
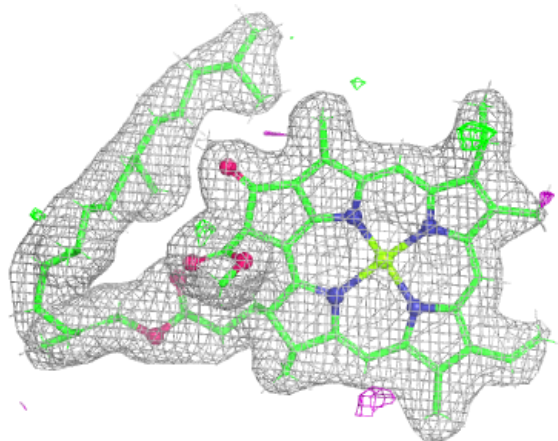
Electron density around CLA B 609:

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



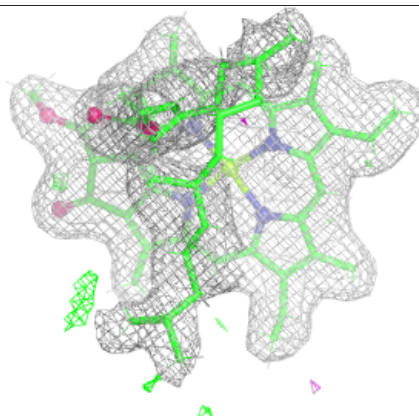
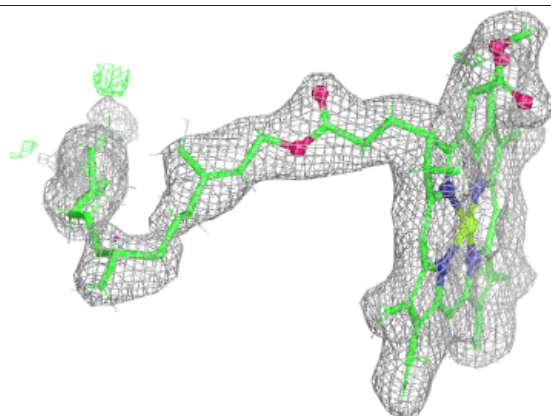
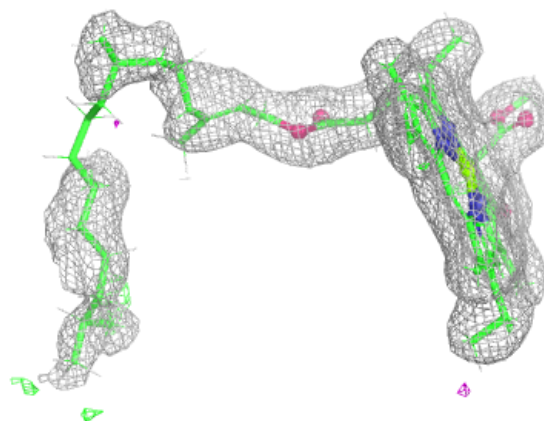
Electron density around CLA B 610:

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

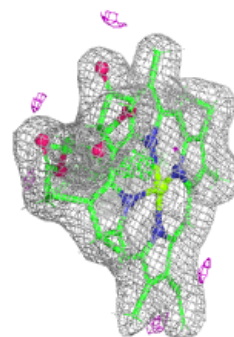
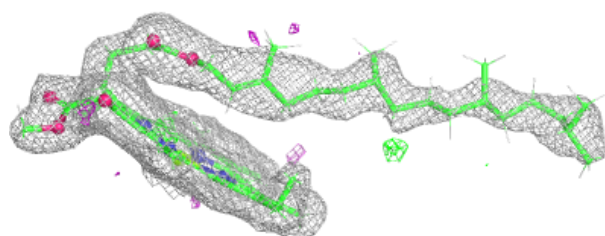
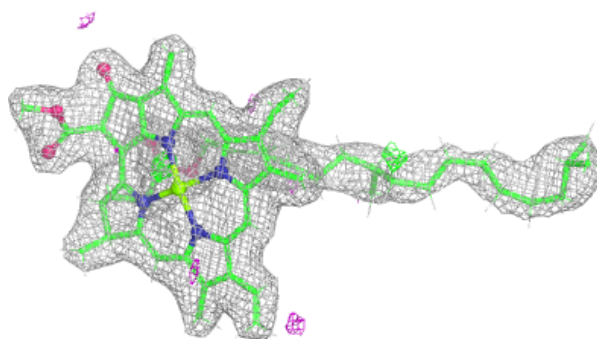


Electron density around CLA a 404:

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

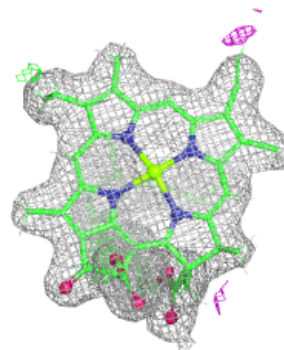
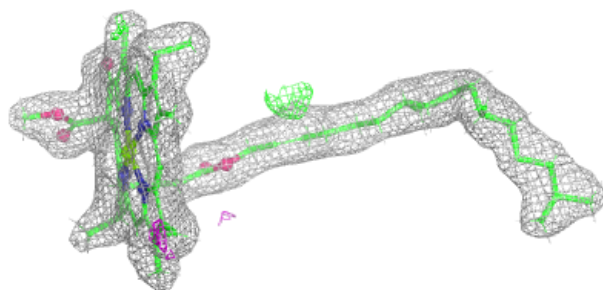
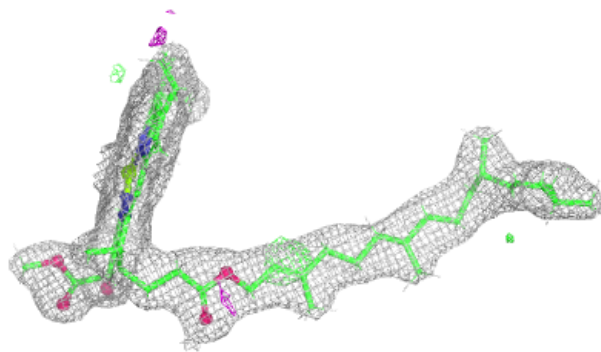
**Electron density around CLA B 614:**

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



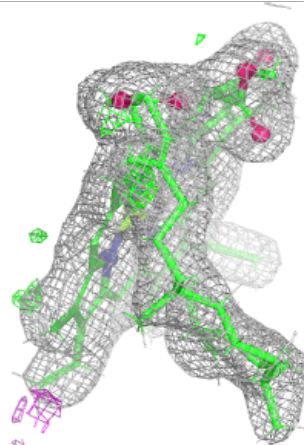
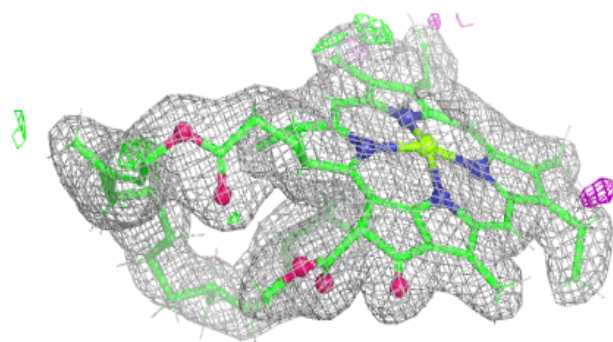
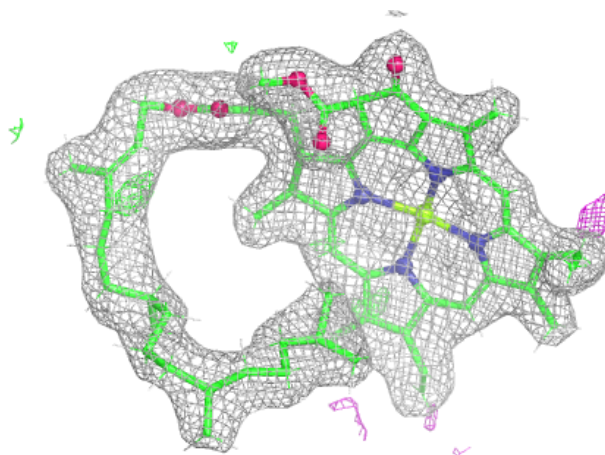
Electron density around CLA b 605:

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



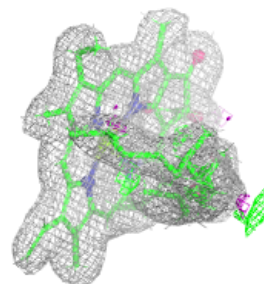
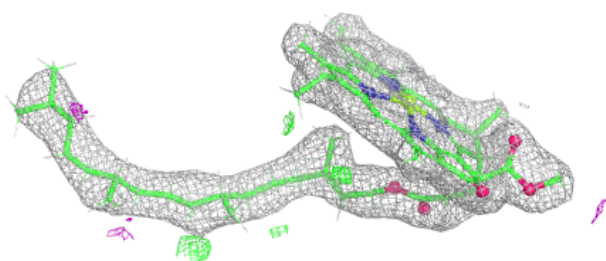
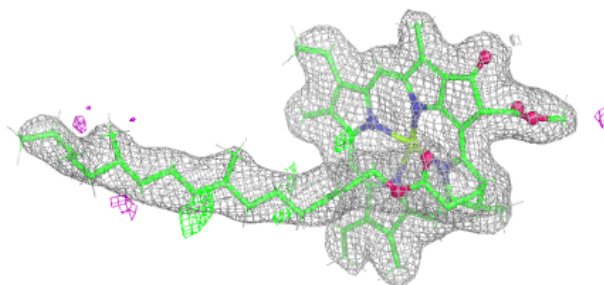
Electron density around CLA B 615:

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

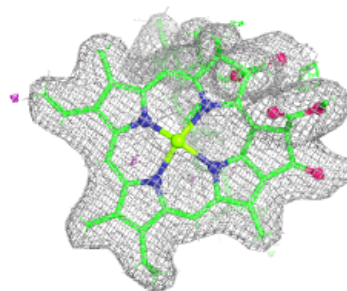
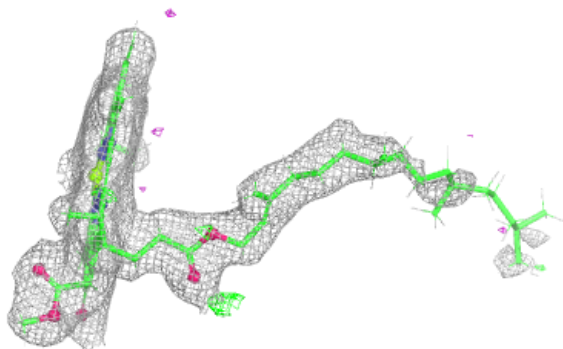
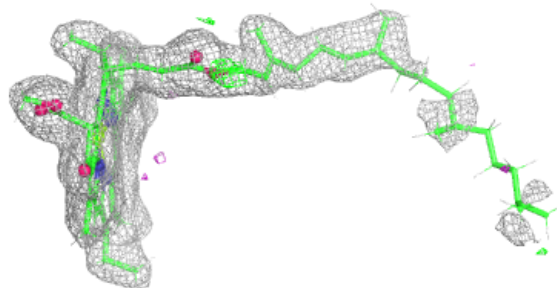


Electron density around CLA b 608:

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

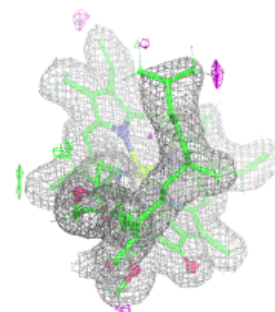
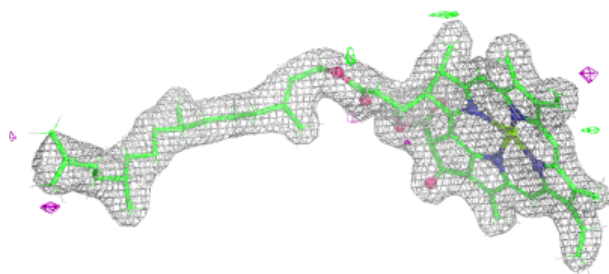
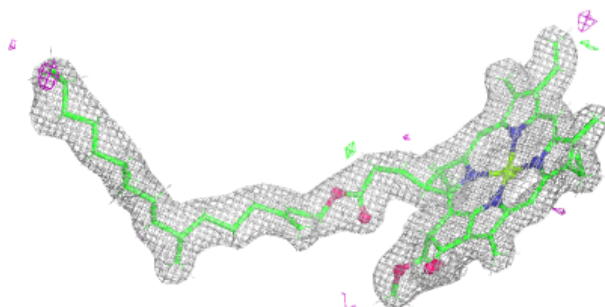
**Electron density around CLA D 404:**

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

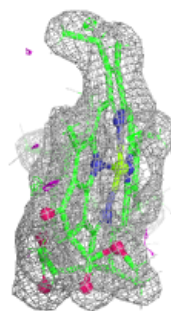
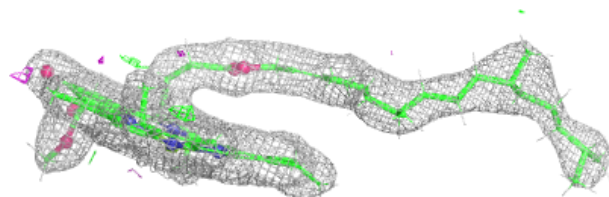
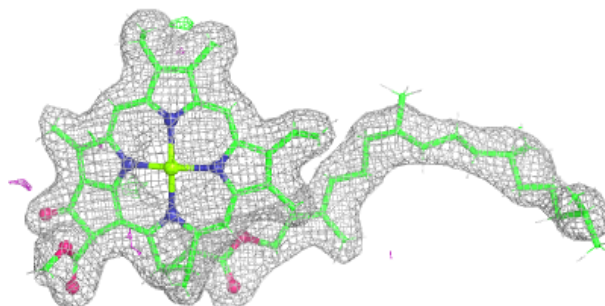


Electron density around CLA a 402:

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

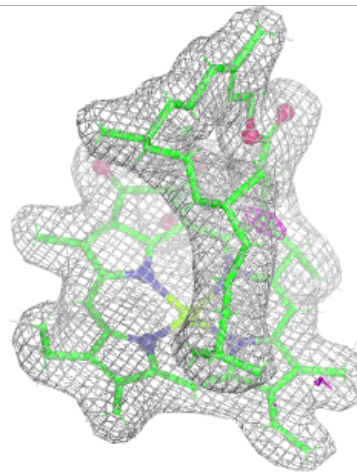
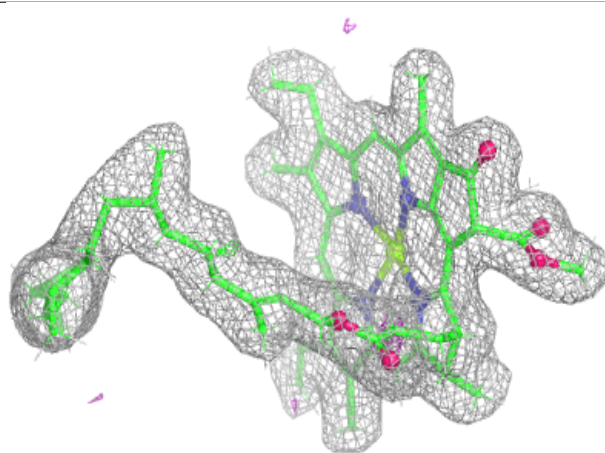
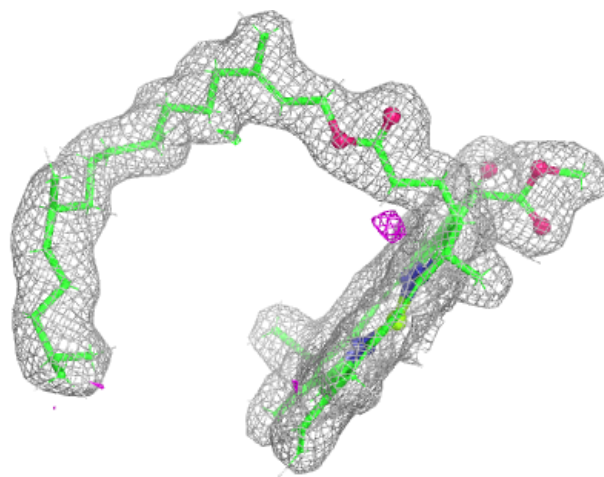
**Electron density around CLA B 603:**

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



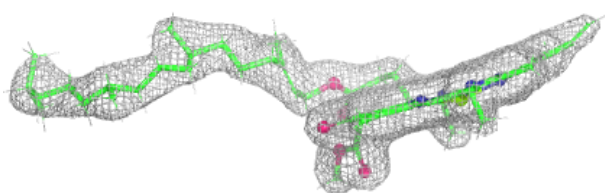
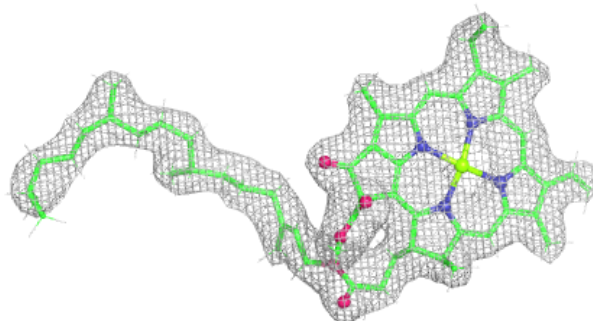
Electron density around CLA B 611:

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

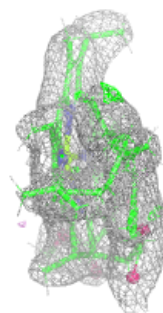
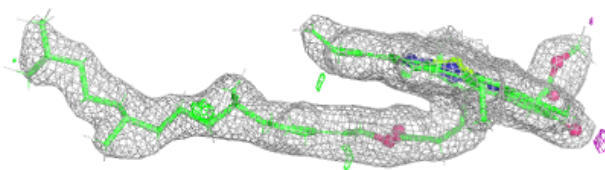
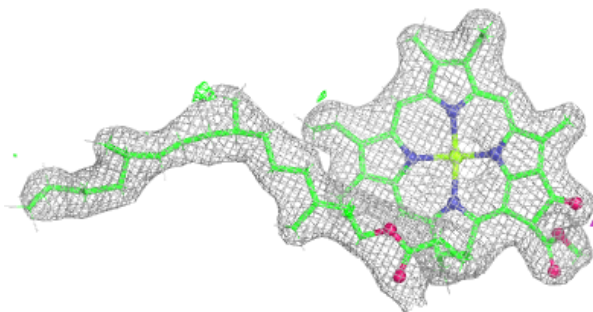


Electron density around CLA b 602:

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

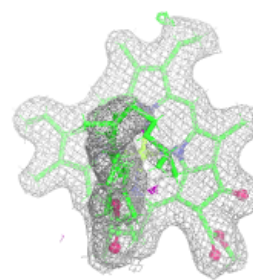
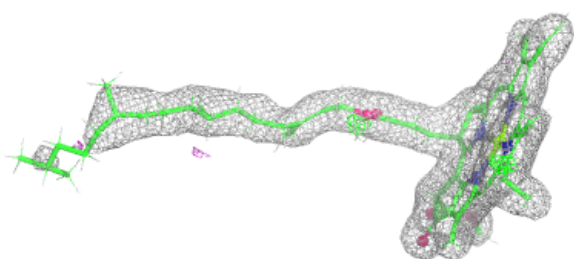
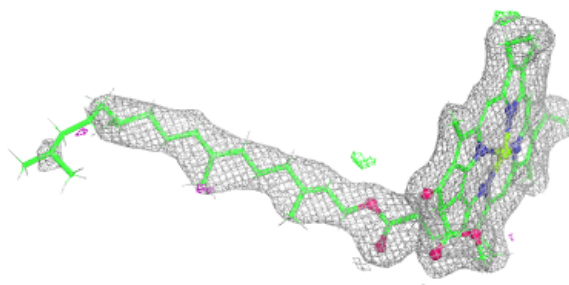
**Electron density around CLA b 603:**

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

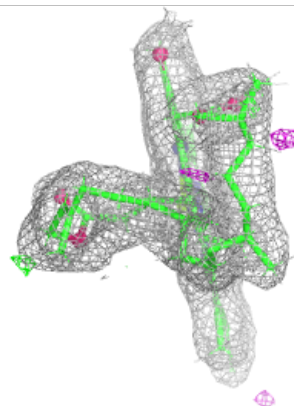
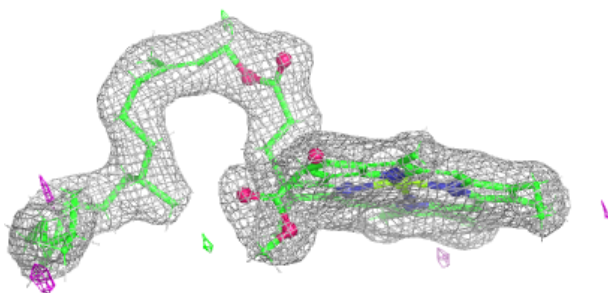
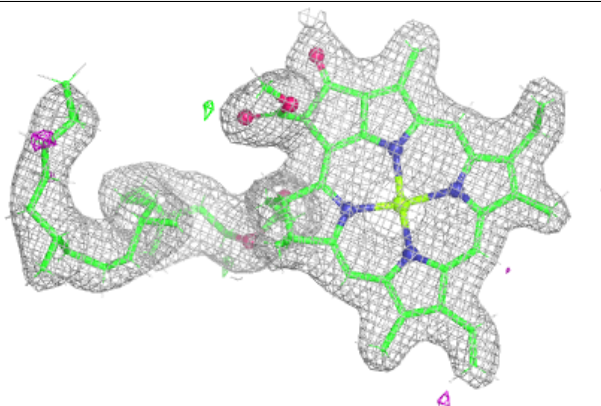


Electron density around CLA b 604:

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

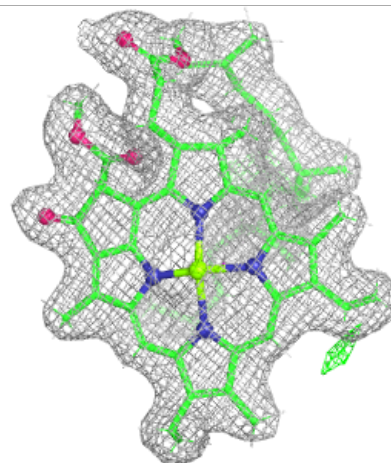
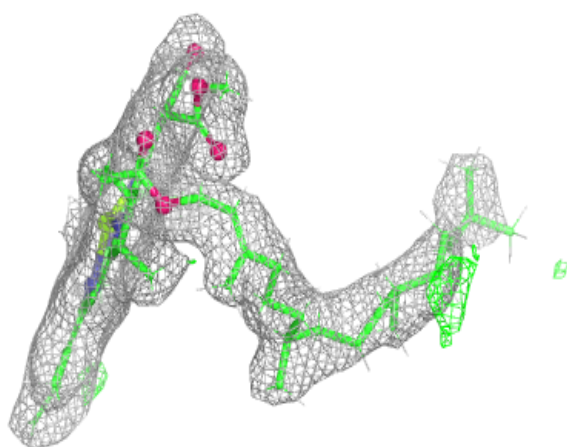
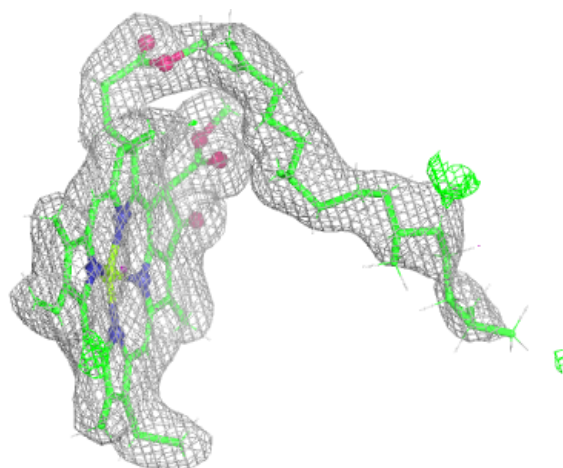
**Electron density around CLA B 612:**

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



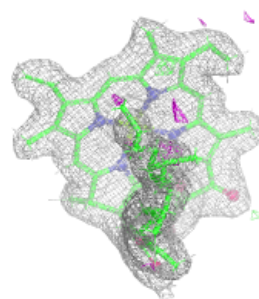
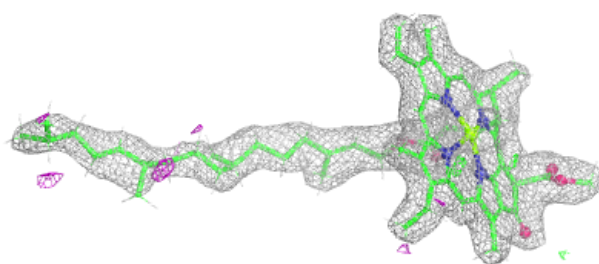
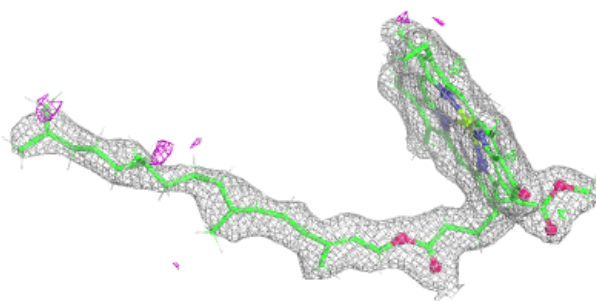
Electron density around CLA B 613:

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

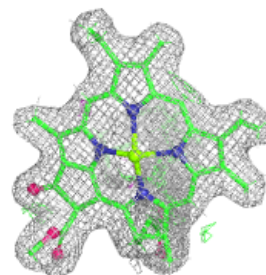
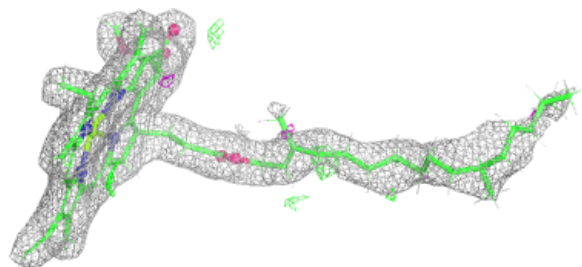
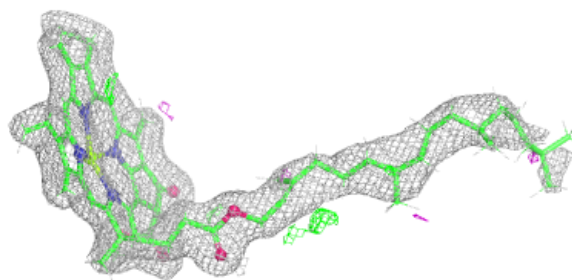


Electron density around CLA b 607:

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

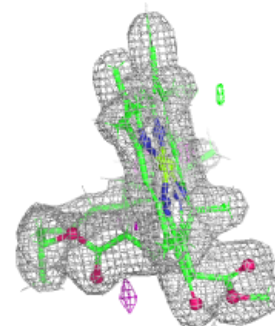
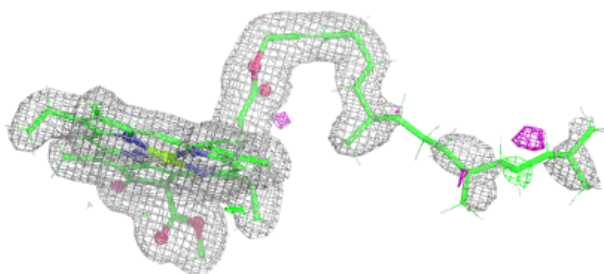
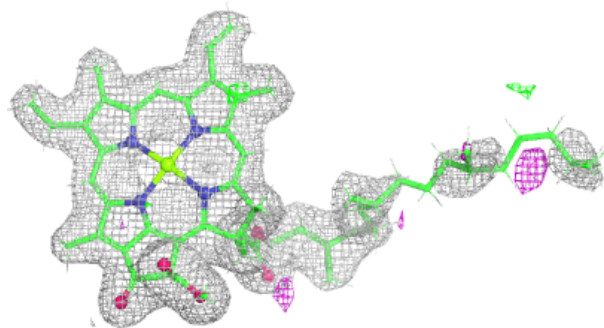
**Electron density around CLA B 604:**

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

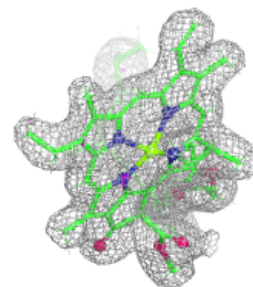
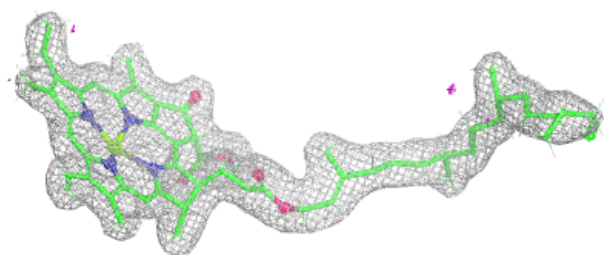
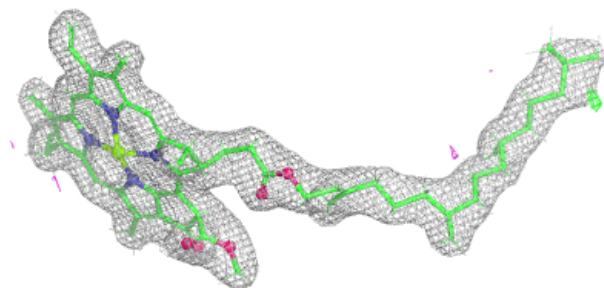


Electron density around CLA A 403:

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

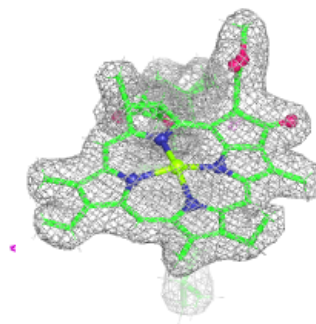
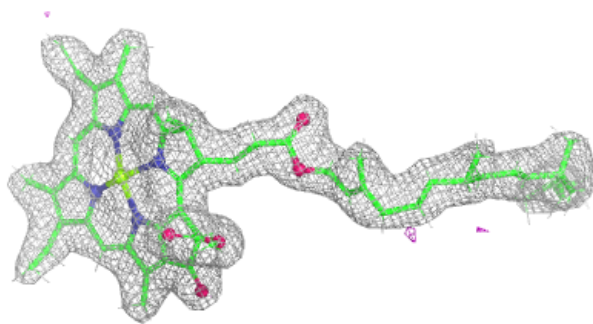
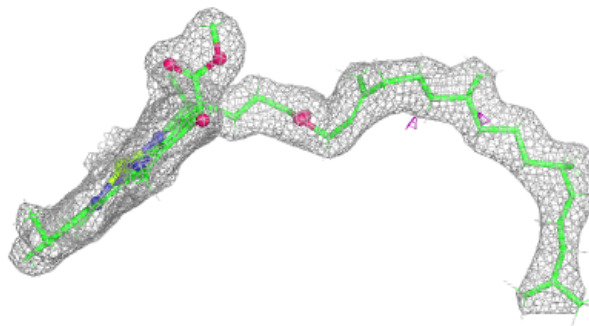
**Electron density around CLA A 402:**

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



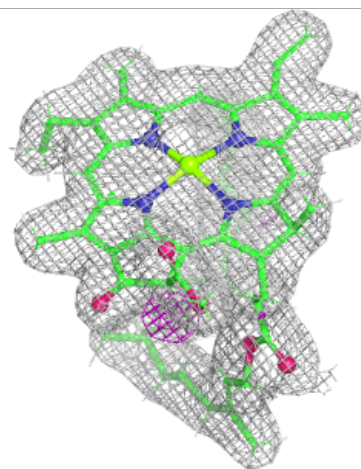
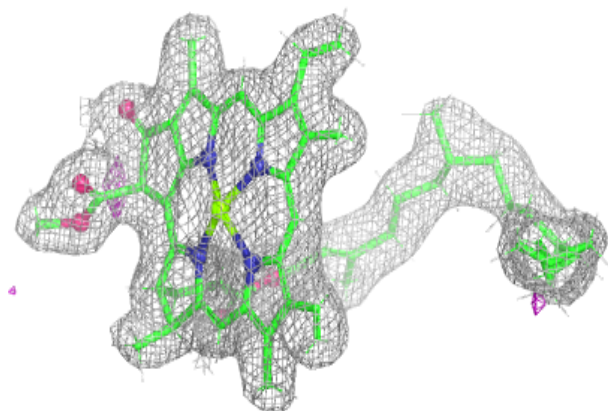
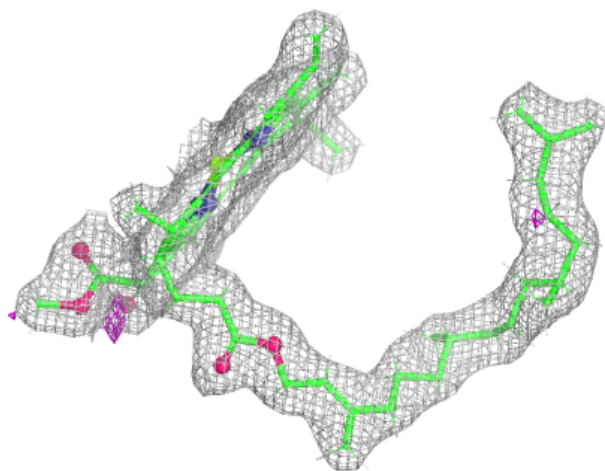
Electron density around CLA d 403:

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



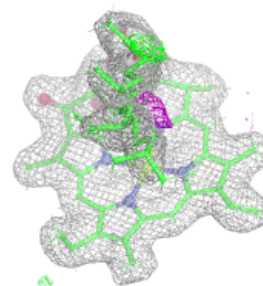
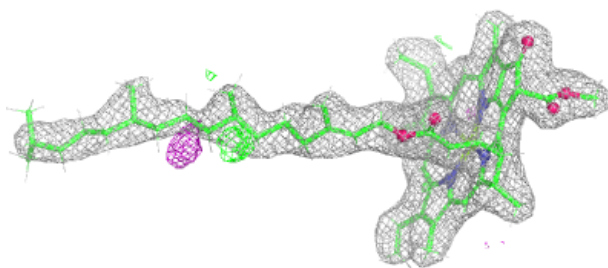
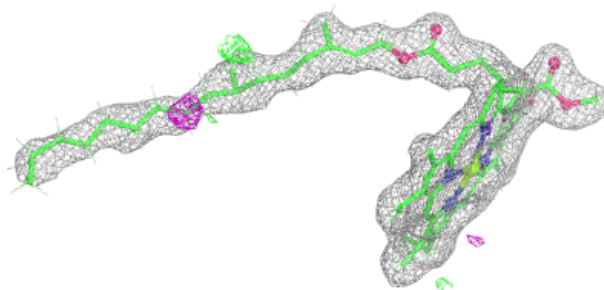
Electron density around CLA b 611:

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



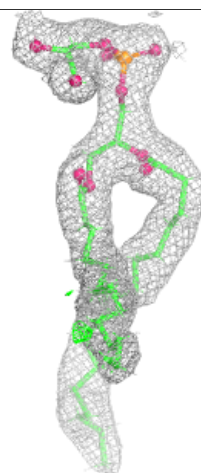
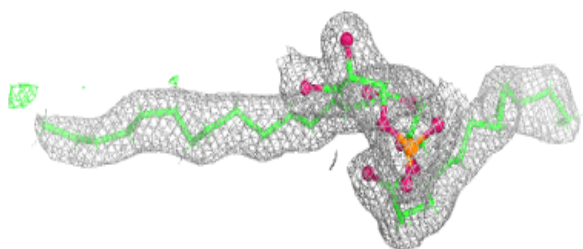
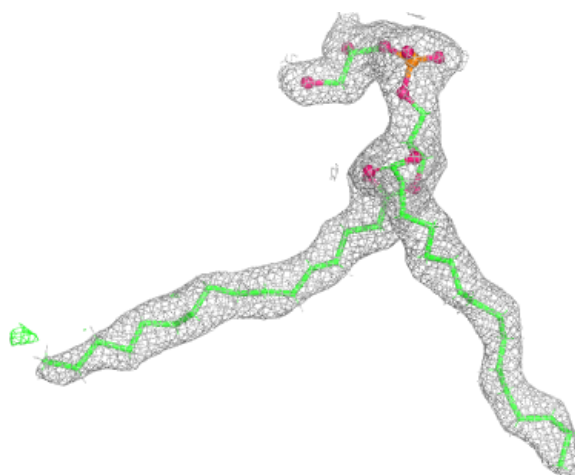
Electron density around CLA B 607:

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



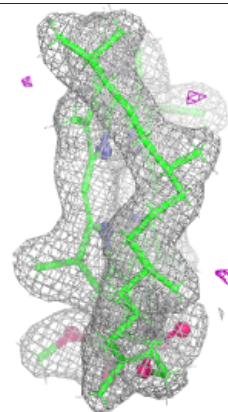
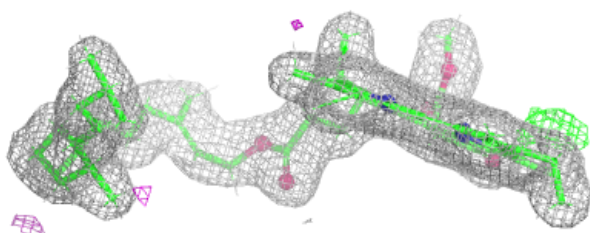
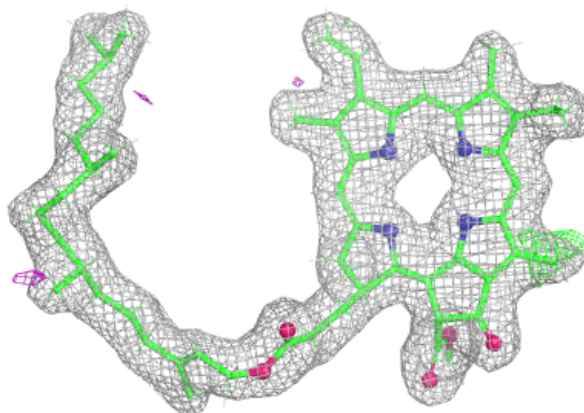
Electron density around LHG B 621:

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

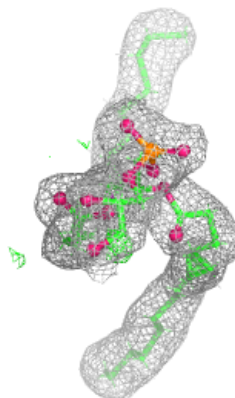
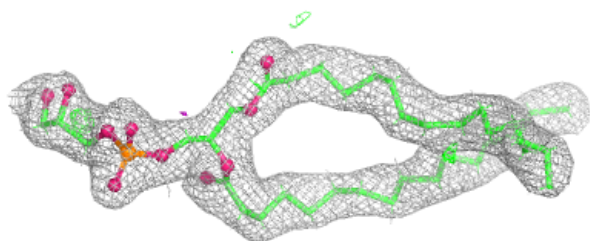
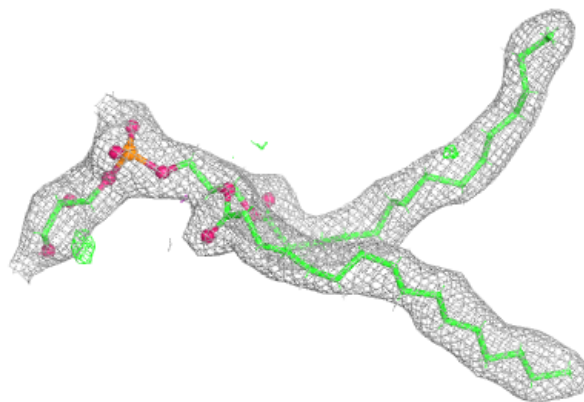


Electron density around PHO A 404:

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

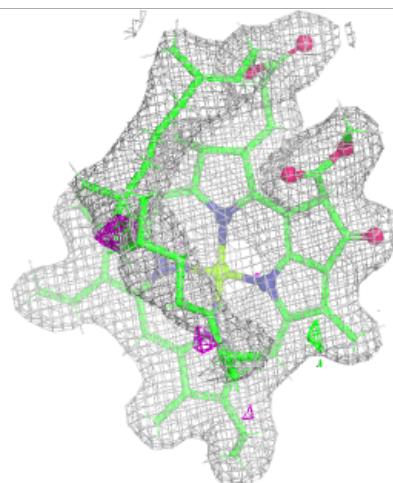
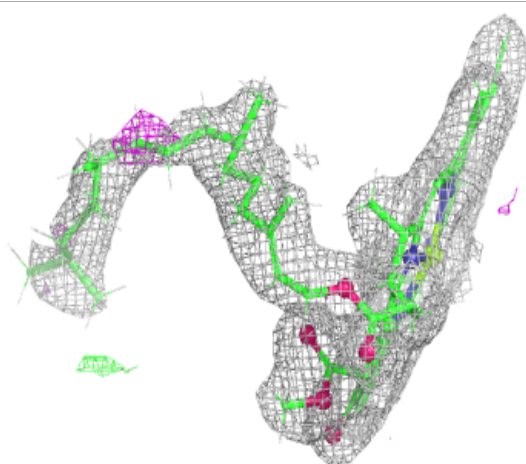
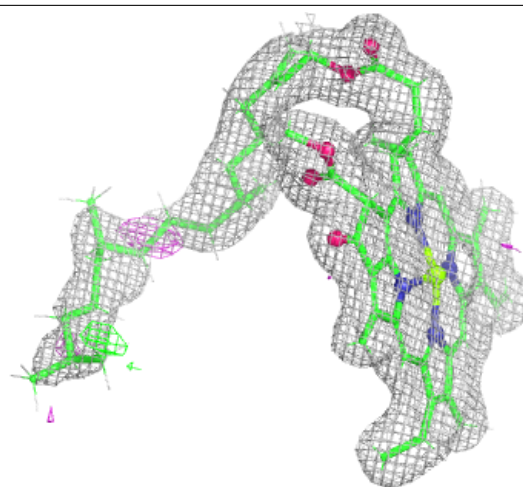
**Electron density around LHG D 409:**

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



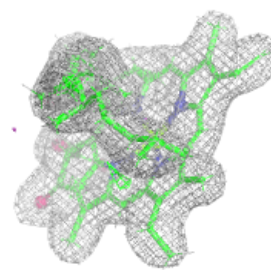
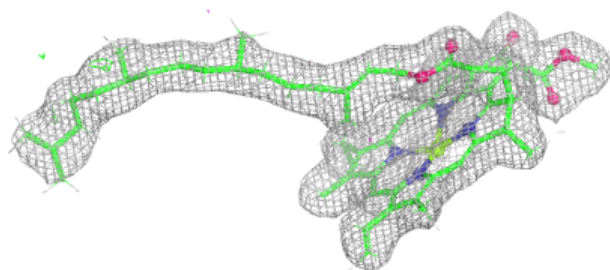
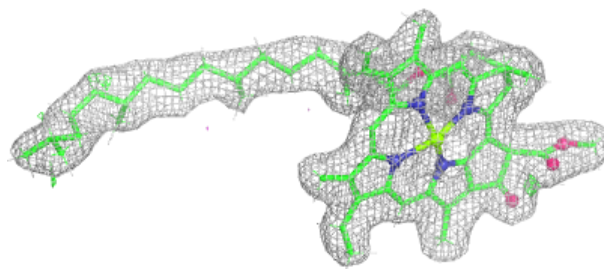
Electron density around CLA b 613:

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

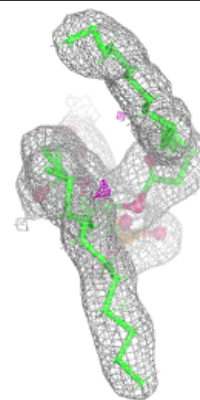
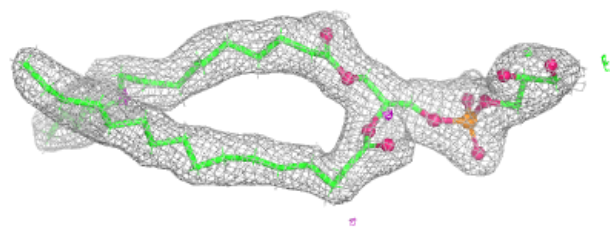
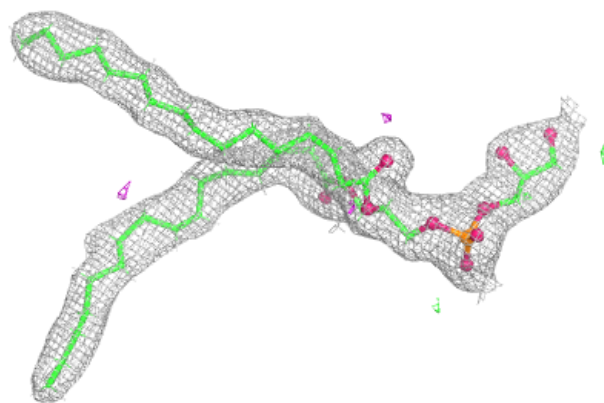


Electron density around CLA B 608:

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

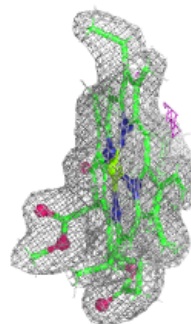
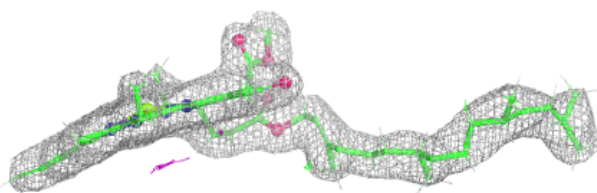
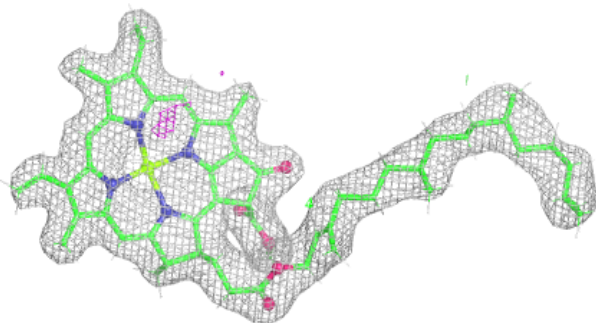
**Electron density around LHG d 408:**

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

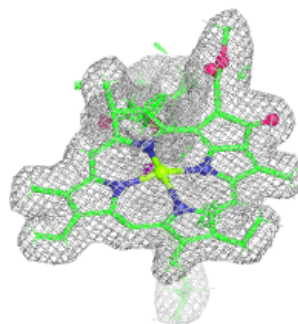
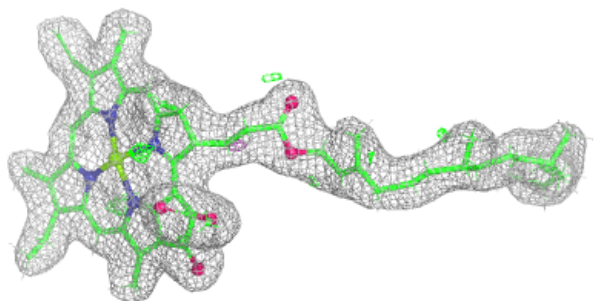
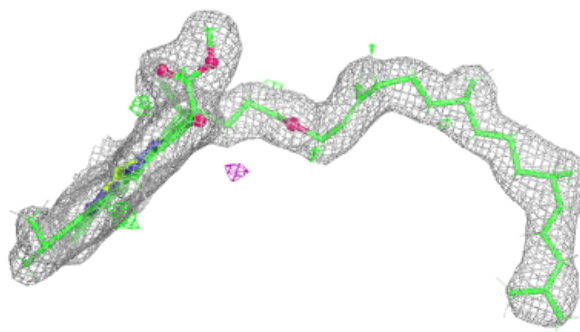


Electron density around CLA B 602:

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

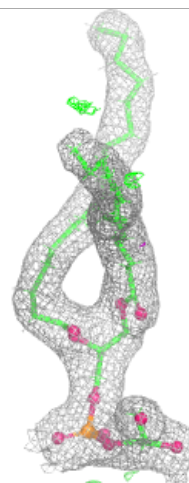
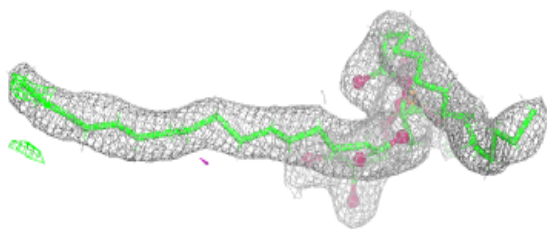
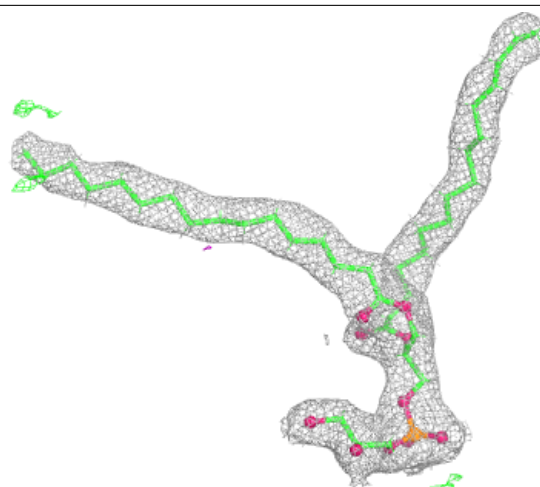
**Electron density around CLA D 402:**

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



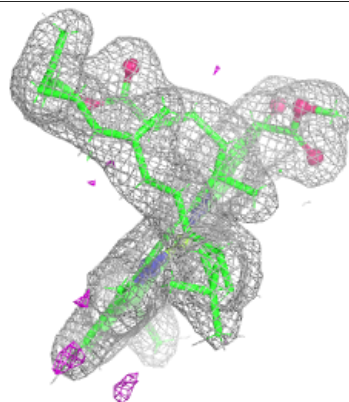
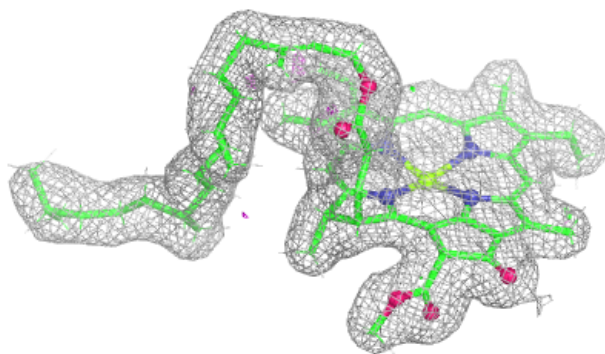
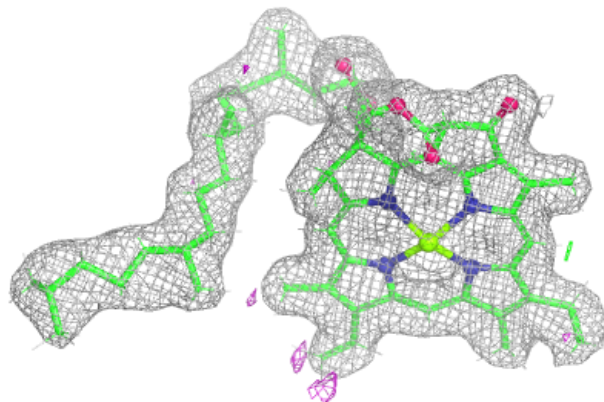
Electron density around LHG 1 101:

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



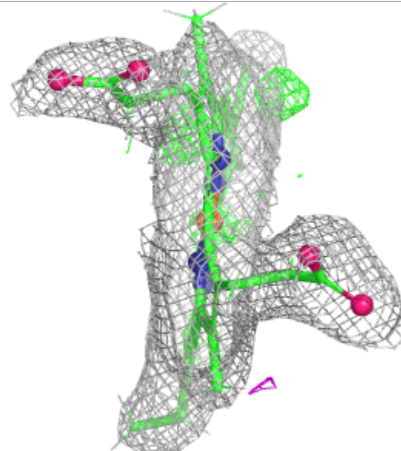
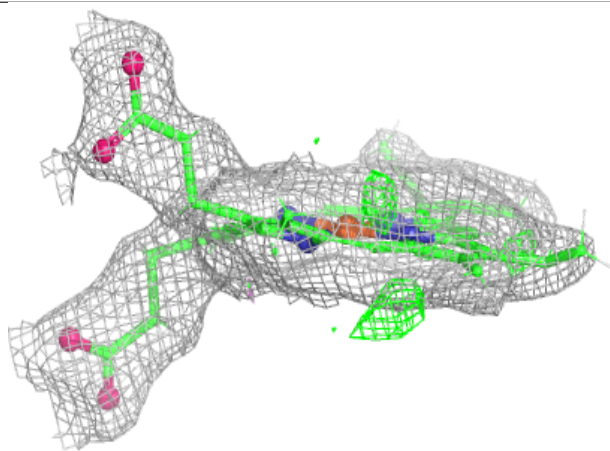
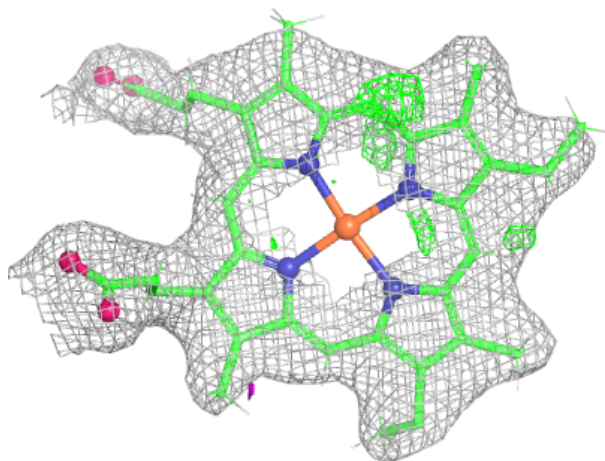
Electron density around CLA D 403:

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



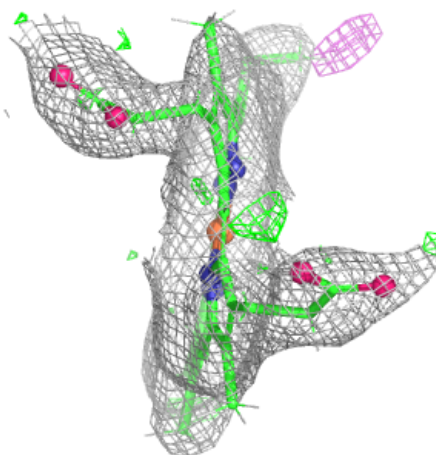
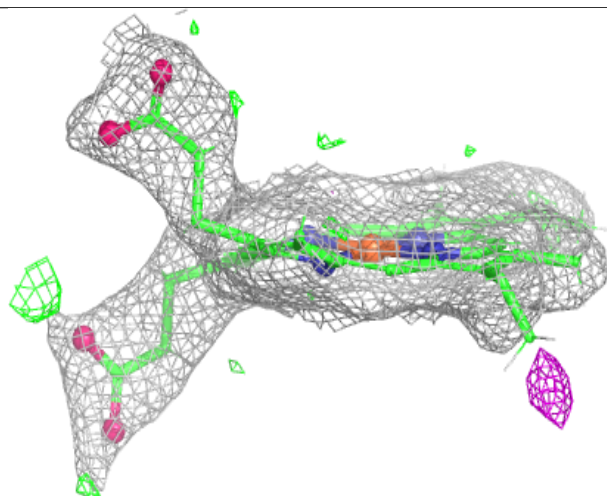
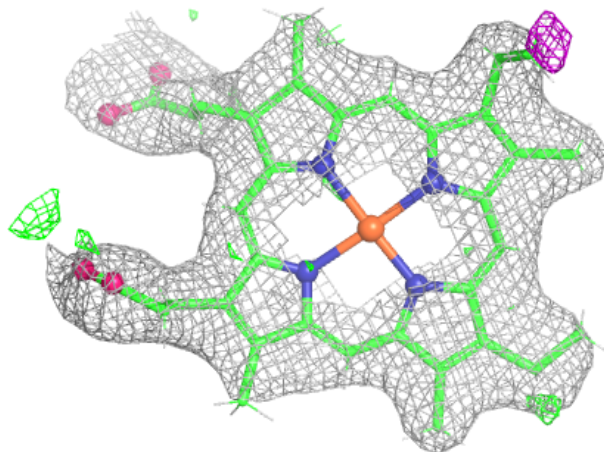
Electron density around HEC F 101:

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



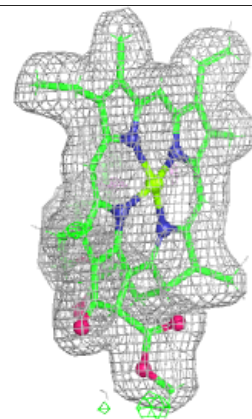
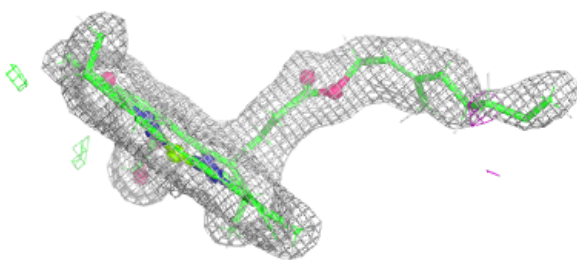
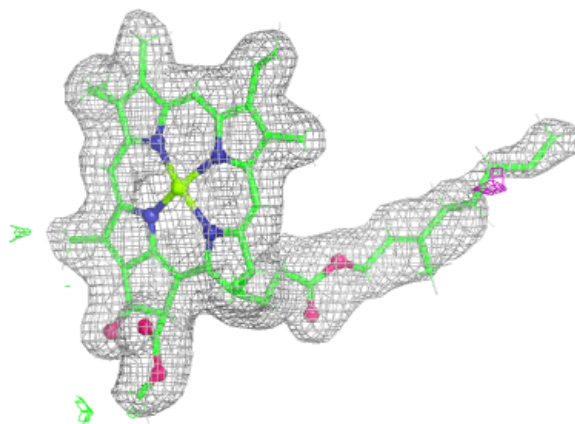
Electron density around HEC f 101:

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



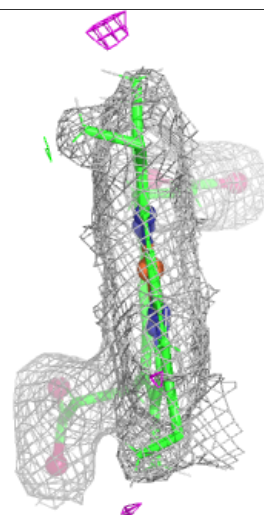
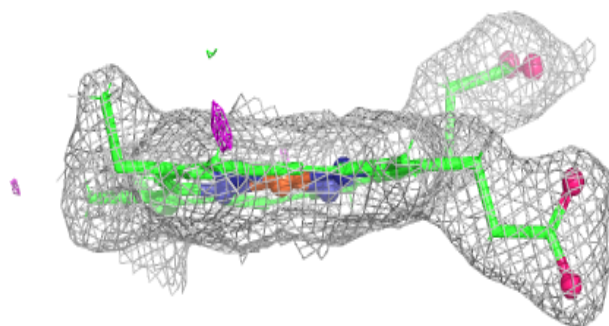
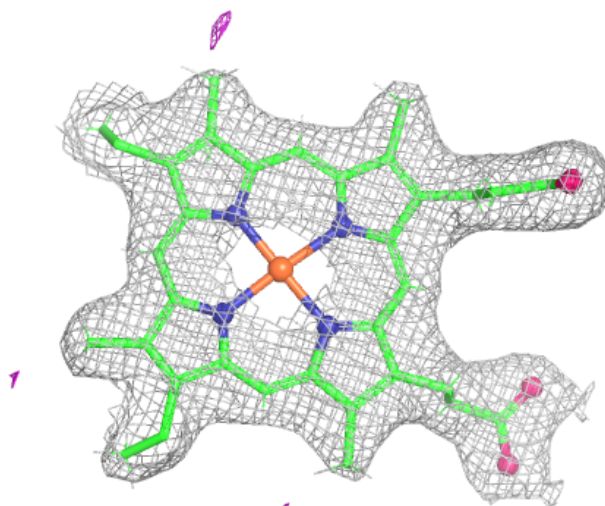
Electron density around CLA A 406:

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



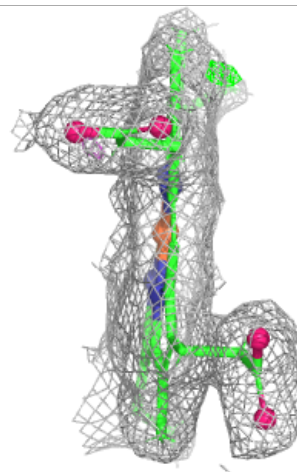
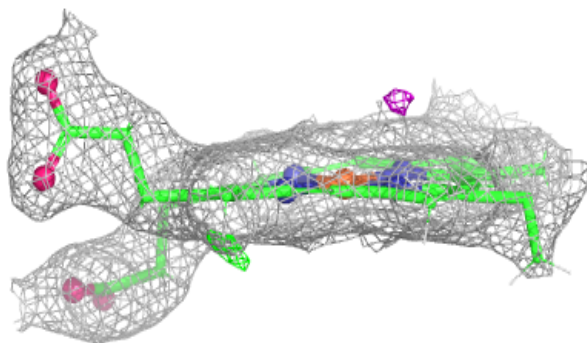
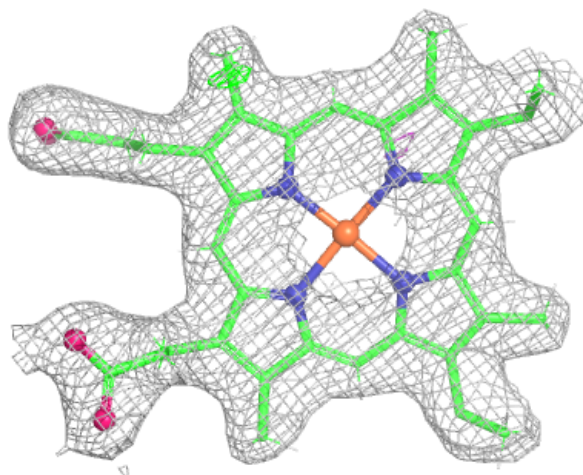
Electron density around HEC v 201:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.