



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:17 PM EDT

PDB ID : 7RF6 / pdb_00007rf6
Title : RT XFEL structure of Photosystem II 250 microseconds after the second illumination at 2.01 Angstrom resolution
Authors : Hussein, R.; Ibrahim, M.; Bhowmick, A.; Simon, P.S.; Chatterjee, R.; Lassalle, L.; Doyle, M.D.; Bogacz, I.; Kim, I.-S.; Cheah, M.H.; Gul, S.; de Lichtenberg, C.; Chernev, P.; Pham, C.C.; Young, I.D.; Carbajo, S.; Fuller, F.D.; Alonso-Mori, R.; Batyuk, A.; Sutherlin, K.D.; Brewster, A.S.; Bolotovskii, R.; Mendez, D.; Holton, J.M.; Moriarty, N.W.; Adams, P.D.; Bergmann, U.; Sauter, N.K.; Dobbek, H.; Messinger, J.; Zouni, A.; Kern, J.; Yachandra, V.K.; Yano, J.
Deposited on : 2021-07-13
Resolution : 2.01 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)
CCP4	: 9.0.015 (Gargrove)

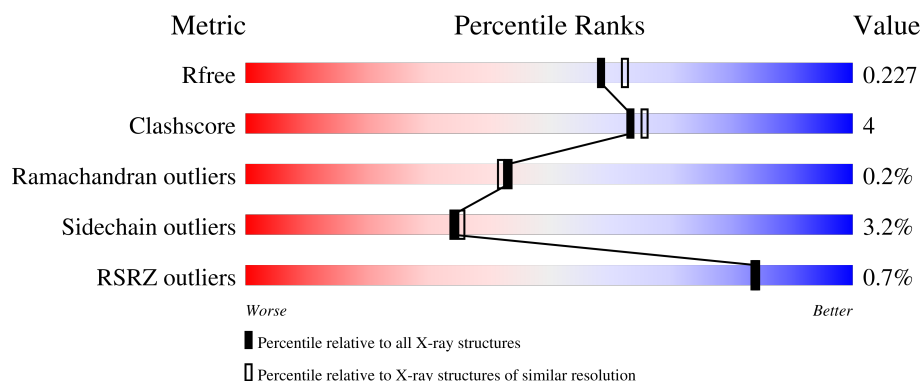
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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)

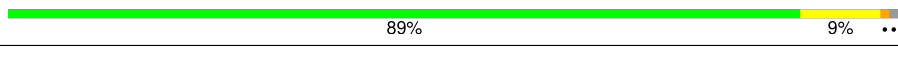
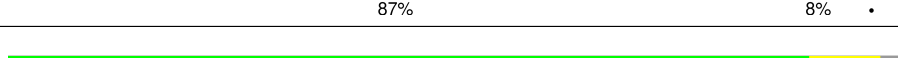
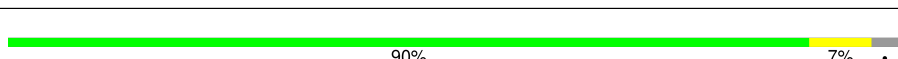
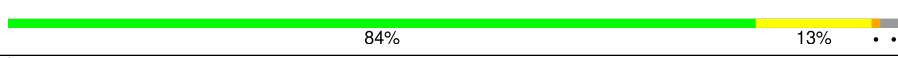
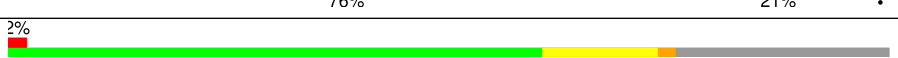
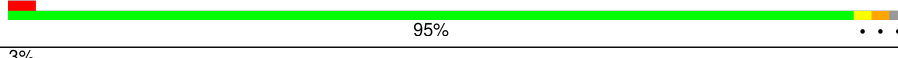
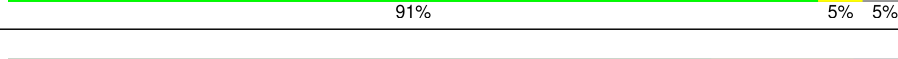
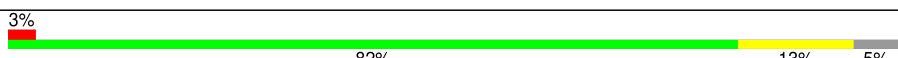
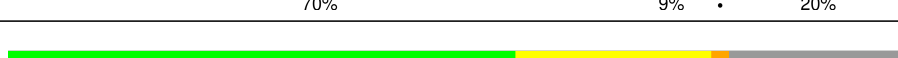
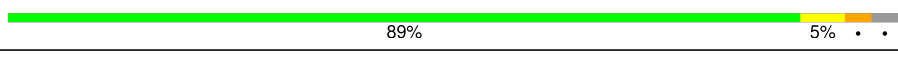
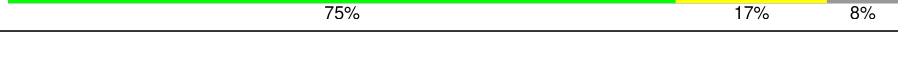
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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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Density-Fitness : 1.0.12
 Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.50

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

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

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

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

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 106128 atoms, of which 52762 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	H	N	O S	0	0	0
			557	187	282	45	42 1			
6	f	34	Total	C	H	N	O S	0	0	0
			557	187	282	45	42 1			

- 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 S	0	0	0
			1042	341	532	82	85 2			
7	h	63	Total	C	H	N	O S	0	0	0
			1016	333	518	80	83 2			

- 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 S	0	0	0
			607	200	311	46	49 1			
8	i	36	Total	C	H	N	O S	0	0	0
			607	200	311	46	49 1			

- 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 S	0	0	0
			525	174	268	40	42 1			
9	j	36	Total	C	H	N	O S	0	0	0
			525	174	268	40	42 1			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	H	N	O	S	0	0
			620	202	316	48	53	1		
11	l	36	Total	C	H	N	O		0	0
			600	197	304	47	52			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	H	N	O	S	0	0
			525	171	269	37	47	1		
12	m	32	Total	C	H	N	O	S	0	0
			518	168	267	36	46	1		

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	244	Total	C	H	N	O	S	0	1
			3700	1168	1830	313	385	4		0
13	o	244	Total	C	H	N	O	S	0	0
			3720	1170	1846	317	383	4		0

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

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

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

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

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

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

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

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

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

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

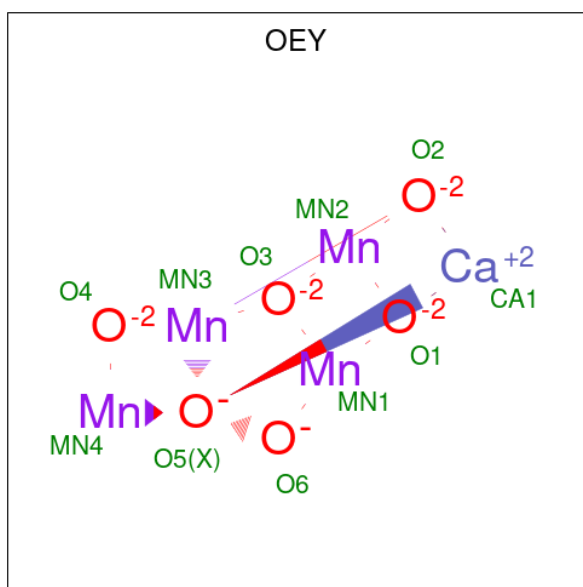
- Molecule 19 is a protein called Photosystem II reaction center protein Ycf12.

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

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

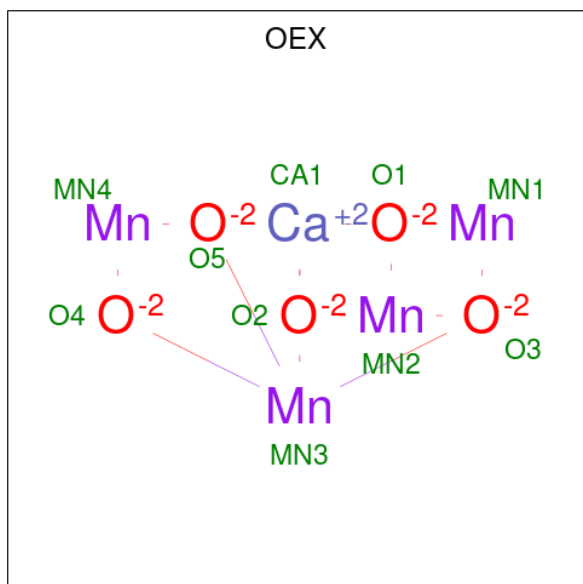
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Z	62	Total	C	H	N	O	S	0	0
			995	328	516	72	77	2		
20	z	62	Total	C	H	N	O	S	0	0
			986	326	509	72	77	2		

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

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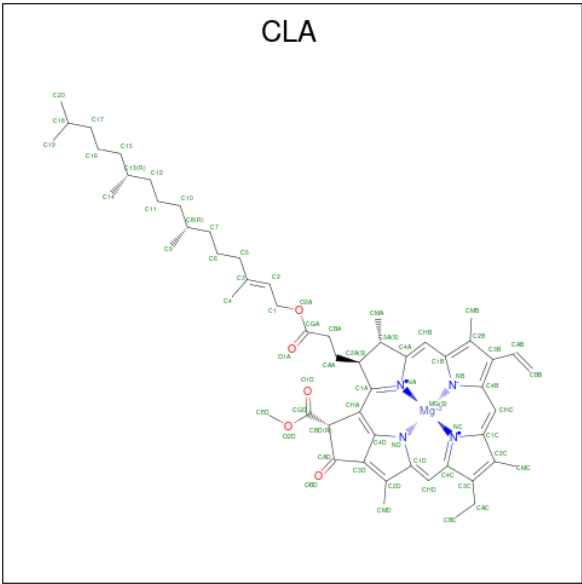
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

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

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

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



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

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

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

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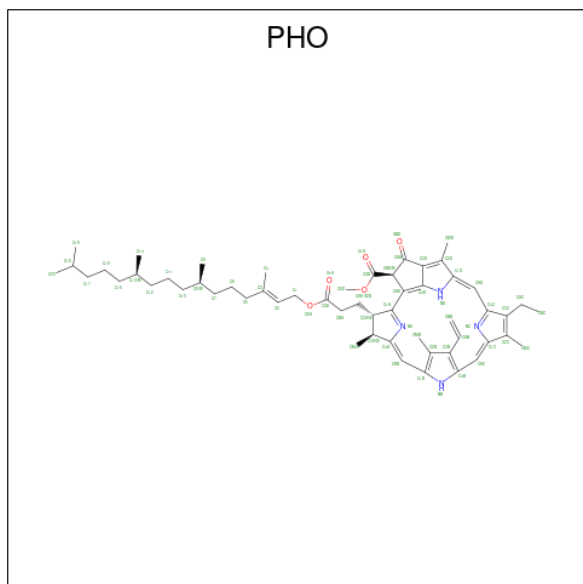
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
24	b	1	Total	C	H	Mg	N	O	0	0
			137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

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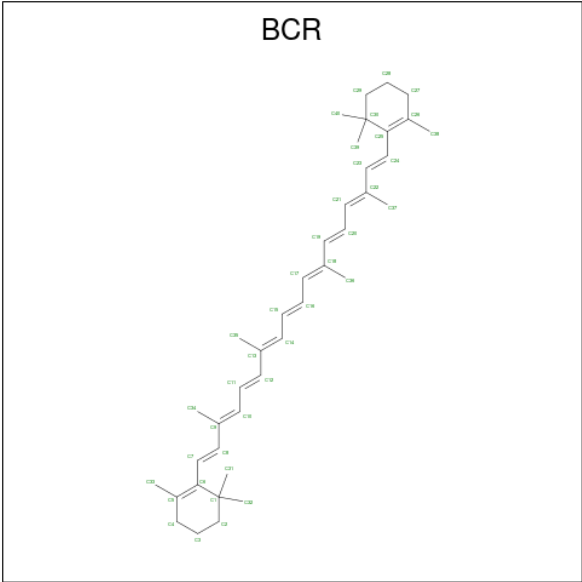
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
24	d	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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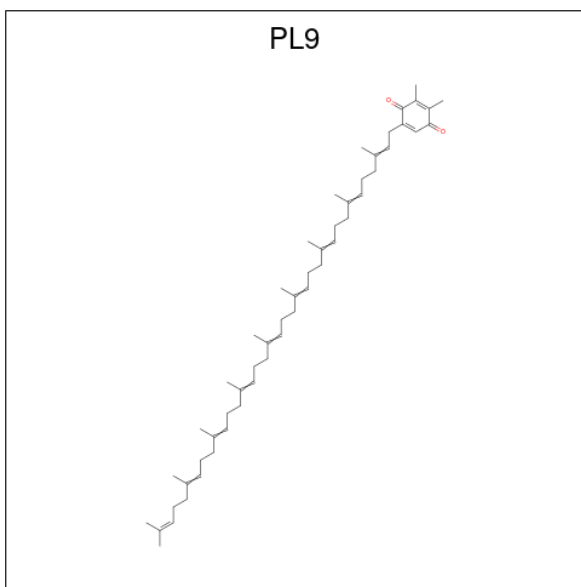
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	b	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	c	1	Total	C	H	0	0
			96	40	56		
26	d	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40	56		
26	k	1	Total	C	H	0	0
			96	40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

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

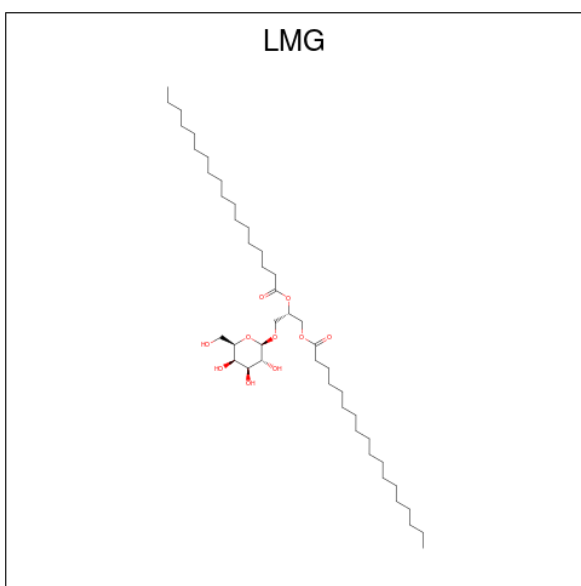
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	2	Total	Cl	0	0
			2	2		
27	a	2	Total	Cl	0	0
			2	2		

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



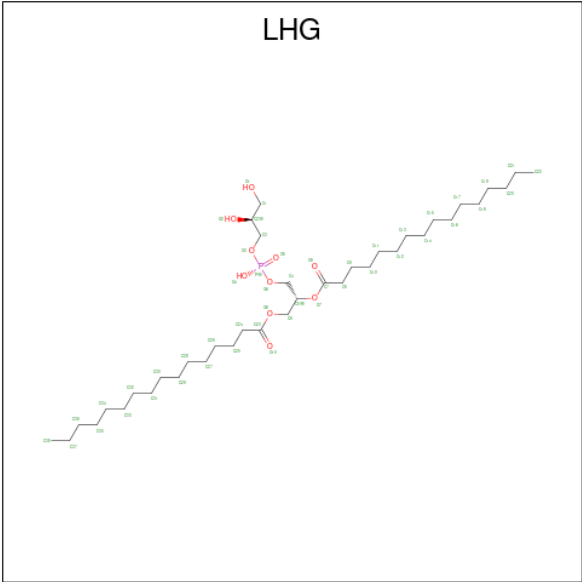
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	H	O	0	0
			135	53	80	2		
28	D	1	Total	C	H	O	0	0
			135	53	80	2		
28	a	1	Total	C	H	O	0	0
			135	53	80	2		
28	d	1	Total	C	H	O	0	0
			135	53	80	2		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



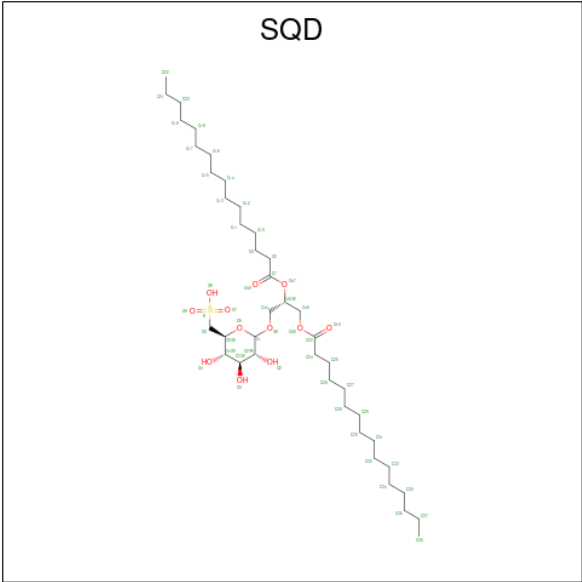
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
29	A	1	Total	C	H	O	0	0
			114	38	66	10		
29	C	1	Total	C	H	O	0	0
			114	38	66	10		
29	D	1	Total	C	H	O	0	0
			123	41	72	10		
29	D	1	Total	C	H	O	0	0
			78	27	45	6		
29	D	1	Total	C	H	O	0	0
			68	24	40	4		
29	M	1	Total	C	H	O	0	0
			123	41	72	10		
29	a	1	Total	C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

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



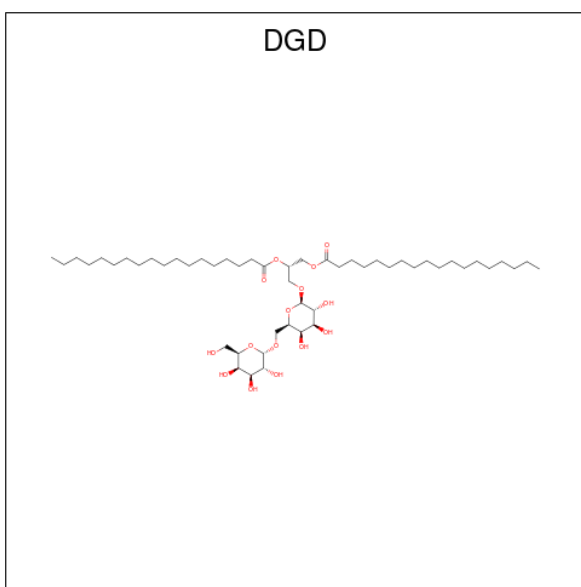
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
30	A	1	Total	C	H	O	P	0	0
			114	36	67	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	B	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	D	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	E	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
30	d	1	Total	C	H	O	P	0	0
			123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

- Molecule 31 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



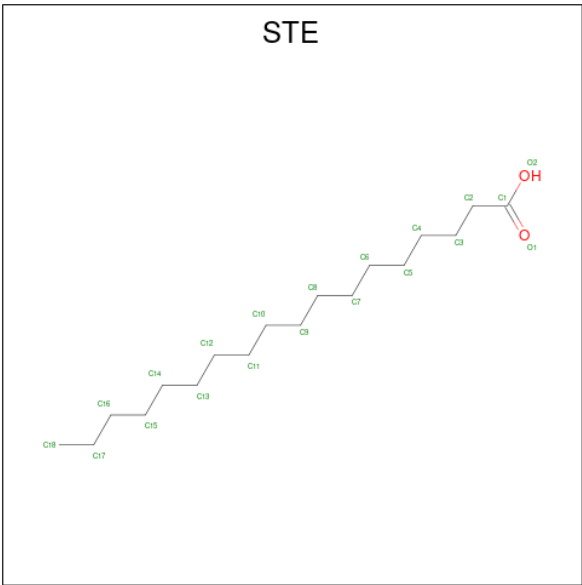
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	A	1	Total	C	H	O	S	0	0
			123	39	71	12	1		
31	A	1	Total	C	H	O		0	0
			104	35	65	4			
31	B	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
31	D	1	Total	C	H	O	S	0	0
			82	25	46	10	1		
31	a	1	Total	C	H	O	S	0	0
			132	41	78	12	1		
31	a	1	Total	C	H	O		0	0
			92	31	56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

- Molecule 32 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



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

- Molecule 33 is STEARIC ACID (CCD ID: STE) (formula: $C_{18}H_{36}O_2$).



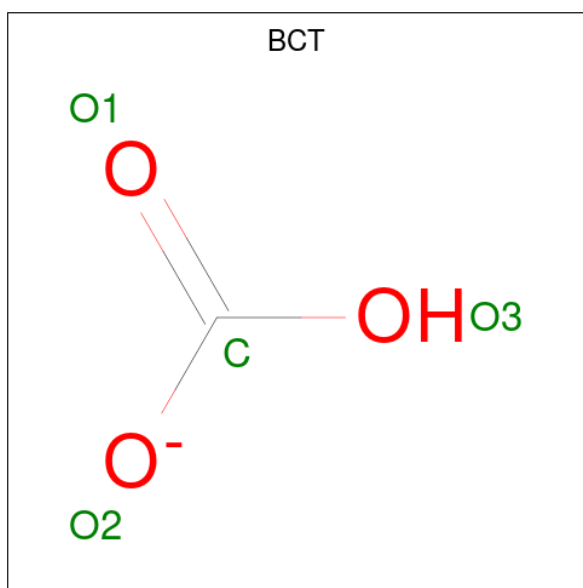
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	B	1	Total	C	H	O	0	0
			43	15	26	2		
33	B	1	Total	C	H	O	0	0
			34	12	20	2		
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	B	1	Total	C	H		0	0
			47	16	31			
33	B	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	C	1	Total	C	H		0	0
			47	16	31			
33	C	1	Total	C	H	O	0	0
			28	10	16	2		
33	D	1	Total	C	H	O	0	0
			55	18	35	2		
33	E	1	Total	C	H	O	0	0
			28	10	16	2		
33	H	1	Total	C	H		0	0
			53	18	35			
33	I	1	Total	C	H		0	0
			41	15	26			
33	J	1	Total	C	H	O	0	0
			28	10	16	2		
33	M	1	Total	C	H	O	0	0
			37	13	22	2		

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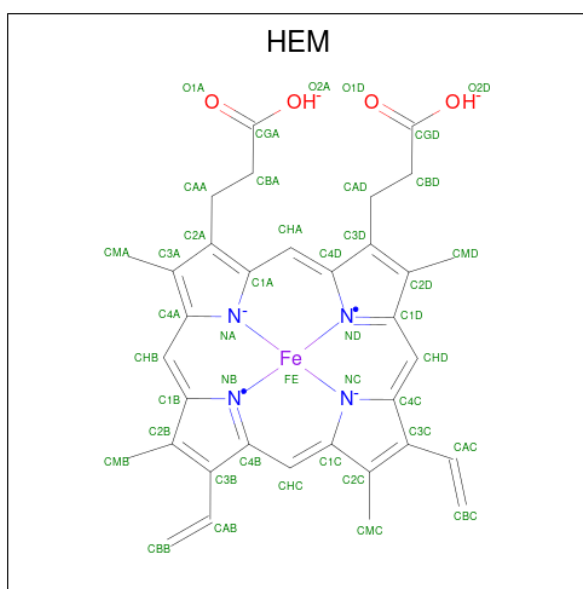
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	M	1	Total	C	H	0	0
			26	10	16		
33	T	1	Total	C	H	0	0
			47	16	31		
33	T	1	Total	C	H	0	0
			44	15	29		
33	Z	1	Total	C	H	0	0
			20	8	12		
33	a	1	Total	C	H	0	0
			26	10	16		
33	a	1	Total	C	H	O	0
			28	10	16	2	0
33	a	1	Total	C	H	0	0
			41	15	26		
33	b	1	Total	C	H	O	0
			55	18	35	2	0
33	b	1	Total	C	H	O	0
			40	14	24	2	0
33	b	1	Total	C	H	O	0
			55	18	35	2	0
33	b	1	Total	C	H	0	0
			26	10	16		
33	b	1	Total	C	H	0	0
			41	14	27		
33	c	1	Total	C	H	O	0
			55	18	35	2	0
33	d	1	Total	C	H	O	0
			43	15	26	2	0
33	d	1	Total	C	H	O	0
			55	18	35	2	0
33	j	1	Total	C	H	O	0
			28	10	16	2	0
33	k	1	Total	C	H	O	0
			28	10	16	2	0
33	l	1	Total	C	H	0	0
			53	18	35		
33	m	1	Total	C	H	O	0
			28	10	16	2	0
33	t	1	Total	C	H	O	0
			46	16	28	2	0
33	x	1	Total	C	H	O	0
			55	18	35	2	0

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



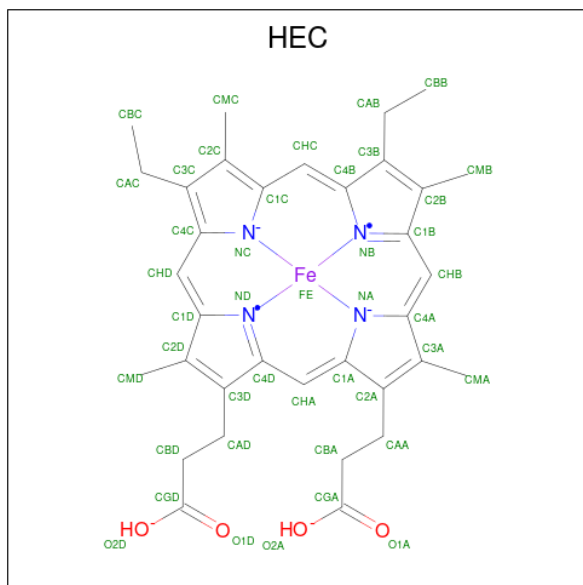
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	D	1	Total	C	H	O	0	0
			5	1	1	3		
34	a	1	Total	C	H	O	0	0
			5	1	1	3		

- Molecule 35 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$).



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

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



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	28	Total O 28 28	0	0
37	I	6	Total O 6 6	0	0
37	J	13	Total O 13 13	0	0
37	K	4	Total O 4 4	0	0
37	L	12	Total O 12 12	0	0
37	M	8	Total O 8 8	0	0
37	O	96	Total O 96 96	0	0
37	R	5	Total O 5 5	0	0
37	T	12	Total O 12 12	0	0
37	U	47	Total O 47 47	0	0
37	V	78	Total O 78 78	0	0
37	X	11	Total O 11 11	0	0
37	Y	2	Total O 2 2	0	0
37	Z	7	Total O 7 7	0	0
37	a	131	Total O 131 131	0	0
37	b	207	Total O 207 207	0	0
37	c	162	Total O 162 162	0	0
37	d	123	Total O 123 123	0	0
37	e	29	Total O 29 29	0	0
37	f	7	Total O 7 7	0	0
37	h	22	Total O 22 22	0	0

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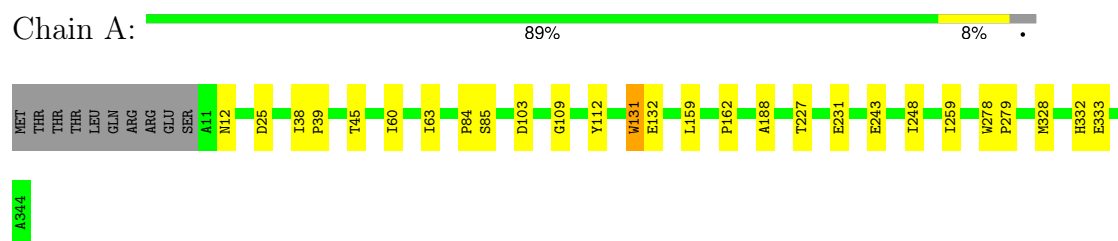
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	i	7	Total 7	O 7	0	0
37	j	8	Total 8	O 8	0	0
37	k	11	Total 11	O 11	0	0
37	l	8	Total 8	O 8	0	0
37	m	9	Total 9	O 9	0	0
37	o	104	Total 104	O 104	0	0
37	r	5	Total 5	O 5	0	0
37	t	9	Total 9	O 9	0	0
37	u	68	Total 68	O 68	0	0
37	v	59	Total 59	O 59	0	0
37	x	8	Total 8	O 8	0	0
37	y	3	Total 3	O 3	0	0
37	z	7	Total 7	O 7	0	0

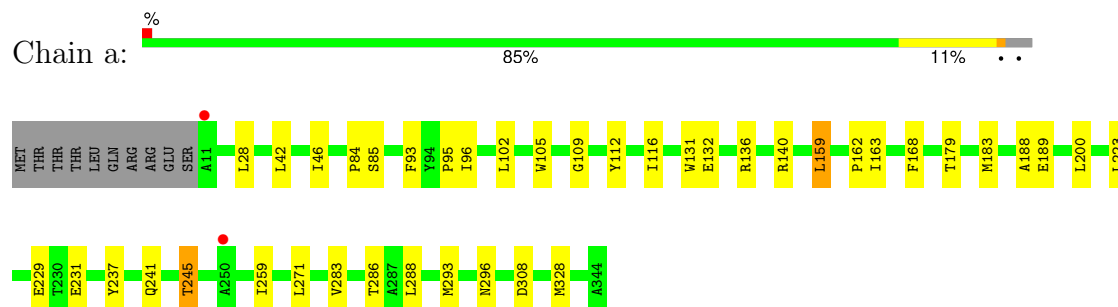
3 Residue-property plots

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

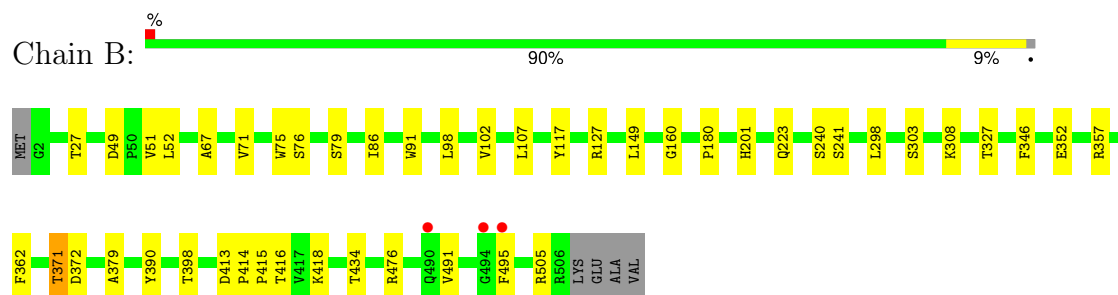
- Molecule 1: Photosystem II protein D1 1



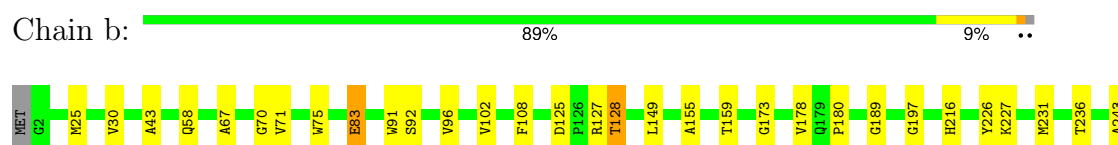
- Molecule 1: Photosystem II protein D1 1



- Molecule 2: Photosystem II CP47 reaction center protein



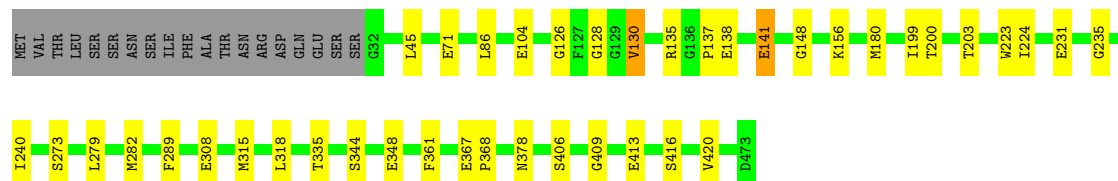
- Molecule 2: Photosystem II CP47 reaction center protein





- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 87% 8% .



- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 90% 8% .



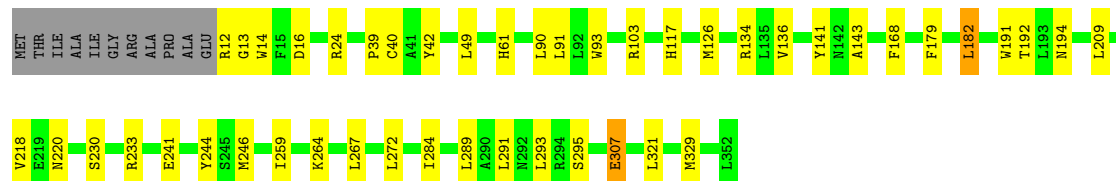
- Molecule 4: Photosystem II D2 protein

Chain D: 90% 7% .



- Molecule 4: Photosystem II D2 protein

Chain d: 84% 13% ..

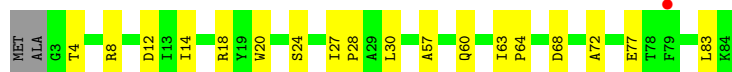
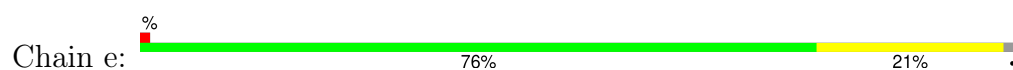


- Molecule 5: Cytochrome b559 subunit alpha

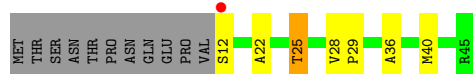
Chain E: 82% 15% .



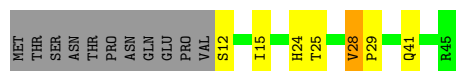
- Molecule 5: Cytochrome b559 subunit alpha



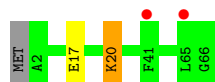
- Molecule 6: Cytochrome b559 subunit beta



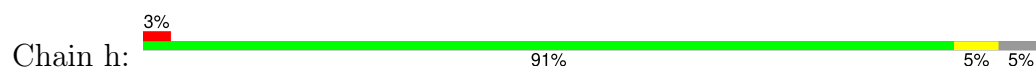
- Molecule 6: Cytochrome b559 subunit beta



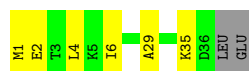
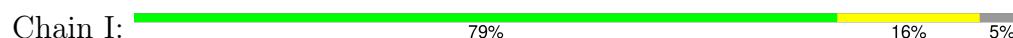
- Molecule 7: Photosystem II reaction center protein H



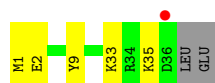
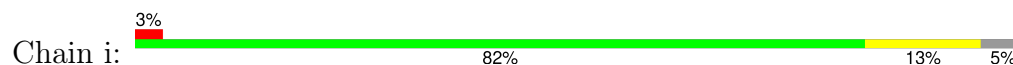
- Molecule 7: Photosystem II reaction center protein H



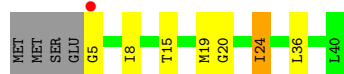
- Molecule 8: Photosystem II reaction center protein I



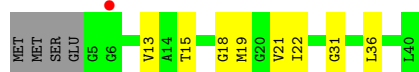
- Molecule 8: Photosystem II reaction center protein I



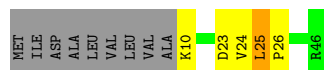
- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



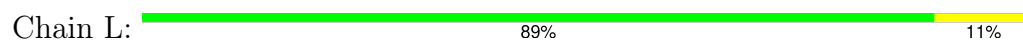
- Molecule 10: Photosystem II reaction center protein K



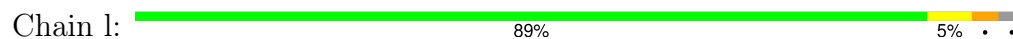
- Molecule 10: Photosystem II reaction center protein K



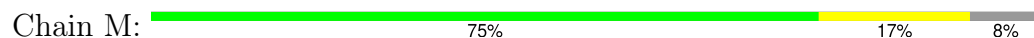
- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M



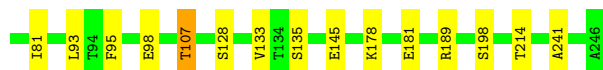
- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 11% 11%



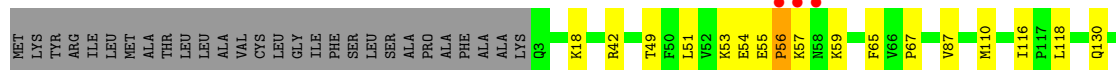
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  78% 10% 10%



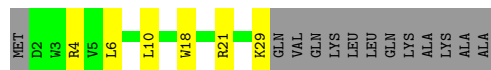
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  81% 8% 10%



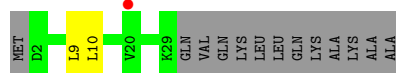
- Molecule 14: Photosystem II protein Y

Chain R:  54% 15% 32%



- Molecule 14: Photosystem II protein Y

Chain r:  2% 63% 5% 32%

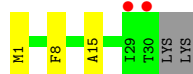
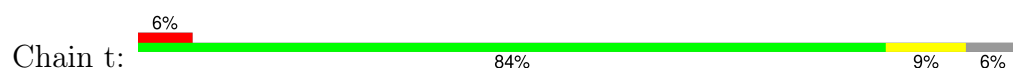


- Molecule 15: Photosystem II reaction center protein T

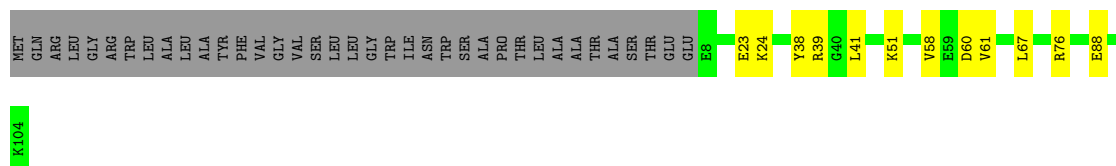
Chain T:  3% 81% 12% 6%



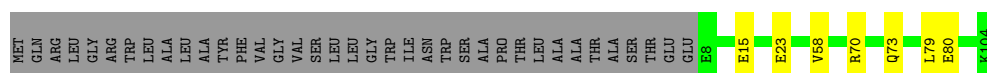
- Molecule 15: Photosystem II reaction center protein T



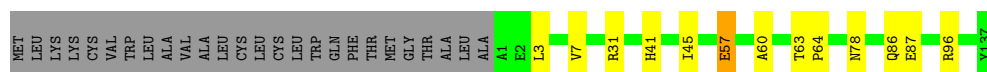
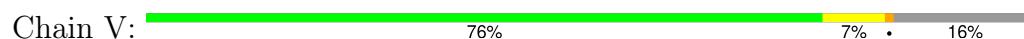
- Molecule 16: Photosystem II 12 kDa extrinsic protein



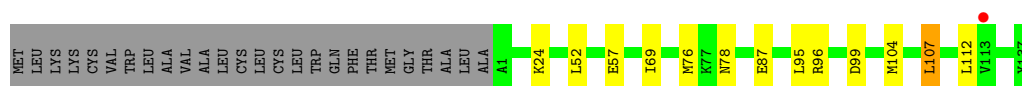
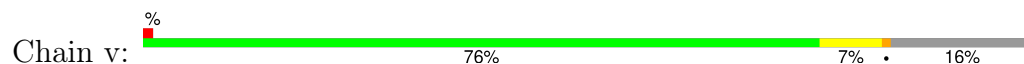
- Molecule 16: Photosystem II 12 kDa extrinsic protein



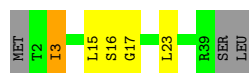
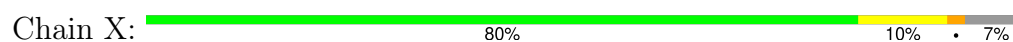
- Molecule 17: Cytochrome c-550



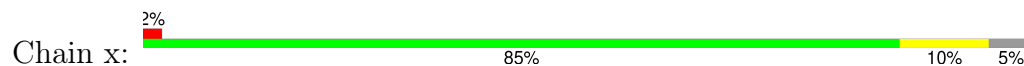
- Molecule 17: Cytochrome c-550

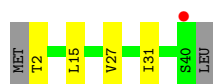


- Molecule 18: Photosystem II reaction center X protein

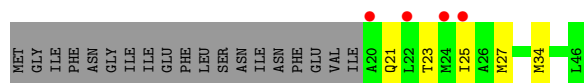


- Molecule 18: Photosystem II reaction center X protein

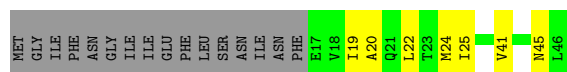




- Molecule 19: Photosystem II reaction center protein Ycf12



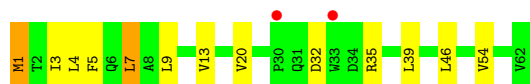
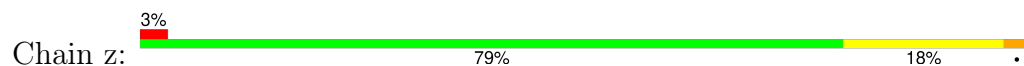
- Molecule 19: Photosystem II reaction center protein Ycf12



- Molecule 20: Photosystem II reaction center protein Z



- Molecule 20: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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 1.19.2_4158	Depositor
R, R_{free}	0.180 , 0.227 0.180 , 0.227	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 , 58.7	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	106128	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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, BCR, HEC, PL9, CLA, PHO, OEY, CL, LHG, HEM, LMG, SQD, OEX, FE2, DGD, 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	0.52	0/3227	0.60	1/4397 (0.0%)
1	a	0.48	0/3224	0.59	1/4393 (0.0%)
2	B	0.55	0/4161	0.62	0/5669
2	b	0.52	0/4118	0.60	0/5611
3	C	0.53	0/3647	0.60	0/4965
3	c	0.49	0/3719	0.59	0/5061
4	D	0.59	0/2825	0.65	0/3847
4	d	0.54	0/2834	0.63	0/3859
5	E	0.46	0/688	0.53	0/940
5	e	0.40	0/683	0.52	0/932
6	F	0.45	0/284	0.55	0/387
6	f	0.44	0/284	0.62	0/387
7	H	0.56	0/523	0.58	0/713
7	h	0.48	0/511	0.59	0/697
8	I	0.51	0/293	0.58	0/396
8	i	0.52	0/293	0.57	0/396
9	J	0.39	0/263	0.55	0/356
9	j	0.39	0/263	0.51	0/356
10	K	0.39	0/303	0.54	0/416
10	k	0.39	0/303	0.50	0/416
11	L	0.56	0/311	0.59	0/422
11	l	0.57	0/303	0.60	0/412
12	M	0.58	0/249	0.64	0/341
12	m	0.57	0/244	0.67	0/334
13	O	0.52	0/1904	0.61	0/2585
13	o	0.53	0/1905	0.60	0/2583
14	R	0.33	0/227	0.42	0/313
14	r	0.28	0/227	0.38	0/313
15	T	0.59	0/257	0.64	0/349
15	t	0.61	0/255	0.55	0/346
16	U	0.46	0/785	0.56	0/1064

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	u	0.49	0/785	0.59	0/1064
17	V	0.51	0/1085	0.62	0/1473
17	v	0.48	0/1085	0.55	0/1473
18	X	0.41	0/284	0.48	0/384
18	x	0.38	0/289	0.47	0/391
19	Y	0.38	0/197	0.45	0/264
19	y	0.35	0/219	0.47	0/294
20	Z	0.35	0/490	0.49	0/669
20	z	0.27	0/488	0.39	0/666
All	All	0.51	0/44035	0.59	2/59934 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	131	TRP	CA-CB-CG	-5.19	103.73	113.60
1	A	131	TRP	CA-CB-CG	-5.02	104.06	113.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	V	63	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	2985	2963	15	0
1	a	3110	2976	2954	22	0
2	B	4005	3873	3867	31	0
2	b	3978	3836	3836	32	0
3	C	3509	3432	3409	22	0
3	c	3583	3503	3492	27	0
4	D	2731	2637	2637	17	0
4	d	2737	2643	2643	36	0
5	E	666	651	651	8	0
5	e	664	648	648	10	0
6	F	275	282	282	5	0
6	f	275	282	282	7	0
7	H	510	532	532	1	0
7	h	498	518	518	2	0
8	I	296	311	311	2	0
8	i	296	311	311	2	0
9	J	257	268	268	5	0
9	j	257	268	268	4	0
10	K	293	305	305	3	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	5	0
12	m	251	267	267	3	0
13	O	1870	1830	1830	22	0
13	o	1874	1846	1846	16	0
14	R	221	238	238	2	0
14	r	221	238	238	0	0
15	T	258	261	261	2	0
15	t	256	256	256	4	0
16	U	774	773	773	8	0
16	u	774	773	773	3	0
17	V	1064	1071	1073	5	0
17	v	1064	1071	1073	8	0
18	X	281	312	312	4	0
18	x	286	316	314	2	0
19	Y	196	217	217	3	0
19	y	218	241	241	2	0
20	Z	479	516	516	8	0
20	z	477	509	509	7	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	a	10	0	0	0	0
23	A	1	0	0	0	0
23	a	1	0	0	0	0
24	A	249	264	264	5	0
24	B	1035	1139	1139	19	0
24	C	839	922	922	6	0
24	D	130	144	144	3	0
24	a	195	216	216	0	0
24	b	1035	1139	1139	13	0
24	c	839	919	919	12	0
24	d	195	216	216	1	0
25	A	128	148	148	1	0
25	a	64	74	74	0	0
25	d	64	74	74	1	0
26	A	40	56	56	0	0
26	B	120	168	168	4	0
26	C	80	112	112	0	0
26	D	40	56	56	1	0
26	H	40	56	56	1	0
26	K	40	56	56	0	0
26	T	40	56	56	1	0
26	Y	40	56	56	1	0
26	a	40	56	56	1	0
26	b	120	168	168	2	0
26	c	80	112	112	1	0
26	d	40	56	56	2	0
26	k	80	112	112	0	0
26	t	40	56	56	3	0
26	x	40	56	56	0	0
27	A	2	0	0	0	0
27	a	2	0	0	0	0
28	A	55	80	80	2	0
28	D	55	80	80	0	0
28	a	55	80	80	2	0
28	d	55	80	80	0	0
29	A	48	66	66	0	0
29	C	48	66	66	0	0
29	D	112	157	157	2	0
29	M	51	72	72	1	0
29	a	55	86	86	5	0
29	b	106	158	158	1	0
29	c	134	181	181	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	d	44	58	58	0	0
30	A	47	67	67	1	0
30	B	98	148	148	1	0
30	D	49	74	74	3	0
30	E	49	74	74	1	0
30	d	137	199	199	5	0
30	e	42	57	57	0	0
30	l	49	74	74	1	0
31	A	91	136	134	2	0
31	B	54	78	76	2	0
31	D	36	46	45	1	0
31	a	90	134	132	0	0
31	b	49	65	64	1	0
31	f	41	48	47	1	0
32	A	66	96	96	3	0
32	C	186	246	245	0	0
32	H	62	82	81	0	0
32	c	186	246	244	2	0
32	h	62	82	79	0	0
33	B	71	109	109	3	0
33	C	40	63	63	0	0
33	D	20	35	35	6	0
33	E	12	16	16	1	0
33	H	18	35	35	1	0
33	I	15	26	26	0	0
33	J	12	16	16	0	0
33	M	25	38	38	1	0
33	T	31	60	60	1	0
33	Z	8	12	12	0	0
33	a	37	58	58	1	0
33	b	80	137	137	4	0
33	c	20	35	35	1	0
33	d	37	61	61	1	0
33	j	12	16	16	0	0
33	k	12	16	16	0	0
33	l	18	35	35	1	0
33	m	12	16	16	1	0
33	t	18	28	28	2	0
33	x	20	35	35	0	0
34	D	4	1	1	1	0
34	a	4	1	1	0	0
35	F	43	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	e	43	30	30	4	0
36	V	43	30	30	1	0
36	v	43	30	30	1	0
37	A	149	0	0	3	0
37	B	200	0	0	9	0
37	C	166	0	0	4	0
37	D	124	0	0	2	0
37	E	24	0	0	1	0
37	F	10	0	0	1	0
37	H	28	0	0	0	0
37	I	6	0	0	0	0
37	J	13	0	0	2	0
37	K	4	0	0	0	0
37	L	12	0	0	1	0
37	M	8	0	0	3	0
37	O	96	0	0	7	0
37	R	5	0	0	0	0
37	T	12	0	0	1	0
37	U	47	0	0	4	0
37	V	78	0	0	2	0
37	X	11	0	0	0	0
37	Y	2	0	0	0	0
37	Z	7	0	0	0	0
37	a	131	0	0	0	0
37	b	207	0	0	4	0
37	c	162	0	0	6	0
37	d	123	0	0	10	0
37	e	29	0	0	0	0
37	f	7	0	0	1	0
37	h	22	0	0	0	0
37	i	7	0	0	0	0
37	j	8	0	0	1	0
37	k	11	0	0	1	0
37	l	8	0	0	0	0
37	m	9	0	0	1	0
37	o	104	0	0	6	0
37	r	5	0	0	0	0
37	t	9	0	0	0	0
37	u	68	0	0	1	0
37	v	59	0	0	1	0
37	x	8	0	0	0	0
37	y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	z	7	0	0	1	0
All	All	53366	52762	52664	415	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 4.

All (415) 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)
3:c:315:MET:SD	37:c:746:HOH:O	2.15	1.04
13:o:54:GLU:HA	37:o:302:HOH:O	1.61	0.98
4:d:307:GLU:OE1	37:d:501:HOH:O	1.83	0.94
12:M:5:GLN:O	37:M:201:HOH:O	1.84	0.94
3:C:231:GLU:OE1	37:C:601:HOH:O	1.86	0.93
3:C:378:ASN:OD1	37:C:602:HOH:O	1.90	0.88
16:U:88:GLU:OE2	37:U:201:HOH:O	1.90	0.88
2:b:372:ASP:OD2	37:b:701:HOH:O	1.90	0.88
1:A:25:ASP:OD1	37:A:701:HOH:O	1.92	0.88
33:B:624:STE:O2	37:B:701:HOH:O	1.90	0.88
10:k:19:ASP:OD1	37:k:201:HOH:O	1.93	0.87
4:d:13:GLY:N	37:d:502:HOH:O	2.02	0.87
13:o:55:GLU:N	37:o:302:HOH:O	2.07	0.86
33:M:102:STE:O1	37:M:202:HOH:O	1.93	0.85
13:o:54:GLU:CA	37:o:302:HOH:O	2.22	0.85
3:c:391[A]:ARG:NE	37:c:601:HOH:O	2.14	0.81
33:B:625:STE:O1	37:B:702:HOH:O	1.98	0.81
13:O:98:GLU:OE1	37:O:301:HOH:O	1.99	0.80
13:o:54:GLU:C	37:o:302:HOH:O	2.24	0.79
2:B:223:GLN:OE1	37:B:703:HOH:O	2.02	0.77
9:j:36:LEU:O	37:j:201:HOH:O	2.02	0.76
13:O:37:THR:HA	37:O:310:HOH:O	1.86	0.75
11:L:8:GLN:OE1	37:L:101:HOH:O	2.04	0.74
16:U:76:ARG:NE	37:U:202:HOH:O	1.96	0.74
2:B:413:ASP:OD1	37:B:705:HOH:O	2.06	0.74
31:b:620:SQD:O9	37:b:703:HOH:O	2.07	0.73
21:A:601[B]:OEY:O5	21:A:601[B]:OEY:O6	2.06	0.73
3:c:391[A]:ARG:NH1	37:c:603:HOH:O	2.22	0.72
17:V:87:GLU:OE2	37:V:301:HOH:O	2.09	0.71
9:J:36:LEU:O	37:J:201:HOH:O	2.09	0.70
5:e:8:ARG:NH1	5:e:12:ASP:OD2	2.23	0.70
12:m:30:GLU:OE2	37:m:201:HOH:O	2.10	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:30:THR:OG1	37:T:201:HOH:O	2.09	0.69
3:c:391[B]:ARG:NH1	37:c:605:HOH:O	2.25	0.69
5:e:57:ALA:H	5:e:60:GLN:HE21	1.40	0.69
2:B:352:GLU:OE1	37:B:706:HOH:O	2.11	0.69
17:v:57:GLU:OE2	37:v:301:HOH:O	2.11	0.67
2:B:352:GLU:OE1	37:B:707:HOH:O	2.12	0.67
3:C:148:GLY:O	3:C:156:LYS:NZ	2.27	0.67
4:d:12:ARG:CA	37:d:502:HOH:O	2.42	0.66
16:u:80:GLU:OE1	37:u:201:HOH:O	2.13	0.66
33:E:102:STE:O1	37:E:201:HOH:O	2.13	0.66
28:A:612:PL9:H361	6:F:25:THR:HG21	1.78	0.66
9:J:5:GLY:N	37:J:202:HOH:O	2.29	0.65
31:B:623:SQD:O2	37:B:708:HOH:O	2.15	0.64
4:d:42:TYR:CZ	6:f:25:THR:HG22	2.32	0.64
6:f:28:VAL:HG22	6:f:29:PRO:HD3	1.79	0.63
1:A:188[A]:ALA:HB2	1:A:328[A]:MET:HB2	1.81	0.63
35:F:101:HEM:HBC2	35:F:101:HEM:HHD	1.80	0.63
35:e:101:HEM:HHC	35:e:101:HEM:HBB2	1.80	0.63
2:B:371:THR:HG23	2:B:372:ASP:O	2.00	0.62
5:E:45:ASP:OD2	14:R:4:ARG:NH2	2.27	0.62
4:d:12:ARG:HA	37:d:502:HOH:O	2.00	0.62
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.83	0.61
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.84	0.60
24:c:504:CLA:H91	24:c:508:CLA:H172	1.84	0.60
13:o:194:LYS:NZ	37:o:301:HOH:O	1.96	0.60
2:B:75:TRP:HB3	29:a:618:LMG:HC91	1.84	0.59
3:c:315:MET:HE3	3:c:365:TRP:HZ3	1.68	0.59
3:C:141:GLU:OE2	37:C:603:HOH:O	2.17	0.59
13:O:27:ARG:O	13:O:27:ARG:HG2	2.02	0.59
3:c:391[B]:ARG:NE	3:c:391[B]:ARG:HA	2.16	0.59
4:d:126:MET:HE3	4:d:143:ALA:O	2.01	0.59
37:A:746:HOH:O	13:O:107:THR:HG22	2.01	0.59
3:c:315:MET:HE3	3:c:365:TRP:CZ3	2.38	0.59
24:c:508:CLA:H191	32:c:517:DGD:HA91	1.85	0.58
29:D:406:LMG:H112	37:D:562:HOH:O	2.03	0.58
20:z:1:MET:HB3	20:z:4:LEU:HB3	1.85	0.58
13:O:6:THR:HG22	13:O:9:ASP:OD2	2.03	0.58
24:b:615:CLA:HHC	24:b:615:CLA:HBB1	1.85	0.58
4:d:103:ARG:NH2	37:d:509:HOH:O	2.37	0.58
24:B:607:CLA:H193	11:L:27:LEU:HD11	1.86	0.58
4:d:230:SER:HB2	37:d:561:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:189[B]:GLU:OE1	21:a:601[B]:OEY:O6	2.23	0.57
16:U:38:TYR:HB2	16:U:41:LEU:HD12	1.85	0.57
24:c:501:CLA:H192	24:c:507:CLA:HBB1	1.86	0.56
8:i:33:LYS:O	8:i:35:LYS:NZ	2.39	0.56
4:D:264:LYS:NZ	34:D:401:BCT:O3	2.38	0.56
2:b:102:VAL:HG11	24:b:606:CLA:H142	1.88	0.56
16:U:60:ASP:OD2	37:U:203:HOH:O	2.18	0.56
19:Y:23:THR:HG22	19:Y:27:MET:HE3	1.88	0.56
1:A:103:ASP:OD1	32:A:618:DGD:O2E	2.24	0.56
1:A:63[B]:ILE:HB	3:C:335:THR:HG21	1.88	0.56
6:f:12:SER:N	37:f:201:HOH:O	2.39	0.56
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.86	0.55
1:A:227:THR:HB	1:A:231:GLU:HG3	1.89	0.55
20:Z:51:VAL:O	20:Z:54:VAL:O	2.23	0.55
16:U:58:VAL:O	16:U:61:VAL:HG22	2.05	0.55
30:D:408:LHG:H321	15:T:21:ILE:HD11	1.89	0.55
16:U:39:ARG:NH2	17:V:60:ALA:O	2.39	0.54
30:A:615:LHG:H151	31:A:616:SQD:H272	1.88	0.54
3:c:315:MET:CE	3:c:366:LEU:HD13	2.38	0.53
17:V:57:GLU:OE2	37:V:302:HOH:O	2.19	0.53
5:e:27:ILE:HB	5:e:28:PRO:HD3	1.90	0.53
3:C:406:SER:HA	3:C:420:VAL:HG23	1.91	0.53
2:b:127:ARG:NH2	7:h:18:TYR:O	2.39	0.53
1:a:179[A]:THR:O	1:a:183[A]:MET:HG3	2.09	0.53
36:V:201:HEC:HMC1	36:V:201:HEC:HBC3	1.90	0.53
20:Z:55:GLY:HA2	20:Z:58:ASN:HB3	1.91	0.53
2:b:476:ARG:HD2	37:b:745:HOH:O	2.09	0.53
12:M:6:LEU:HA	37:M:201:HOH:O	2.08	0.53
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.44	0.52
30:d:407:LHG:H111	30:l:101:LHG:H102	1.90	0.52
6:f:24:HIS:O	6:f:28:VAL:HG13	2.09	0.52
2:B:414:PRO:O	2:B:418:LYS:HG3	2.09	0.52
10:k:26:PRO:O	10:k:29:PRO:HD2	2.09	0.52
29:a:618:LMG:HC92	29:a:618:LMG:O9	2.09	0.52
15:t:15:ALA:HB2	26:t:101:BCR:H14C	1.91	0.52
2:B:117:TYR:HA	11:L:1:MET:HE1	1.91	0.52
4:d:91:LEU:O	37:d:503:HOH:O	2.19	0.52
3:c:178:LYS:NZ	3:c:184:GLY:O	2.42	0.52
2:B:303:SER:OG	37:B:711:HOH:O	2.19	0.52
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.92	0.52
8:I:29:ALA:O	8:I:35:LYS:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:30:VAL:HG12	24:b:605:CLA:HHD	1.92	0.51
4:d:241:GLU:CD	4:d:241:GLU:H	2.18	0.51
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.92	0.51
1:a:102:LEU:HB2	29:a:618:LMG:H111	1.92	0.51
17:v:76:MET:HE2	17:v:112:LEU:HD22	1.93	0.51
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.92	0.51
4:d:246:MET:HE3	4:d:264:LYS:HG2	1.93	0.51
17:v:104:MET:HA	17:v:107:LEU:HD22	1.93	0.51
2:b:492:GLU:OE2	2:b:495:PHE:CE1	2.64	0.51
4:d:267:LEU:C	4:d:267:LEU:HD23	2.36	0.51
3:c:406:SER:HA	3:c:420:VAL:HG23	1.91	0.51
20:z:3:ILE:HG22	20:z:7:LEU:HD23	1.92	0.50
4:D:209:LEU:HD23	4:D:209:LEU:C	2.36	0.50
3:c:391[B]:ARG:CZ	37:c:605:HOH:O	2.60	0.50
13:O:145:GLU:HG2	37:O:330:HOH:O	2.11	0.50
37:A:807:HOH:O	13:O:107:THR:HG21	2.10	0.50
6:F:12:SER:N	37:F:202:HOH:O	2.44	0.50
3:C:45:LEU:HD22	3:C:138:GLU:HG2	1.93	0.50
2:B:149[B]:LEU:HG	24:B:604:CLA:H18	1.94	0.50
9:J:15:THR:HG22	9:J:19:MET:HE2	1.91	0.50
26:T:101:BCR:H321	26:T:101:BCR:HC8	1.92	0.50
2:b:505:ARG:HG3	2:b:506:ARG:N	2.27	0.50
12:M:8:LEU:HD11	33:T:103:STE:H141	1.94	0.50
2:b:492:GLU:OE2	2:b:495:PHE:CD1	2.64	0.49
5:e:14:ILE:O	5:e:20:TRP:NE1	2.44	0.49
37:C:683:HOH:O	4:D:230:SER:HB2	2.12	0.49
25:A:607:PHO:HBC3	4:D:279:LEU:HD22	1.94	0.49
4:d:42:TYR:CE1	6:f:25:THR:HG22	2.47	0.49
24:B:610:CLA:HHC	24:B:610:CLA:CBB	2.43	0.49
26:b:618:BCR:H331	26:b:618:BCR:C8	2.42	0.49
20:Z:29:SER:HB3	20:Z:31:GLN:HE21	1.77	0.48
2:b:159:THR:O	2:b:180:PRO:HB3	2.13	0.48
33:D:411:STE:H121	33:D:411:STE:H92	1.67	0.48
2:b:91:TRP:HE1	33:b:622:STE:H111	1.77	0.48
24:b:615:CLA:H2	24:b:616:CLA:HBB2	1.96	0.48
35:e:101:HEM:HMC1	35:e:101:HEM:HBC2	1.94	0.48
2:B:102:VAL:HA	26:B:618:BCR:C40	2.44	0.48
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.77	0.48
24:b:602:CLA:H43	7:h:45:ILE:HG22	1.94	0.48
2:b:226:TYR:HA	2:b:231:MET:HG3	1.94	0.48
3:c:166:ILE:HG21	24:c:512:CLA:H202	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:t:8:PHE:CE2	33:t:102:STE:H151	2.49	0.48
26:D:404:BCR:H392	26:D:404:BCR:H23C	1.95	0.48
13:O:56:PRO:O	13:O:58:ASN:N	2.44	0.48
5:e:20:TRP:O	5:e:24:SER:OG	2.22	0.48
1:a:84:PRO:HA	1:a:112:TYR:CG	2.49	0.47
13:O:78:LEU:HB3	13:O:81:ILE:HD11	1.95	0.47
1:a:237:TYR:HB2	1:a:245:THR:HG21	1.96	0.47
4:D:85:MET:HE1	5:E:72:ALA:HB2	1.96	0.47
4:d:272:LEU:C	4:d:272:LEU:HD23	2.40	0.47
3:C:135:ARG:O	3:C:135:ARG:HD3	2.14	0.47
9:j:18:GLY:O	9:j:22:ILE:HD13	2.15	0.47
10:K:24:VAL:HG13	19:Y:25:ILE:HD13	1.96	0.47
4:d:194:ASN:HA	4:d:295:SER:OG	2.14	0.47
2:B:51:VAL:HG13	2:B:308:LYS:HB2	1.96	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.47
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.96	0.47
24:b:613:CLA:H172	30:d:407:LHG:H212	1.96	0.47
4:d:61:HIS:CE1	4:d:168:PHE:CE1	3.03	0.47
5:e:30:LEU:HD11	35:e:101:HEM:CBB	2.45	0.47
4:d:24:ARG:O	37:d:504:HOH:O	2.20	0.47
24:D:403:CLA:H141	18:X:15:LEU:HD13	1.96	0.47
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.97	0.47
4:d:14:TRP:N	37:d:511:HOH:O	2.48	0.47
17:v:99:ASP:N	17:v:99:ASP:OD1	2.47	0.47
19:y:20:ALA:O	19:y:24:MET:HG2	2.14	0.46
2:B:414:PRO:N	2:B:415:PRO:HD2	2.29	0.46
5:E:68:ASP:O	5:E:72:ALA:HB2	2.15	0.46
16:u:58:VAL:HG12	16:u:79:LEU:HD22	1.98	0.46
4:D:266:TRP:CD1	30:D:408:LHG:HC31	2.50	0.46
32:c:517:DGD:HA51	32:c:517:DGD:HA81	1.77	0.46
13:O:189:ARG:NH2	37:O:303:HOH:O	2.35	0.46
2:b:91:TRP:HE1	33:b:622:STE:H141	1.79	0.46
2:b:155:ALA:HB1	29:b:623:LMG:H122	1.98	0.46
19:y:22:LEU:HA	19:y:25:ILE:HG22	1.97	0.46
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	1.98	0.46
2:B:357:ARG:NE	37:B:709:HOH:O	2.18	0.46
1:A:131:TRP:CE3	1:A:132:GLU:HA	2.51	0.46
2:B:241:SER:HB3	24:B:612:CLA:HED3	1.98	0.46
26:Y:101:BCR:H322	20:Z:17:PHE:CE2	2.51	0.46
4:d:12:ARG:HH11	4:d:16:ASP:HB3	1.80	0.46
24:A:604:CLA:H201	30:D:408:LHG:H182	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:THR:HG21	29:M:101:LMG:H291	1.96	0.46
3:C:126:GLY:O	3:C:130:VAL:HG13	2.16	0.46
3:C:137:PRO:HD3	24:C:513:CLA:HED2	1.98	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.98	0.46
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.98	0.46
28:a:611:PL9:H371	28:a:611:PL9:H351	1.81	0.46
24:b:607:CLA:H191	30:d:407:LHG:H141	1.97	0.46
4:d:218:VAL:HG13	4:d:244:TYR:CD1	2.51	0.46
2:B:67:ALA:HA	2:B:71:VAL:O	2.16	0.45
2:b:58:GLN:C	2:b:329:PRO:HB3	2.41	0.45
4:d:93:TRP:O	37:d:505:HOH:O	2.20	0.45
35:F:101:HEM:HBB2	35:F:101:HEM:HMB1	1.98	0.45
17:v:78:ASN:OD1	17:v:96:ARG:NH1	2.46	0.45
24:c:504:CLA:H142	24:c:508:CLA:H121	1.98	0.45
13:O:189:ARG:NE	37:O:303:HOH:O	2.29	0.45
1:a:241:GLN:NE2	1:a:245:THR:HG23	2.32	0.45
3:c:42:LEU:HD21	24:c:511:CLA:H2A	1.98	0.45
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.99	0.45
13:O:133:VAL:C	13:O:135:SER:H	2.25	0.45
20:Z:31:GLN:NE2	20:Z:32:ASP:HB2	2.32	0.45
1:a:112:TYR:O	1:a:116:ILE:HG12	2.17	0.45
2:b:83:GLU:H	2:b:83:GLU:HG2	1.63	0.45
3:c:45:LEU:HA	3:c:139:THR:HG22	1.98	0.45
4:d:49:LEU:HD13	26:d:405:BCR:C15	2.46	0.45
26:d:405:BCR:C8	26:d:405:BCR:H331	2.47	0.45
26:H:101:BCR:H331	26:H:101:BCR:C8	2.46	0.45
31:B:623:SQD:H383	31:B:623:SQD:H352	1.83	0.44
3:C:308:GLU:HB2	3:C:361:PHE:CE1	2.52	0.44
3:C:409:GLY:HA3	3:C:413[B]:GLU:HG3	1.99	0.44
9:J:20:GLY:O	9:J:24:ILE:HG13	2.17	0.44
10:k:18:PHE:HE2	20:z:13:VAL:HG21	1.82	0.44
2:B:413:ASP:OD2	2:B:416:THR:OG1	2.26	0.44
3:C:348:GLU:OE2	13:O:11:VAL:HA	2.17	0.44
20:Z:34:ASP:O	20:Z:37:LYS:HG2	2.17	0.44
1:a:283:VAL:HA	1:a:286:THR:HG22	2.00	0.44
2:b:125:ASP:OD2	2:b:128:THR:HG23	2.17	0.44
5:e:63:ILE:HG23	5:e:64:PRO:HD2	1.98	0.44
2:B:149[A]:LEU:HD21	24:B:606:CLA:HBB2	1.98	0.44
16:U:76:ARG:NH2	37:U:202:HOH:O	2.51	0.44
29:a:618:LMG:H151	29:a:618:LMG:H182	1.79	0.44
2:b:451:PHE:CE2	2:b:455:HIS:CE1	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:315:MET:HE1	3:c:366:LEU:HD13	1.99	0.44
5:e:18:ARG:HH22	6:f:15:ILE:HD11	1.82	0.44
24:D:403:CLA:ND	33:D:411:STE:H122	2.33	0.44
13:O:54:GLU:O	13:O:63:ALA:HB3	2.18	0.44
16:U:23:GLU:HG3	16:U:24:LYS:HG2	1.98	0.44
33:D:411:STE:H142	18:X:17:GLY:HA2	2.00	0.44
4:d:246:MET:HE3	4:d:264:LYS:CG	2.47	0.44
1:A:279:PRO:HG2	4:D:212:ALA:HB2	2.00	0.44
10:K:25:LEU:N	10:K:26:PRO:HD2	2.33	0.44
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.47	0.44
33:D:411:STE:H52	33:D:411:STE:H81	1.74	0.44
33:b:625:STE:H122	33:b:625:STE:H151	1.84	0.44
2:B:49:ASP:OD2	13:o:57:LYS:HD2	2.17	0.44
24:B:601:CLA:HAB	33:H:103:STE:H142	1.99	0.44
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.52	0.44
4:d:134:ARG:HG2	33:d:411:STE:O1	2.18	0.44
13:o:53:LYS:HE3	13:o:65:PHE:CZ	2.52	0.44
2:b:357:ARG:NE	37:b:702:HOH:O	1.93	0.43
4:d:141:TYR:OH	30:d:407:LHG:O4	2.23	0.43
31:f:101:SQD:H312	18:x:27:VAL:HG11	2.00	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.53	0.43
24:c:501:CLA:C3D	24:c:503:CLA:H2	2.48	0.43
4:d:179:PHE:HA	4:d:182:LEU:HD22	2.00	0.43
13:o:216:GLU:OE2	13:o:234:LYS:HD2	2.17	0.43
4:D:307:GLU:HG3	37:D:529:HOH:O	2.18	0.43
28:a:611:PL9:C49	4:d:39:PRO:HG3	2.48	0.43
24:c:508:CLA:H171	29:c:519:LMG:H372	2.00	0.43
24:B:601:CLA:HBA1	24:B:601:CLA:HBD	2.00	0.43
3:c:334:PRO:HA	13:o:153:THR:OG1	2.19	0.43
1:A:38:ILE:HB	1:A:39:PRO:HD3	2.00	0.43
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.00	0.43
35:e:101:HEM:HBC2	35:e:101:HEM:CMC	2.47	0.43
13:o:54:GLU:O	13:o:56:PRO:HD3	2.18	0.43
4:D:32:TRP:CD2	29:D:409:LMG:H161	2.53	0.43
24:B:614:CLA:H42	33:m:101:STE:H22	2.01	0.43
2:b:189:GLY:O	2:b:197:GLY:HA3	2.18	0.43
4:d:12:ARG:NH1	4:d:16:ASP:HB3	2.33	0.43
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.43
7:H:17:GLU:OE2	7:H:20:LYS:NZ	2.45	0.43
17:V:41:HIS:HA	17:V:45:ILE:O	2.19	0.43
2:B:52:LEU:HD12	13:o:59:LYS:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:PHE:CD2	30:E:101:LHG:HC81	2.54	0.43
17:v:95:LEU:HD11	17:v:112:LEU:HD11	2.00	0.43
2:B:201:HIS:HB2	24:B:602:CLA:CHB	2.49	0.43
24:B:614:CLA:H18	24:B:614:CLA:H152	1.79	0.43
24:C:509:CLA:H91	24:C:509:CLA:H112	1.82	0.43
13:O:178:LYS:HD2	13:O:181:GLU:OE2	2.19	0.43
18:X:3:ILE:O	18:X:3:ILE:HG13	2.19	0.43
31:A:617:SQD:H301	26:b:619:BCR:H363	2.00	0.42
3:C:180:MET:HG2	3:C:199:ILE:O	2.20	0.42
24:D:403:CLA:C1D	33:D:411:STE:H122	2.49	0.42
33:D:411:STE:H91	18:X:16:SER:HB3	2.00	0.42
17:V:78:ASN:OD1	17:V:96:ARG:NH1	2.42	0.42
5:e:68:ASP:O	5:e:72:ALA:HB2	2.19	0.42
4:D:61:HIS:HE1	4:D:80:THR:O	2.02	0.42
13:O:42:ARG:O	13:O:241:ALA:HA	2.20	0.42
24:b:601:CLA:H141	24:b:601:CLA:H161	1.91	0.42
24:b:604:CLA:H42	24:b:605:CLA:H2	2.01	0.42
24:b:605:CLA:H62	24:b:605:CLA:H41	1.86	0.42
3:c:160:ILE:HG21	24:c:509:CLA:H203	2.01	0.42
4:d:209:LEU:HD23	4:d:209:LEU:C	2.44	0.42
24:B:614:CLA:H41	24:B:614:CLA:H61	1.80	0.42
3:C:71:GLU:HB3	3:C:86:LEU:HD22	2.01	0.42
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.42
3:c:367:GLU:N	3:c:368:PRO:CD	2.82	0.42
4:d:103:ARG:NH1	5:e:77:GLU:HG3	2.34	0.42
15:t:15:ALA:HA	26:t:101:BCR:H12C	2.00	0.42
17:v:76:MET:HE3	36:v:201:HEC:HBB3	2.00	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.42
3:C:279:LEU:HD23	3:C:282:MET:HE3	2.01	0.42
32:A:618:DGD:HD5	2:b:75:TRP:HB3	2.00	0.42
26:B:618:BCR:C8	26:B:618:BCR:H331	2.49	0.42
20:Z:23:VAL:HG22	20:Z:40:ILE:HD12	2.01	0.42
1:a:229:GLU:CD	1:a:229:GLU:H	2.28	0.42
13:O:37:THR:CA	37:O:310:HOH:O	2.58	0.42
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.54	0.42
11:l:7:ARG:HH11	33:l:102:STE:C1	2.33	0.42
16:u:70:ARG:NH1	16:u:73:GLN:OE1	2.53	0.42
1:A:45:THR:HG23	24:A:613:CLA:H191	2.01	0.42
1:A:159[A]:LEU:C	1:A:162[A]:PRO:HD2	2.45	0.42
1:a:85:SER:HA	1:a:109:GLY:HA3	2.02	0.42
1:a:140:ARG:HB2	4:d:220:ASN:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:364:PRO:HG2	3:c:391[A]:ARG:HH12	1.83	0.42
10:k:15:TYR:CZ	20:z:5:PHE:HZ	2.36	0.42
24:B:606:CLA:H72	26:B:619:BCR:H311	2.01	0.42
3:C:344:SER:O	13:O:75:THR:HG22	2.20	0.42
2:b:92:SER:O	2:b:96:VAL:HG23	2.19	0.42
2:b:227:LYS:HB3	2:b:227:LYS:HE2	1.94	0.42
3:c:26:ARG:HA	24:c:511:CLA:OBD	2.19	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.42
1:A:85:SER:HA	1:A:109:GLY:HA3	2.02	0.41
2:B:495:PHE:HD1	2:B:505:ARG:NH1	2.18	0.41
24:C:504:CLA:H62	24:C:504:CLA:H41	1.92	0.41
24:C:507:CLA:H142	24:C:507:CLA:H111	1.96	0.41
4:D:13:GLY:O	4:D:17:ILE:HG12	2.20	0.41
3:c:128:GLY:HA3	24:c:513:CLA:C3C	2.50	0.41
4:d:192:THR:HG23	24:d:403:CLA:HBC2	2.00	0.41
1:A:84:PRO:HA	1:A:112:TYR:CG	2.55	0.41
2:B:91:TRP:HE1	33:B:620:STE:H32	1.85	0.41
24:B:611:CLA:H203	24:B:613:CLA:H8	2.02	0.41
5:E:25:ILE:HG13	14:R:18:TRP:NE1	2.35	0.41
18:x:27:VAL:O	18:x:31:ILE:HG13	2.20	0.41
24:B:615:CLA:H2	24:B:616:CLA:HBB2	2.02	0.41
13:O:93:LEU:O	13:O:128:SER:HA	2.20	0.41
20:Z:28:ALA:O	20:Z:30:PRO:HD3	2.20	0.41
2:b:43:ALA:HA	33:b:625:STE:H22	2.02	0.41
24:b:614:CLA:H111	24:b:614:CLA:H152	1.93	0.41
13:o:56:PRO:O	37:o:303:HOH:O	2.21	0.41
24:B:610:CLA:HHC	24:B:610:CLA:HBB1	2.03	0.41
4:D:267:LEU:C	4:D:267:LEU:HD23	2.46	0.41
1:a:296:ASN:HB3	3:c:401:LEU:HA	2.02	0.41
29:a:618:LMG:O9	29:a:618:LMG:C9	2.68	0.41
9:j:15:THR:HG22	9:j:19:MET:HE2	2.00	0.41
13:o:110:MET:HE2	13:o:116:ILE:HD11	2.02	0.41
24:A:613:CLA:HBA1	24:A:613:CLA:C4A	2.50	0.41
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.51	0.41
1:a:159[B]:LEU:O	1:a:163[B]:ILE:HG13	2.20	0.41
3:c:109:PHE:N	3:c:110:PRO:CD	2.83	0.41
29:c:522:LMG:HC2	8:i:9:TYR:OH	2.20	0.41
10:k:25:LEU:N	10:k:26:PRO:CD	2.83	0.41
24:C:501:CLA:CAD	24:C:503:CLA:H12	2.51	0.41
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.41
2:B:434:THR:OG1	13:O:178:LYS:NZ	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
3:c:318:LEU:C	3:c:318:LEU:HD23	2.45	0.41
26:c:515:BCR:H11C	26:c:515:BCR:H341	1.97	0.41
17:v:87:GLU:CD	17:v:96:ARG:HH12	2.28	0.41
32:A:618:DGD:HB42	32:A:618:DGD:HB91	2.03	0.41
24:B:606:CLA:H93	24:B:606:CLA:H112	1.89	0.41
1:a:241:GLN:HE22	1:a:245:THR:HG23	1.85	0.41
2:b:25:MET:HE1	2:b:108:PHE:CD1	2.56	0.41
3:c:121:SER:CB	33:c:520:STE:H172	2.51	0.41
30:d:409:LHG:H272	30:d:409:LHG:H242	1.79	0.41
1:A:332[B]:HIS:O	1:A:333[B]:GLU:C	2.64	0.41
24:B:613:CLA:HBB1	24:B:613:CLA:HMB1	2.02	0.41
24:B:613:CLA:H143	24:B:613:CLA:H111	1.96	0.41
26:B:618:BCR:H20C	26:B:618:BCR:H361	1.90	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.41
10:K:23:ASP:OD2	19:Y:21:GLN:NE2	2.53	0.41
1:a:46:ILE:HD12	26:a:607:BCR:H15C	2.03	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.41
2:b:67:ALA:HA	2:b:71:VAL:O	2.21	0.41
24:c:504:CLA:H92	24:c:504:CLA:H62	1.83	0.41
4:d:40:CYS:HB3	4:d:117:HIS:O	2.21	0.41
25:d:402:PHO:HHD	25:d:402:PHO:HBC2	2.03	0.41
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.41
3:C:128:GLY:HA3	24:C:513:CLA:C3C	2.51	0.41
4:D:24:ARG:NH2	31:D:407:SQD:O4	2.54	0.41
8:I:2:GLU:O	8:I:6:ILE:HG12	2.22	0.41
13:O:18:LYS:HE2	37:O:323:HOH:O	2.19	0.41
3:c:308:GLU:HB2	3:c:361:PHE:CE1	2.56	0.41
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.20	0.41
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	2.02	0.40
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.40
3:C:367:GLU:N	3:C:368:PRO:CD	2.84	0.40
29:c:521:LMG:H371	29:c:521:LMG:H402	1.98	0.40
2:B:346:PHE:HA	2:B:398:THR:O	2.22	0.40
30:B:621:LHG:HC41	30:B:622:LHG:O1	2.21	0.40
24:b:615:CLA:H3A	24:b:615:CLA:HBA1	1.89	0.40
3:c:338:GLY:HA3	3:c:341:LEU:O	2.21	0.40
15:t:8:PHE:CD2	33:t:102:STE:H151	2.56	0.40
1:A:278:TRP:HB3	1:A:279:PRO:HD3	2.02	0.40
2:b:216:HIS:HE1	24:b:609:CLA:C1A	2.35	0.40
24:B:601:CLA:H93	24:B:601:CLA:H62	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:308:ASP:OD1	1:a:308:ASP:C	2.65	0.40
29:c:521:LMG:H382	29:c:521:LMG:H351	1.96	0.40
10:k:18:PHE:CE2	20:z:13:VAL:HG21	2.56	0.40
13:o:51:LEU:HD23	13:o:67:PRO:HA	2.04	0.40
20:z:9:LEU:HD13	20:z:54:VAL:HG11	2.02	0.40
20:z:35:ARG:NH2	37:z:101:HOH:O	2.54	0.40
28:A:612:PL9:H351	6:F:22:ALA:HA	2.04	0.40
24:A:613:CLA:H161	24:A:613:CLA:H141	1.83	0.40
24:A:613:CLA:H162	24:A:613:CLA:H193	1.87	0.40
5:E:15:THR:HB	9:J:8:ILE:O	2.21	0.40
6:F:36:ALA:O	6:F:40:MET:HG3	2.21	0.40
33:a:617:STE:H91	33:a:617:STE:H121	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/344 (115%)	392 (99%)	4 (1%)	1 (0%)	36	35
1	a	397/344 (115%)	390 (98%)	6 (2%)	1 (0%)	36	35
2	B	508/510 (100%)	498 (98%)	10 (2%)	0	100	100
2	b	503/510 (99%)	494 (98%)	9 (2%)	0	100	100
3	C	454/461 (98%)	442 (97%)	11 (2%)	1 (0%)	43	42
3	c	463/461 (100%)	448 (97%)	14 (3%)	1 (0%)	43	42
4	D	340/352 (97%)	329 (97%)	11 (3%)	0	100	100
4	d	341/352 (97%)	334 (98%)	7 (2%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	80/84 (95%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	32/45 (71%)	32 (100%)	0	0	100	100
6	f	32/45 (71%)	31 (97%)	1 (3%)	0	100	100
7	H	63/66 (96%)	59 (94%)	4 (6%)	0	100	100
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%)	1 (3%)	0	100	100
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
12	M	31/36 (86%)	31 (100%)	0	0	100	100
12	m	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
13	O	243/272 (89%)	230 (95%)	11 (4%)	2 (1%)	16	11
13	o	242/272 (89%)	234 (97%)	7 (3%)	1 (0%)	30	27
14	R	26/41 (63%)	26 (100%)	0	0	100	100
14	r	26/41 (63%)	26 (100%)	0	0	100	100
15	T	28/32 (88%)	28 (100%)	0	0	100	100
15	t	28/32 (88%)	28 (100%)	0	0	100	100
16	U	95/134 (71%)	93 (98%)	2 (2%)	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%)	130 (96%)	5 (4%)	0	100	100
18	X	36/41 (88%)	35 (97%)	1 (3%)	0	100	100
18	x	37/41 (90%)	36 (97%)	1 (3%)	0	100	100
19	Y	25/46 (54%)	22 (88%)	3 (12%)	0	100	100
19	y	28/46 (61%)	26 (93%)	2 (7%)	0	100	100
20	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
20	z	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
All	All	5387/5700 (94%)	5245 (97%)	134 (2%)	8 (0%)	43	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
17	V	64	PRO
3	c	416	SER
13	O	58	ASN
13	O	62	GLU
1	A	259	ILE
1	a	259	ILE
13	o	56	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	324/280 (116%)	319 (98%)	5 (2%)	57	64
1	a	323/280 (115%)	313 (97%)	10 (3%)	35	37
2	B	408/407 (100%)	399 (98%)	9 (2%)	45	50
2	b	402/407 (99%)	394 (98%)	8 (2%)	48	54
3	C	356/362 (98%)	348 (98%)	8 (2%)	45	50
3	c	364/362 (101%)	355 (98%)	9 (2%)	42	45
4	D	277/283 (98%)	274 (99%)	3 (1%)	65	73
4	d	278/283 (98%)	269 (97%)	9 (3%)	34	35
5	E	72/73 (99%)	67 (93%)	5 (7%)	14	11
5	e	71/73 (97%)	69 (97%)	2 (3%)	38	41
6	F	28/39 (72%)	27 (96%)	1 (4%)	31	31
6	f	28/39 (72%)	27 (96%)	1 (4%)	31	31
7	H	54/55 (98%)	53 (98%)	1 (2%)	50	56
7	h	53/55 (96%)	52 (98%)	1 (2%)	50	56
8	I	32/34 (94%)	31 (97%)	1 (3%)	35	37
8	i	32/34 (94%)	31 (97%)	1 (3%)	35	37
9	J	24/28 (86%)	23 (96%)	1 (4%)	26	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	j	24/28 (86%)	22 (92%)	2 (8%)	10	7
10	K	30/37 (81%)	28 (93%)	2 (7%)	15	11
10	k	30/37 (81%)	24 (80%)	6 (20%)	1	0
11	L	35/35 (100%)	34 (97%)	1 (3%)	37	40
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%)	201 (98%)	5 (2%)	43	47
13	o	207/228 (91%)	201 (97%)	6 (3%)	37	40
14	R	22/33 (67%)	18 (82%)	4 (18%)	2	1
14	r	22/33 (67%)	20 (91%)	2 (9%)	9	6
15	T	26/28 (93%)	25 (96%)	1 (4%)	29	29
15	t	25/28 (89%)	25 (100%)	0	100	100
16	U	84/112 (75%)	82 (98%)	2 (2%)	43	47
16	u	84/112 (75%)	82 (98%)	2 (2%)	43	47
17	V	117/138 (85%)	112 (96%)	5 (4%)	26	25
17	v	117/138 (85%)	113 (97%)	4 (3%)	32	33
18	X	31/34 (91%)	29 (94%)	2 (6%)	15	12
18	x	31/34 (91%)	29 (94%)	2 (6%)	15	12
19	Y	19/37 (51%)	18 (95%)	1 (5%)	20	18
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%)	45 (88%)	6 (12%)	5	3
All	All	4451/4654 (96%)	4308 (97%)	143 (3%)	34	35

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	60[A]	ILE
1	A	60[B]	ILE
1	A	243	GLU
1	A	248	ILE
2	B	76	SER

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Mol	Chain	Res	Type
2	B	79	SER
2	B	86	ILE
2	B	98	LEU
2	B	127	ARG
2	B	240	SER
2	B	362	PHE
2	B	371	THR
2	B	476	ARG
3	C	104	GLU
3	C	130	VAL
3	C	141	GLU
3	C	200	THR
3	C	240	ILE
3	C	273	SER
3	C	289	PHE
3	C	315	MET
4	D	43	LEU
4	D	154	VAL
4	D	259	ILE
5	E	11	SER
5	E	22[A]	ILE
5	E	22[B]	ILE
5	E	61	ARG
5	E	81	GLU
6	F	25	THR
7	H	20	LYS
8	I	4	LEU
9	J	24	ILE
10	K	10	LYS
10	K	25	LEU
11	L	2	GLU
12	M	25	LEU
13	O	57	LYS
13	O	78	LEU
13	O	107	THR
13	O	198	SER
13	O	214	THR
14	R	6	LEU
14	R	10	LEU
14	R	21	ARG
14	R	29	LYS
15	T	25	GLU

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Mol	Chain	Res	Type
16	U	51	LYS
16	U	67	LEU
17	V	3	LEU
17	V	7	VAL
17	V	31	ARG
17	V	57	GLU
17	V	86	GLN
18	X	3	ILE
18	X	23	LEU
19	Y	34	MET
20	Z	2	THR
20	Z	15	LEU
20	Z	19	MET
20	Z	32	ASP
20	Z	35	ARG
20	Z	50	LEU
1	a	28	LEU
1	a	42	LEU
1	a	159[A]	LEU
1	a	159[B]	LEU
1	a	200	LEU
1	a	223	LEU
1	a	231	GLU
1	a	245	THR
1	a	271	LEU
1	a	288	LEU
2	b	83	GLU
2	b	128	THR
2	b	149	LEU
2	b	236	THR
2	b	362	PHE
2	b	485	GLU
2	b	492	GLU
2	b	506	ARG
3	c	24	THR
3	c	72	LEU
3	c	99	VAL
3	c	124	VAL
3	c	125	LEU
3	c	165	LEU
3	c	240	ILE
3	c	289	PHE

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Mol	Chain	Res	Type
3	c	416	SER
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	4	THR
5	e	83	LEU
6	f	28	VAL
7	h	7	LEU
8	i	2	GLU
9	j	13	VAL
9	j	21	VAL
10	k	10	LYS
10	k	13	GLU
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
13	o	49	THR
13	o	87	VAL
13	o	118	LEU
13	o	130	GLN
13	o	207	ARG
14	r	9	LEU
14	r	10	LEU
16	u	15	GLU
16	u	23	GLU
17	v	24	LYS
17	v	52	LEU
17	v	69	ILE
17	v	107	LEU

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Mol	Chain	Res	Type
18	x	2	THR
18	x	15	LEU
19	y	19	ILE
19	y	41	VAL
19	y	45	ASN
20	z	1	MET
20	z	7	LEU
20	z	20	VAL
20	z	32	ASP
20	z	39	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	223	GLN
2	B	331	ASN
2	B	497	GLN
3	C	385	GLN
3	C	415	ASN
4	D	61	HIS
4	D	332	GLN
5	E	60	GLN
12	M	5	GLN
13	O	36	GLN
13	O	88	ASN
13	O	155	ASN
14	R	22	ASN
16	U	37	GLN
16	U	78	ASN
17	V	86	GLN
18	X	38	GLN
20	Z	31	GLN
1	a	19	ASN
1	a	234	ASN
2	b	14	ASN
2	b	179	GLN
3	c	322	GLN
3	c	382	ASN
4	d	250	ASN
4	d	350	ASN
5	e	60	GLN

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Mol	Chain	Res	Type
5	e	82	GLN
7	h	59	ASN
13	o	80	GLN
13	o	155	ASN
18	x	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	FME	T	1	15	8,9,10	0.97	1 (12%)	8,9,11	1.37	1 (12%)
12	FME	M	1	12	8,9,10	1.02	1 (12%)	8,9,11	0.97	0
15	FME	t	1	15	8,9,10	1.46	1 (12%)	8,9,11	1.03	1 (12%)
8	FME	I	1	8	8,9,10	1.01	1 (12%)	8,9,11	0.94	0
12	FME	m	1	12	8,9,10	0.97	0	8,9,11	0.73	0
8	FME	i	1	8	8,9,10	1.07	1 (12%)	8,9,11	0.84	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
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	-3.55	1.41	1.46
8	i	1	FME	CA-N	-2.27	1.43	1.46
8	I	1	FME	CA-N	-2.14	1.43	1.46
15	T	1	FME	CA-N	-2.05	1.43	1.46
12	M	1	FME	CA-N	-2.01	1.43	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	1	FME	O1-CN-N	-2.44	119.02	125.32
15	t	1	FME	CB-CA-N	2.22	114.56	110.52

There are no chirality outliers.

All (6) 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	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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$
24	CLA	b	611	2	69,73,73	1.29	8 (11%)	82,113,113	1.40	8 (9%)
24	CLA	d	403	4	69,73,73	1.33	11 (15%)	82,113,113	1.45	7 (8%)
26	BCR	k	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.05	4 (7%)
24	CLA	a	606	1	69,73,73	1.57	11 (15%)	82,113,113	1.30	8 (9%)
24	CLA	B	612	2	69,73,73	1.32	8 (11%)	82,113,113	1.49	11 (13%)
26	BCR	b	619	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
24	CLA	B	614	2	69,73,73	1.19	6 (8%)	82,113,113	1.38	11 (13%)
33	STE	t	102	-	17,17,19	0.57	0	17,17,19	1.19	1 (5%)
33	STE	I	101	-	14,14,19	0.45	0	13,13,19	0.64	0
26	BCR	A	609	-	41,41,41	1.22	5 (12%)	56,56,56	1.42	9 (16%)
26	BCR	c	515	-	41,41,41	1.27	4 (9%)	56,56,56	1.35	8 (14%)
32	DGD	C	517	-	63,63,67	1.19	6 (9%)	77,77,81	1.35	8 (10%)
24	CLA	B	604	2	69,73,73	1.19	7 (10%)	82,113,113	1.48	7 (8%)
24	CLA	a	612	37	69,73,73	1.76	11 (15%)	82,113,113	1.48	8 (9%)
24	CLA	b	616	2	64,68,73	1.18	9 (14%)	76,107,113	1.41	8 (10%)
24	CLA	B	615	2	69,73,73	1.33	8 (11%)	82,113,113	1.27	7 (8%)
33	STE	b	627	-	13,13,19	0.49	0	12,12,19	0.54	0
29	LMG	b	623	-	55,55,55	0.87	3 (5%)	63,63,63	1.40	8 (12%)
30	LHG	B	621	-	48,48,48	0.85	1 (2%)	51,54,54	1.19	6 (11%)
28	PL9	D	405	-	55,55,55	1.51	9 (16%)	68,69,69	1.66	16 (23%)
24	CLA	b	613	2	69,73,73	1.22	8 (11%)	82,113,113	1.31	8 (9%)
22	OEX	A	602[A]	37,1,3	0,14,14	-	-	-	-	-
21	OXY	a	601[B]	37,1,3	0,16,16	-	-	-	-	-
33	STE	k	103	-	11,11,19	0.82	0	11,11,19	0.94	0
29	LMG	b	621	-	51,51,55	0.95	3 (5%)	59,59,63	1.49	10 (16%)
32	DGD	C	518	-	63,63,67	1.12	5 (7%)	77,77,81	1.34	8 (10%)
29	LMG	D	406	-	51,51,55	0.96	3 (5%)	59,59,63	1.27	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	b	602	2	69,73,73	1.19	8 (11%)	82,113,113	1.56	11 (13%)
24	CLA	c	512	3	69,73,73	1.12	7 (10%)	82,113,113	1.34	6 (7%)
24	CLA	b	610	37	69,73,73	1.33	7 (10%)	82,113,113	1.46	11 (13%)
29	LMG	c	519	-	37,37,55	1.23	6 (16%)	45,45,63	1.35	6 (13%)
24	CLA	C	510	3	69,73,73	1.23	10 (14%)	82,113,113	1.47	10 (12%)
26	BCR	B	618	-	41,41,41	1.23	4 (9%)	56,56,56	1.17	4 (7%)
28	PL9	a	611	-	55,55,55	1.13	6 (10%)	68,69,69	1.67	14 (20%)
30	LHG	A	615	-	46,46,48	1.14	4 (8%)	49,52,54	1.39	5 (10%)
24	CLA	B	608	2	69,73,73	1.07	5 (7%)	82,113,113	1.27	10 (12%)
24	CLA	B	603	2	69,73,73	1.33	8 (11%)	82,113,113	1.60	11 (13%)
24	CLA	C	503	3	69,73,73	1.31	7 (10%)	82,113,113	1.69	11 (13%)
31	SQD	B	623	-	52,54,54	0.97	3 (5%)	62,65,65	1.96	14 (22%)
26	BCR	B	617	-	41,41,41	1.14	3 (7%)	56,56,56	1.33	9 (16%)
32	DGD	c	518	-	63,63,67	1.10	6 (9%)	77,77,81	1.42	14 (18%)
24	CLA	b	609	2	69,73,73	1.47	8 (11%)	82,113,113	1.60	12 (14%)
22	OEX	a	602[A]	37,1,3	0,14,14	-	-	-	-	-
33	STE	E	102	-	11,11,19	0.88	0	11,11,19	1.18	1 (9%)
24	CLA	b	607	37	69,73,73	1.26	8 (11%)	82,113,113	1.23	8 (9%)
24	CLA	c	504	37	64,68,73	1.23	7 (10%)	76,107,113	1.24	9 (11%)
35	HEM	F	101	6,5	50,50,50	1.35	4 (8%)	67,82,82	1.20	6 (8%)
33	STE	H	103	-	17,17,19	0.51	0	16,16,19	0.69	0
25	PHO	A	606	-	58,69,69	1.78	14 (24%)	55,99,99	1.73	10 (18%)
24	CLA	B	610	37	69,73,73	1.40	10 (14%)	82,113,113	1.43	8 (9%)
26	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
33	STE	a	617	-	14,14,19	0.43	0	13,13,19	0.80	0
32	DGD	c	517	-	63,63,67	1.22	8 (12%)	77,77,81	1.40	15 (19%)
24	CLA	B	606	2	69,73,73	1.31	12 (17%)	82,113,113	1.42	12 (14%)
33	STE	M	103	-	9,9,19	0.41	0	8,8,19	0.88	0
26	BCR	C	514	-	41,41,41	1.24	3 (7%)	56,56,56	1.36	8 (14%)
24	CLA	C	508	3	69,73,73	1.51	10 (14%)	82,113,113	1.47	11 (13%)
31	SQD	f	101	-	39,41,54	1.12	4 (10%)	49,52,65	1.94	11 (22%)
32	DGD	h	101	-	63,63,67	1.16	7 (11%)	77,77,81	1.38	12 (15%)
24	CLA	b	612	2	69,73,73	1.58	10 (14%)	82,113,113	1.27	10 (12%)
24	CLA	D	402	4	69,73,73	1.21	10 (14%)	82,113,113	1.34	8 (9%)
33	STE	B	626	-	15,15,19	0.46	0	14,14,19	0.67	0
24	CLA	b	614	2	69,73,73	1.43	9 (13%)	82,113,113	1.48	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	SQD	a	613	-	52,54,54	1.05	5 (9%)	62,65,65	1.87	11 (17%)
24	CLA	A	605	37	69,73,73	1.29	7 (10%)	82,113,113	1.46	11 (13%)
31	SQD	b	620	-	47,49,54	0.99	3 (6%)	57,60,65	1.87	14 (24%)
24	CLA	C	506	3	69,73,73	1.72	10 (14%)	82,113,113	1.22	7 (8%)
24	CLA	b	604	2	69,73,73	1.16	7 (10%)	82,113,113	1.48	15 (18%)
30	LHG	d	409	-	38,38,48	0.93	1 (2%)	41,44,54	1.19	2 (4%)
34	BCT	D	401	23	3,3,3	0.99	0	2,3,3	3.31	1 (50%)
33	STE	T	103	-	14,14,19	0.45	0	13,13,19	0.79	0
24	CLA	B	605	2	69,73,73	1.19	5 (7%)	82,113,113	1.31	9 (10%)
33	STE	B	620	-	16,16,19	0.74	0	16,16,19	1.08	0
33	STE	d	412	-	19,19,19	0.55	0	19,19,19	1.14	0
24	CLA	c	511	3	69,73,73	1.49	9 (13%)	82,113,113	1.29	4 (4%)
24	CLA	C	502	3	69,73,73	1.22	7 (10%)	82,113,113	1.36	7 (8%)
29	LMG	d	410	-	44,44,55	1.02	3 (6%)	52,52,63	1.26	6 (11%)
29	LMG	D	410	-	26,26,55	0.60	0	26,26,63	1.25	1 (3%)
29	LMG	c	522	-	49,49,55	0.88	2 (4%)	57,57,63	1.30	6 (10%)
33	STE	B	625	-	11,11,19	0.80	0	11,11,19	1.09	0
33	STE	m	101	-	11,11,19	0.66	0	11,11,19	1.35	1 (9%)
26	BCR	D	404	-	41,41,41	1.21	2 (4%)	56,56,56	1.22	4 (7%)
28	PL9	d	406	-	55,55,55	1.54	7 (12%)	68,69,69	1.75	14 (20%)
33	STE	x	102	-	19,19,19	0.77	1 (5%)	19,19,19	1.09	1 (5%)
24	CLA	C	505	3	69,73,73	1.33	7 (10%)	82,113,113	1.40	8 (9%)
26	BCR	b	618	-	41,41,41	1.28	4 (9%)	56,56,56	1.18	7 (12%)
33	STE	J	101	-	11,11,19	0.74	0	11,11,19	1.34	1 (9%)
33	STE	b	624	-	15,15,19	0.83	1 (6%)	15,15,19	0.78	0
24	CLA	b	608	2	69,73,73	1.28	10 (14%)	82,113,113	1.30	12 (14%)
30	LHG	d	407	-	48,48,48	0.88	4 (8%)	51,54,54	1.46	7 (13%)
24	CLA	c	508	3	68,72,73	1.41	7 (10%)	80,111,113	1.45	10 (12%)
26	BCR	x	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	5 (8%)
33	STE	C	521	-	15,15,19	0.37	0	14,14,19	0.86	0
26	BCR	C	515	-	41,41,41	1.24	3 (7%)	56,56,56	1.25	5 (8%)
31	SQD	A	617	-	38,38,54	0.97	3 (7%)	40,40,65	1.46	4 (10%)
33	STE	M	102	-	14,14,19	0.62	0	14,14,19	1.14	1 (7%)
25	PHO	a	605	-	58,69,69	1.90	12 (20%)	55,99,99	1.62	10 (18%)
24	CLA	b	606	2	69,73,73	1.73	8 (11%)	82,113,113	1.61	9 (10%)
30	LHG	D	408	-	48,48,48	1.14	4 (8%)	51,54,54	1.27	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	613	2	69,73,73	1.24	8 (11%)	82,113,113	1.12	7 (8%)
33	STE	d	411	-	16,16,19	0.60	0	16,16,19	1.43	1 (6%)
24	CLA	c	513	3	69,73,73	1.26	9 (13%)	82,113,113	1.23	9 (10%)
33	STE	b	626	-	9,9,19	0.46	0	8,8,19	0.64	0
30	LHG	B	622	-	48,48,48	0.92	3 (6%)	51,54,54	1.35	8 (15%)
30	LHG	e	102	-	41,41,48	0.89	2 (4%)	44,47,54	1.33	5 (11%)
24	CLA	c	502	3	69,73,73	1.19	9 (13%)	82,113,113	1.34	8 (9%)
26	BCR	K	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.18	4 (7%)
24	CLA	D	403	4	69,73,73	1.56	10 (14%)	82,113,113	1.31	6 (7%)
26	BCR	b	617	-	41,41,41	1.12	3 (7%)	56,56,56	1.40	8 (14%)
24	CLA	b	615	2	69,73,73	1.55	10 (14%)	82,113,113	1.60	13 (15%)
28	PL9	A	612	-	55,55,55	1.13	4 (7%)	68,69,69	1.57	11 (16%)
33	STE	B	624	-	13,13,19	0.70	0	13,13,19	1.12	1 (7%)
24	CLA	A	613	37	69,73,73	1.30	11 (15%)	82,113,113	1.40	7 (8%)
24	CLA	b	605	2	69,73,73	1.19	8 (11%)	82,113,113	1.49	12 (14%)
33	STE	b	622	-	19,19,19	0.59	0	19,19,19	1.04	1 (5%)
24	CLA	d	404	4	69,73,73	1.44	10 (14%)	82,113,113	1.18	8 (9%)
24	CLA	d	401	37	69,73,73	1.32	12 (17%)	82,113,113	1.37	10 (12%)
33	STE	C	522	-	11,11,19	0.70	0	11,11,19	1.36	2 (18%)
36	HEC	v	201	17	50,50,50	1.69	5 (10%)	68,82,82	1.31	7 (10%)
24	CLA	c	510	3	69,73,73	1.54	10 (14%)	82,113,113	1.47	11 (13%)
24	CLA	c	503	3	69,73,73	1.25	8 (11%)	82,113,113	1.17	5 (6%)
24	CLA	C	507	37	69,73,73	1.24	7 (10%)	82,113,113	1.50	11 (13%)
33	STE	b	625	-	19,19,19	0.66	0	19,19,19	1.00	1 (5%)
24	CLA	A	604	1	69,73,73	1.26	7 (10%)	82,113,113	1.24	10 (12%)
24	CLA	A	608	1	58,62,73	1.37	8 (13%)	68,99,113	1.30	6 (8%)
33	STE	D	411	-	19,19,19	0.57	0	19,19,19	1.24	1 (5%)
24	CLA	B	601	37	69,73,73	1.27	6 (8%)	82,113,113	1.38	9 (10%)
24	CLA	B	607	37	69,73,73	1.16	8 (11%)	82,113,113	1.34	6 (7%)
24	CLA	b	603	2	69,73,73	1.36	7 (10%)	82,113,113	1.43	12 (14%)
32	DGD	c	516	-	63,63,67	1.17	8 (12%)	77,77,81	1.38	11 (14%)
31	SQD	a	614	-	35,35,54	1.04	2 (5%)	37,37,65	1.52	6 (16%)
24	CLA	C	513	3	69,73,73	1.14	5 (7%)	82,113,113	1.43	10 (12%)
26	BCR	T	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	6 (10%)
24	CLA	C	501	3	69,73,73	1.40	8 (11%)	82,113,113	1.54	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	D	409	-	31,31,55	0.98	2 (6%)	33,33,63	1.11	1 (3%)
21	OEY	A	601[B]	37,1,3	0,16,16	-	-	-		
30	LHG	E	101	-	48,48,48	0.90	2 (4%)	51,54,54	1.28	5 (9%)
29	LMG	A	614	-	48,48,55	1.04	4 (8%)	56,56,63	1.41	6 (10%)
31	SQD	D	407	-	34,36,54	1.01	3 (8%)	42,45,65	2.09	10 (23%)
24	CLA	C	509	3	69,73,73	1.23	7 (10%)	82,113,113	1.46	8 (9%)
33	STE	c	520	-	19,19,19	0.63	0	19,19,19	0.98	0
33	STE	j	101	-	11,11,19	0.85	0	11,11,19	0.99	1 (9%)
29	LMG	a	618	-	55,55,55	1.06	5 (9%)	63,63,63	1.45	8 (12%)
24	CLA	c	505	3	69,73,73	1.19	10 (14%)	82,113,113	1.31	7 (8%)
24	CLA	B	616	2	64,68,73	1.36	8 (12%)	76,107,113	1.56	8 (10%)
26	BCR	t	101	-	41,41,41	1.15	5 (12%)	56,56,56	1.39	8 (14%)
33	STE	C	520	-	11,11,19	0.92	0	11,11,19	1.03	0
36	HEC	V	201	17	50,50,50	1.56	4 (8%)	68,82,82	1.32	9 (13%)
29	LMG	c	521	-	48,48,55	1.09	6 (12%)	56,56,63	1.27	3 (5%)
32	DGD	H	102	-	63,63,67	1.35	13 (20%)	77,77,81	1.38	8 (10%)
26	BCR	Y	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.18	5 (8%)
26	BCR	a	607	-	41,41,41	1.08	4 (9%)	56,56,56	1.23	6 (10%)
24	CLA	a	604	1	69,73,73	1.25	8 (11%)	82,113,113	1.28	6 (7%)
24	CLA	c	507	37	69,73,73	1.19	5 (7%)	82,113,113	1.39	10 (12%)
29	LMG	C	519	-	48,48,55	0.90	3 (6%)	56,56,63	1.38	7 (12%)
34	BCT	a	610	23	3,3,3	0.97	0	2,3,3	3.21	1 (50%)
25	PHO	d	402	-	58,69,69	2.11	8 (13%)	55,99,99	1.53	7 (12%)
26	BCR	k	102	-	41,41,41	1.17	3 (7%)	56,56,56	1.18	4 (7%)
33	STE	a	616	-	11,11,19	0.86	0	11,11,19	1.28	2 (18%)
24	CLA	B	611	2	69,73,73	1.35	7 (10%)	82,113,113	1.66	11 (13%)
32	DGD	C	516	-	63,63,67	1.29	9 (14%)	77,77,81	1.39	9 (11%)
35	HEM	e	101	6,5	50,50,50	1.39	8 (16%)	67,82,82	1.23	6 (8%)
24	CLA	c	506	3	69,73,73	1.43	11 (15%)	82,113,113	1.39	8 (9%)
24	CLA	B	602	2	69,73,73	1.42	9 (13%)	82,113,113	1.27	10 (12%)
29	LMG	M	101	-	51,51,55	1.08	4 (7%)	59,59,63	1.50	7 (11%)
33	STE	B	627	-	11,11,19	0.83	0	11,11,19	1.06	1 (9%)
24	CLA	B	609	2	69,73,73	1.46	9 (13%)	82,113,113	1.41	12 (14%)
24	CLA	C	511	3	69,73,73	1.54	9 (13%)	82,113,113	1.32	7 (8%)
26	BCR	d	405	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	C	512	3	69,73,73	1.15	6 (8%)	82,113,113	1.35	9 (10%)
31	SQD	A	616	-	50,52,54	1.12	6 (12%)	60,63,65	2.05	11 (18%)
33	STE	Z	101	-	7,7,19	0.48	0	6,6,19	0.46	0
33	STE	l	102	-	17,17,19	0.37	0	16,16,19	0.90	0
24	CLA	b	601	37	69,73,73	1.27	8 (11%)	82,113,113	1.40	6 (7%)
24	CLA	c	501	3	69,73,73	1.09	3 (4%)	82,113,113	1.39	9 (10%)
25	PHO	A	607	-	58,69,69	2.01	9 (15%)	55,99,99	1.46	9 (16%)
32	DGD	A	618	-	67,67,67	1.22	7 (10%)	81,81,81	1.38	9 (11%)
30	LHG	d	408	-	48,48,48	0.86	1 (2%)	51,54,54	1.23	4 (7%)
24	CLA	c	509	3	69,73,73	1.30	5 (7%)	82,113,113	1.48	8 (9%)
26	BCR	c	514	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	8 (14%)
33	STE	T	102	-	15,15,19	0.41	0	14,14,19	0.83	0
26	BCR	B	619	-	41,41,41	1.27	5 (12%)	56,56,56	1.28	4 (7%)
33	STE	a	615	-	9,9,19	0.57	0	8,8,19	0.48	0
24	CLA	C	504	37	63,67,73	1.17	6 (9%)	74,105,113	1.35	7 (9%)
30	LHG	l	101	-	48,48,48	0.88	1 (2%)	51,54,54	1.29	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	611	2	-	5/39/115/115	-
24	CLA	d	403	4	-	5/39/115/115	-
26	BCR	k	101	-	-	12/29/63/63	0/2/2/2
24	CLA	a	606	1	-	8/39/115/115	-
24	CLA	B	612	2	-	8/39/115/115	-
26	BCR	b	619	-	-	2/29/63/63	0/2/2/2
24	CLA	B	614	2	-	15/39/115/115	-
33	STE	t	102	-	-	9/15/15/17	-
33	STE	I	101	-	-	4/12/12/17	-
26	BCR	A	609	-	-	8/29/63/63	0/2/2/2
26	BCR	c	515	-	-	3/29/63/63	0/2/2/2
32	DGD	C	517	-	-	23/51/91/95	0/2/2/2
24	CLA	B	604	2	-	8/39/115/115	-
24	CLA	a	612	37	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	616	2	-	10/33/109/115	-
24	CLA	B	615	2	-	12/39/115/115	-
33	STE	b	627	-	-	6/11/11/17	-
29	LMG	b	623	-	-	25/50/70/70	0/1/1/1
30	LHG	B	621	-	-	25/53/53/53	-
28	PL9	D	405	-	-	10/53/73/73	0/1/1/1
24	CLA	b	613	2	-	7/39/115/115	-
33	STE	k	103	-	-	4/9/9/17	-
29	LMG	b	621	-	-	24/46/66/70	0/1/1/1
32	DGD	C	518	-	-	18/51/91/95	0/2/2/2
29	LMG	D	406	-	-	14/46/66/70	0/1/1/1
24	CLA	b	602	2	-	4/39/115/115	-
24	CLA	c	512	3	-	20/39/115/115	-
24	CLA	b	610	37	-	4/39/115/115	-
29	LMG	c	519	-	-	11/31/51/70	0/1/1/1
24	CLA	C	510	3	-	9/39/115/115	-
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
28	PL9	a	611	-	-	22/53/73/73	0/1/1/1
30	LHG	A	615	-	-	20/51/51/53	-
24	CLA	B	608	2	-	2/39/115/115	-
24	CLA	B	603	2	-	7/39/115/115	-
24	CLA	C	503	3	-	2/39/115/115	-
31	SQD	B	623	-	-	22/49/69/69	0/1/1/1
26	BCR	B	617	-	-	7/29/63/63	0/2/2/2
32	DGD	c	518	-	-	12/51/91/95	0/2/2/2
24	CLA	b	609	2	-	9/39/115/115	-
33	STE	E	102	-	-	4/9/9/17	-
24	CLA	b	607	37	-	12/39/115/115	-
24	CLA	c	504	37	-	7/33/109/115	-
35	HEM	F	101	6,5	-	2/14/54/54	-
33	STE	H	103	-	-	9/15/15/17	-
25	PHO	A	606	-	-	1/37/103/103	0/5/6/6
24	CLA	B	610	37	-	5/39/115/115	-
26	BCR	H	101	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	a	617	-	-	8/12/12/17	-
32	DGD	c	517	-	-	18/51/91/95	0/2/2/2
24	CLA	B	606	2	-	11/39/115/115	-
33	STE	M	103	-	-	1/7/7/17	-
26	BCR	C	514	-	-	8/29/63/63	0/2/2/2
24	CLA	C	508	3	-	7/39/115/115	-
31	SQD	f	101	-	-	13/36/56/69	0/1/1/1
32	DGD	h	101	-	-	15/51/91/95	0/2/2/2
24	CLA	b	612	2	-	6/39/115/115	-
24	CLA	D	402	4	-	5/39/115/115	-
33	STE	B	626	-	-	8/13/13/17	-
24	CLA	b	614	2	-	12/39/115/115	-
31	SQD	a	613	-	-	22/49/69/69	0/1/1/1
24	CLA	A	605	37	-	11/39/115/115	-
31	SQD	b	620	-	-	20/44/64/69	0/1/1/1
24	CLA	C	506	3	-	9/39/115/115	-
24	CLA	b	604	2	-	7/39/115/115	-
30	LHG	d	409	-	-	14/43/43/53	-
33	STE	T	103	-	-	11/12/12/17	-
24	CLA	B	605	2	-	9/39/115/115	-
33	STE	B	620	-	-	5/14/14/17	-
33	STE	d	412	-	-	11/17/17/17	-
24	CLA	c	511	3	-	11/39/115/115	-
24	CLA	C	502	3	-	5/39/115/115	-
29	LMG	d	410	-	-	11/39/59/70	0/1/1/1
29	LMG	D	410	-	-	14/22/22/70	-
29	LMG	c	522	-	-	20/44/64/70	0/1/1/1
33	STE	B	625	-	-	5/9/9/17	-
33	STE	m	101	-	-	3/9/9/17	-
26	BCR	D	404	-	-	5/29/63/63	0/2/2/2
28	PL9	d	406	-	-	11/53/73/73	0/1/1/1
33	STE	x	102	-	-	6/17/17/17	-
24	CLA	C	505	3	-	7/39/115/115	-
26	BCR	b	618	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	STE	J	101	-	-	7/9/9/17	-
33	STE	b	624	-	-	10/13/13/17	-
24	CLA	b	608	2	-	1/39/115/115	-
30	LHG	d	407	-	-	21/53/53/53	-
24	CLA	c	508	3	-	7/38/114/115	-
26	BCR	x	101	-	-	7/29/63/63	0/2/2/2
33	STE	C	521	-	-	7/13/13/17	-
26	BCR	C	515	-	-	4/29/63/63	0/2/2/2
31	SQD	A	617	-	-	13/39/39/69	-
33	STE	M	102	-	-	5/12/12/17	-
25	PHO	a	605	-	-	1/37/103/103	0/5/6/6
24	CLA	b	606	2	-	9/39/115/115	-
30	LHG	D	408	-	-	23/53/53/53	-
24	CLA	B	613	2	-	14/39/115/115	-
33	STE	d	411	-	-	8/14/14/17	-
24	CLA	c	513	3	-	6/39/115/115	-
33	STE	b	626	-	-	5/7/7/17	-
30	LHG	B	622	-	-	14/53/53/53	-
30	LHG	e	102	-	-	26/46/46/53	-
24	CLA	c	502	3	-	3/39/115/115	-
26	BCR	K	101	-	-	8/29/63/63	0/2/2/2
24	CLA	D	403	4	-	9/39/115/115	-
26	BCR	b	617	-	-	6/29/63/63	0/2/2/2
24	CLA	b	615	2	-	8/39/115/115	-
28	PL9	A	612	-	-	24/53/73/73	0/1/1/1
33	STE	B	624	-	-	3/11/11/17	-
24	CLA	A	613	37	-	4/39/115/115	-
24	CLA	b	605	2	-	7/39/115/115	-
33	STE	b	622	-	-	10/17/17/17	-
24	CLA	d	404	4	-	11/39/115/115	-
24	CLA	d	401	37	-	12/39/115/115	-
33	STE	C	522	-	-	3/9/9/17	-
36	HEC	v	201	17	1/1/7/7	4/14/54/54	-
24	CLA	c	510	3	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	503	3	-	6/39/115/115	-
24	CLA	C	507	37	-	11/39/115/115	-
33	STE	b	625	-	-	12/17/17/17	-
24	CLA	A	604	1	-	4/39/115/115	-
24	CLA	A	608	1	-	2/26/102/115	-
33	STE	D	411	-	-	11/17/17/17	-
24	CLA	B	601	37	-	15/39/115/115	-
24	CLA	B	607	37	-	4/39/115/115	-
24	CLA	b	603	2	-	8/39/115/115	-
32	DGD	c	516	-	-	28/51/91/95	0/2/2/2
31	SQD	a	614	-	-	18/37/37/69	-
24	CLA	C	513	3	-	5/39/115/115	-
26	BCR	T	101	-	-	8/29/63/63	0/2/2/2
24	CLA	C	501	3	-	3/39/115/115	-
29	LMG	D	409	-	-	16/33/33/70	-
30	LHG	E	101	-	-	22/53/53/53	-
33	STE	c	520	-	-	10/17/17/17	-
29	LMG	A	614	-	-	21/43/63/70	0/1/1/1
31	SQD	D	407	-	-	14/28/48/69	0/1/1/1
24	CLA	C	509	3	-	16/39/115/115	-
33	STE	j	101	-	-	4/9/9/17	-
29	LMG	a	618	-	-	30/50/70/70	0/1/1/1
24	CLA	c	505	3	-	11/39/115/115	-
24	CLA	B	616	2	-	8/33/109/115	-
26	BCR	t	101	-	-	6/29/63/63	0/2/2/2
33	STE	C	520	-	-	6/9/9/17	-
36	HEC	V	201	17	1/1/7/7	6/14/54/54	-
29	LMG	c	521	-	-	23/43/63/70	0/1/1/1
32	DGD	H	102	-	-	19/51/91/95	0/2/2/2
26	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
26	BCR	a	607	-	-	1/29/63/63	0/2/2/2
24	CLA	a	604	1	-	4/39/115/115	-
24	CLA	c	507	37	-	10/39/115/115	-
29	LMG	C	519	-	-	17/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PHO	d	402	-	-	1/37/103/103	0/5/6/6
26	BCR	k	102	-	-	7/29/63/63	0/2/2/2
33	STE	a	616	-	-	3/9/9/17	-
24	CLA	B	611	2	-	6/39/115/115	-
32	DGD	C	516	-	-	19/51/91/95	0/2/2/2
35	HEM	e	101	6,5	-	3/14/54/54	-
24	CLA	c	506	3	-	13/39/115/115	-
24	CLA	B	602	2	-	6/39/115/115	-
29	LMG	M	101	-	-	24/46/66/70	0/1/1/1
33	STE	B	627	-	-	5/9/9/17	-
24	CLA	B	609	2	-	3/39/115/115	-
24	CLA	C	511	3	-	3/39/115/115	-
26	BCR	d	405	-	-	5/29/63/63	0/2/2/2
24	CLA	C	512	3	-	12/39/115/115	-
31	SQD	A	616	-	-	15/47/67/69	0/1/1/1
33	STE	Z	101	-	-	2/5/5/17	-
33	STE	l	102	-	-	9/15/15/17	-
24	CLA	b	601	37	-	16/39/115/115	-
24	CLA	c	501	3	-	1/39/115/115	-
25	PHO	A	607	-	-	1/37/103/103	0/5/6/6
32	DGD	A	618	-	-	27/55/95/95	0/2/2/2
30	LHG	d	408	-	-	18/53/53/53	-
24	CLA	c	509	3	-	11/39/115/115	-
26	BCR	c	514	-	-	10/29/63/63	0/2/2/2
33	STE	T	102	-	-	8/13/13/17	-
26	BCR	B	619	-	-	5/29/63/63	0/2/2/2
33	STE	a	615	-	-	4/7/7/17	-
24	CLA	C	504	37	-	7/32/108/115	-
30	LHG	l	101	-	-	15/53/53/53	-

All (899) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	606	CLA	MG-NA	9.48	2.28	2.06
25	d	402	PHO	C1B-C2B	9.37	1.49	1.39
25	A	607	PHO	C3B-C4B	9.23	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402	PHO	C3B-C4B	9.22	1.50	1.41
24	a	606	CLA	MG-ND	-8.26	1.89	2.05
25	A	607	PHO	C1B-C2B	8.11	1.48	1.39
25	a	605	PHO	C1B-C2B	8.00	1.48	1.39
24	C	506	CLA	MG-ND	-7.96	1.90	2.05
24	a	612	CLA	MG-NA	7.78	2.24	2.06
24	c	511	CLA	MG-NA	7.69	2.24	2.06
24	D	403	CLA	MG-NB	-7.43	1.91	2.05
24	c	510	CLA	MG-NA	7.43	2.23	2.06
25	A	606	PHO	C1B-C2B	7.35	1.47	1.39
36	v	201	HEC	C3D-C2D	7.29	1.52	1.36
24	b	612	CLA	MG-NC	-7.19	1.89	2.06
24	B	611	CLA	MG-NA	7.14	2.23	2.06
24	B	610	CLA	MG-ND	-6.97	1.92	2.05
24	C	501	CLA	MG-NA	6.56	2.21	2.06
24	b	614	CLA	MG-ND	-6.47	1.93	2.05
36	V	201	HEC	C3D-C2D	6.33	1.50	1.36
24	b	609	CLA	MG-NA	6.23	2.21	2.06
24	C	511	CLA	MG-NA	6.03	2.20	2.06
24	C	505	CLA	MG-NA	5.97	2.20	2.06
24	B	616	CLA	MG-NA	5.94	2.20	2.06
24	C	508	CLA	MG-NA	5.93	2.20	2.06
24	B	609	CLA	MG-NA	5.93	2.20	2.06
28	d	406	PL9	C6-C1	-5.92	1.38	1.48
24	a	612	CLA	MG-NB	5.83	2.17	2.05
25	a	605	PHO	C3B-C4B	5.83	1.47	1.41
24	b	615	CLA	MG-NB	5.82	2.17	2.05
24	C	503	CLA	MG-NA	5.81	2.20	2.06
24	b	611	CLA	MG-NB	5.45	2.16	2.05
24	d	404	CLA	MG-NB	-5.28	1.95	2.05
24	C	507	CLA	MG-NA	5.28	2.18	2.06
24	c	506	CLA	MG-NB	5.25	2.16	2.05
24	C	506	CLA	MG-NB	5.09	2.15	2.05
24	d	404	CLA	MG-NA	4.95	2.18	2.06
24	b	610	CLA	MG-ND	-4.89	1.96	2.05
24	B	609	CLA	MG-NB	-4.87	1.96	2.05
24	B	602	CLA	C1D-ND	4.86	1.44	1.37
24	B	612	CLA	MG-NC	4.84	2.17	2.06
24	c	508	CLA	MG-NA	4.83	2.17	2.06
24	B	603	CLA	MG-NA	4.81	2.17	2.06
30	D	408	LHG	O7-C5	-4.75	1.35	1.46
24	c	513	CLA	MG-ND	-4.74	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	MG-NA	4.73	2.17	2.06
24	b	609	CLA	MG-ND	-4.71	1.96	2.05
24	A	608	CLA	MG-ND	-4.71	1.96	2.05
24	A	608	CLA	C1D-ND	4.68	1.44	1.37
36	V	201	HEC	FE-ND	4.67	2.09	1.94
24	b	612	CLA	MG-NB	4.67	2.15	2.05
28	d	406	PL9	C53-C6	-4.62	1.41	1.50
24	c	509	CLA	MG-NB	4.62	2.14	2.05
24	C	511	CLA	MG-ND	4.59	2.14	2.05
25	a	605	PHO	C1D-C2D	4.57	1.44	1.39
24	B	604	CLA	MG-NC	4.56	2.17	2.06
24	b	603	CLA	MG-NA	4.55	2.17	2.06
24	c	509	CLA	C1D-ND	4.51	1.43	1.37
24	b	606	CLA	MG-NB	-4.48	1.96	2.05
24	B	602	CLA	MG-NB	-4.47	1.96	2.05
24	b	610	CLA	C1D-ND	4.44	1.43	1.37
24	C	502	CLA	MG-NA	4.39	2.16	2.06
26	c	515	BCR	C1-C6	-4.37	1.48	1.53
32	A	618	DGD	O5D-C6D	-4.35	1.36	1.43
24	B	606	CLA	MG-NA	4.35	2.16	2.06
26	B	618	BCR	C30-C25	-4.33	1.48	1.53
24	C	506	CLA	MG-NA	4.32	2.16	2.06
26	Y	101	BCR	C30-C25	-4.31	1.48	1.53
24	C	511	CLA	MG-NB	-4.31	1.97	2.05
24	d	403	CLA	C4B-NB	4.30	1.43	1.37
24	b	602	CLA	MG-NB	4.26	2.14	2.05
24	c	507	CLA	MG-ND	4.20	2.14	2.05
24	C	509	CLA	C1D-ND	4.19	1.43	1.37
36	v	201	HEC	FE-NA	4.14	2.08	1.95
26	C	515	BCR	C1-C6	-4.13	1.48	1.53
30	A	615	LHG	O3-C3	-4.09	1.29	1.44
24	C	508	CLA	MG-NC	-4.09	1.96	2.06
25	A	606	PHO	C3B-C4B	4.09	1.45	1.41
24	a	612	CLA	C1D-ND	4.06	1.43	1.37
24	c	508	CLA	MG-NB	4.04	2.13	2.05
24	A	605	CLA	MG-NB	-4.01	1.97	2.05
24	b	601	CLA	MG-NA	4.01	2.15	2.06
28	D	405	PL9	C3-C4	-4.01	1.43	1.49
24	C	508	CLA	MG-ND	4.01	2.13	2.05
32	C	518	DGD	O2G-C2G	-4.00	1.37	1.46
26	c	514	BCR	C1-C6	-3.98	1.48	1.53
26	H	101	BCR	C30-C25	-3.95	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	D	404	BCR	C30-C25	-3.94	1.48	1.53
24	b	607	CLA	C1B-NB	-3.94	1.32	1.37
24	B	615	CLA	MG-NA	3.93	2.15	2.06
29	a	618	LMG	C4-C5	3.93	1.61	1.53
29	D	409	LMG	C7-C8	3.92	1.60	1.51
24	c	504	CLA	C4B-NB	3.89	1.43	1.37
24	b	603	CLA	C4B-NB	3.86	1.42	1.37
26	C	514	BCR	C1-C6	-3.85	1.48	1.53
26	B	619	BCR	C1-C6	-3.82	1.48	1.53
24	c	504	CLA	MG-ND	-3.82	1.98	2.05
26	K	101	BCR	C30-C25	-3.81	1.48	1.53
26	T	101	BCR	C30-C25	-3.79	1.48	1.53
26	d	405	BCR	C30-C25	-3.79	1.48	1.53
24	b	606	CLA	C1D-ND	3.79	1.42	1.37
24	c	506	CLA	C1B-NB	-3.79	1.32	1.37
24	b	615	CLA	C1B-C2B	3.77	1.52	1.43
24	b	612	CLA	MG-ND	-3.74	1.98	2.05
24	c	510	CLA	MG-NC	-3.71	1.97	2.06
24	c	506	CLA	MG-ND	-3.71	1.98	2.05
32	c	518	DGD	O3G-C3G	-3.70	1.37	1.43
31	b	620	SQD	O48-C23	3.70	1.44	1.33
26	C	514	BCR	C30-C25	-3.69	1.49	1.53
24	B	605	CLA	C1B-C2B	3.69	1.51	1.43
30	B	621	LHG	O7-C5	-3.68	1.38	1.46
24	c	501	CLA	C1D-ND	3.65	1.42	1.37
24	B	612	CLA	C4B-NB	3.64	1.42	1.37
24	b	609	CLA	C1D-ND	3.64	1.42	1.37
26	k	101	BCR	C30-C25	-3.62	1.49	1.53
24	D	403	CLA	C1D-ND	3.62	1.42	1.37
24	c	508	CLA	C1D-ND	3.60	1.42	1.37
24	B	605	CLA	MG-NB	3.60	2.12	2.05
24	A	604	CLA	MG-NC	3.59	2.14	2.06
32	C	517	DGD	O5D-C6D	-3.59	1.37	1.43
28	D	405	PL9	C7-C3	-3.58	1.46	1.51
28	d	406	PL9	C31-C29	-3.57	1.43	1.51
31	a	613	SQD	O48-C23	3.57	1.43	1.33
31	a	614	SQD	O48-C23	3.55	1.43	1.33
29	A	614	LMG	O1-C7	-3.55	1.37	1.43
30	A	615	LHG	P-O6	3.53	1.73	1.59
25	d	402	PHO	CMC-C2C	-3.53	1.45	1.50
24	b	603	CLA	MG-NB	-3.52	1.98	2.05
24	b	612	CLA	MG-NA	3.51	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	405	PL9	C6-C1	-3.51	1.42	1.48
24	a	604	CLA	MG-ND	-3.50	1.98	2.05
24	c	502	CLA	MG-NB	-3.49	1.98	2.05
26	k	102	BCR	C30-C25	-3.49	1.49	1.53
26	b	618	BCR	C1-C6	-3.49	1.49	1.53
24	d	401	CLA	MG-NB	3.48	2.12	2.05
29	c	521	LMG	O1-C1	3.48	1.46	1.40
24	A	605	CLA	C1D-ND	3.48	1.42	1.37
26	c	514	BCR	C30-C25	-3.48	1.49	1.53
24	C	506	CLA	C1D-ND	3.46	1.42	1.37
28	D	405	PL9	C26-C24	-3.45	1.44	1.51
24	B	602	CLA	C4B-NB	3.45	1.42	1.37
29	c	519	LMG	C1-C2	3.44	1.62	1.52
25	A	606	PHO	C3D-C4D	3.44	1.45	1.41
24	B	601	CLA	C1D-ND	3.42	1.42	1.37
24	B	609	CLA	C1D-ND	3.42	1.42	1.37
24	A	604	CLA	C4B-NB	3.42	1.42	1.37
24	B	612	CLA	C1D-ND	3.42	1.42	1.37
24	b	613	CLA	C1D-ND	3.41	1.42	1.37
26	B	617	BCR	C1-C6	-3.40	1.49	1.53
24	D	403	CLA	MG-NC	3.40	2.14	2.06
26	C	515	BCR	C30-C25	-3.40	1.49	1.53
25	a	605	PHO	C3D-C4D	3.39	1.45	1.41
24	B	601	CLA	MG-ND	-3.39	1.99	2.05
24	b	613	CLA	MG-ND	-3.39	1.99	2.05
24	A	613	CLA	C1D-ND	3.39	1.42	1.37
32	C	517	DGD	C4D-C3D	3.39	1.61	1.52
26	b	618	BCR	C30-C25	-3.37	1.49	1.53
24	C	501	CLA	C1D-ND	3.37	1.42	1.37
24	b	601	CLA	C1D-ND	3.37	1.42	1.37
24	A	604	CLA	C1D-ND	3.36	1.42	1.37
30	d	407	LHG	C24-C23	3.36	1.60	1.50
25	A	606	PHO	C4D-ND	-3.36	1.33	1.38
25	A	606	PHO	CMC-C2C	-3.34	1.45	1.50
31	B	623	SQD	O47-C7	3.33	1.43	1.34
26	b	617	BCR	C30-C25	-3.33	1.49	1.53
24	b	605	CLA	C1B-C2B	3.32	1.50	1.43
24	C	513	CLA	C1D-ND	3.32	1.42	1.37
24	d	403	CLA	MG-ND	-3.31	1.99	2.05
24	B	614	CLA	C4B-NB	3.31	1.42	1.37
26	x	101	BCR	C30-C25	-3.31	1.49	1.53
24	b	614	CLA	C1D-ND	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C4B-NB	3.30	1.42	1.37
26	c	515	BCR	C30-C25	-3.30	1.49	1.53
31	D	407	SQD	O48-C23	3.30	1.43	1.33
28	d	406	PL9	C3-C4	-3.30	1.44	1.49
24	c	505	CLA	MG-NA	3.29	2.14	2.06
24	b	601	CLA	C1B-C2B	3.27	1.50	1.43
24	b	615	CLA	C1D-ND	3.27	1.42	1.37
24	B	615	CLA	C4B-NB	3.27	1.42	1.37
24	a	604	CLA	MG-NC	3.26	2.14	2.06
32	c	517	DGD	C3E-C2E	3.26	1.60	1.52
24	B	602	CLA	MG-NA	3.25	2.14	2.06
29	d	410	LMG	C4-C5	3.25	1.60	1.53
24	a	606	CLA	C1D-ND	3.25	1.42	1.37
24	b	615	CLA	C3B-C4B	3.25	1.52	1.42
24	A	613	CLA	MG-NB	3.24	2.12	2.05
24	d	401	CLA	MG-NC	3.22	2.13	2.06
26	Y	101	BCR	C1-C6	-3.22	1.49	1.53
24	c	510	CLA	C1D-ND	3.22	1.42	1.37
24	c	503	CLA	C1D-ND	3.21	1.42	1.37
24	B	616	CLA	C1D-ND	3.21	1.42	1.37
31	a	614	SQD	O47-C7	3.20	1.43	1.34
24	b	613	CLA	C1B-NB	-3.20	1.33	1.37
32	h	101	DGD	O2D-C2D	-3.20	1.35	1.43
24	B	613	CLA	CMD-C2D	-3.20	1.44	1.50
24	A	613	CLA	MG-NA	3.20	2.13	2.06
24	B	615	CLA	C1D-ND	3.18	1.42	1.37
24	c	507	CLA	MG-NB	-3.18	1.99	2.05
24	B	607	CLA	C1D-ND	3.18	1.42	1.37
32	C	516	DGD	C6D-C5D	3.18	1.61	1.51
30	E	101	LHG	P-O6	3.17	1.71	1.59
28	a	611	PL9	C3-C4	-3.17	1.44	1.49
32	H	102	DGD	O3G-C1D	3.17	1.45	1.40
30	B	622	LHG	O7-C5	-3.17	1.39	1.46
31	B	623	SQD	O48-C23	3.17	1.42	1.33
24	B	607	CLA	MG-NA	3.16	2.13	2.06
26	b	619	BCR	C30-C25	-3.16	1.49	1.53
32	A	618	DGD	C4D-C3D	3.16	1.60	1.52
24	C	509	CLA	MG-NB	-3.15	1.99	2.05
24	c	511	CLA	MG-NC	-3.15	1.98	2.06
32	H	102	DGD	O2D-C2D	-3.15	1.35	1.43
24	B	604	CLA	MG-NA	3.15	2.13	2.06
26	A	609	BCR	C33-C5	-3.15	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	405	BCR	C1-C6	-3.15	1.49	1.53
24	d	403	CLA	C1B-C2B	3.14	1.50	1.43
31	A	617	SQD	O47-C7	3.14	1.43	1.34
26	t	101	BCR	C30-C25	-3.14	1.49	1.53
24	B	603	CLA	C1D-ND	3.13	1.42	1.37
24	C	511	CLA	C3B-C4B	3.13	1.51	1.42
25	a	605	PHO	C4D-ND	-3.13	1.33	1.38
32	H	102	DGD	O5D-C1E	3.13	1.45	1.40
24	A	605	CLA	C4B-NB	3.12	1.42	1.37
32	A	618	DGD	C3E-C2E	3.12	1.60	1.52
24	b	616	CLA	C1D-ND	3.12	1.42	1.37
26	b	619	BCR	C1-C6	-3.11	1.49	1.53
24	C	507	CLA	MG-NB	-3.10	1.99	2.05
24	b	603	CLA	C1D-ND	3.09	1.41	1.37
31	A	616	SQD	O48-C23	3.08	1.42	1.33
24	a	612	CLA	MG-ND	-3.08	1.99	2.05
24	B	603	CLA	CMB-C2B	-3.07	1.44	1.50
24	C	509	CLA	C3B-C4B	3.07	1.51	1.42
31	f	101	SQD	O48-C23	3.07	1.42	1.33
24	B	615	CLA	C1B-C2B	3.07	1.50	1.43
32	c	516	DGD	O2G-C2G	-3.07	1.39	1.46
24	B	601	CLA	C4B-NB	3.07	1.41	1.37
24	b	606	CLA	MG-ND	3.07	2.11	2.05
24	b	604	CLA	MG-NC	3.06	2.13	2.06
32	C	516	DGD	O5D-C1E	3.06	1.45	1.40
24	b	608	CLA	MG-ND	3.05	2.11	2.05
24	c	509	CLA	C1B-C2B	3.05	1.50	1.43
24	C	510	CLA	C1D-ND	3.05	1.41	1.37
26	A	609	BCR	C1-C6	-3.05	1.49	1.53
26	B	619	BCR	C30-C25	-3.04	1.49	1.53
24	D	402	CLA	MG-NB	-3.04	1.99	2.05
24	B	613	CLA	MG-ND	-3.04	1.99	2.05
35	F	101	HEM	FE-NC	3.04	2.05	1.95
32	C	516	DGD	C6E-C5E	3.04	1.62	1.51
24	a	612	CLA	MG-NC	-3.03	1.99	2.06
24	b	613	CLA	C4B-NB	3.03	1.41	1.37
25	A	607	PHO	CMB-C2B	-3.03	1.45	1.51
24	C	506	CLA	MG-NC	-3.03	1.99	2.06
24	C	511	CLA	C1D-ND	3.02	1.41	1.37
32	C	517	DGD	C6E-C5E	3.02	1.61	1.51
24	C	505	CLA	C1B-C2B	3.01	1.50	1.43
24	b	615	CLA	C4B-NB	3.01	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	617	BCR	C1-C6	-3.01	1.49	1.53
26	k	102	BCR	C1-C6	-3.01	1.49	1.53
24	C	505	CLA	C4B-NB	3.01	1.41	1.37
24	a	604	CLA	C1B-C2B	3.01	1.50	1.43
24	B	612	CLA	C1B-C2B	3.00	1.50	1.43
24	C	501	CLA	CHC-C1C	3.00	1.44	1.38
28	a	611	PL9	C52-C5	-2.99	1.44	1.50
31	b	620	SQD	O47-C7	2.99	1.42	1.34
24	C	504	CLA	MG-NB	2.99	2.11	2.05
31	a	613	SQD	O2-C2	-2.98	1.35	1.43
24	B	611	CLA	C1B-C2B	2.98	1.50	1.43
29	a	618	LMG	C4-C3	2.97	1.60	1.52
24	c	507	CLA	C1B-NB	-2.97	1.34	1.37
24	c	503	CLA	MG-NC	2.97	2.13	2.06
28	a	611	PL9	C53-C6	-2.97	1.44	1.50
24	a	612	CLA	C1B-C2B	2.97	1.50	1.43
24	b	602	CLA	C1D-ND	2.97	1.41	1.37
31	f	101	SQD	O47-C7	2.97	1.42	1.34
24	B	609	CLA	C4B-NB	2.96	1.41	1.37
24	C	513	CLA	MG-NA	2.96	2.13	2.06
24	B	615	CLA	CMB-C2B	-2.96	1.44	1.50
31	A	617	SQD	O48-C23	2.96	1.42	1.33
24	D	403	CLA	C1B-C2B	2.95	1.50	1.43
24	d	401	CLA	C1D-ND	2.95	1.41	1.37
32	C	516	DGD	O2E-C2E	-2.94	1.35	1.43
28	A	612	PL9	C3-C4	-2.94	1.45	1.49
32	c	518	DGD	O2G-C2G	-2.94	1.39	1.46
32	H	102	DGD	C4E-C5E	2.94	1.59	1.53
32	C	518	DGD	O5D-C1E	2.94	1.45	1.40
32	H	102	DGD	C3E-C2E	2.93	1.59	1.52
24	C	508	CLA	C1D-ND	2.93	1.41	1.37
35	e	101	HEM	FE-NA	2.93	2.04	1.95
24	c	502	CLA	CMD-C2D	-2.93	1.44	1.50
24	c	507	CLA	C1D-ND	2.92	1.41	1.37
24	a	606	CLA	C1B-C2B	2.92	1.50	1.43
24	C	505	CLA	CHC-C1C	2.92	1.44	1.38
24	c	508	CLA	C1B-C2B	2.91	1.50	1.43
24	D	402	CLA	CHC-C1C	2.91	1.44	1.38
26	D	404	BCR	C1-C6	-2.91	1.50	1.53
26	B	617	BCR	C33-C5	-2.91	1.46	1.50
24	A	605	CLA	C1B-C2B	2.91	1.50	1.43
26	T	101	BCR	C1-C6	-2.91	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C1B-NB	-2.90	1.34	1.37
26	B	617	BCR	C30-C25	-2.90	1.50	1.53
32	h	101	DGD	C4E-C5E	2.90	1.59	1.53
24	a	606	CLA	MG-NB	-2.90	2.00	2.05
24	D	402	CLA	C1B-C2B	2.90	1.49	1.43
24	c	505	CLA	C4B-NB	2.90	1.41	1.37
24	B	606	CLA	C1D-ND	2.90	1.41	1.37
24	C	512	CLA	MG-NA	2.89	2.13	2.06
24	B	610	CLA	C4B-NB	2.89	1.41	1.37
24	c	506	CLA	C1D-ND	2.88	1.41	1.37
24	B	614	CLA	MG-ND	-2.88	2.00	2.05
24	c	513	CLA	C1D-ND	2.87	1.41	1.37
36	v	201	HEC	FE-ND	2.87	2.03	1.94
24	A	613	CLA	CHC-C1C	2.87	1.44	1.38
24	b	614	CLA	MG-NA	2.87	2.13	2.06
24	B	603	CLA	MG-ND	2.87	2.11	2.05
28	d	406	PL9	C21-C19	-2.86	1.45	1.51
30	d	409	LHG	P-O6	2.86	1.70	1.59
24	a	606	CLA	CMC-C2C	-2.86	1.44	1.50
24	B	601	CLA	C1B-C2B	2.85	1.49	1.43
28	A	612	PL9	C7-C8	-2.85	1.46	1.50
25	A	606	PHO	C3B-C2B	-2.85	1.36	1.40
26	b	617	BCR	C33-C5	-2.85	1.46	1.50
32	h	101	DGD	C4D-C3D	2.85	1.59	1.52
29	c	521	LMG	C3-C2	2.84	1.59	1.52
24	B	607	CLA	MG-NB	-2.84	2.00	2.05
24	b	603	CLA	CMC-C2C	-2.84	1.45	1.50
24	c	511	CLA	C1B-C2B	2.84	1.49	1.43
30	l	101	LHG	O7-C5	-2.84	1.39	1.46
24	C	501	CLA	C4B-NB	2.84	1.41	1.37
25	d	402	PHO	CMD-C2D	-2.83	1.46	1.51
24	d	404	CLA	MG-ND	-2.83	2.00	2.05
32	C	516	DGD	C4D-C3D	2.83	1.59	1.52
24	B	604	CLA	C3B-C4B	2.83	1.51	1.42
24	C	508	CLA	CHC-C1C	2.83	1.44	1.38
24	C	511	CLA	C1B-C2B	2.83	1.49	1.43
24	b	607	CLA	CMD-C2D	-2.83	1.45	1.50
24	b	615	CLA	CMB-C2B	-2.83	1.45	1.50
24	b	607	CLA	MG-NC	2.83	2.13	2.06
24	a	606	CLA	CMD-C2D	-2.82	1.45	1.50
24	b	607	CLA	C1B-C2B	2.82	1.49	1.43
24	B	612	CLA	C3B-C4B	2.82	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	615	CLA	CMD-C2D	-2.81	1.45	1.50
31	a	613	SQD	O47-C7	2.81	1.42	1.34
24	C	512	CLA	CMD-C2D	-2.81	1.45	1.50
24	b	608	CLA	MG-NB	-2.81	2.00	2.05
28	D	405	PL9	C30-C29	-2.81	1.43	1.50
24	b	608	CLA	CMB-C2B	-2.81	1.45	1.50
24	d	404	CLA	CMD-C2D	-2.80	1.45	1.50
24	b	607	CLA	MG-NA	2.80	2.12	2.06
24	b	612	CLA	CMB-C2B	-2.80	1.45	1.50
31	A	617	SQD	O47-C45	-2.80	1.42	1.47
24	b	610	CLA	C1B-C2B	2.80	1.49	1.43
24	D	403	CLA	C4B-NB	2.80	1.41	1.37
25	d	402	PHO	CAC-C3C	-2.79	1.46	1.51
25	A	607	PHO	C1D-C2D	2.79	1.42	1.39
26	a	607	BCR	C1-C6	-2.79	1.50	1.53
24	C	511	CLA	C4B-NB	2.78	1.41	1.37
24	B	602	CLA	CMB-C2B	-2.78	1.45	1.50
26	a	607	BCR	C27-C26	-2.77	1.45	1.51
24	B	601	CLA	CMB-C2B	-2.77	1.45	1.50
24	d	401	CLA	C1B-NB	-2.77	1.34	1.37
24	C	503	CLA	C1B-C2B	2.76	1.49	1.43
32	c	516	DGD	O2E-C2E	-2.76	1.36	1.43
25	A	606	PHO	C1D-C2D	2.76	1.42	1.39
24	b	614	CLA	MG-NB	2.76	2.11	2.05
36	V	201	HEC	CMB-C2B	2.75	1.56	1.50
24	B	616	CLA	CMC-C2C	-2.75	1.45	1.50
25	A	607	PHO	C4D-CHA	2.75	1.43	1.39
24	B	608	CLA	C1D-ND	2.75	1.41	1.37
24	c	510	CLA	CMB-C2B	-2.75	1.45	1.50
24	b	606	CLA	MG-NC	-2.75	1.99	2.06
24	D	403	CLA	C1B-NB	-2.75	1.34	1.37
35	F	101	HEM	FE-NA	2.75	2.04	1.95
25	a	605	PHO	C3B-C2B	-2.75	1.36	1.40
24	c	512	CLA	C1D-ND	2.74	1.41	1.37
24	B	603	CLA	CMC-C2C	-2.74	1.45	1.50
24	b	601	CLA	C4B-NB	2.74	1.41	1.37
24	C	502	CLA	C1B-C2B	2.74	1.49	1.43
32	C	516	DGD	O5D-C6D	-2.74	1.39	1.43
24	B	605	CLA	C3B-C4B	2.73	1.50	1.42
24	d	401	CLA	C1B-C2B	2.73	1.49	1.43
30	D	408	LHG	P-O3	2.72	1.70	1.59
24	c	513	CLA	C4B-NB	2.72	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	508	CLA	C3B-C4B	2.72	1.50	1.42
29	M	101	LMG	C4-C5	2.72	1.58	1.53
24	A	605	CLA	CMD-C2D	-2.72	1.45	1.50
24	C	504	CLA	C1D-ND	2.72	1.41	1.37
29	D	406	LMG	C4-C5	2.71	1.58	1.53
24	b	607	CLA	C1D-ND	2.71	1.41	1.37
24	C	513	CLA	C1B-C2B	2.71	1.49	1.43
26	A	609	BCR	C30-C25	-2.71	1.50	1.53
24	d	403	CLA	C1D-ND	2.71	1.41	1.37
29	b	621	LMG	C4-C3	2.71	1.59	1.52
24	d	404	CLA	CMC-C2C	-2.71	1.45	1.50
28	A	612	PL9	C6-C1	-2.70	1.44	1.48
24	a	612	CLA	CMB-C2B	-2.70	1.45	1.50
24	C	508	CLA	C1D-C2D	2.70	1.50	1.45
24	b	608	CLA	MG-NA	2.70	2.12	2.06
32	C	516	DGD	O2G-C1B	2.70	1.41	1.34
24	C	508	CLA	C3B-C4B	2.70	1.50	1.42
24	C	501	CLA	CMC-C2C	-2.70	1.45	1.50
31	D	407	SQD	O2-C2	-2.69	1.36	1.43
24	B	608	CLA	MG-NA	2.69	2.12	2.06
24	D	402	CLA	CMD-C2D	-2.69	1.45	1.50
31	A	616	SQD	O2-C2	-2.69	1.36	1.43
26	k	101	BCR	C1-C6	-2.69	1.50	1.53
24	b	604	CLA	C4B-NB	2.69	1.41	1.37
28	D	405	PL9	C10-C9	-2.69	1.44	1.50
30	e	102	LHG	P-O6	2.68	1.69	1.59
24	a	612	CLA	C1B-NB	-2.68	1.34	1.37
24	D	403	CLA	CMB-C2B	-2.68	1.45	1.50
24	b	610	CLA	CMD-C2D	-2.68	1.45	1.50
24	d	403	CLA	MG-NA	2.68	2.12	2.06
24	b	616	CLA	CMC-C2C	-2.67	1.45	1.50
24	B	608	CLA	CMD-C2D	-2.67	1.45	1.50
24	d	401	CLA	C4B-NB	2.67	1.41	1.37
26	K	101	BCR	C1-C6	-2.66	1.50	1.53
25	a	605	PHO	O2D-CGD	2.66	1.39	1.33
24	a	604	CLA	C4B-NB	2.65	1.41	1.37
24	b	612	CLA	CMC-C2C	-2.65	1.45	1.50
24	B	606	CLA	C4B-NB	2.65	1.41	1.37
25	A	607	PHO	C4D-ND	-2.64	1.34	1.38
24	C	507	CLA	C1D-ND	2.64	1.41	1.37
24	a	606	CLA	C4B-NB	2.64	1.41	1.37
24	b	603	CLA	CMB-C2B	-2.64	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	621	LMG	O7-C8	-2.64	1.40	1.46
29	M	101	LMG	O7-C8	-2.64	1.40	1.46
28	a	611	PL9	C6-C1	-2.64	1.44	1.48
24	b	615	CLA	MG-ND	-2.64	2.00	2.05
35	F	101	HEM	CAB-C3B	2.64	1.54	1.47
31	f	101	SQD	O2-C2	-2.64	1.36	1.43
24	B	613	CLA	CMC-C2C	-2.63	1.45	1.50
32	c	516	DGD	C4D-C5D	2.63	1.58	1.53
32	c	517	DGD	O3G-C1D	-2.63	1.35	1.40
29	c	522	LMG	C4-C5	2.63	1.58	1.53
32	c	517	DGD	O3E-C3E	-2.63	1.36	1.43
32	c	516	DGD	C6D-C5D	2.63	1.59	1.51
30	A	615	LHG	O7-C7	2.63	1.41	1.34
24	c	506	CLA	CHC-C1C	2.63	1.43	1.38
24	D	402	CLA	C4B-NB	2.62	1.41	1.37
24	B	616	CLA	C1B-NB	-2.62	1.34	1.37
24	c	510	CLA	CMC-C2C	-2.62	1.45	1.50
24	B	609	CLA	MG-ND	2.62	2.11	2.05
24	b	609	CLA	C1B-C2B	2.62	1.49	1.43
25	d	402	PHO	C1D-C2D	2.62	1.42	1.39
32	H	102	DGD	C1E-C2E	2.62	1.60	1.52
32	c	517	DGD	C4D-C3D	2.61	1.59	1.52
24	c	505	CLA	CHC-C1C	2.61	1.43	1.38
31	B	623	SQD	O2-C2	-2.61	1.36	1.43
31	A	616	SQD	O47-C7	2.61	1.41	1.34
24	b	610	CLA	MG-NB	-2.60	2.00	2.05
25	A	607	PHO	CMC-C2C	-2.60	1.46	1.50
24	B	614	CLA	C1B-NB	-2.60	1.34	1.37
32	C	517	DGD	C1E-C2E	2.60	1.60	1.52
24	B	613	CLA	C1B-C2B	2.60	1.49	1.43
24	B	610	CLA	C1D-ND	2.59	1.41	1.37
30	E	101	LHG	O7-C5	-2.59	1.40	1.46
28	D	405	PL9	C5-C4	-2.59	1.38	1.47
24	A	604	CLA	C1B-C2B	2.59	1.49	1.43
24	B	609	CLA	C1B-C2B	2.58	1.49	1.43
24	A	608	CLA	MG-NB	-2.58	2.00	2.05
26	K	101	BCR	C33-C5	-2.58	1.46	1.50
24	d	403	CLA	CMD-C2D	-2.57	1.45	1.50
24	b	604	CLA	C1D-ND	2.57	1.41	1.37
24	b	609	CLA	C4B-NB	2.57	1.41	1.37
24	c	511	CLA	CHC-C1C	2.57	1.43	1.38
24	B	614	CLA	C1D-ND	2.57	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	CHC-C1C	2.57	1.43	1.38
30	A	615	LHG	C8-C7	-2.57	1.43	1.50
24	b	611	CLA	C1B-C2B	2.57	1.49	1.43
29	c	519	LMG	C4-C3	2.56	1.59	1.52
24	C	505	CLA	C1B-NB	-2.56	1.34	1.37
24	c	505	CLA	C1B-C2B	2.56	1.49	1.43
24	C	507	CLA	C1B-C2B	2.56	1.49	1.43
24	B	612	CLA	C1B-NB	-2.56	1.34	1.37
24	A	605	CLA	C3B-C4B	2.56	1.50	1.42
24	c	503	CLA	C5-C3	-2.55	1.46	1.51
24	A	613	CLA	C3D-C4D	2.55	1.49	1.44
26	a	607	BCR	C30-C25	-2.55	1.50	1.53
24	c	513	CLA	C1B-C2B	2.55	1.49	1.43
26	t	101	BCR	C33-C5	-2.55	1.46	1.50
24	C	504	CLA	C3B-C4B	2.55	1.50	1.42
24	C	509	CLA	C1B-C2B	2.54	1.49	1.43
24	b	612	CLA	C1D-ND	2.54	1.41	1.37
24	c	508	CLA	CHC-C1C	2.54	1.43	1.38
29	c	521	LMG	C4-C3	2.54	1.58	1.52
24	b	614	CLA	CMB-C2B	-2.54	1.45	1.50
24	b	602	CLA	MG-NA	-2.54	2.00	2.06
24	b	606	CLA	C1B-C2B	2.54	1.49	1.43
24	C	505	CLA	MG-NC	-2.54	2.00	2.06
24	b	601	CLA	CHC-C1C	2.54	1.43	1.38
24	c	502	CLA	C1B-C2B	2.53	1.49	1.43
24	C	510	CLA	O2A-CGA	2.53	1.40	1.33
24	b	616	CLA	C1B-C2B	2.53	1.49	1.43
24	B	606	CLA	MG-NC	2.53	2.12	2.06
36	V	201	HEC	FE-NB	2.52	2.02	1.94
35	e	101	HEM	C3B-C2B	-2.52	1.32	1.37
24	c	510	CLA	C4B-NB	2.52	1.41	1.37
30	B	622	LHG	C24-C23	2.52	1.58	1.50
29	A	614	LMG	C4-C3	2.52	1.58	1.52
25	A	606	PHO	C4D-CHA	2.52	1.43	1.39
24	C	504	CLA	CMD-C2D	-2.52	1.45	1.50
24	b	610	CLA	CHC-C4B	-2.52	1.33	1.39
32	H	102	DGD	C6E-C5E	2.52	1.60	1.51
32	A	618	DGD	C3G-C2G	2.52	1.58	1.50
29	M	101	LMG	O1-C7	-2.51	1.39	1.43
25	A	607	PHO	CMD-C2D	-2.51	1.46	1.51
24	d	404	CLA	C4B-NB	2.51	1.41	1.37
32	h	101	DGD	O2E-C2E	-2.51	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	616	SQD	O3-C3	-2.51	1.36	1.43
24	c	510	CLA	C1B-C2B	2.51	1.49	1.43
24	B	605	CLA	C1B-NB	-2.51	1.34	1.37
24	b	614	CLA	CMC-C2C	-2.50	1.45	1.50
24	B	612	CLA	CHC-C1C	2.50	1.43	1.38
26	k	101	BCR	C33-C5	-2.50	1.47	1.50
28	d	406	PL9	C45-C44	-2.50	1.44	1.50
24	C	513	CLA	C3B-C4B	2.49	1.50	1.42
24	B	611	CLA	CMC-C2C	-2.49	1.45	1.50
29	b	623	LMG	C7-C8	2.49	1.58	1.50
24	B	615	CLA	CHC-C4B	-2.49	1.33	1.39
24	B	615	CLA	C1B-NB	-2.49	1.34	1.37
24	b	612	CLA	C1B-C2B	2.49	1.49	1.43
31	A	616	SQD	O47-C45	-2.49	1.40	1.46
24	b	611	CLA	CMC-C2C	-2.48	1.45	1.50
24	c	506	CLA	CAC-C3C	-2.48	1.44	1.51
32	H	102	DGD	O2G-C2G	-2.48	1.40	1.46
24	D	402	CLA	CAA-C2A	-2.48	1.49	1.54
30	d	408	LHG	O7-C5	-2.48	1.40	1.46
24	B	611	CLA	C3B-C4B	2.48	1.49	1.42
24	b	602	CLA	CAC-C3C	-2.47	1.44	1.51
32	A	618	DGD	C4D-C5D	2.47	1.58	1.53
24	b	604	CLA	C1B-C2B	2.47	1.48	1.43
24	b	611	CLA	CHC-C1C	2.47	1.43	1.38
24	b	612	CLA	C3B-C4B	2.47	1.49	1.42
24	b	614	CLA	C3B-C4B	2.47	1.49	1.42
24	D	403	CLA	CMC-C2C	-2.47	1.45	1.50
25	a	605	PHO	CMC-C2C	-2.47	1.46	1.50
24	b	601	CLA	C3B-C4B	2.47	1.49	1.42
24	C	508	CLA	C1B-C2B	2.47	1.48	1.43
26	c	515	BCR	C33-C5	-2.47	1.47	1.50
24	b	605	CLA	MG-NB	-2.47	2.00	2.05
32	c	517	DGD	C6E-C5E	2.47	1.60	1.51
32	c	517	DGD	C4D-C5D	2.47	1.58	1.53
32	C	518	DGD	O3G-C1D	-2.46	1.36	1.40
35	e	101	HEM	FE-ND	2.46	2.02	1.94
29	C	519	LMG	C4-C5	2.46	1.58	1.53
24	B	607	CLA	C3B-C4B	2.46	1.49	1.42
24	b	608	CLA	C1B-C2B	2.46	1.48	1.43
32	C	517	DGD	C6D-C5D	2.46	1.58	1.51
24	c	504	CLA	C1B-C2B	2.45	1.48	1.43
24	B	609	CLA	O2D-CGD	2.45	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	CMB-C2B	-2.45	1.45	1.50
30	D	408	LHG	C8-C7	-2.45	1.43	1.50
31	a	613	SQD	O4-C4	-2.44	1.36	1.43
24	b	605	CLA	C3B-C4B	2.44	1.49	1.42
24	B	606	CLA	CHC-C4B	-2.44	1.33	1.39
24	B	610	CLA	CHC-C1C	2.44	1.43	1.38
24	c	508	CLA	CMD-C2D	-2.43	1.45	1.50
24	c	509	CLA	C3B-C4B	2.43	1.49	1.42
32	c	518	DGD	O1G-C1G	-2.43	1.39	1.45
31	b	620	SQD	O2-C2	-2.43	1.36	1.43
24	d	401	CLA	CHC-C1C	2.43	1.43	1.38
24	C	502	CLA	CMB-C2B	-2.43	1.45	1.50
24	B	613	CLA	MG-NC	2.42	2.12	2.06
24	d	401	CLA	CMB-C2B	-2.42	1.45	1.50
29	c	519	LMG	O1-C1	2.42	1.44	1.40
29	M	101	LMG	C29-C28	-2.42	1.43	1.50
24	c	513	CLA	C3B-C4B	2.42	1.49	1.42
24	B	609	CLA	CMD-C2D	-2.41	1.45	1.50
32	c	518	DGD	O5D-C6D	-2.41	1.39	1.43
24	c	511	CLA	C1D-ND	2.41	1.41	1.37
25	d	402	PHO	CAA-C2A	-2.41	1.49	1.54
24	C	510	CLA	C4B-NB	2.41	1.41	1.37
24	B	605	CLA	CHC-C1C	2.41	1.43	1.38
24	B	616	CLA	C1B-C2B	2.41	1.48	1.43
24	c	510	CLA	CHC-C1C	2.41	1.43	1.38
24	B	616	CLA	CMD-C2D	-2.41	1.45	1.50
24	B	613	CLA	C3B-C4B	2.41	1.49	1.42
24	b	610	CLA	CMB-C2B	-2.40	1.45	1.50
24	b	602	CLA	C3B-C4B	2.40	1.49	1.42
29	D	406	LMG	C7-C8	2.40	1.58	1.50
24	C	510	CLA	C3D-C4D	2.40	1.49	1.44
32	C	518	DGD	C6D-C5D	2.40	1.58	1.51
24	C	510	CLA	C1B-C2B	2.40	1.48	1.43
24	C	512	CLA	C1B-C2B	2.40	1.48	1.43
24	b	605	CLA	C1B-NB	-2.40	1.34	1.37
24	b	608	CLA	C3B-C4B	2.40	1.49	1.42
24	C	507	CLA	C1B-NB	-2.40	1.34	1.37
24	C	510	CLA	CMC-C2C	-2.39	1.45	1.50
32	c	516	DGD	O3G-C3G	-2.39	1.39	1.43
24	c	503	CLA	C1B-NB	-2.39	1.34	1.37
24	c	503	CLA	C4B-NB	2.39	1.41	1.37
24	A	613	CLA	C1B-C2B	2.39	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	606	CLA	CHC-C1C	2.39	1.43	1.38
26	a	607	BCR	C33-C5	-2.38	1.47	1.50
35	e	101	HEM	CHB-C4A	-2.37	1.34	1.39
24	C	511	CLA	CMB-C2B	-2.37	1.45	1.50
24	b	605	CLA	MG-NA	2.37	2.11	2.06
24	d	403	CLA	MG-NC	2.37	2.11	2.06
24	c	502	CLA	C1D-ND	2.37	1.41	1.37
24	b	611	CLA	MG-ND	-2.37	2.01	2.05
24	B	603	CLA	C1B-C2B	2.36	1.48	1.43
31	f	101	SQD	O3-C3	-2.36	1.37	1.43
28	A	612	PL9	C37-C38	2.36	1.57	1.50
24	d	404	CLA	C3B-C4B	2.36	1.49	1.42
24	C	506	CLA	C4B-NB	2.36	1.41	1.37
24	C	509	CLA	CMD-C2D	-2.36	1.45	1.50
24	A	613	CLA	CMD-C2D	-2.35	1.45	1.50
24	A	608	CLA	C4B-NB	2.35	1.41	1.37
24	c	511	CLA	C4B-NB	2.35	1.41	1.37
24	c	512	CLA	C3B-C4B	2.35	1.49	1.42
29	A	614	LMG	C4-C5	2.35	1.58	1.53
24	c	504	CLA	CMD-C2D	-2.35	1.46	1.50
26	x	101	BCR	C1-C6	-2.35	1.50	1.53
24	d	403	CLA	C3B-C4B	2.35	1.49	1.42
24	A	604	CLA	MG-NB	-2.34	2.01	2.05
24	b	605	CLA	CHC-C1C	2.34	1.43	1.38
24	a	604	CLA	C3B-C4B	2.34	1.49	1.42
24	b	614	CLA	C4B-NB	2.33	1.40	1.37
24	c	506	CLA	CMC-C2C	-2.33	1.46	1.50
24	b	608	CLA	C1B-NB	-2.33	1.34	1.37
24	B	606	CLA	C1B-C2B	2.33	1.48	1.43
24	c	501	CLA	C1B-C2B	2.32	1.48	1.43
30	d	407	LHG	O7-C5	-2.32	1.41	1.46
24	b	609	CLA	C3B-C4B	2.32	1.49	1.42
24	c	503	CLA	C1B-C2B	2.32	1.48	1.43
24	c	512	CLA	CMD-C2D	-2.32	1.46	1.50
24	B	607	CLA	CMB-C2B	-2.32	1.46	1.50
26	t	101	BCR	C27-C26	-2.32	1.46	1.51
35	e	101	HEM	CAB-C3B	2.31	1.53	1.47
28	D	405	PL9	C7-C8	-2.31	1.46	1.50
29	b	623	LMG	C3-C2	2.31	1.58	1.52
24	B	610	CLA	C1B-C2B	2.31	1.48	1.43
26	A	609	BCR	C38-C26	-2.31	1.47	1.50
24	B	602	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	621	LMG	C1-C2	2.31	1.59	1.52
24	C	512	CLA	CMC-C2C	-2.31	1.46	1.50
24	c	512	CLA	C1B-C2B	2.31	1.48	1.43
24	A	604	CLA	CMD-C2D	-2.30	1.46	1.50
24	c	511	CLA	C3B-C4B	2.30	1.49	1.42
24	c	502	CLA	C4B-NB	2.30	1.40	1.37
24	b	616	CLA	CMB-C2B	-2.30	1.46	1.50
24	d	403	CLA	CMB-C2B	-2.30	1.46	1.50
24	B	602	CLA	C1B-C2B	2.30	1.48	1.43
24	a	606	CLA	CHC-C4B	-2.30	1.34	1.39
24	C	503	CLA	C4B-NB	2.29	1.40	1.37
29	d	410	LMG	O1-C1	2.29	1.44	1.40
32	c	516	DGD	O3D-C3D	-2.29	1.37	1.43
24	b	616	CLA	CMD-C2D	-2.29	1.46	1.50
28	a	611	PL9	C46-C44	-2.29	1.46	1.51
24	B	610	CLA	C3B-C4B	2.29	1.49	1.42
24	C	501	CLA	C1B-NB	-2.29	1.34	1.37
24	b	616	CLA	MG-NA	2.29	2.11	2.06
24	c	504	CLA	CHC-C1C	2.29	1.43	1.38
24	c	506	CLA	CMD-C2D	-2.29	1.46	1.50
32	H	102	DGD	C6D-C5D	2.28	1.58	1.51
32	c	518	DGD	O3D-C3D	-2.28	1.37	1.43
24	b	604	CLA	C3D-C4D	2.28	1.49	1.44
24	b	613	CLA	CMC-C2C	-2.28	1.46	1.50
32	A	618	DGD	O3D-C3D	-2.28	1.37	1.43
25	d	402	PHO	C4D-ND	-2.28	1.35	1.38
24	B	608	CLA	C1B-C2B	2.28	1.48	1.43
24	c	501	CLA	MG-NB	-2.28	2.01	2.05
24	B	615	CLA	C1D-C2D	2.28	1.49	1.45
29	c	521	LMG	O7-C8	-2.28	1.41	1.46
24	b	601	CLA	O2A-CGA	2.27	1.40	1.33
30	D	408	LHG	O8-C6	-2.27	1.40	1.45
24	c	512	CLA	MG-NB	2.27	2.10	2.05
24	B	606	CLA	CAB-C3B	-2.27	1.41	1.47
24	b	604	CLA	MG-NB	-2.27	2.01	2.05
35	e	101	HEM	CMC-C2C	2.27	1.55	1.50
24	C	510	CLA	C3B-C4B	2.27	1.49	1.42
24	b	606	CLA	C3B-C4B	2.27	1.49	1.42
32	H	102	DGD	C4D-C5D	2.27	1.57	1.53
24	B	613	CLA	C1B-NB	-2.27	1.34	1.37
26	B	619	BCR	C31-C1	-2.27	1.49	1.53
25	a	605	PHO	CMB-C2B	-2.27	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	502	CLA	MG-NC	2.26	2.11	2.06
26	B	618	BCR	C27-C26	-2.26	1.46	1.51
24	a	612	CLA	CHB-C1B	2.26	1.44	1.39
26	C	515	BCR	C33-C5	-2.26	1.47	1.50
24	A	613	CLA	CMB-C2B	-2.26	1.46	1.50
24	d	403	CLA	CHC-C4B	-2.26	1.34	1.39
29	c	519	LMG	O2-C2	-2.26	1.37	1.43
24	C	512	CLA	CMB-C2B	-2.25	1.46	1.50
24	b	611	CLA	O2D-CGD	2.25	1.38	1.33
24	c	505	CLA	CMC-C2C	-2.25	1.46	1.50
24	C	502	CLA	MG-NC	2.25	2.11	2.06
24	b	605	CLA	CHC-C4B	-2.25	1.34	1.39
24	c	513	CLA	CMB-C2B	-2.25	1.46	1.50
24	B	610	CLA	CMB-C2B	-2.25	1.46	1.50
24	b	602	CLA	CMD-C2D	-2.25	1.46	1.50
24	B	604	CLA	CHC-C1C	2.24	1.43	1.38
24	B	608	CLA	C3B-C4B	2.24	1.49	1.42
24	D	403	CLA	CHC-C4B	-2.24	1.34	1.39
33	b	624	STE	O1-C1	2.24	1.29	1.22
24	B	604	CLA	CMC-C2C	-2.24	1.46	1.50
36	v	201	HEC	FE-NC	2.23	2.02	1.95
24	a	612	CLA	C3B-C4B	2.23	1.49	1.42
24	c	505	CLA	C3B-C4B	2.23	1.49	1.42
24	C	508	CLA	CMC-C2C	-2.23	1.46	1.50
24	C	501	CLA	C3B-C4B	2.23	1.49	1.42
30	B	622	LHG	P-O4	-2.23	1.45	1.55
24	d	401	CLA	C3B-C4B	2.23	1.49	1.42
26	b	618	BCR	C27-C26	-2.23	1.46	1.51
24	c	503	CLA	CMB-C2B	-2.23	1.46	1.50
24	B	603	CLA	C3B-C4B	2.23	1.49	1.42
24	B	610	CLA	MG-NA	2.23	2.11	2.06
24	b	612	CLA	CHC-C1C	2.23	1.42	1.38
24	B	607	CLA	CHC-C1C	2.22	1.42	1.38
24	C	507	CLA	CMD-C2D	-2.22	1.46	1.50
24	C	511	CLA	CMC-C2C	-2.22	1.46	1.50
32	C	517	DGD	O1G-C1G	-2.22	1.40	1.45
24	b	603	CLA	C1B-C2B	2.22	1.48	1.43
29	D	406	LMG	O7-C10	2.22	1.40	1.34
24	c	507	CLA	C1B-C2B	2.22	1.48	1.43
24	A	613	CLA	C1B-NB	-2.22	1.34	1.37
24	A	613	CLA	C4B-NB	2.22	1.40	1.37
24	c	502	CLA	C3B-C4B	2.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	608	CLA	CMD-C2D	-2.21	1.46	1.50
24	C	510	CLA	CMB-C2B	-2.21	1.46	1.50
32	C	516	DGD	C3G-C2G	2.21	1.57	1.50
25	A	606	PHO	CAC-C3C	-2.21	1.47	1.51
24	b	613	CLA	MG-NB	-2.20	2.01	2.05
24	a	606	CLA	CMA-C3A	-2.20	1.48	1.53
24	C	507	CLA	CMB-C2B	-2.20	1.46	1.50
26	B	618	BCR	C1-C6	-2.20	1.51	1.53
24	c	504	CLA	CMC-C2C	-2.20	1.46	1.50
32	c	516	DGD	O3E-C3E	-2.20	1.37	1.43
24	c	506	CLA	O2D-CGD	2.20	1.38	1.33
25	a	605	PHO	CAC-C3C	-2.20	1.47	1.51
29	a	618	LMG	C7-C8	2.19	1.57	1.50
24	c	513	CLA	CMC-C2C	-2.19	1.46	1.50
24	C	510	CLA	CMD-C2D	-2.19	1.46	1.50
24	D	403	CLA	CMD-C2D	-2.19	1.46	1.50
26	t	101	BCR	C31-C1	-2.19	1.49	1.53
24	C	502	CLA	C3B-C4B	2.19	1.49	1.42
25	A	606	PHO	CHA-CBD	-2.18	1.49	1.51
24	c	505	CLA	MG-ND	2.18	2.10	2.05
29	b	623	LMG	O6-C1	2.18	1.47	1.41
24	b	613	CLA	C1B-C2B	2.18	1.48	1.43
29	A	614	LMG	O7-C8	-2.18	1.41	1.46
24	C	503	CLA	CMD-C2D	-2.18	1.46	1.50
24	B	607	CLA	CAC-C3C	-2.18	1.45	1.51
24	c	511	CLA	CMB-C2B	-2.18	1.46	1.50
28	D	405	PL9	C52-C5	-2.17	1.46	1.50
24	b	602	CLA	C1B-C2B	2.17	1.48	1.43
29	a	618	LMG	C1-C2	2.17	1.58	1.52
26	d	405	BCR	C33-C5	-2.17	1.47	1.50
32	H	102	DGD	O1G-C1G	-2.17	1.40	1.45
24	B	611	CLA	C4B-NB	2.17	1.40	1.37
24	B	606	CLA	MG-NB	-2.17	2.01	2.05
24	C	502	CLA	MG-ND	2.17	2.10	2.05
24	C	506	CLA	C3D-C4D	2.16	1.49	1.44
24	b	616	CLA	O2D-CED	-2.16	1.40	1.45
28	a	611	PL9	C30-C29	-2.16	1.45	1.50
24	b	609	CLA	CMB-C2B	-2.16	1.46	1.50
24	B	610	CLA	MG-NB	-2.16	2.01	2.05
31	A	616	SQD	O4-C4	-2.16	1.37	1.43
26	t	101	BCR	C1-C6	-2.16	1.51	1.53
24	B	602	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	CHC-C4B	-2.16	1.34	1.39
24	C	505	CLA	CMC-C2C	-2.16	1.46	1.50
24	d	401	CLA	CMD-C2D	-2.16	1.46	1.50
24	c	502	CLA	CHC-C1C	2.15	1.42	1.38
32	h	101	DGD	C1E-C2E	2.15	1.58	1.52
29	C	519	LMG	O7-C8	-2.15	1.41	1.46
31	D	407	SQD	O3-C3	-2.15	1.37	1.43
24	b	608	CLA	C1D-ND	2.15	1.40	1.37
24	a	612	CLA	C4B-NB	2.15	1.40	1.37
32	H	102	DGD	C4E-C3E	2.15	1.57	1.52
24	B	614	CLA	MG-NA	2.14	2.11	2.06
26	b	618	BCR	C33-C5	-2.14	1.47	1.50
24	c	505	CLA	CMB-C2B	-2.14	1.46	1.50
24	d	404	CLA	C1B-C2B	2.14	1.48	1.43
24	c	504	CLA	C3B-C4B	2.14	1.49	1.42
24	C	504	CLA	CHC-C1C	2.14	1.42	1.38
25	a	605	PHO	C4D-CHA	2.14	1.42	1.39
24	C	506	CLA	C1B-C2B	2.14	1.48	1.43
24	c	511	CLA	C3D-C4D	2.14	1.49	1.44
24	B	604	CLA	C3C-C2C	2.14	1.41	1.36
35	e	101	HEM	CAC-C3C	2.13	1.53	1.47
24	c	503	CLA	CMC-C2C	-2.13	1.46	1.50
36	v	201	HEC	CMA-C3A	2.13	1.55	1.50
29	c	519	LMG	C7-C8	2.13	1.57	1.50
29	c	521	LMG	C7-C8	2.13	1.57	1.50
24	c	505	CLA	MG-NC	2.13	2.11	2.06
24	c	505	CLA	C1D-ND	2.13	1.40	1.37
24	b	611	CLA	CMD-C2D	-2.13	1.46	1.50
26	B	619	BCR	C27-C26	-2.13	1.47	1.51
24	b	611	CLA	C3B-C4B	2.13	1.48	1.42
30	d	407	LHG	P-O6	2.12	1.67	1.59
24	C	501	CLA	C1B-C2B	2.12	1.48	1.43
24	b	601	CLA	C1D-C2D	2.12	1.49	1.45
24	B	601	CLA	CMC-C2C	-2.12	1.46	1.50
29	d	410	LMG	O7-C8	-2.12	1.41	1.46
24	B	614	CLA	CAA-C2A	-2.12	1.50	1.54
32	A	618	DGD	O6E-C5E	-2.12	1.39	1.44
26	A	609	BCR	C37-C22	-2.11	1.46	1.50
32	H	102	DGD	O6E-C1E	2.11	1.47	1.41
24	b	614	CLA	CAC-C3C	-2.11	1.45	1.51
35	F	101	HEM	CMA-C3A	2.11	1.55	1.50
32	c	517	DGD	O3D-C3D	-2.11	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3D-C4D	2.11	1.48	1.44
25	A	606	PHO	C1D-ND	2.11	1.42	1.38
24	D	402	CLA	MG-ND	2.11	2.10	2.05
30	e	102	LHG	O8-C23	2.11	1.39	1.33
24	B	606	CLA	C3B-C2B	-2.11	1.34	1.41
24	C	506	CLA	C1B-NB	-2.11	1.35	1.37
24	c	513	CLA	CMD-C2D	-2.10	1.46	1.50
24	C	503	CLA	C3B-C4B	2.10	1.48	1.42
24	b	616	CLA	CAC-C3C	-2.10	1.45	1.51
24	D	402	CLA	MG-NC	2.10	2.11	2.06
29	a	618	LMG	C3-C2	2.10	1.57	1.52
24	A	604	CLA	C1D-C2D	2.10	1.49	1.45
29	C	519	LMG	C4-C3	2.10	1.57	1.52
24	C	503	CLA	O2D-CED	-2.10	1.40	1.45
32	h	101	DGD	O4D-C4D	-2.09	1.37	1.43
24	c	509	CLA	C1B-NB	-2.09	1.35	1.37
24	d	401	CLA	CHC-C4B	-2.09	1.34	1.39
25	A	607	PHO	C1C-NC	-2.09	1.31	1.37
24	b	616	CLA	C3B-C4B	2.09	1.48	1.42
24	b	604	CLA	CHC-C1C	2.09	1.42	1.38
24	B	602	CLA	MG-ND	-2.09	2.01	2.05
24	A	608	CLA	CHC-C4B	-2.09	1.34	1.39
26	c	514	BCR	C33-C5	-2.09	1.47	1.50
24	a	606	CLA	C3B-C4B	2.08	1.48	1.42
24	b	608	CLA	CHC-C1C	2.08	1.42	1.38
31	a	613	SQD	O3-C3	-2.08	1.37	1.43
29	c	519	LMG	C3-C2	2.08	1.57	1.52
25	A	606	PHO	CBD-CGD	-2.08	1.49	1.52
24	C	512	CLA	C3D-C4D	2.08	1.48	1.44
26	c	515	BCR	C27-C26	-2.08	1.47	1.51
24	d	403	CLA	CHC-C1C	2.08	1.42	1.38
24	B	607	CLA	CMD-C2D	-2.08	1.46	1.50
26	k	102	BCR	C27-C26	-2.08	1.47	1.51
24	B	609	CLA	C3B-C4B	2.08	1.48	1.42
24	c	513	CLA	CHC-C1C	2.08	1.42	1.38
24	A	605	CLA	MG-NC	2.08	2.11	2.06
24	c	512	CLA	CHC-C1C	2.07	1.42	1.38
24	c	510	CLA	CHC-C4B	-2.07	1.34	1.39
24	C	509	CLA	C4B-NB	2.07	1.40	1.37
24	c	502	CLA	CMC-C2C	-2.07	1.46	1.50
24	C	502	CLA	CMC-C2C	-2.07	1.46	1.50
24	d	404	CLA	CAC-C3C	-2.07	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	607	CLA	C3B-C4B	2.07	1.48	1.42
24	B	606	CLA	CMB-C2B	-2.07	1.46	1.50
24	A	608	CLA	C1B-C2B	2.06	1.48	1.43
32	C	516	DGD	O1G-C1A	2.06	1.39	1.33
26	H	101	BCR	C33-C5	-2.06	1.47	1.50
25	A	606	PHO	CMB-C2B	-2.06	1.47	1.51
24	C	506	CLA	CMB-C2B	-2.06	1.46	1.50
24	B	610	CLA	C1A-CHA	-2.06	1.34	1.43
24	c	506	CLA	C1B-C2B	2.06	1.48	1.43
24	A	613	CLA	C3B-C4B	2.05	1.48	1.42
24	b	607	CLA	CHC-C1C	2.05	1.42	1.38
24	b	609	CLA	MG-NB	2.05	2.09	2.05
24	B	616	CLA	CAB-C3B	-2.05	1.41	1.47
24	b	606	CLA	C3D-C4D	2.05	1.48	1.44
35	e	101	HEM	CMA-C3A	2.05	1.55	1.50
29	c	522	LMG	O1-C7	-2.04	1.40	1.43
32	c	516	DGD	O4D-C4D	-2.04	1.37	1.43
32	h	101	DGD	O2G-C2G	-2.04	1.41	1.46
24	d	401	CLA	CMC-C2C	-2.04	1.46	1.50
24	a	604	CLA	C1B-NB	-2.04	1.35	1.37
26	B	618	BCR	C33-C5	-2.04	1.47	1.50
24	C	509	CLA	CMB-C2B	-2.04	1.46	1.50
25	a	605	PHO	C4C-NC	2.04	1.44	1.37
26	C	514	BCR	C33-C5	-2.04	1.47	1.50
24	C	504	CLA	C1B-NB	-2.04	1.35	1.37
24	D	402	CLA	C3B-C4B	2.04	1.48	1.42
24	a	604	CLA	MG-NB	2.04	2.09	2.05
24	c	512	CLA	C1D-C2D	2.04	1.49	1.45
25	A	606	PHO	CMA-C3A	-2.04	1.49	1.53
24	A	608	CLA	C3D-C4D	2.04	1.48	1.44
24	a	606	CLA	C1C-NC	-2.04	1.34	1.37
24	B	606	CLA	C3B-C4B	2.03	1.48	1.42
24	B	611	CLA	C1D-ND	2.03	1.40	1.37
24	B	604	CLA	C1B-C2B	2.03	1.47	1.43
24	B	616	CLA	C4B-NB	2.03	1.40	1.37
24	B	603	CLA	C3D-C4D	2.03	1.48	1.44
24	C	503	CLA	CAC-C3C	-2.02	1.45	1.51
24	C	513	CLA	CHC-C4B	-2.02	1.34	1.39
26	B	619	BCR	C33-C5	-2.02	1.47	1.50
32	c	517	DGD	C4E-C5E	2.02	1.57	1.53
24	b	608	CLA	CMD-C2D	-2.02	1.46	1.50
32	c	518	DGD	O3E-C3E	-2.02	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	602	CLA	CHC-C1C	2.02	1.42	1.38
24	b	605	CLA	C1A-CHA	-2.02	1.34	1.43
24	b	615	CLA	CMC-C2C	-2.01	1.46	1.50
24	D	402	CLA	C1C-NC	-2.01	1.34	1.37
29	D	409	LMG	O8-C28	2.01	1.39	1.33
24	a	604	CLA	O2D-CED	-2.01	1.40	1.45
30	d	407	LHG	P-O4	-2.01	1.46	1.55
24	c	510	CLA	O2D-CED	-2.01	1.40	1.45
28	d	406	PL9	C27-C28	-2.01	1.44	1.50
33	x	102	STE	C2-C1	2.01	1.55	1.50
29	c	521	LMG	O2-C2	2.01	1.47	1.43
32	C	518	DGD	C1D-C2D	2.00	1.58	1.52
24	c	506	CLA	CMB-C2B	-2.00	1.46	1.50
24	B	612	CLA	C1C-NC	-2.00	1.34	1.37

All (1204) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	503	CLA	C4A-NA-C1A	9.98	111.23	106.68
24	b	615	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	a	613	SQD	O6-C1-C2	9.24	122.30	108.27
24	B	611	CLA	C4A-NA-C1A	9.16	110.86	106.68
24	B	603	CLA	C4A-NA-C1A	8.54	110.57	106.68
24	b	606	CLA	C4A-NA-C1A	8.41	110.52	106.68
24	B	616	CLA	C4A-NA-C1A	8.40	110.51	106.68
31	D	407	SQD	O6-C1-C2	8.37	120.98	108.27
24	B	604	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	B	623	SQD	O6-C1-C2	8.13	120.61	108.27
24	C	507	CLA	C4A-NA-C1A	8.02	110.34	106.68
24	b	601	CLA	C4A-NA-C1A	7.97	110.32	106.68
24	d	403	CLA	C4A-NA-C1A	7.93	110.30	106.68
24	B	612	CLA	C4A-NA-C1A	7.82	110.25	106.68
24	b	609	CLA	C4A-NA-C1A	7.79	110.23	106.68
24	A	613	CLA	C4A-NA-C1A	7.76	110.22	106.68
24	c	510	CLA	C4A-NA-C1A	7.61	110.15	106.68
24	C	501	CLA	C4A-NA-C1A	7.51	110.11	106.68
24	C	511	CLA	C4A-NA-C1A	7.37	110.04	106.68
24	A	605	CLA	C4A-NA-C1A	7.35	110.03	106.68
24	c	509	CLA	C4A-NA-C1A	7.29	110.00	106.68
24	c	511	CLA	C4A-NA-C1A	7.29	110.00	106.68
31	A	616	SQD	O7-S-C6	7.21	117.53	106.76
24	B	601	CLA	C4A-NA-C1A	7.15	109.94	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	C4A-NA-C1A	7.09	109.91	106.68
24	b	614	CLA	C4A-NA-C1A	7.05	109.90	106.68
31	b	620	SQD	O6-C1-C2	6.97	118.86	108.27
25	A	606	PHO	C4D-CHA-CBD	-6.91	105.14	108.45
24	b	616	CLA	C4A-NA-C1A	6.86	109.81	106.68
24	c	508	CLA	C4A-NA-C1A	6.84	109.80	106.68
31	f	101	SQD	O6-C1-C2	6.80	118.60	108.27
24	a	612	CLA	C4A-NA-C1A	6.71	109.74	106.68
24	C	513	CLA	C4A-NA-C1A	6.67	109.72	106.68
31	A	616	SQD	O6-C1-C2	6.57	118.26	108.27
24	D	403	CLA	C4A-NA-C1A	6.42	109.61	106.68
24	C	502	CLA	C4A-NA-C1A	6.39	109.60	106.68
24	B	606	CLA	C4A-NA-C1A	6.31	109.56	106.68
24	c	502	CLA	C4A-NA-C1A	6.25	109.53	106.68
24	c	506	CLA	C4A-NA-C1A	6.18	109.50	106.68
24	B	609	CLA	C4A-NA-C1A	6.14	109.48	106.68
25	a	605	PHO	C4D-CHA-CBD	-6.13	105.52	108.45
24	b	602	CLA	C4A-NA-C1A	6.08	109.45	106.68
24	C	510	CLA	C4A-NA-C1A	6.06	109.44	106.68
24	C	508	CLA	C4A-NA-C1A	5.99	109.41	106.68
24	C	505	CLA	C4A-NA-C1A	5.97	109.40	106.68
24	B	607	CLA	C4A-NA-C1A	5.86	109.35	106.68
28	d	406	PL9	C7-C3-C4	5.67	121.58	116.91
24	d	401	CLA	C4A-NA-C1A	5.64	109.25	106.68
24	a	604	CLA	C4A-NA-C1A	5.60	109.23	106.68
28	a	611	PL9	C7-C3-C4	5.58	121.51	116.91
24	B	615	CLA	C4A-NA-C1A	5.54	109.21	106.68
24	C	512	CLA	C4A-NA-C1A	5.54	109.21	106.68
31	A	616	SQD	O9-S-O7	-5.54	95.80	113.82
31	A	617	SQD	C45-O47-C7	5.39	125.55	117.78
24	c	501	CLA	O2D-CGD-O1D	-5.30	113.53	123.85
24	b	606	CLA	O2D-CGD-O1D	-5.25	113.62	123.85
24	c	512	CLA	C4A-NA-C1A	5.24	109.07	106.68
24	B	610	CLA	O2D-CGD-O1D	-5.22	113.68	123.85
31	f	101	SQD	O7-S-C6	5.21	114.54	106.76
24	b	610	CLA	C4A-NA-C1A	5.19	109.05	106.68
24	C	501	CLA	O2D-CGD-O1D	-5.15	113.82	123.85
24	B	605	CLA	C4A-NA-C1A	5.07	108.99	106.68
31	a	614	SQD	O47-C7-C8	5.06	122.44	111.48
31	A	616	SQD	C1-C2-C3	-5.01	99.47	110.01
24	C	510	CLA	O2D-CGD-O1D	-5.01	114.10	123.85
28	d	406	PL9	C40-C39-C41	5.01	123.92	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	501	CLA	C4A-NA-C1A	4.98	108.95	106.68
24	b	607	CLA	C4A-NA-C1A	4.96	108.94	106.68
24	b	604	CLA	C4A-NA-C1A	4.94	108.93	106.68
24	B	611	CLA	O2D-CGD-O1D	-4.94	114.24	123.85
24	c	504	CLA	C4A-NA-C1A	4.91	108.92	106.68
24	A	613	CLA	C3B-C4B-NB	-4.89	106.17	110.53
25	d	402	PHO	C4D-CHA-CBD	-4.87	106.12	108.45
24	c	505	CLA	C4A-NA-C1A	4.86	108.90	106.68
36	V	201	HEC	C1D-ND-C4D	4.83	110.93	105.21
24	D	402	CLA	C4A-NA-C1A	4.80	108.87	106.68
29	a	618	LMG	C1-C2-C3	-4.78	99.95	110.01
24	c	507	CLA	C4A-NA-C1A	4.76	108.85	106.68
24	b	602	CLA	O2D-CGD-O1D	-4.74	114.62	123.85
24	C	501	CLA	O2D-CGD-CBD	4.68	119.42	111.23
30	A	615	LHG	O4-P-O5	4.65	134.08	112.44
24	B	614	CLA	C3B-C4B-NB	-4.64	106.39	110.53
24	b	605	CLA	O2D-CGD-O1D	-4.59	114.90	123.85
30	E	101	LHG	O4-P-O5	4.55	133.62	112.44
24	b	611	CLA	O2D-CGD-CBD	4.55	119.19	111.23
24	C	508	CLA	CHD-C1D-ND	-4.49	118.48	124.80
24	D	402	CLA	C3B-C4B-NB	-4.47	106.54	110.53
31	A	616	SQD	C1-O5-C5	-4.40	105.12	113.72
24	c	513	CLA	C4A-NA-C1A	4.39	108.68	106.68
24	C	506	CLA	C4A-NA-C1A	4.37	108.67	106.68
31	f	101	SQD	O9-S-O7	-4.37	99.62	113.82
30	d	409	LHG	O4-P-O5	4.34	132.65	112.44
34	D	401	BCT	O2-C-O1	4.34	130.78	119.68
25	d	402	PHO	O1D-CGD-CBD	4.30	131.24	124.72
30	e	102	LHG	O4-P-O5	4.30	132.43	112.44
30	B	622	LHG	O4-P-O5	4.29	132.41	112.44
28	a	611	PL9	C35-C34-C36	4.28	122.67	115.23
35	e	101	HEM	CBD-CAD-C3D	-4.28	100.69	112.53
24	B	610	CLA	C4A-NA-C1A	4.26	108.62	106.68
24	c	509	CLA	CHB-C4A-NA	4.26	130.55	124.40
24	b	610	CLA	O2D-CGD-O1D	-4.25	115.57	123.85
30	d	408	LHG	O4-P-O5	4.24	132.19	112.44
28	a	611	PL9	C7-C3-C2	-4.23	118.40	123.39
24	a	606	CLA	C4A-NA-C1A	4.23	108.61	106.68
29	b	621	LMG	O7-C10-O9	-4.22	113.83	123.70
24	C	513	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
24	C	510	CLA	O2D-CGD-CBD	4.20	118.57	111.23
30	d	407	LHG	O4-P-O5	4.19	131.92	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	O1D-CGD-CBD	4.16	132.73	124.52
30	D	408	LHG	O4-P-O5	4.16	131.80	112.44
34	a	610	BCT	O2-C-O1	4.14	130.27	119.68
24	b	603	CLA	C4A-NA-C1A	4.12	108.56	106.68
26	b	617	BCR	C2-C1-C6	4.11	116.41	110.44
31	b	620	SQD	O7-S-C6	4.11	112.89	106.76
24	a	612	CLA	CMB-C2B-C1B	-4.08	119.21	125.42
24	b	602	CLA	O2D-CGD-CBD	4.08	118.36	111.23
24	C	505	CLA	CMB-C2B-C1B	-4.06	119.24	125.42
24	B	608	CLA	O2D-CGD-O1D	-4.05	115.96	123.85
25	A	606	PHO	C2B-C1B-NB	-4.03	106.51	109.43
31	D	407	SQD	O8-S-C6	4.03	113.76	105.97
24	B	614	CLA	O2D-CGD-O1D	-4.03	116.01	123.85
32	C	518	DGD	O6D-C1D-O3G	-4.02	100.54	110.04
24	b	609	CLA	CMB-C2B-C1B	-4.01	119.31	125.42
29	b	623	LMG	C1-O6-C5	-4.01	105.90	113.72
32	H	102	DGD	O3G-C3G-C2G	-4.01	101.08	110.82
26	B	619	BCR	C2-C1-C6	3.99	116.23	110.44
31	D	407	SQD	O9-S-C6	3.99	112.71	106.76
24	B	602	CLA	O2D-CGD-CBD	3.98	118.19	111.23
24	b	603	CLA	O2D-CGD-O1D	-3.98	116.10	123.85
24	C	509	CLA	CMB-C2B-C1B	-3.98	119.36	125.42
25	d	402	PHO	C1-C2-C3	-3.97	119.69	126.20
35	F	101	HEM	CBD-CAD-C3D	-3.95	101.61	112.53
24	A	608	CLA	O2D-CGD-O1D	-3.94	116.19	123.85
25	A	607	PHO	O1D-CGD-CBD	3.93	130.69	124.72
30	l	101	LHG	O4-P-O5	3.92	130.66	112.44
28	d	406	PL9	C7-C3-C2	-3.89	118.80	123.39
28	A	612	PL9	C40-C39-C41	3.88	121.97	115.23
24	b	611	CLA	C4A-NA-C1A	3.88	108.45	106.68
24	b	602	CLA	CHB-C4A-NA	3.87	129.99	124.40
24	C	504	CLA	C4A-NA-C1A	3.87	108.44	106.68
24	B	607	CLA	C3B-C4B-NB	-3.86	107.08	110.53
30	d	407	LHG	O8-C23-O10	-3.86	113.98	123.63
26	C	515	BCR	C15-C16-C17	-3.86	115.63	123.52
32	C	518	DGD	O3G-C3G-C2G	-3.85	101.44	110.82
31	A	616	SQD	O47-C7-C8	3.85	119.81	111.48
24	B	606	CLA	C3B-C4B-NB	-3.84	107.11	110.53
24	A	605	CLA	CED-O2D-CGD	-3.83	107.22	115.92
36	v	201	HEC	C1D-ND-C4D	3.82	109.73	105.21
28	a	611	PL9	C25-C24-C26	3.81	121.84	115.23
30	B	621	LHG	O4-P-O5	3.79	130.08	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	C3B-C4B-NB	-3.78	107.15	110.53
32	C	516	DGD	O3G-C3G-C2G	-3.78	101.62	110.82
24	b	608	CLA	C3B-C4B-NB	-3.77	107.17	110.53
26	A	609	BCR	C27-C26-C25	3.75	127.77	122.70
24	B	604	CLA	C3B-C4B-NB	-3.74	107.19	110.53
24	C	506	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
32	c	518	DGD	O3G-C3G-C2G	-3.71	101.79	110.82
26	c	515	BCR	C27-C26-C25	3.70	127.70	122.70
24	d	403	CLA	O2D-CGD-CBD	3.70	117.69	111.23
32	c	516	DGD	O3G-C3G-C2G	-3.69	101.85	110.82
24	a	612	CLA	O2D-CGD-CBD	3.67	117.65	111.23
24	d	403	CLA	O2D-CGD-O1D	-3.67	116.70	123.85
24	b	614	CLA	CMB-C2B-C1B	-3.67	119.83	125.42
28	D	405	PL9	C27-C28-C29	-3.66	119.24	127.62
24	B	601	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
24	c	513	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
24	b	605	CLA	C4-C3-C5	3.66	121.58	115.23
24	C	504	CLA	C3B-C4B-NB	-3.65	107.27	110.53
31	a	614	SQD	O48-C23-C24	3.64	122.94	111.83
29	M	101	LMG	C1-O6-C5	-3.64	106.61	113.72
24	c	506	CLA	C3B-C4B-NB	-3.63	107.29	110.53
31	B	623	SQD	C1-O5-C5	-3.63	106.64	113.72
24	C	512	CLA	C1-C2-C3	-3.62	120.27	126.20
31	B	623	SQD	O5-C5-C4	3.61	116.21	109.70
24	B	613	CLA	C1-C2-C3	-3.59	120.31	126.20
24	d	401	CLA	CHB-C4A-NA	3.58	129.57	124.40
24	C	508	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
26	C	514	BCR	C2-C1-C6	3.58	115.64	110.44
28	D	405	PL9	C30-C29-C31	-3.57	109.03	115.23
31	B	623	SQD	O47-C7-C8	3.57	119.19	111.48
25	A	606	PHO	O2D-CGD-CBD	3.57	114.86	110.95
24	c	512	CLA	C3B-C4B-NB	-3.56	107.35	110.53
24	b	611	CLA	C3B-C4B-NB	-3.55	107.36	110.53
24	c	509	CLA	O2A-CGA-O1A	-3.55	114.76	123.63
31	B	623	SQD	O7-S-C6	3.54	112.04	106.76
28	A	612	PL9	C7-C3-C4	3.54	119.82	116.91
31	a	613	SQD	O9-S-O7	-3.53	102.33	113.82
25	A	607	PHO	O2D-CGD-O1D	-3.53	116.97	123.85
30	e	102	LHG	O8-C23-C24	3.53	122.59	111.83
26	B	617	BCR	C2-C1-C6	3.52	115.56	110.44
31	f	101	SQD	C1-C2-C3	-3.52	102.61	110.01
28	D	405	PL9	C7-C3-C4	3.52	119.81	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	612	PL9	O1-C4-C3	-3.51	117.02	120.73
24	B	603	CLA	O2D-CGD-O1D	-3.51	117.01	123.85
24	C	509	CLA	CMB-C2B-C3B	3.51	134.81	126.55
24	B	616	CLA	CMB-C2B-C1B	-3.51	120.08	125.42
24	b	613	CLA	C1-C2-C3	-3.51	120.45	126.20
28	A	612	PL9	C20-C19-C21	3.50	121.31	115.23
30	d	407	LHG	O8-C23-C24	3.50	122.51	111.83
24	c	512	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
24	c	501	CLA	CED-O2D-CGD	-3.49	108.00	115.92
31	B	623	SQD	O48-C23-C24	3.49	122.47	111.83
28	d	406	PL9	C37-C38-C39	-3.48	119.66	127.62
24	a	604	CLA	C3B-C4B-NB	-3.48	107.43	110.53
24	c	505	CLA	C3B-C4B-NB	-3.48	107.43	110.53
24	B	612	CLA	C3B-C4B-NB	-3.47	107.43	110.53
25	A	607	PHO	C2B-C1B-NB	-3.47	106.92	109.43
24	b	608	CLA	CMB-C2B-C1B	-3.46	120.15	125.42
24	c	512	CLA	C1-C2-C3	-3.46	120.53	126.20
35	e	101	HEM	CHB-C1B-NB	3.46	128.65	124.37
28	D	405	PL9	C36-C34-C33	-3.45	113.43	121.17
24	A	608	CLA	O2D-CGD-CBD	3.45	117.25	111.23
24	B	602	CLA	C4A-NA-C1A	3.44	108.25	106.68
28	A	612	PL9	C22-C23-C24	-3.44	119.76	127.62
24	b	601	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
32	h	101	DGD	O2D-C2D-C1D	-3.42	101.91	110.08
24	A	604	CLA	C4A-NA-C1A	3.42	108.24	106.68
24	D	403	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
24	b	604	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
31	B	623	SQD	O48-C23-O10	-3.39	115.14	123.63
29	c	522	LMG	O6-C1-O1	-3.39	102.04	110.04
24	B	614	CLA	O1D-CGD-CBD	3.38	131.18	124.52
24	b	613	CLA	CHB-C4A-NA	3.37	129.27	124.40
26	d	405	BCR	C27-C26-C25	3.37	127.25	122.70
26	A	609	BCR	C37-C22-C21	-3.36	117.37	122.82
24	C	503	CLA	O1D-CGD-CBD	3.36	131.15	124.52
24	c	510	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
26	H	101	BCR	C2-C1-C6	3.35	115.31	110.44
29	M	101	LMG	O1-C1-C2	-3.33	103.22	108.27
26	b	619	BCR	C29-C30-C25	3.32	115.27	110.44
24	B	611	CLA	O2D-CGD-CBD	3.32	117.03	111.23
28	D	405	PL9	C42-C43-C44	-3.31	120.04	127.62
31	a	613	SQD	C1-C2-C3	-3.31	103.04	110.01
24	C	503	CLA	C7-C6-C5	-3.31	104.43	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	v	201	HEC	CHB-C1B-NB	3.31	127.99	124.42
24	c	502	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
24	B	603	CLA	C3B-C4B-NB	-3.31	107.58	110.53
24	C	510	CLA	C3B-C4B-NB	-3.30	107.58	110.53
24	A	604	CLA	CHB-C4A-NA	3.30	129.16	124.40
29	A	614	LMG	O6-C1-O1	-3.30	102.25	110.04
24	c	501	CLA	O2D-CGD-CBD	3.28	116.97	111.23
24	b	606	CLA	O2D-CGD-CBD	3.28	116.97	111.23
24	b	610	CLA	O1D-CGD-CBD	3.28	130.99	124.52
29	D	406	LMG	O6-C1-O1	-3.28	102.30	110.04
24	b	614	CLA	O2A-CGA-O1A	-3.27	115.44	123.63
24	c	508	CLA	CHB-C4A-NA	3.27	129.12	124.40
25	A	607	PHO	C4D-CHA-CBD	-3.27	106.89	108.45
32	h	101	DGD	O3G-C3G-C2G	-3.27	102.86	110.82
28	D	405	PL9	C35-C34-C36	3.27	120.90	115.23
24	C	504	CLA	C4-C3-C5	3.26	120.89	115.23
24	B	605	CLA	O2D-CGD-O1D	-3.26	117.51	123.85
25	a	605	PHO	C2B-C1B-NB	-3.25	107.08	109.43
24	d	401	CLA	C2D-C1D-ND	-3.25	106.91	110.13
24	b	612	CLA	CHB-C4A-NA	3.25	129.09	124.40
32	C	517	DGD	O3G-C3G-C2G	-3.24	102.94	110.82
24	c	503	CLA	C3B-C4B-NB	-3.24	107.64	110.53
24	C	506	CLA	O1D-CGD-CBD	3.24	130.90	124.52
24	b	601	CLA	CHB-C4A-NA	3.23	129.06	124.40
32	C	516	DGD	C3D-C4D-C5D	-3.23	104.38	110.23
24	B	610	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
30	d	409	LHG	C26-C25-C24	3.21	124.93	113.13
25	a	605	PHO	CMB-C2B-C3B	3.21	131.10	124.68
24	d	404	CLA	CMB-C2B-C1B	-3.21	120.53	125.42
24	C	502	CLA	C4D-CHA-C1A	3.21	125.07	121.24
31	B	623	SQD	C3-C4-C5	3.20	116.04	110.23
24	B	603	CLA	C4-C3-C5	3.20	120.79	115.23
24	a	612	CLA	CHB-C4A-NA	3.20	129.02	124.40
31	a	613	SQD	C1-O5-C5	-3.19	107.49	113.72
24	B	604	CLA	CHB-C4A-NA	3.18	129.00	124.40
24	C	502	CLA	C3B-C4B-NB	-3.18	107.69	110.53
24	b	615	CLA	CHB-C4A-NA	3.18	128.99	124.40
32	C	516	DGD	O6D-C1D-O3G	-3.18	102.54	110.04
25	d	402	PHO	C2B-C1B-NB	-3.18	107.14	109.43
25	A	607	PHO	CMB-C2B-C3B	3.18	131.03	124.68
24	b	602	CLA	CMB-C2B-C1B	-3.17	120.59	125.42
24	B	616	CLA	CMB-C2B-C3B	3.17	134.01	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	101	BCR	C27-C26-C25	3.16	126.98	122.70
24	B	602	CLA	CMB-C2B-C1B	-3.16	120.60	125.42
31	b	620	SQD	O5-C5-C4	3.16	115.40	109.70
24	c	507	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
26	t	101	BCR	C1-C6-C5	-3.16	118.31	122.64
31	b	620	SQD	O48-C23-C24	3.16	121.47	111.83
24	B	616	CLA	O2A-CGA-O1A	-3.16	115.72	123.63
24	b	614	CLA	C4-C3-C5	3.16	120.71	115.23
26	b	617	BCR	C27-C26-C25	3.15	126.95	122.70
24	B	602	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
24	D	402	CLA	CED-O2D-CGD	3.14	123.04	115.92
24	b	616	CLA	CHB-C4A-NA	3.13	128.92	124.40
31	B	623	SQD	O8-S-C6	3.13	112.01	105.97
36	v	201	HEC	CHA-C4D-ND	3.13	127.79	124.42
31	A	617	SQD	O48-C23-C24	3.12	121.36	111.83
24	c	502	CLA	C3B-C4B-NB	-3.12	107.74	110.53
24	a	604	CLA	CMB-C2B-C1B	-3.12	120.66	125.42
28	d	406	PL9	C7-C8-C9	-3.12	121.45	126.83
24	c	507	CLA	CHB-C4A-NA	3.12	128.90	124.40
29	a	618	LMG	C9-C8-C7	-3.12	104.52	111.78
24	C	504	CLA	O2A-CGA-O1A	-3.12	115.83	123.63
24	c	512	CLA	CHB-C4A-NA	3.11	128.90	124.40
24	c	503	CLA	C7-C6-C5	-3.11	104.96	113.26
28	D	405	PL9	C22-C23-C24	-3.11	120.50	127.62
24	b	612	CLA	C1-C2-C3	-3.11	121.10	126.20
33	D	411	STE	C3-C2-C1	-3.10	106.41	114.51
24	b	603	CLA	CHB-C1B-NB	3.10	128.71	124.05
24	b	611	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
31	D	407	SQD	C1-C2-C3	-3.10	103.49	110.01
24	B	615	CLA	CHC-C4B-NB	3.10	128.69	124.05
24	C	505	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
26	T	101	BCR	C35-C13-C14	-3.09	117.80	122.82
24	a	606	CLA	CHB-C4A-NA	3.09	128.87	124.40
31	b	620	SQD	C1-C2-C3	-3.09	103.50	110.01
24	C	513	CLA	C1-O2A-CGA	-3.09	109.18	116.65
29	b	623	LMG	O1-C1-C2	-3.09	103.59	108.27
24	C	512	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
24	C	507	CLA	C3B-C4B-NB	-3.07	107.79	110.53
24	b	603	CLA	CMB-C2B-C1B	-3.07	120.74	125.42
28	A	612	PL9	C36-C34-C33	-3.07	114.28	121.17
32	c	517	DGD	O3G-C3G-C2G	-3.06	103.37	110.82
24	C	512	CLA	CHB-C4A-NA	3.06	128.82	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Y	101	BCR	C27-C26-C25	3.06	126.84	122.70
26	D	404	BCR	C27-C26-C25	3.06	126.84	122.70
24	b	605	CLA	C4A-NA-C1A	3.06	108.08	106.68
28	d	406	PL9	C42-C43-C44	-3.06	120.62	127.62
26	T	101	BCR	C7-C8-C9	-3.06	121.72	126.23
25	A	607	PHO	C3B-C4B-NB	-3.05	105.47	107.46
24	b	610	CLA	CAC-C3C-C4C	3.05	128.76	124.79
24	B	610	CLA	O2D-CGD-CBD	3.05	116.56	111.23
32	c	518	DGD	C3D-C4D-C5D	-3.05	104.71	110.23
24	b	602	CLA	C3B-C4B-NB	-3.05	107.81	110.53
24	b	614	CLA	C1-C2-C3	-3.04	121.22	126.20
31	b	620	SQD	O9-S-C6	3.04	111.29	106.76
24	c	511	CLA	C3B-C4B-NB	-3.04	107.82	110.53
26	C	514	BCR	C27-C26-C25	3.04	126.81	122.70
32	C	517	DGD	O6D-C1D-O3G	-3.04	102.87	110.04
31	a	613	SQD	O47-C7-C8	3.03	118.04	111.48
24	c	508	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
29	d	410	LMG	O2-C2-C1	-3.02	102.88	110.08
24	B	612	CLA	CMB-C2B-C1B	-3.02	120.82	125.42
24	d	401	CLA	C1D-ND-C4D	3.02	108.43	106.31
31	a	613	SQD	O7-S-C6	3.02	111.26	106.76
31	a	614	SQD	O48-C23-O10	-3.01	116.09	123.63
24	b	608	CLA	CMB-C2B-C3B	3.01	133.64	126.55
24	c	505	CLA	C1-C2-C3	-3.01	121.26	126.20
24	b	609	CLA	O1D-CGD-CBD	3.01	130.46	124.52
24	b	605	CLA	CHB-C1B-NB	3.01	128.56	124.05
24	B	614	CLA	C4A-NA-C1A	3.01	108.05	106.68
24	a	612	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
30	d	407	LHG	C11-C10-C9	-3.00	99.19	114.37
24	a	606	CLA	O2D-CGD-CBD	3.00	116.48	111.23
24	c	503	CLA	C4A-NA-C1A	3.00	108.05	106.68
29	b	621	LMG	C9-C8-C7	-3.00	104.79	111.78
24	C	507	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
31	a	613	SQD	O9-S-C6	3.00	111.23	106.76
31	A	616	SQD	O5-C1-O6	2.99	117.12	110.04
24	D	402	CLA	CMD-C2D-C1D	-2.99	119.46	124.73
24	C	507	CLA	O2D-CGD-CBD	2.98	116.45	111.23
32	C	517	DGD	C6D-O5D-C1E	2.98	120.19	113.80
26	A	609	BCR	C2-C1-C6	2.98	114.77	110.44
24	B	607	CLA	CHB-C1B-NB	2.98	128.52	124.05
25	a	605	PHO	OBD-CAD-CBD	-2.98	121.45	125.82
24	b	602	CLA	CMB-C2B-C3B	2.98	133.55	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	618	DGD	C3G-C2G-C1G	-2.98	104.84	111.78
30	B	622	LHG	O8-C23-C24	2.98	120.91	111.83
24	B	602	CLA	C1-C2-C3	-2.98	121.32	126.20
31	b	620	SQD	O9-S-O7	-2.97	104.16	113.82
24	c	510	CLA	O2A-CGA-O1A	-2.97	116.20	123.63
29	c	521	LMG	O3-C3-C2	-2.97	103.38	110.38
25	A	606	PHO	OBD-CAD-CBD	-2.96	121.48	125.82
26	c	514	BCR	C27-C26-C25	2.96	126.70	122.70
33	C	522	STE	C3-C2-C1	-2.96	106.79	114.51
24	b	604	CLA	C3B-C4B-NB	-2.95	107.89	110.53
28	A	612	PL9	C27-C28-C29	-2.95	120.88	127.62
25	d	402	PHO	CMB-C2B-C3B	2.95	130.57	124.68
24	b	613	CLA	C4A-NA-C1A	2.95	108.02	106.68
31	D	407	SQD	O48-C23-C24	2.94	120.80	111.83
24	c	506	CLA	CHB-C4A-NA	2.94	128.64	124.40
24	A	605	CLA	CMB-C2B-C1B	-2.94	120.95	125.42
26	d	405	BCR	C38-C26-C25	-2.94	121.28	124.48
32	A	618	DGD	O3G-C3G-C2G	-2.93	103.69	110.82
24	c	513	CLA	CMB-C2B-C1B	-2.92	120.97	125.42
31	a	613	SQD	O48-C23-C24	2.92	120.73	111.83
24	C	508	CLA	C3B-C4B-NB	-2.92	107.93	110.53
24	C	510	CLA	CMB-C2B-C1B	-2.92	120.98	125.42
24	C	509	CLA	CHB-C4A-NA	2.92	128.61	124.40
30	E	101	LHG	O8-C23-C24	2.91	120.72	111.83
33	d	411	STE	O2-C1-C2	2.91	123.20	114.00
36	V	201	HEC	CBD-CAD-C3D	-2.91	104.49	112.53
24	d	404	CLA	CMB-C2B-C3B	2.91	133.39	126.55
24	c	509	CLA	CHC-C1C-NC	2.90	128.69	124.31
28	D	405	PL9	C20-C19-C21	2.90	120.26	115.23
24	c	506	CLA	CBC-CAC-C3C	-2.90	104.56	112.42
31	b	620	SQD	C3-C4-C5	2.90	115.48	110.23
29	d	410	LMG	O1-C1-C2	-2.90	103.88	108.27
24	c	505	CLA	CMB-C2B-C1B	-2.89	121.02	125.42
29	b	621	LMG	C38-C37-C36	-2.89	99.76	114.37
24	c	504	CLA	CHB-C4A-NA	2.89	128.57	124.40
24	B	611	CLA	C3B-C4B-NB	-2.89	107.95	110.53
25	a	605	PHO	C3D-C4D-ND	2.88	111.41	107.71
31	D	407	SQD	C1-O5-C5	-2.88	108.09	113.72
26	t	101	BCR	C7-C8-C9	-2.88	121.97	126.23
32	C	518	DGD	O3D-C3D-C4D	-2.88	103.59	110.38
24	b	609	CLA	CMB-C2B-C3B	2.88	133.31	126.55
24	B	609	CLA	O2D-CGD-O1D	-2.87	118.26	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	x	101	BCR	C38-C26-C25	-2.87	121.35	124.48
24	c	507	CLA	C4-C3-C5	2.87	120.21	115.23
24	C	503	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
29	A	614	LMG	C9-C8-C7	-2.87	105.09	111.78
31	A	616	SQD	O47-C7-O49	-2.87	117.00	123.70
24	b	610	CLA	O2A-CGA-O1A	-2.87	116.46	123.63
24	B	614	CLA	C4-C3-C5	2.86	120.20	115.23
29	C	519	LMG	O6-C1-O1	-2.86	103.28	110.04
24	d	401	CLA	CAC-C3C-C4C	2.86	128.51	124.79
24	b	613	CLA	CMB-C2B-C1B	-2.85	121.07	125.42
24	A	605	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	c	505	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
26	d	405	BCR	C2-C1-C6	2.85	114.58	110.44
29	b	623	LMG	C3-C4-C5	-2.85	105.06	110.23
24	C	505	CLA	CMB-C2B-C3B	2.85	133.25	126.55
32	c	516	DGD	O2D-C2D-C3D	-2.84	103.68	110.38
24	b	615	CLA	O2D-CGD-CBD	2.84	116.19	111.23
24	C	513	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
24	b	615	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
24	c	511	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	C	506	CLA	CHB-C4A-NA	2.83	128.48	124.40
24	B	606	CLA	CHA-C1A-NA	-2.82	119.99	126.39
36	V	201	HEC	CMC-C2C-C1C	-2.82	121.13	125.42
32	C	518	DGD	CDB-CCB-CBB	-2.82	100.14	114.37
24	b	610	CLA	CHB-C4A-NA	2.81	128.46	124.40
24	b	611	CLA	CHD-C1D-ND	-2.81	120.84	124.80
32	c	518	DGD	O6D-C1D-O3G	-2.81	103.40	110.04
31	D	407	SQD	O5-C1-C2	-2.81	104.60	110.37
30	D	408	LHG	O8-C23-C24	2.81	120.39	111.83
29	b	621	LMG	O3-C3-C2	-2.80	103.78	110.38
33	a	616	STE	C3-C2-C1	-2.79	107.22	114.51
24	c	513	CLA	CHB-C4A-NA	2.79	128.42	124.40
24	b	610	CLA	C1-C2-C3	-2.79	121.63	126.20
24	C	503	CLA	C3B-C4B-NB	-2.79	108.04	110.53
26	c	515	BCR	C2-C1-C6	2.79	114.48	110.44
26	c	515	BCR	C7-C8-C9	-2.78	122.12	126.23
31	f	101	SQD	O5-C1-C2	-2.78	104.65	110.37
24	A	604	CLA	O1D-CGD-CBD	2.78	130.00	124.52
24	b	606	CLA	CMB-C2B-C1B	-2.78	121.18	125.42
26	k	102	BCR	C29-C30-C25	2.78	114.48	110.44
31	b	620	SQD	C45-O47-C7	2.78	124.44	117.80
24	b	604	CLA	C6-C5-C3	-2.78	106.71	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CHB-C4A-NA	2.78	128.41	124.40
24	a	604	CLA	CAC-C3C-C4C	2.77	128.40	124.79
24	b	615	CLA	C3B-C4B-NB	-2.77	108.06	110.53
29	b	623	LMG	O6-C5-C6	2.77	113.30	106.44
24	b	615	CLA	C11-C10-C8	-2.77	106.77	115.97
29	b	623	LMG	O2-C2-C1	-2.77	103.49	110.08
26	C	515	BCR	C36-C18-C17	-2.76	118.34	122.82
29	b	621	LMG	C1-O6-C5	-2.76	108.33	113.72
33	m	101	STE	O2-C1-C2	2.76	122.72	114.00
28	D	405	PL9	C40-C39-C38	-2.76	116.54	123.63
24	b	604	CLA	C1-C2-C3	-2.76	121.68	126.20
26	b	617	BCR	C15-C16-C17	-2.76	117.88	123.52
26	t	101	BCR	C36-C18-C19	2.76	122.30	118.09
29	M	101	LMG	O3-C3-C2	-2.75	103.89	110.38
24	B	606	CLA	C1-C2-C3	-2.75	121.69	126.20
24	a	606	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
24	B	605	CLA	C16-C15-C13	-2.75	106.83	115.97
32	C	516	DGD	O2D-C2D-C1D	-2.75	103.53	110.08
24	C	505	CLA	CHB-C1B-NB	2.74	128.16	124.05
26	B	619	BCR	C29-C30-C25	2.74	114.41	110.44
24	C	502	CLA	C1D-ND-C4D	2.74	108.23	106.31
32	A	618	DGD	C4E-C3E-C2E	-2.73	106.03	110.83
24	B	613	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	C	508	CLA	CHD-C1D-C2D	2.73	131.17	125.49
32	C	517	DGD	O5D-C6D-C5D	-2.73	103.27	109.42
26	k	101	BCR	C38-C26-C25	-2.73	121.51	124.48
24	b	603	CLA	CHC-C4B-NB	2.73	128.14	124.05
25	d	402	PHO	O2D-CGD-O1D	-2.72	118.55	123.85
31	b	620	SQD	O2-C2-C1	2.72	116.56	110.08
32	H	102	DGD	O2D-C2D-C1D	-2.72	103.59	110.08
24	b	602	CLA	CHC-C1C-NC	2.72	128.41	124.31
25	a	605	PHO	OBD-CAD-C3D	2.72	132.13	127.89
24	C	511	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
35	e	101	HEM	C3B-C2B-C1B	2.71	108.45	106.41
30	d	408	LHG	O8-C23-C24	2.71	120.10	111.83
26	C	514	BCR	C11-C10-C9	-2.71	123.48	127.28
24	D	402	CLA	CMD-C2D-C3D	2.71	133.90	127.69
26	A	609	BCR	C36-C18-C17	-2.71	118.43	122.82
24	C	512	CLA	C3B-C4B-NB	-2.70	108.12	110.53
24	B	615	CLA	CAC-C3C-C4C	2.70	128.30	124.79
36	V	201	HEC	CHA-C4D-ND	2.70	127.33	124.42
31	a	613	SQD	C3-C4-C5	2.70	115.12	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	609	BCR	C38-C26-C25	-2.70	121.54	124.48
32	H	102	DGD	C3D-C4D-C5D	-2.69	105.35	110.23
24	C	508	CLA	C1-C2-C3	-2.69	121.79	126.20
26	b	617	BCR	C38-C26-C25	-2.69	121.55	124.48
31	a	614	SQD	O49-C7-C8	-2.69	113.26	123.78
24	b	608	CLA	C4A-NA-C1A	2.69	107.91	106.68
28	d	406	PL9	C20-C19-C21	2.69	119.89	115.23
24	b	612	CLA	CMB-C2B-C1B	-2.69	121.33	125.42
24	C	509	CLA	CED-O2D-CGD	2.68	122.00	115.92
26	B	617	BCR	C29-C30-C25	2.68	114.34	110.44
24	B	611	CLA	C1-C2-C3	-2.68	121.80	126.20
24	a	606	CLA	C1D-ND-C4D	-2.68	104.43	106.31
26	C	514	BCR	C38-C26-C25	-2.68	121.56	124.48
24	A	604	CLA	CMB-C2B-C3B	2.68	132.85	126.55
30	l	101	LHG	C20-C19-C18	-2.68	100.83	114.37
24	b	609	CLA	O2A-CGA-O1A	-2.68	116.93	123.63
32	A	618	DGD	CDB-CCB-CBB	-2.68	100.83	114.37
24	b	603	CLA	O2D-CGD-CBD	2.68	115.91	111.23
26	Y	101	BCR	C39-C30-C25	-2.68	106.05	110.24
32	A	618	DGD	C1D-C2D-C3D	-2.67	104.38	110.01
24	c	510	CLA	CMB-C2B-C1B	-2.67	121.35	125.42
32	C	516	DGD	O5D-C6D-C5D	-2.67	103.40	109.42
32	c	517	DGD	O6D-C1D-O3G	-2.67	103.74	110.04
24	B	601	CLA	C3B-C4B-NB	-2.67	108.15	110.53
32	H	102	DGD	O3E-C3E-C2E	-2.66	104.09	110.38
24	b	616	CLA	CMB-C2B-C3B	2.66	132.81	126.55
24	B	614	CLA	CHC-C4B-NB	2.66	128.04	124.05
24	B	612	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
26	D	404	BCR	C2-C1-C6	2.66	114.30	110.44
24	B	605	CLA	C3B-C4B-NB	-2.66	108.16	110.53
29	b	621	LMG	O1-C1-C2	-2.66	104.23	108.27
26	a	607	BCR	C37-C22-C23	2.66	122.15	118.09
25	A	606	PHO	CMB-C2B-C3B	2.66	129.99	124.68
24	B	610	CLA	O1D-CGD-CBD	2.66	129.76	124.52
29	b	621	LMG	O1-C7-C8	-2.66	104.36	110.82
24	a	612	CLA	C3B-C4B-NB	-2.65	108.16	110.53
24	A	613	CLA	CHB-C4A-NA	2.65	128.22	124.40
28	D	405	PL9	C8-C7-C3	2.65	118.88	112.03
29	c	519	LMG	O6-C1-O1	-2.65	103.79	110.04
32	c	518	DGD	O3D-C3D-C4D	-2.65	104.14	110.38
24	b	616	CLA	C3B-C4B-NB	-2.65	108.17	110.53
24	C	507	CLA	CHC-C4B-NB	2.65	128.02	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C3B-C4B-NB	-2.64	108.17	110.53
24	B	616	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
24	C	512	CLA	CMB-C2B-C3B	2.64	132.75	126.55
24	b	613	CLA	C7-C6-C5	-2.64	106.23	113.26
24	C	501	CLA	CHB-C1B-NB	2.64	128.00	124.05
24	D	403	CLA	CMB-C2B-C1B	-2.63	121.41	125.42
26	t	101	BCR	C15-C16-C17	-2.63	118.13	123.52
36	V	201	HEC	CMD-C2D-C1D	2.63	129.15	125.03
26	b	618	BCR	C37-C22-C21	-2.63	118.56	122.82
24	C	509	CLA	C3B-C4B-NB	-2.62	108.19	110.53
33	x	102	STE	O2-C1-O1	-2.62	116.59	123.33
24	B	616	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	b	612	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
26	H	101	BCR	C37-C22-C21	-2.62	118.57	122.82
26	C	515	BCR	C27-C26-C25	2.62	126.24	122.70
24	b	601	CLA	C3B-C4B-NB	-2.62	108.19	110.53
24	b	607	CLA	C1-O2A-CGA	2.62	122.99	116.65
24	A	605	CLA	CMB-C2B-C3B	2.61	132.70	126.55
24	B	606	CLA	CGD-CBD-CAD	-2.61	102.39	110.85
32	c	516	DGD	O6E-C5E-C4E	2.61	114.41	109.70
32	C	517	DGD	C1D-C2D-C3D	-2.61	104.51	110.01
31	B	623	SQD	O5-C1-C2	-2.61	105.01	110.37
24	B	601	CLA	O2D-CGD-CBD	2.61	115.79	111.23
26	H	101	BCR	C16-C15-C14	-2.61	118.18	123.52
24	c	508	CLA	CHD-C1D-ND	-2.61	121.13	124.80
26	H	101	BCR	C27-C26-C25	2.61	126.23	122.70
26	c	514	BCR	C15-C16-C17	-2.61	118.19	123.52
30	l	101	LHG	C11-C10-C9	-2.61	101.19	114.37
29	A	614	LMG	O3-C3-C2	-2.60	104.24	110.38
24	c	507	CLA	O2A-CGA-O1A	-2.60	117.11	123.63
24	C	513	CLA	O2D-CGD-CBD	2.60	115.78	111.23
32	C	517	DGD	C3E-C4E-C5E	-2.60	105.52	110.23
24	B	611	CLA	CHB-C4A-NA	2.60	128.15	124.40
31	D	407	SQD	O5-C5-C4	2.60	114.38	109.70
24	B	604	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
26	B	618	BCR	C7-C8-C9	-2.60	122.39	126.23
24	a	612	CLA	CMB-C2B-C3B	2.60	132.66	126.55
26	H	101	BCR	C1-C6-C5	-2.60	119.09	122.64
31	f	101	SQD	C3-C4-C5	2.59	114.94	110.23
30	l	101	LHG	C18-C17-C16	-2.59	101.25	114.37
24	b	612	CLA	C11-C12-C13	-2.59	107.36	115.97
24	C	504	CLA	O2D-CGD-O1D	-2.59	118.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C3B-C4B-NB	-2.59	108.22	110.53
24	B	609	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
28	D	405	PL9	C37-C38-C39	-2.59	121.70	127.62
26	D	404	BCR	C38-C26-C25	-2.59	121.66	124.48
24	b	612	CLA	CAC-C3C-C4C	2.58	128.15	124.79
30	D	408	LHG	C11-C10-C9	-2.58	101.31	114.37
24	c	501	CLA	CHB-C4A-NA	2.58	128.13	124.40
24	A	608	CLA	C4-C3-C5	2.58	119.71	115.23
26	c	514	BCR	C2-C1-C6	2.58	114.18	110.44
24	c	508	CLA	CHD-C4C-NC	2.58	128.23	124.23
24	A	605	CLA	O2D-CGD-CBD	2.58	115.73	111.23
24	d	403	CLA	O2A-CGA-O1A	-2.58	117.19	123.63
24	C	511	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
24	B	609	CLA	C3B-C4B-NB	-2.57	108.23	110.53
24	B	606	CLA	C4-C3-C5	2.57	119.69	115.23
24	D	402	CLA	CHB-C4A-NA	2.57	128.11	124.40
24	b	615	CLA	CHC-C1C-NC	2.57	128.19	124.31
32	C	516	DGD	CDB-CCB-CBB	-2.57	101.36	114.37
29	c	519	LMG	C9-C8-C7	-2.57	105.79	111.78
24	c	502	CLA	C1-C2-C3	-2.57	121.99	126.20
24	B	612	CLA	C11-C12-C13	-2.57	107.43	115.97
31	A	616	SQD	O48-C23-C24	2.57	119.66	111.83
30	D	408	LHG	C20-C19-C18	-2.57	101.39	114.37
24	a	606	CLA	O2A-CGA-O1A	-2.57	117.21	123.63
26	k	102	BCR	C27-C26-C25	2.56	126.17	122.70
26	b	619	BCR	C27-C26-C25	2.56	126.17	122.70
24	B	613	CLA	C3B-C4B-NB	-2.56	108.24	110.53
26	b	617	BCR	C36-C18-C19	2.56	122.00	118.09
26	x	101	BCR	C27-C26-C25	2.56	126.16	122.70
24	b	616	CLA	CMB-C2B-C1B	-2.56	121.53	125.42
24	B	612	CLA	CMB-C2B-C3B	2.55	132.56	126.55
24	B	605	CLA	C7-C6-C5	-2.55	106.46	113.26
35	e	101	HEM	C4C-C3C-C2C	2.55	109.03	106.81
29	d	410	LMG	O6-C1-O1	-2.55	104.01	110.04
24	C	506	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	b	605	CLA	CHD-C1D-ND	-2.55	121.21	124.80
24	b	605	CLA	C3B-C4B-NB	-2.55	108.25	110.53
24	C	510	CLA	CMB-C2B-C3B	2.55	132.54	126.55
24	b	611	CLA	CHD-C1D-C2D	2.55	130.78	125.49
24	B	613	CLA	CHA-C1A-NA	-2.55	120.63	126.39
26	a	607	BCR	C29-C30-C25	2.54	114.13	110.44
26	k	101	BCR	C27-C26-C25	2.54	126.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	CHB-C4A-NA	2.54	128.07	124.40
32	c	516	DGD	CDB-CCB-CBB	-2.54	101.53	114.37
30	B	622	LHG	C11-C10-C9	-2.53	101.55	114.37
24	b	602	CLA	C1-C2-C3	-2.53	122.04	126.20
24	c	510	CLA	C7-C6-C5	-2.53	106.51	113.26
24	c	513	CLA	CMB-C2B-C3B	2.53	132.51	126.55
32	c	518	DGD	O5D-C1E-C2E	2.53	112.12	108.27
24	b	610	CLA	CHA-C1A-NA	-2.53	120.66	126.39
24	c	502	CLA	CMB-C2B-C1B	-2.53	121.57	125.42
24	c	511	CLA	O2D-CGD-CBD	2.53	115.65	111.23
25	A	606	PHO	C2D-C1D-ND	2.53	111.25	109.43
24	a	604	CLA	CMB-C2B-C3B	2.52	132.49	126.55
35	F	101	HEM	CHB-C1B-NB	2.52	127.49	124.37
24	b	612	CLA	CHD-C1D-ND	-2.52	121.25	124.80
24	C	509	CLA	C1-C2-C3	-2.52	122.07	126.20
24	B	603	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
24	B	605	CLA	CHD-C1D-ND	-2.52	121.26	124.80
32	H	102	DGD	C3E-C4E-C5E	-2.52	105.67	110.23
31	D	407	SQD	O9-S-O7	-2.52	105.64	113.82
24	c	507	CLA	CHD-C1D-ND	-2.52	121.26	124.80
24	c	508	CLA	O2D-CGD-CBD	2.52	115.63	111.23
32	H	102	DGD	O5D-C1E-C2E	2.51	112.09	108.27
26	B	617	BCR	C27-C26-C25	2.51	126.10	122.70
24	b	606	CLA	CHB-C1B-NB	2.51	127.82	124.05
31	b	620	SQD	O47-C45-C46	2.51	117.36	108.34
26	B	618	BCR	C29-C30-C25	2.51	114.08	110.44
24	b	616	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
26	c	514	BCR	C37-C22-C23	2.51	121.92	118.09
32	h	101	DGD	C4E-C3E-C2E	-2.51	106.43	110.83
24	b	614	CLA	CMB-C2B-C3B	2.51	132.45	126.55
24	b	613	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
26	K	101	BCR	C27-C26-C25	2.51	126.09	122.70
24	b	615	CLA	CMB-C2B-C1B	-2.50	121.61	125.42
24	b	610	CLA	C2A-C1A-CHA	2.50	128.21	123.87
24	B	602	CLA	O2A-CGA-O1A	-2.50	117.37	123.63
31	b	620	SQD	O8-S-C6	2.50	110.80	105.97
33	J	101	STE	C3-C2-C1	-2.50	107.99	114.51
24	b	604	CLA	CMA-C3A-C4A	2.50	118.49	111.77
24	C	508	CLA	CMB-C2B-C1B	-2.50	121.62	125.42
32	A	618	DGD	O5D-C6D-C5D	-2.49	103.80	109.42
28	a	611	PL9	C27-C28-C29	-2.49	121.92	127.62
24	C	513	CLA	C3B-C4B-NB	-2.49	108.31	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	404	CLA	CHA-C1A-NA	-2.49	120.75	126.39
24	d	401	CLA	CHD-C1D-C2D	2.49	130.66	125.49
32	h	101	DGD	C3D-C4D-C5D	-2.49	105.72	110.23
24	C	507	CLA	C2A-C1A-CHA	2.48	128.18	123.87
29	b	623	LMG	O1-C7-C8	-2.48	104.78	110.82
24	c	501	CLA	O1D-CGD-CBD	2.48	129.41	124.52
24	b	605	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
24	C	513	CLA	CMB-C2B-C3B	2.48	132.37	126.55
26	c	515	BCR	C1-C6-C5	-2.47	119.26	122.64
26	a	607	BCR	C27-C26-C25	2.47	126.04	122.70
35	e	101	HEM	CHD-C4C-NC	2.47	127.14	124.45
24	b	604	CLA	O1D-CGD-CBD	2.47	129.38	124.52
26	C	514	BCR	C33-C5-C6	-2.47	121.79	124.48
30	d	407	LHG	C18-C17-C16	-2.46	101.91	114.37
24	C	501	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
24	a	604	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
32	h	101	DGD	O3E-C3E-C2E	-2.46	104.58	110.38
24	b	601	CLA	CHD-C1D-ND	-2.46	121.34	124.80
24	b	614	CLA	CHB-C4A-NA	2.46	127.95	124.40
24	B	603	CLA	CHD-C4C-NC	2.46	128.04	124.23
24	C	507	CLA	C1-C2-C3	-2.46	122.17	126.20
24	B	604	CLA	CGD-CBD-CAD	-2.46	102.90	110.85
24	d	401	CLA	CHC-C1C-NC	2.45	128.01	124.31
26	b	619	BCR	C2-C1-C6	2.45	114.00	110.44
24	B	606	CLA	OBD-CAD-C3D	2.45	134.14	128.42
26	B	617	BCR	C3-C4-C5	-2.45	109.69	114.06
30	A	615	LHG	O8-C6-C5	-2.44	101.35	108.40
24	B	608	CLA	CMB-C2B-C3B	2.44	132.30	126.55
36	V	201	HEC	CAC-C3C-C2C	2.44	130.76	126.89
24	C	508	CLA	CHB-C4A-NA	2.44	127.93	124.40
24	A	613	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
29	c	519	LMG	O2-C2-C1	-2.44	104.26	110.08
29	A	614	LMG	O8-C28-O10	-2.44	117.52	123.63
24	b	607	CLA	C4D-CHA-C1A	2.44	124.15	121.24
30	d	408	LHG	C20-C19-C18	-2.44	102.04	114.37
32	C	518	DGD	C1D-C2D-C3D	-2.44	104.88	110.01
26	t	101	BCR	C2-C1-C6	2.44	113.98	110.44
24	c	509	CLA	CMB-C2B-C3B	2.44	132.28	126.55
24	c	501	CLA	C3B-C4B-NB	-2.44	108.36	110.53
32	c	518	DGD	O6E-C1E-O5D	-2.43	104.29	110.04
26	c	514	BCR	C7-C8-C9	-2.43	122.63	126.23
29	c	522	LMG	C38-C37-C36	-2.43	102.07	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	O2D-CGD-CBD	2.43	115.48	111.23
24	C	507	CLA	CHB-C4A-NA	2.43	127.91	124.40
33	B	624	STE	C3-C2-C1	-2.43	108.16	114.51
24	B	603	CLA	O1D-CGD-CBD	2.43	129.31	124.52
29	c	519	LMG	C3-C4-C5	-2.43	105.83	110.23
31	A	617	SQD	O47-C7-C8	2.43	116.73	111.48
28	a	611	PL9	O2-C1-C6	2.43	124.34	120.48
24	c	506	CLA	OBD-CAD-C3D	2.43	134.09	128.42
36	V	201	HEC	CAC-C3C-C4C	-2.43	121.57	124.91
31	D	407	SQD	C44-O6-C1	2.42	117.82	113.68
24	C	506	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
24	B	608	CLA	CHB-C4A-NA	2.42	127.90	124.40
24	d	403	CLA	CHB-C4A-NA	2.42	127.90	124.40
25	A	607	PHO	C1-C2-C3	-2.42	122.23	126.20
24	c	509	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
24	B	612	CLA	C1-C2-C3	-2.42	122.23	126.20
29	A	614	LMG	C12-C11-C10	-2.42	104.83	113.69
24	A	604	CLA	C3B-C4B-NB	-2.42	108.37	110.53
24	A	608	CLA	CHB-C4A-NA	2.42	127.89	124.40
24	B	604	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
24	C	504	CLA	CHD-C1D-ND	-2.42	121.40	124.80
24	B	605	CLA	O1D-CGD-CBD	2.41	129.28	124.52
28	d	406	PL9	C22-C23-C24	-2.41	122.10	127.62
26	b	619	BCR	C7-C8-C9	-2.41	122.67	126.23
29	C	519	LMG	O7-C10-O9	-2.41	118.07	123.70
24	c	501	CLA	CMB-C2B-C3B	2.41	132.22	126.55
24	C	513	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
26	Y	101	BCR	C38-C26-C25	-2.41	121.86	124.48
24	A	604	CLA	O2D-CGD-CBD	-2.41	107.02	111.23
24	c	508	CLA	C7-C6-C5	-2.41	106.84	113.26
29	a	618	LMG	C40-C39-C38	-2.41	102.20	114.37
24	c	506	CLA	C4-C3-C2	-2.40	117.45	123.63
26	c	515	BCR	C8-C9-C10	2.40	122.79	119.01
26	C	515	BCR	C2-C1-C6	2.40	113.93	110.44
26	T	101	BCR	C1-C6-C5	-2.40	119.36	122.64
24	c	502	CLA	O1D-CGD-CBD	2.40	129.25	124.52
24	C	508	CLA	O2D-CGD-CBD	2.40	115.42	111.23
29	C	519	LMG	O2-C2-C1	-2.39	104.37	110.08
24	b	610	CLA	CAA-CBA-CGA	-2.39	106.41	113.21
32	c	517	DGD	C3E-C4E-C5E	-2.39	105.90	110.23
25	a	605	PHO	C3B-C4B-NB	-2.39	105.91	107.46
24	c	507	CLA	C1D-ND-C4D	2.39	107.99	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	c	517	DGD	O3G-C1D-C2D	-2.39	104.64	108.27
24	b	605	CLA	C4D-CHA-C1A	2.39	124.09	121.24
26	T	101	BCR	C38-C26-C27	-2.39	108.51	113.60
28	a	611	PL9	C12-C13-C14	-2.39	122.16	127.62
25	a	605	PHO	O2A-CGA-O1A	-2.39	117.66	123.63
24	B	610	CLA	C1-C2-C3	-2.39	122.29	126.20
28	a	611	PL9	C22-C23-C24	-2.39	122.16	127.62
29	c	521	LMG	O2-C2-C1	-2.39	104.39	110.08
32	H	102	DGD	CDB-CCB-CBB	-2.38	102.32	114.37
24	b	604	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
24	b	613	CLA	CHA-C1A-NA	-2.38	121.00	126.39
26	b	617	BCR	C29-C30-C25	2.38	113.90	110.44
24	d	401	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
24	C	502	CLA	CHA-C1A-NA	-2.38	121.00	126.39
24	C	508	CLA	CMB-C2B-C3B	2.38	132.15	126.55
33	E	102	STE	O2-C1-C2	2.38	121.52	114.00
24	b	612	CLA	CMD-C2D-C3D	2.38	133.14	127.69
31	a	614	SQD	O48-C46-C45	2.38	115.25	108.40
29	b	621	LMG	O6-C1-O1	-2.38	104.43	110.04
29	c	521	LMG	O6-C1-O1	-2.38	104.43	110.04
32	A	618	DGD	CBB-CAB-C9B	-2.38	102.36	114.37
24	b	615	CLA	C1-O2A-CGA	2.38	122.40	116.65
28	A	612	PL9	C26-C24-C23	-2.37	115.84	121.17
32	c	518	DGD	O6E-C5E-C4E	2.37	113.97	109.70
24	B	615	CLA	CHD-C1D-ND	-2.37	121.46	124.80
24	B	604	CLA	O2D-CGD-CBD	2.37	115.38	111.23
32	C	516	DGD	O1G-C1A-C2A	-2.37	104.61	111.83
24	b	604	CLA	C11-C12-C13	-2.37	108.09	115.97
24	d	404	CLA	CHB-C1B-NB	2.37	127.60	124.05
24	b	603	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
24	b	602	CLA	C4-C3-C5	2.37	119.34	115.23
26	B	617	BCR	C15-C16-C17	-2.37	118.68	123.52
24	b	609	CLA	CHA-C1A-NA	-2.37	121.03	126.39
24	C	513	CLA	CHB-C4A-NA	2.37	127.81	124.40
26	H	101	BCR	C37-C22-C23	2.36	121.70	118.09
32	c	518	DGD	CDB-CCB-CBB	-2.36	102.42	114.37
24	C	504	CLA	CHC-C1C-NC	2.36	127.87	124.31
26	x	101	BCR	C37-C22-C21	-2.36	118.99	122.82
33	B	627	STE	O2-C1-C2	2.36	121.46	114.00
30	B	622	LHG	C20-C19-C18	-2.36	102.44	114.37
24	c	510	CLA	C3B-C4B-NB	-2.36	108.43	110.53
30	B	622	LHG	O8-C23-O10	-2.36	117.73	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	E	101	LHG	C18-C17-C16	-2.35	102.47	114.37
26	t	101	BCR	C4-C5-C6	2.35	125.88	122.70
32	h	101	DGD	O5E-C6E-C5E	-2.35	103.33	111.33
29	D	406	LMG	O3-C3-C2	-2.35	104.83	110.38
24	B	601	CLA	CHC-C4B-NB	2.35	127.57	124.05
29	M	101	LMG	O1-C7-C8	-2.35	105.11	110.82
26	A	609	BCR	C15-C16-C17	-2.35	118.72	123.52
24	C	502	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
30	e	102	LHG	C11-C10-C9	-2.35	102.51	114.37
24	b	608	CLA	CHB-C1B-NB	2.34	127.56	124.05
24	C	510	CLA	C11-C10-C8	-2.34	108.17	115.97
24	c	502	CLA	CMB-C2B-C3B	2.34	132.06	126.55
26	C	514	BCR	C15-C16-C17	-2.34	118.72	123.52
24	B	606	CLA	C2A-C1A-CHA	2.34	127.93	123.87
24	c	508	CLA	CHD-C1D-C2D	2.34	130.36	125.49
24	B	608	CLA	C4A-NA-C1A	2.34	107.75	106.68
26	a	607	BCR	C37-C22-C21	-2.34	119.03	122.82
32	c	517	DGD	C3D-C4D-C5D	-2.34	105.99	110.23
24	C	503	CLA	CHC-C4B-NB	2.34	127.56	124.05
29	D	409	LMG	O1-C7-C8	-2.34	105.76	111.77
24	b	608	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
25	d	402	PHO	C3D-C4D-ND	2.33	110.70	107.71
24	B	605	CLA	CHB-C4A-NA	2.33	127.76	124.40
32	c	516	DGD	O3E-C3E-C2E	-2.33	104.89	110.38
26	d	405	BCR	C3-C4-C5	-2.33	109.90	114.06
29	a	618	LMG	O6-C5-C4	2.33	113.89	109.70
24	A	613	CLA	O2D-CGD-CBD	2.33	115.30	111.23
28	d	406	PL9	C8-C7-C3	2.32	118.04	112.03
24	b	603	CLA	CHD-C1D-ND	-2.32	121.53	124.80
24	B	609	CLA	C6-C5-C3	2.32	119.12	113.47
24	B	602	CLA	C3B-C4B-NB	-2.32	108.46	110.53
24	c	505	CLA	CAC-C3C-C4C	2.32	127.81	124.79
28	a	611	PL9	C36-C34-C33	-2.32	115.96	121.17
26	x	101	BCR	C2-C1-C6	2.32	113.80	110.44
28	a	611	PL9	C20-C19-C21	2.31	119.25	115.23
25	A	606	PHO	O2D-CGD-O1D	-2.31	119.34	123.85
24	B	609	CLA	CHA-C1A-NA	-2.31	121.15	126.39
24	A	605	CLA	C1-O2A-CGA	2.31	122.25	116.65
24	b	606	CLA	O1D-CGD-CBD	2.31	129.08	124.52
24	c	512	CLA	O1D-CGD-CBD	2.31	129.08	124.52
26	d	405	BCR	C24-C23-C22	-2.31	122.82	126.23
31	b	620	SQD	O10-C23-C24	-2.31	114.75	123.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	F	101	HEM	C4C-C3C-C2C	2.31	108.81	106.81
24	b	603	CLA	C4-C3-C5	2.31	119.23	115.23
24	b	614	CLA	CAC-C3C-C4C	2.31	127.79	124.79
24	d	404	CLA	CHB-C1B-C2B	-2.31	120.73	127.43
29	A	614	LMG	C1-O6-C5	-2.31	109.22	113.72
24	D	402	CLA	C6-C5-C3	2.30	119.08	113.47
33	C	522	STE	C4-C3-C2	-2.30	104.66	113.13
24	C	511	CLA	C1-C2-C3	-2.30	122.43	126.20
24	B	612	CLA	CHB-C4A-NA	2.30	127.72	124.40
30	A	615	LHG	C27-C26-C25	-2.30	102.75	114.37
24	B	605	CLA	CHD-C1D-C2D	2.30	130.27	125.49
24	b	603	CLA	CMB-C2B-C3B	2.30	131.95	126.55
36	v	201	HEC	C1B-C2B-C3B	2.30	109.40	106.98
26	Y	101	BCR	C30-C25-C26	-2.30	119.50	122.64
31	f	101	SQD	O5-C5-C4	2.30	113.83	109.70
32	C	517	DGD	CDB-CCB-CBB	-2.29	102.78	114.37
32	c	516	DGD	CBB-CAB-C9B	-2.29	102.78	114.37
24	B	607	CLA	CHD-C4C-NC	2.29	127.78	124.23
32	c	517	DGD	C4E-C3E-C2E	-2.29	106.81	110.83
32	c	518	DGD	O2D-C2D-C1D	-2.29	104.63	110.08
24	B	608	CLA	O1D-CGD-CBD	2.28	129.02	124.52
30	A	615	LHG	C3-C2-C1	-2.28	104.08	111.77
29	M	101	LMG	C1-C2-C3	-2.28	105.21	110.01
24	b	607	CLA	CHA-C1A-NA	-2.28	121.22	126.39
24	B	601	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
24	A	608	CLA	C1-C2-C3	-2.28	122.46	126.20
26	b	618	BCR	C15-C16-C17	-2.28	118.85	123.52
32	h	101	DGD	O6E-C5E-C4E	2.28	113.81	109.70
24	b	612	CLA	CMB-C2B-C3B	2.28	131.91	126.55
28	D	405	PL9	C32-C33-C34	-2.28	122.41	127.62
32	c	517	DGD	C8B-C7B-C6B	-2.28	102.85	114.37
24	b	609	CLA	C11-C10-C8	-2.28	108.40	115.97
24	b	605	CLA	C1-C2-C3	-2.27	122.47	126.20
30	A	615	LHG	O8-C23-C24	2.27	118.77	111.83
24	C	509	CLA	C2A-C3A-C4A	2.27	105.54	101.87
28	a	611	PL9	C7-C8-C9	-2.27	122.92	126.83
24	b	607	CLA	C2A-C1A-CHA	2.27	127.81	123.87
26	b	618	BCR	C36-C18-C17	-2.27	119.14	122.82
30	E	101	LHG	C11-C10-C9	-2.27	102.90	114.37
24	B	612	CLA	CHD-C1D-ND	-2.27	121.61	124.80
26	b	619	BCR	C38-C26-C25	-2.26	122.01	124.48
24	B	614	CLA	CAC-C3C-C4C	2.26	127.74	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	617	BCR	C36-C18-C17	-2.26	119.15	122.82
33	b	625	STE	C4-C3-C2	-2.26	104.82	113.13
26	B	618	BCR	C15-C16-C17	-2.26	118.89	123.52
24	B	602	CLA	CHA-C4D-ND	2.26	137.21	132.55
24	C	502	CLA	CHD-C1D-ND	-2.26	121.62	124.80
24	d	403	CLA	C2A-C1A-CHA	2.26	127.79	123.87
28	a	611	PL9	O2-C1-C2	-2.26	116.69	121.83
25	A	606	PHO	CBC-CAC-C3C	2.26	116.10	112.87
35	e	101	HEM	CAB-C3B-C2B	-2.26	121.10	128.43
32	C	516	DGD	C5B-C4B-C3B	-2.26	102.97	114.37
32	c	518	DGD	CBB-CAB-C9B	-2.25	102.99	114.37
26	b	618	BCR	C15-C14-C13	-2.25	124.12	127.28
24	b	608	CLA	CHD-C1D-ND	-2.25	121.64	124.80
30	D	408	LHG	C27-C26-C25	-2.25	103.00	114.37
26	b	617	BCR	C36-C18-C17	-2.25	119.17	122.82
30	d	408	LHG	C18-C17-C16	-2.25	103.00	114.37
24	B	611	CLA	C9-C8-C10	-2.25	103.27	111.27
30	l	101	LHG	O8-C23-C24	2.25	118.68	111.83
31	f	101	SQD	C46-C45-C44	-2.25	106.55	111.78
32	h	101	DGD	CDB-CCB-CBB	-2.24	103.03	114.37
32	c	517	DGD	O2E-C2E-C1E	-2.24	104.73	110.08
25	A	607	PHO	C3D-C4D-ND	2.24	110.58	107.71
24	b	607	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
24	d	401	CLA	C3B-C4B-NB	-2.24	108.53	110.53
28	A	612	PL9	O2-C1-C2	-2.24	116.74	121.83
29	D	406	LMG	C38-C37-C36	-2.24	103.06	114.37
24	c	504	CLA	O1A-CGA-CBA	2.23	132.52	123.78
32	h	101	DGD	C6D-C5D-C4D	2.23	116.75	112.07
24	b	606	CLA	O2A-CGA-O1A	-2.23	118.04	123.63
24	A	613	CLA	CHC-C4B-NB	2.23	127.40	124.05
24	c	507	CLA	C2C-C1C-NC	2.23	112.33	109.98
32	c	516	DGD	C5B-C4B-C3B	-2.23	103.10	114.37
32	c	516	DGD	O1G-C1A-C2A	-2.23	105.04	111.83
32	C	518	DGD	O3E-C3E-C2E	-2.23	105.13	110.38
24	b	616	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
24	c	504	CLA	O2D-CGD-CBD	2.23	115.12	111.23
24	c	507	CLA	CMB-C2B-C3B	2.23	131.79	126.55
29	c	519	LMG	C1-O6-C5	-2.22	109.38	113.72
24	B	615	CLA	C6-C7-C8	-2.22	108.58	115.97
24	b	605	CLA	O1A-CGA-CBA	2.22	132.46	123.78
24	c	509	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
26	B	619	BCR	C36-C18-C17	-2.22	119.22	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	CHB-C4A-NA	2.22	127.60	124.40
24	A	605	CLA	C2D-C1D-ND	-2.22	107.93	110.13
30	l	101	LHG	C27-C26-C25	-2.22	103.16	114.37
24	b	604	CLA	C6-C7-C8	-2.22	108.59	115.97
26	C	514	BCR	C24-C23-C22	-2.22	122.95	126.23
30	d	407	LHG	C20-C19-C18	-2.22	103.17	114.37
29	a	618	LMG	C42-C41-C40	-2.21	103.17	114.37
24	C	511	CLA	CHB-C4A-NA	2.21	127.59	124.40
26	T	101	BCR	C4-C5-C6	2.21	125.69	122.70
28	a	611	PL9	C37-C38-C39	-2.21	122.56	127.62
28	D	405	PL9	C50-C49-C48	-2.21	116.03	122.66
29	M	101	LMG	C31-C30-C29	-2.21	105.02	113.13
32	c	518	DGD	O5E-C6E-C5E	-2.21	103.82	111.33
24	c	506	CLA	C4-C3-C5	2.20	119.05	115.23
24	B	608	CLA	CHD-C1D-ND	-2.20	121.70	124.80
24	C	512	CLA	C6-C5-C3	-2.20	108.10	113.47
24	b	604	CLA	CHB-C1B-NB	2.20	127.35	124.05
30	E	101	LHG	C20-C19-C18	-2.20	103.24	114.37
24	B	601	CLA	C2A-C1A-CHA	2.20	127.69	123.87
24	b	604	CLA	CAC-C3C-C4C	2.20	127.65	124.79
24	b	604	CLA	C3A-C2A-C1A	2.20	104.63	101.34
24	a	612	CLA	C2B-C1B-NB	-2.20	108.05	110.33
24	c	502	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	C	512	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
24	B	609	CLA	CHC-C4B-NB	2.20	127.34	124.05
26	x	101	BCR	C16-C15-C14	-2.19	119.03	123.52
26	d	405	BCR	C30-C25-C26	-2.19	119.64	122.64
24	b	611	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	A	604	CLA	CHC-C4B-NB	2.19	127.34	124.05
24	A	604	CLA	CAA-CBA-CGA	-2.19	106.98	113.21
24	B	606	CLA	CHC-C4B-NB	2.19	127.33	124.05
29	c	522	LMG	C8-O7-C10	2.19	123.04	117.80
24	b	610	CLA	C2C-C1C-NC	2.19	112.28	109.98
35	F	101	HEM	C3B-C4B-NB	2.19	111.04	109.47
29	b	623	LMG	C40-C39-C38	-2.19	103.31	114.37
30	B	621	LHG	C20-C19-C18	-2.19	103.31	114.37
32	c	517	DGD	O4E-C4E-C3E	-2.19	105.22	110.38
24	B	601	CLA	CHB-C4A-NA	2.19	127.56	124.40
24	B	612	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
24	a	606	CLA	CHA-C1A-NA	-2.18	121.44	126.39
24	b	615	CLA	C6-C5-C3	-2.18	108.15	113.47
24	b	604	CLA	CGD-CBD-CAD	-2.18	103.78	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C6-C7-C8	-2.18	108.71	115.97
26	B	618	BCR	C2-C1-C6	2.18	113.61	110.44
24	A	605	CLA	CHB-C4A-NA	2.18	127.55	124.40
28	A	612	PL9	C7-C3-C2	-2.18	120.82	123.39
36	v	201	HEC	CHD-C1D-ND	2.18	127.06	124.37
26	H	101	BCR	C29-C30-C25	2.18	113.60	110.44
26	c	514	BCR	C33-C5-C6	-2.18	122.11	124.48
24	b	606	CLA	CMB-C2B-C3B	2.18	131.67	126.55
24	b	601	CLA	O2D-CGD-CBD	2.17	115.03	111.23
24	c	509	CLA	CHD-C1D-ND	-2.17	121.74	124.80
24	A	613	CLA	C7-C6-C5	-2.17	107.47	113.26
28	D	405	PL9	C12-C13-C14	-2.17	122.65	127.62
26	K	101	BCR	C37-C22-C21	-2.17	119.30	122.82
26	c	515	BCR	C15-C16-C17	-2.17	119.08	123.52
32	H	102	DGD	C1E-O6E-C5E	2.17	117.96	113.72
24	d	404	CLA	C1-C2-C3	-2.17	122.64	126.20
33	M	102	STE	C3-C2-C1	-2.17	108.85	114.51
24	B	614	CLA	CHB-C1B-NB	2.17	127.30	124.05
24	B	609	CLA	C2C-C1C-NC	2.17	112.26	109.98
26	c	515	BCR	C36-C18-C17	-2.16	119.31	122.82
24	B	608	CLA	O2D-CGD-CBD	2.16	115.01	111.23
24	b	608	CLA	C11-C10-C8	-2.16	108.78	115.97
29	C	519	LMG	O8-C28-O10	-2.16	118.23	123.63
24	A	605	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
26	C	515	BCR	C1-C6-C5	-2.16	119.69	122.64
28	D	405	PL9	C7-C3-C2	-2.16	120.85	123.39
24	c	506	CLA	CHD-C1D-ND	-2.16	121.77	124.80
33	t	102	STE	C3-C2-C1	-2.16	108.88	114.51
24	c	501	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
24	C	507	CLA	CHA-C1A-NA	-2.15	121.51	126.39
32	c	517	DGD	O3E-C3E-C4E	-2.15	105.30	110.38
26	D	404	BCR	C7-C8-C9	-2.15	123.05	126.23
24	B	608	CLA	CMB-C2B-C1B	-2.15	122.14	125.42
32	c	518	DGD	C3G-C2G-C1G	-2.15	106.77	111.78
31	B	623	SQD	C25-C24-C23	-2.15	105.81	113.69
24	C	503	CLA	C3A-C2A-C1A	2.15	104.56	101.34
24	B	611	CLA	C14-C13-C15	-2.15	103.61	111.27
26	b	617	BCR	C3-C4-C5	-2.15	110.22	114.06
25	a	605	PHO	O2D-CGD-O1D	-2.15	119.66	123.85
35	F	101	HEM	CHC-C1C-NC	2.15	126.79	124.45
24	A	608	CLA	CAA-CBA-CGA	-2.15	107.11	113.21
32	h	101	DGD	C4D-C3D-C2D	-2.15	107.06	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	C3B-C4B-NB	-2.15	108.61	110.53
24	B	603	CLA	C5-C3-C2	-2.15	116.35	121.17
24	D	403	CLA	O2D-CGD-CBD	2.15	114.98	111.23
24	b	612	CLA	C4D-C3D-CAD	-2.15	105.78	108.11
24	b	614	CLA	O1A-CGA-CBA	2.15	132.17	123.78
29	d	410	LMG	O3-C3-C2	-2.14	105.32	110.38
24	B	612	CLA	C16-C15-C13	-2.14	108.84	115.97
24	c	507	CLA	CHD-C1D-C2D	2.14	129.94	125.49
24	c	508	CLA	C3B-C4B-NB	-2.14	108.62	110.53
24	d	404	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
24	A	604	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
32	c	517	DGD	C1D-C2D-C3D	-2.14	105.51	110.01
26	k	101	BCR	C1-C6-C5	-2.14	119.71	122.64
24	b	603	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
24	B	613	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
24	c	510	CLA	O1A-CGA-CBA	2.13	132.13	123.78
29	c	522	LMG	C40-C39-C38	-2.13	103.59	114.37
26	c	514	BCR	C38-C26-C25	-2.13	122.16	124.48
24	C	503	CLA	O2A-C1-C2	-2.13	99.90	108.11
24	B	603	CLA	CHC-C1C-NC	2.13	127.52	124.31
24	c	510	CLA	CHB-C1B-NB	2.13	127.25	124.05
36	V	201	HEC	O1D-CGD-CBD	-2.13	116.34	123.09
24	c	505	CLA	CMD-C2D-C3D	2.13	132.57	127.69
24	c	504	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	B	609	CLA	C1D-ND-C4D	-2.13	104.82	106.31
24	b	608	CLA	CHA-C1A-NA	-2.13	121.58	126.39
26	B	617	BCR	C11-C10-C9	-2.13	124.30	127.28
31	f	101	SQD	O5-C1-O6	2.13	115.07	110.04
26	Y	101	BCR	C1-C6-C5	-2.12	119.73	122.64
24	b	615	CLA	CHA-C4D-ND	2.12	136.93	132.55
25	a	605	PHO	O2D-CGD-CBD	2.12	113.28	110.95
24	C	510	CLA	CHD-C1D-ND	-2.12	121.81	124.80
26	b	618	BCR	C7-C8-C9	-2.12	123.09	126.23
24	B	614	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	B	611	CLA	C11-C12-C13	-2.12	108.92	115.97
24	C	510	CLA	C16-C15-C13	-2.12	108.92	115.97
24	C	508	CLA	C4D-C3D-CAD	-2.12	105.81	108.11
30	B	622	LHG	C13-C12-C11	-2.12	103.67	114.37
31	f	101	SQD	O9-S-C6	2.12	109.92	106.76
30	B	622	LHG	O3-P-O5	-2.12	100.55	108.94
24	c	504	CLA	CHD-C1D-ND	-2.12	121.83	124.80
24	b	608	CLA	O2D-CGD-CBD	2.11	114.93	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	623	SQD	C27-C26-C25	-2.11	103.69	114.37
26	b	618	BCR	C27-C26-C25	2.11	125.56	122.70
26	A	609	BCR	C40-C30-C39	-2.11	102.58	108.63
29	d	410	LMG	C40-C39-C38	-2.11	103.69	114.37
24	b	614	CLA	CHB-C1B-NB	2.11	127.22	124.05
24	C	501	CLA	C3A-C2A-C1A	2.11	104.50	101.34
31	B	623	SQD	O9-S-O7	-2.11	106.96	113.82
30	l	101	LHG	C5-O7-C7	-2.11	112.75	117.80
24	B	613	CLA	O1D-CGD-CBD	2.11	128.67	124.52
24	C	505	CLA	C3B-C4B-NB	-2.11	108.65	110.53
24	b	604	CLA	CHC-C1C-C2C	-2.11	120.96	126.95
24	b	611	CLA	C11-C12-C13	-2.11	108.97	115.97
31	f	101	SQD	O48-C23-C24	2.11	118.25	111.83
26	t	101	BCR	C15-C14-C13	-2.10	124.33	127.28
28	d	406	PL9	C36-C34-C33	-2.10	116.44	121.17
24	d	401	CLA	CMA-C3A-C4A	-2.10	106.12	111.77
24	B	611	CLA	O1D-CGD-CBD	2.10	128.66	124.52
32	A	618	DGD	O5E-C6E-C5E	-2.10	104.17	111.33
28	d	406	PL9	C32-C33-C34	-2.10	122.81	127.62
24	C	511	CLA	C4-C3-C5	2.10	118.88	115.23
32	c	516	DGD	CAB-C9B-C8B	-2.10	103.74	114.37
24	c	503	CLA	C4D-C3D-CAD	-2.10	105.83	108.11
28	d	406	PL9	C12-C13-C14	-2.10	122.82	127.62
26	k	102	BCR	C1-C6-C5	-2.10	119.77	122.64
29	C	519	LMG	O1-C7-C8	-2.10	105.72	110.82
28	D	405	PL9	C31-C29-C28	2.10	125.87	121.17
31	a	614	SQD	C9-C8-C7	-2.10	106.02	113.69
24	b	614	CLA	C4-C3-C2	-2.09	118.25	123.63
30	B	622	LHG	C18-C17-C16	-2.09	103.79	114.37
36	V	201	HEC	CHD-C4C-NC	2.09	127.66	123.86
24	B	602	CLA	CMB-C2B-C3B	2.09	131.47	126.55
30	e	102	LHG	O8-C23-O10	-2.09	118.40	123.63
29	c	522	LMG	O2-C2-C3	-2.09	105.45	110.38
24	D	402	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
24	B	616	CLA	C4D-CHA-C1A	2.09	123.74	121.24
36	v	201	HEC	CBA-CAA-C2A	-2.09	106.76	112.53
32	c	517	DGD	O2D-C2D-C1D	-2.09	105.10	110.08
32	c	516	DGD	C8B-C7B-C6B	-2.09	103.81	114.37
26	H	101	BCR	C38-C26-C25	-2.09	122.21	124.48
30	B	621	LHG	O7-C7-O9	-2.09	118.83	123.70
31	a	613	SQD	O8-S-C6	2.08	110.00	105.97
24	B	608	CLA	C3B-C4B-NB	-2.08	108.67	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	C2A-C3A-C4A	2.08	105.23	101.87
24	B	614	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	A	605	CLA	CAC-C3C-C4C	2.08	127.50	124.79
24	b	608	CLA	CHD-C1D-C2D	2.08	129.82	125.49
24	c	513	CLA	C3B-C4B-NB	-2.08	108.67	110.53
24	c	513	CLA	CHD-C1D-ND	-2.08	121.88	124.80
30	d	407	LHG	O3-P-O5	-2.08	100.69	108.94
26	t	101	BCR	C27-C26-C25	2.08	125.51	122.70
29	d	410	LMG	C38-C37-C36	-2.08	103.86	114.37
30	e	102	LHG	C20-C19-C18	-2.08	103.86	114.37
24	B	609	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
26	b	619	BCR	C36-C18-C17	-2.08	119.45	122.82
25	A	606	PHO	OBD-CAD-C3D	2.08	131.13	127.89
24	B	614	CLA	C1-C2-C3	-2.08	122.80	126.20
24	D	403	CLA	CHB-C4A-NA	2.08	127.40	124.40
32	C	518	DGD	O5E-C6E-C5E	-2.07	104.27	111.33
24	b	615	CLA	CHC-C1C-C2C	-2.07	121.05	126.95
24	B	606	CLA	O1A-CGA-CBA	2.07	131.89	123.78
24	B	615	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	b	609	CLA	C1-C2-C3	-2.07	122.80	126.20
29	D	410	LMG	O7-C10-O9	-2.07	118.00	123.33
24	B	602	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	b	615	CLA	CHB-C1B-NB	2.07	127.16	124.05
28	d	406	PL9	C40-C39-C38	-2.07	118.31	123.63
30	B	621	LHG	O8-C23-C24	2.07	118.15	111.83
24	b	609	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	C	503	CLA	CMB-C2B-C3B	2.07	131.41	126.55
26	B	619	BCR	C38-C26-C25	-2.07	122.23	124.48
29	C	519	LMG	C40-C39-C38	-2.07	103.93	114.37
24	B	606	CLA	C4D-CHA-C1A	2.06	123.71	121.24
24	b	607	CLA	CMB-C2B-C3B	2.06	131.41	126.55
24	a	606	CLA	CHC-C4B-NB	2.06	127.15	124.05
24	b	606	CLA	C2C-C1C-NC	2.06	112.15	109.98
28	A	612	PL9	O2-C1-C6	2.06	123.76	120.48
32	C	517	DGD	O2D-C2D-C1D	-2.06	105.16	110.08
24	b	609	CLA	C1D-ND-C4D	2.06	107.76	106.31
24	b	605	CLA	CHA-C1A-NA	-2.06	121.73	126.39
32	c	517	DGD	CBB-CAB-C9B	-2.06	103.97	114.37
30	B	621	LHG	C18-C17-C16	-2.06	103.97	114.37
31	A	617	SQD	O48-C23-O10	-2.06	118.48	123.63
33	b	622	STE	C3-C2-C1	-2.06	109.14	114.51
29	b	623	LMG	C38-C37-C36	-2.06	103.98	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C11-C10-C8	-2.06	109.13	115.97
24	C	511	CLA	C3B-C4B-NB	-2.05	108.70	110.53
24	c	504	CLA	CMB-C2B-C1B	-2.05	122.29	125.42
24	B	601	CLA	C4-C3-C5	2.05	118.79	115.23
26	a	607	BCR	C8-C7-C6	-2.05	121.51	127.00
24	c	504	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
36	v	201	HEC	CBD-CAD-C3D	-2.05	106.86	112.53
24	B	606	CLA	CHB-C1B-NB	2.05	127.13	124.05
26	k	102	BCR	C2-C1-C6	2.05	113.42	110.44
24	b	602	CLA	CHC-C1C-C2C	-2.05	121.12	126.95
33	a	616	STE	O2-C1-C2	2.05	120.47	114.00
24	c	503	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
24	b	607	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
24	B	609	CLA	CHD-C1D-ND	-2.05	121.92	124.80
32	h	101	DGD	O3G-C1D-C2D	-2.05	105.17	108.27
24	B	611	CLA	C7-C6-C5	-2.04	107.81	113.26
24	C	507	CLA	CHD-C1D-ND	-2.04	121.92	124.80
24	B	603	CLA	C2A-C1A-CHA	2.04	127.42	123.87
26	B	617	BCR	C8-C7-C6	-2.04	121.54	127.00
29	c	519	LMG	C40-C39-C38	-2.04	104.04	114.37
31	A	616	SQD	O8-S-O9	2.04	116.51	111.40
31	b	620	SQD	O48-C23-O10	-2.04	118.52	123.63
24	B	607	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
24	D	403	CLA	C11-C10-C8	-2.04	109.18	115.97
26	A	609	BCR	C16-C15-C14	-2.04	119.34	123.52
24	d	403	CLA	C4-C3-C5	2.04	118.77	115.23
24	c	513	CLA	C1-C2-C3	-2.04	122.85	126.20
30	l	101	LHG	C29-C28-C27	-2.04	104.05	114.37
24	C	505	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	d	404	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
29	b	621	LMG	O8-C28-O10	-2.04	118.53	123.63
32	c	518	DGD	CAB-C9B-C8B	-2.04	104.06	114.37
28	d	406	PL9	C35-C34-C36	2.04	118.77	115.23
24	b	609	CLA	CHB-C1B-NB	2.04	127.11	124.05
24	B	616	CLA	C1-O2A-CGA	-2.04	111.72	116.65
24	C	507	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
24	C	503	CLA	C2C-C1C-NC	2.04	112.12	109.98
29	a	618	LMG	O6-C1-C2	-2.04	106.19	110.37
32	C	516	DGD	C6B-C5B-C4B	-2.03	104.08	114.37
31	B	623	SQD	C1-C2-C3	-2.03	105.73	110.01
24	c	508	CLA	CMB-C2B-C3B	2.03	131.33	126.55
24	C	513	CLA	O1D-CGD-CBD	2.03	128.53	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	CHD-C4C-NC	2.03	127.38	124.23
32	c	518	DGD	C5B-C4B-C3B	-2.03	104.10	114.37
26	b	618	BCR	C29-C30-C25	2.03	113.39	110.44
24	c	510	CLA	O1D-CGD-CBD	2.03	128.52	124.52
25	A	607	PHO	CAC-C3C-C2C	2.03	131.29	127.56
31	a	613	SQD	O4-C4-C3	-2.03	105.59	110.38
24	c	504	CLA	C3B-C4B-NB	-2.03	108.72	110.53
26	K	101	BCR	C29-C30-C25	2.03	113.38	110.44
31	A	616	SQD	O9-S-C6	2.03	109.78	106.76
24	C	503	CLA	CHD-C1D-ND	-2.03	121.95	124.80
24	B	615	CLA	C2C-C1C-NC	2.03	112.11	109.98
24	B	607	CLA	CHD-C1D-ND	-2.02	121.95	124.80
26	a	607	BCR	C7-C8-C9	-2.02	123.24	126.23
29	M	101	LMG	C6-C5-C4	-2.02	108.05	113.02
26	A	609	BCR	C4-C5-C6	2.02	125.44	122.70
32	c	517	DGD	CDB-CCB-CBB	-2.02	104.14	114.37
29	a	618	LMG	O7-C10-O9	-2.02	118.98	123.70
32	c	517	DGD	O6E-C1E-O5D	-2.02	105.27	110.04
32	c	516	DGD	O6D-C1D-O3G	-2.02	105.27	110.04
24	C	506	CLA	CHD-C1D-ND	-2.02	121.96	124.80
24	b	613	CLA	CMB-C2B-C3B	2.02	131.30	126.55
26	C	514	BCR	C36-C18-C17	-2.02	119.55	122.82
29	C	519	LMG	C38-C37-C36	-2.02	104.18	114.37
25	A	606	PHO	C1A-C2A-C3A	-2.01	100.92	102.84
26	B	617	BCR	C37-C22-C23	2.01	121.16	118.09
28	a	611	PL9	O1-C4-C3	-2.01	118.61	120.73
24	C	510	CLA	CHB-C4A-NA	2.01	127.31	124.40
35	F	101	HEM	O2D-CGD-CBD	2.01	120.36	114.00
24	b	609	CLA	C7-C6-C5	-2.01	107.90	113.26
30	B	621	LHG	C27-C26-C25	-2.01	104.20	114.37
26	c	514	BCR	C37-C22-C21	-2.01	119.56	122.82
24	C	512	CLA	CMA-C3A-C2A	-2.01	106.21	113.98
24	B	608	CLA	CED-O2D-CGD	-2.01	111.36	115.92
24	A	604	CLA	C7-C6-C5	-2.01	107.91	113.26
29	c	522	LMG	C30-C29-C28	-2.01	106.34	113.69
24	c	510	CLA	C9-C8-C7	-2.01	104.12	111.27
26	K	101	BCR	C8-C7-C6	-2.01	121.64	127.00
29	b	621	LMG	C22-C21-C20	-2.01	104.23	114.37
33	j	101	STE	O2-C1-O1	-2.01	118.17	123.33
32	h	101	DGD	O6D-C1D-O3G	-2.01	105.31	110.04
32	C	518	DGD	O6D-C5D-C4D	-2.00	106.09	109.70
32	A	618	DGD	C8B-C7B-C6B	-2.00	104.25	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	618	LMG	O6-C1-O1	-2.00	105.31	110.04
26	c	515	BCR	C21-C20-C19	-2.00	117.40	123.20
26	k	101	BCR	C4-C5-C6	2.00	125.41	122.70
24	B	613	CLA	CAC-C3C-C4C	2.00	127.39	124.79

All (2) chirality outliers are listed below:

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

All (1749) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	601	CLA	C1A-C2A-CAA-CBA
24	B	601	CLA	CAD-CBD-CGD-O1D
24	B	601	CLA	CAD-CBD-CGD-O2D
24	B	603	CLA	C4-C3-C5-C6
24	B	606	CLA	C2B-C3B-CAB-CBB
24	B	606	CLA	C4B-C3B-CAB-CBB
24	B	614	CLA	CAD-CBD-CGD-O1D
24	B	614	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	C11-C10-C8-C9
24	b	605	CLA	C4B-C3B-CAB-CBB
24	b	614	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	c	512	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C35-C13-C14-C15
26	C	514	BCR	C11-C12-C13-C35
26	C	515	BCR	C11-C12-C13-C14
26	D	404	BCR	C21-C22-C23-C24
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	K	101	BCR	C37-C22-C23-C24
26	T	101	BCR	C11-C12-C13-C35
26	Y	101	BCR	C5-C6-C7-C8
26	b	617	BCR	C21-C22-C23-C24
26	c	514	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
26	d	405	BCR	C37-C22-C23-C24
26	k	101	BCR	C5-C6-C7-C8
28	A	612	PL9	C12-C13-C14-C15
28	A	612	PL9	C12-C13-C14-C16
28	A	612	PL9	C22-C23-C24-C26
28	A	612	PL9	C37-C38-C39-C40
28	A	612	PL9	C37-C38-C39-C41
28	A	612	PL9	C40-C39-C41-C42
28	D	405	PL9	C32-C33-C34-C36
28	D	405	PL9	C37-C38-C39-C40
28	a	611	PL9	C12-C13-C14-C15
28	a	611	PL9	C17-C18-C19-C21
28	a	611	PL9	C20-C19-C21-C22
28	a	611	PL9	C22-C23-C24-C25
28	a	611	PL9	C22-C23-C24-C26
28	a	611	PL9	C25-C24-C26-C27
28	d	406	PL9	C32-C33-C34-C36
28	d	406	PL9	C38-C39-C41-C42
28	d	406	PL9	C42-C43-C44-C45
29	A	614	LMG	O9-C10-O7-C8
29	D	409	LMG	O1-C7-C8-C9
29	D	409	LMG	O1-C7-C8-O7
29	b	623	LMG	C11-C10-O7-C8
29	c	522	LMG	O6-C1-O1-C7
30	A	615	LHG	C3-O3-P-O6
30	B	621	LHG	C4-O6-P-O3
30	B	621	LHG	C4-O6-P-O5
30	D	408	LHG	O1-C1-C2-C3
30	D	408	LHG	C1-C2-C3-O3
30	D	408	LHG	O2-C2-C3-O3
30	D	408	LHG	C3-O3-P-O5
30	D	408	LHG	C3-O3-P-O6
30	D	408	LHG	C4-O6-P-O3
30	D	408	LHG	C4-O6-P-O4
30	E	101	LHG	O1-C1-C2-C3
30	E	101	LHG	O10-C23-O8-C6
30	E	101	LHG	C24-C23-O8-C6
30	d	407	LHG	C3-O3-P-O4
30	d	407	LHG	C3-O3-P-O6
30	d	408	LHG	O1-C1-C2-C3
30	d	408	LHG	C3-O3-P-O4
30	d	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C4-O6-P-O3
30	d	408	LHG	C4-O6-P-O4
30	d	409	LHG	C4-O6-P-O4
30	e	102	LHG	C1-C2-C3-O3
30	e	102	LHG	C3-O3-P-O5
30	e	102	LHG	C3-O3-P-O6
30	e	102	LHG	C4-O6-P-O5
30	e	102	LHG	O6-C4-C5-O7
30	e	102	LHG	O10-C23-O8-C6
30	e	102	LHG	C24-C23-O8-C6
30	l	101	LHG	C4-O6-P-O3
31	A	617	SQD	C46-C45-O47-C7
31	B	623	SQD	O5-C1-O6-C44
31	B	623	SQD	O6-C44-C45-O47
31	B	623	SQD	O49-C7-O47-C45
31	D	407	SQD	O5-C1-O6-C44
31	D	407	SQD	O10-C23-O48-C46
31	a	613	SQD	O6-C44-C45-O47
31	a	614	SQD	O6-C44-C45-C46
31	a	614	SQD	O6-C44-C45-O47
31	a	614	SQD	C8-C7-O47-C45
31	a	614	SQD	O10-C23-O48-C46
31	a	614	SQD	C24-C23-O48-C46
31	f	101	SQD	C2-C1-O6-C44
31	f	101	SQD	O5-C1-O6-C44
32	A	618	DGD	C2B-C1B-O2G-C2G
32	A	618	DGD	O1B-C1B-O2G-C2G
36	V	201	HEC	C2C-C3C-CAC-CBC
24	c	513	CLA	CBD-CGD-O2D-CED
29	c	522	LMG	O10-C28-O8-C9
24	B	614	CLA	C15-C16-C17-C18
31	D	407	SQD	C24-C23-O48-C46
31	f	101	SQD	C24-C23-O48-C46
29	M	101	LMG	O10-C28-O8-C9
29	c	521	LMG	O10-C28-O8-C9
31	f	101	SQD	O10-C23-O48-C46
29	D	409	LMG	O9-C10-O7-C8
29	b	623	LMG	O9-C10-O7-C8
31	a	614	SQD	O49-C7-O47-C45
24	B	614	CLA	C3-C5-C6-C7
29	c	522	LMG	C29-C28-O8-C9
31	b	620	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
24	C	509	CLA	CBD-CGD-O2D-CED
29	A	614	LMG	C11-C10-O7-C8
29	a	618	LMG	C11-C10-O7-C8
31	B	623	SQD	C8-C7-O47-C45
31	b	620	SQD	O10-C23-O48-C46
24	A	608	CLA	C4-C3-C5-C6
24	B	614	CLA	C4-C3-C5-C6
24	C	504	CLA	C4-C3-C5-C6
24	b	603	CLA	C4-C3-C5-C6
24	b	605	CLA	C4-C3-C5-C6
24	c	507	CLA	C4-C3-C5-C6
28	a	611	PL9	C35-C34-C36-C37
28	d	406	PL9	C40-C39-C41-C42
24	A	608	CLA	C2-C3-C5-C6
24	B	603	CLA	C2-C3-C5-C6
24	B	614	CLA	C2-C3-C5-C6
24	C	504	CLA	C2-C3-C5-C6
24	C	507	CLA	C2-C3-C5-C6
24	b	603	CLA	C2-C3-C5-C6
28	A	612	PL9	C43-C44-C46-C47
28	D	405	PL9	C33-C34-C36-C37
28	a	611	PL9	C23-C24-C26-C27
24	b	601	CLA	C3-C5-C6-C7
24	b	602	CLA	C3-C5-C6-C7
24	d	404	CLA	C3-C5-C6-C7
24	B	616	CLA	CBA-CGA-O2A-C1
29	c	521	LMG	C29-C28-O8-C9
28	A	612	PL9	C22-C23-C24-C25
28	d	406	PL9	C32-C33-C34-C35
28	a	611	PL9	C42-C43-C44-C46
31	B	623	SQD	O10-C23-O48-C46
28	A	612	PL9	C47-C48-C49-C51
30	e	102	LHG	O2-C2-C3-O3
24	c	513	CLA	O1D-CGD-O2D-CED
24	B	601	CLA	CBA-CGA-O2A-C1
24	C	511	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	C11-C10-O7-C8
29	D	409	LMG	C11-C10-O7-C8
32	A	618	DGD	O6E-C5E-C6E-O5E
29	A	614	LMG	O6-C5-C6-O5
29	M	101	LMG	C29-C28-O8-C9
24	C	507	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C2-C3-C5-C6
24	b	614	CLA	C2-C3-C5-C6
24	c	507	CLA	C2-C3-C5-C6
28	A	612	PL9	C23-C24-C26-C27
33	T	102	STE	C5-C6-C7-C8
28	A	612	PL9	C9-C11-C12-C13
28	A	612	PL9	C34-C36-C37-C38
28	a	611	PL9	C19-C21-C22-C23
28	a	611	PL9	C24-C26-C27-C28
28	a	611	PL9	C34-C36-C37-C38
32	A	618	DGD	C4E-C5E-C6E-O5E
24	C	501	CLA	CBD-CGD-O2D-CED
24	B	616	CLA	O1A-CGA-O2A-C1
31	B	623	SQD	C24-C23-O48-C46
29	a	618	LMG	O6-C5-C6-O5
28	D	405	PL9	C27-C28-C29-C30
24	B	601	CLA	O1A-CGA-O2A-C1
36	V	201	HEC	C4C-C3C-CAC-CBC
24	c	508	CLA	CBD-CGD-O2D-CED
28	d	406	PL9	C47-C48-C49-C51
30	d	409	LHG	C30-C31-C32-C33
24	c	506	CLA	CBA-CGA-O2A-C1
24	B	612	CLA	CBD-CGD-O2D-CED
30	d	409	LHG	C24-C25-C26-C27
24	b	614	CLA	C4-C3-C5-C6
28	a	611	PL9	C33-C34-C36-C37
24	A	605	CLA	C14-C13-C15-C16
24	B	610	CLA	C14-C13-C15-C16
24	B	613	CLA	C11-C12-C13-C14
24	B	614	CLA	C6-C7-C8-C9
24	B	614	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C9
24	C	512	CLA	C11-C10-C8-C9
24	D	403	CLA	C11-C12-C13-C14
24	b	601	CLA	C14-C13-C15-C16
24	b	602	CLA	C11-C10-C8-C9
24	b	613	CLA	C11-C12-C13-C14
24	b	616	CLA	C11-C10-C8-C9
24	c	509	CLA	C6-C7-C8-C9
24	c	509	CLA	C11-C12-C13-C14
24	c	512	CLA	C6-C7-C8-C9
24	d	404	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	A	614	LMG	C4-C5-C6-O5
29	a	618	LMG	C4-C5-C6-O5
26	C	515	BCR	C36-C18-C19-C20
26	H	101	BCR	C11-C12-C13-C35
26	K	101	BCR	C36-C18-C19-C20
26	T	101	BCR	C7-C8-C9-C34
26	Y	101	BCR	C37-C22-C23-C24
26	b	619	BCR	C11-C12-C13-C35
26	b	619	BCR	C37-C22-C23-C24
26	k	101	BCR	C7-C8-C9-C34
26	k	102	BCR	C37-C22-C23-C24
26	t	101	BCR	C7-C8-C9-C34
26	t	101	BCR	C11-C12-C13-C35
26	x	101	BCR	C7-C8-C9-C34
28	A	612	PL9	C47-C48-C49-C50
24	C	509	CLA	O1D-CGD-O2D-CED
33	B	627	STE	C1-C2-C3-C4
33	C	522	STE	C4-C5-C6-C7
24	B	611	CLA	C13-C15-C16-C17
24	C	513	CLA	C15-C16-C17-C18
28	A	612	PL9	C32-C33-C34-C36
24	B	611	CLA	C12-C13-C15-C16
24	b	613	CLA	C11-C10-C8-C7
24	C	510	CLA	C15-C16-C17-C18
28	A	612	PL9	C44-C46-C47-C48
33	D	411	STE	C11-C12-C13-C14
24	c	503	CLA	C8-C10-C11-C12
32	C	518	DGD	C8A-C9A-CAA-CBA
31	B	623	SQD	C45-C46-O48-C23
29	b	623	LMG	C28-C29-C30-C31
29	d	410	LMG	C10-C11-C12-C13
30	E	101	LHG	C23-C24-C25-C26
30	d	407	LHG	C23-C24-C25-C26
30	d	409	LHG	C23-C24-C25-C26
32	c	518	DGD	C1A-C2A-C3A-C4A
33	C	520	STE	C1-C2-C3-C4
33	E	102	STE	C1-C2-C3-C4
29	c	521	LMG	C11-C10-O7-C8
24	B	605	CLA	C15-C16-C17-C18
24	B	613	CLA	C8-C10-C11-C12
24	D	402	CLA	C15-C16-C17-C18
24	c	512	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	b	606	CLA	C2A-CAA-CBA-CGA
26	c	514	BCR	C18-C19-C20-C21
24	B	609	CLA	C13-C15-C16-C17
24	B	614	CLA	C13-C15-C16-C17
24	a	606	CLA	C10-C11-C12-C13
24	a	606	CLA	C15-C16-C17-C18
29	D	406	LMG	C10-C11-C12-C13
29	D	409	LMG	C28-C29-C30-C31
30	B	622	LHG	C23-C24-C25-C26
30	d	407	LHG	C7-C8-C9-C10
33	d	412	STE	C7-C8-C9-C10
24	A	604	CLA	C15-C16-C17-C18
24	B	601	CLA	C5-C6-C7-C8
24	B	602	CLA	C13-C15-C16-C17
24	B	606	CLA	C15-C16-C17-C18
24	B	616	CLA	C5-C6-C7-C8
24	C	503	CLA	C5-C6-C7-C8
24	C	506	CLA	C8-C10-C11-C12
24	C	510	CLA	C10-C11-C12-C13
24	b	611	CLA	C15-C16-C17-C18
24	b	614	CLA	C5-C6-C7-C8
24	c	505	CLA	C5-C6-C7-C8
24	c	509	CLA	C13-C15-C16-C17
24	c	511	CLA	C15-C16-C17-C18
30	d	407	LHG	O2-C2-C3-O3
24	c	506	CLA	O1A-CGA-O2A-C1
29	c	519	LMG	C28-C29-C30-C31
33	b	624	STE	C1-C2-C3-C4
24	B	612	CLA	C13-C15-C16-C17
24	C	508	CLA	C15-C16-C17-C18
24	b	615	CLA	C10-C11-C12-C13
24	C	506	CLA	C15-C16-C17-C18
24	b	607	CLA	C10-C11-C12-C13
24	c	511	CLA	CBD-CGD-O2D-CED
29	c	521	LMG	C10-C11-C12-C13
24	C	512	CLA	C13-C15-C16-C17
24	b	611	CLA	C13-C15-C16-C17
24	c	509	CLA	C10-C11-C12-C13
24	c	511	CLA	C13-C15-C16-C17
24	c	512	CLA	C8-C10-C11-C12
29	a	618	LMG	C29-C28-O8-C9
29	b	621	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	C13-C15-C16-C17
26	c	514	BCR	C13-C14-C15-C16
32	c	518	DGD	O1A-C1A-O1G-C1G
31	B	623	SQD	C29-C30-C31-C32
36	v	201	HEC	C2C-C3C-CAC-CBC
29	M	101	LMG	O9-C10-O7-C8
30	e	102	LHG	O9-C7-O7-C5
30	d	407	LHG	C1-C2-C3-O3
31	D	407	SQD	C44-C45-C46-O48
24	C	513	CLA	CBA-CGA-O2A-C1
24	C	509	CLA	C10-C11-C12-C13
24	C	512	CLA	C10-C11-C12-C13
24	D	403	CLA	C10-C11-C12-C13
24	b	611	CLA	C8-C10-C11-C12
24	b	615	CLA	C15-C16-C17-C18
24	c	506	CLA	C15-C16-C17-C18
29	d	410	LMG	C28-C29-C30-C31
30	e	102	LHG	C7-C8-C9-C10
24	C	509	CLA	C13-C15-C16-C17
24	b	601	CLA	C8-C10-C11-C12
24	c	503	CLA	C5-C6-C7-C8
24	b	607	CLA	C8-C10-C11-C12
31	b	620	SQD	C8-C7-O47-C45
29	c	522	LMG	C2-C1-O1-C7
31	B	623	SQD	C2-C1-O6-C44
32	C	517	DGD	C2E-C1E-O5D-C6D
32	c	517	DGD	C2E-C1E-O5D-C6D
24	a	606	CLA	C5-C6-C7-C8
24	B	606	CLA	C16-C17-C18-C19
26	A	609	BCR	C11-C10-C9-C34
26	A	609	BCR	C35-C13-C14-C15
26	A	609	BCR	C20-C21-C22-C37
26	B	617	BCR	C11-C10-C9-C34
26	D	404	BCR	C20-C21-C22-C37
26	K	101	BCR	C11-C10-C9-C34
26	b	617	BCR	C20-C21-C22-C37
26	b	618	BCR	C16-C17-C18-C36
26	c	514	BCR	C16-C17-C18-C36
26	k	101	BCR	C35-C13-C14-C15
26	t	101	BCR	C35-C13-C14-C15
26	t	101	BCR	C20-C21-C22-C37
32	c	516	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
26	A	609	BCR	C36-C18-C19-C20
26	A	609	BCR	C37-C22-C23-C24
26	B	619	BCR	C11-C12-C13-C35
26	B	619	BCR	C37-C22-C23-C24
26	C	515	BCR	C11-C12-C13-C35
26	b	618	BCR	C37-C22-C23-C24
26	C	514	BCR	C11-C12-C13-C14
26	T	101	BCR	C7-C8-C9-C10
26	Y	101	BCR	C21-C22-C23-C24
24	B	606	CLA	C2A-CAA-CBA-CGA
24	c	512	CLA	C2A-CAA-CBA-CGA
24	b	614	CLA	C8-C10-C11-C12
30	d	407	LHG	O1-C1-C2-C3
30	d	409	LHG	O1-C1-C2-C3
24	B	614	CLA	C16-C17-C18-C20
24	D	403	CLA	C16-C17-C18-C19
24	a	604	CLA	C16-C17-C18-C19
24	c	504	CLA	C11-C12-C13-C14
24	c	511	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C19
24	d	403	CLA	C16-C17-C18-C20
24	b	603	CLA	C13-C15-C16-C17
26	B	618	BCR	C20-C21-C22-C23
26	B	619	BCR	C11-C10-C9-C8
26	B	619	BCR	C12-C13-C14-C15
26	C	514	BCR	C11-C10-C9-C8
26	K	101	BCR	C11-C10-C9-C8
26	K	101	BCR	C20-C21-C22-C23
26	T	101	BCR	C12-C13-C14-C15
26	b	617	BCR	C20-C21-C22-C23
26	b	618	BCR	C20-C21-C22-C23
26	c	514	BCR	C20-C21-C22-C23
26	k	101	BCR	C11-C10-C9-C8
26	k	102	BCR	C11-C10-C9-C8
26	x	101	BCR	C11-C10-C9-C8
26	x	101	BCR	C12-C13-C14-C15
26	x	101	BCR	C16-C17-C18-C19
32	C	517	DGD	O6E-C1E-O5D-C6D
32	c	517	DGD	O6E-C1E-O5D-C6D
29	c	522	LMG	C11-C10-O7-C8
29	b	621	LMG	C29-C28-O8-C9
24	B	611	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	C	511	CLA	O1D-CGD-O2D-CED
24	B	615	CLA	C16-C17-C18-C20
24	c	510	CLA	C16-C17-C18-C19
24	c	511	CLA	C16-C17-C18-C20
24	C	505	CLA	C10-C11-C12-C13
29	c	521	LMG	C33-C34-C35-C36
30	E	101	LHG	C9-C10-C11-C12
33	C	520	STE	C6-C7-C8-C9
26	C	514	BCR	C14-C15-C16-C17
30	A	615	LHG	C11-C12-C13-C14
30	D	408	LHG	C30-C31-C32-C33
32	c	516	DGD	C7A-C8A-C9A-CAA
32	h	101	DGD	C5B-C6B-C7B-C8B
33	B	620	STE	C4-C5-C6-C7
33	T	102	STE	C7-C8-C9-C10
33	t	102	STE	C2-C3-C4-C5
29	a	618	LMG	C12-C13-C14-C15
29	c	519	LMG	C33-C34-C35-C36
33	b	627	STE	C11-C12-C13-C14
33	l	102	STE	C14-C15-C16-C17
29	a	618	LMG	O10-C28-O8-C9
29	A	614	LMG	C14-C15-C16-C17
29	D	410	LMG	C14-C15-C16-C17
29	M	101	LMG	C36-C37-C38-C39
29	c	521	LMG	C40-C41-C42-C43
29	c	522	LMG	C12-C13-C14-C15
29	d	410	LMG	C36-C37-C38-C39
30	A	615	LHG	C12-C13-C14-C15
30	B	621	LHG	C31-C32-C33-C34
30	E	101	LHG	C27-C28-C29-C30
30	d	407	LHG	C10-C11-C12-C13
31	a	614	SQD	C12-C13-C14-C15
32	C	518	DGD	C9A-CAA-CBA-CCA
32	c	517	DGD	CAB-CBB-CCB-CDB
33	B	626	STE	C4-C5-C6-C7
33	T	103	STE	C13-C14-C15-C16
33	x	102	STE	C11-C12-C13-C14
29	c	521	LMG	O9-C10-O7-C8
30	D	408	LHG	O1-C1-C2-O2
30	E	101	LHG	O1-C1-C2-O2
30	d	407	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
29	A	614	LMG	C13-C14-C15-C16
29	b	621	LMG	C32-C33-C34-C35
29	d	410	LMG	C33-C34-C35-C36
30	B	621	LHG	C17-C18-C19-C20
30	E	101	LHG	C28-C29-C30-C31
32	h	101	DGD	C9A-CAA-CBA-CCA
33	d	412	STE	C14-C15-C16-C17
24	C	501	CLA	O1D-CGD-O2D-CED
24	B	601	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C4B-C3B-CAB-CBB
32	c	516	DGD	C1B-C2B-C3B-C4B
33	m	101	STE	C1-C2-C3-C4
33	x	102	STE	C1-C2-C3-C4
32	c	517	DGD	CCA-CDA-CEA-CFA
24	a	604	CLA	C16-C17-C18-C20
24	b	601	CLA	C16-C17-C18-C20
24	b	607	CLA	C16-C17-C18-C20
29	c	521	LMG	C30-C31-C32-C33
30	d	408	LHG	C32-C33-C34-C35
31	a	614	SQD	C10-C11-C12-C13
32	c	517	DGD	CBB-CCB-CDB-CEB
33	b	627	STE	C9-C10-C11-C12
33	t	102	STE	C5-C6-C7-C8
24	b	607	CLA	C5-C6-C7-C8
24	c	506	CLA	C8-C10-C11-C12
30	E	101	LHG	C24-C25-C26-C27
33	T	102	STE	C6-C7-C8-C9
30	A	615	LHG	C32-C33-C34-C35
29	A	614	LMG	C28-C29-C30-C31
24	C	505	CLA	C5-C6-C7-C8
29	d	410	LMG	O6-C5-C6-O5
29	b	621	LMG	C14-C15-C16-C17
29	c	519	LMG	C39-C40-C41-C42
31	a	613	SQD	C25-C26-C27-C28
33	b	624	STE	C10-C11-C12-C13
33	b	625	STE	C4-C5-C6-C7
24	c	512	CLA	C3A-C2A-CAA-CBA
29	a	618	LMG	C36-C37-C38-C39
29	c	521	LMG	C39-C40-C41-C42
32	H	102	DGD	CCB-CDB-CEB-CFB
33	B	624	STE	C6-C7-C8-C9
33	b	622	STE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	k	103	STE	C6-C7-C8-C9
33	H	103	STE	C11-C12-C13-C14
33	M	102	STE	C11-C10-C9-C8
24	b	613	CLA	C13-C15-C16-C17
24	d	401	CLA	C8-C10-C11-C12
29	b	623	LMG	C10-C11-C12-C13
24	B	606	CLA	C16-C17-C18-C20
24	B	607	CLA	C16-C17-C18-C20
24	B	614	CLA	C16-C17-C18-C19
29	A	614	LMG	C38-C39-C40-C41
29	M	101	LMG	C29-C30-C31-C32
31	B	623	SQD	C33-C34-C35-C36
31	a	613	SQD	C24-C25-C26-C27
29	b	623	LMG	C11-C12-C13-C14
30	E	101	LHG	C33-C34-C35-C36
31	B	623	SQD	C11-C12-C13-C14
31	f	101	SQD	C29-C30-C31-C32
24	B	612	CLA	O1D-CGD-O2D-CED
29	d	410	LMG	C32-C33-C34-C35
31	A	617	SQD	C12-C13-C14-C15
31	a	613	SQD	C34-C35-C36-C37
32	C	516	DGD	C3B-C4B-C5B-C6B
32	H	102	DGD	C8B-C9B-CAB-CBB
32	c	516	DGD	C4B-C5B-C6B-C7B
33	D	411	STE	C2-C3-C4-C5
33	b	627	STE	C7-C8-C9-C10
29	M	101	LMG	C28-C29-C30-C31
29	A	614	LMG	C11-C12-C13-C14
29	A	614	LMG	C35-C36-C37-C38
29	c	521	LMG	C41-C42-C43-C44
30	B	621	LHG	C12-C13-C14-C15
32	H	102	DGD	C6B-C7B-C8B-C9B
32	c	516	DGD	C3A-C4A-C5A-C6A
32	c	517	DGD	C7B-C8B-C9B-CAB
33	T	103	STE	C5-C6-C7-C8
33	k	103	STE	C2-C3-C4-C5
24	C	513	CLA	O1A-CGA-O2A-C1
29	D	410	LMG	C29-C30-C31-C32
31	A	616	SQD	C30-C31-C32-C33
32	h	101	DGD	C6B-C7B-C8B-C9B
33	H	103	STE	C13-C14-C15-C16
29	b	621	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	b	623	LMG	C13-C14-C15-C16
30	A	615	LHG	C29-C30-C31-C32
32	h	101	DGD	O6E-C5E-C6E-O5E
29	A	614	LMG	C17-C18-C19-C20
29	c	519	LMG	C38-C39-C40-C41
30	l	101	LHG	C29-C30-C31-C32
32	A	618	DGD	C5B-C6B-C7B-C8B
32	C	516	DGD	C5B-C6B-C7B-C8B
33	C	521	STE	C7-C8-C9-C10
33	d	411	STE	C4-C5-C6-C7
24	C	509	CLA	C16-C17-C18-C19
30	B	622	LHG	C7-C8-C9-C10
24	B	601	CLA	C2B-C3B-CAB-CBB
24	b	605	CLA	C2B-C3B-CAB-CBB
26	Y	101	BCR	C1-C6-C7-C8
26	k	101	BCR	C1-C6-C7-C8
29	b	621	LMG	C18-C19-C20-C21
30	d	409	LHG	C26-C27-C28-C29
29	M	101	LMG	C11-C10-O7-C8
30	e	102	LHG	C8-C7-O7-C5
24	C	512	CLA	C3-C5-C6-C7
29	c	521	LMG	C16-C17-C18-C19
32	C	517	DGD	C7B-C8B-C9B-CAB
32	c	517	DGD	C6A-C7A-C8A-C9A
33	c	520	STE	C2-C3-C4-C5
24	c	508	CLA	O1D-CGD-O2D-CED
29	D	410	LMG	C30-C31-C32-C33
29	c	521	LMG	C31-C32-C33-C34
31	A	617	SQD	C10-C11-C12-C13
32	C	516	DGD	C8A-C9A-CAA-CBA
29	D	410	LMG	C28-C29-C30-C31
32	c	517	DGD	C1B-C2B-C3B-C4B
29	b	623	LMG	C37-C38-C39-C40
30	d	409	LHG	C32-C33-C34-C35
31	A	616	SQD	C9-C10-C11-C12
31	B	623	SQD	C34-C35-C36-C37
33	a	617	STE	C10-C11-C12-C13
30	B	622	LHG	C29-C30-C31-C32
30	e	102	LHG	C26-C27-C28-C29
32	C	516	DGD	CCB-CDB-CEB-CFB
33	a	617	STE	C5-C6-C7-C8
29	D	410	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	a	613	SQD	C29-C30-C31-C32
32	C	517	DGD	C5A-C6A-C7A-C8A
26	B	619	BCR	C10-C11-C12-C13
24	B	612	CLA	C10-C11-C12-C13
28	A	612	PL9	C18-C19-C21-C22
29	a	618	LMG	C13-C14-C15-C16
29	b	621	LMG	C17-C18-C19-C20
31	b	620	SQD	C25-C26-C27-C28
33	H	103	STE	C2-C3-C4-C5
33	j	101	STE	C4-C5-C6-C7
33	x	102	STE	C6-C7-C8-C9
31	a	613	SQD	C24-C23-O48-C46
24	B	606	CLA	C11-C12-C13-C14
24	C	503	CLA	C11-C10-C8-C9
24	b	607	CLA	C11-C10-C8-C9
24	c	511	CLA	C14-C13-C15-C16
25	A	607	PHO	C6-C7-C8-C9
29	M	101	LMG	C17-C18-C19-C20
30	d	407	LHG	C30-C31-C32-C33
32	c	516	DGD	C5B-C6B-C7B-C8B
33	B	620	STE	C11-C12-C13-C14
24	B	603	CLA	C8-C10-C11-C12
30	A	615	LHG	C27-C28-C29-C30
30	l	101	LHG	C14-C15-C16-C17
26	b	617	BCR	C14-C15-C16-C17
29	b	623	LMG	C21-C22-C23-C24
29	d	410	LMG	C30-C31-C32-C33
30	D	408	LHG	C11-C12-C13-C14
33	J	101	STE	C5-C6-C7-C8
33	c	520	STE	C9-C10-C11-C12
31	D	407	SQD	C2-C1-O6-C44
24	C	510	CLA	CBD-CGD-O2D-CED
29	A	614	LMG	C31-C32-C33-C34
30	D	408	LHG	C34-C35-C36-C37
30	d	408	LHG	C33-C34-C35-C36
32	C	517	DGD	CAB-CBB-CCB-CDB
33	B	626	STE	C14-C15-C16-C17
33	b	625	STE	C5-C6-C7-C8
33	d	412	STE	C9-C10-C11-C12
29	D	406	LMG	C17-C18-C19-C20
30	B	622	LHG	C27-C28-C29-C30
32	c	516	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
32	c	518	DGD	C3A-C4A-C5A-C6A
33	x	102	STE	C3-C4-C5-C6
29	C	519	LMG	C32-C33-C34-C35
29	b	623	LMG	C41-C42-C43-C44
32	A	618	DGD	C4B-C5B-C6B-C7B
32	C	517	DGD	C9A-CAA-CBA-CCA
32	H	102	DGD	C5B-C6B-C7B-C8B
33	B	626	STE	C5-C6-C7-C8
24	D	403	CLA	C16-C17-C18-C20
32	A	618	DGD	C2A-C3A-C4A-C5A
33	H	103	STE	C10-C11-C12-C13
30	B	621	LHG	C14-C15-C16-C17
30	e	102	LHG	C13-C14-C15-C16
24	b	602	CLA	C8-C10-C11-C12
31	f	101	SQD	O49-C7-O47-C45
29	D	406	LMG	C32-C33-C34-C35
29	c	519	LMG	C36-C37-C38-C39
30	B	622	LHG	C14-C15-C16-C17
30	d	407	LHG	C25-C26-C27-C28
33	T	103	STE	C14-C15-C16-C17
29	C	519	LMG	C15-C16-C17-C18
30	A	615	LHG	C9-C10-C11-C12
31	D	407	SQD	C31-C32-C33-C34
26	k	101	BCR	C37-C22-C23-C24
30	d	408	LHG	C29-C30-C31-C32
29	a	618	LMG	C8-C7-O1-C1
30	D	408	LHG	C25-C26-C27-C28
32	h	101	DGD	CCA-CDA-CEA-CFA
33	d	411	STE	C10-C11-C12-C13
24	b	616	CLA	C11-C12-C13-C14
24	b	616	CLA	C11-C12-C13-C15
24	c	510	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C20
29	A	614	LMG	C16-C17-C18-C19
29	A	614	LMG	C36-C37-C38-C39
29	b	623	LMG	C23-C24-C25-C26
29	c	522	LMG	C15-C16-C17-C18
30	e	102	LHG	C16-C17-C18-C19
33	a	617	STE	C12-C13-C14-C15
29	M	101	LMG	C11-C12-C13-C14
31	D	407	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	a	613	SQD	C17-C18-C19-C20
33	B	620	STE	C9-C10-C11-C12
33	C	522	STE	C6-C7-C8-C9
33	b	625	STE	C7-C8-C9-C10
32	h	101	DGD	C2B-C3B-C4B-C5B
30	B	621	LHG	C29-C30-C31-C32
24	A	613	CLA	C13-C15-C16-C17
29	b	621	LMG	C12-C13-C14-C15
31	a	614	SQD	C11-C12-C13-C14
33	d	411	STE	C11-C12-C13-C14
29	b	621	LMG	O9-C10-O7-C8
29	b	623	LMG	O6-C5-C6-O5
29	c	521	LMG	C14-C15-C16-C17
29	c	522	LMG	C33-C34-C35-C36
32	H	102	DGD	C7A-C8A-C9A-CAA
24	b	609	CLA	CBD-CGD-O2D-CED
24	A	613	CLA	C15-C16-C17-C18
24	C	509	CLA	C16-C17-C18-C20
30	e	102	LHG	C11-C10-C9-C8
33	B	627	STE	C5-C6-C7-C8
29	A	614	LMG	C33-C34-C35-C36
32	c	518	DGD	C8B-C9B-CAB-CBB
24	C	513	CLA	C5-C6-C7-C8
24	b	604	CLA	C5-C6-C7-C8
29	M	101	LMG	C14-C15-C16-C17
29	c	522	LMG	C30-C31-C32-C33
31	B	623	SQD	C28-C29-C30-C31
33	E	102	STE	C3-C4-C5-C6
29	D	406	LMG	O6-C5-C6-O5
31	A	616	SQD	O6-C44-C45-O47
32	A	618	DGD	O2G-C2G-C3G-O3G
29	c	522	LMG	C37-C38-C39-C40
33	t	102	STE	C7-C8-C9-C10
33	t	102	STE	C11-C12-C13-C14
29	D	409	LMG	C31-C32-C33-C34
30	A	615	LHG	C30-C31-C32-C33
33	t	102	STE	C4-C5-C6-C7
24	b	607	CLA	C16-C17-C18-C19
24	c	507	CLA	C5-C6-C7-C8
29	D	409	LMG	C14-C15-C16-C17
30	e	102	LHG	C27-C28-C29-C30
33	T	103	STE	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	B	624	STE	C11-C10-C9-C8
24	B	605	CLA	C3-C5-C6-C7
24	B	616	CLA	C3-C5-C6-C7
29	b	623	LMG	C16-C17-C18-C19
29	c	522	LMG	C17-C18-C19-C20
30	e	102	LHG	C18-C19-C20-C21
32	C	517	DGD	C4A-C5A-C6A-C7A
32	h	101	DGD	C3B-C4B-C5B-C6B
33	T	103	STE	C6-C7-C8-C9
28	a	611	PL9	C42-C43-C44-C45
30	d	408	LHG	C28-C29-C30-C31
32	A	618	DGD	C5A-C6A-C7A-C8A
33	b	622	STE	C7-C8-C9-C10
32	H	102	DGD	C7B-C8B-C9B-CAB
32	A	618	DGD	CAA-CBA-CCA-CDA
29	C	519	LMG	C16-C17-C18-C19
30	l	101	LHG	C27-C28-C29-C30
29	b	623	LMG	O10-C28-O8-C9
29	a	618	LMG	C35-C36-C37-C38
24	c	513	CLA	C1A-C2A-CAA-CBA
32	C	517	DGD	CBA-CCA-CDA-CEA
32	h	101	DGD	C7A-C8A-C9A-CAA
33	D	411	STE	C5-C6-C7-C8
29	b	621	LMG	C16-C17-C18-C19
29	b	621	LMG	C30-C31-C32-C33
30	B	622	LHG	C28-C29-C30-C31
33	b	622	STE	C5-C6-C7-C8
30	B	621	LHG	O6-C4-C5-C6
32	C	516	DGD	O6E-C5E-C6E-O5E
29	C	519	LMG	O9-C10-O7-C8
29	c	522	LMG	O9-C10-O7-C8
30	B	621	LHG	C27-C28-C29-C30
32	A	618	DGD	CEB-CFB-CGB-CHB
32	C	518	DGD	CBA-CCA-CDA-CEA
32	c	517	DGD	C7A-C8A-C9A-CAA
33	b	627	STE	C10-C11-C12-C13
24	A	605	CLA	C11-C12-C13-C15
24	B	603	CLA	C12-C13-C15-C16
24	C	507	CLA	C11-C10-C8-C7
24	C	510	CLA	C12-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C10
24	c	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	c	513	CLA	C11-C12-C13-C15
24	d	401	CLA	C11-C10-C8-C7
24	d	404	CLA	C11-C12-C13-C15
24	d	404	CLA	C12-C13-C15-C16
30	E	101	LHG	C11-C12-C13-C14
24	B	616	CLA	C11-C12-C13-C15
24	b	615	CLA	C16-C17-C18-C19
24	B	608	CLA	C15-C16-C17-C18
24	C	509	CLA	C5-C6-C7-C8
32	c	517	DGD	C1A-C2A-C3A-C4A
28	D	405	PL9	C45-C44-C46-C47
24	c	505	CLA	C2-C3-C5-C6
24	A	605	CLA	C11-C12-C13-C14
24	B	604	CLA	C11-C12-C13-C14
24	C	510	CLA	C14-C13-C15-C16
24	b	604	CLA	C14-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C14
24	b	609	CLA	C14-C13-C15-C16
24	c	506	CLA	C6-C7-C8-C9
24	c	506	CLA	C11-C12-C13-C14
24	d	404	CLA	C14-C13-C15-C16
29	D	409	LMG	C15-C16-C17-C18
29	D	409	LMG	C16-C17-C18-C19
30	B	621	LHG	C34-C35-C36-C37
29	D	406	LMG	C30-C31-C32-C33
33	B	625	STE	C3-C4-C5-C6
24	c	512	CLA	CBA-CGA-O2A-C1
28	a	611	PL9	C17-C18-C19-C20
33	E	102	STE	C4-C5-C6-C7
29	a	618	LMG	O9-C10-O7-C8
24	B	605	CLA	C8-C10-C11-C12
24	b	615	CLA	C5-C6-C7-C8
31	A	617	SQD	C9-C10-C11-C12
29	M	101	LMG	C7-C8-C9-O8
29	c	521	LMG	O1-C7-C8-C9
29	c	522	LMG	O1-C7-C8-C9
31	A	616	SQD	O6-C44-C45-C46
31	B	623	SQD	O6-C44-C45-C46
31	b	620	SQD	C44-C45-C46-O48
32	A	618	DGD	C1G-C2G-C3G-O3G
29	C	519	LMG	C17-C18-C19-C20
30	E	101	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	E	101	LHG	C32-C33-C34-C35
32	C	517	DGD	C6A-C7A-C8A-C9A
32	c	516	DGD	CBB-CCB-CDB-CEB
29	c	521	LMG	C11-C12-C13-C14
24	b	609	CLA	C15-C16-C17-C18
30	D	408	LHG	C28-C29-C30-C31
32	C	518	DGD	CAB-CBB-CCB-CDB
32	c	516	DGD	O6E-C5E-C6E-O5E
24	B	607	CLA	C16-C17-C18-C19
24	B	613	CLA	C16-C17-C18-C20
31	b	620	SQD	C27-C28-C29-C30
33	d	412	STE	C12-C13-C14-C15
30	D	408	LHG	C17-C18-C19-C20
32	c	517	DGD	C8B-C9B-CAB-CBB
33	T	102	STE	C9-C10-C11-C12
29	D	406	LMG	C34-C35-C36-C37
32	C	518	DGD	C5A-C6A-C7A-C8A
26	D	404	BCR	C11-C10-C9-C34
24	b	601	CLA	C13-C15-C16-C17
31	B	623	SQD	C35-C36-C37-C38
33	B	620	STE	C2-C3-C4-C5
33	b	622	STE	C10-C11-C12-C13
30	d	407	LHG	C14-C15-C16-C17
24	C	505	CLA	C4-C3-C5-C6
24	c	505	CLA	C4-C3-C5-C6
24	C	505	CLA	C2-C3-C5-C6
28	a	611	PL9	C38-C39-C41-C42
24	D	402	CLA	C10-C11-C12-C13
24	b	614	CLA	C15-C16-C17-C18
26	k	101	BCR	C36-C18-C19-C20
33	T	103	STE	C11-C12-C13-C14
33	a	617	STE	C11-C12-C13-C14
24	b	601	CLA	C10-C11-C12-C13
29	b	623	LMG	C32-C33-C34-C35
30	A	615	LHG	C25-C26-C27-C28
32	C	516	DGD	C3A-C4A-C5A-C6A
33	d	412	STE	C2-C3-C4-C5
29	C	519	LMG	C30-C31-C32-C33
31	B	623	SQD	C9-C10-C11-C12
30	B	621	LHG	C7-C8-C9-C10
31	a	613	SQD	C23-C24-C25-C26
29	a	618	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
32	c	516	DGD	C6B-C7B-C8B-C9B
24	C	513	CLA	O2A-C1-C2-C3
29	a	618	LMG	C9-C8-O7-C10
29	M	101	LMG	C31-C32-C33-C34
32	C	516	DGD	O6D-C5D-C6D-O5D
24	C	506	CLA	C13-C15-C16-C17
24	C	509	CLA	C8-C10-C11-C12
31	a	613	SQD	C18-C19-C20-C21
32	A	618	DGD	C9B-CAB-CBB-CCB
32	C	517	DGD	C9B-CAB-CBB-CCB
33	B	627	STE	C2-C3-C4-C5
26	T	101	BCR	C13-C14-C15-C16
24	C	507	CLA	C16-C17-C18-C20
32	C	516	DGD	C8B-C9B-CAB-CBB
33	M	102	STE	C9-C10-C11-C12
26	a	607	BCR	C12-C13-C14-C15
26	c	514	BCR	C16-C17-C18-C19
24	d	404	CLA	C13-C15-C16-C17
29	b	621	LMG	C37-C38-C39-C40
33	C	522	STE	C5-C6-C7-C8
31	D	407	SQD	C30-C31-C32-C33
33	b	622	STE	C13-C14-C15-C16
31	a	614	SQD	C31-C32-C33-C34
29	b	621	LMG	C39-C40-C41-C42
31	A	616	SQD	C16-C17-C18-C19
33	C	521	STE	C4-C5-C6-C7
24	B	610	CLA	C15-C16-C17-C18
30	B	622	LHG	C19-C20-C21-C22
32	C	518	DGD	CDA-CEA-CFA-CGA
29	b	621	LMG	C11-C12-C13-C14
31	A	617	SQD	C16-C17-C18-C19
32	A	618	DGD	C2B-C3B-C4B-C5B
33	B	626	STE	C6-C7-C8-C9
29	A	614	LMG	C34-C35-C36-C37
29	c	521	LMG	C34-C35-C36-C37
29	c	521	LMG	C38-C39-C40-C41
33	d	411	STE	C5-C6-C7-C8
29	a	618	LMG	C33-C34-C35-C36
29	c	522	LMG	C31-C32-C33-C34
30	d	408	LHG	C12-C13-C14-C15
33	J	101	STE	C6-C7-C8-C9
33	Z	101	STE	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
33	a	615	STE	C5-C6-C7-C8
31	a	613	SQD	O47-C45-C46-O48
30	E	101	LHG	O2-C2-C3-O3
30	B	621	LHG	C30-C31-C32-C33
30	B	622	LHG	C18-C19-C20-C21
33	b	626	STE	C4-C5-C6-C7
29	b	621	LMG	C22-C23-C24-C25
30	l	101	LHG	C13-C14-C15-C16
32	c	516	DGD	C3B-C4B-C5B-C6B
33	m	101	STE	C7-C8-C9-C10
31	B	623	SQD	C13-C14-C15-C16
32	C	518	DGD	CCA-CDA-CEA-CFA
33	a	615	STE	C2-C3-C4-C5
31	A	616	SQD	C17-C18-C19-C20
32	c	516	DGD	O6D-C5D-C6D-O5D
24	C	507	CLA	C10-C11-C12-C13
33	b	625	STE	C3-C4-C5-C6
24	b	601	CLA	C16-C17-C18-C19
32	C	517	DGD	CDB-CEB-CFB-CGB
33	B	625	STE	C7-C8-C9-C10
24	b	609	CLA	O1D-CGD-O2D-CED
24	c	512	CLA	O1A-CGA-O2A-C1
30	E	101	LHG	C19-C20-C21-C22
33	C	521	STE	C3-C4-C5-C6
31	D	407	SQD	C27-C28-C29-C30
31	a	613	SQD	C27-C28-C29-C30
32	C	516	DGD	C2A-C3A-C4A-C5A
33	d	412	STE	C6-C7-C8-C9
29	C	519	LMG	C29-C28-O8-C9
29	a	618	LMG	C16-C17-C18-C19
29	c	519	LMG	C31-C32-C33-C34
32	c	518	DGD	C4B-C5B-C6B-C7B
32	c	518	DGD	C5B-C6B-C7B-C8B
32	H	102	DGD	CDB-CEB-CFB-CGB
31	b	620	SQD	C11-C12-C13-C14
32	h	101	DGD	CBA-CCA-CDA-CEA
24	C	512	CLA	C8-C10-C11-C12
32	c	516	DGD	O1A-C1A-O1G-C1G
29	b	621	LMG	C38-C39-C40-C41
30	d	407	LHG	C28-C29-C30-C31
24	B	604	CLA	C2C-C3C-CAC-CBC
32	C	517	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
24	c	510	CLA	C8-C10-C11-C12
24	B	616	CLA	C11-C12-C13-C14
28	d	406	PL9	C45-C44-C46-C47
29	A	614	LMG	C40-C41-C42-C43
29	c	522	LMG	C8-C9-O8-C28
29	C	519	LMG	C31-C32-C33-C34
29	D	406	LMG	C21-C22-C23-C24
29	D	409	LMG	C34-C35-C36-C37
29	b	623	LMG	C42-C43-C44-C45
30	e	102	LHG	C28-C29-C30-C31
33	T	102	STE	C15-C16-C17-C18
30	d	407	LHG	C15-C16-C17-C18
32	C	518	DGD	C8B-C9B-CAB-CBB
33	d	412	STE	C5-C6-C7-C8
36	V	201	HEC	C2B-C3B-CAB-CBB
29	a	618	LMG	C34-C35-C36-C37
30	D	408	LHG	C33-C34-C35-C36
32	C	516	DGD	C9B-CAB-CBB-CCB
33	b	624	STE	C6-C7-C8-C9
30	d	409	LHG	O1-C1-C2-O2
31	D	407	SQD	C45-C44-O6-C1
24	A	613	CLA	C14-C13-C15-C16
24	B	603	CLA	C14-C13-C15-C16
24	C	509	CLA	C11-C12-C13-C14
24	D	402	CLA	C11-C10-C8-C9
24	b	606	CLA	C14-C13-C15-C16
24	b	607	CLA	C6-C7-C8-C9
24	b	607	CLA	C14-C13-C15-C16
24	b	615	CLA	C11-C10-C8-C9
24	c	510	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C12-C13-C14
24	d	401	CLA	C11-C10-C8-C9
24	d	401	CLA	C14-C13-C15-C16
24	d	404	CLA	C11-C12-C13-C14
24	b	612	CLA	C10-C11-C12-C13
24	c	504	CLA	C5-C6-C7-C8
24	B	605	CLA	C4B-C3B-CAB-CBB
24	d	401	CLA	C4B-C3B-CAB-CBB
29	b	623	LMG	C22-C23-C24-C25
33	b	625	STE	C11-C10-C9-C8
24	C	510	CLA	O1D-CGD-O2D-CED
29	c	519	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C16-C17-C18-C19
24	b	615	CLA	C16-C17-C18-C20
29	a	618	LMG	C17-C18-C19-C20
29	D	406	LMG	C38-C39-C40-C41
31	A	617	SQD	C14-C15-C16-C17
33	C	520	STE	C2-C3-C4-C5
33	I	101	STE	C4-C5-C6-C7
33	Z	101	STE	C13-C14-C15-C16
24	C	509	CLA	C3-C5-C6-C7
31	a	614	SQD	C19-C20-C21-C22
31	b	620	SQD	C19-C20-C21-C22
30	e	102	LHG	O6-C4-C5-C6
29	b	623	LMG	C18-C19-C20-C21
30	B	622	LHG	C25-C26-C27-C28
32	H	102	DGD	CCA-CDA-CEA-CFA
29	D	406	LMG	C14-C15-C16-C17
24	B	604	CLA	C11-C12-C13-C15
24	B	613	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C12-C13-C15
24	C	512	CLA	C12-C13-C15-C16
24	b	601	CLA	C12-C13-C15-C16
24	b	604	CLA	C12-C13-C15-C16
24	b	607	CLA	C11-C12-C13-C15
24	b	614	CLA	C12-C13-C15-C16
24	b	615	CLA	C11-C10-C8-C7
24	c	505	CLA	C6-C7-C8-C10
24	c	506	CLA	C6-C7-C8-C10
24	c	506	CLA	C11-C12-C13-C15
24	c	509	CLA	C6-C7-C8-C10
24	c	512	CLA	C12-C13-C15-C16
24	d	401	CLA	C12-C13-C15-C16
24	C	512	CLA	C15-C16-C17-C18
24	b	604	CLA	C13-C15-C16-C17
31	D	407	SQD	O6-C44-C45-C46
29	A	614	LMG	C30-C31-C32-C33
32	h	101	DGD	C5A-C6A-C7A-C8A
30	d	408	LHG	O9-C7-O7-C5
32	c	517	DGD	C5B-C6B-C7B-C8B
32	h	101	DGD	CAB-CBB-CCB-CDB
30	E	101	LHG	C29-C30-C31-C32
31	a	613	SQD	C28-C29-C30-C31
28	a	611	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
29	c	519	LMG	C4-C5-C6-O5
24	D	403	CLA	C5-C6-C7-C8
32	C	516	DGD	C4D-C5D-C6D-O5D
30	e	102	LHG	C10-C11-C12-C13
33	M	102	STE	C4-C5-C6-C7
24	a	606	CLA	CBA-CGA-O2A-C1
26	T	101	BCR	C9-C10-C11-C12
32	C	516	DGD	CDA-CEA-CFA-CGA
33	T	102	STE	C3-C4-C5-C6
29	M	101	LMG	C39-C40-C41-C42
29	a	618	LMG	C23-C24-C25-C26
33	l	102	STE	C2-C3-C4-C5
26	k	101	BCR	C17-C18-C19-C20
29	b	621	LMG	C20-C21-C22-C23
32	C	516	DGD	CBA-CCA-CDA-CEA
30	E	101	LHG	C4-C5-C6-O8
31	a	613	SQD	O6-C44-C45-C46
31	a	613	SQD	C44-C45-C46-O48
32	A	618	DGD	O1G-C1G-C2G-C3G
32	c	516	DGD	O1G-C1G-C2G-C3G
29	M	101	LMG	C38-C39-C40-C41
30	D	408	LHG	C11-C10-C9-C8
33	E	102	STE	C6-C7-C8-C9
30	e	102	LHG	C14-C15-C16-C17
32	c	517	DGD	C9B-CAB-CBB-CCB
32	C	517	DGD	CDA-CEA-CFA-CGA
24	A	605	CLA	C16-C17-C18-C19
29	C	519	LMG	C12-C13-C14-C15
32	C	517	DGD	C3A-C4A-C5A-C6A
33	b	622	STE	C4-C5-C6-C7
33	b	624	STE	C11-C10-C9-C8
33	T	103	STE	C7-C8-C9-C10
28	a	611	PL9	C40-C39-C41-C42
33	j	101	STE	C1-C2-C3-C4
33	j	101	STE	C2-C3-C4-C5
24	c	511	CLA	O1D-CGD-O2D-CED
31	A	617	SQD	C31-C32-C33-C34
31	a	614	SQD	C17-C18-C19-C20
24	B	604	CLA	C16-C17-C18-C20
30	B	621	LHG	O9-C7-O7-C5
24	d	401	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	k	102	BCR	C1-C6-C7-C8
32	c	517	DGD	C5A-C6A-C7A-C8A
31	a	613	SQD	C11-C10-C9-C8
33	b	625	STE	C6-C7-C8-C9
24	B	613	CLA	C10-C11-C12-C13
33	l	102	STE	C1-C2-C3-C4
30	d	407	LHG	C32-C33-C34-C35
32	C	518	DGD	C3A-C4A-C5A-C6A
31	A	616	SQD	C24-C25-C26-C27
33	d	412	STE	C4-C5-C6-C7
24	c	504	CLA	C11-C12-C13-C15
29	c	521	LMG	O1-C7-C8-O7
29	c	521	LMG	O7-C8-C9-O8
29	c	522	LMG	O1-C7-C8-O7
31	b	620	SQD	O6-C44-C45-O47
29	b	623	LMG	C24-C25-C26-C27
28	a	611	PL9	C4-C3-C7-C8
30	l	101	LHG	C32-C33-C34-C35
29	M	101	LMG	C40-C41-C42-C43
30	A	615	LHG	C11-C10-C9-C8
33	D	411	STE	C12-C13-C14-C15
26	c	514	BCR	C10-C11-C12-C13
24	B	602	CLA	C8-C10-C11-C12
30	B	621	LHG	C10-C11-C12-C13
32	C	518	DGD	C3B-C4B-C5B-C6B
29	D	406	LMG	C39-C40-C41-C42
30	A	615	LHG	C33-C34-C35-C36
24	b	616	CLA	O1D-CGD-O2D-CED
24	B	604	CLA	C14-C13-C15-C16
24	B	613	CLA	C14-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16
24	C	508	CLA	C11-C10-C8-C9
24	c	512	CLA	C14-C13-C15-C16
30	B	621	LHG	C11-C12-C13-C14
26	A	609	BCR	C14-C15-C16-C17
29	d	410	LMG	C38-C39-C40-C41
33	H	103	STE	C9-C10-C11-C12
30	D	408	LHG	C29-C30-C31-C32
33	l	102	STE	C7-C8-C9-C10
24	c	513	CLA	C13-C15-C16-C17
36	v	201	HEC	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	D	409	LMG	C11-C12-C13-C14
30	A	615	LHG	C34-C35-C36-C37
30	D	408	LHG	C10-C11-C12-C13
31	A	616	SQD	C11-C12-C13-C14
29	c	519	LMG	C30-C31-C32-C33
32	C	518	DGD	O1A-C1A-O1G-C1G
33	d	412	STE	C1-C2-C3-C4
32	A	618	DGD	CCB-CDB-CEB-CFB
26	c	514	BCR	C15-C16-C17-C18
24	B	615	CLA	C16-C17-C18-C19
32	A	618	DGD	CDB-CEB-CFB-CGB
30	d	407	LHG	C16-C17-C18-C19
30	d	408	LHG	C26-C27-C28-C29
33	x	102	STE	C2-C3-C4-C5
33	b	625	STE	C10-C11-C12-C13
24	b	616	CLA	C8-C10-C11-C12
29	a	618	LMG	C29-C30-C31-C32
26	C	514	BCR	C16-C17-C18-C36
26	k	101	BCR	C11-C10-C9-C34
26	x	101	BCR	C16-C17-C18-C36
33	H	103	STE	C1-C2-C3-C4
24	c	509	CLA	CAA-CBA-CGA-O2A
29	D	409	LMG	C33-C34-C35-C36
32	A	618	DGD	CFA-CGA-CHA-CIA
24	B	610	CLA	C16-C17-C18-C19
29	a	618	LMG	C32-C33-C34-C35
33	T	103	STE	C12-C13-C14-C15
33	d	412	STE	C11-C10-C9-C8
33	t	102	STE	C10-C11-C12-C13
24	B	604	CLA	C12-C13-C15-C16
24	B	605	CLA	C11-C10-C8-C7
24	B	613	CLA	C11-C12-C13-C15
24	B	614	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C12-C13-C15
24	C	505	CLA	C6-C7-C8-C10
24	C	508	CLA	C11-C10-C8-C7
24	C	510	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C10-C8-C7
24	b	602	CLA	C11-C10-C8-C7
24	b	609	CLA	C12-C13-C15-C16
24	b	616	CLA	C11-C10-C8-C7
24	c	512	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
33	J	101	STE	C1-C2-C3-C4
33	c	520	STE	C4-C5-C6-C7
29	a	618	LMG	C19-C20-C21-C22
29	a	618	LMG	C21-C22-C23-C24
29	d	410	LMG	C14-C15-C16-C17
32	C	517	DGD	C8B-C9B-CAB-CBB
33	d	411	STE	C7-C8-C9-C10
24	b	616	CLA	CBD-CGD-O2D-CED
33	M	103	STE	C1-C2-C3-C4
26	K	101	BCR	C17-C18-C19-C20
26	k	101	BCR	C21-C22-C23-C24
32	C	517	DGD	C2G-C3G-O3G-C1D
32	C	517	DGD	C5D-C6D-O5D-C1E
32	c	517	DGD	C5D-C6D-O5D-C1E
29	b	623	LMG	C34-C35-C36-C37
31	A	617	SQD	C11-C12-C13-C14
33	H	103	STE	C12-C13-C14-C15
30	B	621	LHG	C18-C19-C20-C21
33	D	411	STE	C6-C7-C8-C9
29	D	410	LMG	C34-C35-C36-C37
24	c	512	CLA	C4-C3-C5-C6
28	A	612	PL9	C25-C24-C26-C27
29	D	410	LMG	C37-C38-C39-C40
30	d	408	LHG	C11-C12-C13-C14
30	d	409	LHG	C35-C36-C37-C38
33	d	411	STE	C12-C13-C14-C15
33	b	627	STE	C5-C6-C7-C8
29	b	623	LMG	C19-C20-C21-C22
24	b	606	CLA	C8-C10-C11-C12
29	c	522	LMG	C9-C8-O7-C10
32	C	517	DGD	O1A-C1A-O1G-C1G
30	E	101	LHG	C31-C32-C33-C34
31	b	620	SQD	C12-C13-C14-C15
30	l	101	LHG	C19-C20-C21-C22
30	D	408	LHG	C32-C33-C34-C35
33	D	411	STE	C9-C10-C11-C12
24	b	604	CLA	C3-C5-C6-C7
33	a	616	STE	C5-C6-C7-C8
33	C	520	STE	C3-C4-C5-C6
28	D	405	PL9	C47-C48-C49-C51
30	l	101	LHG	O6-C4-C5-O7
29	D	406	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	A	615	LHG	C17-C18-C19-C20
28	d	406	PL9	C34-C36-C37-C38
29	c	521	LMG	C7-C8-C9-O8
35	e	101	HEM	C4B-C3B-CAB-CBB
24	B	611	CLA	C16-C17-C18-C20
24	B	613	CLA	C16-C17-C18-C19
33	C	521	STE	C10-C11-C12-C13
33	I	101	STE	C11-C10-C9-C8
33	a	617	STE	C7-C8-C9-C10
33	T	102	STE	C10-C11-C12-C13
24	C	506	CLA	C4-C3-C5-C6
28	D	405	PL9	C43-C44-C46-C47
29	M	101	LMG	C12-C13-C14-C15
33	C	521	STE	C11-C10-C9-C8
32	C	517	DGD	CBB-CCB-CDB-CEB
33	B	626	STE	C9-C10-C11-C12
24	B	606	CLA	C8-C10-C11-C12
31	a	614	SQD	C24-C25-C26-C27
31	a	614	SQD	O47-C45-C46-O48
32	A	618	DGD	O1G-C1G-C2G-O2G
32	c	516	DGD	O1G-C1G-C2G-O2G
32	c	516	DGD	C4D-C5D-C6D-O5D
24	B	605	CLA	C11-C10-C8-C9
24	C	505	CLA	C6-C7-C8-C9
24	b	609	CLA	C6-C7-C8-C9
24	c	512	CLA	C11-C12-C13-C14
24	d	401	CLA	C6-C7-C8-C9
24	B	610	CLA	C16-C17-C18-C20
32	C	516	DGD	C7A-C8A-C9A-CAA
33	b	622	STE	C3-C4-C5-C6
32	c	516	DGD	O1G-C1A-C2A-C3A
29	b	621	LMG	C31-C32-C33-C34
30	B	622	LHG	C9-C10-C11-C12
30	B	622	LHG	C32-C33-C34-C35
31	f	101	SQD	C33-C34-C35-C36
24	a	604	CLA	C15-C16-C17-C18
29	a	618	LMG	C22-C23-C24-C25
29	b	623	LMG	C12-C13-C14-C15
24	c	509	CLA	C15-C16-C17-C18
24	B	609	CLA	C16-C17-C18-C19
24	c	506	CLA	C16-C17-C18-C20
24	B	612	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	b	623	LMG	C20-C21-C22-C23
33	l	102	STE	C4-C5-C6-C7
28	D	405	PL9	C35-C34-C36-C37
24	d	403	CLA	C3-C5-C6-C7
24	C	506	CLA	C2-C3-C5-C6
33	a	617	STE	C13-C14-C15-C16
32	A	618	DGD	CBA-CCA-CDA-CEA
33	I	101	STE	C7-C8-C9-C10
24	c	505	CLA	C15-C16-C17-C18
33	l	102	STE	C10-C11-C12-C13
31	D	407	SQD	C29-C30-C31-C32
33	D	411	STE	C11-C10-C9-C8
28	A	612	PL9	C39-C41-C42-C43
29	D	406	LMG	C37-C38-C39-C40
32	H	102	DGD	C5A-C6A-C7A-C8A
32	c	516	DGD	CBA-CCA-CDA-CEA
24	C	504	CLA	C4B-C3B-CAB-CBB
24	C	508	CLA	C1A-C2A-CAA-CBA
24	b	601	CLA	C4B-C3B-CAB-CBB
24	c	511	CLA	C1A-C2A-CAA-CBA
26	C	514	BCR	C9-C10-C11-C12
33	I	101	STE	C2-C3-C4-C5
30	d	409	LHG	C29-C30-C31-C32
33	H	103	STE	C14-C15-C16-C17
30	l	101	LHG	O6-C4-C5-C6
31	D	407	SQD	C33-C34-C35-C36
31	A	617	SQD	O49-C7-O47-C45
31	A	616	SQD	C14-C15-C16-C17
33	T	103	STE	C9-C10-C11-C12
33	b	624	STE	C11-C12-C13-C14
33	a	615	STE	C4-C5-C6-C7
24	A	605	CLA	C11-C10-C8-C7
24	A	605	CLA	C12-C13-C15-C16
24	B	615	CLA	C6-C7-C8-C10
24	B	616	CLA	C6-C7-C8-C10
24	C	506	CLA	C12-C13-C15-C16
24	C	509	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C10-C8-C7
24	D	403	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C10-C8-C7
24	c	512	CLA	C6-C7-C8-C10
24	d	404	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	B	604	CLA	C16-C17-C18-C19
24	d	404	CLA	C16-C17-C18-C19
32	H	102	DGD	CBA-CCA-CDA-CEA
32	c	516	DGD	C6A-C7A-C8A-C9A
33	a	617	STE	C3-C4-C5-C6
32	A	618	DGD	CEA-CFA-CGA-CHA
24	c	503	CLA	CBA-CGA-O2A-C1
29	C	519	LMG	C37-C38-C39-C40
30	d	407	LHG	C29-C30-C31-C32
33	C	521	STE	C12-C13-C14-C15
31	B	623	SQD	C18-C19-C20-C21
31	a	614	SQD	C13-C14-C15-C16
30	d	409	LHG	C27-C28-C29-C30
32	H	102	DGD	C2B-C3B-C4B-C5B
24	B	615	CLA	C5-C6-C7-C8
24	b	616	CLA	C10-C11-C12-C13
29	M	101	LMG	C13-C14-C15-C16
33	b	625	STE	C14-C15-C16-C17
32	C	518	DGD	O6D-C5D-C6D-O5D
24	C	510	CLA	C11-C10-C8-C9
24	c	508	CLA	C11-C12-C13-C14
29	a	618	LMG	C37-C38-C39-C40
29	a	618	LMG	C41-C42-C43-C44
29	c	519	LMG	C35-C36-C37-C38
29	M	101	LMG	C35-C36-C37-C38
30	d	408	LHG	C31-C32-C33-C34
24	A	605	CLA	C15-C16-C17-C18
24	c	510	CLA	C15-C16-C17-C18
30	E	101	LHG	O7-C5-C6-O8
33	t	102	STE	C13-C14-C15-C16
32	c	518	DGD	C5A-C6A-C7A-C8A
29	a	618	LMG	O1-C7-C8-C9
31	a	614	SQD	C44-C45-C46-O48
24	B	607	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	b	609	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
29	b	621	LMG	C4-C5-C6-O5
24	a	606	CLA	O1A-CGA-O2A-C1
33	J	101	STE	C3-C4-C5-C6
24	d	404	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
24	b	604	CLA	C8-C10-C11-C12
33	b	625	STE	C11-C12-C13-C14
30	A	615	LHG	C14-C15-C16-C17
24	B	607	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	CHA-CBD-CGD-O1D
24	b	616	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
26	C	514	BCR	C13-C14-C15-C16
26	d	405	BCR	C20-C21-C22-C37
30	A	615	LHG	C3-O3-P-O5
30	B	622	LHG	C3-O3-P-O4
30	D	408	LHG	C3-O3-P-O4
30	D	408	LHG	C4-O6-P-O5
30	d	407	LHG	C3-O3-P-O5
30	d	408	LHG	C4-O6-P-O5
30	e	102	LHG	C4-O6-P-O3
30	l	101	LHG	C4-O6-P-O5
29	b	623	LMG	C17-C18-C19-C20
24	b	601	CLA	C2B-C3B-CAB-CBB
26	d	405	BCR	C23-C24-C25-C30
32	C	518	DGD	C4B-C5B-C6B-C7B
28	A	612	PL9	C38-C39-C41-C42
26	B	617	BCR	C11-C12-C13-C35
29	b	621	LMG	O6-C5-C6-O5
30	d	409	LHG	C9-C10-C11-C12
33	b	624	STE	C3-C4-C5-C6
33	c	520	STE	C3-C4-C5-C6
33	D	411	STE	C1-C2-C3-C4
28	A	612	PL9	C4-C3-C7-C8
24	A	605	CLA	C16-C17-C18-C20
29	b	621	LMG	C28-C29-C30-C31
30	d	409	LHG	C25-C26-C27-C28
24	c	503	CLA	O1A-CGA-O2A-C1
24	C	507	CLA	C5-C6-C7-C8
33	b	625	STE	C12-C13-C14-C15
29	D	409	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
31	B	623	SQD	C46-C45-O47-C7
31	b	620	SQD	C46-C45-O47-C7
32	C	518	DGD	C9B-CAB-CBB-CCB
32	C	516	DGD	O1G-C1A-C2A-C3A
24	C	511	CLA	C8-C10-C11-C12
24	c	511	CLA	C8-C10-C11-C12
24	c	512	CLA	C2-C3-C5-C6
30	D	408	LHG	C23-C24-C25-C26
29	D	410	LMG	C13-C14-C15-C16
31	A	616	SQD	C29-C30-C31-C32
33	l	102	STE	C15-C16-C17-C18
24	B	605	CLA	C6-C7-C8-C9
24	C	512	CLA	C14-C13-C15-C16
24	b	614	CLA	C14-C13-C15-C16
24	c	504	CLA	C11-C10-C8-C9
30	B	621	LHG	C13-C14-C15-C16
33	C	521	STE	C11-C12-C13-C14
24	B	615	CLA	C12-C13-C15-C16
24	D	402	CLA	C12-C13-C15-C16
24	b	612	CLA	C11-C10-C8-C7
24	b	615	CLA	C11-C12-C13-C15
24	c	504	CLA	C11-C10-C8-C7
24	d	401	CLA	C6-C7-C8-C10
33	b	624	STE	C5-C6-C7-C8
26	B	617	BCR	C12-C13-C14-C15
26	C	514	BCR	C12-C13-C14-C15
26	H	101	BCR	C12-C13-C14-C15
29	C	519	LMG	C13-C14-C15-C16
30	B	621	LHG	O6-C4-C5-O7
24	b	611	CLA	C16-C17-C18-C19
36	V	201	HEC	C4B-C3B-CAB-CBB
32	h	101	DGD	O2G-C1B-C2B-C3B
29	b	621	LMG	C19-C20-C21-C22
24	b	606	CLA	C15-C16-C17-C18
30	e	102	LHG	C12-C13-C14-C15
32	c	518	DGD	C2A-C1A-O1G-C1G
24	c	505	CLA	C16-C17-C18-C20
32	C	518	DGD	C2A-C3A-C4A-C5A
33	x	102	STE	C10-C11-C12-C13
29	M	101	LMG	O7-C8-C9-O8
29	a	618	LMG	O1-C7-C8-O7
31	b	620	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
32	H	102	DGD	O2G-C1B-C2B-C3B
30	e	102	LHG	C11-C12-C13-C14
30	l	101	LHG	C23-C24-C25-C26
24	B	609	CLA	C16-C17-C18-C20
24	c	506	CLA	C16-C17-C18-C19
31	a	613	SQD	C8-C7-O47-C45
33	d	412	STE	C13-C14-C15-C16
24	c	506	CLA	C2-C1-O2A-CGA
29	C	519	LMG	O1-C7-C8-C9
32	A	618	DGD	CBB-CCB-CDB-CEB
30	A	615	LHG	C24-C25-C26-C27
26	c	515	BCR	C21-C22-C23-C24
28	a	611	PL9	C21-C22-C23-C24
32	c	516	DGD	C5D-C6D-O5D-C1E
31	f	101	SQD	C32-C33-C34-C35
30	e	102	LHG	C24-C25-C26-C27
33	c	520	STE	C1-C2-C3-C4
29	c	522	LMG	C36-C37-C38-C39
30	B	621	LHG	C32-C33-C34-C35
33	B	626	STE	C7-C8-C9-C10
24	B	616	CLA	C6-C7-C8-C9
24	b	601	CLA	C11-C12-C13-C14
24	c	505	CLA	C6-C7-C8-C9
24	c	505	CLA	C11-C10-C8-C9
24	c	507	CLA	C11-C10-C8-C9
32	c	518	DGD	C8A-C9A-CAA-CBA
24	C	505	CLA	C15-C16-C17-C18
29	d	410	LMG	C15-C16-C17-C18
30	l	101	LHG	C12-C13-C14-C15
24	b	610	CLA	C4B-C3B-CAB-CBB
33	k	103	STE	C1-C2-C3-C4
30	d	408	LHG	C19-C20-C21-C22
24	d	401	CLA	C16-C17-C18-C20
33	T	102	STE	C12-C13-C14-C15
29	D	409	LMG	C29-C28-O8-C9
24	a	612	CLA	C2C-C3C-CAC-CBC
24	a	612	CLA	C4C-C3C-CAC-CBC
29	c	522	LMG	C34-C35-C36-C37
31	A	616	SQD	C26-C27-C28-C29
29	C	519	LMG	C18-C19-C20-C21
29	b	623	LMG	C31-C32-C33-C34
24	C	508	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	b	603	CLA	C6-C7-C8-C10
24	b	614	CLA	C11-C12-C13-C15
24	c	505	CLA	C11-C10-C8-C7
32	C	516	DGD	O1A-C1A-O1G-C1G
32	H	102	DGD	C9A-CAA-CBA-CCA
33	D	411	STE	C4-C5-C6-C7
24	B	611	CLA	C16-C17-C18-C19
31	a	613	SQD	C10-C11-C12-C13
24	B	601	CLA	C3A-C2A-CAA-CBA
30	B	621	LHG	C24-C25-C26-C27
29	a	618	LMG	O8-C28-C29-C30
29	c	521	LMG	C42-C43-C44-C45
31	b	620	SQD	C30-C31-C32-C33
24	B	613	CLA	C2-C1-O2A-CGA
24	d	403	CLA	C2-C1-O2A-CGA
30	l	101	LHG	C17-C18-C19-C20
33	b	624	STE	C9-C10-C11-C12
30	A	615	LHG	C2-C3-O3-P
33	b	626	STE	C7-C8-C9-C10
31	a	613	SQD	C19-C20-C21-C22
31	a	614	SQD	C30-C31-C32-C33
28	d	406	PL9	C43-C44-C46-C47
32	h	101	DGD	CDB-CEB-CFB-CGB
32	H	102	DGD	C4E-C5E-C6E-O5E
30	E	101	LHG	C1-C2-C3-O3
30	l	101	LHG	C4-C5-C6-O8
32	A	618	DGD	C6A-C7A-C8A-C9A
32	c	516	DGD	CDB-CEB-CFB-CGB
24	A	604	CLA	C14-C13-C15-C16
24	A	605	CLA	C6-C7-C8-C9
24	A	605	CLA	C11-C10-C8-C9
24	B	606	CLA	C11-C10-C8-C9
24	C	507	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C12-C13-C14
24	b	605	CLA	C11-C10-C8-C9
24	c	507	CLA	C14-C13-C15-C16
24	c	511	CLA	C11-C10-C8-C9
29	M	101	LMG	C20-C21-C22-C23
24	c	505	CLA	C10-C11-C12-C13
33	b	626	STE	C1-C2-C3-C4
31	b	620	SQD	C11-C10-C9-C8
33	B	620	STE	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
25	a	605	PHO	O2A-C1-C2-C3
31	A	617	SQD	C17-C18-C19-C20
32	A	618	DGD	O6D-C5D-C6D-O5D
24	c	508	CLA	C4-C3-C5-C6
28	D	405	PL9	C40-C39-C41-C42
31	D	407	SQD	C23-C24-C25-C26
24	B	601	CLA	C16-C17-C18-C19
24	c	507	CLA	C15-C16-C17-C18
33	l	102	STE	C12-C13-C14-C15
36	v	201	HEC	CAD-CBD-CGD-O1D
29	M	101	LMG	C19-C20-C21-C22
24	c	508	CLA	C1A-C2A-CAA-CBA
26	B	617	BCR	C11-C10-C9-C8
33	M	102	STE	O1-C1-C2-C3
29	C	519	LMG	C28-C29-C30-C31
32	c	516	DGD	C5A-C6A-C7A-C8A
24	B	614	CLA	C8-C10-C11-C12
31	B	623	SQD	C10-C11-C12-C13
33	k	103	STE	C4-C5-C6-C7
24	B	605	CLA	C2B-C3B-CAB-CBB
24	B	615	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	B	617	BCR	C5-C6-C7-C8
26	H	101	BCR	C23-C24-C25-C26
26	H	101	BCR	C23-C24-C25-C30
26	K	101	BCR	C23-C24-C25-C30
26	T	101	BCR	C1-C6-C7-C8
26	b	617	BCR	C1-C6-C7-C8
26	b	617	BCR	C5-C6-C7-C8
26	k	102	BCR	C5-C6-C7-C8
26	k	102	BCR	C23-C24-C25-C30
26	t	101	BCR	C1-C6-C7-C8
26	x	101	BCR	C23-C24-C25-C30
33	b	622	STE	C1-C2-C3-C4
33	B	626	STE	C11-C12-C13-C14
24	a	612	CLA	CBA-CGA-O2A-C1
33	C	520	STE	C4-C5-C6-C7
35	F	101	HEM	CAD-CBD-CGD-O1D
36	v	201	HEC	CAD-CBD-CGD-O2D
24	b	609	CLA	C4-C3-C5-C6
33	a	616	STE	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C15-C16-C17-C18
29	D	410	LMG	O9-C10-C11-C12
33	b	624	STE	O1-C1-C2-C3
24	c	510	CLA	C10-C11-C12-C13
24	A	604	CLA	C12-C13-C15-C16
24	B	614	CLA	C6-C7-C8-C10
24	C	502	CLA	C12-C13-C15-C16
24	b	606	CLA	C11-C10-C8-C7
24	b	606	CLA	C11-C12-C13-C15
24	c	507	CLA	C11-C12-C13-C15
24	b	601	CLA	C2A-CAA-CBA-CGA
33	b	627	STE	C6-C7-C8-C9
33	B	627	STE	C3-C4-C5-C6
33	H	103	STE	C7-C8-C9-C10
33	b	625	STE	O1-C1-C2-C3
29	D	406	LMG	C20-C21-C22-C23
24	b	606	CLA	C10-C11-C12-C13
32	H	102	DGD	O6E-C5E-C6E-O5E
33	j	101	STE	C5-C6-C7-C8
35	e	101	HEM	CAD-CBD-CGD-O1D
24	C	510	CLA	C4-C3-C5-C6
24	a	606	CLA	C4-C3-C5-C6
28	A	612	PL9	C30-C29-C31-C32
28	A	612	PL9	C33-C34-C36-C37
30	e	102	LHG	C25-C26-C27-C28
26	k	101	BCR	C7-C8-C9-C10
30	B	621	LHG	C9-C10-C11-C12
29	A	614	LMG	C19-C20-C21-C22
31	a	614	SQD	C15-C16-C17-C18
24	B	602	CLA	C11-C12-C13-C14
33	c	520	STE	C10-C11-C12-C13
33	J	101	STE	C7-C8-C9-C10
31	b	620	SQD	C10-C11-C12-C13
32	C	518	DGD	C4A-C5A-C6A-C7A
31	a	613	SQD	C35-C36-C37-C38
33	D	411	STE	C15-C16-C17-C18
24	D	403	CLA	C13-C15-C16-C17
30	d	409	LHG	C2-C3-O3-P
25	d	402	PHO	C2C-C3C-CAC-CBC
24	B	605	CLA	C2-C3-C5-C6
24	d	401	CLA	C16-C17-C18-C19
36	V	201	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
32	C	517	DGD	C5B-C6B-C7B-C8B
24	c	508	CLA	C10-C11-C12-C13
33	C	520	STE	C5-C6-C7-C8
32	C	516	DGD	O1G-C1G-C2G-C3G
32	C	518	DGD	C2B-C3B-C4B-C5B
29	a	618	LMG	C24-C25-C26-C27
24	B	614	CLA	C2A-CAA-CBA-CGA
24	b	610	CLA	C2A-CAA-CBA-CGA
24	c	501	CLA	C2A-CAA-CBA-CGA
33	b	626	STE	C5-C6-C7-C8
33	M	102	STE	O2-C1-C2-C3
30	d	408	LHG	C14-C15-C16-C17
24	B	615	CLA	C4-C3-C5-C6
36	V	201	HEC	CAD-CBD-CGD-O1D
24	b	611	CLA	C16-C17-C18-C20
30	E	101	LHG	C10-C11-C12-C13
33	b	625	STE	O2-C1-C2-C3
35	e	101	HEM	CAD-CBD-CGD-O2D
31	A	616	SQD	C31-C32-C33-C34
30	B	622	LHG	C31-C32-C33-C34
26	Y	101	BCR	C16-C17-C18-C36
24	B	612	CLA	O1A-CGA-O2A-C1
35	F	101	HEM	CAD-CBD-CGD-O2D
33	B	625	STE	C6-C7-C8-C9
30	D	408	LHG	O6-C4-C5-C6
24	C	508	CLA	C16-C17-C18-C19
24	b	608	CLA	C4-C3-C5-C6
24	d	404	CLA	C10-C11-C12-C13
33	b	624	STE	O2-C1-C2-C3
28	d	406	PL9	C13-C14-C16-C17
24	d	401	CLA	C15-C16-C17-C18
26	c	515	BCR	C7-C8-C9-C34
24	A	605	CLA	C6-C7-C8-C10
24	c	509	CLA	C11-C12-C13-C15
32	c	518	DGD	O6D-C5D-C6D-O5D
33	T	103	STE	C15-C16-C17-C18
33	t	102	STE	O2-C1-C2-C3
29	D	406	LMG	C18-C19-C20-C21
33	D	411	STE	C13-C14-C15-C16
33	J	101	STE	O2-C1-C2-C3
24	B	615	CLA	C6-C7-C8-C9
24	C	506	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
24	b	603	CLA	C6-C7-C8-C9
24	b	612	CLA	C11-C10-C8-C9
24	c	502	CLA	C6-C7-C8-C9
24	a	612	CLA	O1A-CGA-O2A-C1
29	M	101	LMG	C8-C7-O1-C1
29	b	621	LMG	C8-C7-O1-C1
31	a	613	SQD	C5-C6-S-O8
24	B	601	CLA	C13-C15-C16-C17
24	b	614	CLA	C13-C15-C16-C17
24	D	402	CLA	C2-C1-O2A-CGA
24	B	602	CLA	C3A-C2A-CAA-CBA
29	D	410	LMG	C17-C18-C19-C20
31	b	620	SQD	C13-C14-C15-C16
28	A	612	PL9	C13-C14-C16-C17
32	C	517	DGD	C1B-C2B-C3B-C4B
33	B	625	STE	O2-C1-C2-C3
33	c	520	STE	O2-C1-C2-C3
24	b	612	CLA	C8-C10-C11-C12
30	B	621	LHG	C23-C24-C25-C26
26	d	405	BCR	C18-C19-C20-C21
32	h	101	DGD	CDA-CEA-CFA-CGA
32	c	518	DGD	C7B-C8B-C9B-CAB
30	A	615	LHG	C35-C36-C37-C38
30	B	621	LHG	C35-C36-C37-C38
33	c	520	STE	O1-C1-C2-C3
28	a	611	PL9	C47-C48-C49-C50
24	b	605	CLA	C10-C11-C12-C13
32	C	518	DGD	C1B-C2B-C3B-C4B
29	A	614	LMG	C7-C8-C9-O8
31	b	620	SQD	O6-C44-C45-C46
24	C	508	CLA	O1A-CGA-O2A-C1
24	b	601	CLA	O1A-CGA-O2A-C1
31	f	101	SQD	C24-C25-C26-C27
33	B	627	STE	C4-C5-C6-C7
33	l	102	STE	C9-C10-C11-C12
26	k	101	BCR	C19-C20-C21-C22
24	B	613	CLA	C5-C6-C7-C8
31	A	616	SQD	C25-C26-C27-C28
33	B	625	STE	O1-C1-C2-C3
33	t	102	STE	O1-C1-C2-C3
29	D	409	LMG	C37-C38-C39-C40
30	d	407	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
29	C	519	LMG	O1-C7-C8-O7
24	C	502	CLA	C14-C13-C15-C16
24	a	606	CLA	C11-C10-C8-C9
24	b	604	CLA	C11-C10-C8-C9
24	b	606	CLA	C11-C12-C13-C14
24	c	503	CLA	C11-C10-C8-C9
31	A	617	SQD	C32-C33-C34-C35
30	B	621	LHG	O7-C7-C8-C9
30	E	101	LHG	C26-C27-C28-C29
33	J	101	STE	O1-C1-C2-C3
24	B	603	CLA	C2A-CAA-CBA-CGA
24	B	610	CLA	C2A-CAA-CBA-CGA
24	B	602	CLA	C11-C12-C13-C15
24	B	613	CLA	C11-C10-C8-C7
24	C	512	CLA	C11-C12-C13-C15
24	a	606	CLA	C11-C10-C8-C7
24	b	601	CLA	C11-C12-C13-C15
24	b	603	CLA	C11-C10-C8-C7
24	c	511	CLA	C12-C13-C15-C16
29	D	410	LMG	C33-C34-C35-C36
24	C	509	CLA	C2B-C3B-CAB-CBB
24	b	610	CLA	C2B-C3B-CAB-CBB
26	A	609	BCR	C23-C24-C25-C26
26	A	609	BCR	C23-C24-C25-C30
26	B	618	BCR	C23-C24-C25-C30
26	K	101	BCR	C23-C24-C25-C26
26	T	101	BCR	C5-C6-C7-C8
26	c	514	BCR	C1-C6-C7-C8
26	c	514	BCR	C5-C6-C7-C8
26	d	405	BCR	C23-C24-C25-C26
26	k	102	BCR	C23-C24-C25-C26
26	t	101	BCR	C5-C6-C7-C8
26	x	101	BCR	C23-C24-C25-C26
29	C	519	LMG	C39-C40-C41-C42
30	d	407	LHG	C33-C34-C35-C36
32	c	518	DGD	CAA-CBA-CCA-CDA
32	c	517	DGD	C3B-C4B-C5B-C6B
32	c	517	DGD	C6B-C7B-C8B-C9B
33	a	616	STE	C6-C7-C8-C9
32	A	618	DGD	O6D-C1D-O3G-C3G
33	B	624	STE	C3-C4-C5-C6
24	B	601	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	A	617	SQD	O48-C23-C24-C25
24	b	609	CLA	C2-C3-C5-C6
28	D	405	PL9	C13-C14-C16-C17
32	C	517	DGD	O1B-C1B-O2G-C2G
29	c	522	LMG	C18-C19-C20-C21
24	C	501	CLA	C2A-CAA-CBA-CGA
30	d	407	LHG	C18-C19-C20-C21
29	D	410	LMG	O7-C10-C11-C12
31	B	623	SQD	C31-C32-C33-C34
24	c	509	CLA	CAA-CBA-CGA-O1A
33	T	103	STE	C4-C5-C6-C7
24	B	601	CLA	O1D-CGD-O2D-CED
31	a	613	SQD	O47-C7-C8-C9
32	H	102	DGD	CBB-CCB-CDB-CEB
33	a	615	STE	C3-C4-C5-C6
31	b	620	SQD	C26-C27-C28-C29
24	B	615	CLA	C2-C3-C5-C6
28	d	406	PL9	C18-C19-C21-C22
24	c	509	CLA	C2A-CAA-CBA-CGA
24	B	601	CLA	CBD-CGD-O2D-CED
33	b	622	STE	C9-C10-C11-C12
32	A	618	DGD	CCA-CDA-CEA-CFA
32	H	102	DGD	CDA-CEA-CFA-CGA
28	a	611	PL9	C39-C41-C42-C43
29	c	519	LMG	O1-C7-C8-C9
31	f	101	SQD	O6-C44-C45-C46
32	c	516	DGD	C1G-C2G-C3G-O3G
24	B	612	CLA	C8-C10-C11-C12
24	b	610	CLA	C15-C16-C17-C18
24	B	602	CLA	C1A-C2A-CAA-CBA
24	C	502	CLA	C1A-C2A-CAA-CBA
33	c	520	STE	C11-C10-C9-C8
26	b	618	BCR	C22-C23-C24-C25
32	C	517	DGD	O6D-C1D-O3G-C3G
32	c	516	DGD	O6E-C1E-O5D-C6D
31	A	616	SQD	O47-C7-C8-C9
32	c	516	DGD	O2G-C1B-C2B-C3B
29	A	614	LMG	O1-C7-C8-O7
30	l	101	LHG	O7-C5-C6-O8
31	f	101	SQD	O6-C44-C45-O47
26	c	515	BCR	C13-C14-C15-C16
26	k	102	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
29	M	101	LMG	C33-C34-C35-C36
31	b	620	SQD	O47-C7-C8-C9
31	A	616	SQD	C5-C6-S-O7
31	a	613	SQD	C5-C6-S-O7
24	c	506	CLA	C4-C3-C5-C6
24	B	606	CLA	C11-C12-C13-C15
24	B	608	CLA	C6-C7-C8-C10
24	B	613	CLA	C6-C7-C8-C10
24	b	614	CLA	C11-C10-C8-C7
24	c	503	CLA	C11-C10-C8-C7
24	c	508	CLA	C11-C10-C8-C7
24	c	510	CLA	C11-C10-C8-C7
29	c	521	LMG	C35-C36-C37-C38
24	C	512	CLA	O2A-C1-C2-C3
24	b	612	CLA	CAA-CBA-CGA-O2A
32	c	516	DGD	C2B-C3B-C4B-C5B
33	a	617	STE	C4-C5-C6-C7
30	A	615	LHG	C10-C11-C12-C13
24	A	613	CLA	C16-C17-C18-C19
29	D	410	LMG	O8-C28-C29-C30
32	H	102	DGD	CAA-CBA-CCA-CDA
33	b	626	STE	C3-C4-C5-C6
29	M	101	LMG	C10-C11-C12-C13
24	b	613	CLA	CBD-CGD-O2D-CED
24	b	601	CLA	C4-C3-C5-C6
31	f	101	SQD	C25-C26-C27-C28
30	A	615	LHG	C23-C24-C25-C26
26	C	515	BCR	C11-C10-C9-C8
33	b	622	STE	O1-C1-C2-C3
24	b	613	CLA	C15-C16-C17-C18
24	b	601	CLA	CBA-CGA-O2A-C1
32	h	101	DGD	O1B-C1B-C2B-C3B
24	c	512	CLA	C5-C6-C7-C8
24	B	611	CLA	C6-C7-C8-C9
24	B	613	CLA	C6-C7-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	D	403	CLA	C11-C10-C8-C9
24	a	604	CLA	C14-C13-C15-C16
24	b	603	CLA	C11-C10-C8-C9
24	b	603	CLA	C11-C12-C13-C14
24	b	613	CLA	C11-C10-C8-C9
31	A	617	SQD	O10-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
29	D	409	LMG	C36-C37-C38-C39
30	B	622	LHG	C16-C17-C18-C19
32	c	516	DGD	CAA-CBA-CCA-CDA
24	b	606	CLA	C5-C6-C7-C8
24	b	613	CLA	CAA-CBA-CGA-O2A
29	b	621	LMG	O8-C28-C29-C30
24	B	613	CLA	CAA-CBA-CGA-O2A
29	a	618	LMG	O7-C10-C11-C12
33	d	411	STE	O2-C1-C2-C3
24	c	509	CLA	C8-C10-C11-C12
24	A	604	CLA	C4C-C3C-CAC-CBC
33	c	520	STE	C11-C12-C13-C14
31	b	620	SQD	C45-C44-O6-C1
32	c	517	DGD	C2G-C3G-O3G-C1D
32	C	516	DGD	O1G-C1G-C2G-O2G
32	c	516	DGD	O1B-C1B-C2B-C3B
24	C	504	CLA	C10-C11-C12-C13
28	A	612	PL9	C20-C19-C21-C22
32	H	102	DGD	C3A-C4A-C5A-C6A
24	B	603	CLA	C10-C11-C12-C13
24	B	612	CLA	CAA-CBA-CGA-O2A
30	B	621	LHG	C16-C17-C18-C19
24	b	607	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	B	601	CLA	CAA-CBA-CGA-O2A
33	m	101	STE	C6-C7-C8-C9
24	B	606	CLA	C3-C5-C6-C7
24	b	612	CLA	CAA-CBA-CGA-O1A
25	A	606	PHO	C8-C10-C11-C12
32	A	618	DGD	C4D-C5D-C6D-O5D
29	c	521	LMG	C15-C16-C17-C18
29	d	410	LMG	C37-C38-C39-C40
32	C	516	DGD	O6E-C1E-O5D-C6D
24	B	604	CLA	C13-C15-C16-C17
24	C	506	CLA	C2-C1-O2A-CGA
29	D	410	LMG	O10-C28-C29-C30
29	b	623	LMG	O10-C28-C29-C30
33	B	626	STE	C3-C4-C5-C6
31	f	101	SQD	C30-C31-C32-C33
33	d	411	STE	O1-C1-C2-C3
31	B	623	SQD	O10-C23-C24-C25

There are no ring outliers.

105 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	d	403	CLA	1	0
24	B	612	CLA	1	0
26	b	619	BCR	1	0
24	B	614	CLA	3	0
33	t	102	STE	2	0
26	c	515	BCR	1	0
24	B	604	CLA	1	0
24	b	616	CLA	1	0
24	B	615	CLA	1	0
29	b	623	LMG	1	0
30	B	621	LHG	1	0
24	b	613	CLA	1	0
21	a	601[B]	OEY	1	0
29	D	406	LMG	1	0
24	b	602	CLA	1	0
24	c	512	CLA	1	0
29	c	519	LMG	1	0
26	B	618	BCR	3	0
28	a	611	PL9	2	0
30	A	615	LHG	1	0
24	C	503	CLA	1	0
31	B	623	SQD	2	0
24	b	609	CLA	1	0
33	E	102	STE	1	0
24	b	607	CLA	1	0
24	c	504	CLA	3	0
35	F	101	HEM	2	0
33	H	103	STE	1	0
24	B	610	CLA	2	0
26	H	101	BCR	1	0
33	a	617	STE	1	0
32	c	517	DGD	2	0
24	B	606	CLA	3	0
31	f	101	SQD	1	0
24	b	614	CLA	1	0
31	b	620	SQD	1	0
24	b	604	CLA	1	0
30	d	409	LHG	1	0
34	D	401	BCT	1	0
33	T	103	STE	1	0
33	B	620	STE	1	0
24	c	511	CLA	2	0

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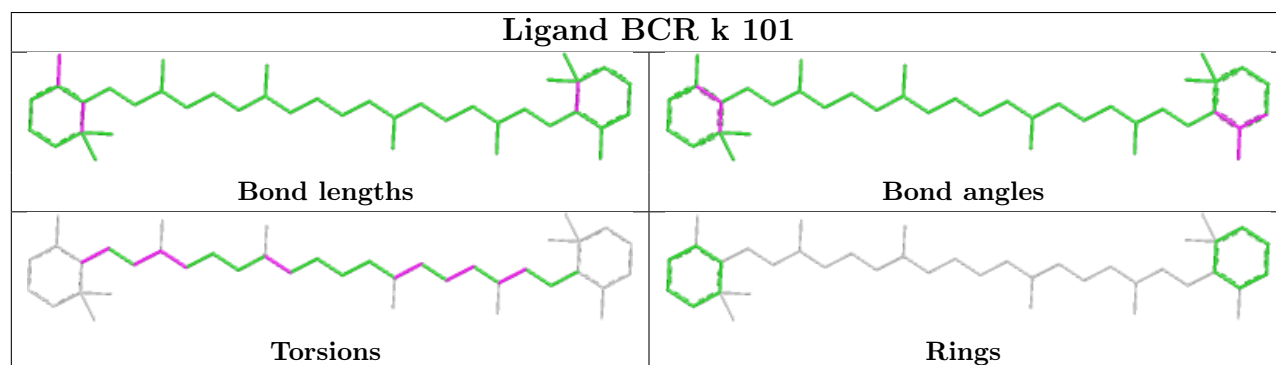
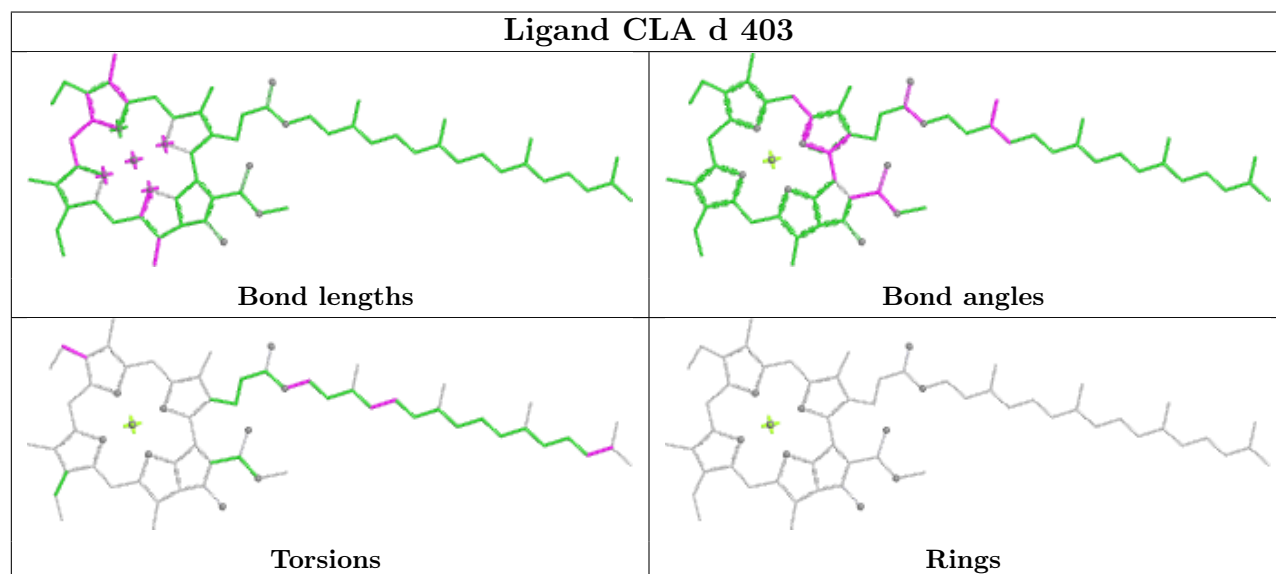
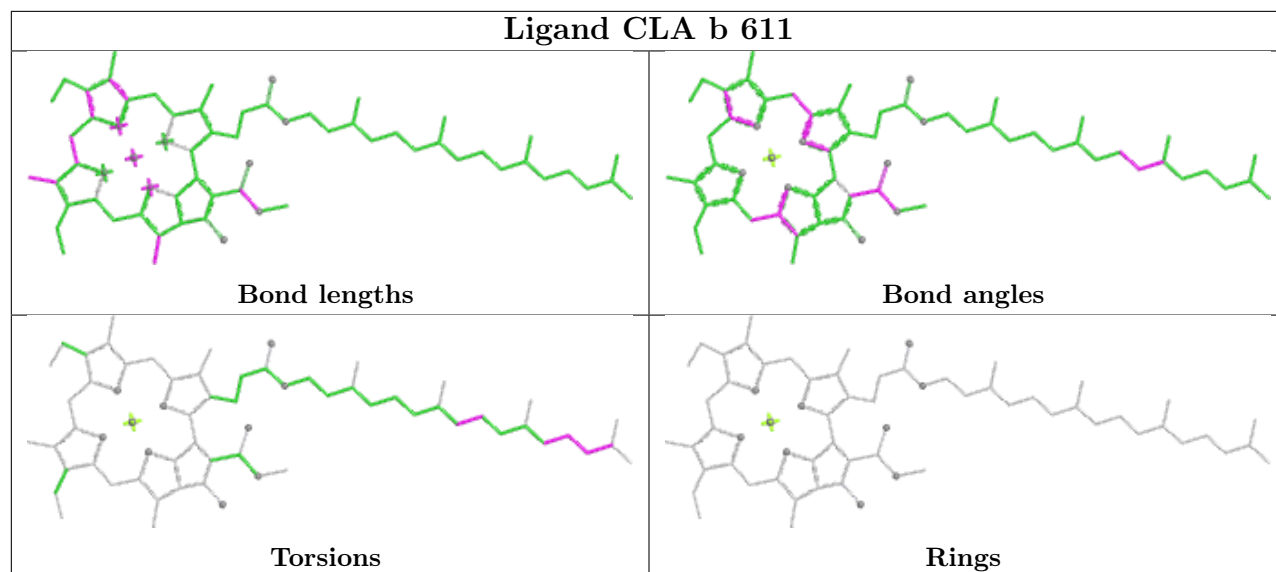
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	c	522	LMG	1	0
33	B	625	STE	1	0
33	m	101	STE	1	0
26	D	404	BCR	1	0
26	b	618	BCR	1	0
30	d	407	LHG	4	0
24	c	508	CLA	4	0
31	A	617	SQD	1	0
33	M	102	STE	1	0
24	b	606	CLA	1	0
30	D	408	LHG	3	0
24	B	613	CLA	3	0
33	d	411	STE	1	0
24	c	513	CLA	1	0
30	B	622	LHG	1	0
24	D	403	CLA	3	0
24	b	615	CLA	3	0
28	A	612	PL9	2	0
33	B	624	STE	1	0
24	A	613	CLA	4	0
24	b	605	CLA	3	0
33	b	622	STE	2	0
36	v	201	HEC	1	0
24	c	503	CLA	1	0
24	C	507	CLA	1	0
33	b	625	STE	2	0
24	A	604	CLA	1	0
33	D	411	STE	6	0
24	B	601	CLA	3	0
24	B	607	CLA	1	0
24	C	513	CLA	2	0
26	T	101	BCR	1	0
24	C	501	CLA	1	0
29	D	409	LMG	1	0
21	A	601[B]	OEY	1	0
30	E	101	LHG	1	0
31	D	407	SQD	1	0
24	C	509	CLA	1	0
33	c	520	STE	1	0
29	a	618	LMG	5	0
24	B	616	CLA	1	0
26	t	101	BCR	3	0

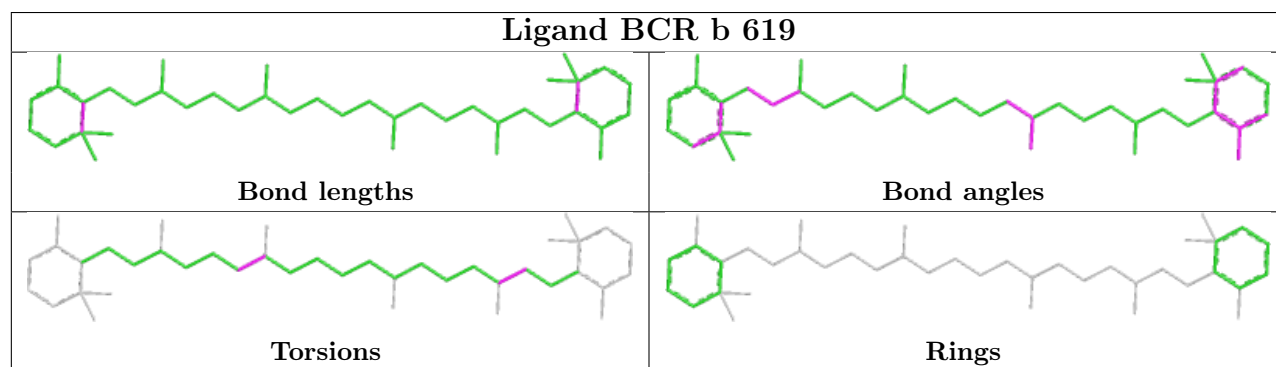
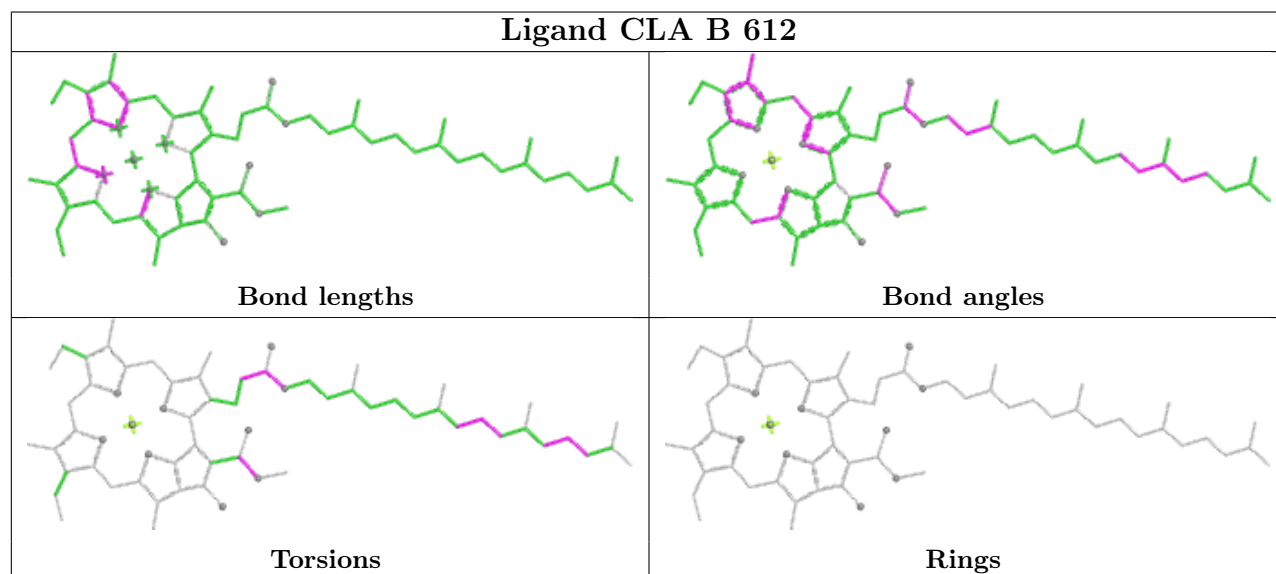
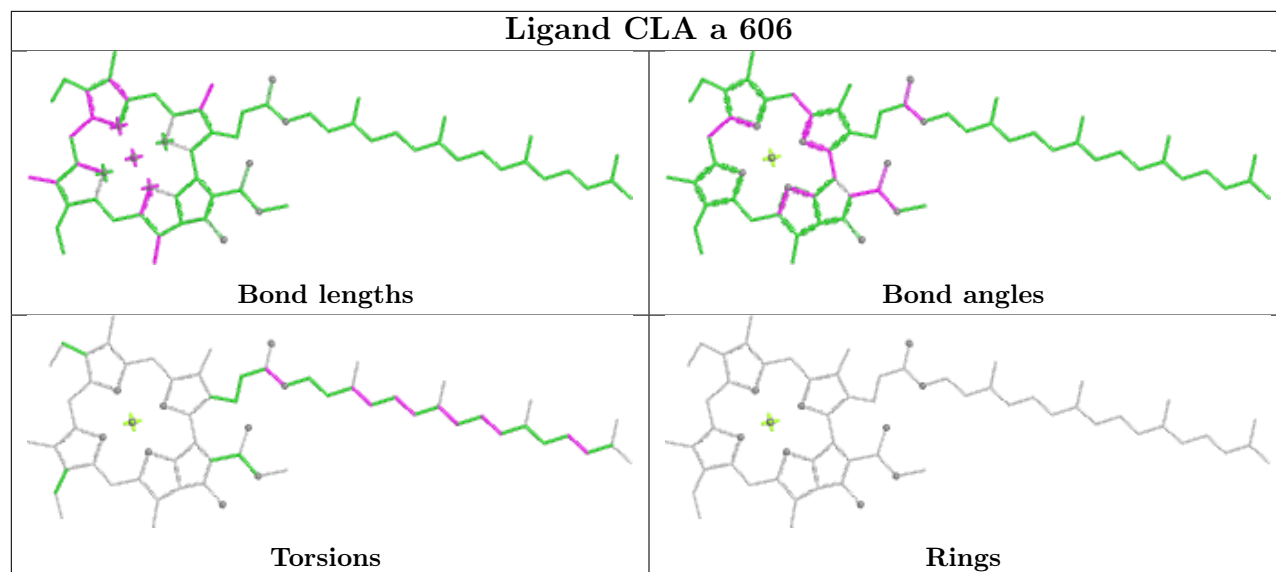
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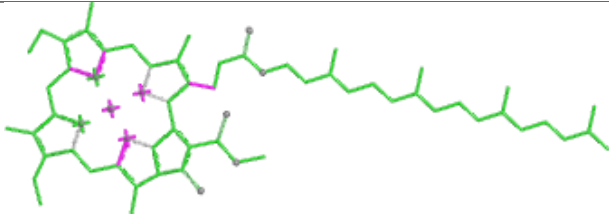
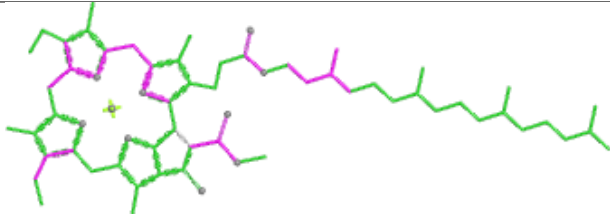
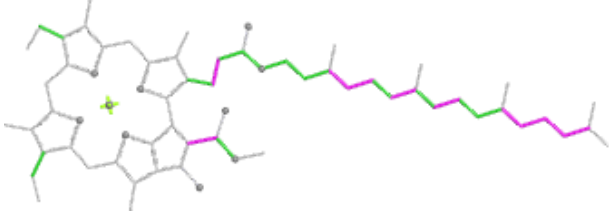
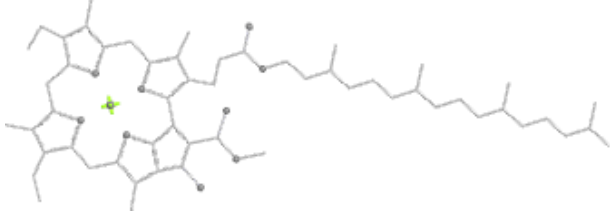
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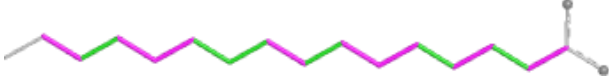
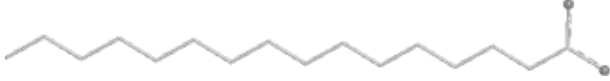
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	V	201	HEC	1	0
29	c	521	LMG	2	0
26	Y	101	BCR	1	0
26	a	607	BCR	1	0
24	c	507	CLA	1	0
25	d	402	PHO	1	0
24	B	611	CLA	1	0
35	e	101	HEM	4	0
24	B	602	CLA	1	0
29	M	101	LMG	1	0
26	d	405	BCR	2	0
31	A	616	SQD	1	0
33	l	102	STE	1	0
24	b	601	CLA	1	0
24	c	501	CLA	2	0
25	A	607	PHO	1	0
32	A	618	DGD	3	0
24	c	509	CLA	1	0
26	B	619	BCR	1	0
24	C	504	CLA	1	0
30	l	101	LHG	1	0

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

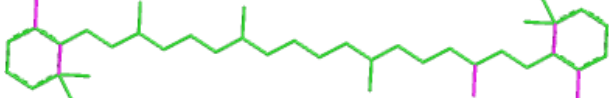
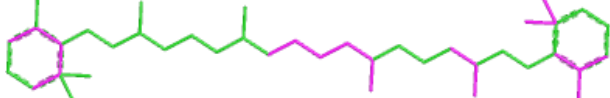
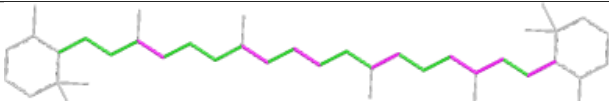
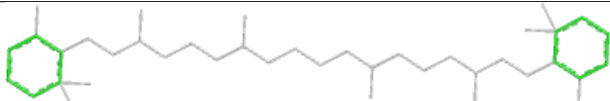


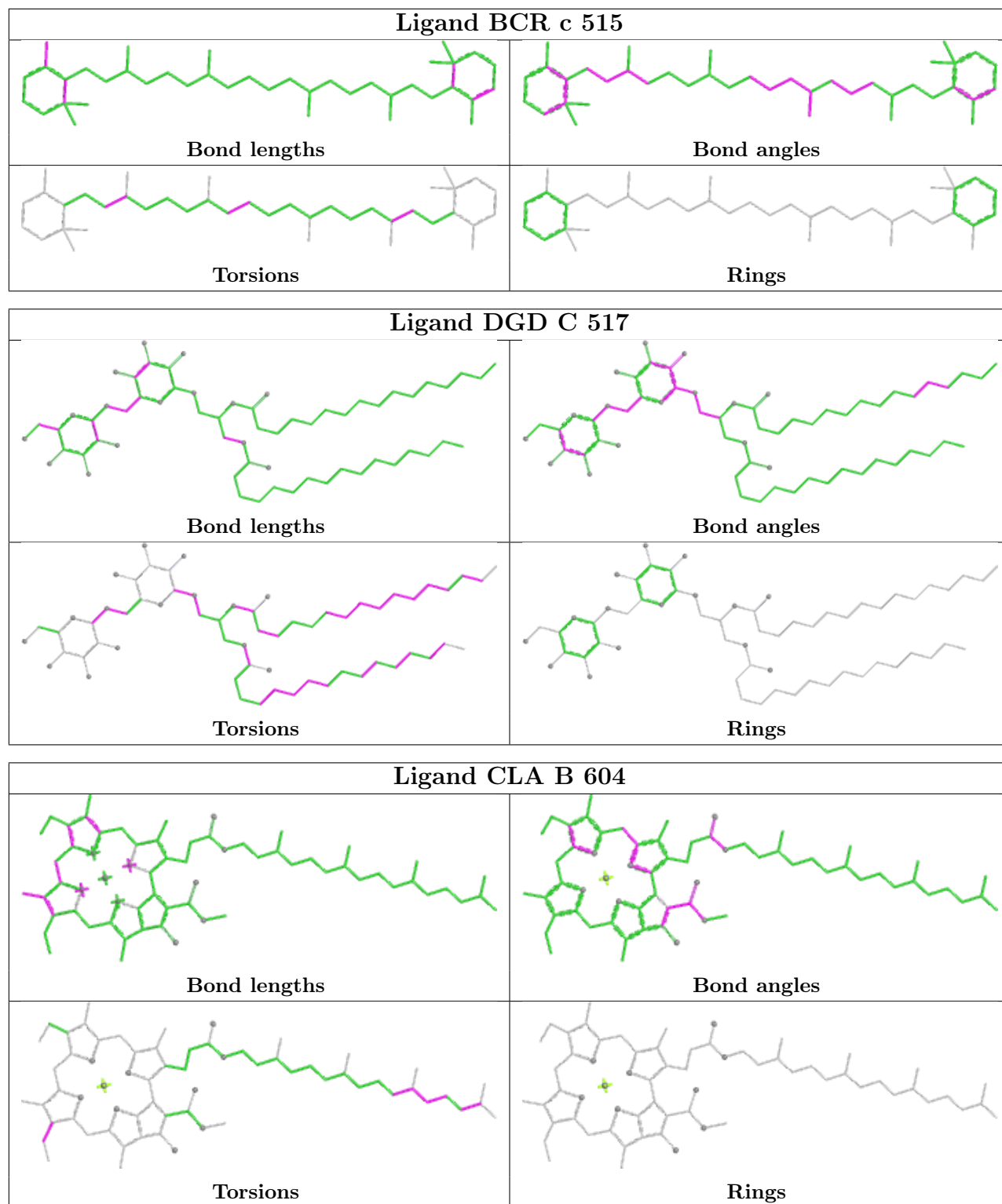


Ligand CLA B 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

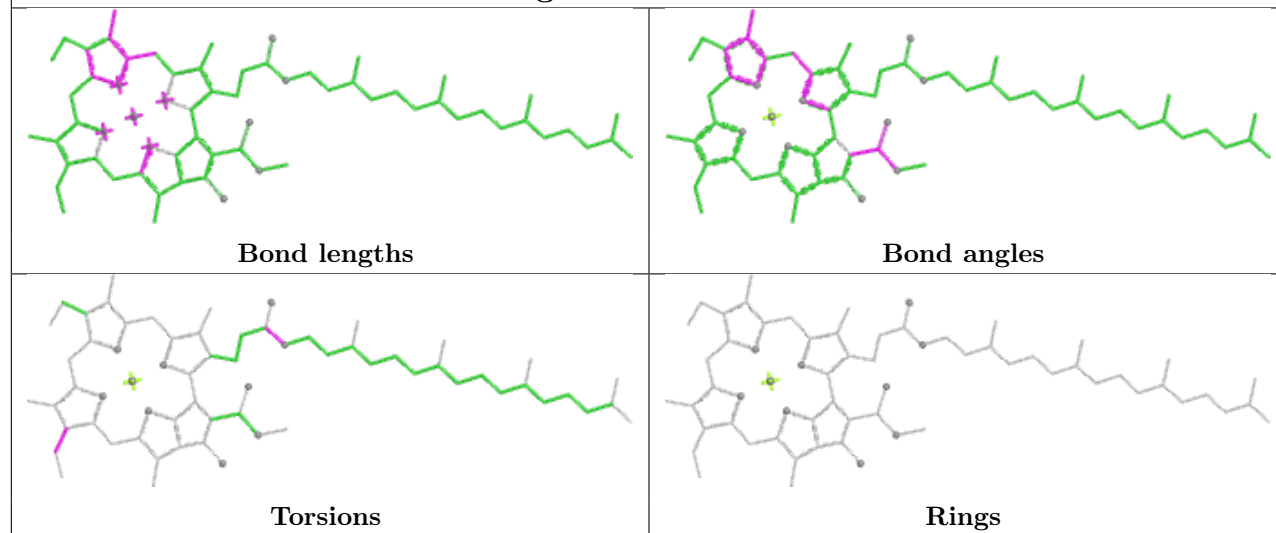
Ligand STE t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE I 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

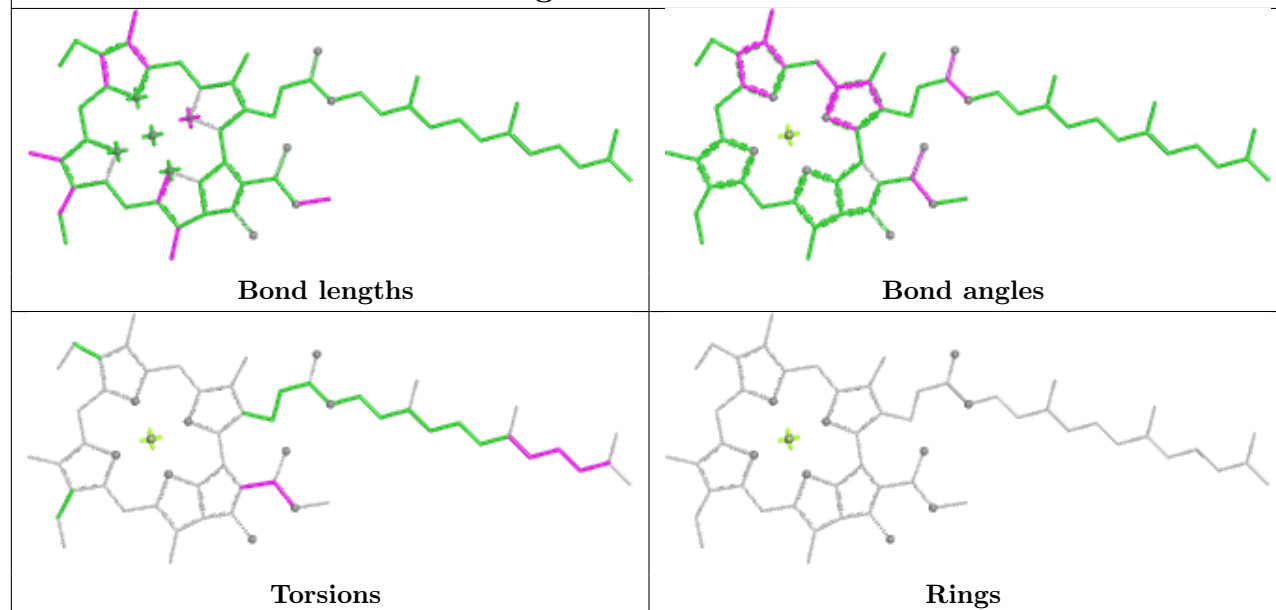
Ligand BCR A 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

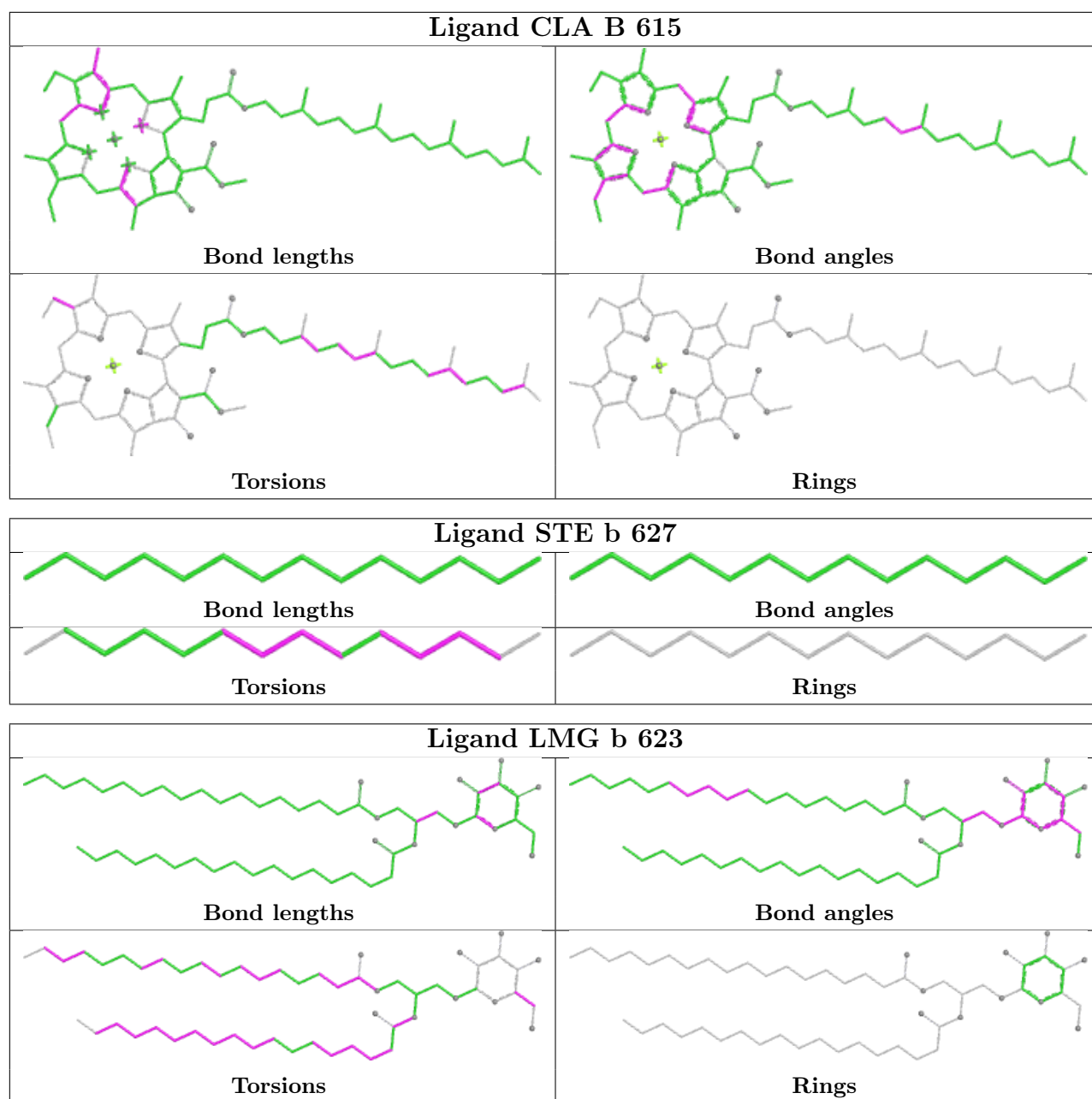


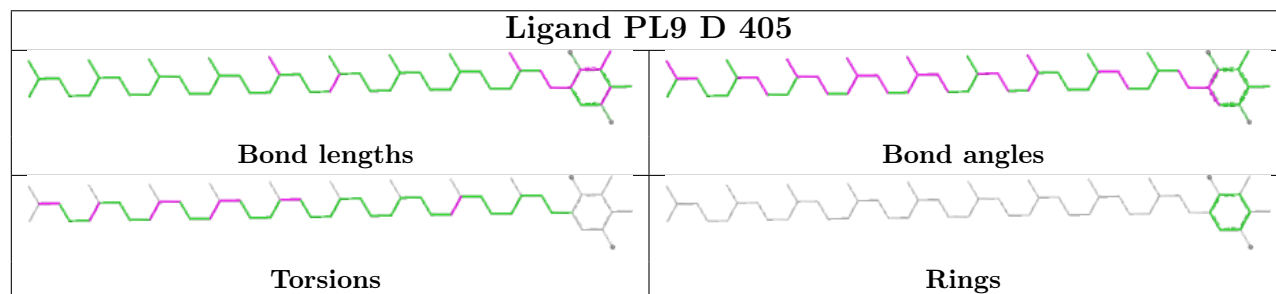
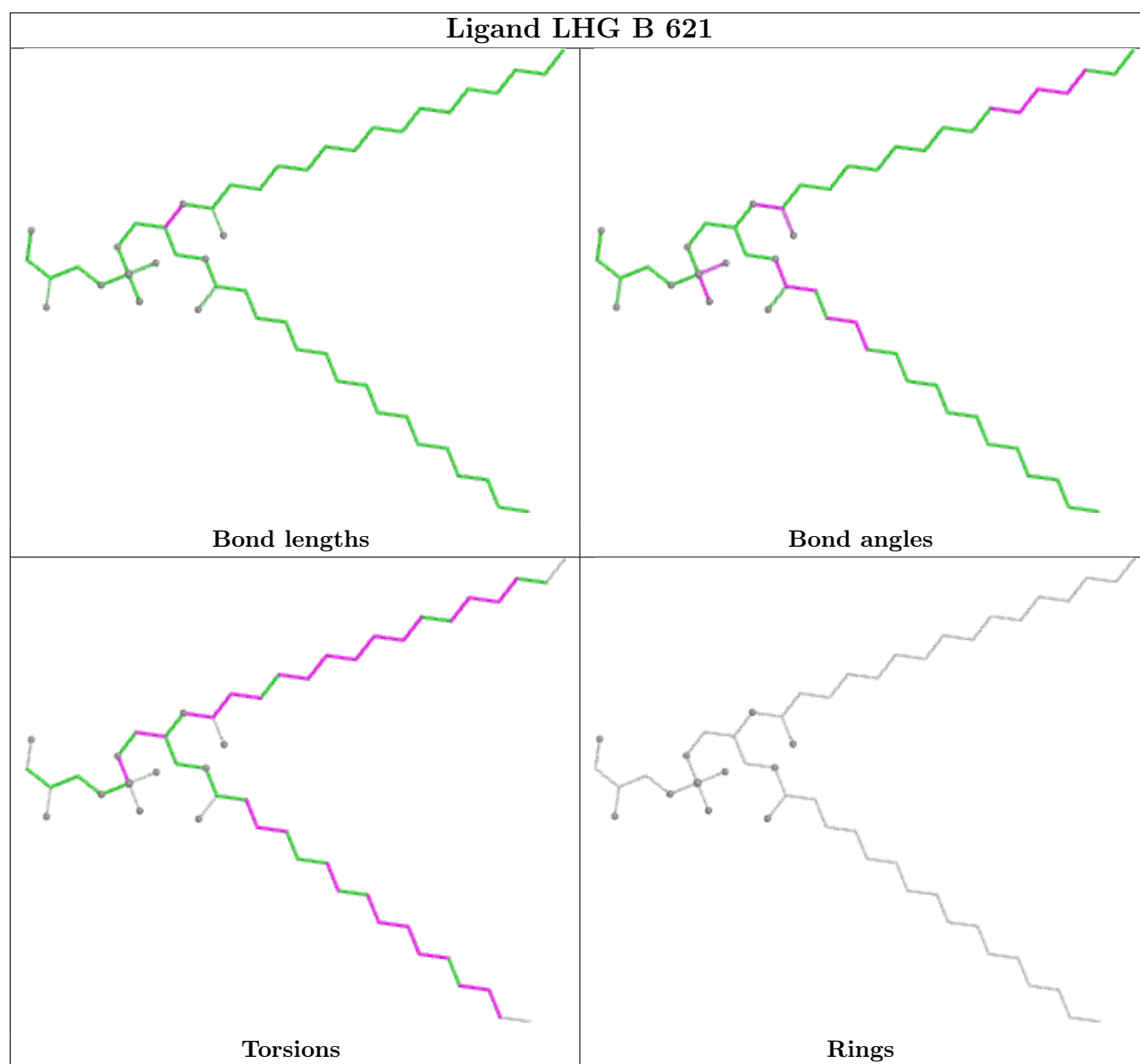
Ligand CLA a 612



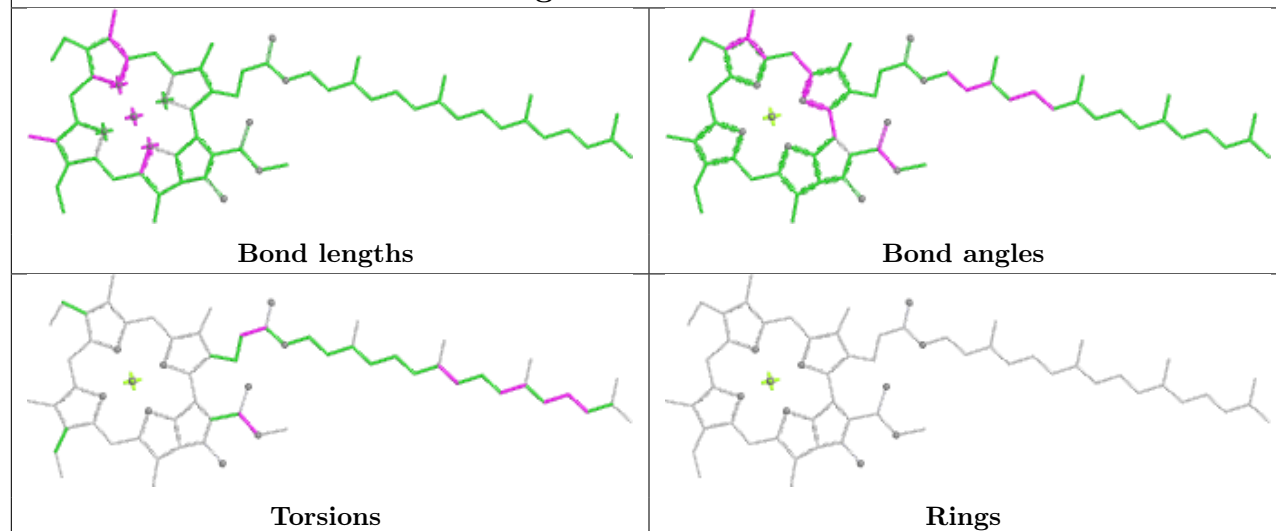
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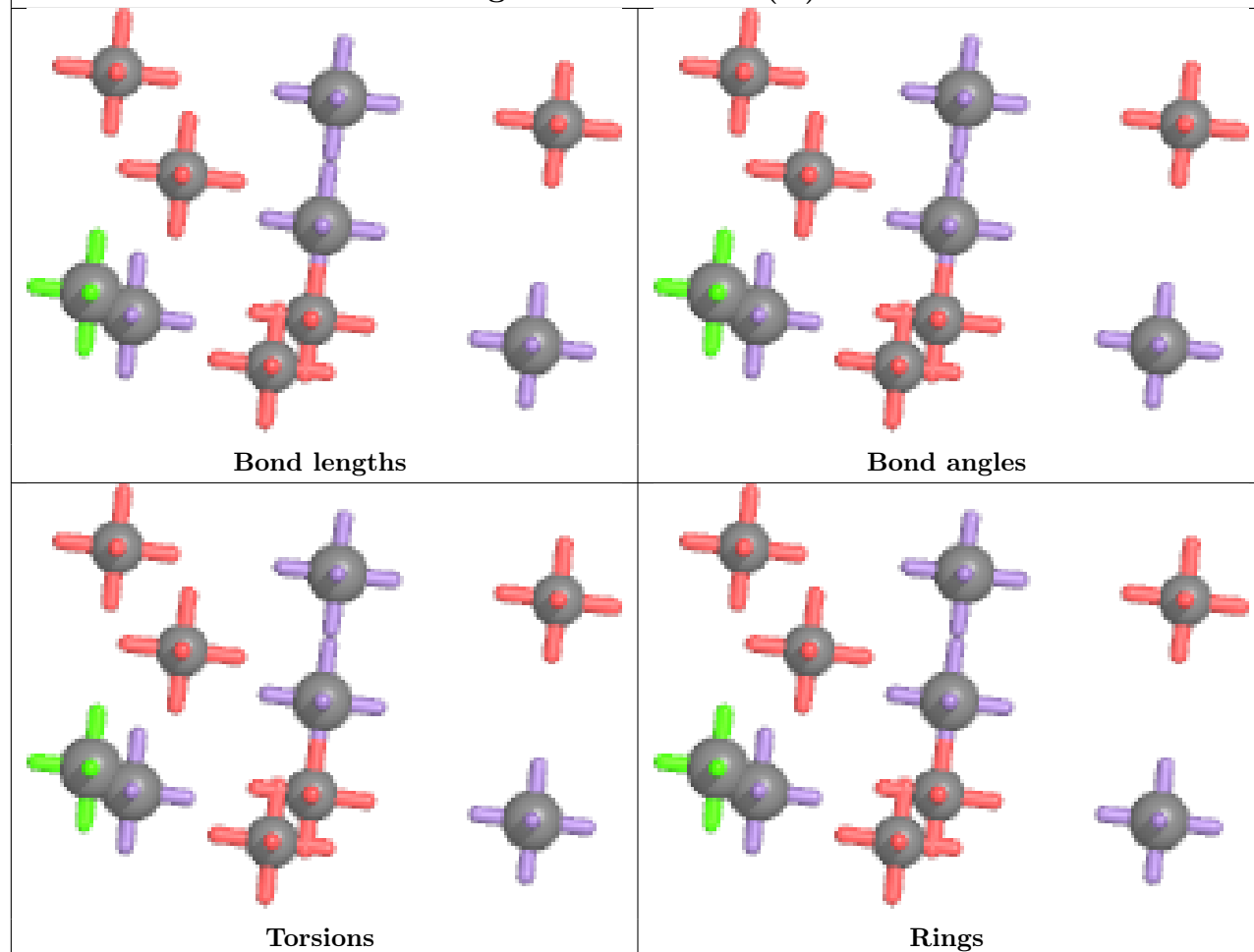




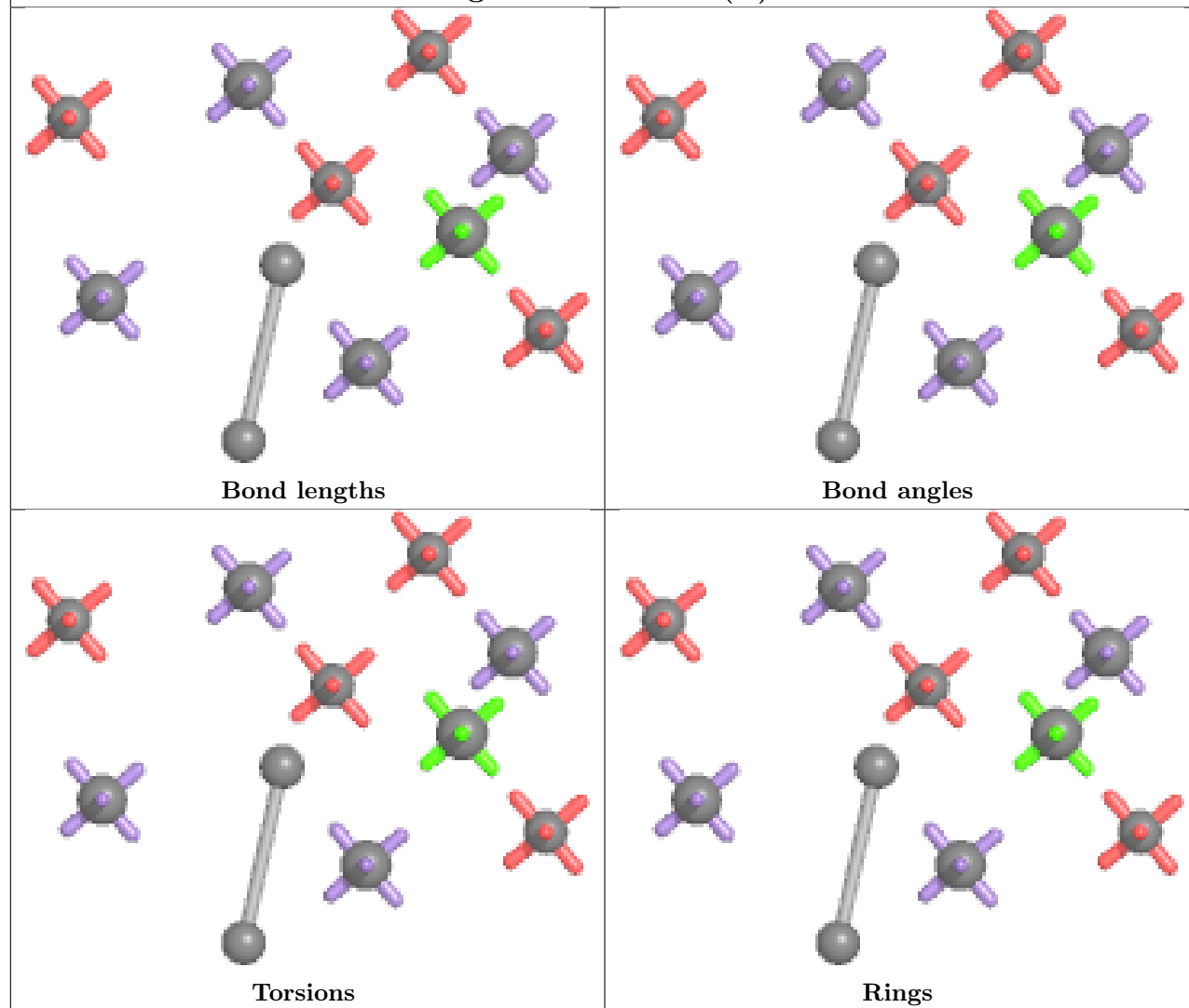
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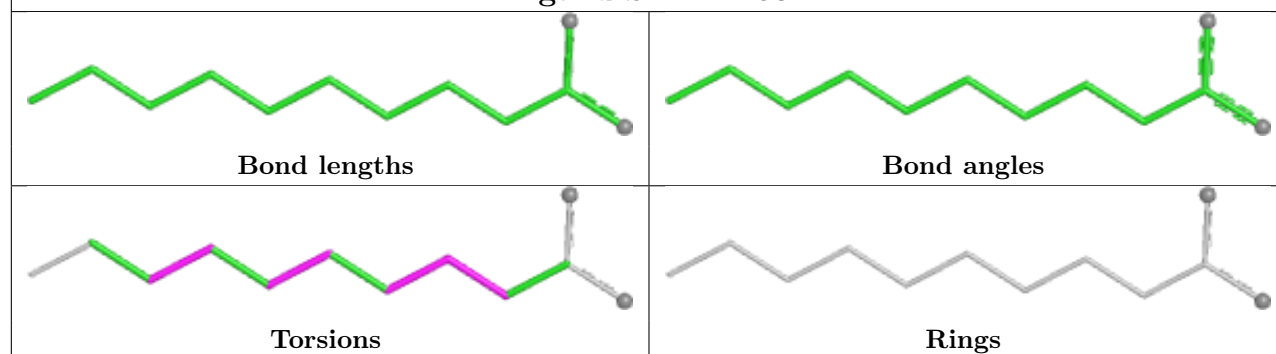
Ligand OEX A 602 (A)

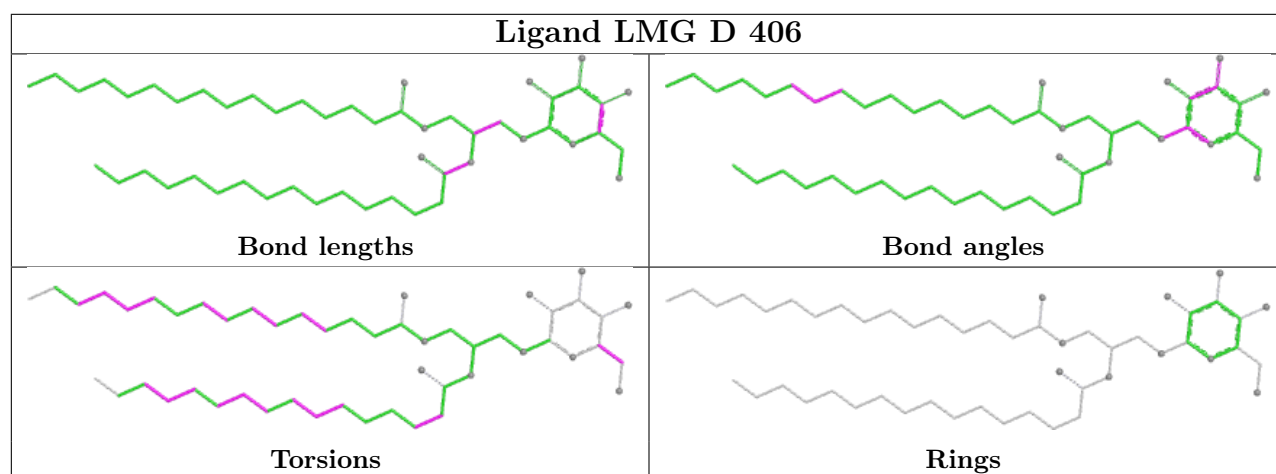
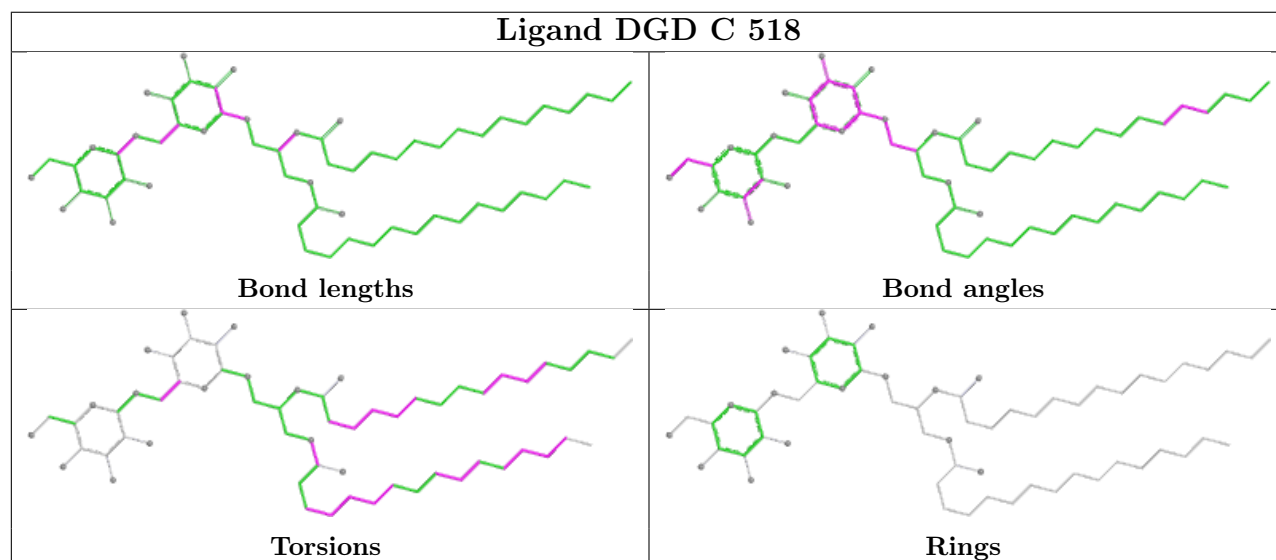
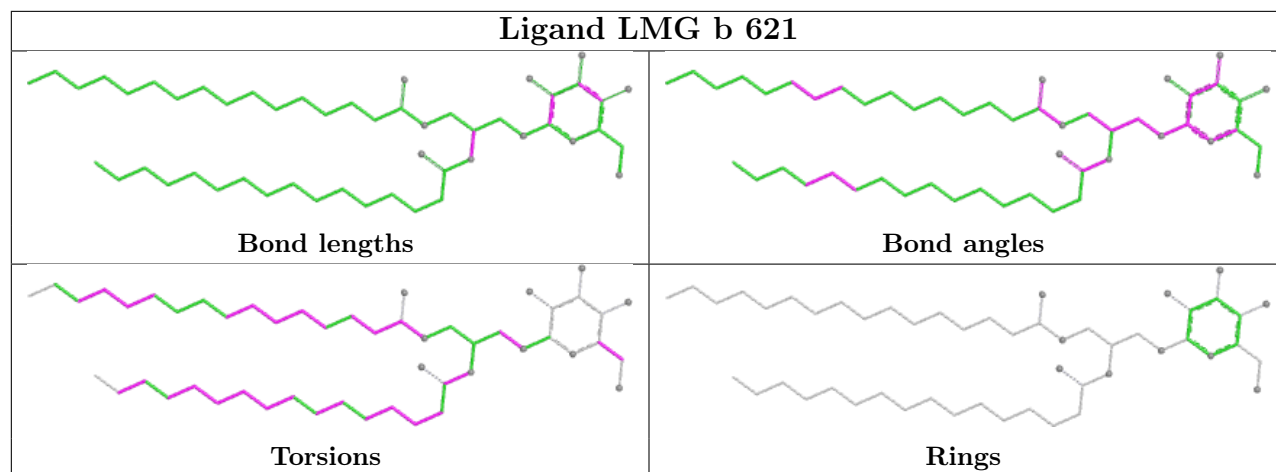


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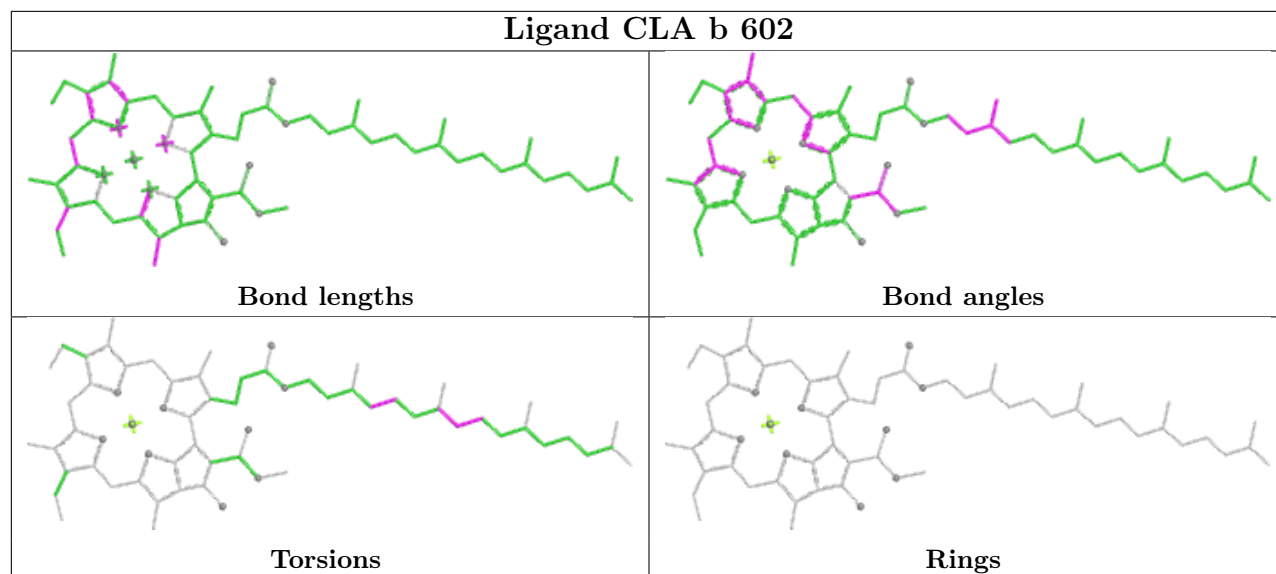


Ligand STE k 103

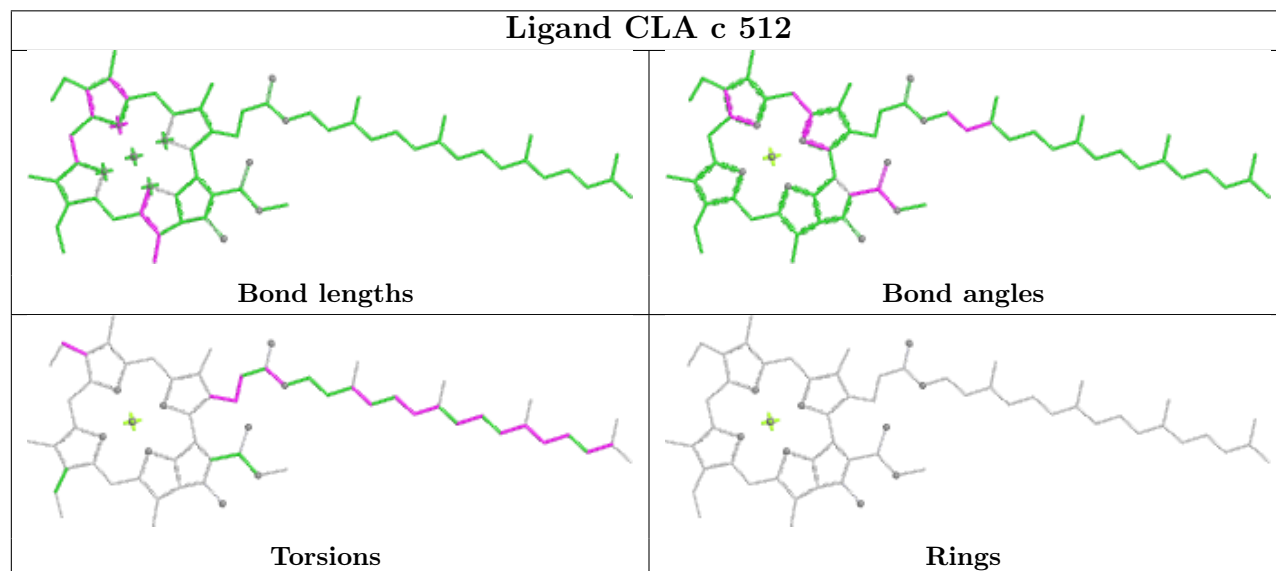




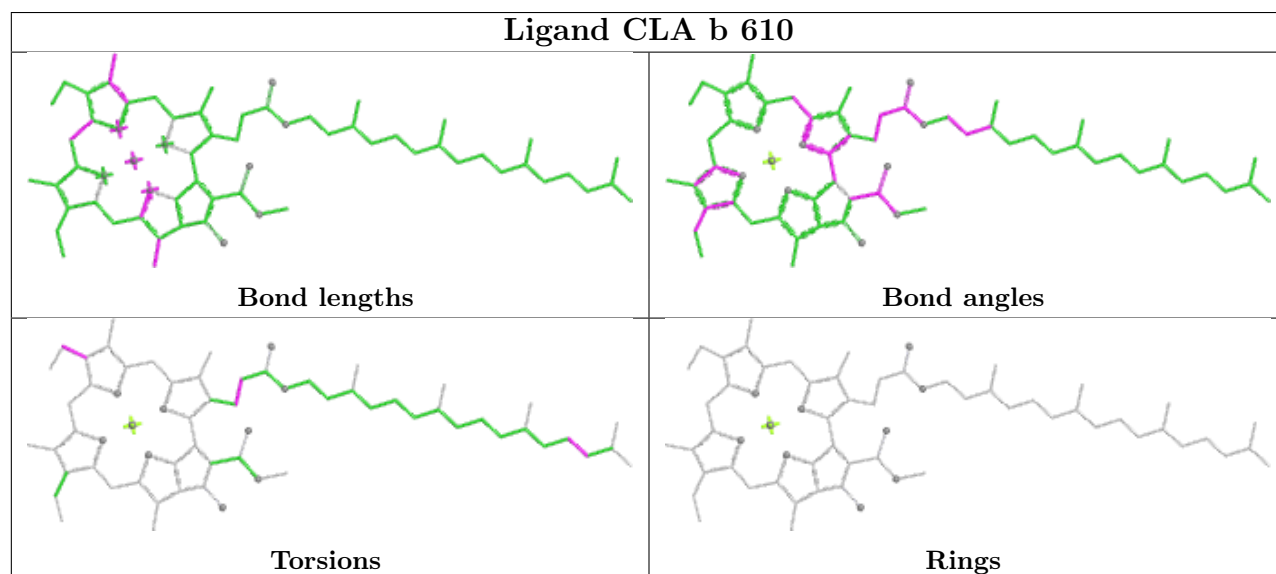
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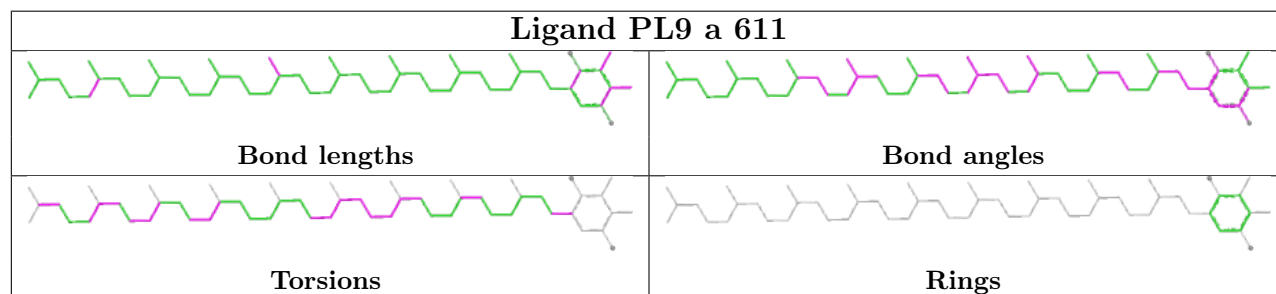
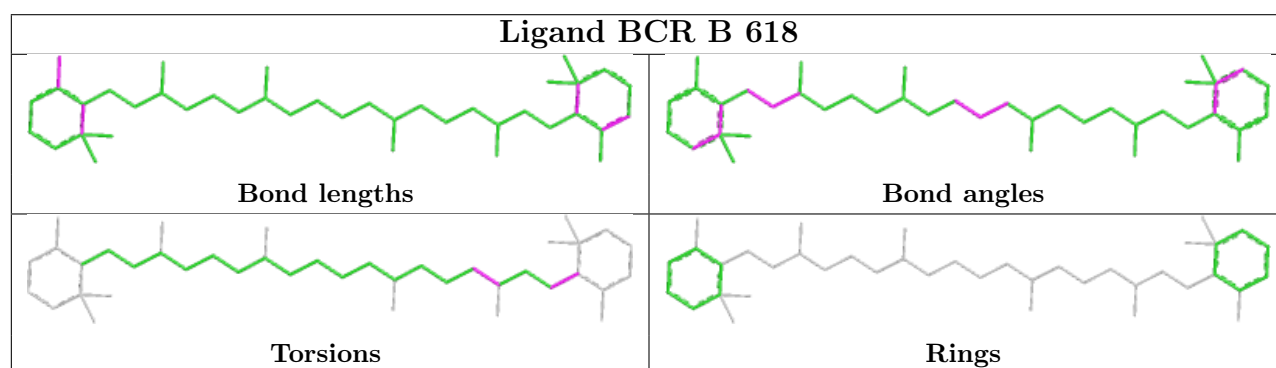
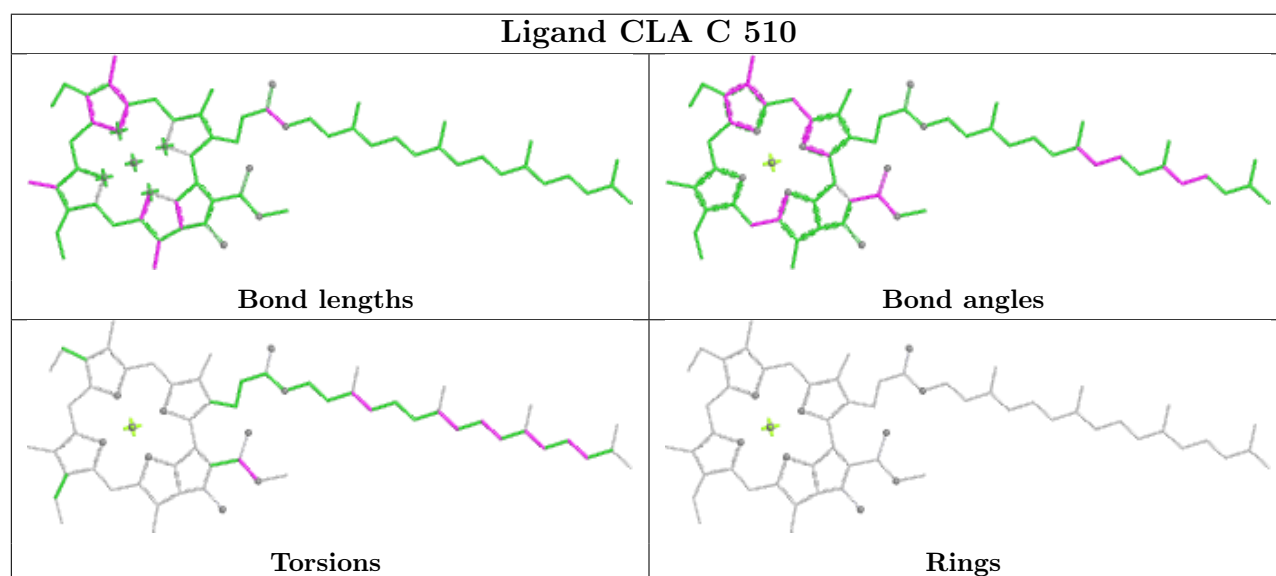
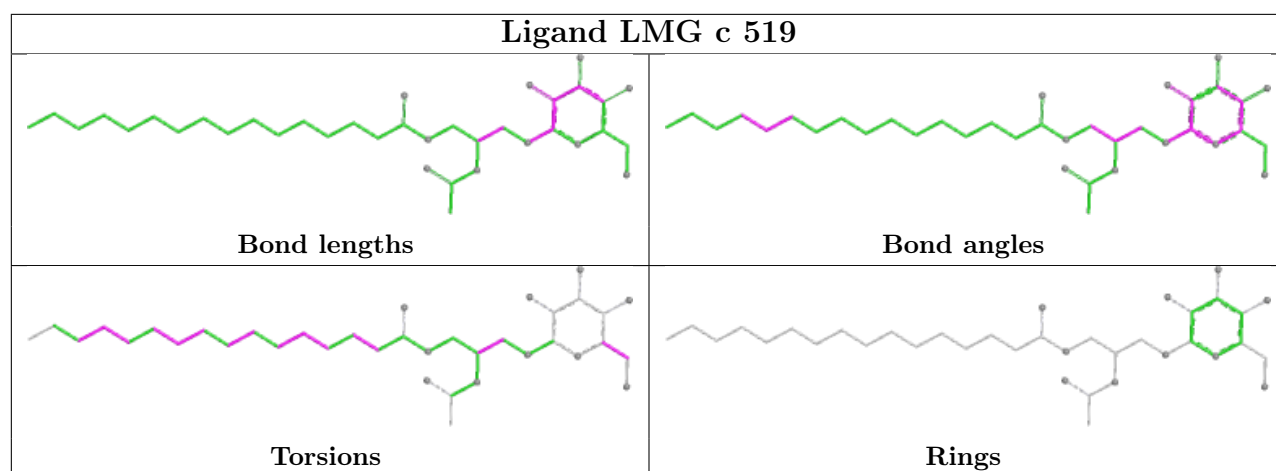


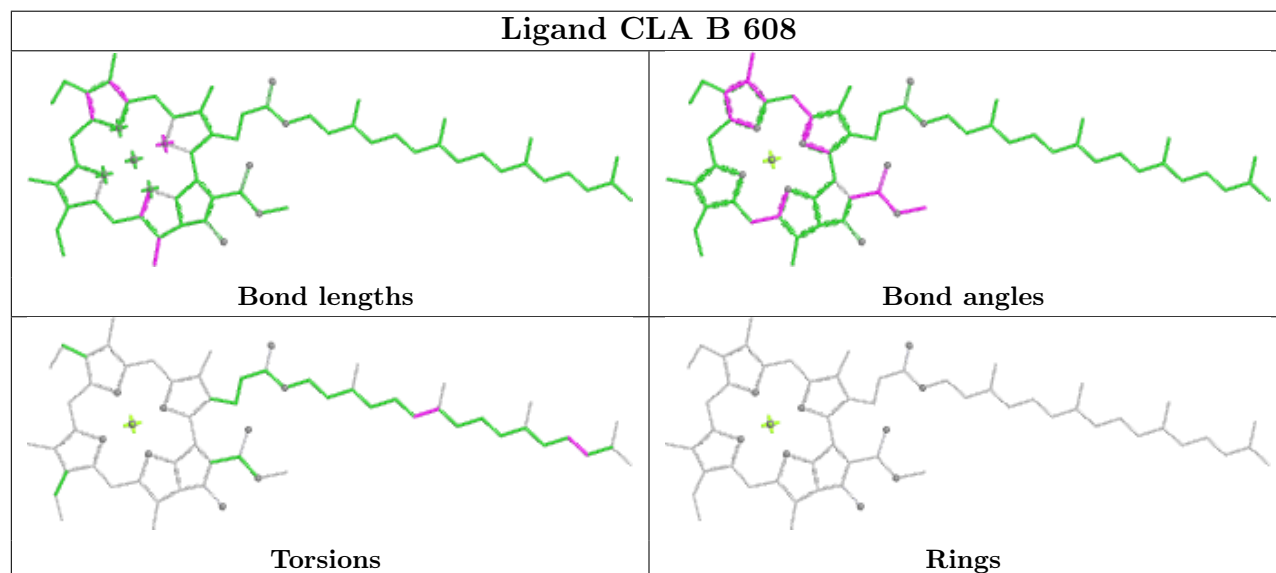
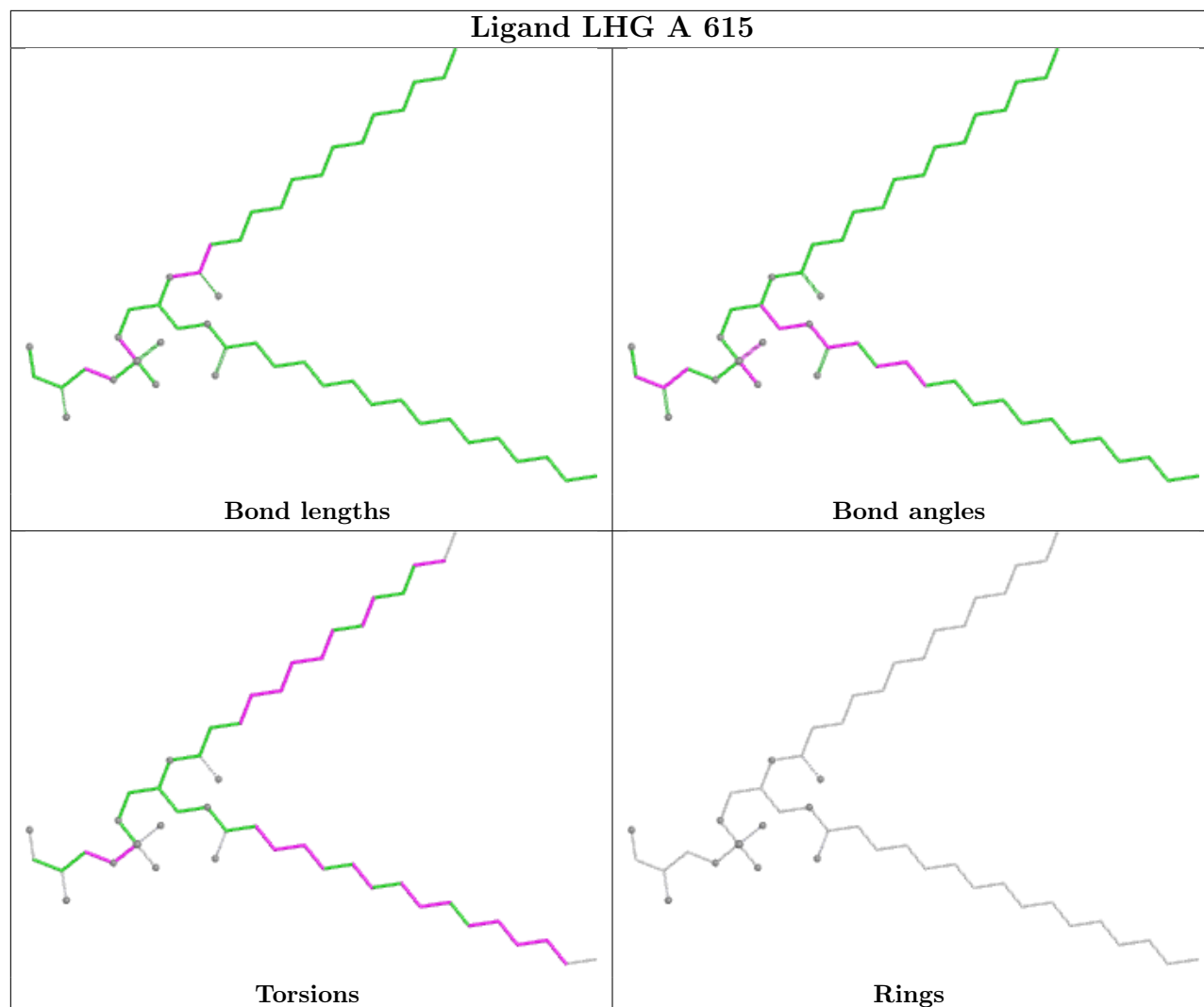
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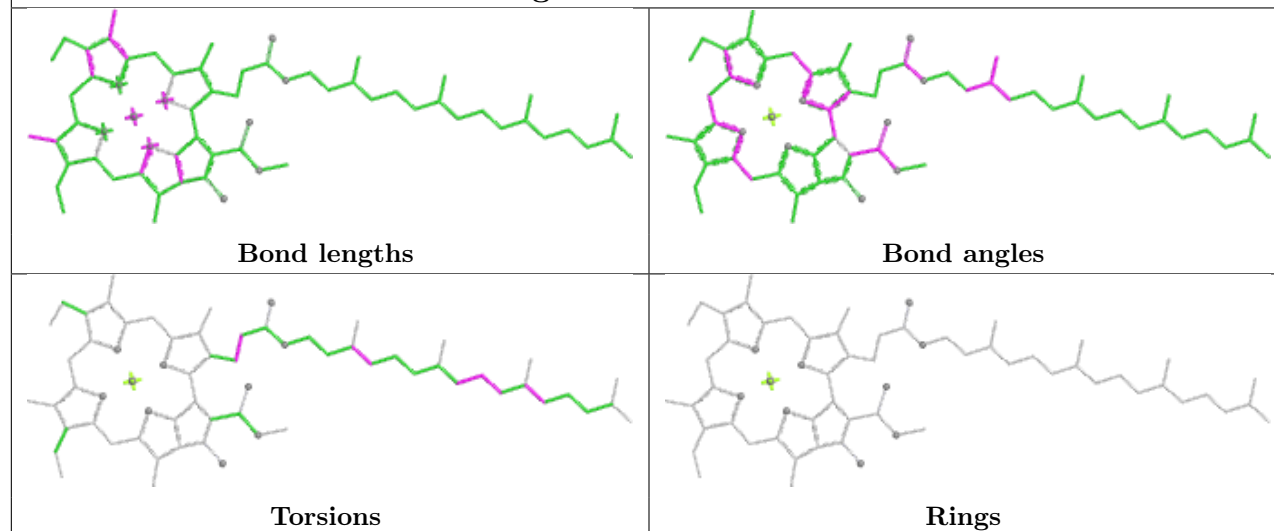
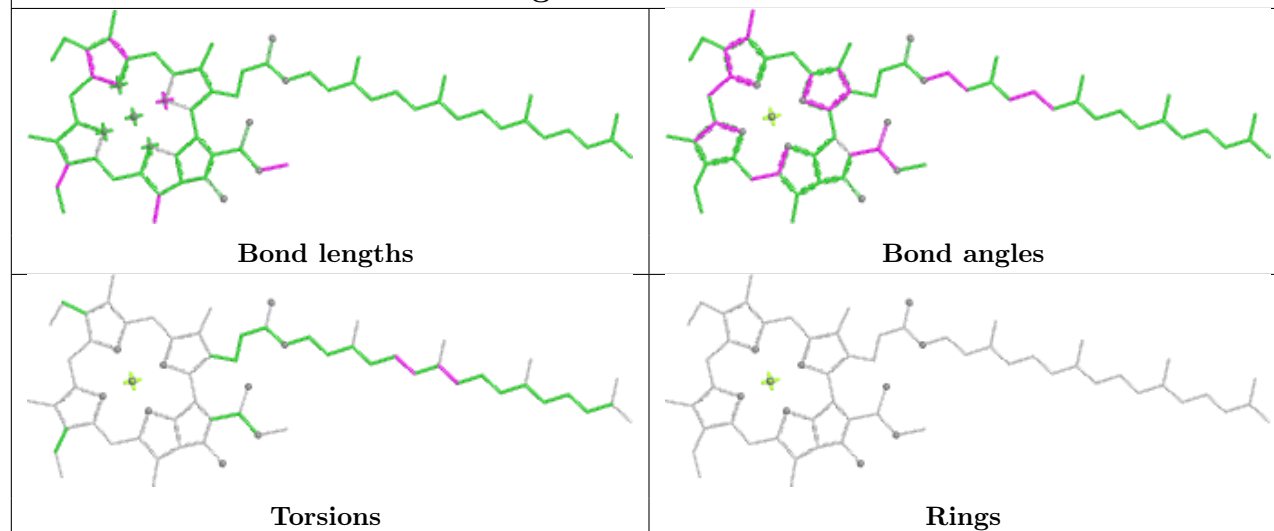


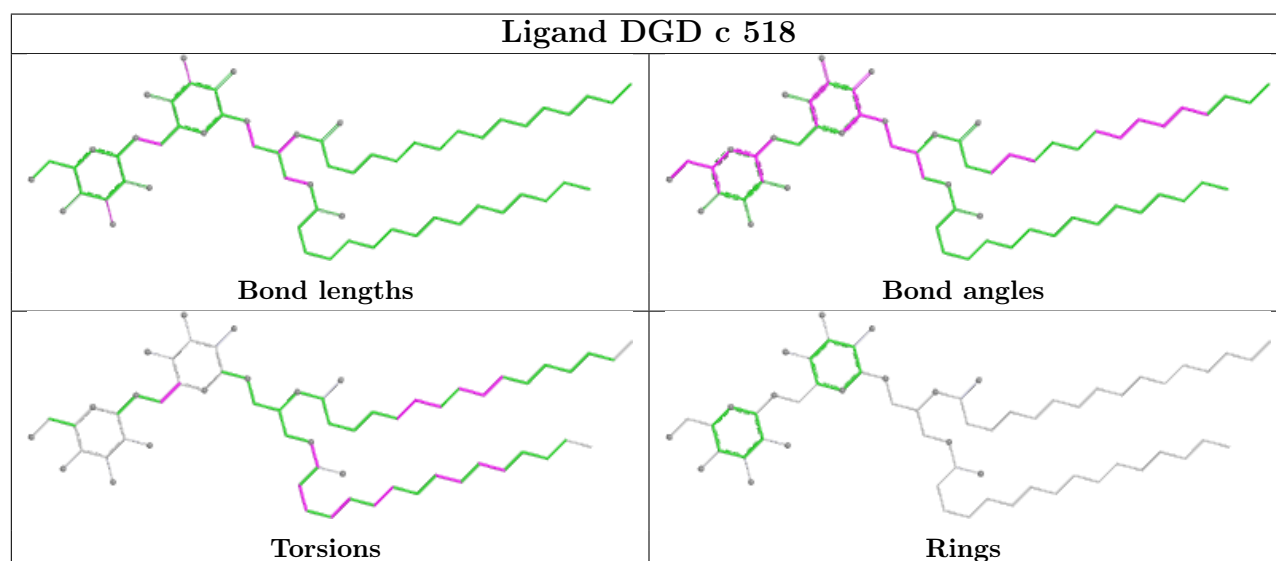
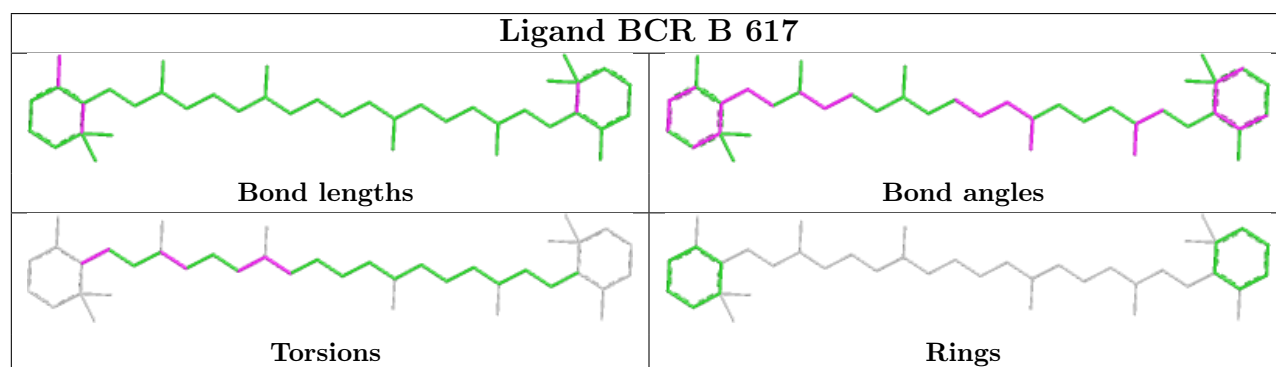
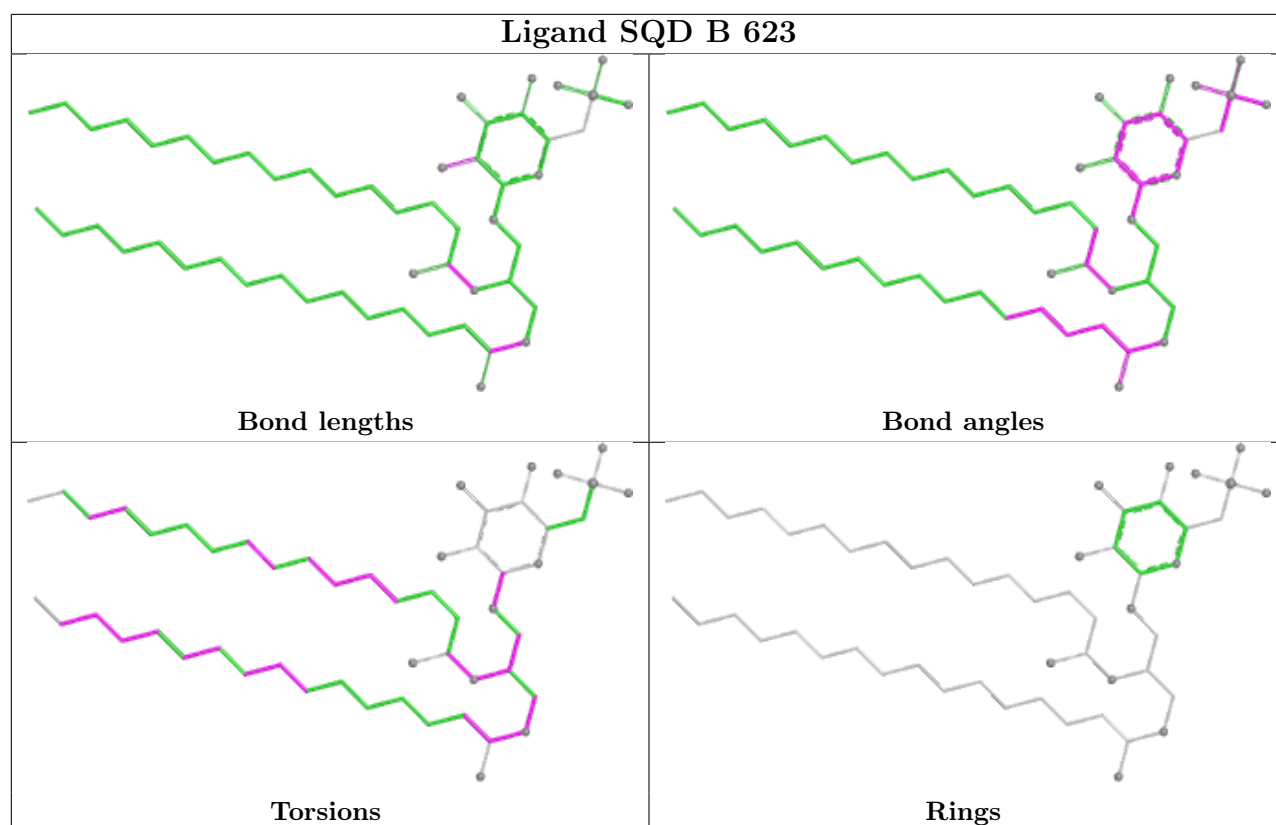
Ligand CLA b 610



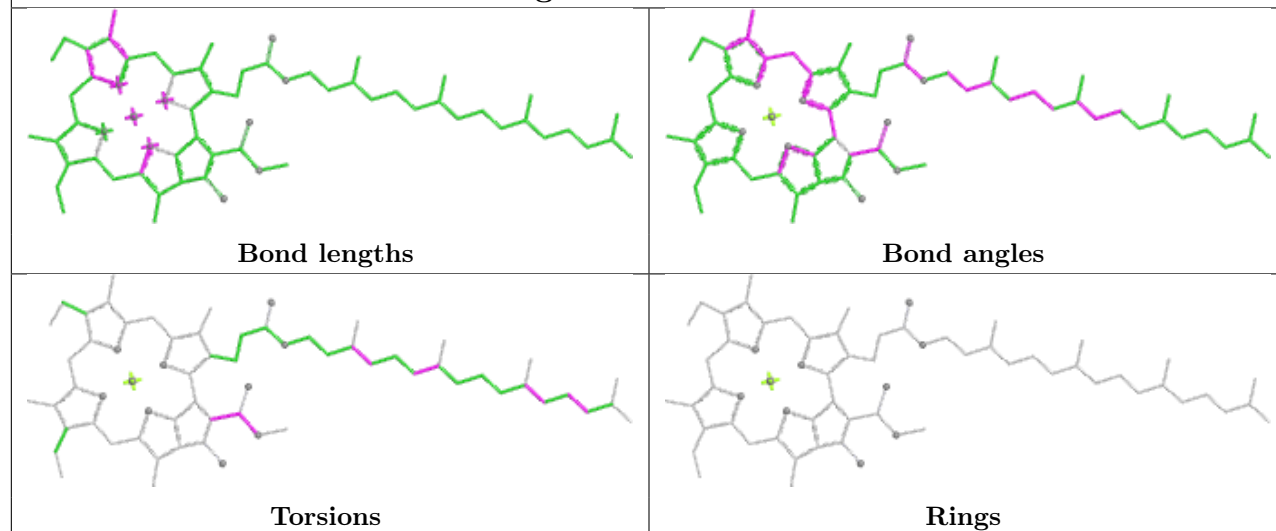




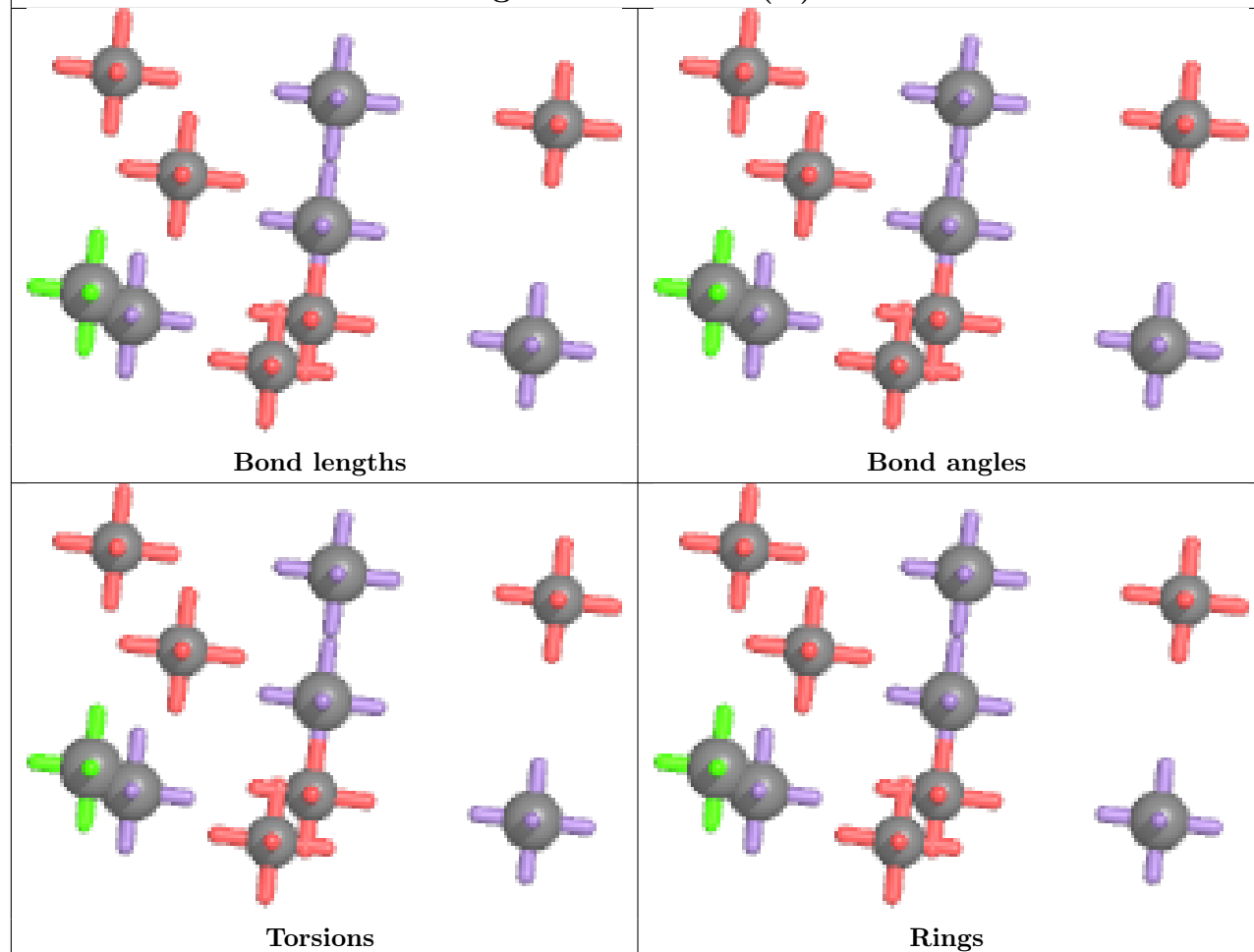
Ligand CLA B 603**Ligand CLA C 503**

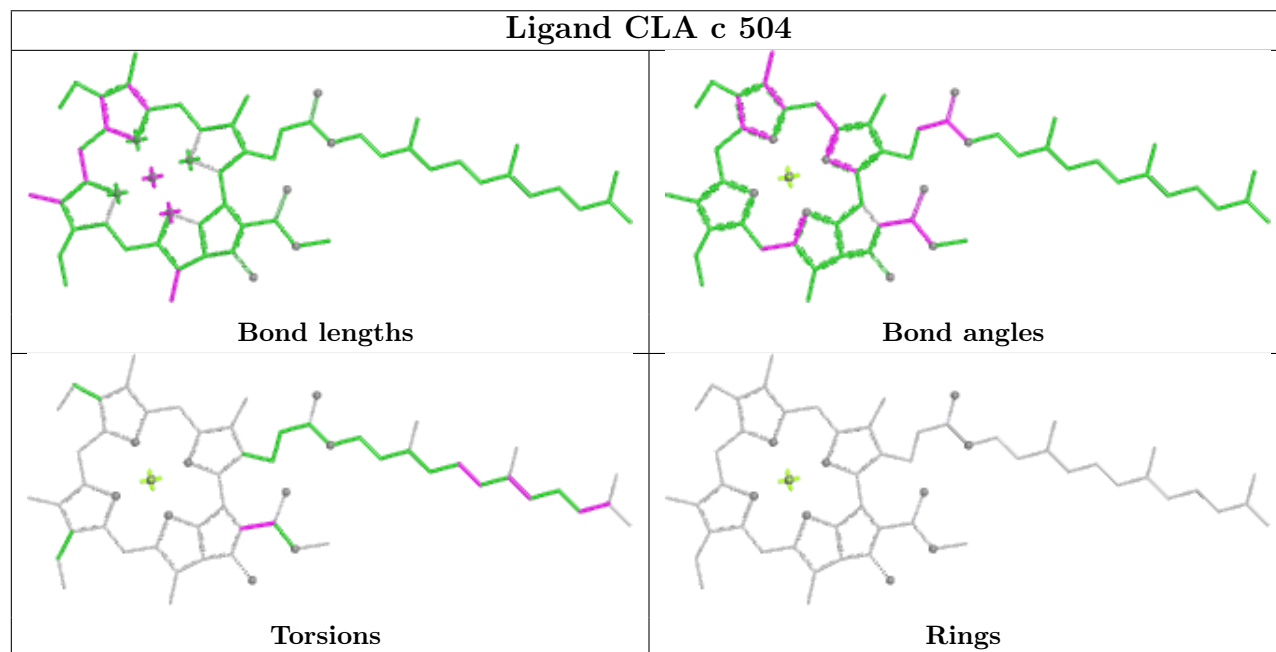
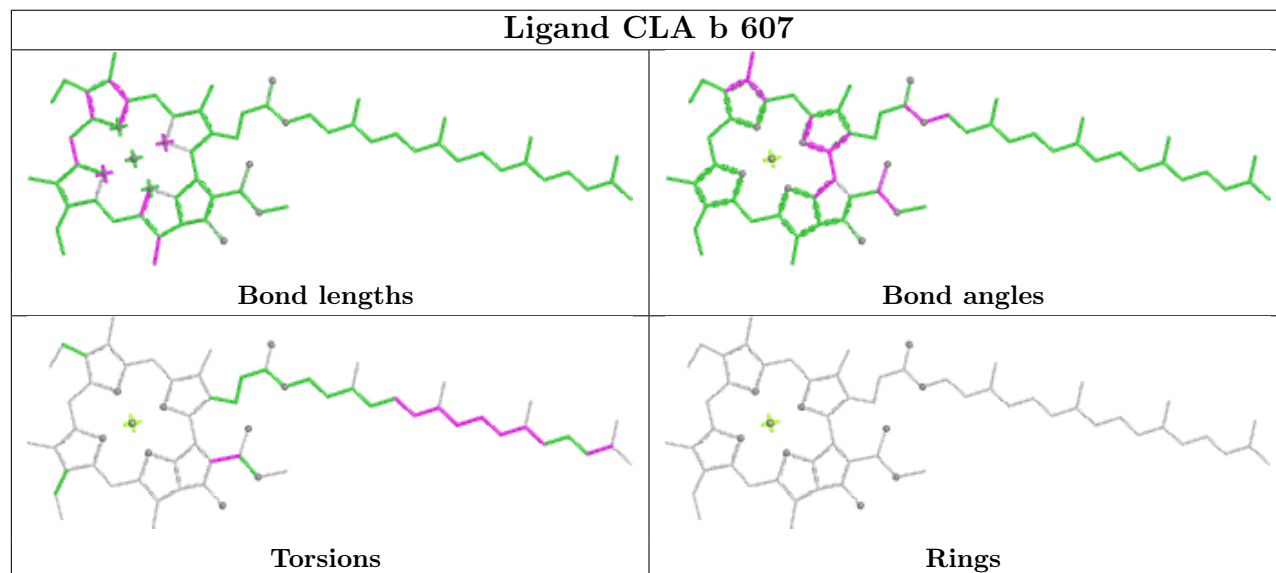
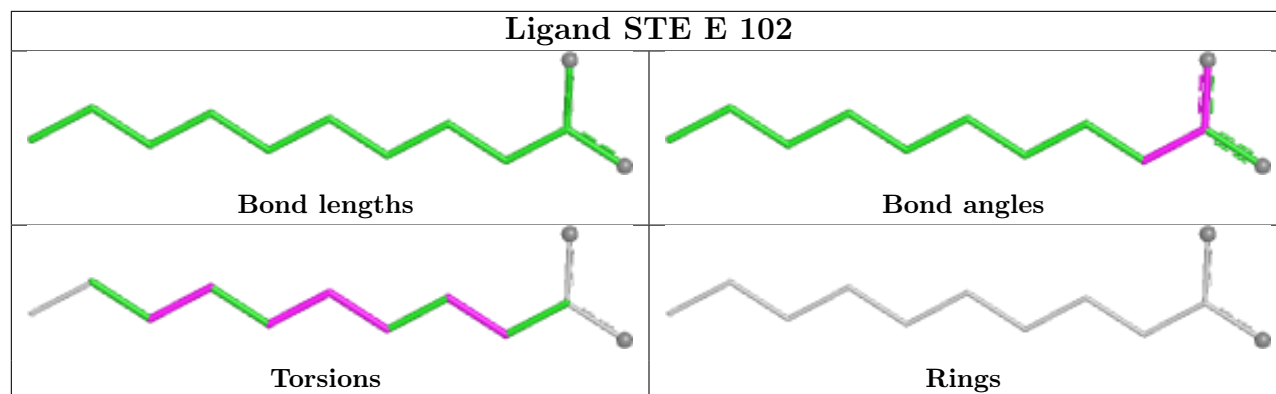


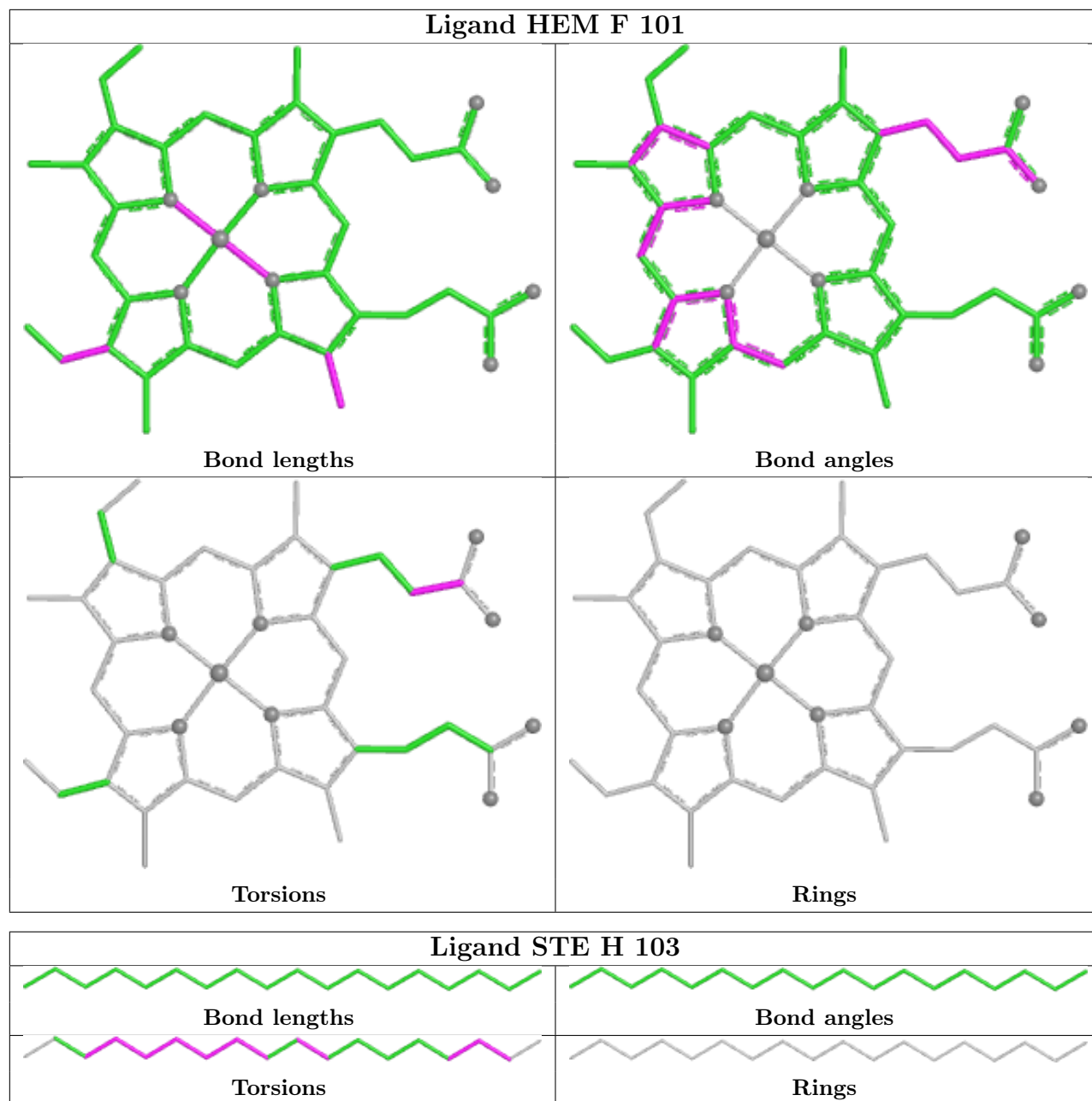
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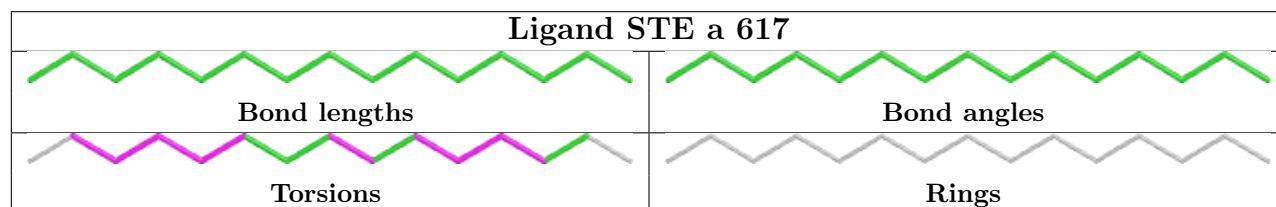
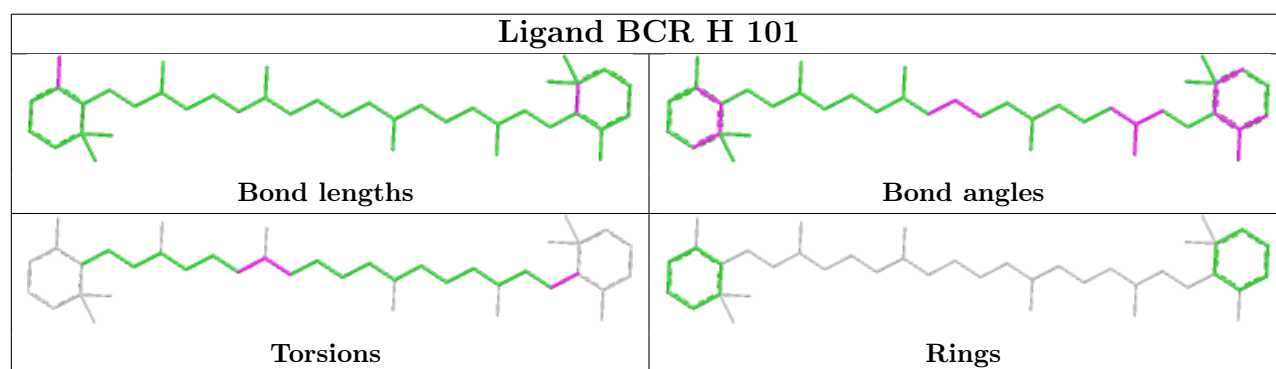
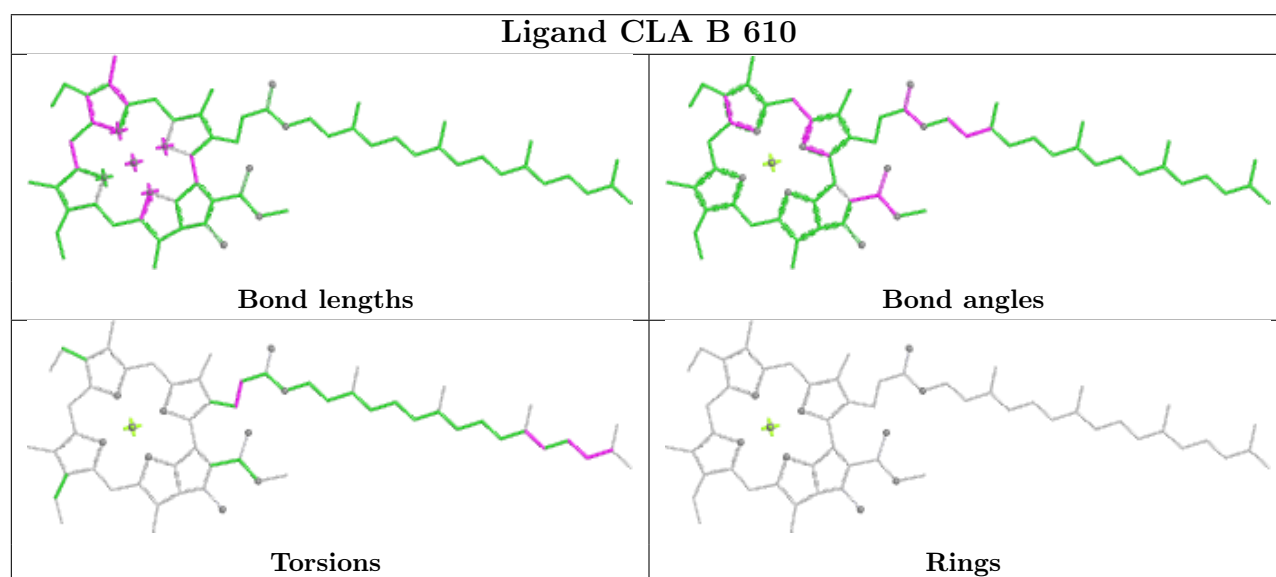
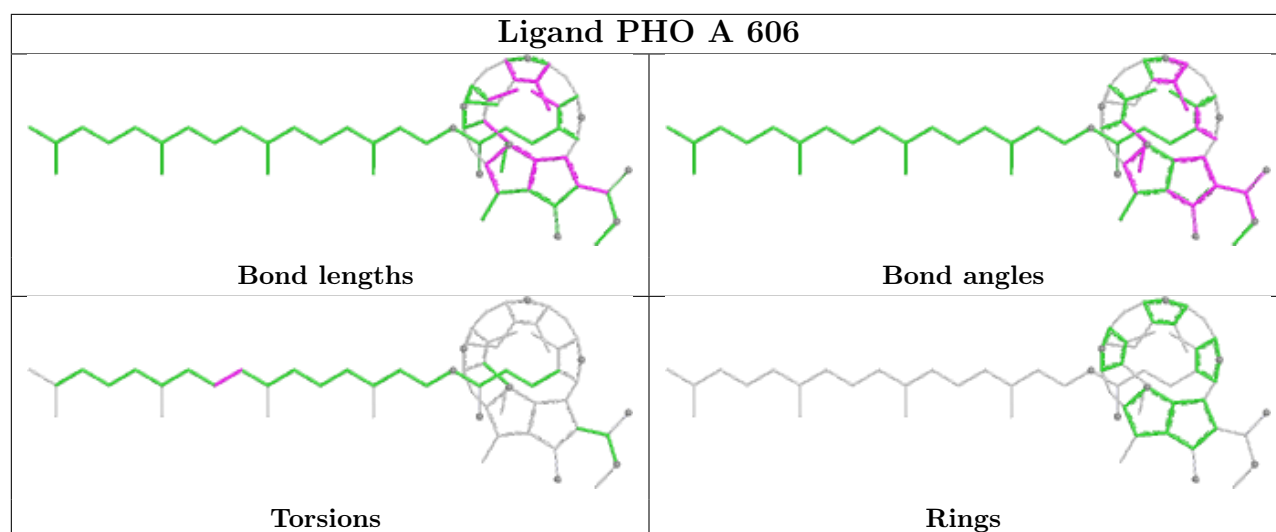


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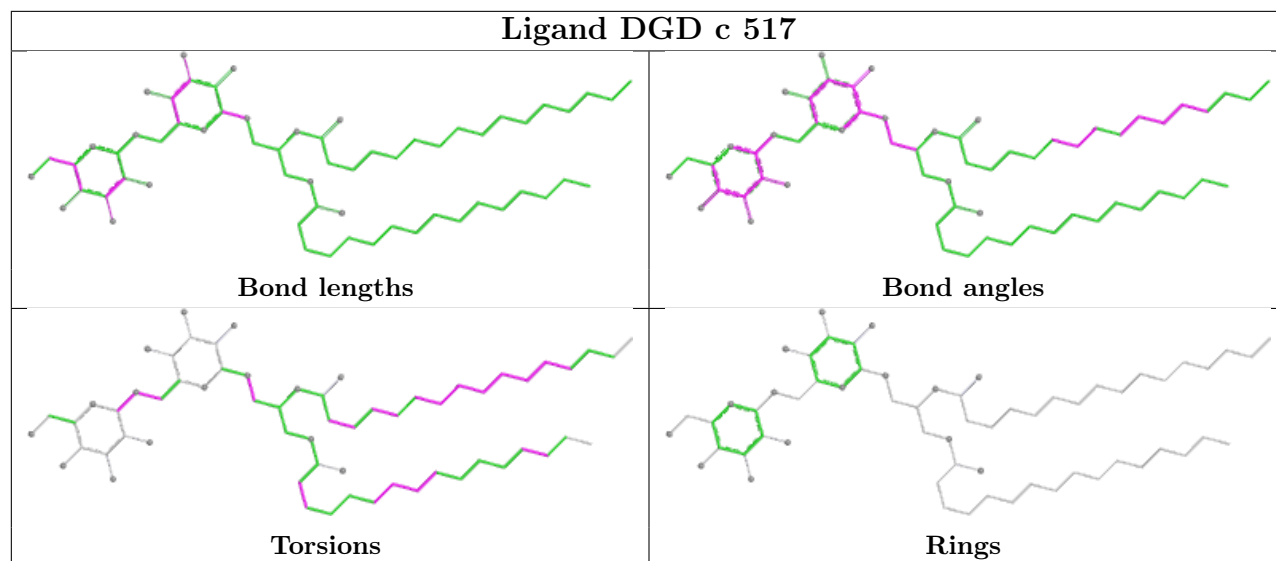




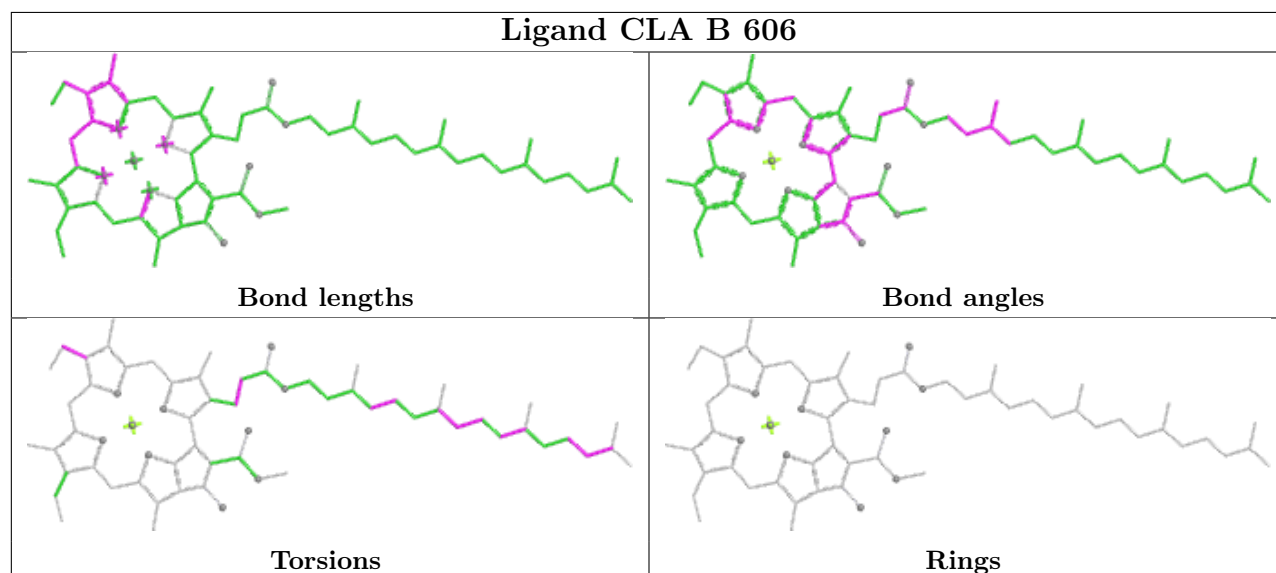




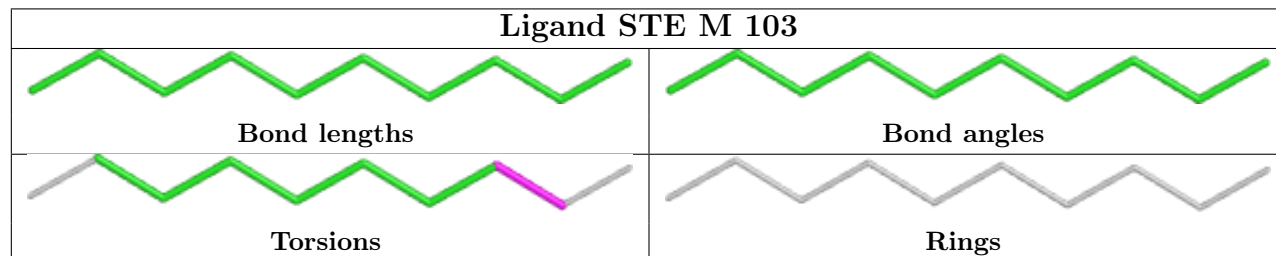
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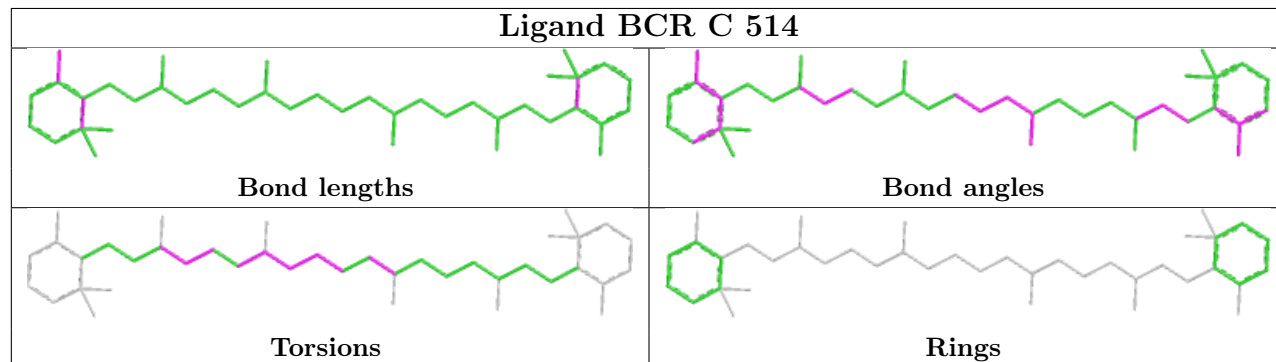
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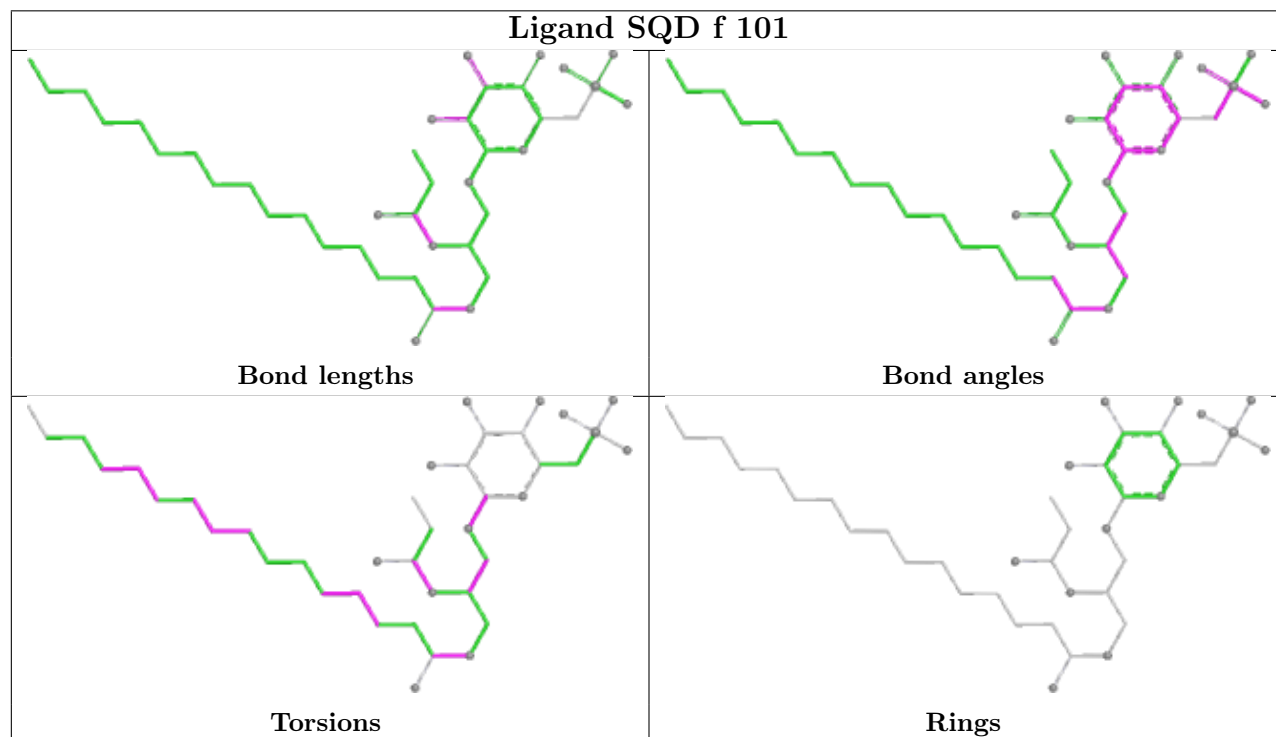
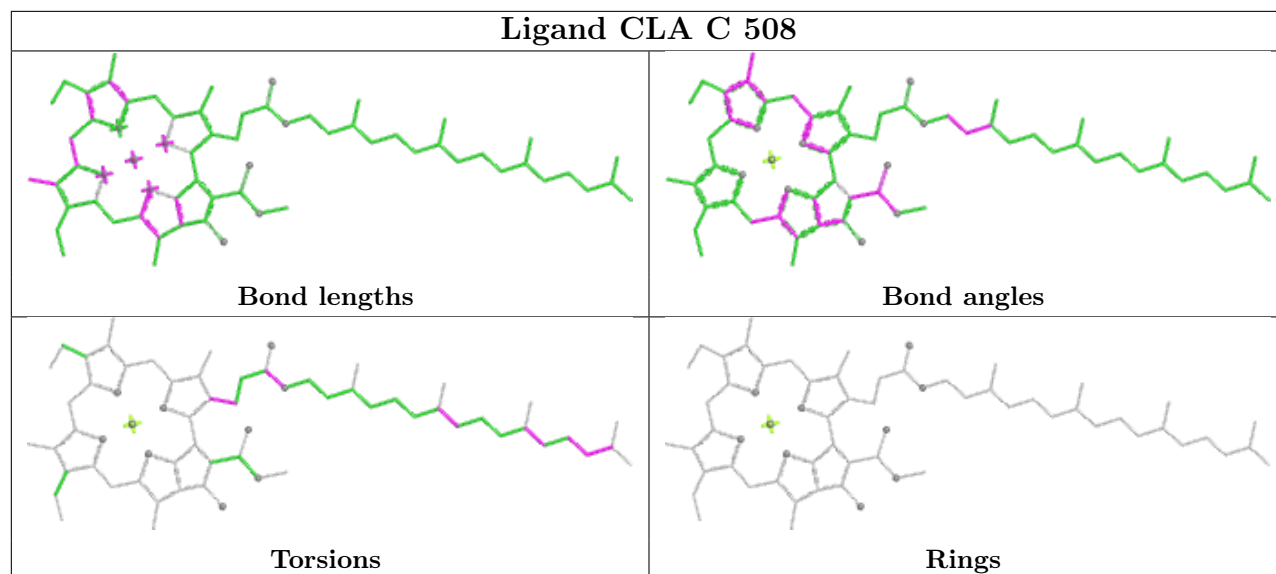


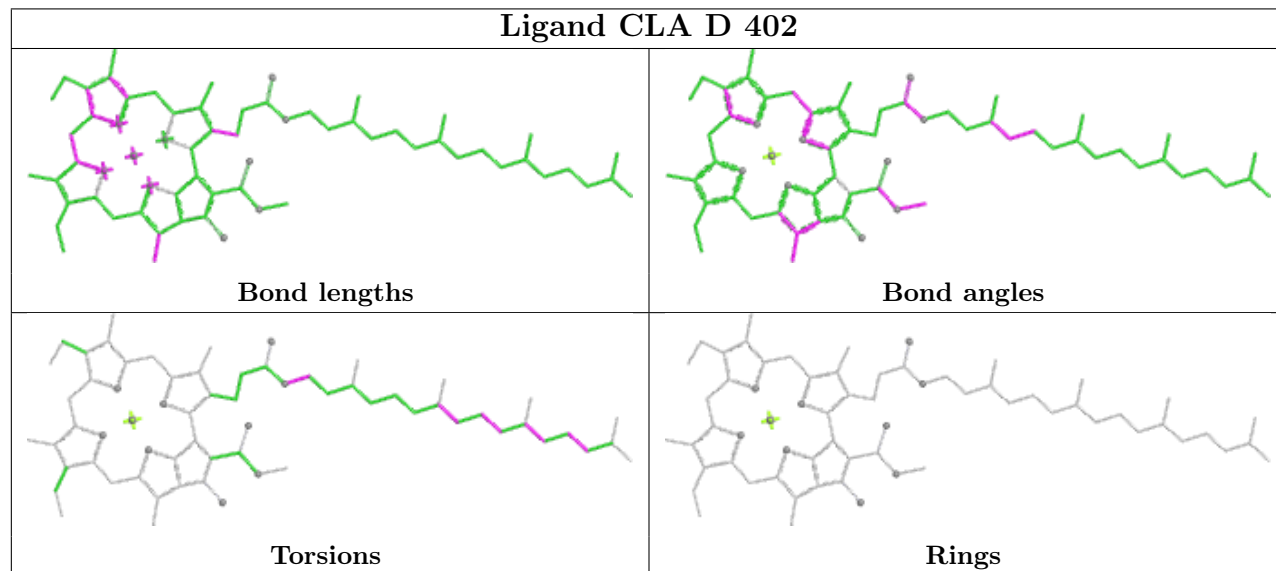
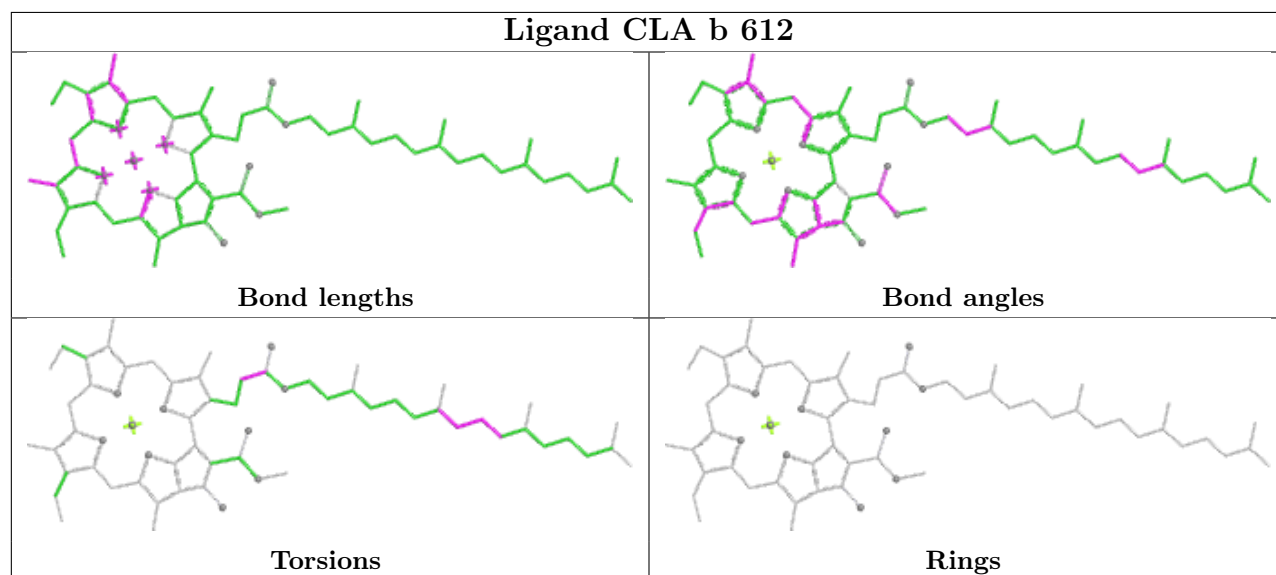
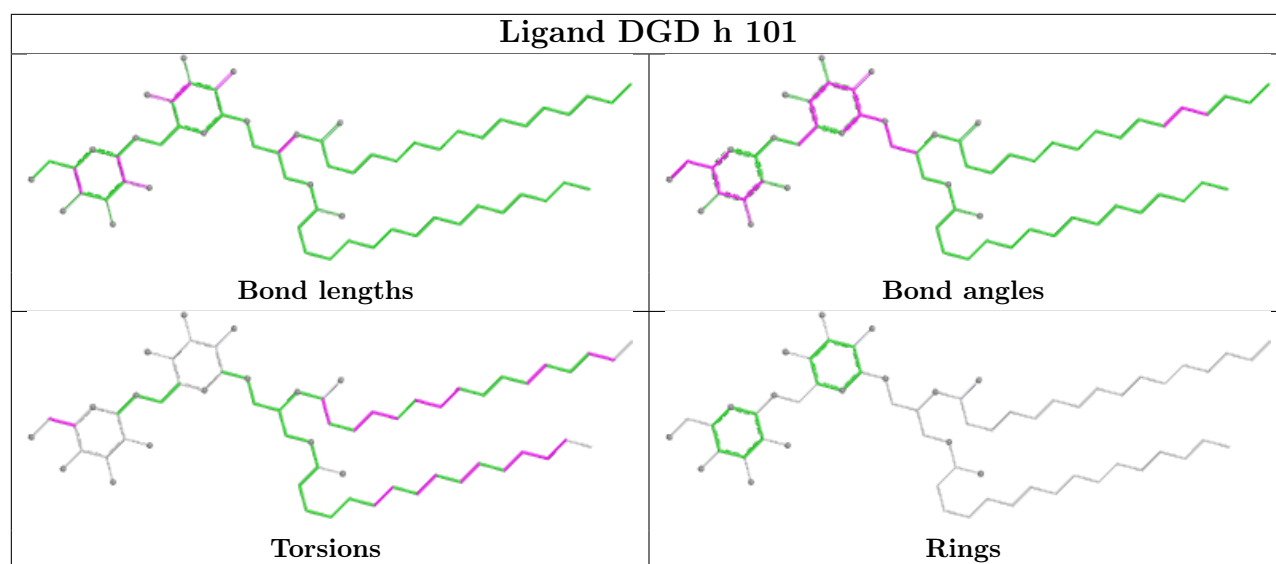
Ligand STE M 103

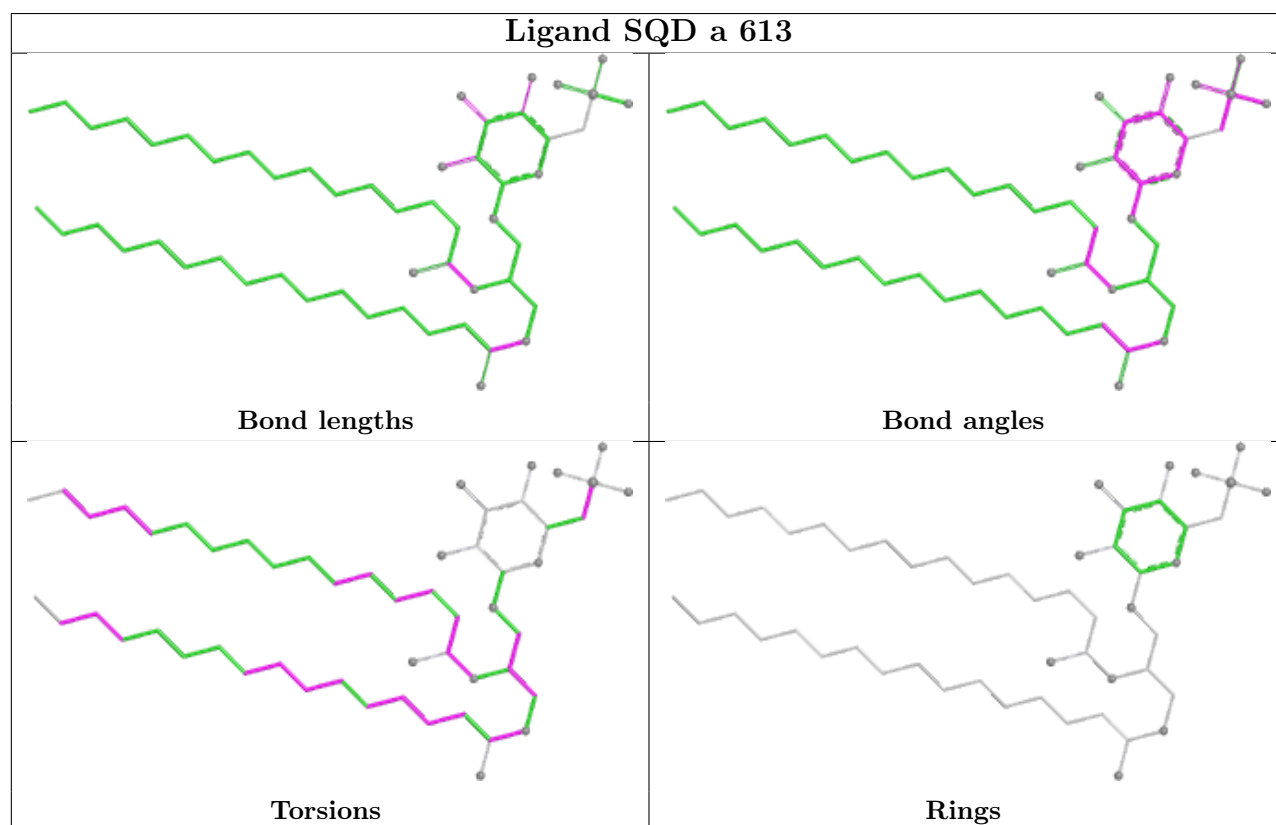
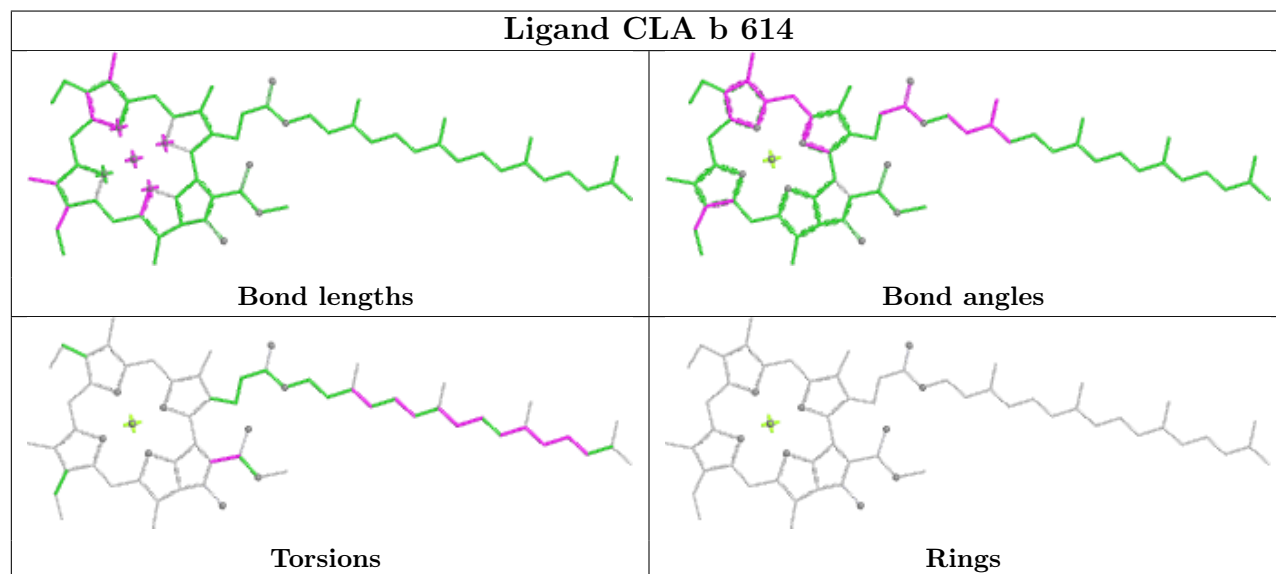
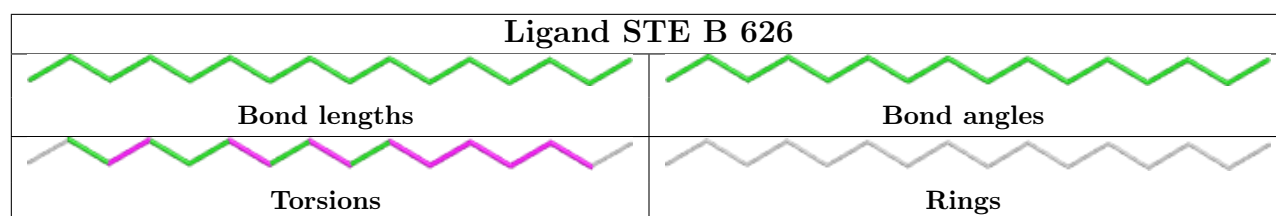


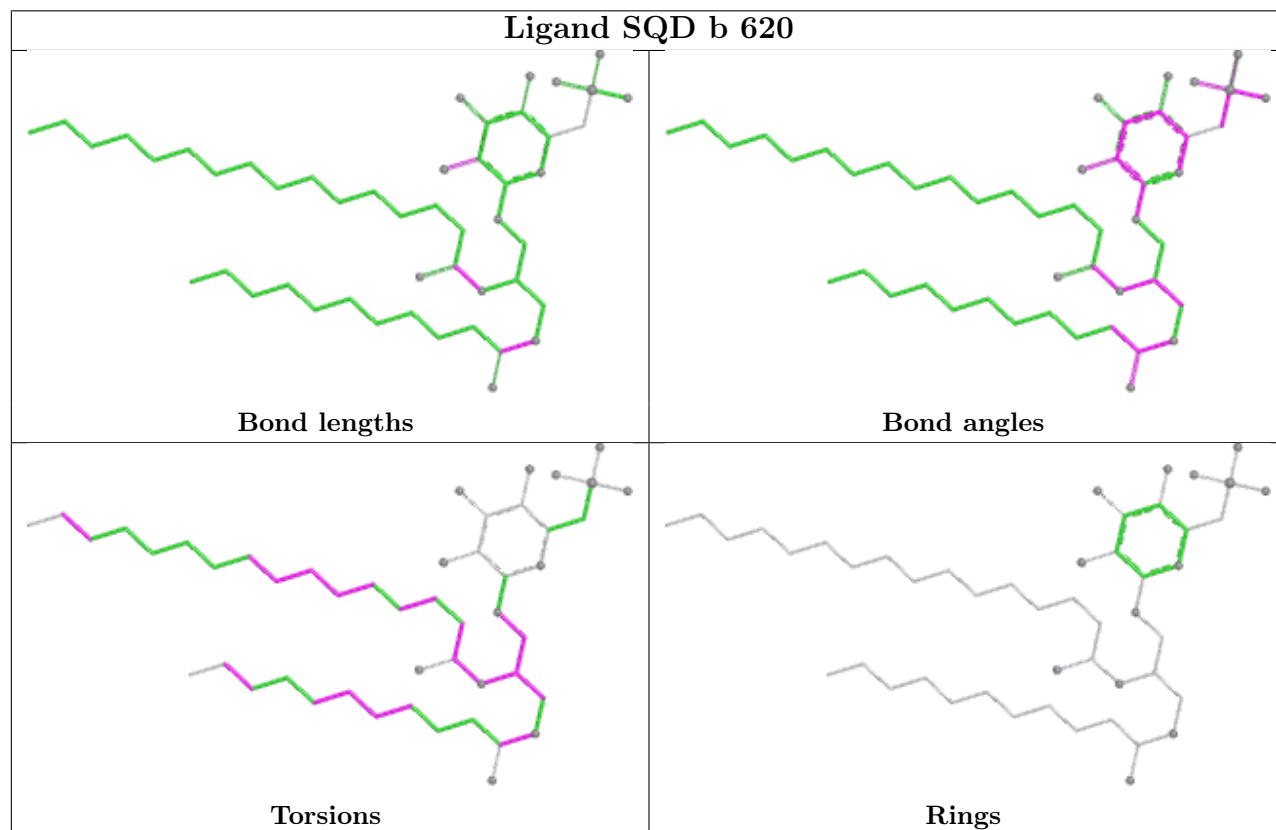
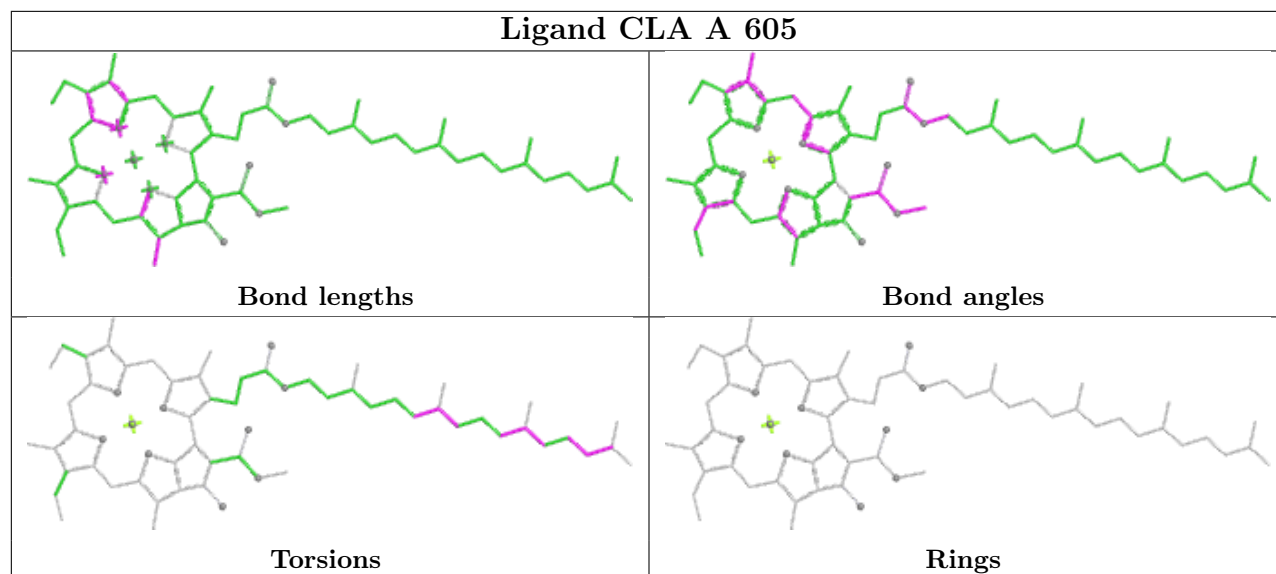
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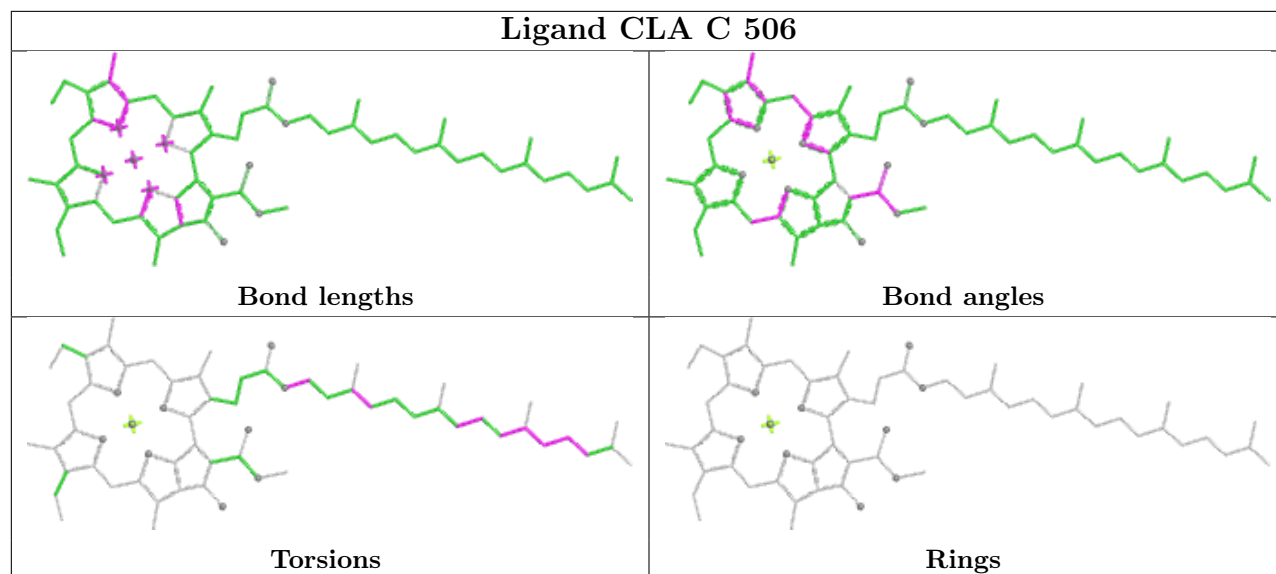




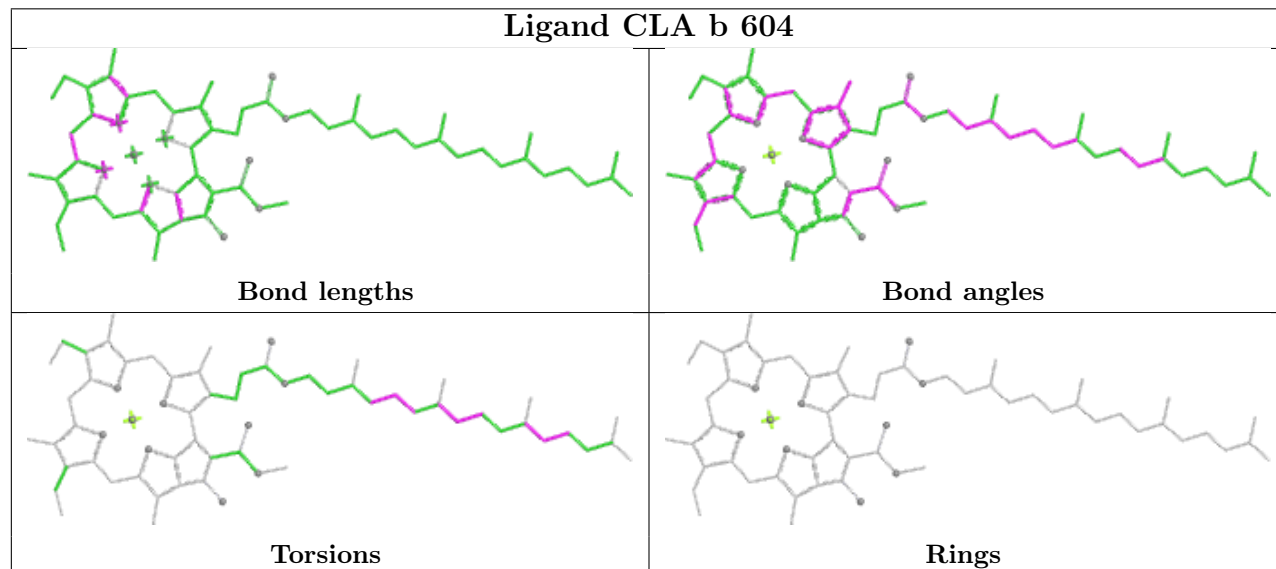


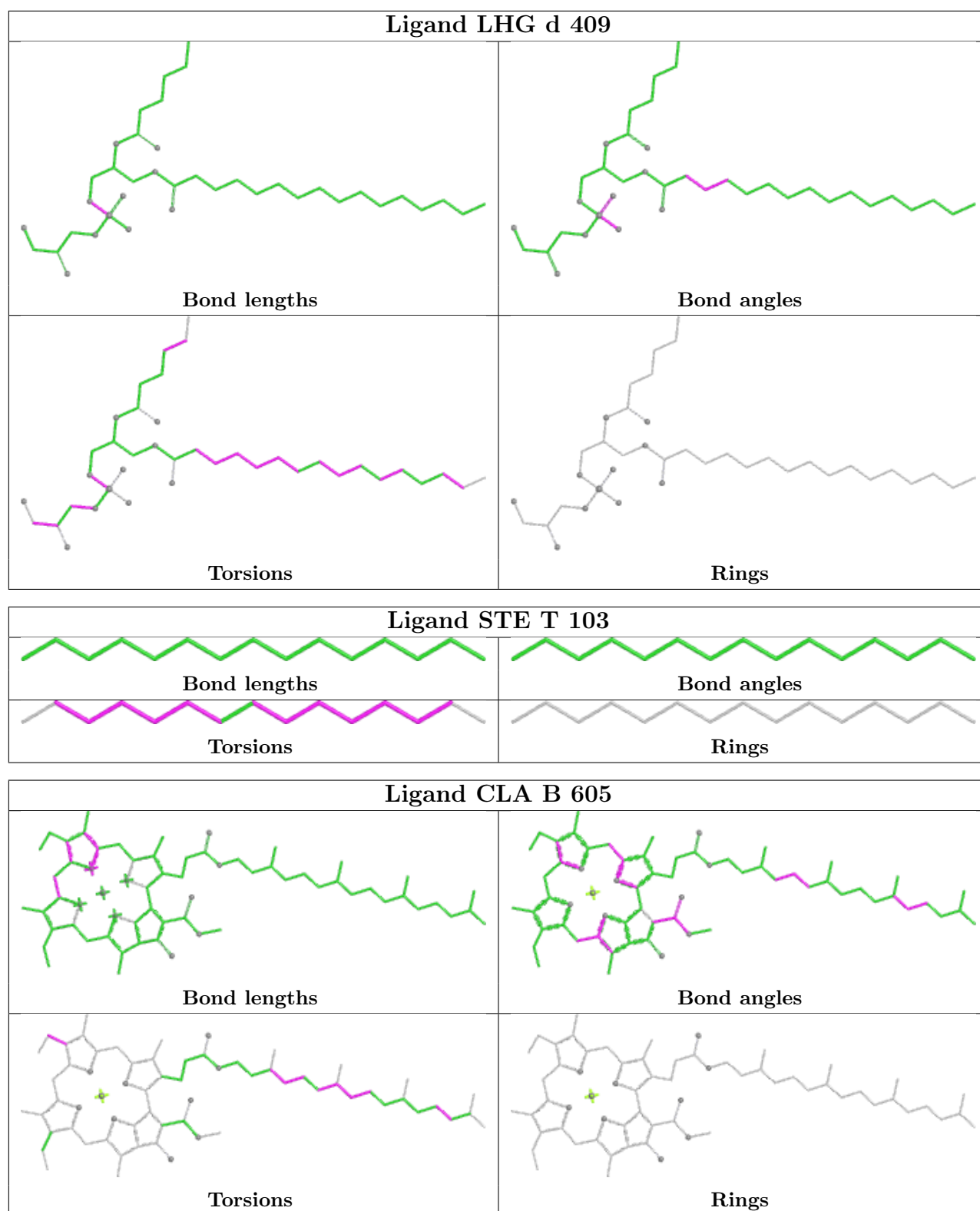


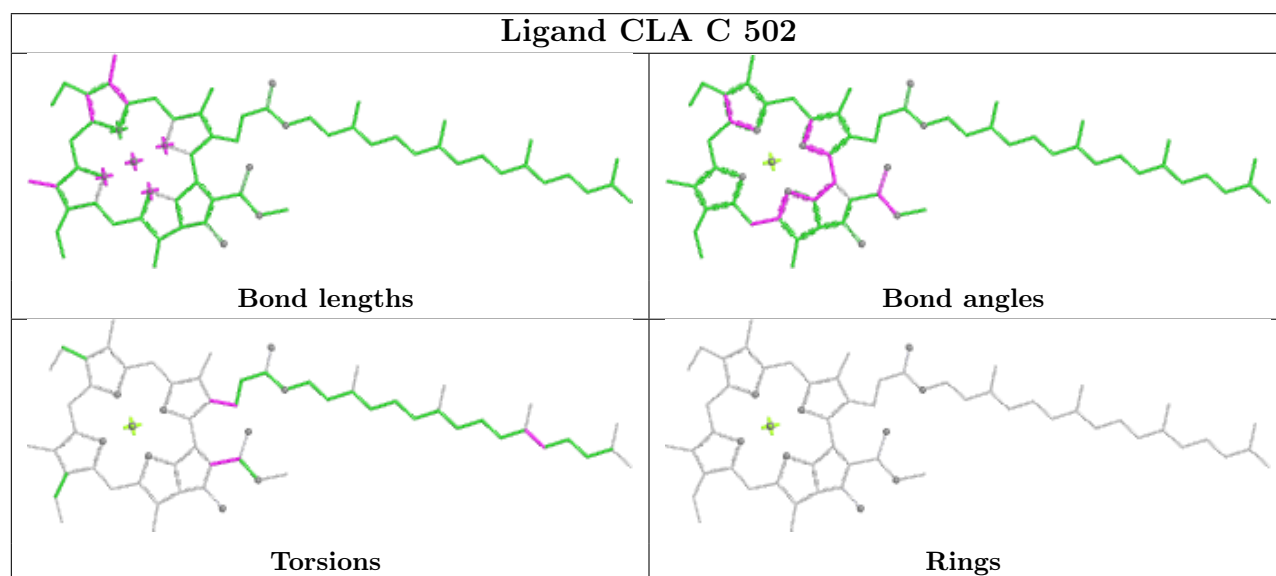
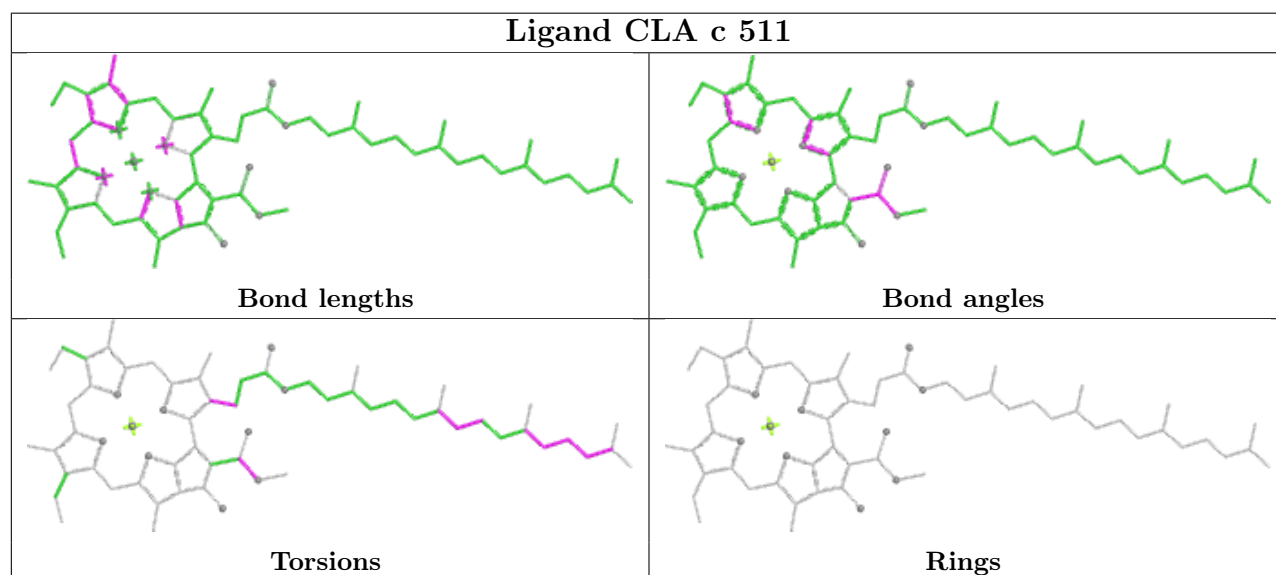
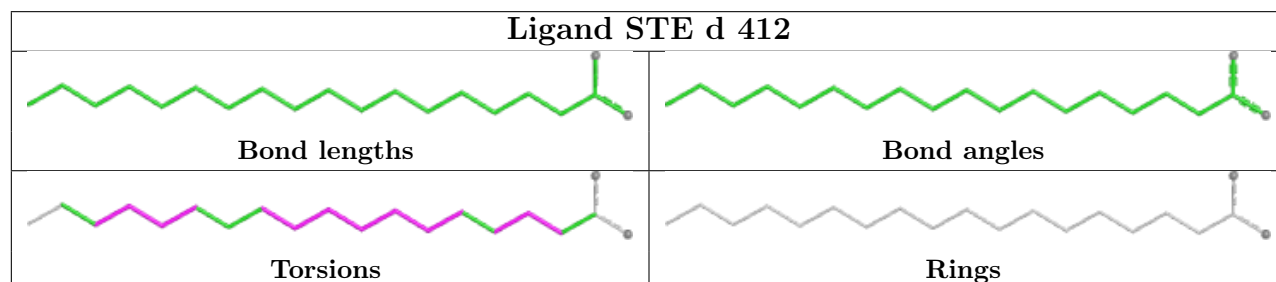
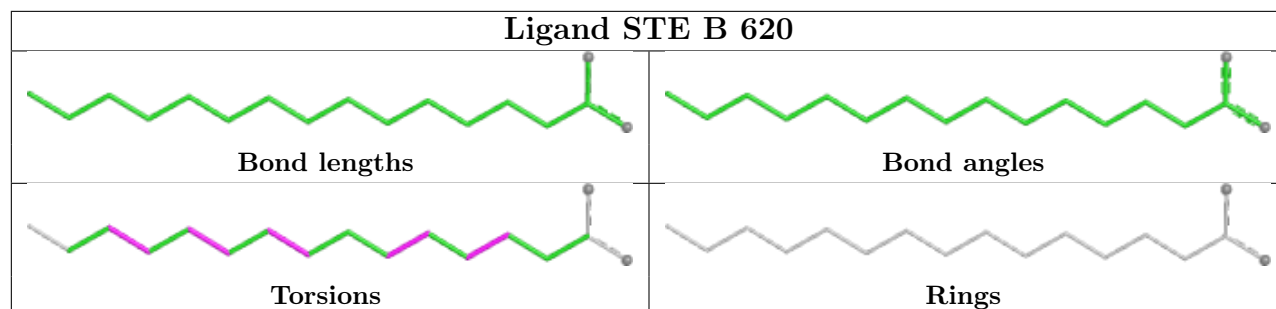
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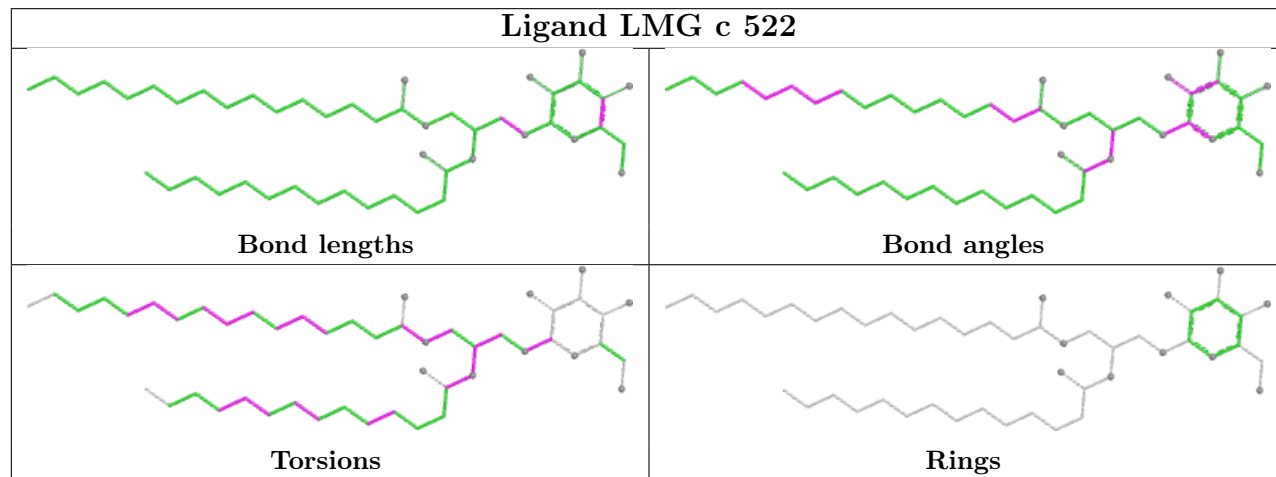
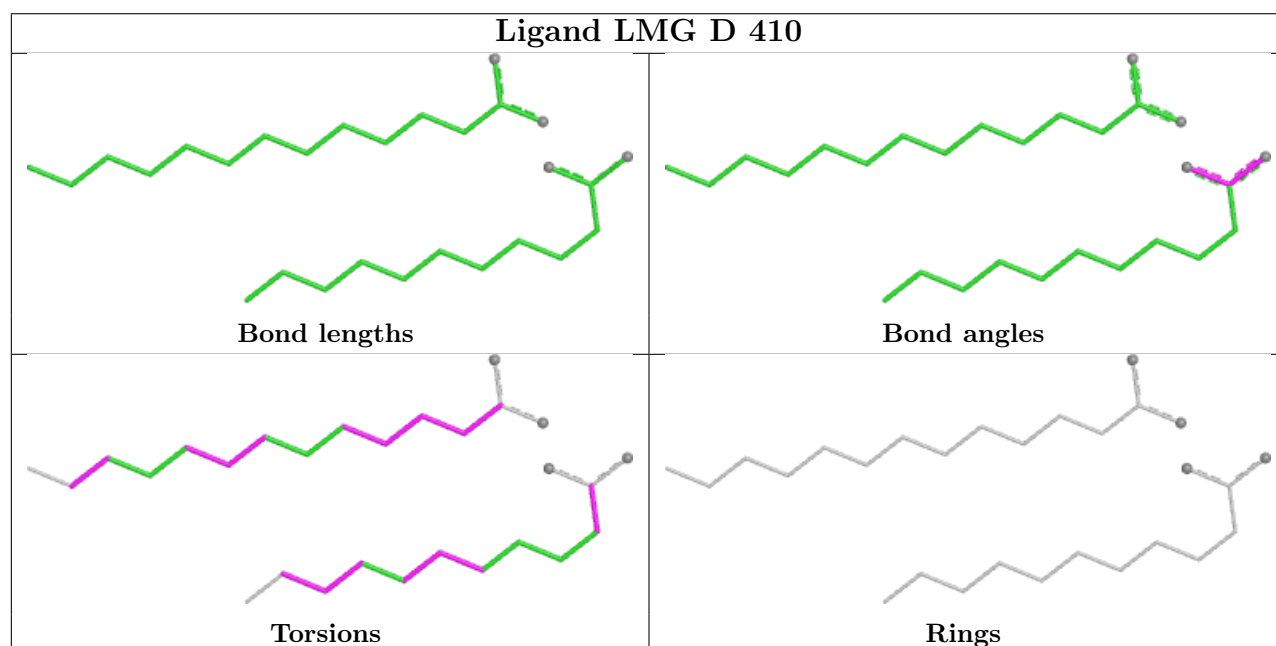
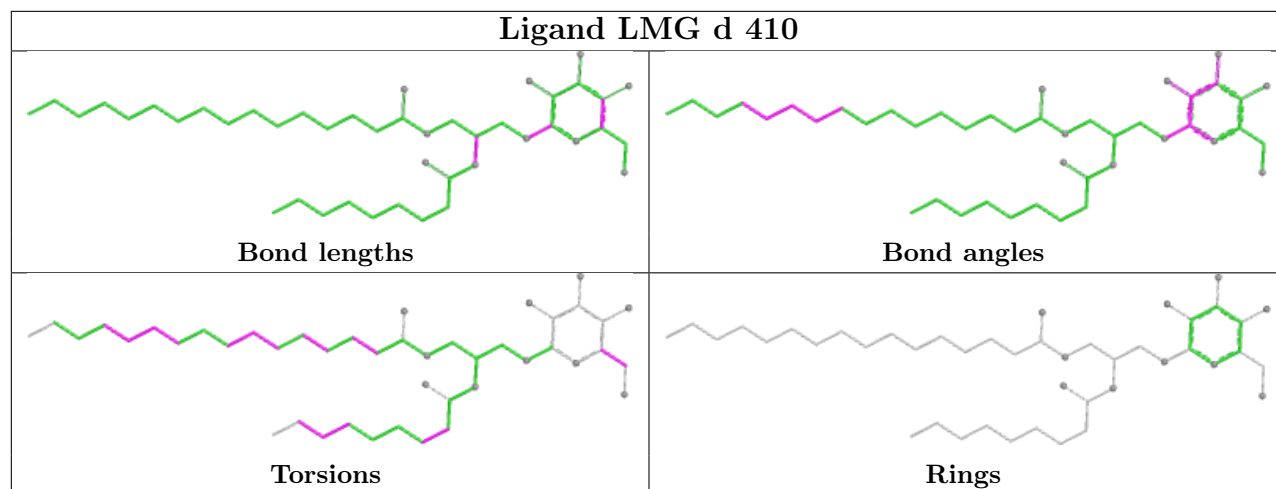


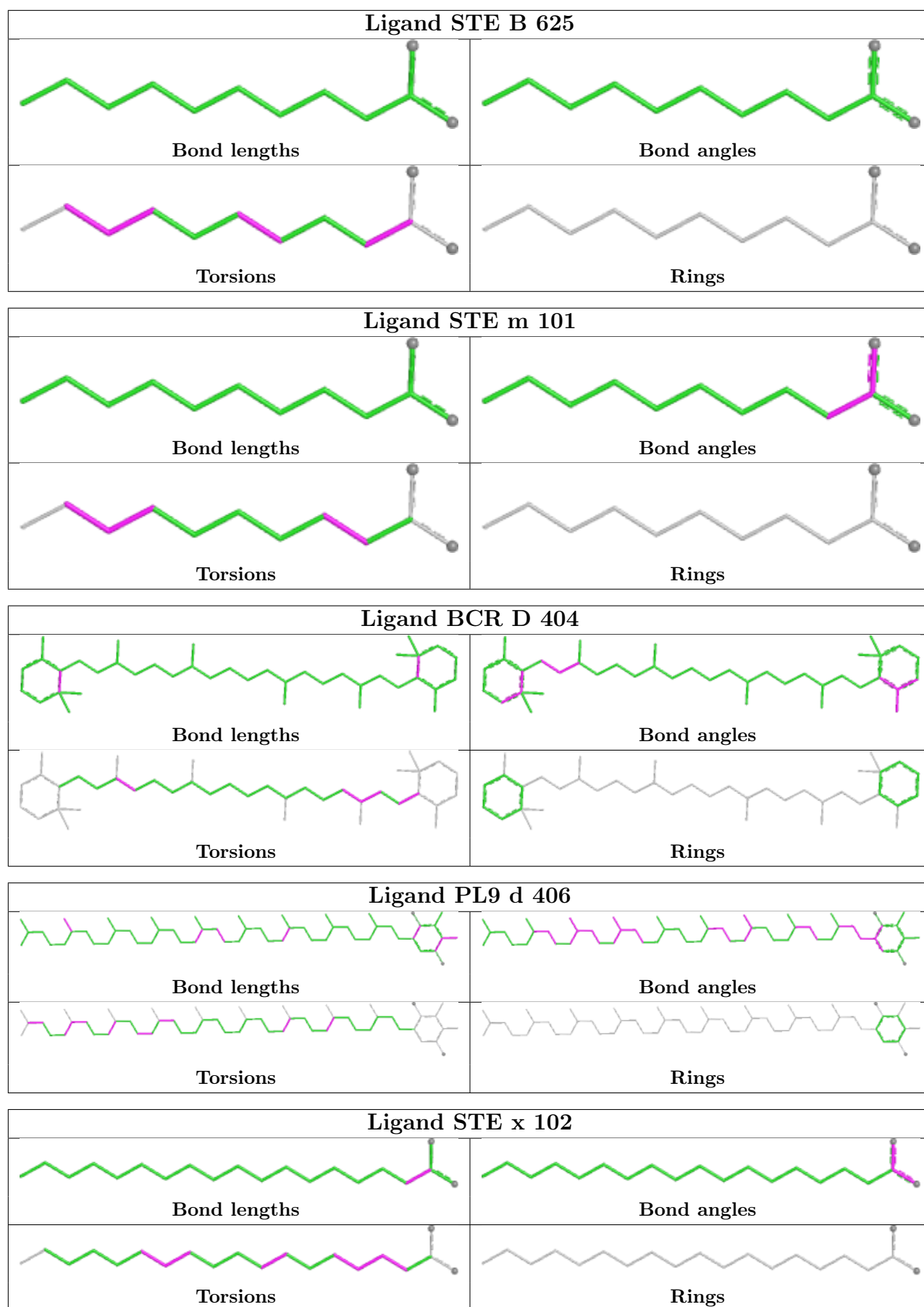
Ligand CLA b 604

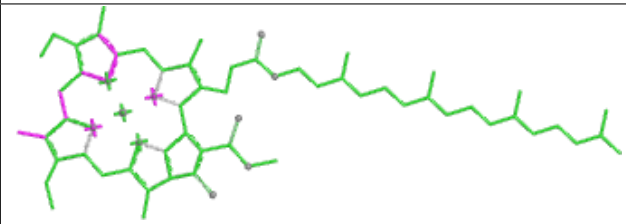
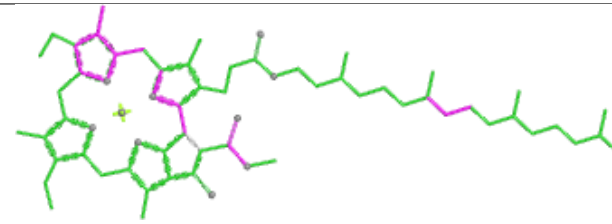
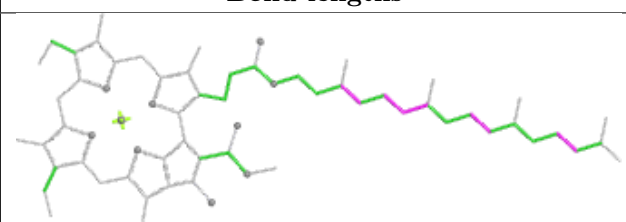
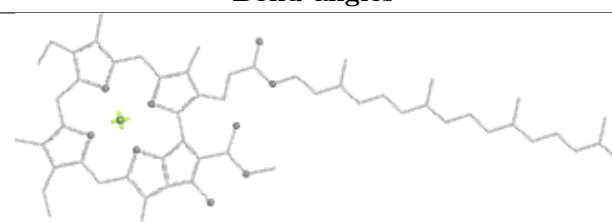


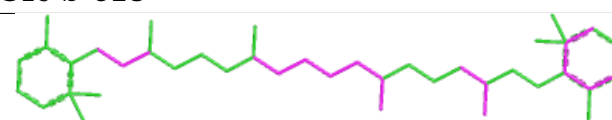
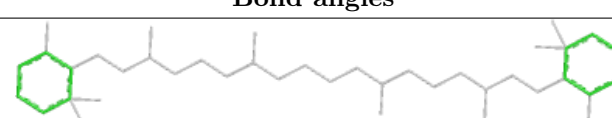


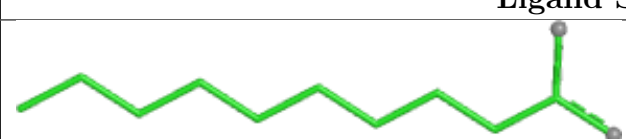
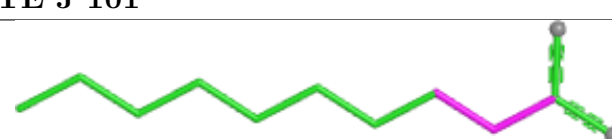
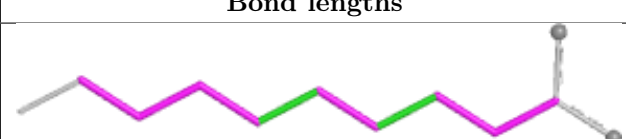
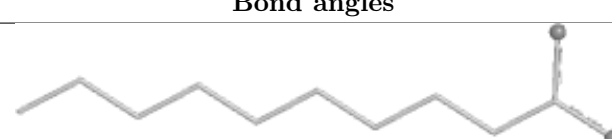


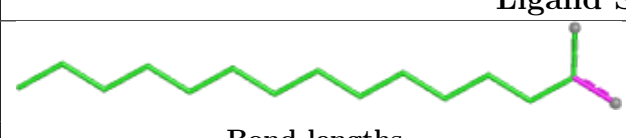
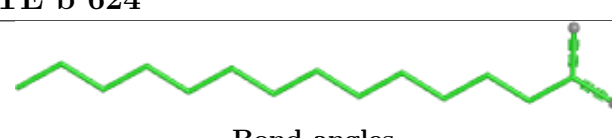
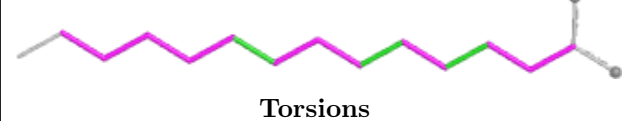
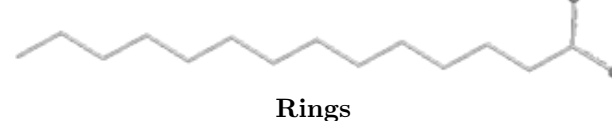


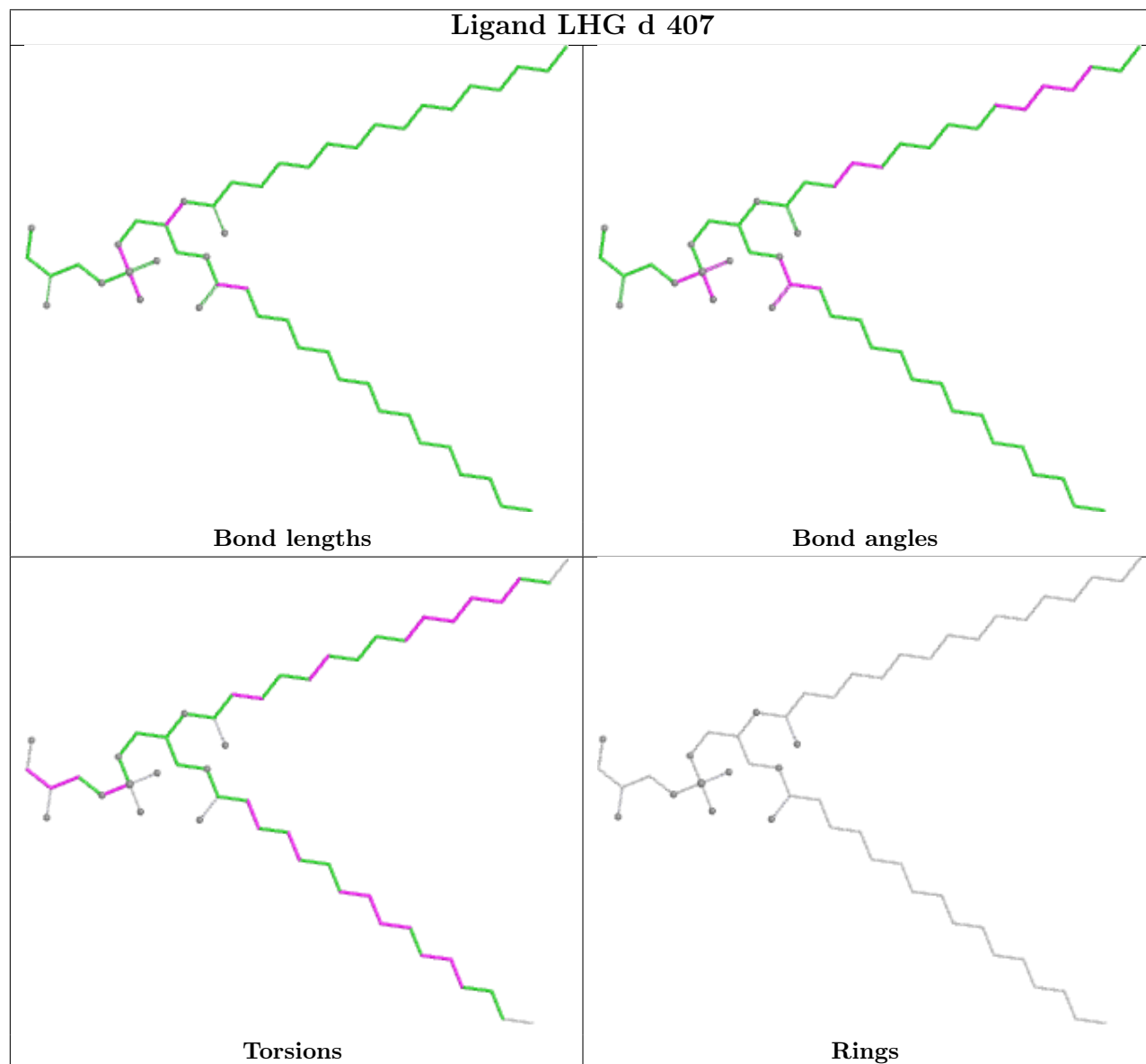
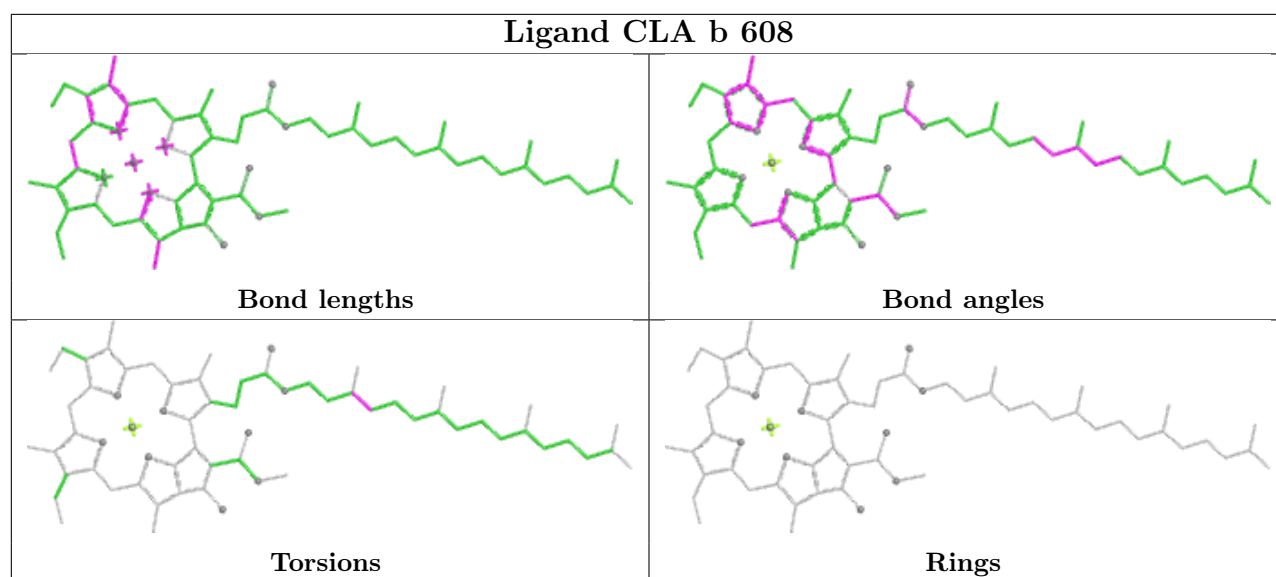


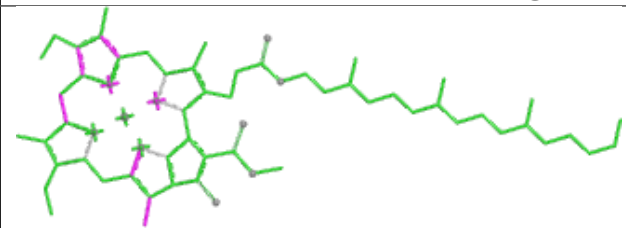
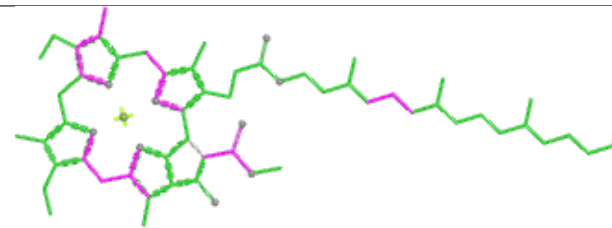
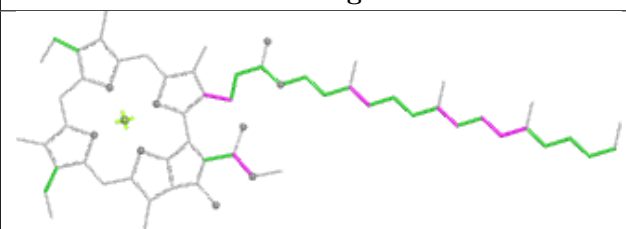
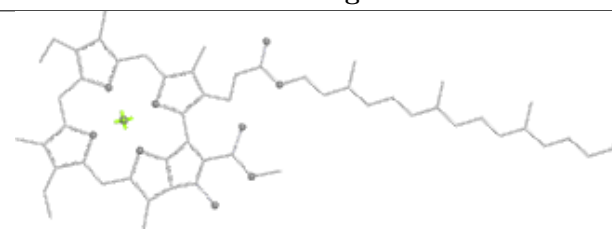
Ligand CLA C 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

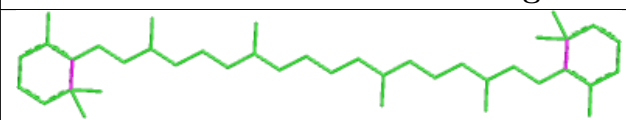
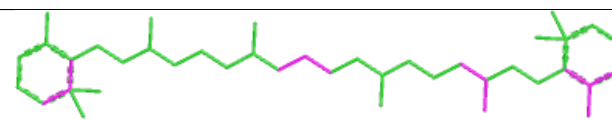
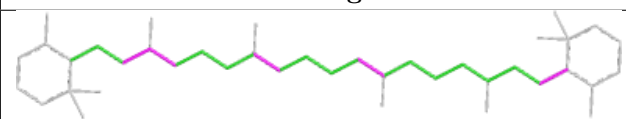
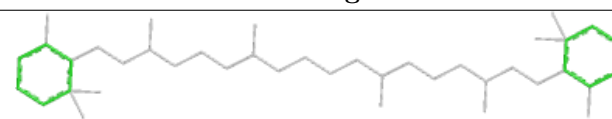
Ligand BCR b 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

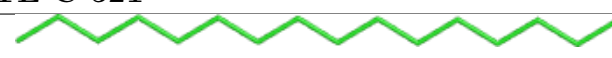
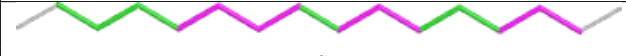
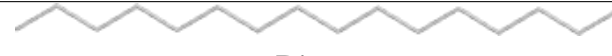
Ligand STE J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

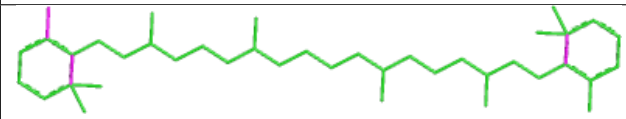
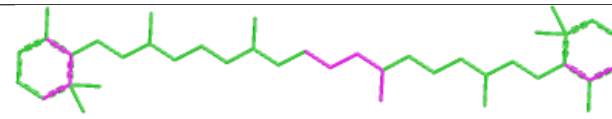
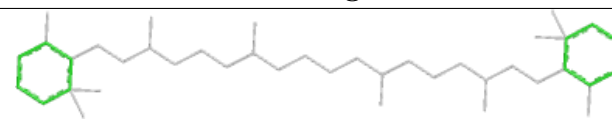
Ligand STE b 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

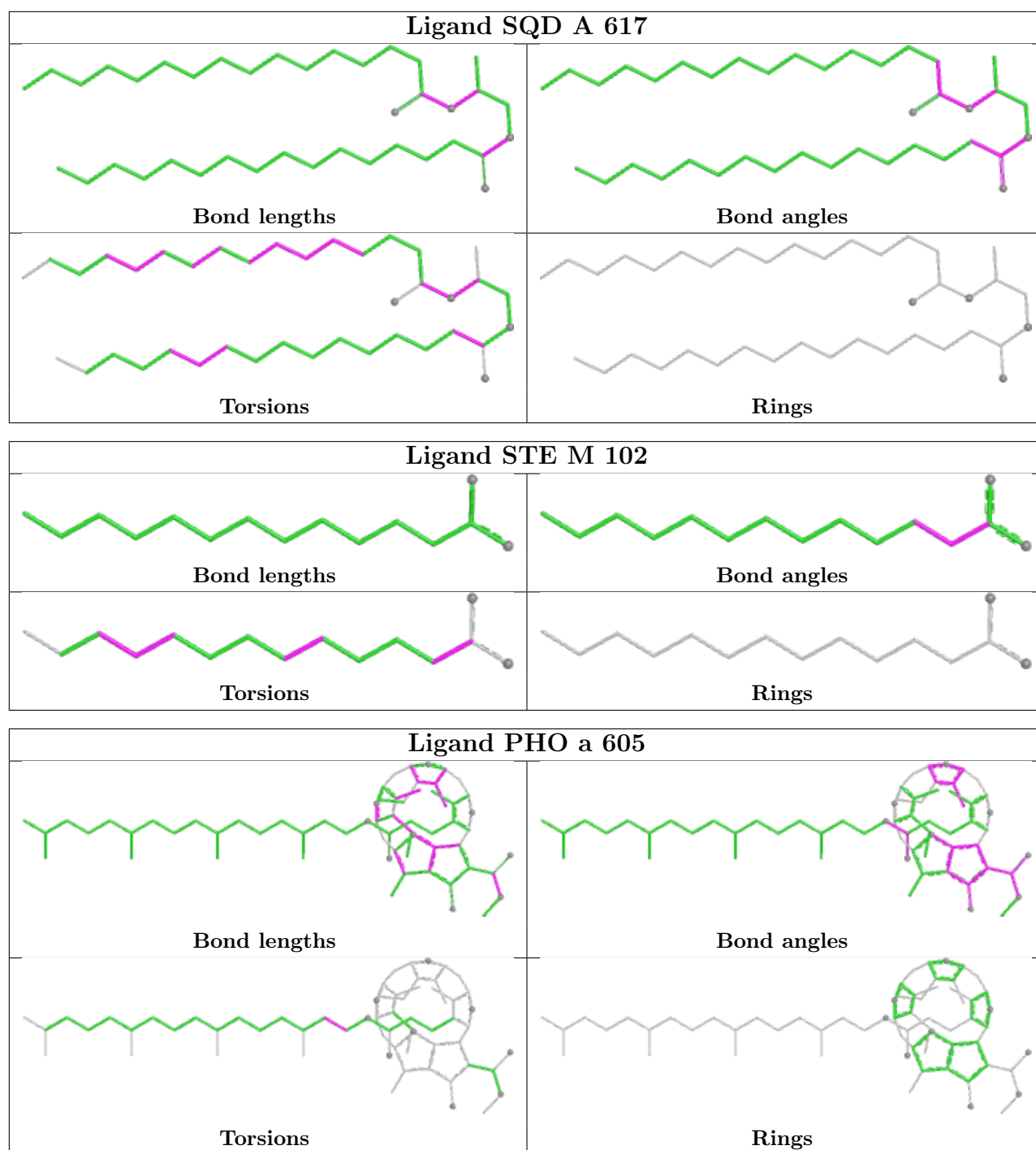


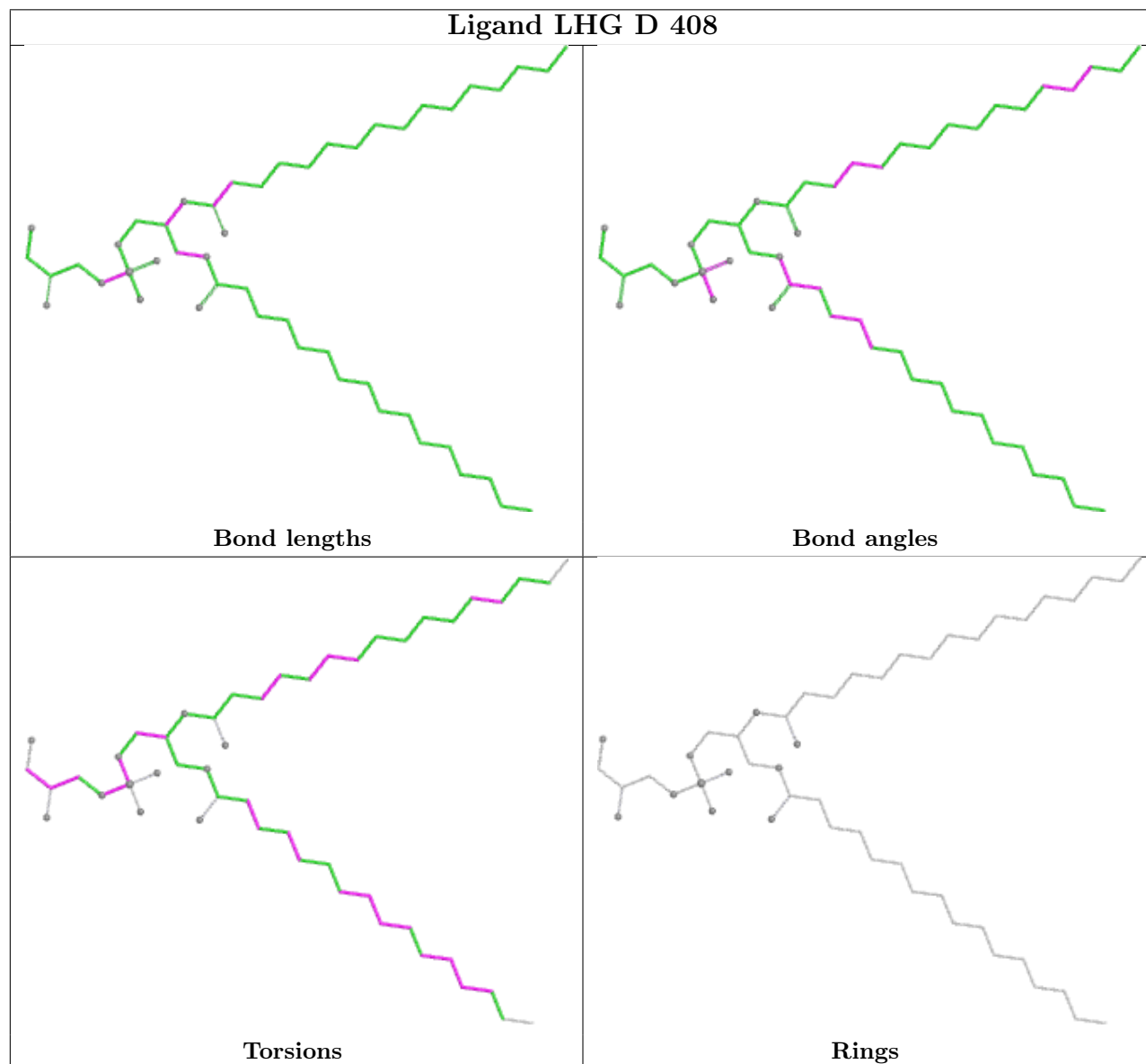
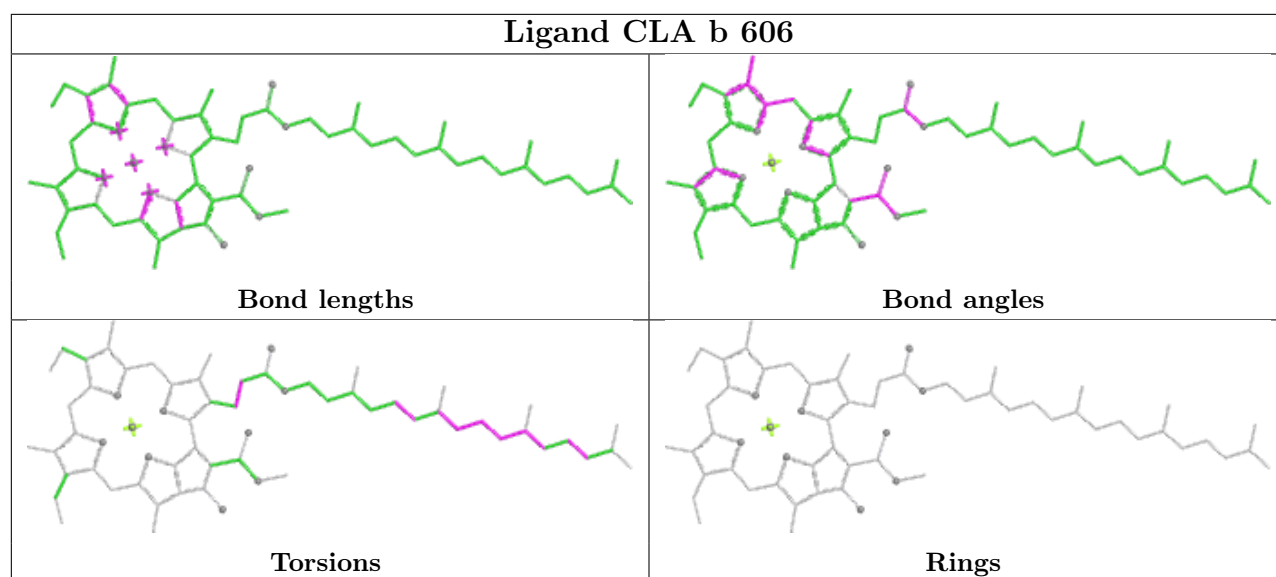
Ligand CLA c 508	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR x 101	
	Bond lengths
	Bond angles
	Torsions
	Rings

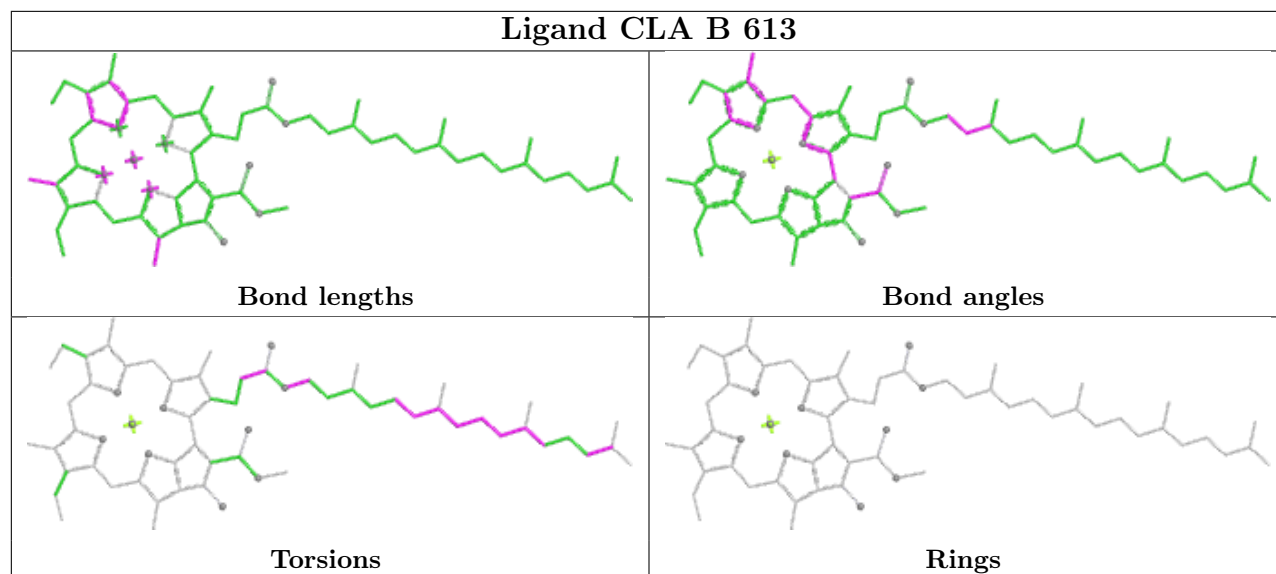
Ligand STE C 521	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR C 515	
	Bond lengths
	Bond angles
	Torsions
	Rings

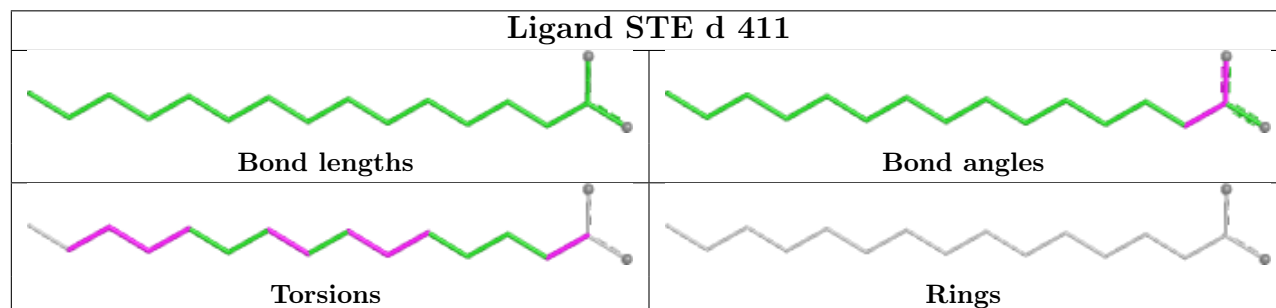




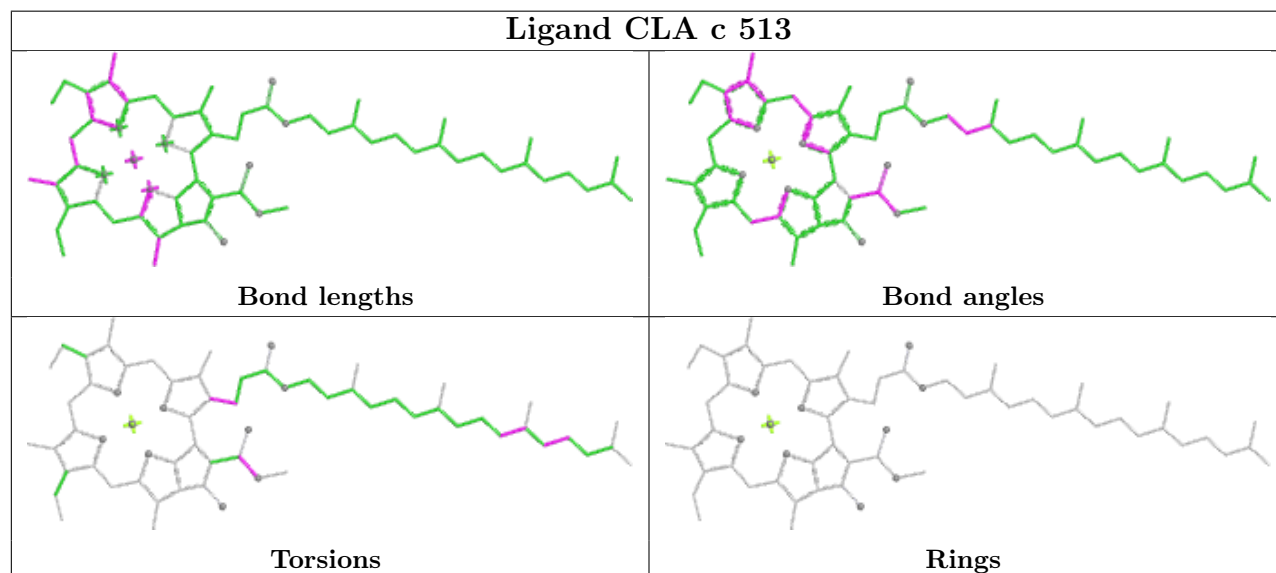
Ligand CLA B 613



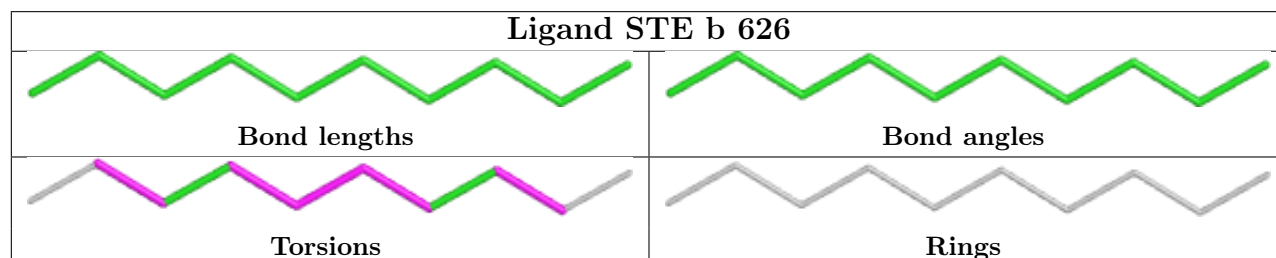
Ligand STE d 411

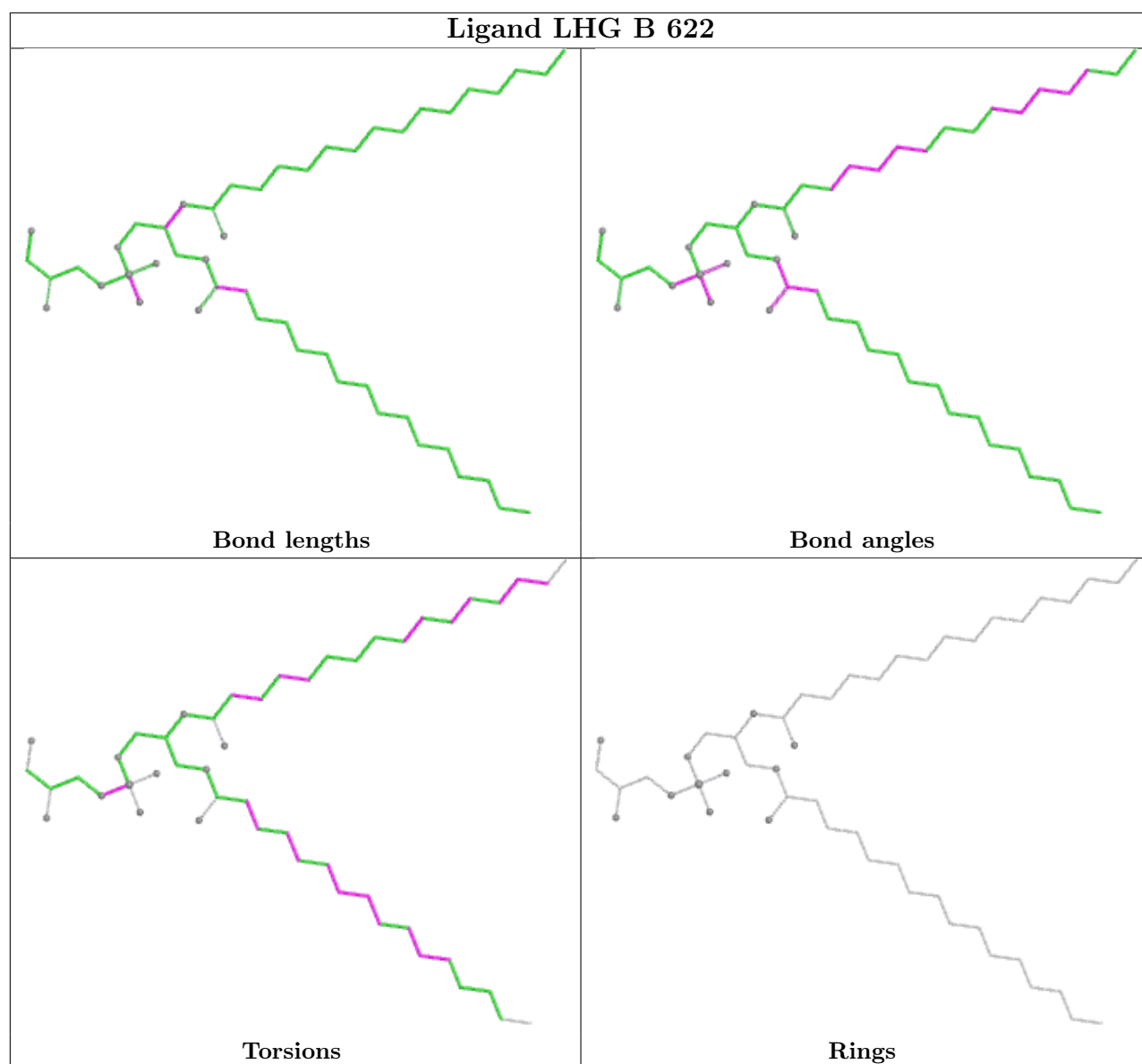


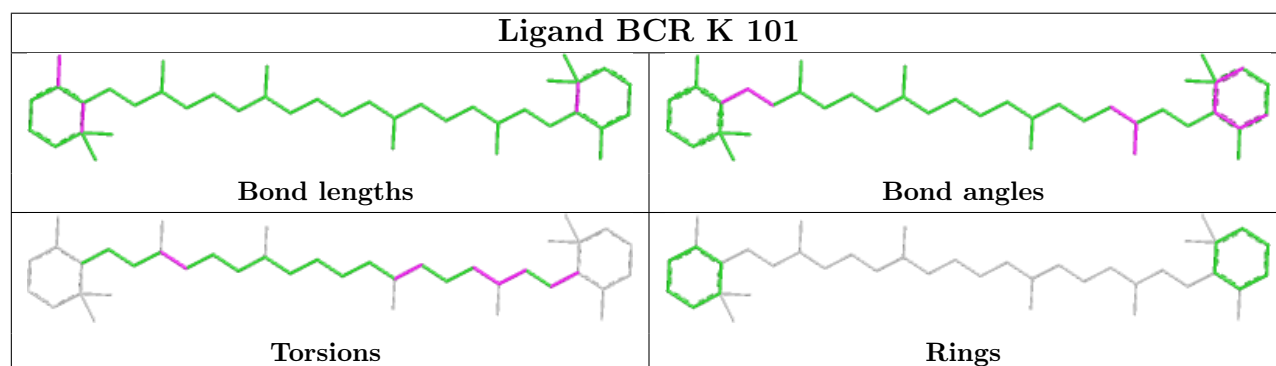
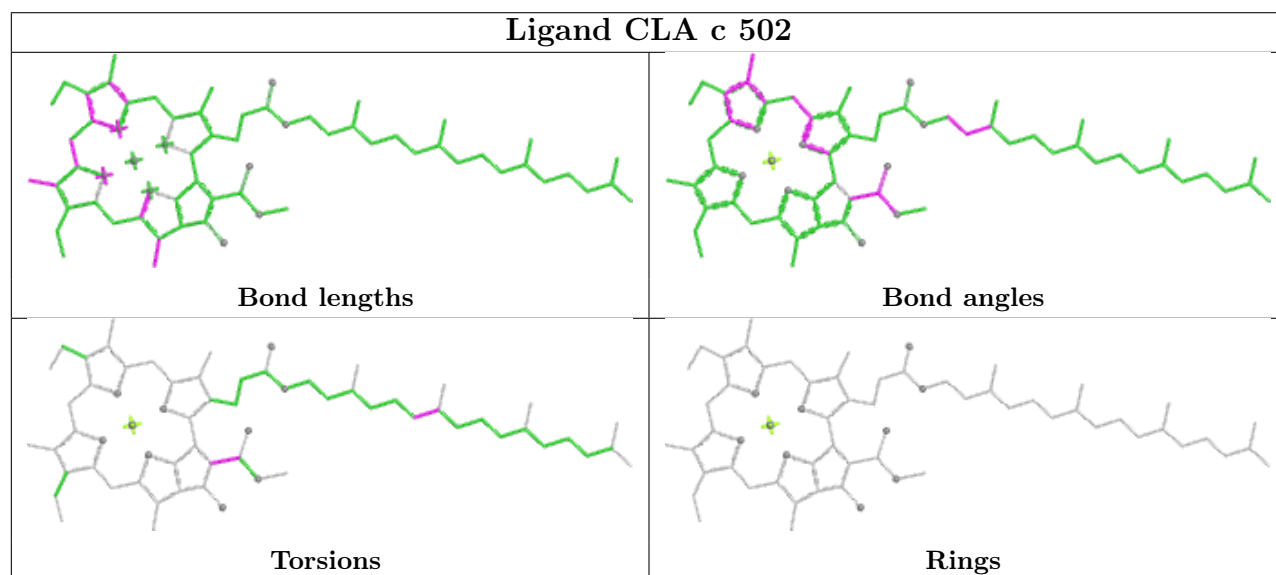
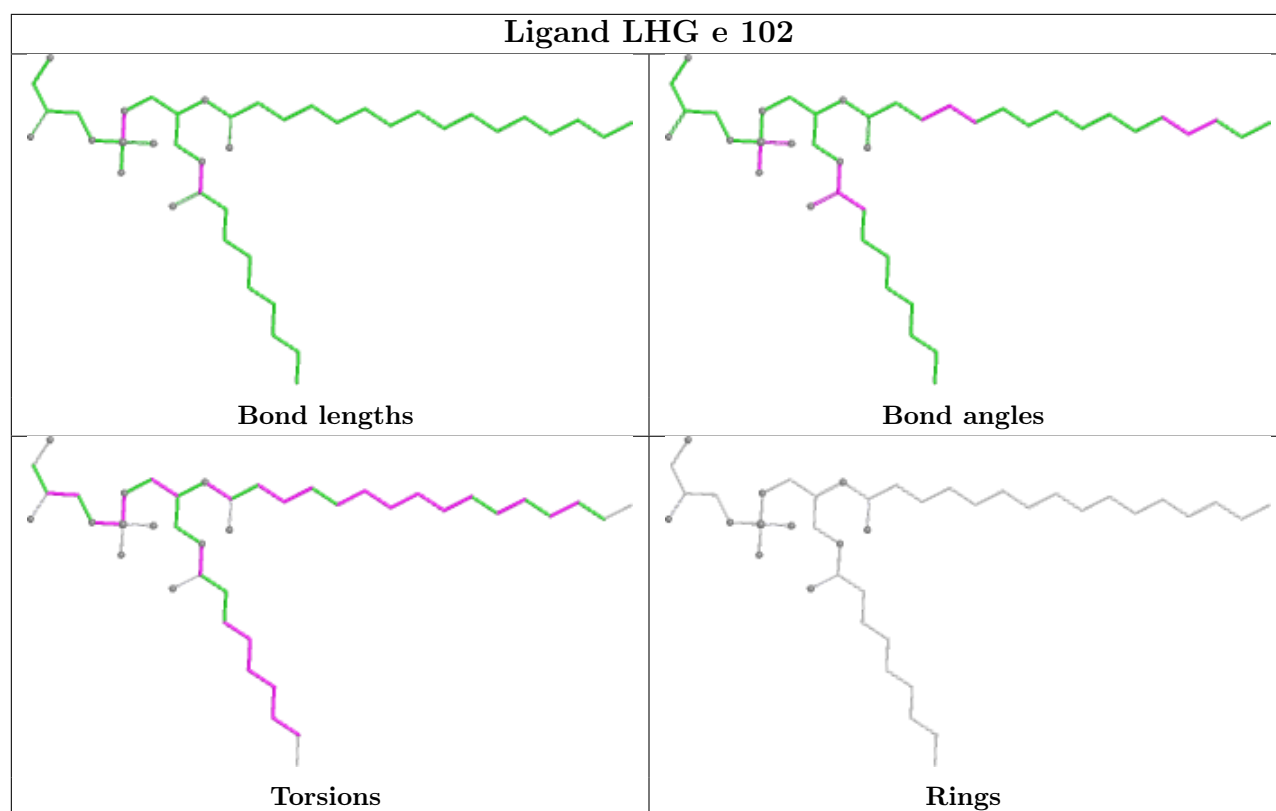
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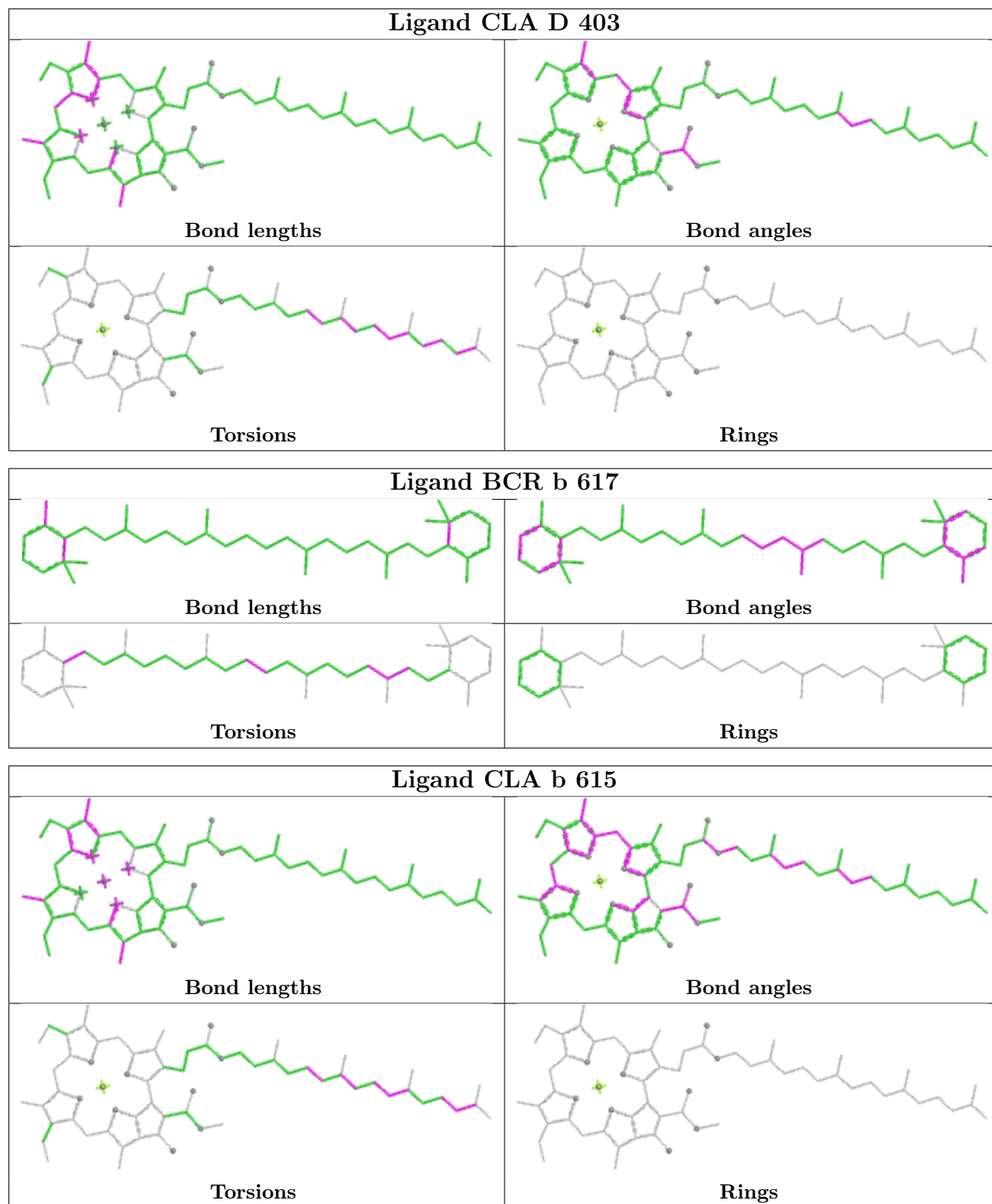


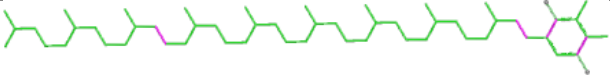
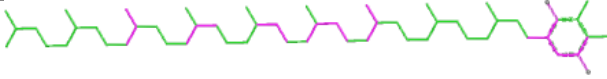
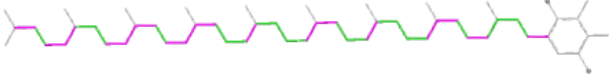
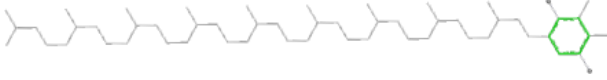
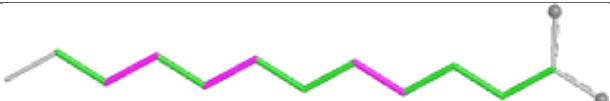
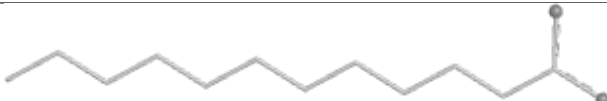
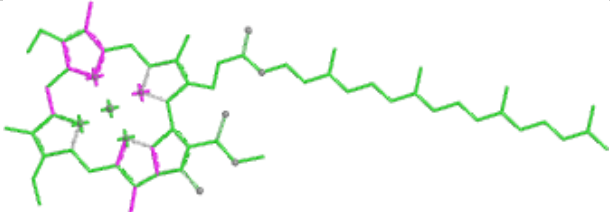
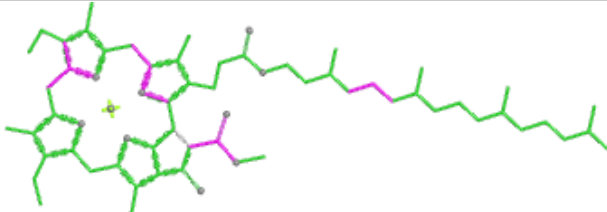
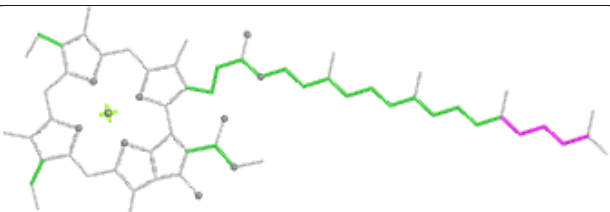
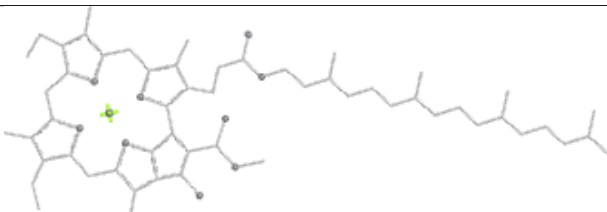
Ligand STE b 626

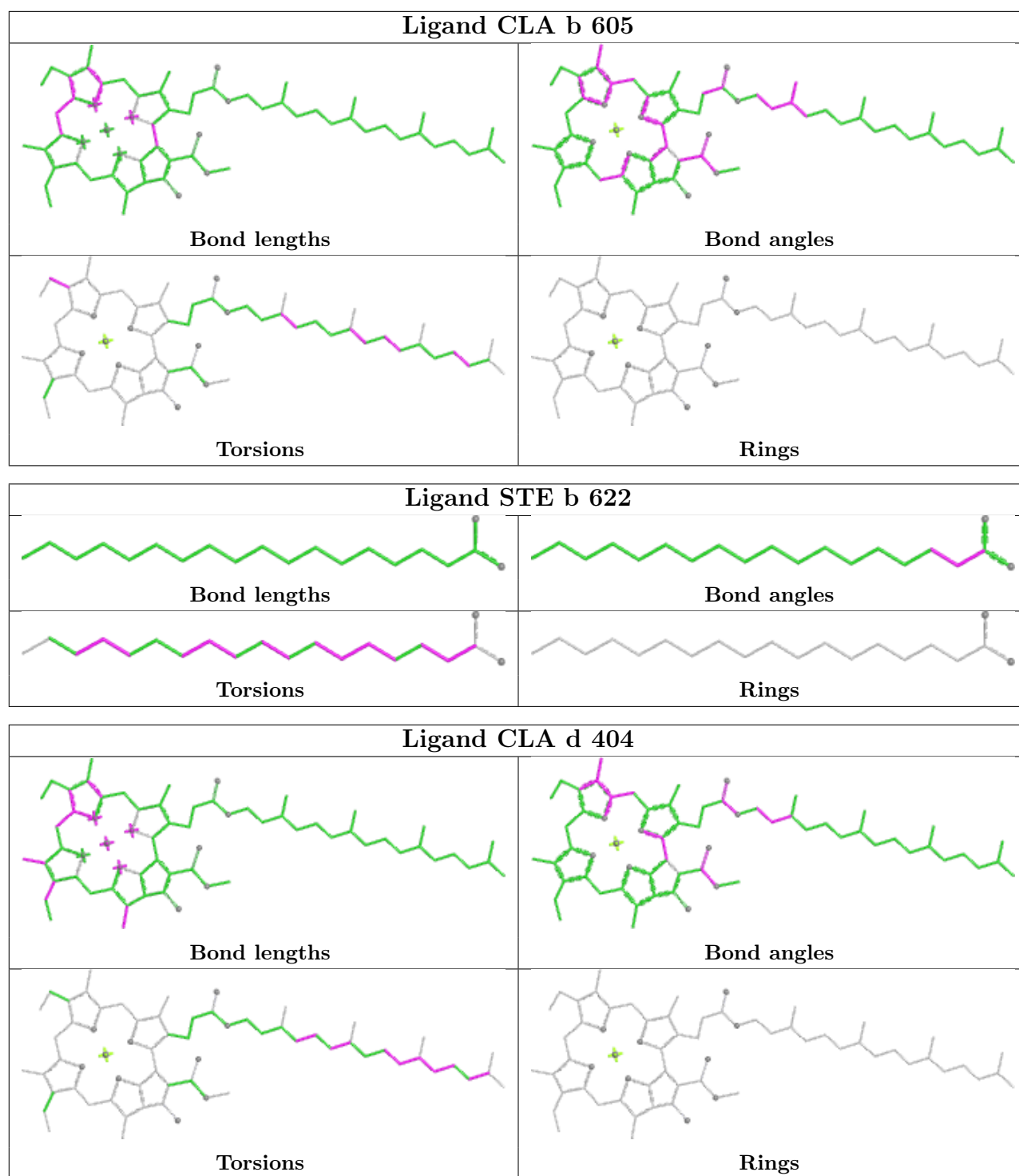


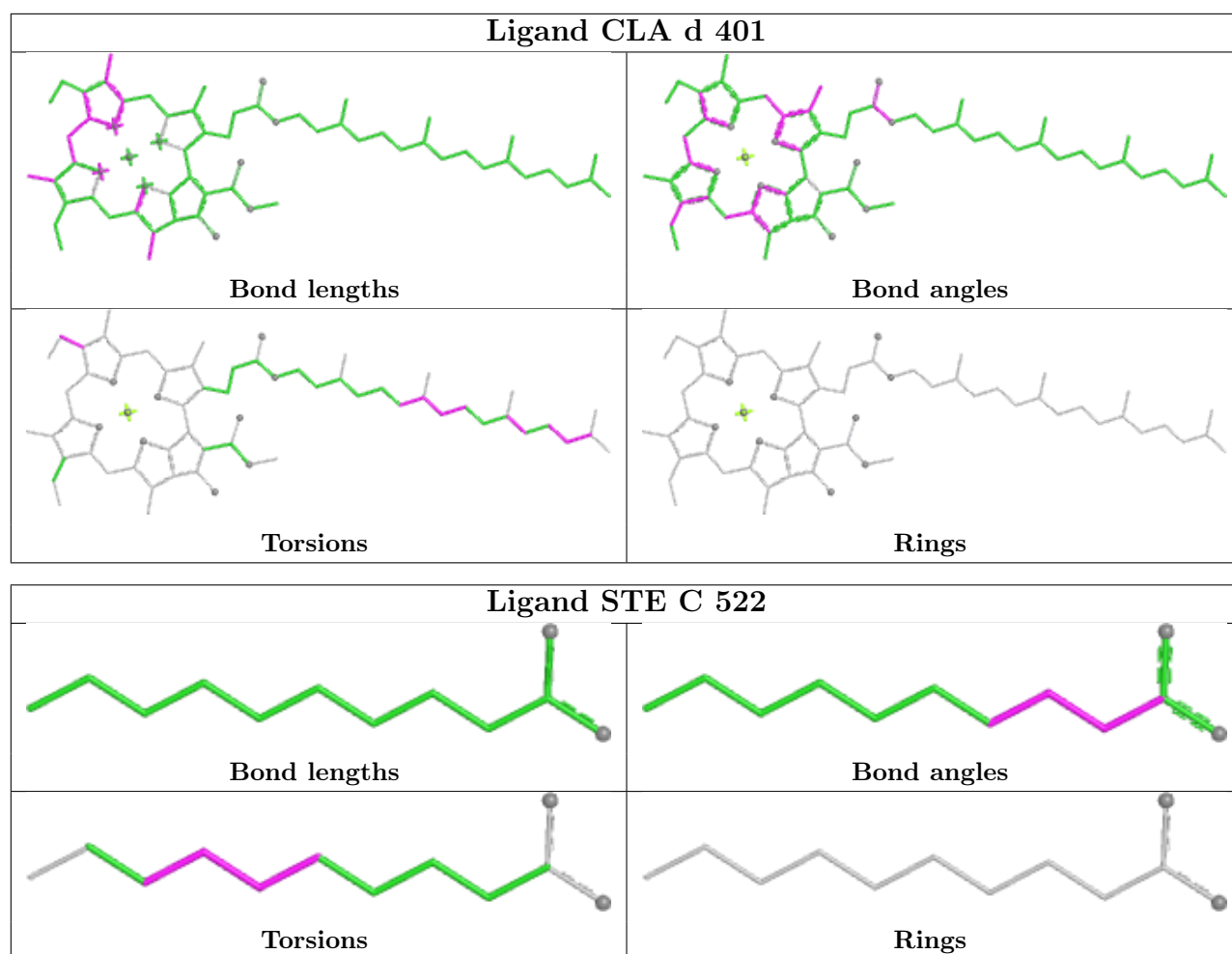




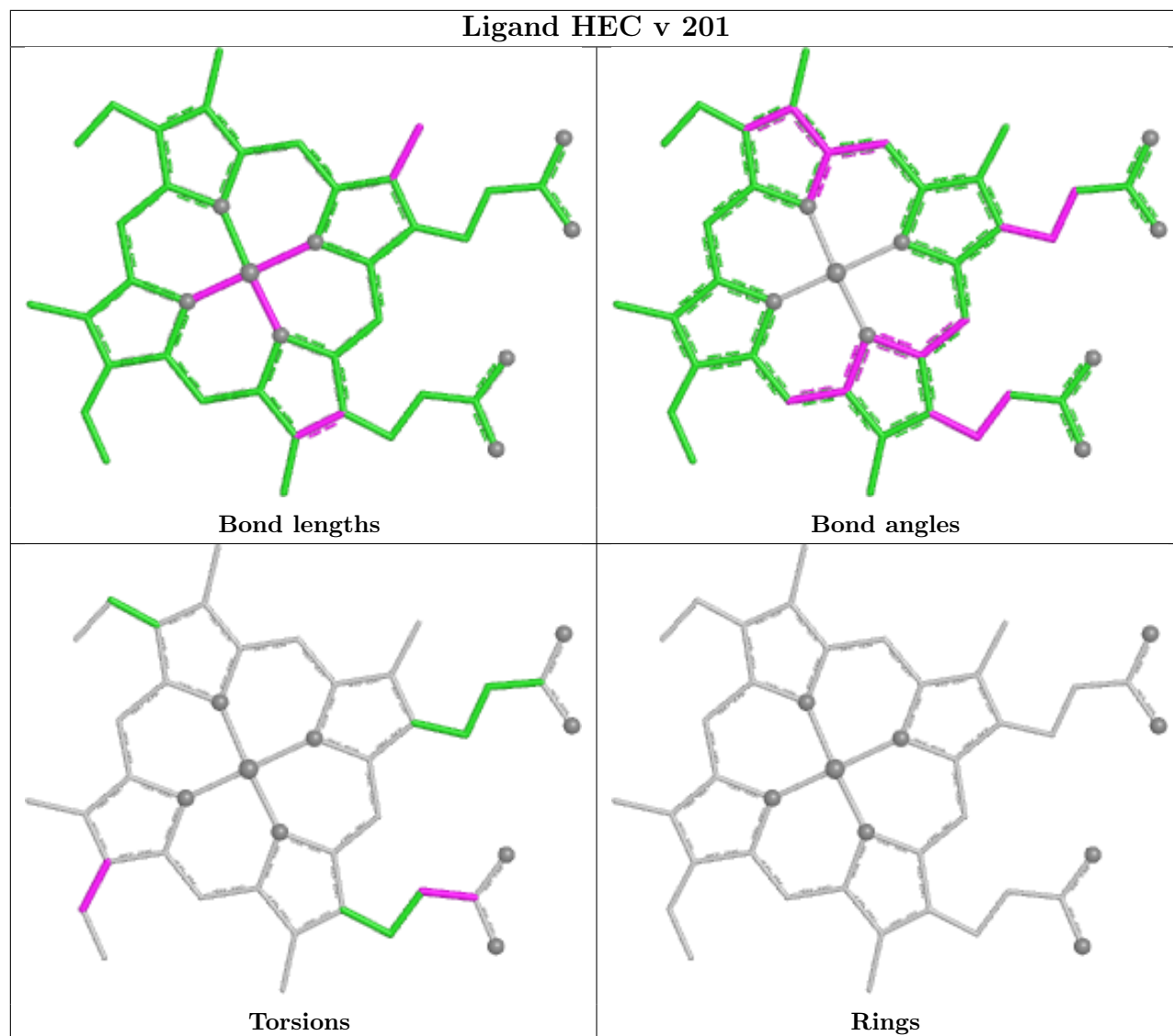


Ligand PL9 A 612	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand STE B 624	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

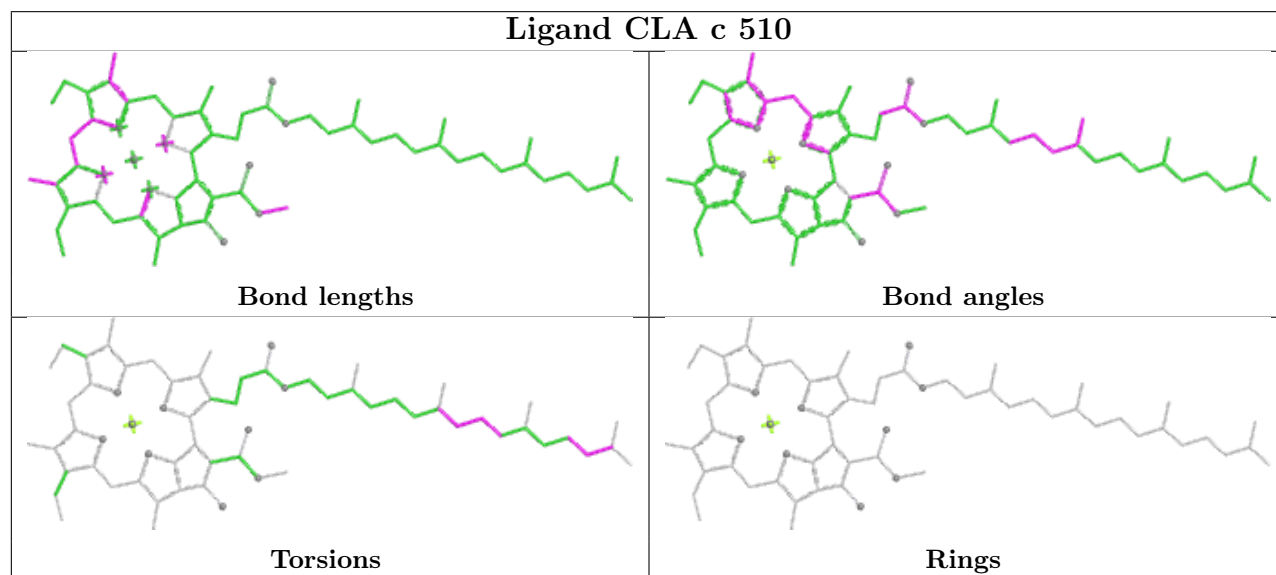


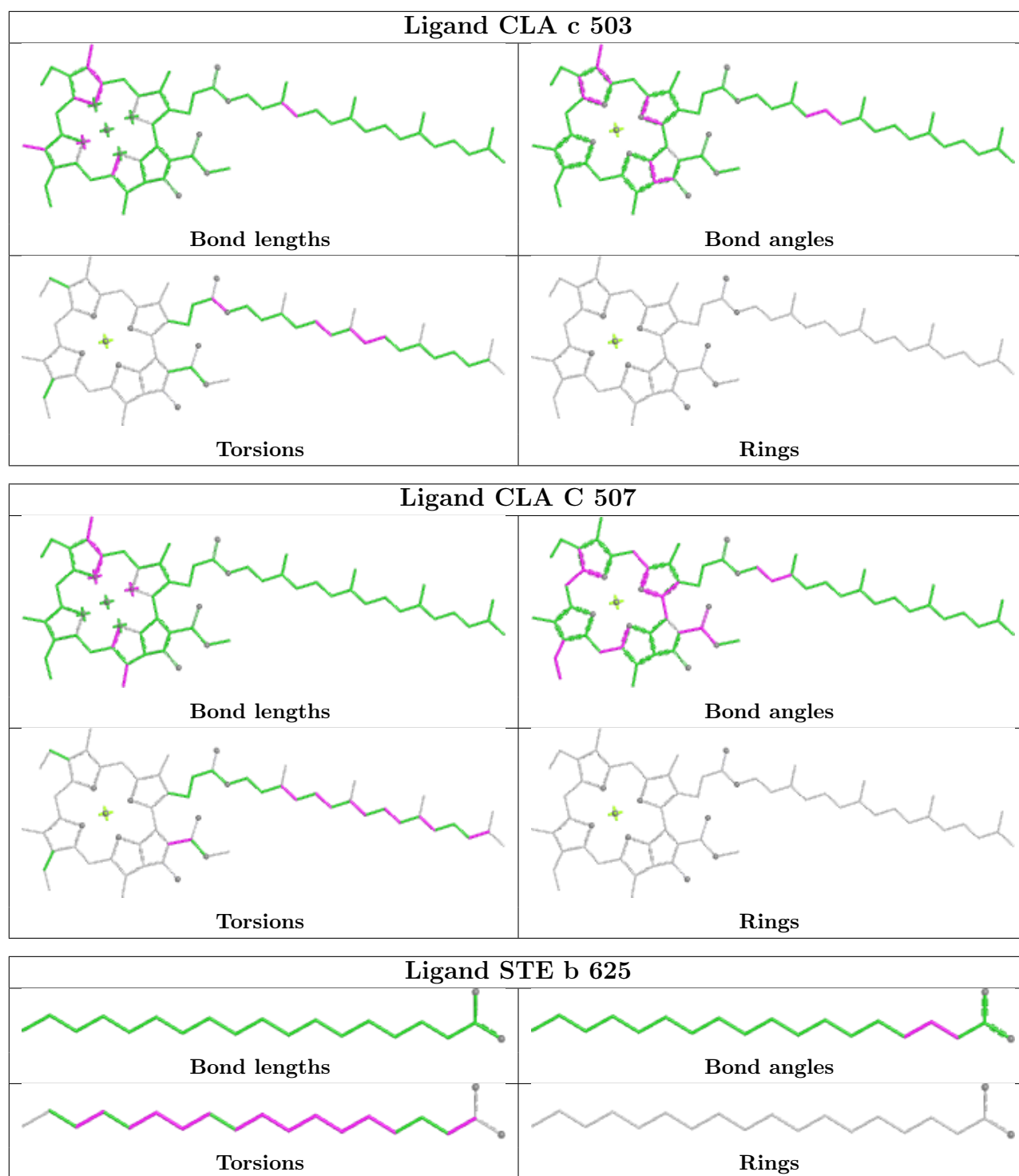


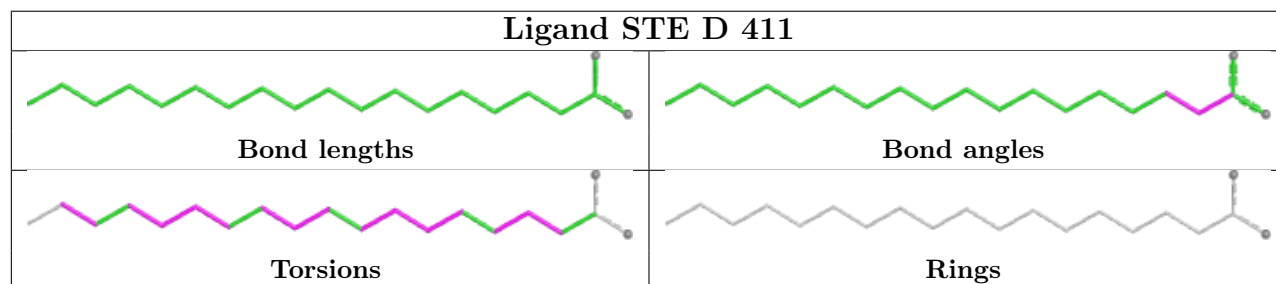
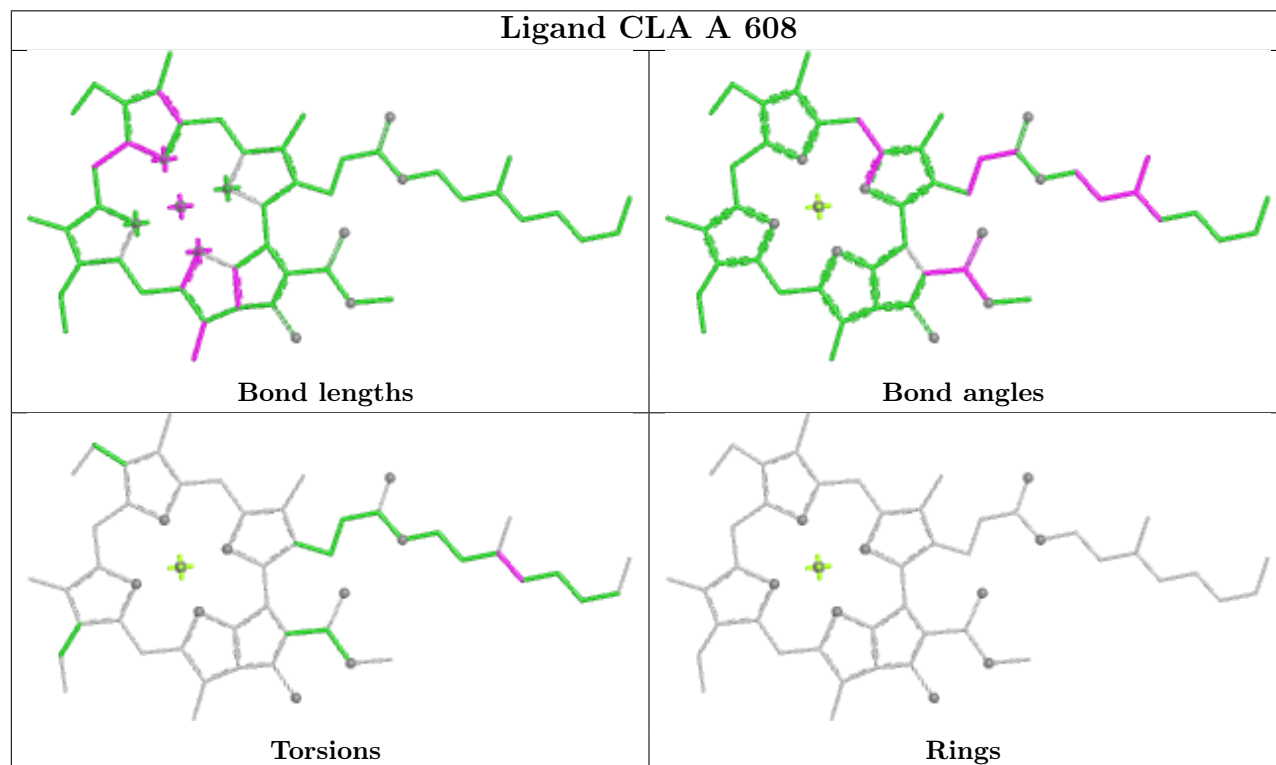
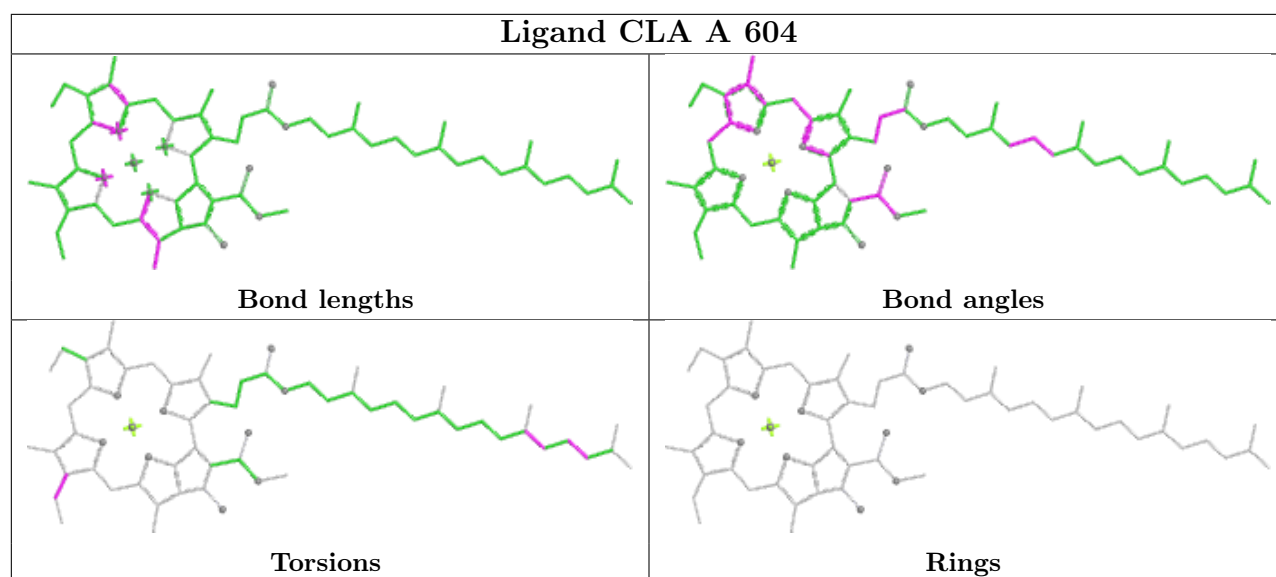
Ligand HEC v 201



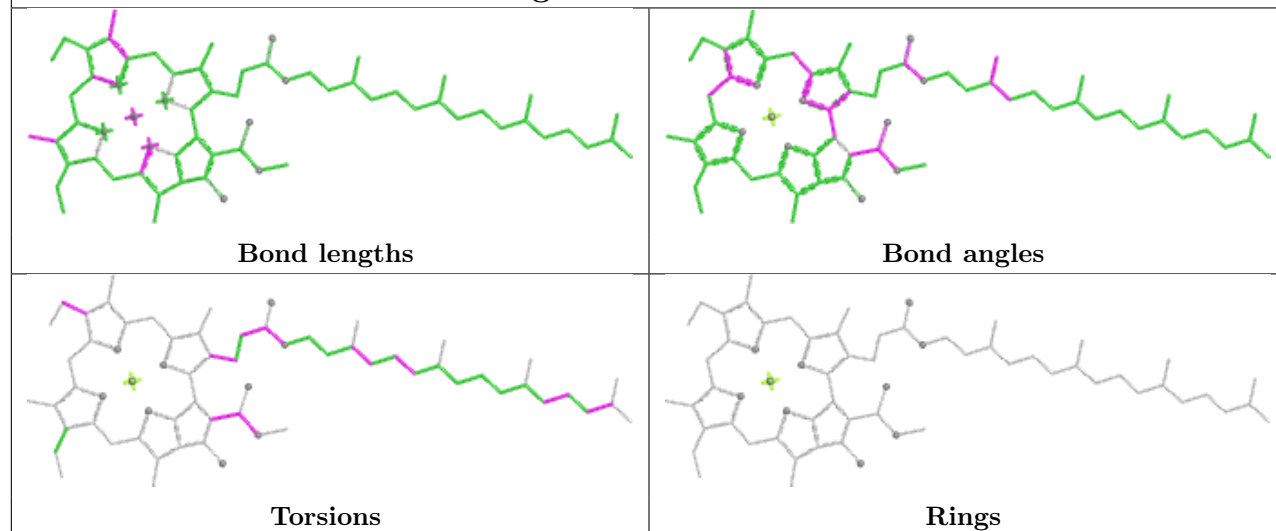
Ligand CLA c 510



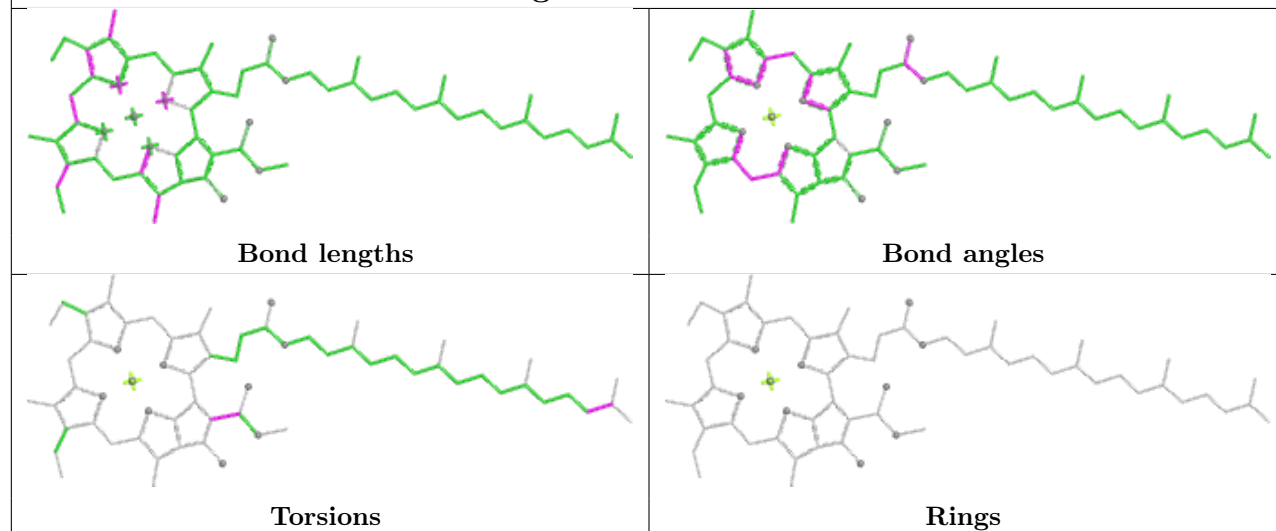




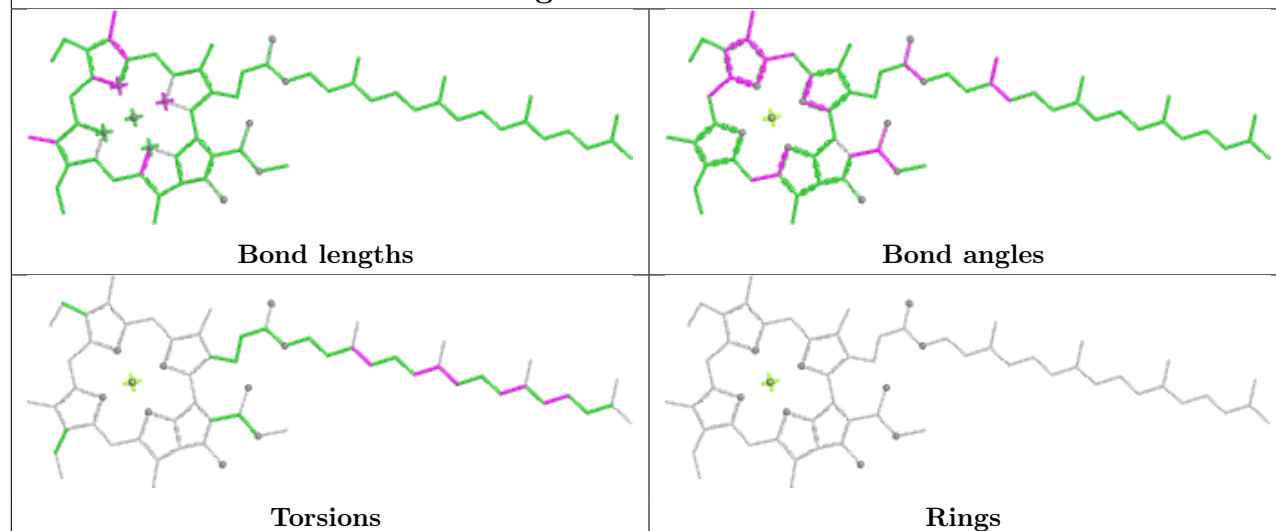
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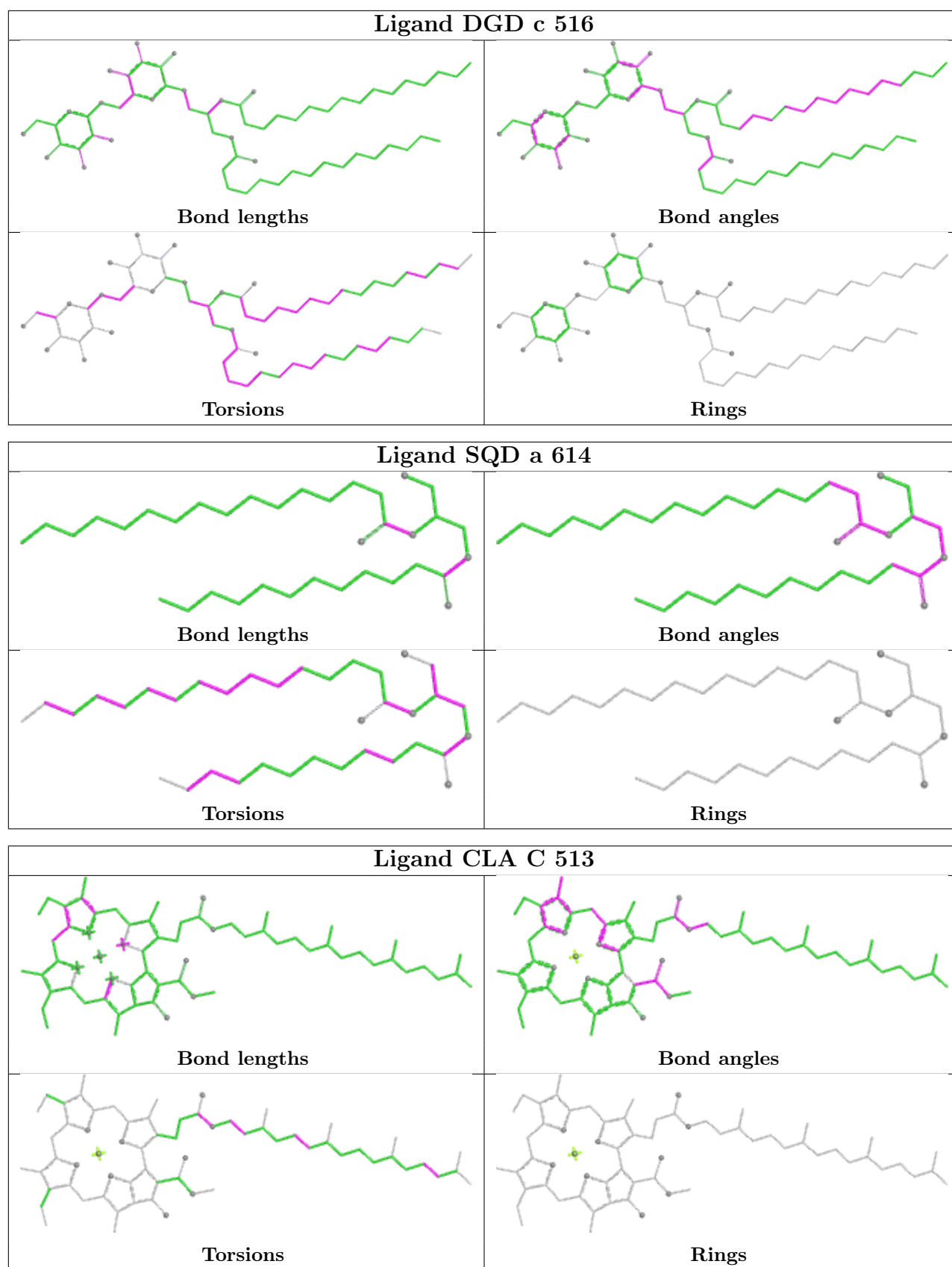


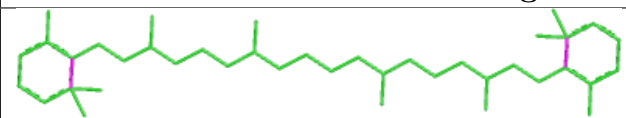
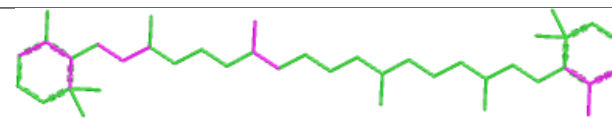
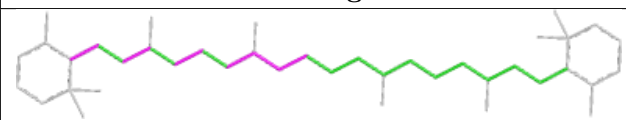
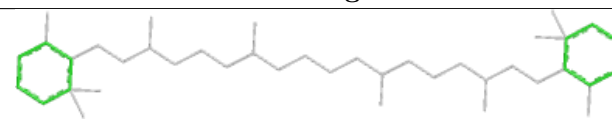
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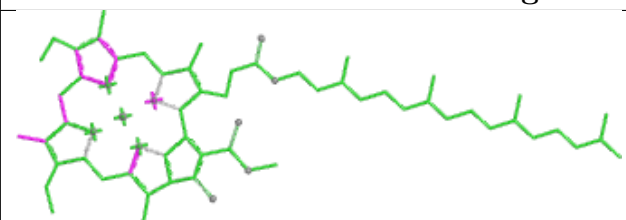
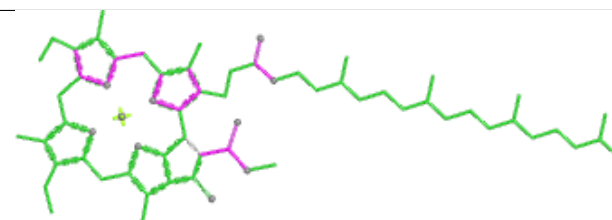
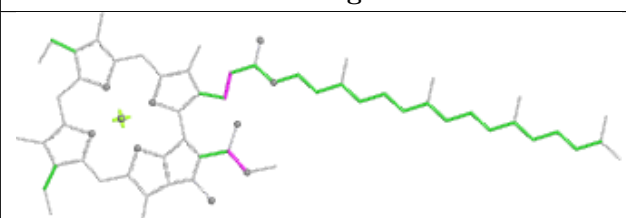
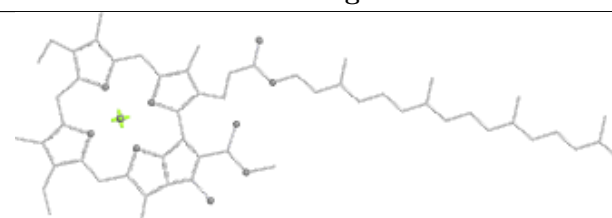


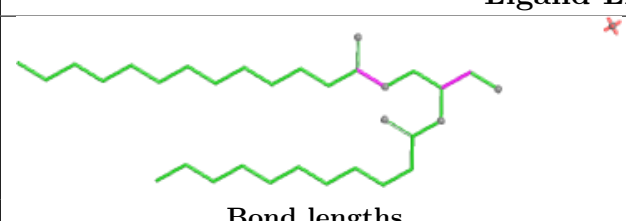
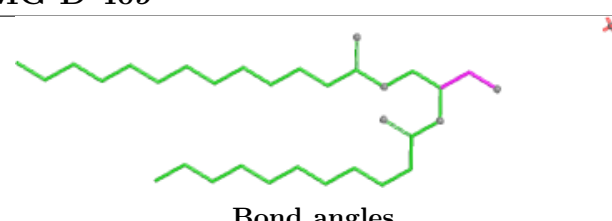
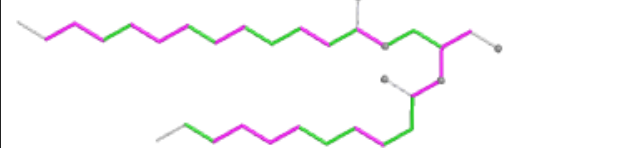
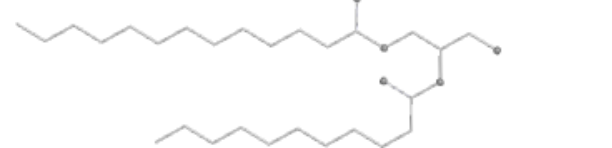
Ligand CLA b 603



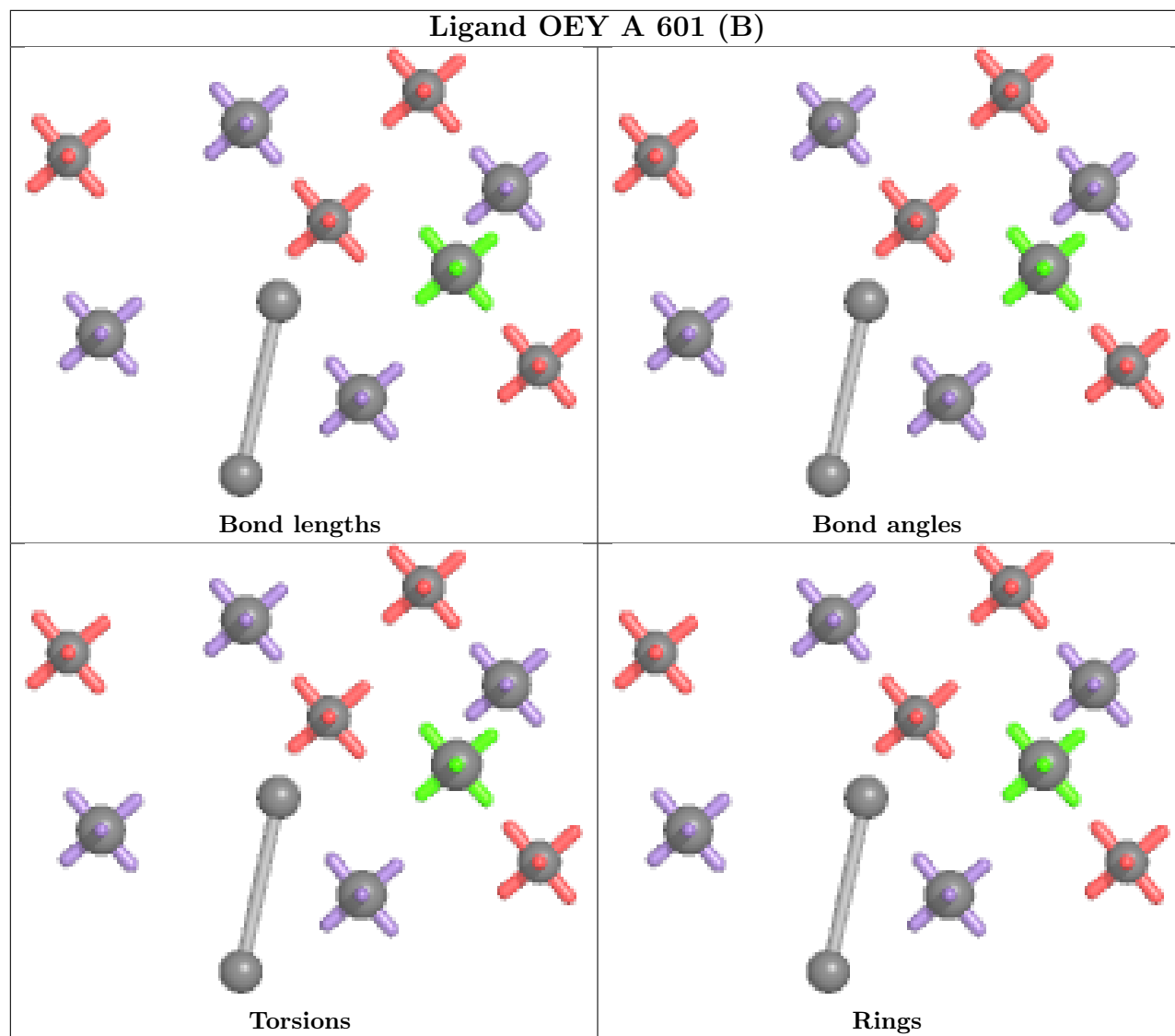


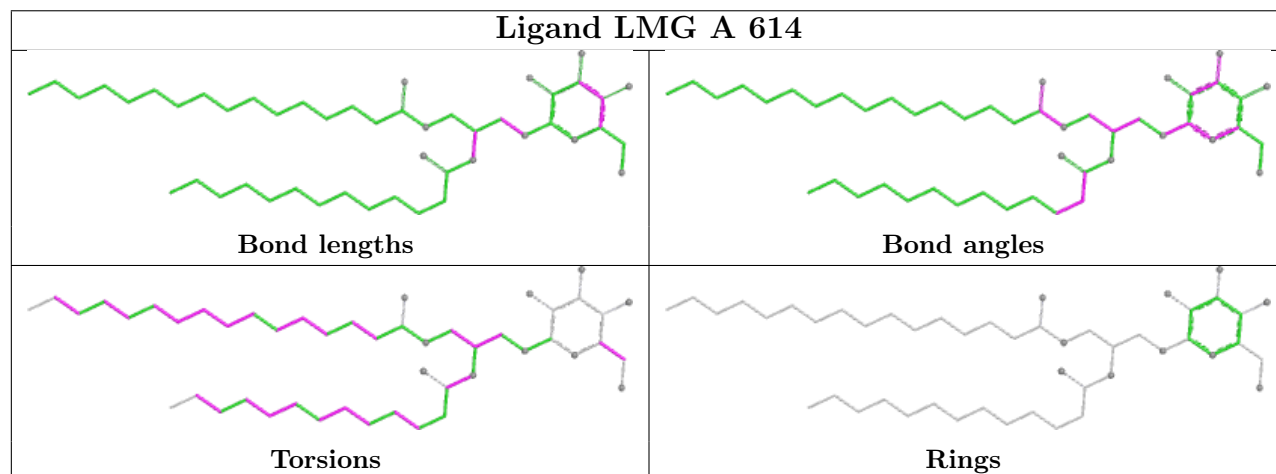
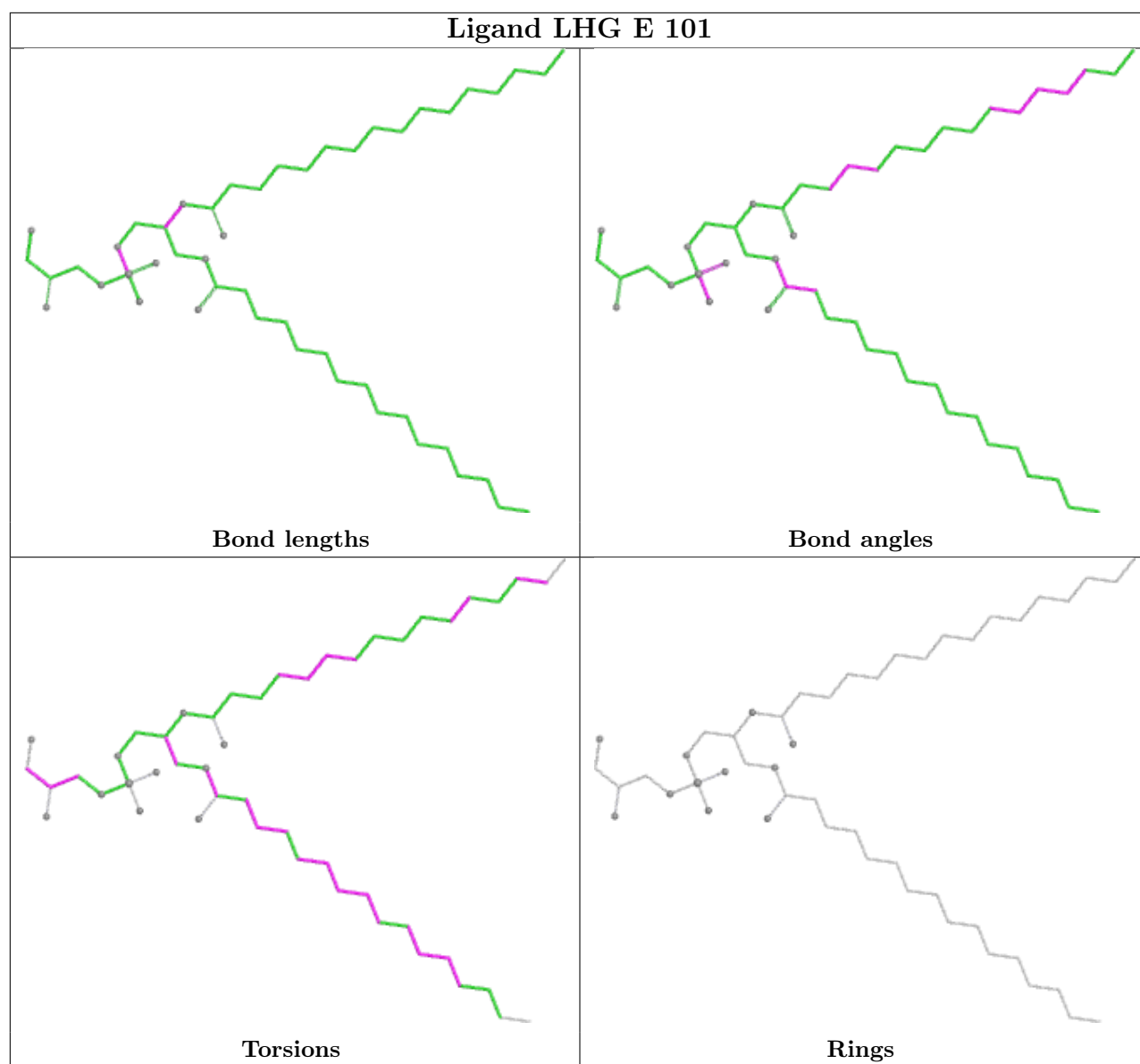
Ligand BCR T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

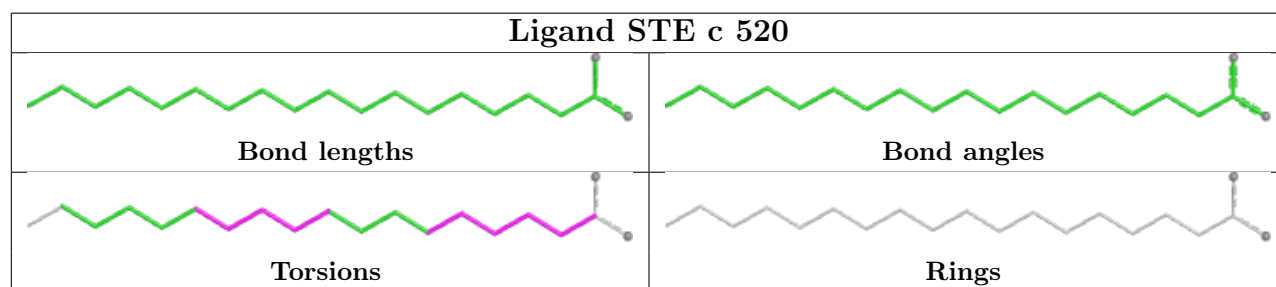
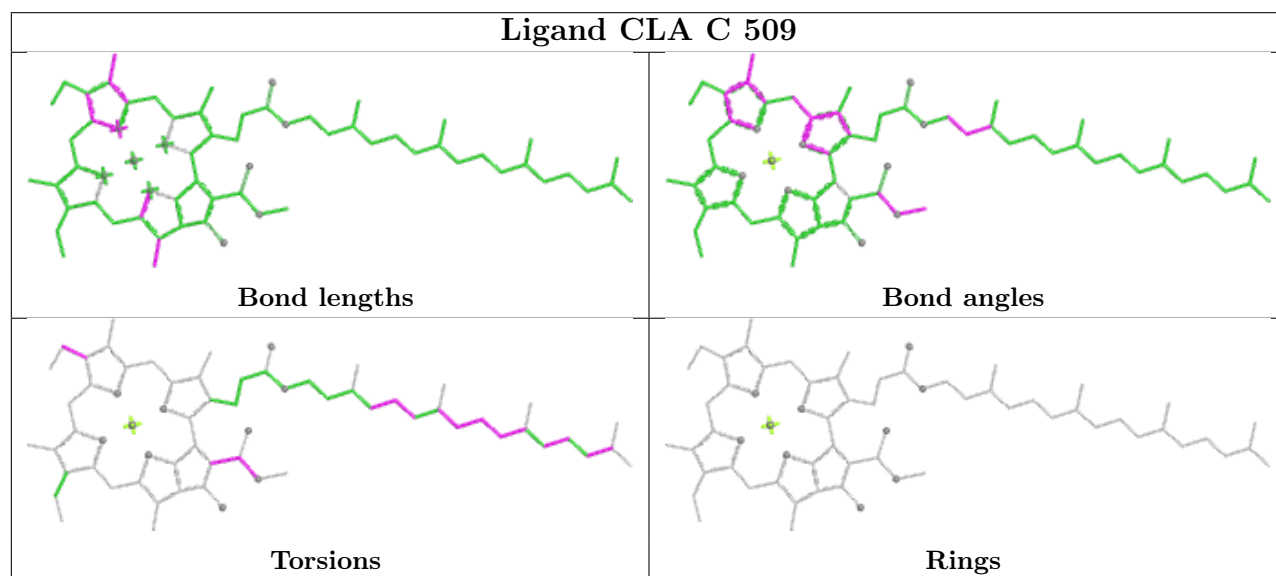
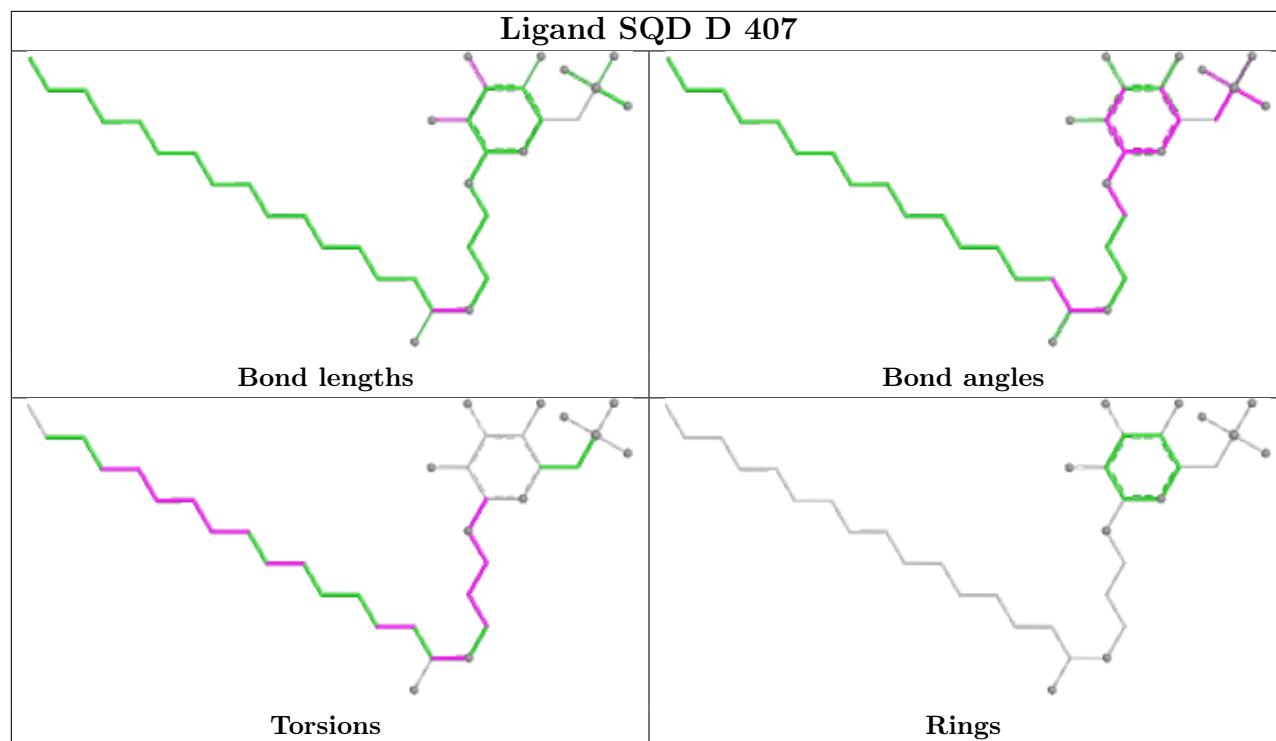
Ligand CLA C 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

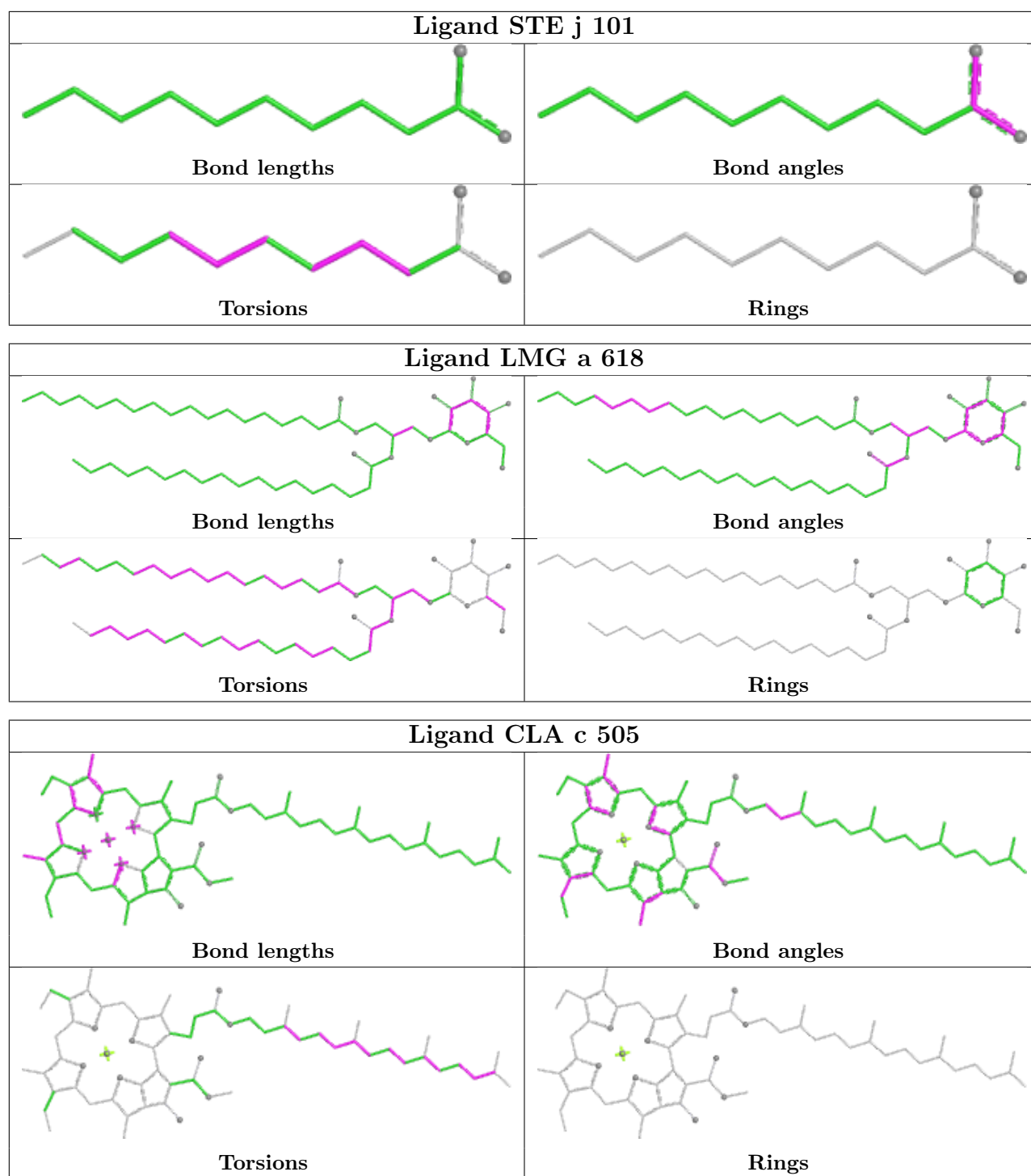
Ligand LMG D 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand OEY A 601 (B)

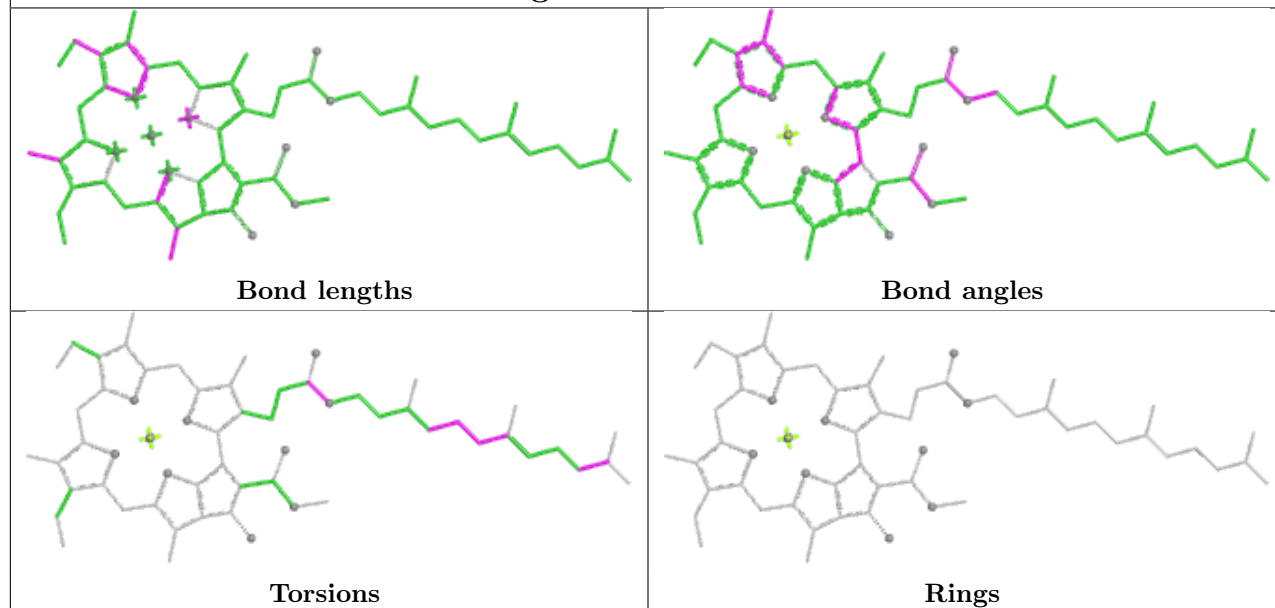




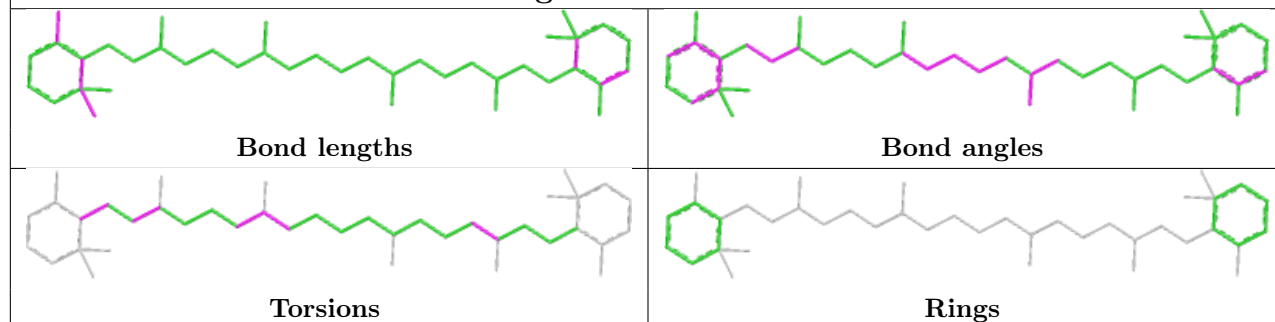




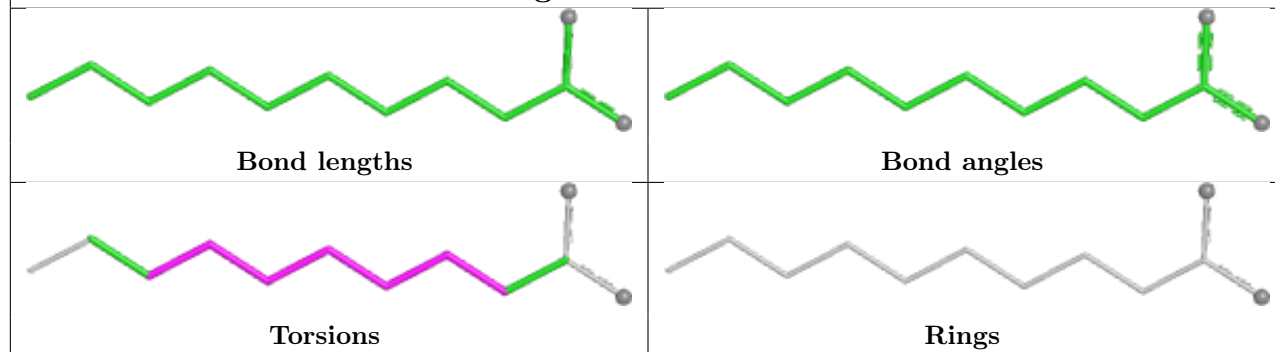
Ligand CLA B 616



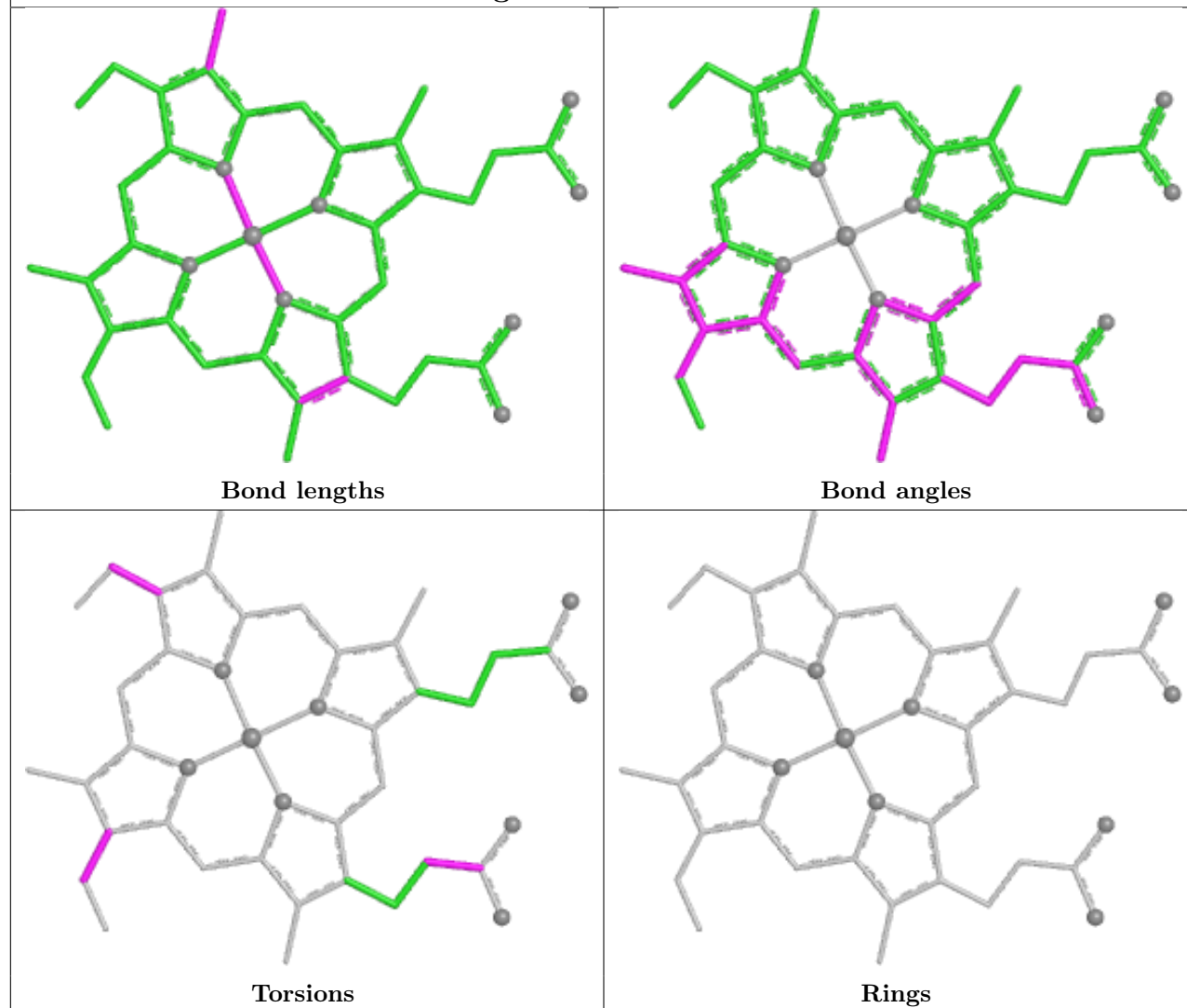
Ligand BCR t 101



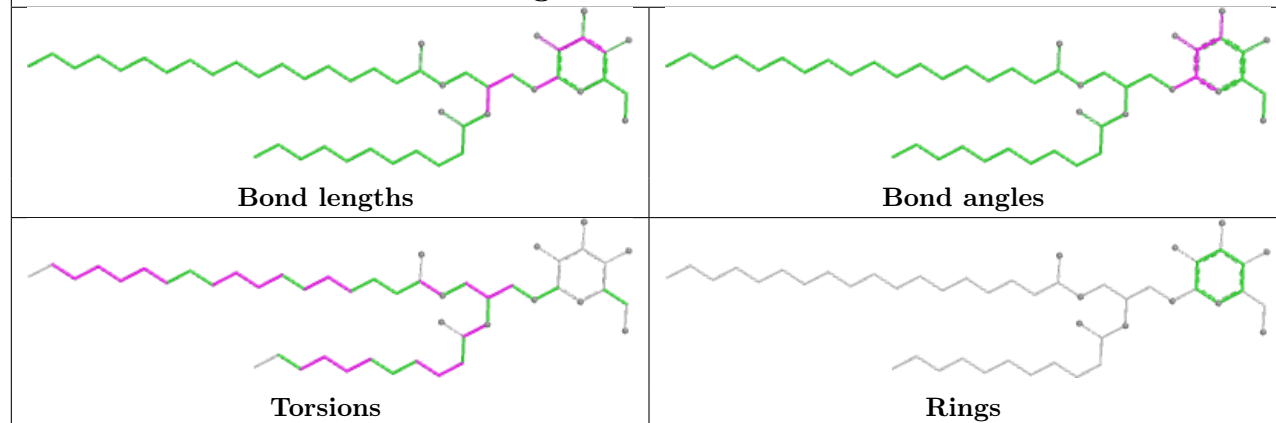
Ligand STE C 520

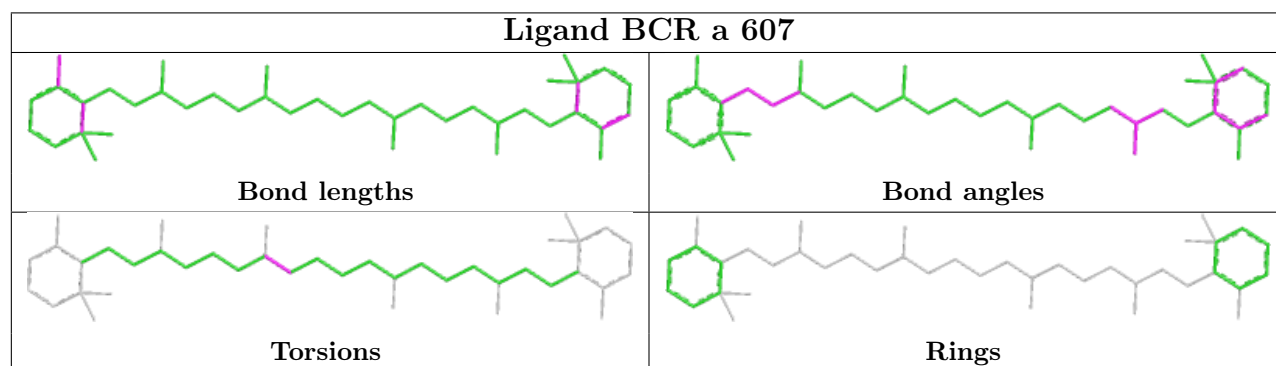
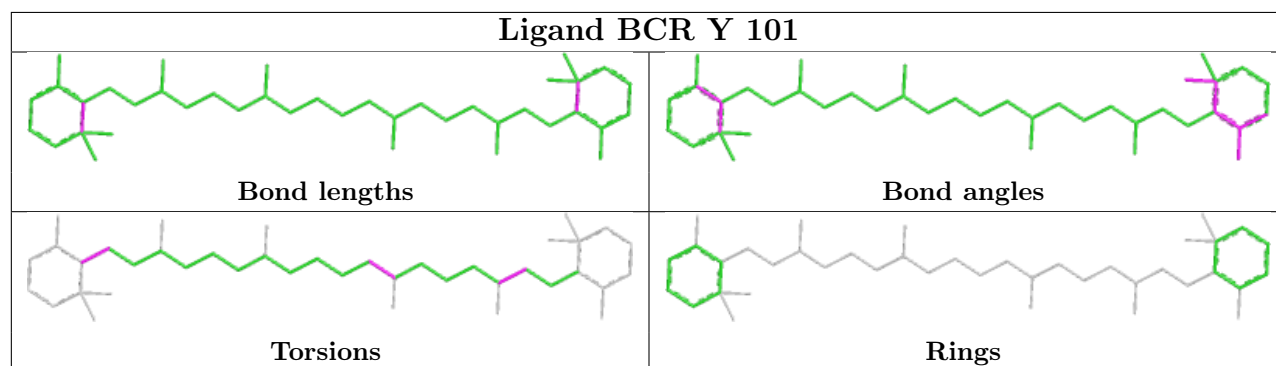
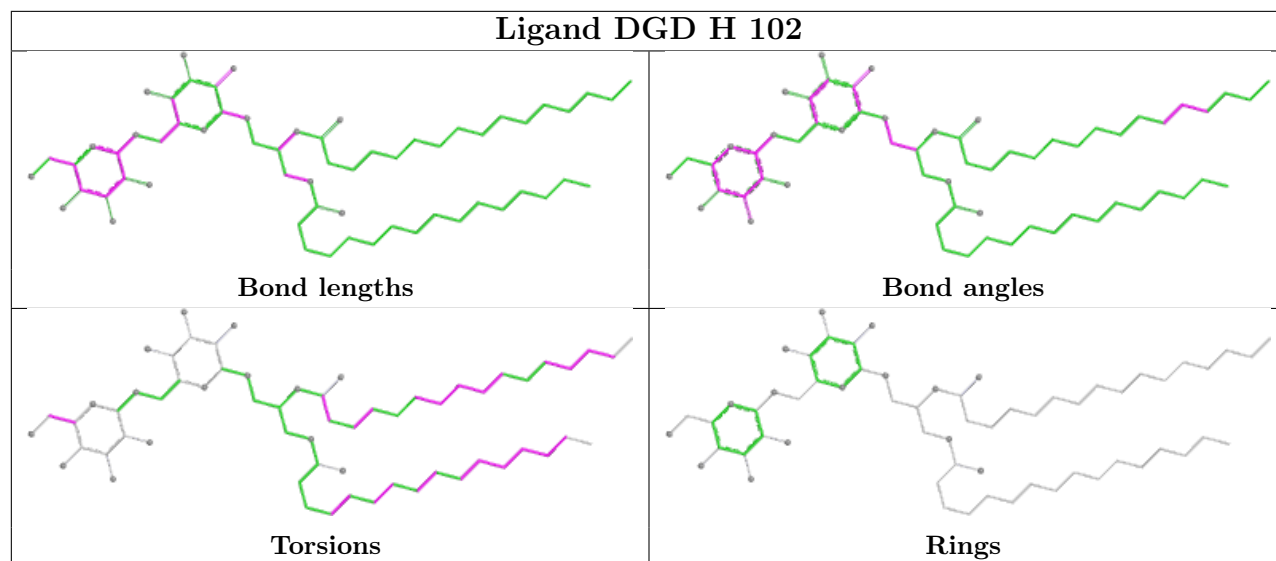


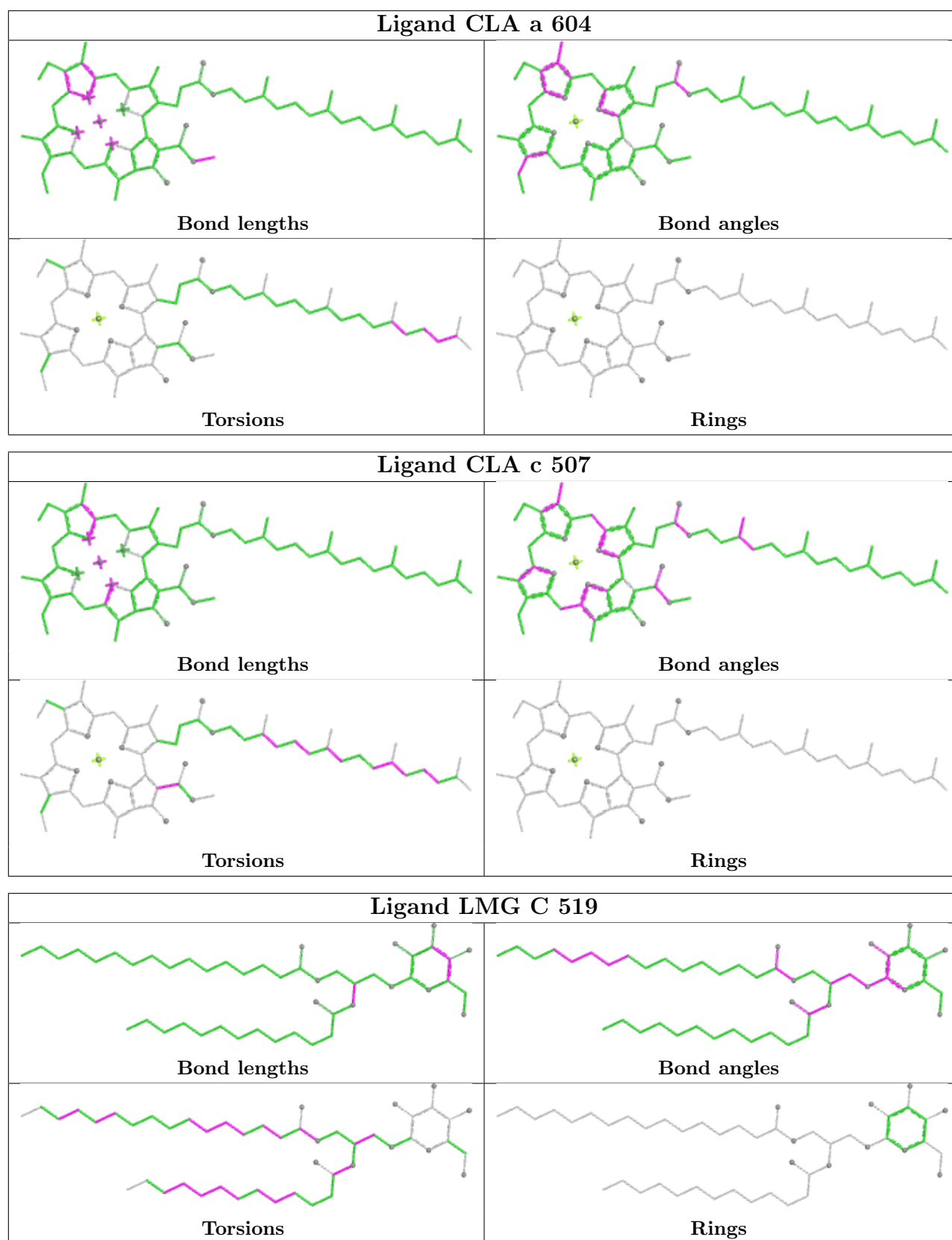
Ligand HEC V 201

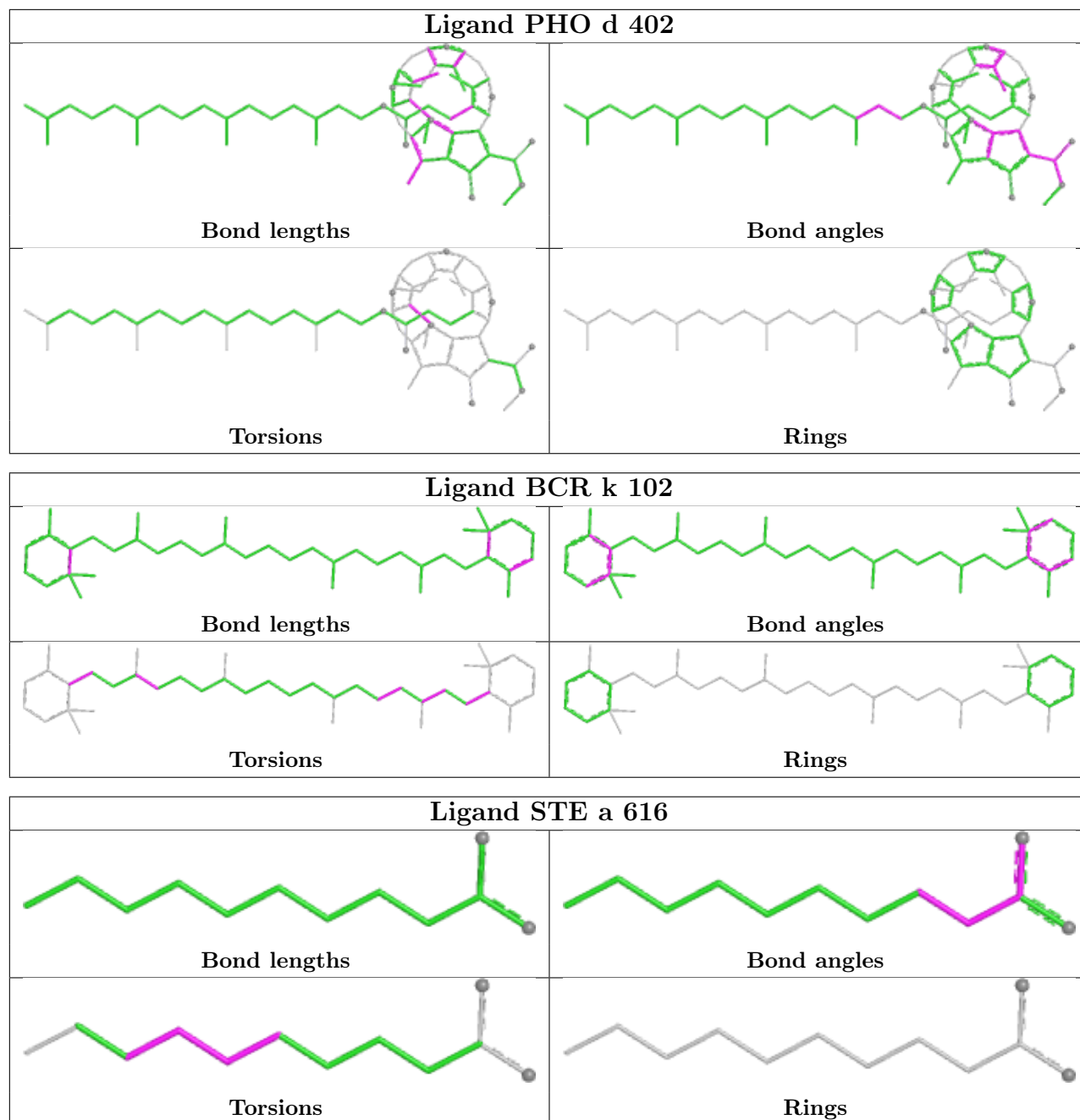


Ligand LMG c 521

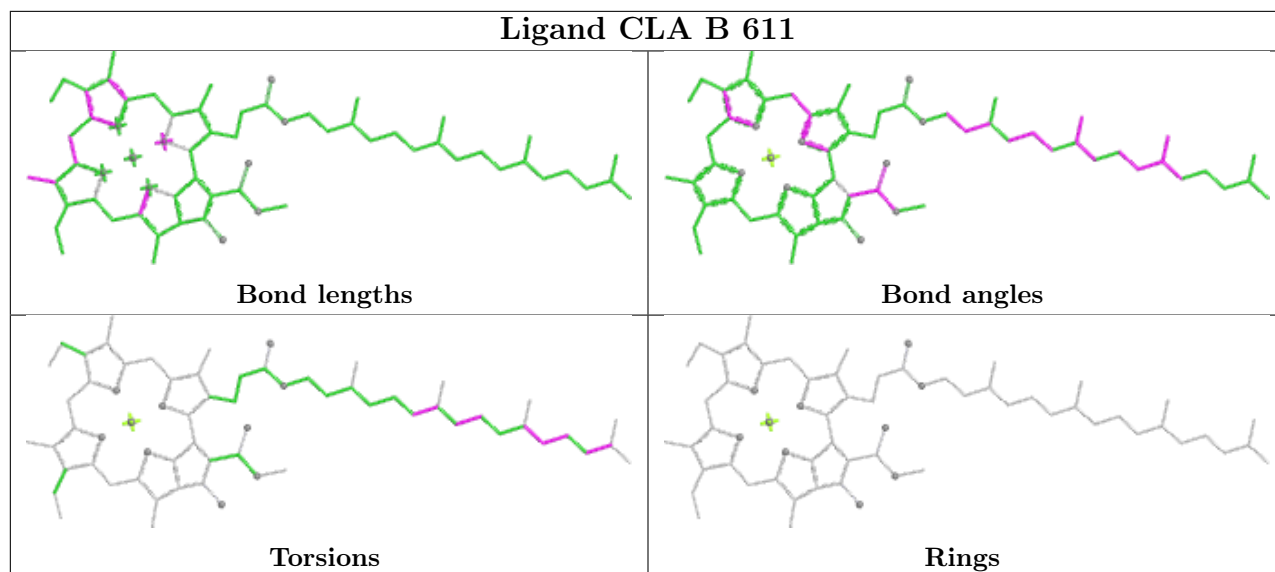




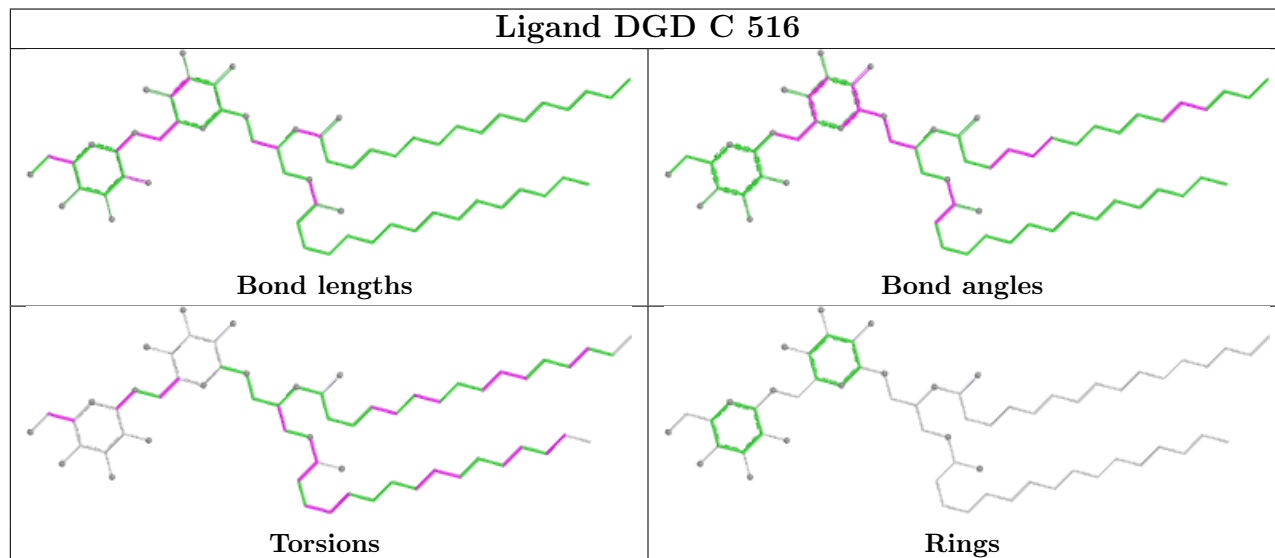




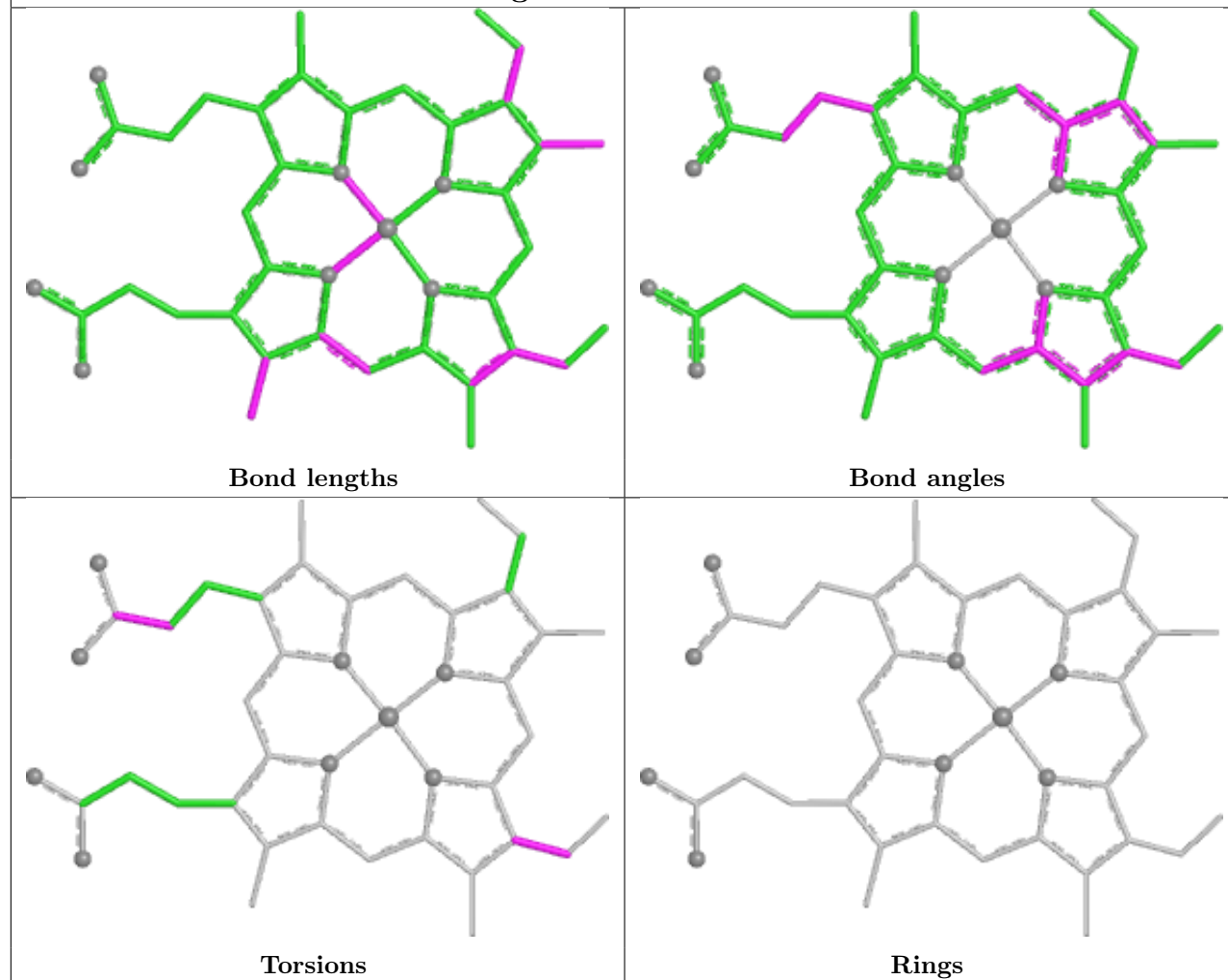
Ligand CLA B 611



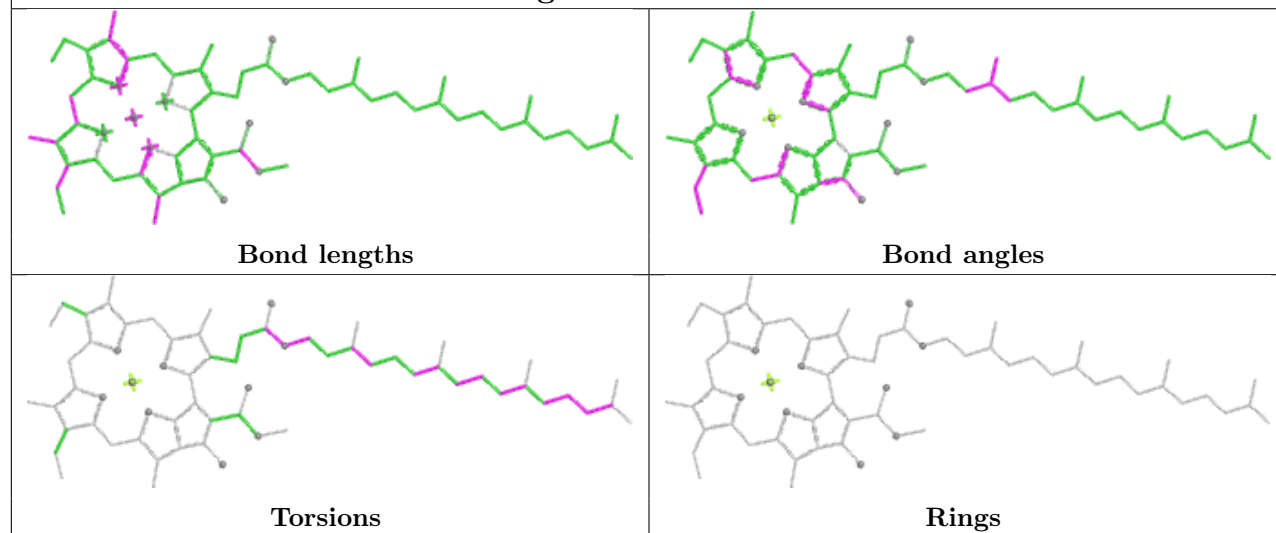
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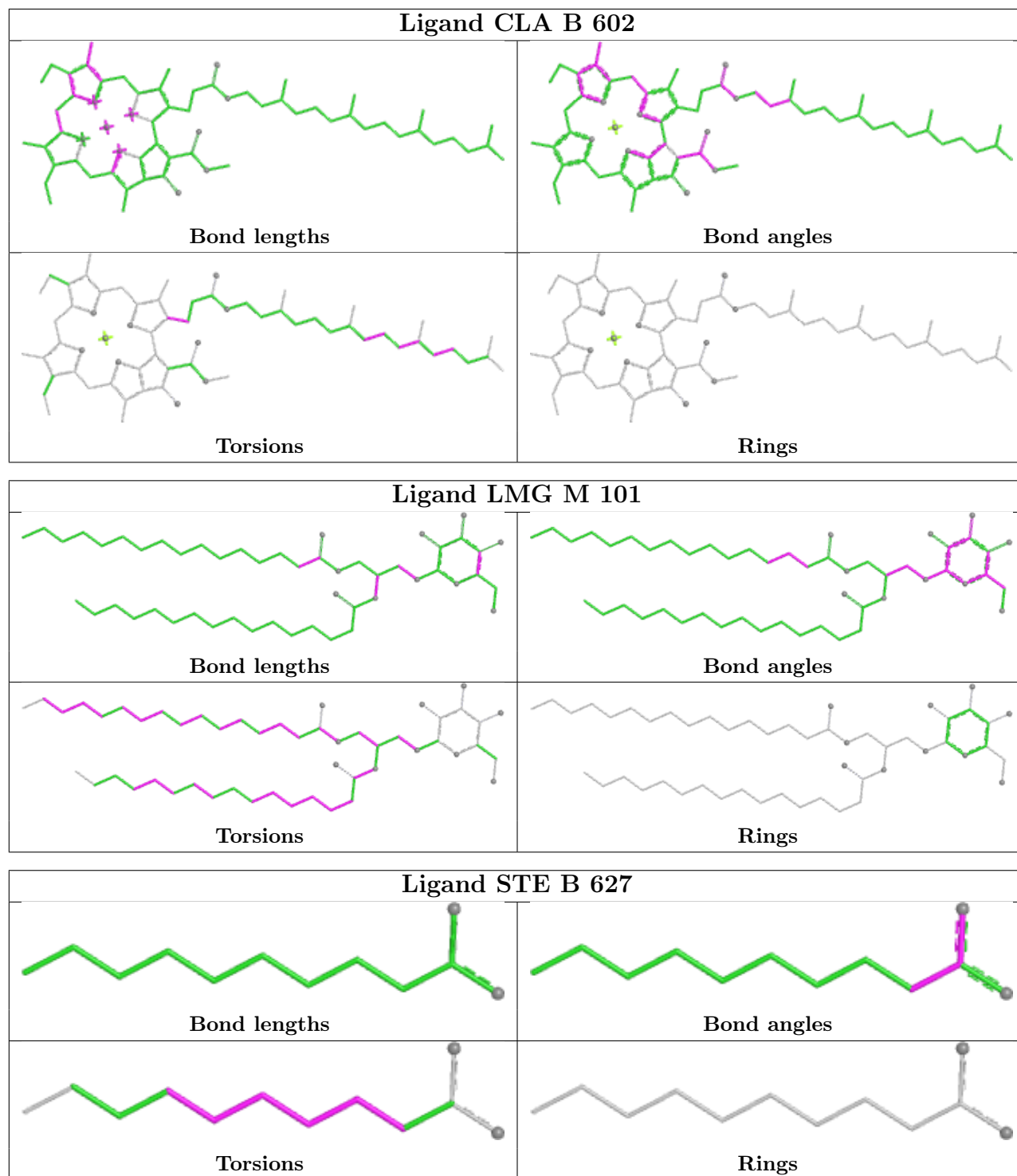


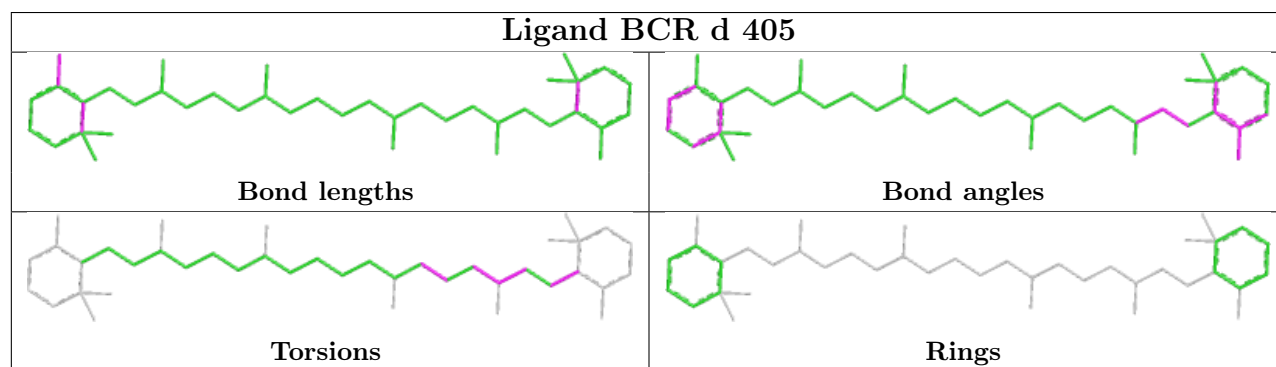
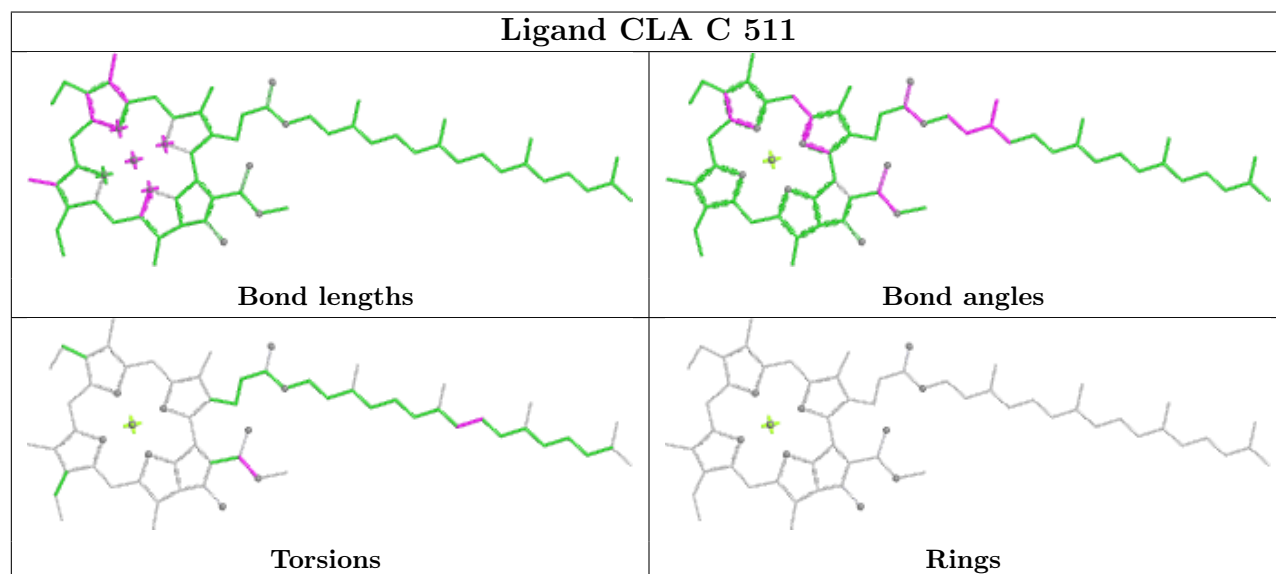
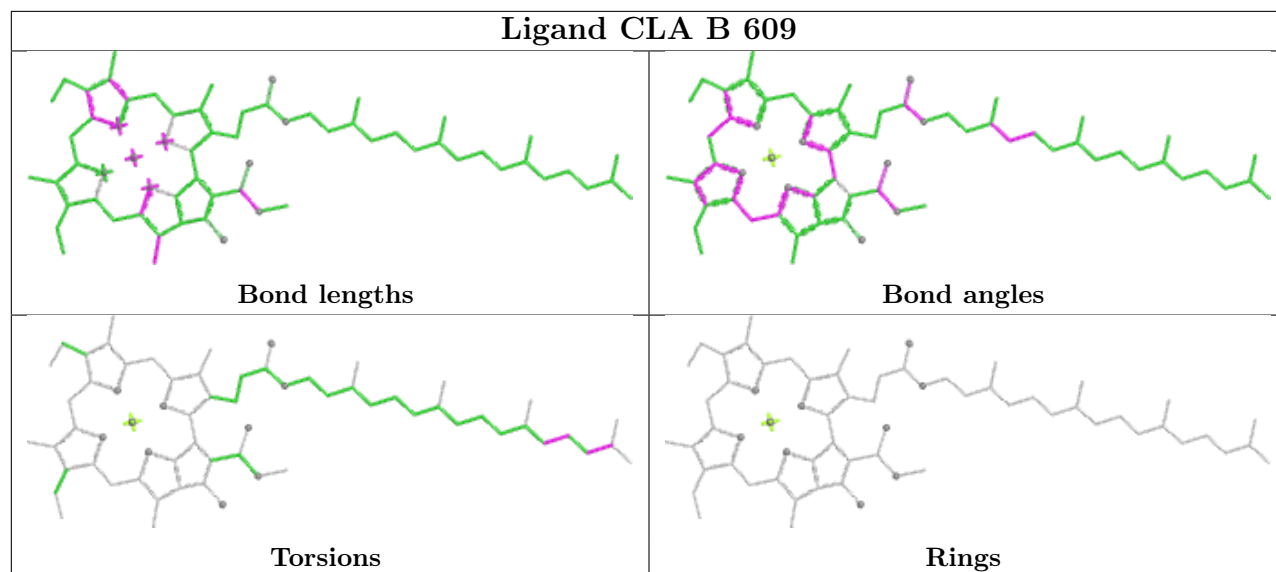
Ligand HEM e 101

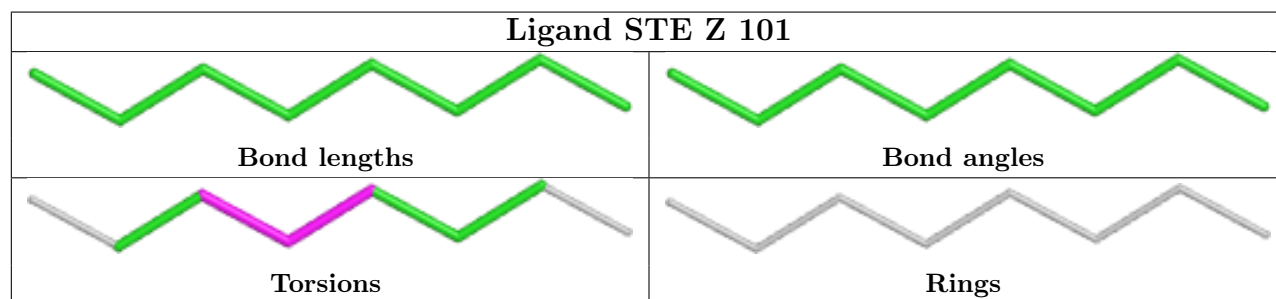
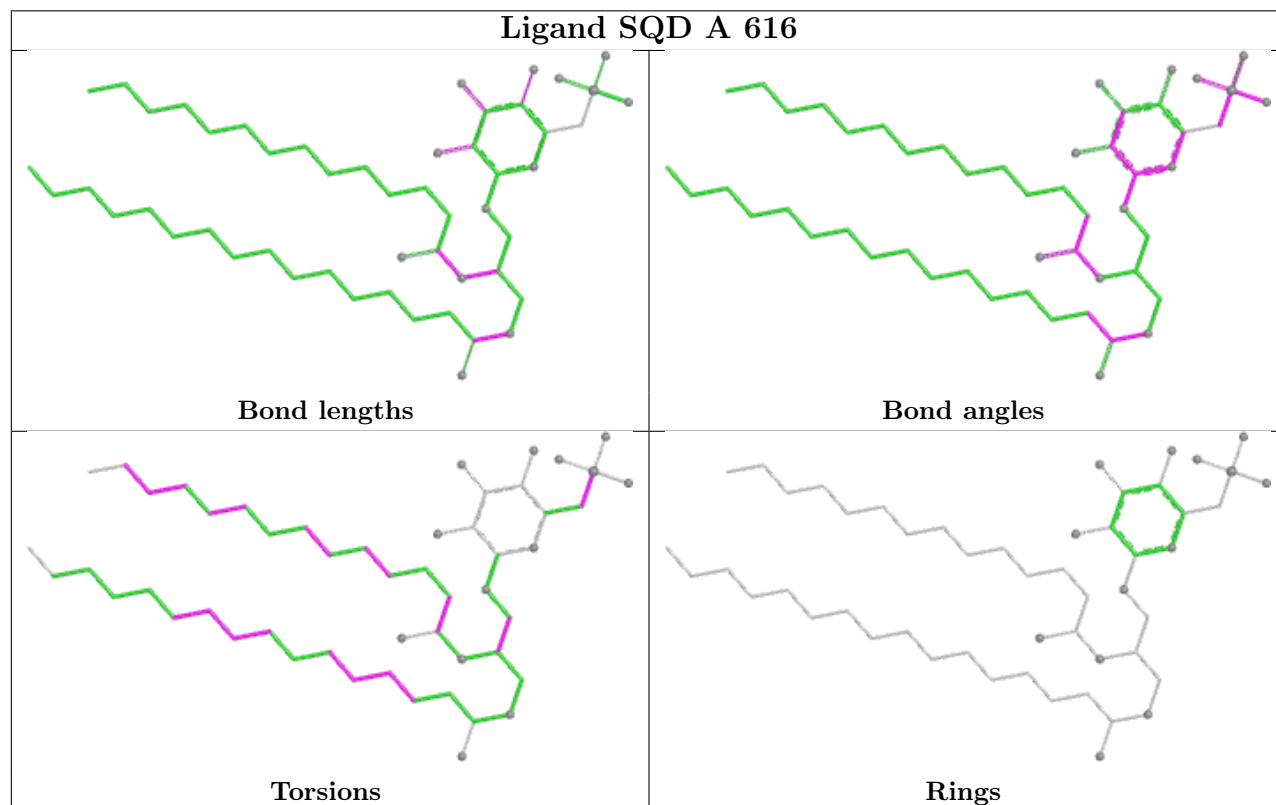
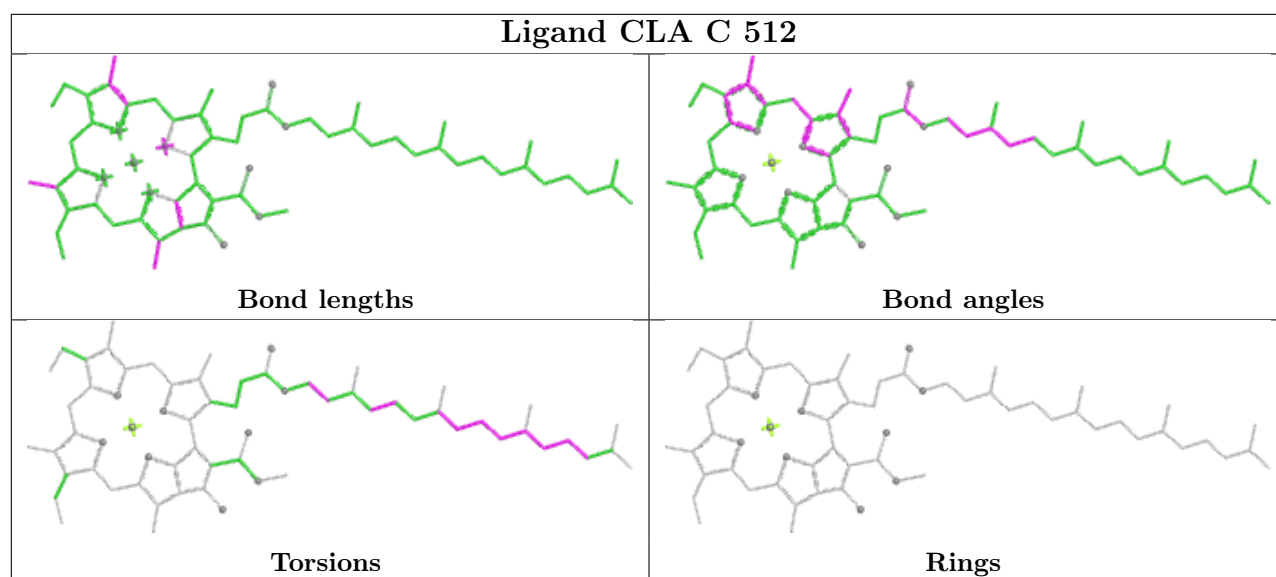


Ligand CLA c 506

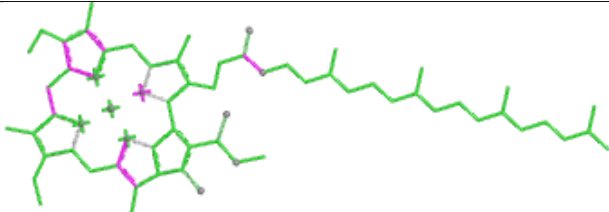
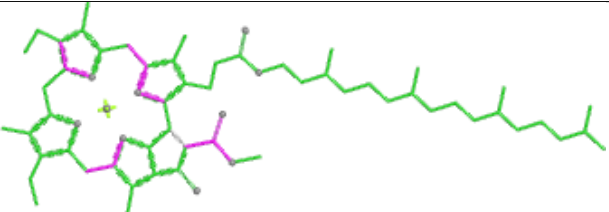
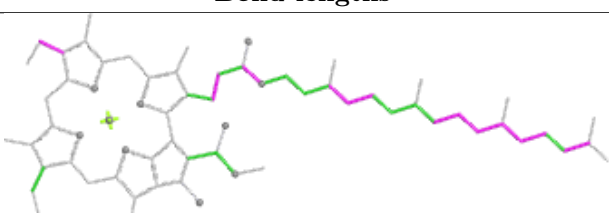
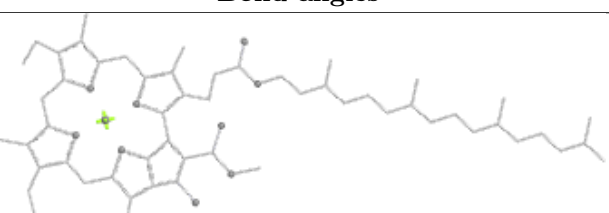


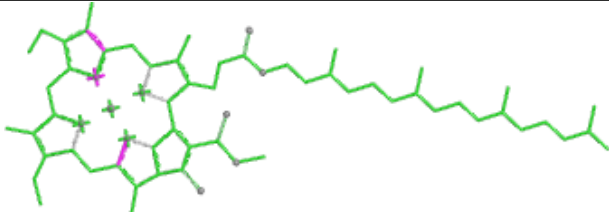
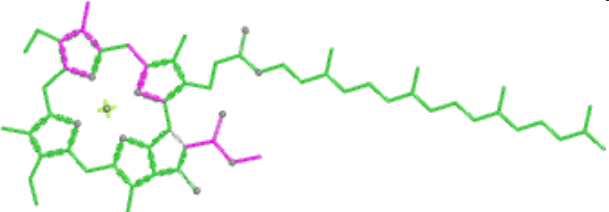
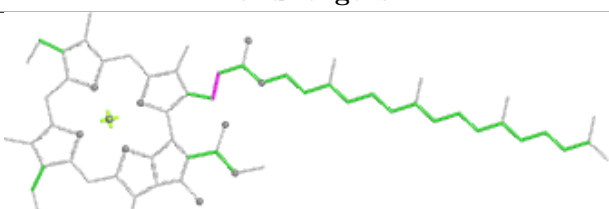
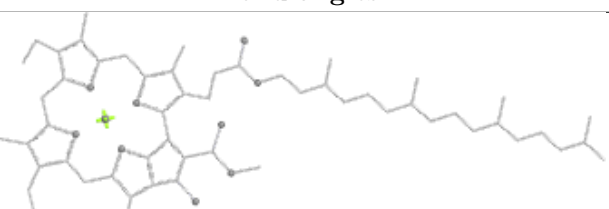


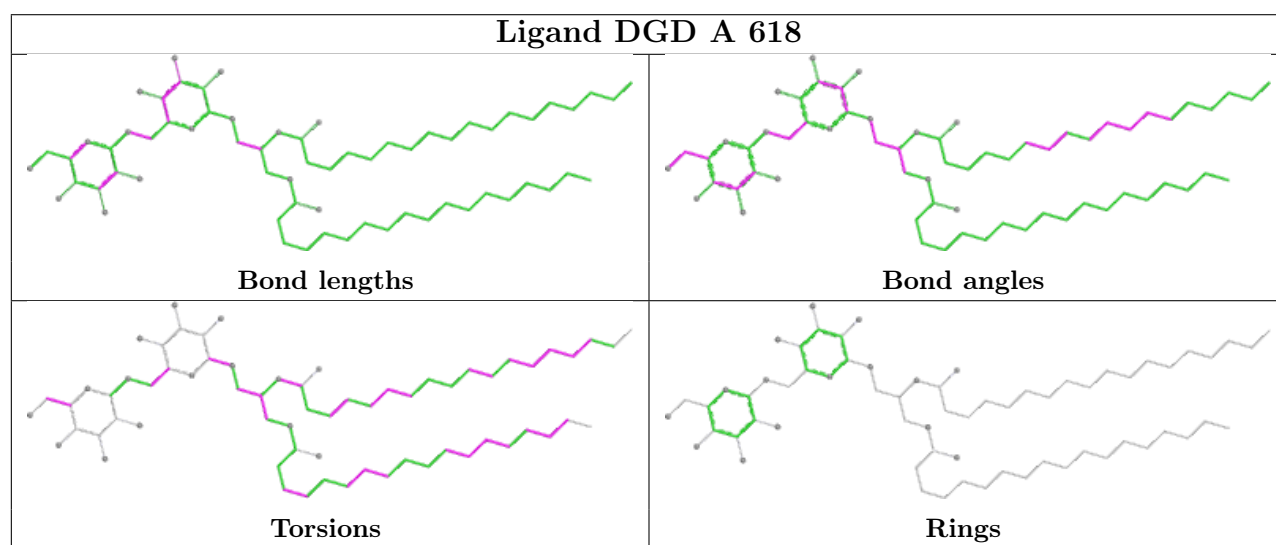
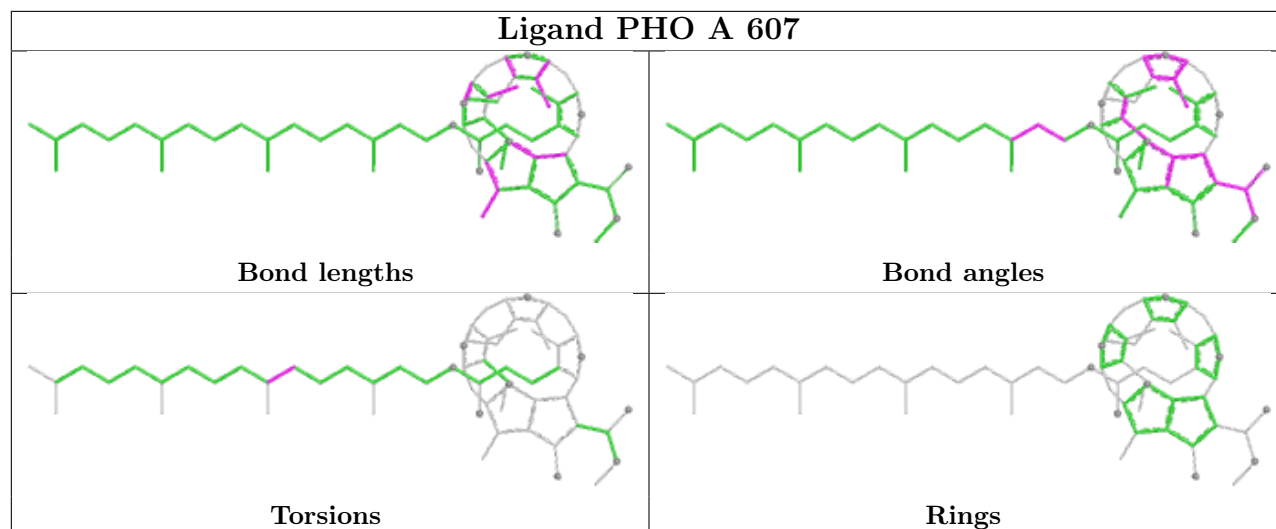


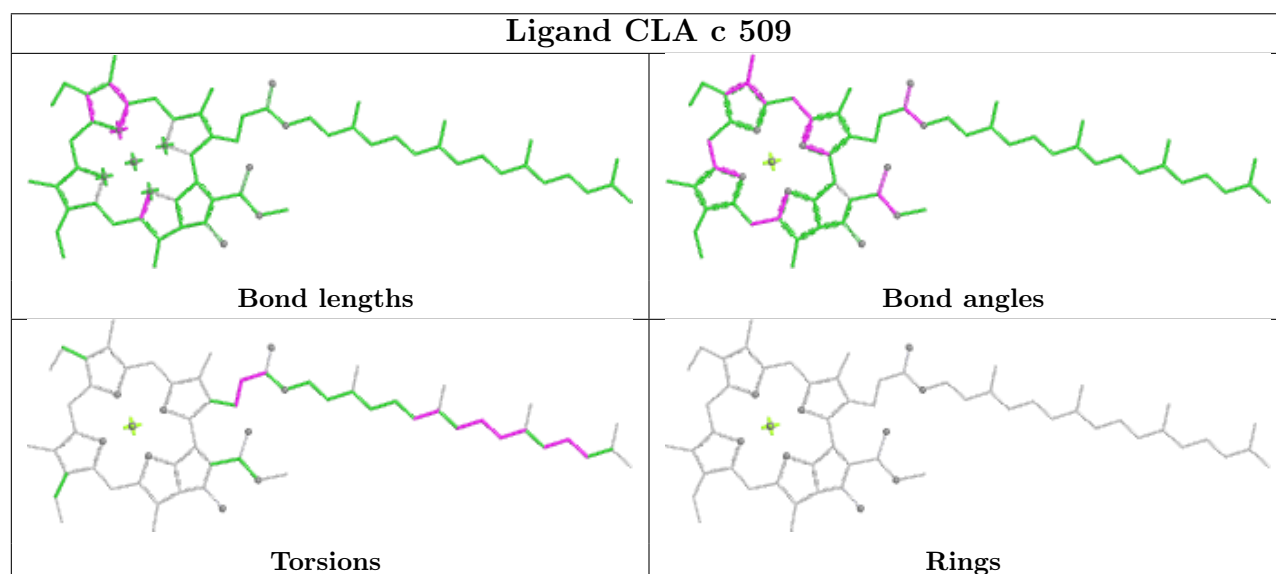
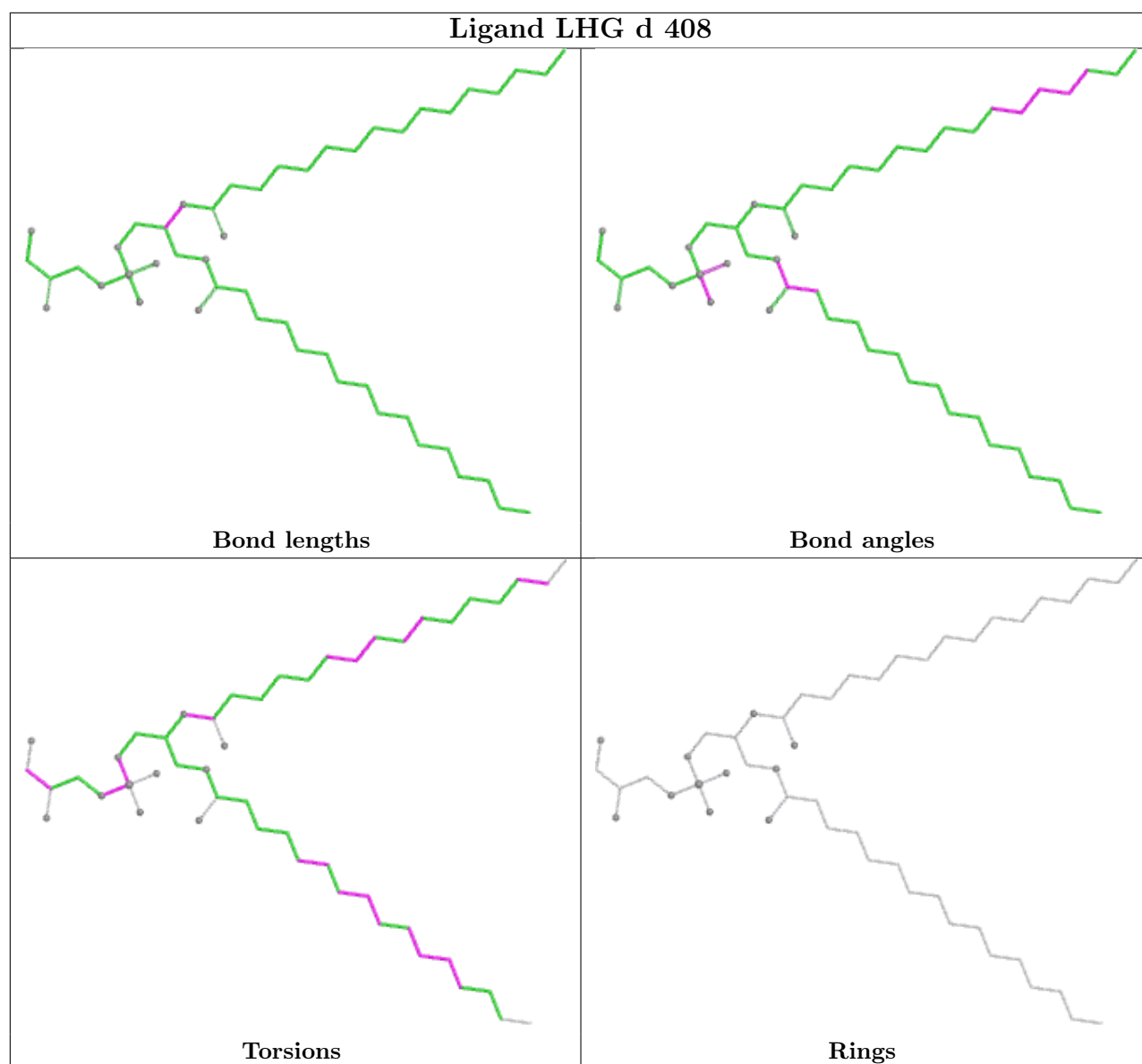


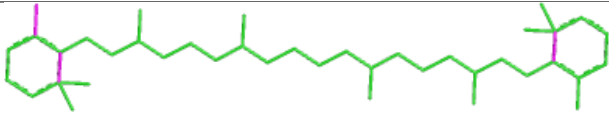
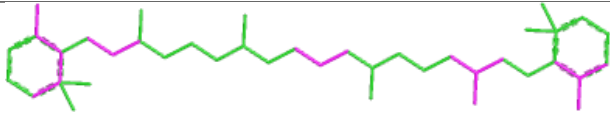
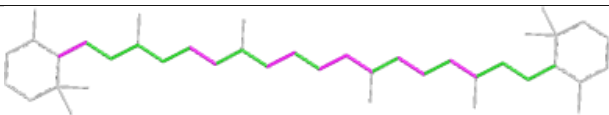
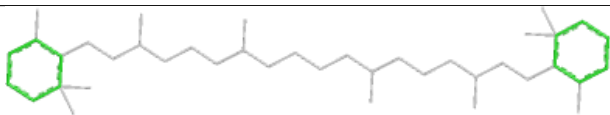
Ligand STE l 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

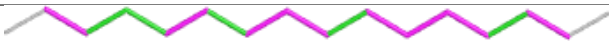
Ligand CLA b 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

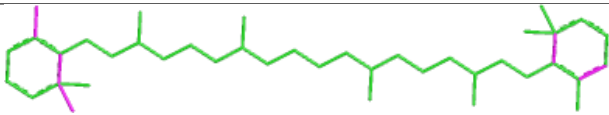
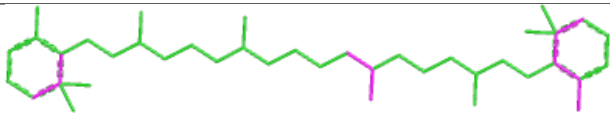
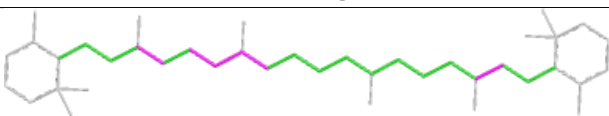
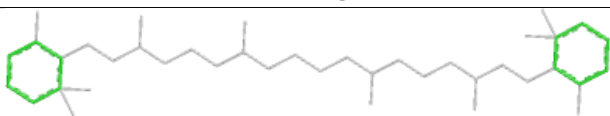
Ligand CLA c 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

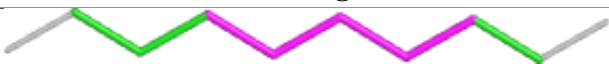


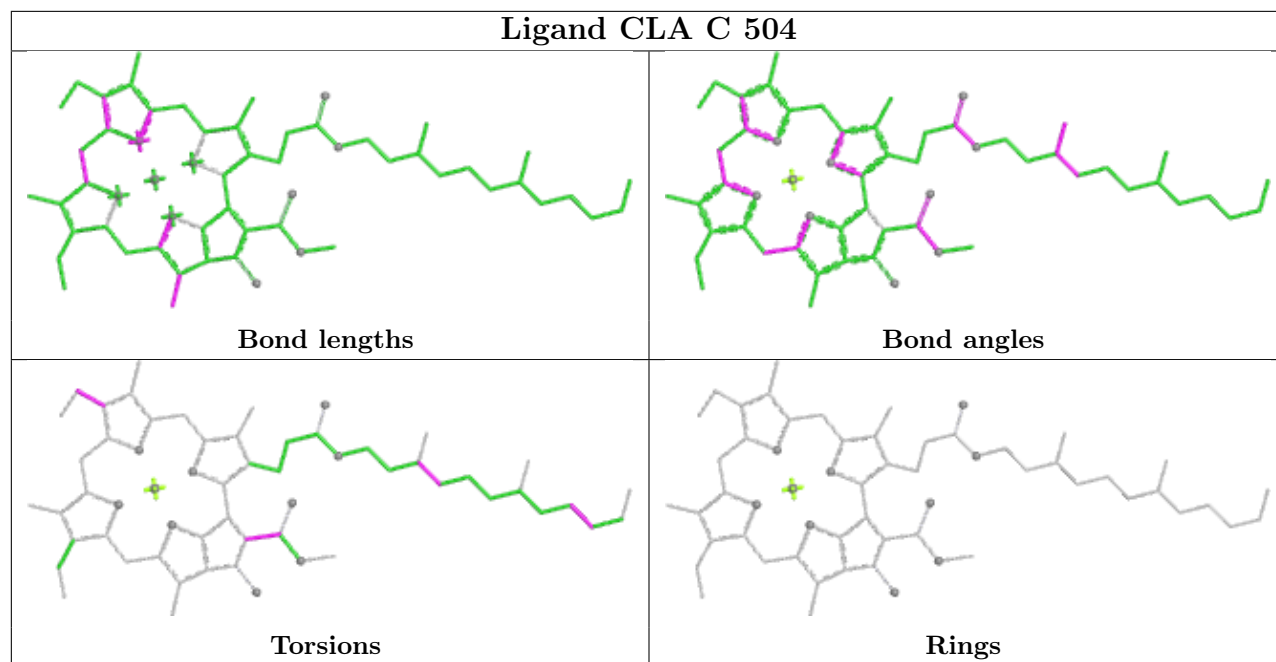


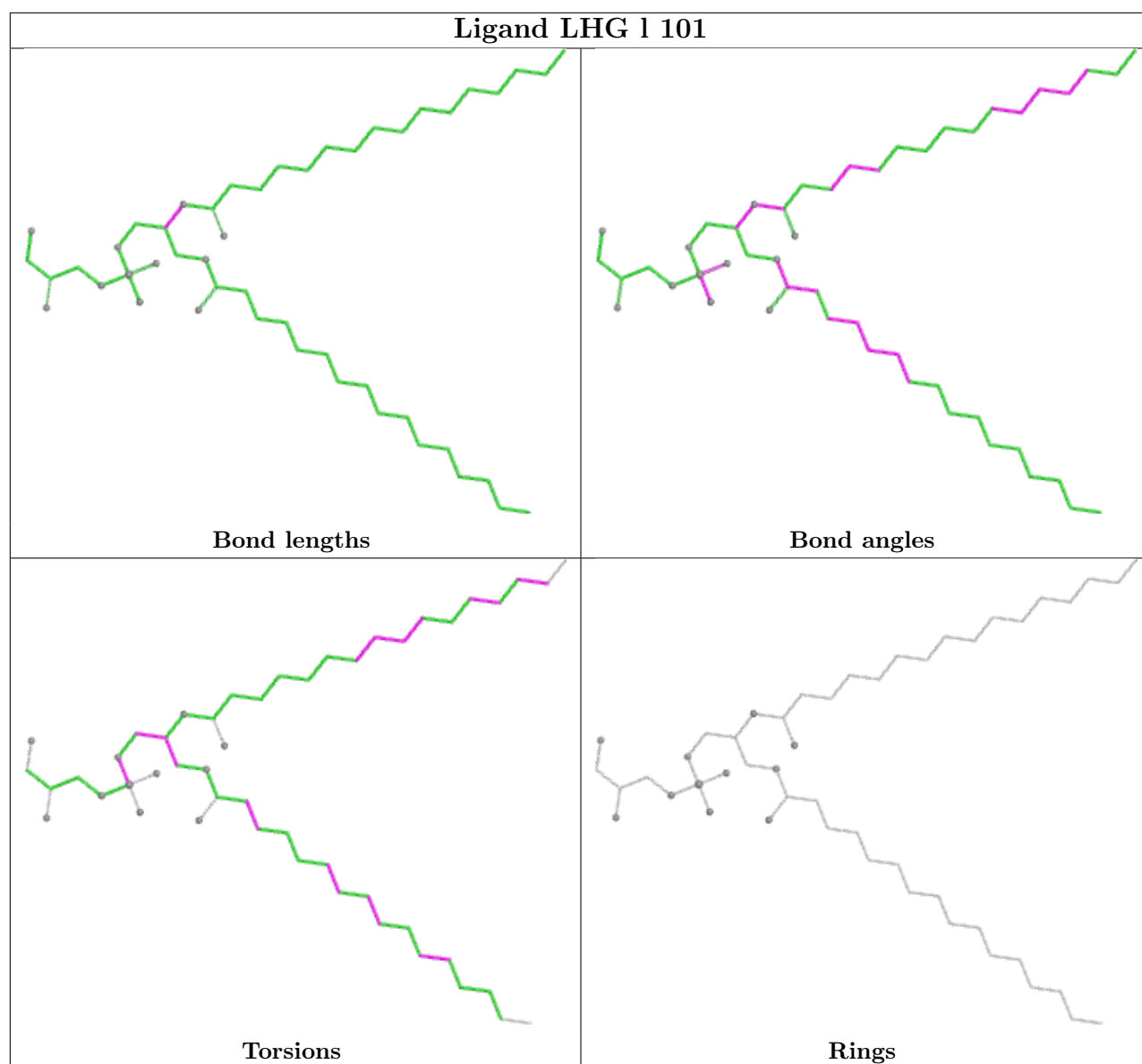
Ligand BCR c 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE T 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand STE a 615	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.58	0 100 100	13, 29, 48, 83	64 (19%)
1	a	334/344 (97%)	-0.47	2 (0%) 85 85	12, 31, 57, 84	64 (19%)
2	B	505/510 (99%)	-0.46	3 (0%) 85 85	16, 34, 61, 87	4 (0%)
2	b	505/510 (99%)	-0.30	2 (0%) 88 88	25, 38, 69, 107	0
3	C	442/461 (95%)	-0.43	0 100 100	14, 37, 53, 80	11 (2%)
3	c	451/461 (97%)	-0.29	1 (0%) 91 90	14, 41, 62, 101	12 (2%)
4	D	341/352 (96%)	-0.65	0 100 100	15, 31, 47, 84	2 (0%)
4	d	341/352 (96%)	-0.46	0 100 100	16, 34, 56, 81	3 (0%)
5	E	82/84 (97%)	0.19	2 (2%) 59 59	30, 51, 69, 85	1 (1%)
5	e	82/84 (97%)	0.36	1 (1%) 76 76	39, 60, 76, 92	0
6	F	34/45 (75%)	-0.17	1 (2%) 53 52	37, 43, 62, 83	0
6	f	34/45 (75%)	0.03	0 100 100	41, 49, 77, 91	0
7	H	65/66 (98%)	-0.29	2 (3%) 51 50	32, 42, 58, 72	0
7	h	63/66 (95%)	0.06	2 (3%) 50 49	39, 51, 65, 73	0
8	I	35/38 (92%)	-0.39	0 100 100	32, 40, 68, 84	0
8	i	35/38 (92%)	-0.18	1 (2%) 53 52	31, 42, 75, 91	0
9	J	36/40 (90%)	-0.08	1 (2%) 55 54	34, 51, 72, 91	0
9	j	36/40 (90%)	0.10	1 (2%) 55 54	38, 53, 91, 107	0
10	K	37/46 (80%)	-0.02	0 100 100	41, 52, 73, 77	0
10	k	37/46 (80%)	0.19	0 100 100	47, 57, 71, 80	0
11	L	37/37 (100%)	-0.57	0 100 100	25, 32, 61, 68	0
11	l	36/37 (97%)	-0.49	0 100 100	26, 32, 74, 90	0
12	M	32/36 (88%)	-0.50	0 100 100	25, 36, 56, 68	0
12	m	31/36 (86%)	-0.47	0 100 100	27, 36, 50, 69	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	244/272 (89%)	-0.14	4 (1%) 70 70	25, 44, 82, 136	1 (0%)
13	o	244/272 (89%)	-0.17	3 (1%) 76 76	26, 42, 78, 135	0
14	R	28/41 (68%)	0.72	0 100 100	61, 71, 87, 91	0
14	r	28/41 (68%)	1.14	1 (3%) 46 45	69, 87, 104, 114	0
15	T	29/32 (90%)	-0.53	1 (3%) 48 47	27, 32, 61, 75	0
15	t	29/32 (90%)	-0.36	2 (6%) 23 21	29, 33, 78, 85	0
16	U	97/134 (72%)	-0.21	0 100 100	33, 44, 72, 88	0
16	u	97/134 (72%)	-0.28	0 100 100	30, 41, 56, 86	0
17	V	137/163 (84%)	-0.36	0 100 100	30, 41, 57, 77	0
17	v	137/163 (84%)	-0.11	1 (0%) 84 84	34, 48, 69, 86	0
18	X	38/41 (92%)	-0.05	0 100 100	37, 50, 67, 77	0
18	x	39/41 (95%)	0.26	1 (2%) 57 56	48, 58, 86, 100	0
19	Y	27/46 (58%)	1.11	4 (14%) 5 5	52, 70, 96, 99	0
19	y	30/46 (65%)	0.84	0 100 100	60, 72, 91, 100	0
20	Z	62/62 (100%)	0.76	1 (1%) 70 70	53, 68, 119, 126	0
20	z	62/62 (100%)	0.76	2 (3%) 50 49	59, 73, 111, 121	0
All	All	5293/5700 (92%)	-0.28	39 (0%) 84 84	12, 39, 74, 136	162 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	58	ASN	5.0
13	O	59	LYS	4.1
5	e	79	PHE	3.7
20	Z	62	VAL	3.7
15	t	30	THR	3.7
2	b	495	PHE	3.4
18	x	40	SER	3.2
14	r	20	VAL	3.1
7	H	41	PHE	3.1
19	Y	22	LEU	3.0
20	z	33	TRP	2.9
19	Y	20	ALA	2.9
2	B	495	PHE	2.9
15	T	30	THR	2.8
5	E	84	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
7	h	41	PHE	2.7
13	O	60	ARG	2.7
19	Y	25	ILE	2.7
3	c	24	THR	2.7
2	B	490	GLN	2.6
1	a	11	ALA	2.6
13	O	58	ASN	2.6
9	J	5	GLY	2.6
1	a	250	ALA	2.3
7	h	64	ALA	2.3
13	o	56	PRO	2.2
17	v	113	VAL	2.2
13	o	57	LYS	2.2
19	Y	24	MET	2.2
6	F	12	SER	2.2
13	O	56	PRO	2.1
20	z	30	PRO	2.1
9	j	6	GLY	2.1
8	i	36	ASP	2.1
15	t	29	ILE	2.1
2	b	487	SER	2.1
5	E	79	PHE	2.0
7	H	65	LEU	2.0
2	B	494	GLY	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	37,48,67,75	0
15	FME	t	1	10/11	0.94	0.08	31,44,66,66	0
8	FME	I	1	10/11	0.95	0.09	35,46,65,66	0
12	FME	m	1	10/11	0.96	0.09	34,42,59,71	0
8	FME	i	1	10/11	0.96	0.08	33,48,59,64	0
15	FME	T	1	10/11	0.97	0.06	28,45,61,61	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	STE	a	616	12/20	0.74	0.15	45,61,68,71	0
33	STE	H	103	18/20	0.75	0.17	49,67,78,81	0
33	STE	b	626	10/20	0.76	0.17	42,54,62,63	0
33	STE	d	412	20/20	0.76	0.16	41,65,84,85	0
33	STE	b	625	20/20	0.78	0.14	47,62,72,76	0
29	LMG	a	618	55/55	0.79	0.14	38,58,72,83	0
33	STE	a	615	10/20	0.79	0.16	40,60,68,69	0
29	LMG	b	623	55/55	0.79	0.16	51,68,87,91	0
33	STE	a	617	15/20	0.80	0.18	38,57,69,77	0
33	STE	m	101	12/20	0.80	0.15	45,61,75,76	0
29	LMG	c	521	48/55	0.81	0.14	50,71,93,96	0
33	STE	b	627	14/20	0.81	0.15	50,65,77,78	0
33	STE	I	101	15/20	0.81	0.15	40,55,75,80	0
30	LHG	e	102	42/49	0.81	0.13	52,77,103,111	0
33	STE	B	627	12/20	0.82	0.15	47,60,73,74	0
33	STE	k	103	12/20	0.82	0.12	49,67,78,80	0
33	STE	E	102	12/20	0.82	0.16	56,72,77,83	0
30	LHG	E	101	49/49	0.83	0.13	46,71,102,108	0
33	STE	B	626	16/20	0.83	0.14	45,58,70,74	0
33	STE	T	103	15/20	0.83	0.14	43,55,68,71	0
31	SQD	a	614	36/54	0.84	0.13	33,61,81,83	0
33	STE	j	101	12/20	0.84	0.12	45,58,67,70	0
33	STE	C	520	12/20	0.84	0.12	44,56,64,64	0
24	CLA	b	601	65/65	0.84	0.12	47,65,83,96	0
33	STE	T	102	16/20	0.85	0.12	30,48,62,65	0
33	STE	b	624	16/20	0.85	0.13	45,61,70,73	0
33	STE	B	620	17/20	0.85	0.12	36,51,64,65	0
33	STE	x	102	20/20	0.85	0.11	38,55,68,71	0
33	STE	C	522	12/20	0.86	0.12	39,49,57,58	0
33	STE	Z	101	8/20	0.86	0.17	41,57,64,64	0
29	LMG	A	614	48/55	0.86	0.11	37,55,74,84	0
31	SQD	A	617	39/54	0.86	0.13	40,59,87,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMG	D	409	33/55	0.86	0.13	37,56,77,84	0
33	STE	J	101	12/20	0.86	0.12	45,55,63,65	0
33	STE	t	102	18/20	0.86	0.12	42,55,72,77	0
32	DGD	A	618	66/66	0.86	0.11	43,61,74,82	0
33	STE	b	622	20/20	0.87	0.11	38,53,67,67	0
29	LMG	c	522	49/55	0.87	0.11	37,56,81,96	0
33	STE	B	624	14/20	0.87	0.11	36,51,61,63	0
33	STE	l	102	18/20	0.87	0.12	36,49,76,78	0
29	LMG	c	519	37/55	0.87	0.12	44,63,80,85	0
28	PL9	A	612	55/55	0.87	0.13	33,62,82,85	0
33	STE	c	520	20/20	0.87	0.11	36,55,71,76	0
28	PL9	a	611	55/55	0.88	0.13	32,65,80,88	0
31	SQD	B	623	54/54	0.88	0.10	39,57,81,90	0
29	LMG	C	519	48/55	0.88	0.12	39,67,85,89	0
33	STE	M	103	10/20	0.89	0.13	33,43,52,58	0
33	STE	C	521	16/20	0.89	0.11	37,51,64,71	0
33	STE	B	625	12/20	0.89	0.10	37,51,59,66	0
26	BCR	C	514	40/40	0.89	0.12	38,55,68,71	0
33	STE	d	411	17/20	0.90	0.11	41,52,64,65	0
29	LMG	D	410	28/55	0.90	0.11	36,50,61,63	0
24	CLA	B	601	65/65	0.90	0.11	32,58,84,95	0
31	SQD	D	407	36/54	0.90	0.11	41,65,80,82	0
33	STE	D	411	20/20	0.90	0.10	35,49,68,72	0
29	LMG	b	621	51/55	0.90	0.10	35,51,70,76	0
31	SQD	b	620	49/54	0.90	0.09	38,54,87,97	0
31	SQD	f	101	41/54	0.90	0.12	54,77,98,101	0
26	BCR	d	405	40/40	0.91	0.10	37,52,87,93	0
31	SQD	a	613	54/54	0.91	0.10	38,60,79,84	0
29	LMG	M	101	51/55	0.91	0.09	31,47,64,73	0
24	CLA	C	513	65/65	0.91	0.10	41,62,84,92	0
26	BCR	D	404	40/40	0.91	0.10	28,43,79,87	0
26	BCR	H	101	40/40	0.92	0.08	30,46,59,63	0
32	DGD	H	102	62/66	0.92	0.08	25,43,55,60	0
26	BCR	k	101	40/40	0.92	0.09	39,56,68,69	0
26	BCR	x	101	40/40	0.92	0.09	37,52,71,75	0
26	BCR	Y	101	40/40	0.92	0.09	32,50,62,69	0
26	BCR	c	514	40/40	0.92	0.09	46,59,68,70	0
32	DGD	c	517	62/66	0.93	0.08	31,51,87,90	0
32	DGD	h	101	62/66	0.93	0.08	31,45,57,64	0
24	CLA	c	512	65/65	0.93	0.10	41,56,88,94	0
24	CLA	c	513	65/65	0.93	0.11	44,65,100,105	0
29	LMG	D	406	51/55	0.93	0.10	26,52,75,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	C	512	65/65	0.93	0.10	33,51,81,86	0
26	BCR	b	617	40/40	0.93	0.07	29,40,51,54	0
29	LMG	d	410	44/55	0.93	0.10	33,51,79,86	0
26	BCR	b	618	40/40	0.93	0.07	26,39,51,54	0
30	LHG	d	407	49/49	0.93	0.11	34,47,70,74	0
32	DGD	C	517	62/66	0.93	0.09	27,47,92,108	0
26	BCR	b	619	40/40	0.93	0.08	26,47,61,69	0
26	BCR	B	618	40/40	0.94	0.07	23,38,49,49	0
24	CLA	c	509	65/65	0.94	0.09	32,46,61,69	0
33	STE	M	102	15/20	0.94	0.08	36,47,59,62	0
26	BCR	C	515	40/40	0.94	0.08	27,40,50,61	0
24	CLA	C	511	65/65	0.94	0.09	30,48,65,70	0
24	CLA	b	606	65/65	0.94	0.08	25,39,70,73	0
26	BCR	k	102	40/40	0.94	0.10	39,51,63,68	0
32	DGD	C	516	62/66	0.94	0.09	21,40,77,80	0
26	BCR	T	101	40/40	0.94	0.07	25,37,50,52	0
31	SQD	A	616	52/54	0.94	0.10	34,54,90,95	0
26	BCR	A	609	40/40	0.94	0.07	21,34,42,44	0
26	BCR	B	617	40/40	0.94	0.07	26,38,56,60	0
30	LHG	d	409	39/49	0.95	0.08	30,44,67,68	0
26	BCR	t	101	40/40	0.95	0.06	27,37,50,54	0
24	CLA	C	507	65/65	0.95	0.07	25,38,53,57	0
26	BCR	B	619	40/40	0.95	0.07	25,41,54,62	0
28	PL9	D	405	55/55	0.95	0.06	19,31,46,47	0
24	CLA	b	608	65/65	0.95	0.08	25,42,61,66	0
28	PL9	d	406	55/55	0.95	0.06	20,34,42,44	0
24	CLA	b	609	65/65	0.95	0.08	29,43,62,68	0
24	CLA	c	504	60/65	0.95	0.08	31,43,78,85	0
24	CLA	c	506	65/65	0.95	0.09	31,48,89,90	0
26	BCR	K	101	40/40	0.95	0.08	34,49,65,65	0
24	CLA	c	508	64/65	0.95	0.09	29,43,83,98	0
24	CLA	C	510	65/65	0.95	0.07	26,41,61,62	0
32	DGD	C	518	62/66	0.95	0.08	24,46,75,85	0
26	BCR	a	607	40/40	0.95	0.06	23,33,43,49	0
32	DGD	c	516	62/66	0.95	0.08	21,41,67,74	0
24	CLA	c	511	65/65	0.95	0.09	33,50,70,75	0
32	DGD	c	518	62/66	0.95	0.09	25,49,80,86	0
24	CLA	B	610	65/65	0.95	0.07	20,32,42,45	0
24	CLA	C	503	65/65	0.95	0.06	27,39,48,51	0
24	CLA	d	404	65/65	0.95	0.09	28,47,81,87	0
26	BCR	c	515	40/40	0.95	0.07	27,42,58,61	0
25	PHO	d	402	64/64	0.95	0.06	26,35,45,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	LHG	A	615	47/49	0.95	0.10	27,48,77,88	0
30	LHG	B	622	49/49	0.95	0.08	29,43,64,69	0
24	CLA	C	504	59/65	0.95	0.08	28,40,79,80	0
24	CLA	C	506	65/65	0.95	0.09	26,42,78,84	0
34	BCT	a	610	4/4	0.95	0.09	28,33,39,47	0
24	CLA	B	605	65/65	0.96	0.07	20,31,47,50	0
24	CLA	c	505	65/65	0.96	0.08	25,38,66,72	0
24	CLA	C	505	65/65	0.96	0.08	23,39,65,81	0
24	CLA	c	507	65/65	0.96	0.07	26,43,58,64	0
24	CLA	B	606	65/65	0.96	0.07	23,34,65,71	0
24	CLA	B	609	65/65	0.96	0.07	24,36,58,66	0
24	CLA	c	510	65/65	0.96	0.07	28,45,58,71	0
24	CLA	C	508	65/65	0.96	0.07	26,38,98,109	0
24	CLA	C	509	65/65	0.96	0.08	26,42,60,64	0
24	CLA	A	604	65/65	0.96	0.06	15,26,44,54	0
24	CLA	d	401	65/65	0.96	0.08	24,37,86,90	0
24	CLA	B	613	65/65	0.96	0.07	17,31,65,70	0
25	PHO	A	606	64/64	0.96	0.05	17,27,35,41	0
25	PHO	A	607	64/64	0.96	0.05	22,31,40,42	0
24	CLA	B	614	65/65	0.96	0.08	20,35,70,80	0
24	CLA	B	615	65/65	0.96	0.07	22,36,59,63	0
24	CLA	a	604	65/65	0.96	0.05	18,28,45,55	0
24	CLA	a	606	65/65	0.96	0.08	19,36,78,84	0
30	LHG	B	621	49/49	0.96	0.07	26,40,54,61	0
24	CLA	a	612	65/65	0.96	0.06	20,29,46,51	0
24	CLA	B	616	60/65	0.96	0.08	23,37,88,95	0
24	CLA	b	602	65/65	0.96	0.07	27,41,57,62	0
24	CLA	b	603	65/65	0.96	0.07	23,36,60,68	0
24	CLA	b	605	65/65	0.96	0.06	21,34,49,54	0
30	LHG	l	101	49/49	0.96	0.06	30,42,51,57	0
24	CLA	C	501	65/65	0.96	0.06	21,35,48,51	0
24	CLA	b	607	65/65	0.96	0.07	20,35,62,68	0
24	CLA	C	502	65/65	0.96	0.06	25,39,52,59	0
24	CLA	B	602	65/65	0.96	0.06	23,35,54,61	0
24	CLA	b	610	65/65	0.96	0.07	22,37,50,54	0
24	CLA	b	611	65/65	0.96	0.06	22,33,52,62	0
24	CLA	b	612	65/65	0.96	0.07	21,34,47,56	0
24	CLA	b	613	65/65	0.96	0.07	17,33,66,74	0
24	CLA	b	614	65/65	0.96	0.07	24,38,68,76	0
24	CLA	b	615	65/65	0.96	0.07	26,39,57,63	0
24	CLA	b	616	60/65	0.96	0.08	26,41,81,83	0
24	CLA	c	501	65/65	0.96	0.06	28,39,51,55	0

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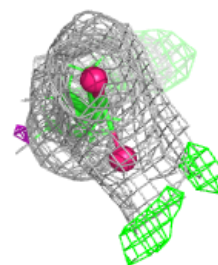
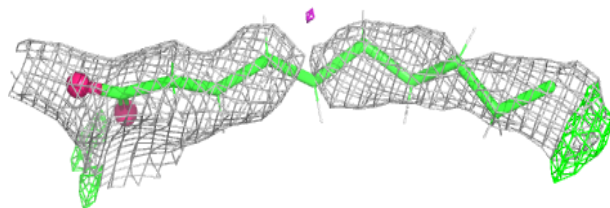
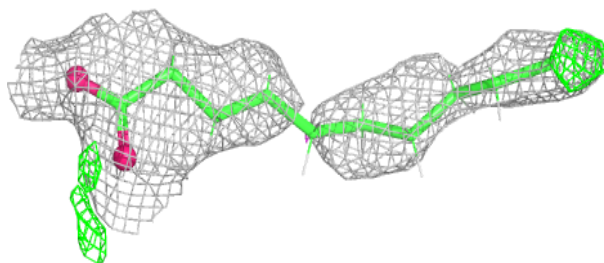
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	CLA	c	502	65/65	0.96	0.06	29,40,55,62	0
24	CLA	c	503	65/65	0.96	0.07	28,42,53,61	0
30	LHG	D	408	49/49	0.97	0.07	21,40,52,57	0
24	CLA	B	612	65/65	0.97	0.06	19,32,49,53	0
24	CLA	A	605	65/65	0.97	0.08	23,33,83,91	0
30	LHG	d	408	49/49	0.97	0.07	24,41,51,60	0
24	CLA	D	402	65/65	0.97	0.06	17,28,54,56	0
24	CLA	D	403	65/65	0.97	0.08	22,42,105,112	0
24	CLA	d	403	65/65	0.97	0.06	20,32,54,64	0
24	CLA	A	613	65/65	0.97	0.06	18,28,47,53	0
24	CLA	B	607	65/65	0.97	0.07	17,32,57,67	0
24	CLA	B	608	65/65	0.97	0.06	18,33,54,56	0
25	PHO	a	605	64/64	0.97	0.05	18,29,37,46	0
24	CLA	B	603	65/65	0.97	0.06	20,32,61,63	0
24	CLA	B	604	65/65	0.97	0.07	21,32,68,71	0
24	CLA	B	611	65/65	0.97	0.06	19,31,49,52	0
34	BCT	D	401	4/4	0.97	0.06	27,28,31,38	0
24	CLA	b	604	65/65	0.97	0.07	19,35,79,89	0
35	HEM	F	101	43/43	0.97	0.08	34,46,60,62	0
35	HEM	e	101	43/43	0.97	0.09	41,53,73,73	0
27	CL	A	611	1/1	0.98	0.05	27,27,27,27	0
24	CLA	A	608	54/65	0.98	0.06	17,32,67,69	0
36	HEC	V	201	43/43	0.98	0.05	23,31,40,40	0
36	HEC	v	201	43/43	0.98	0.06	26,36,46,46	0
22	OEX	a	602[A]	10/10	0.99	0.03	27,32,35,35	10
23	FE2	a	603	1/1	0.99	0.03	29,29,29,29	0
27	CL	A	610	1/1	0.99	0.03	28,28,28,28	0
21	OEY	a	601[B]	11/11	0.99	0.03	15,21,24,26	11
27	CL	a	608	1/1	0.99	0.04	25,25,25,25	0
27	CL	a	609	1/1	0.99	0.06	25,25,25,25	0
22	OEX	A	602[A]	10/10	0.99	0.03	29,31,35,35	10
21	OEY	A	601[B]	11/11	1.00	0.03	15,20,23,26	11
23	FE2	A	603	1/1	1.00	0.01	24,24,24,24	0

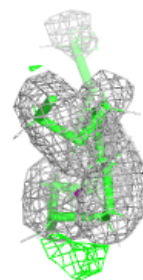
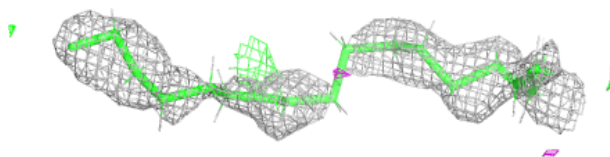
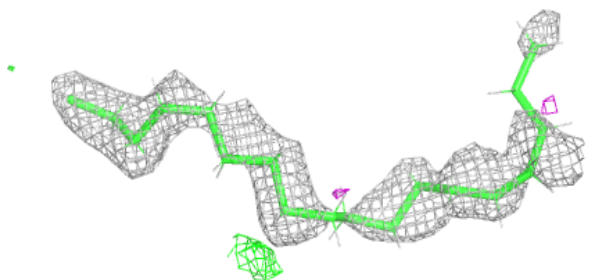
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STE a 616:

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

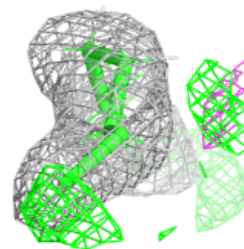
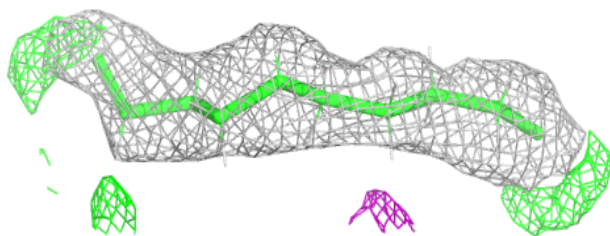
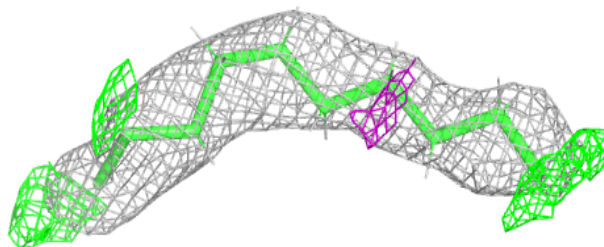
**Electron density around STE H 103:**

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

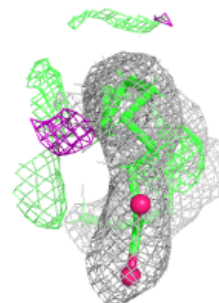
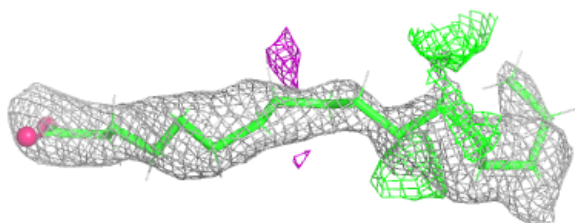
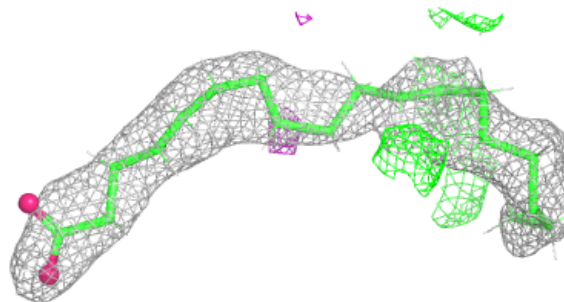


Electron density around STE b 626:

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

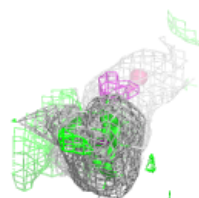
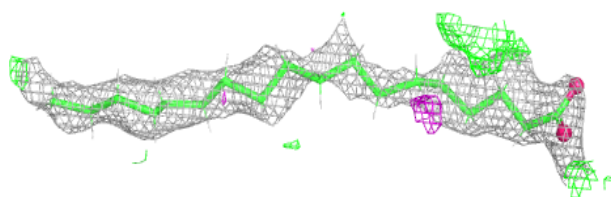
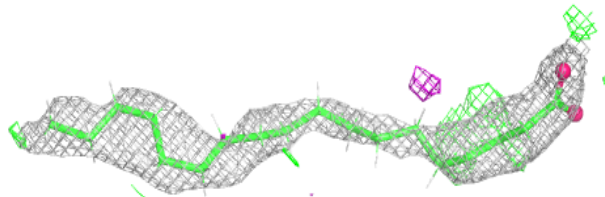
**Electron density around STE d 412:**

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

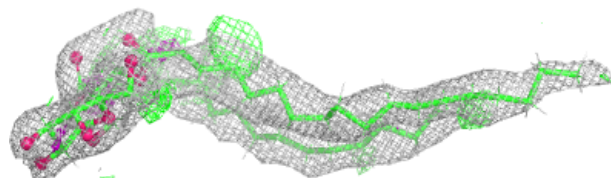
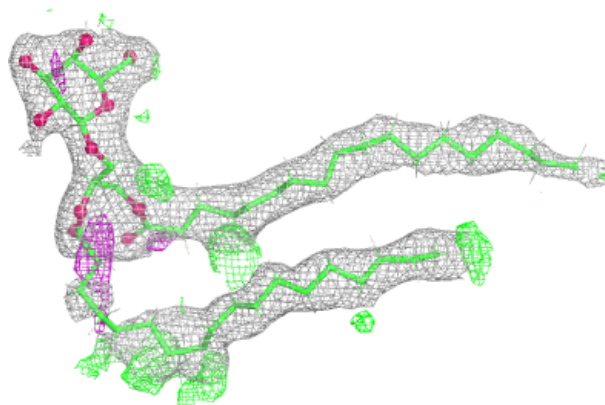


Electron density around STE b 625:

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

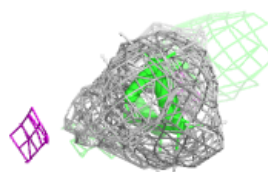
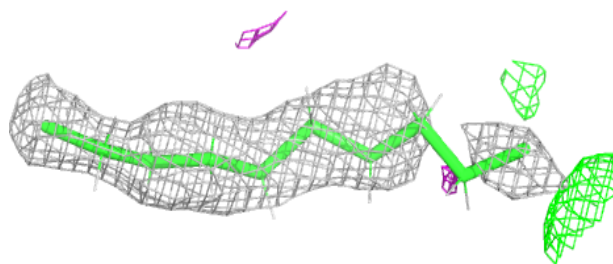
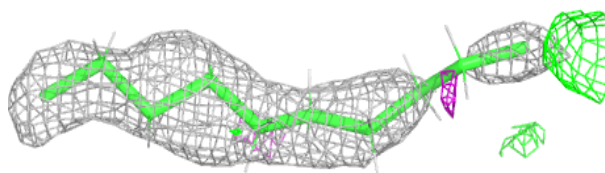
**Electron density around LMG a 618:**

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

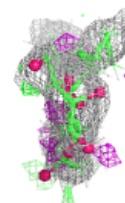
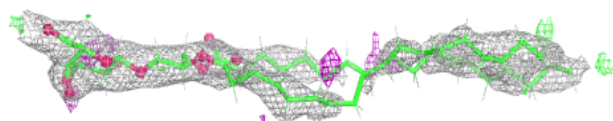
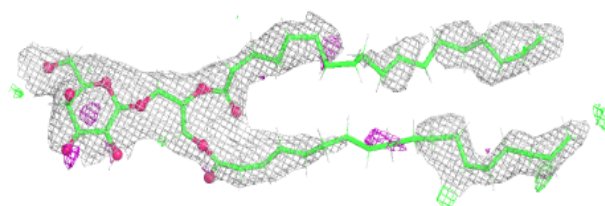


Electron density around STE a 615:

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

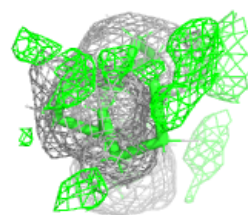
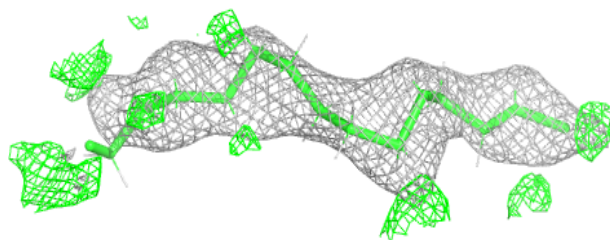
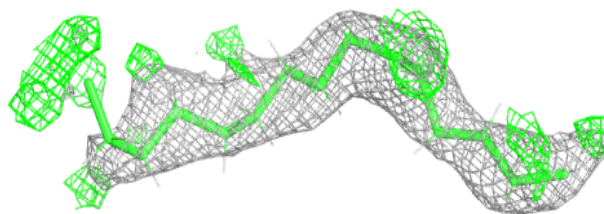
**Electron density around LMG b 623:**

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

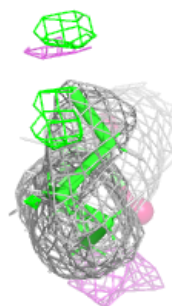
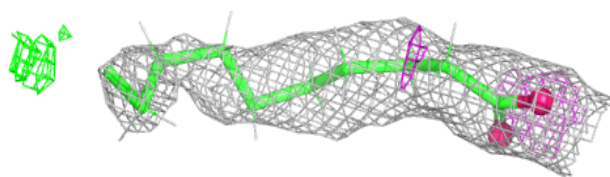
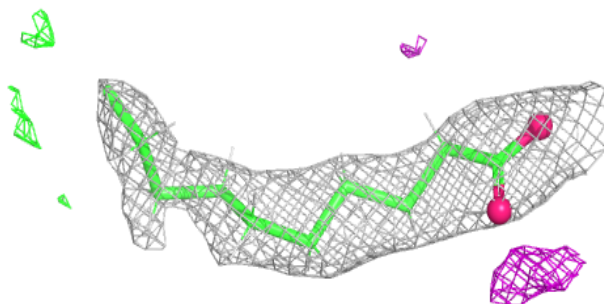


Electron density around STE a 617:

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

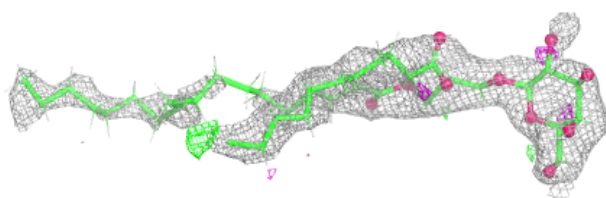
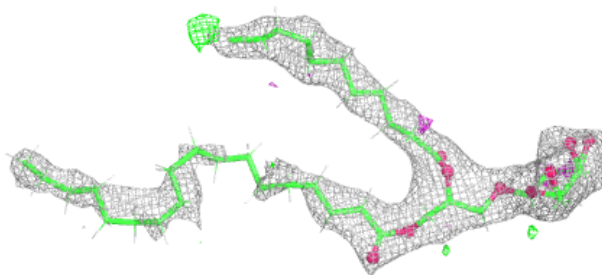
**Electron density around STE m 101:**

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

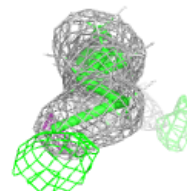
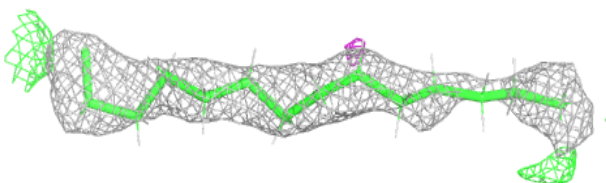
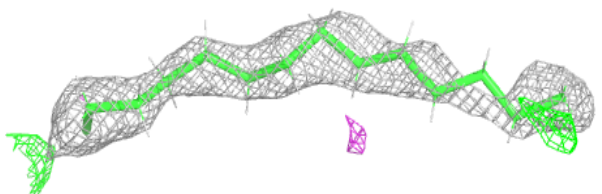


Electron density around LMG c 521:

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

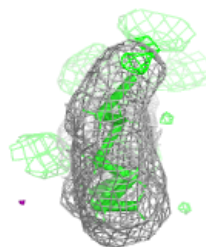
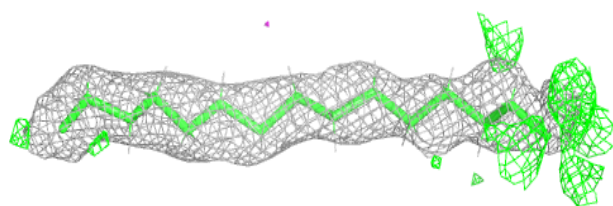
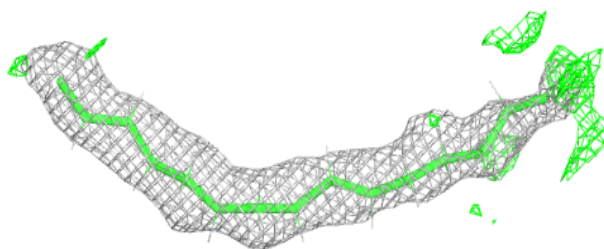
**Electron density around STE b 627:**

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

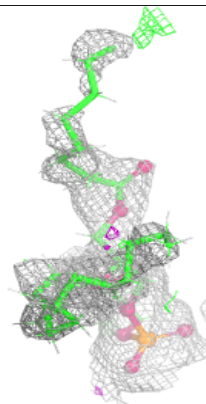
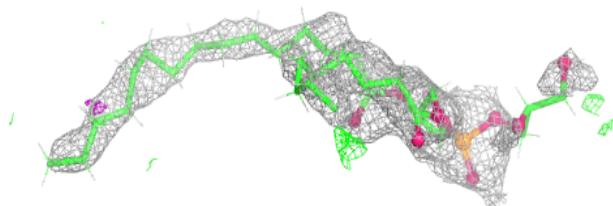
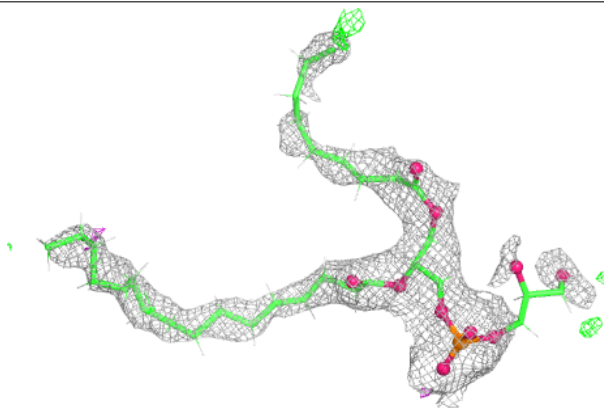


Electron density around STE I 101:

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

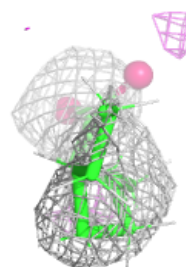
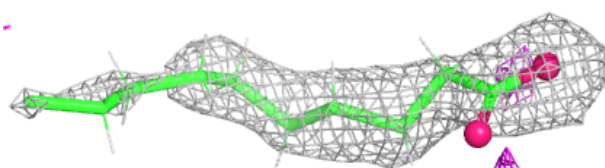
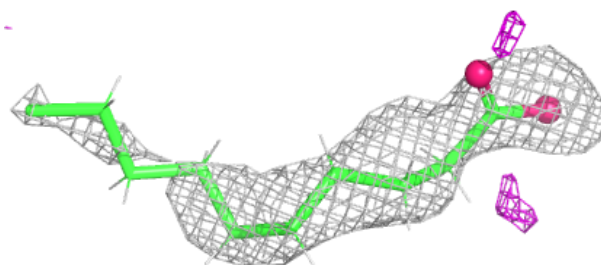
**Electron density around LHG e 102:**

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

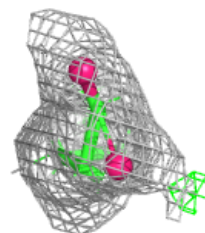
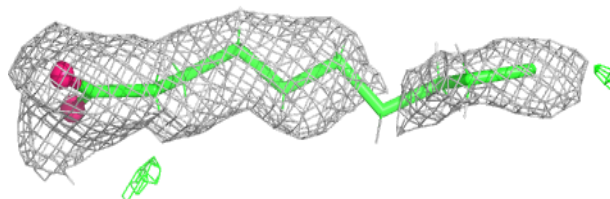
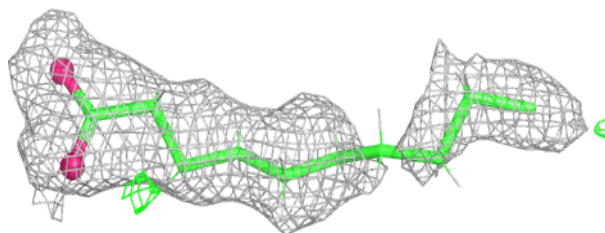


Electron density around STE B 627:

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

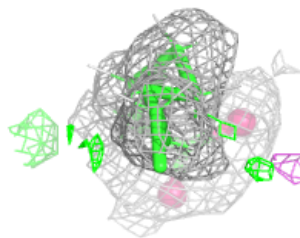
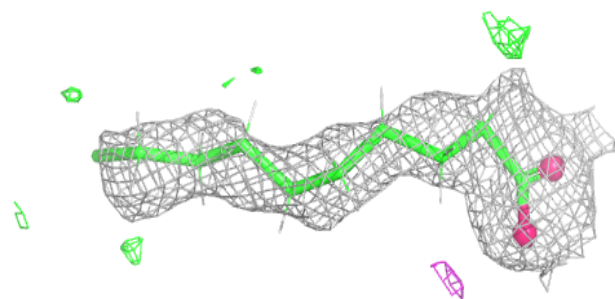
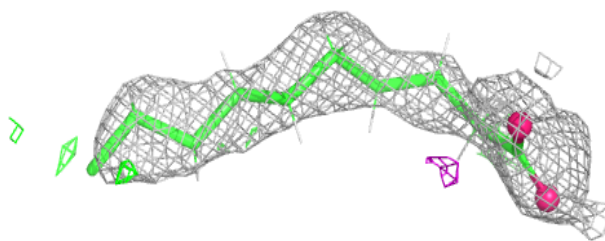
**Electron density around STE k 103:**

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



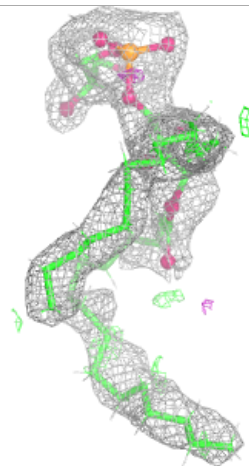
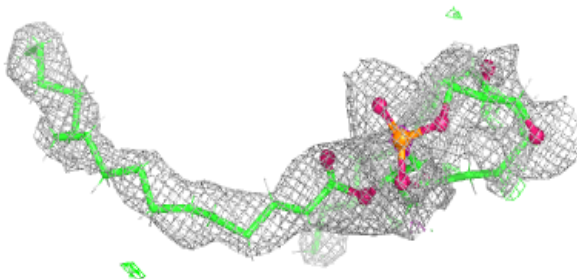
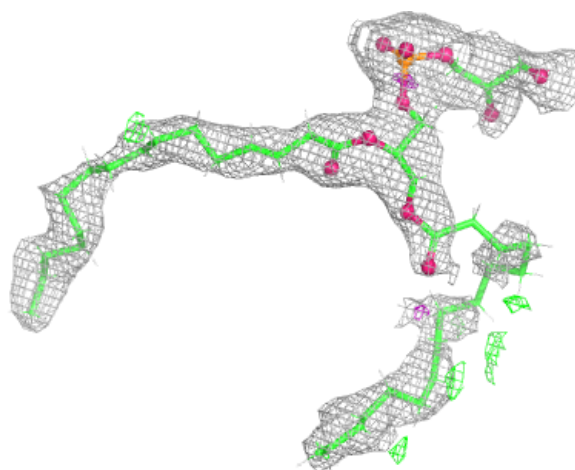
Electron density around STE E 102:

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



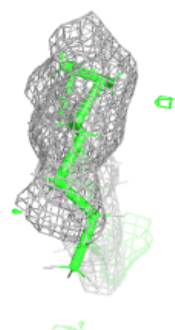
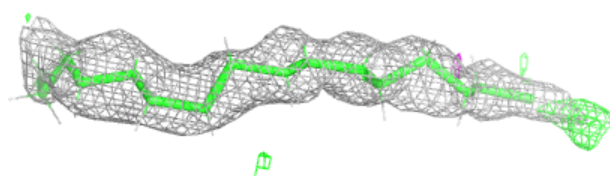
Electron density around LHG E 101:

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

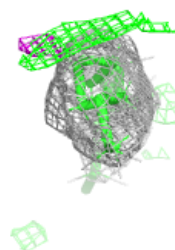
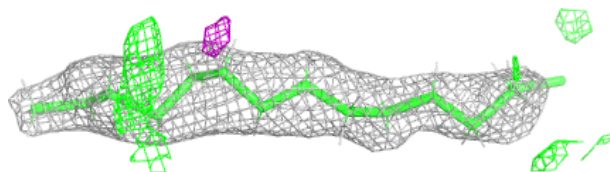
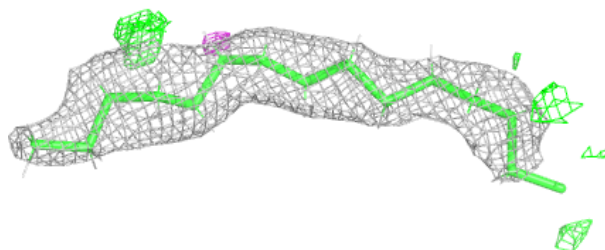


Electron density around STE B 626:

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

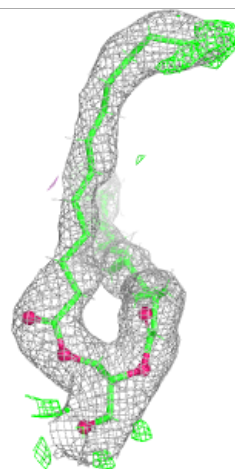
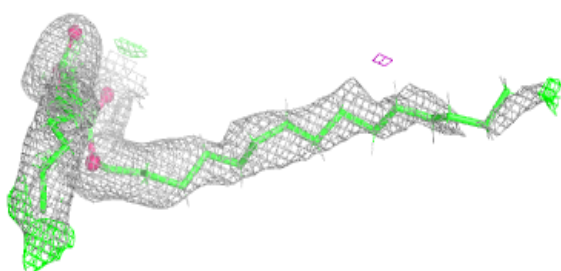
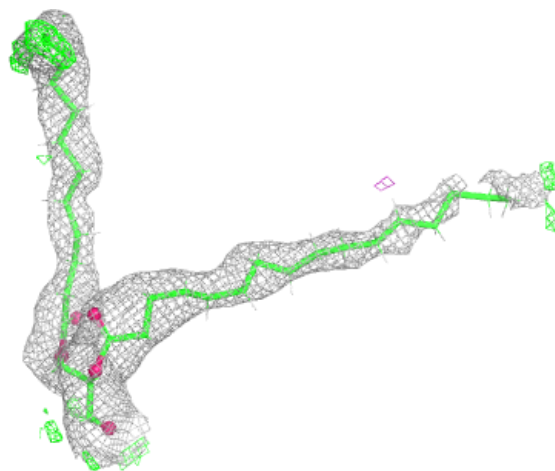
**Electron density around STE T 103:**

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



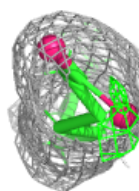
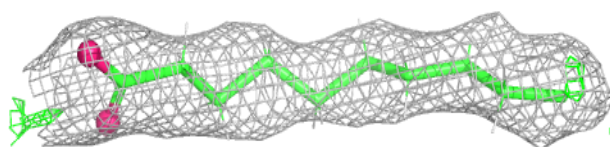
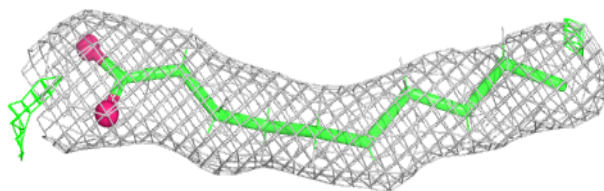
Electron density around SQD a 614:

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

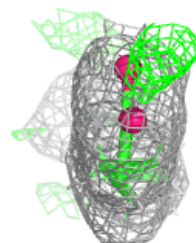
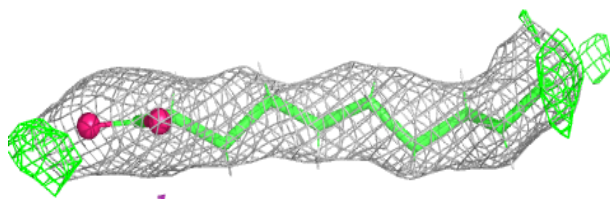
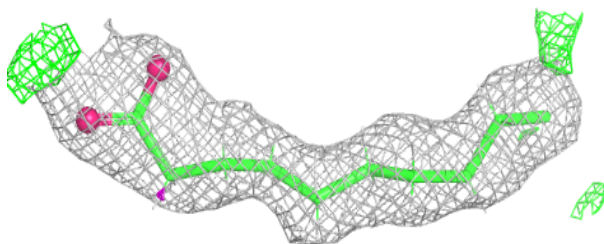


Electron density around STE j 101:

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

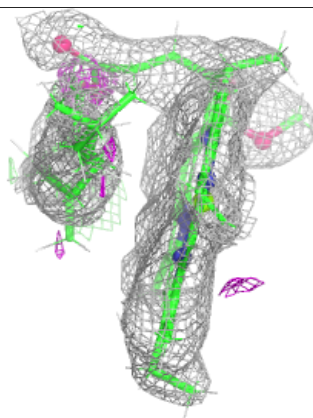
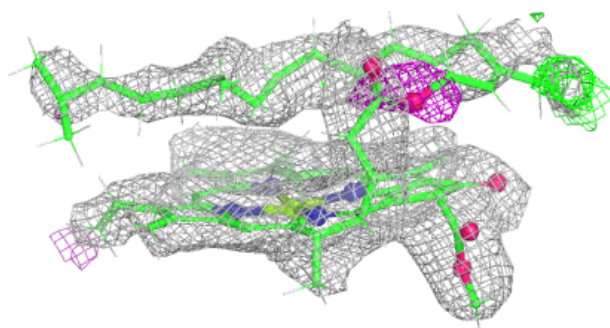
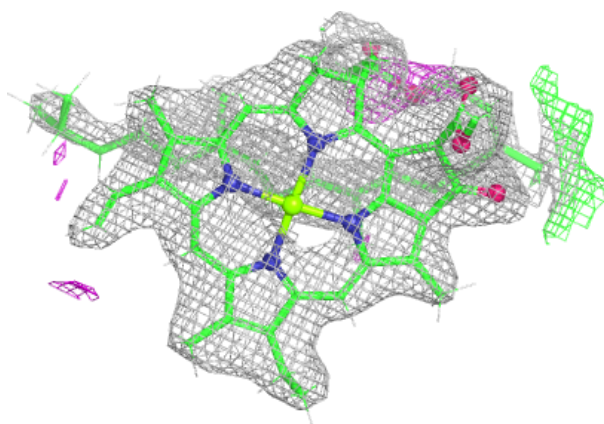
**Electron density around STE C 520:**

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

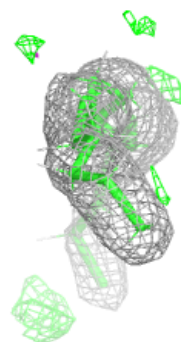
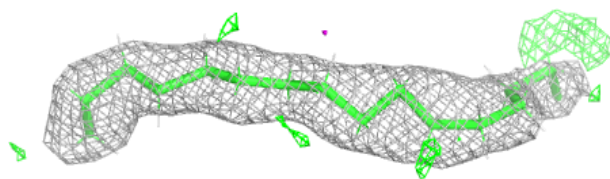
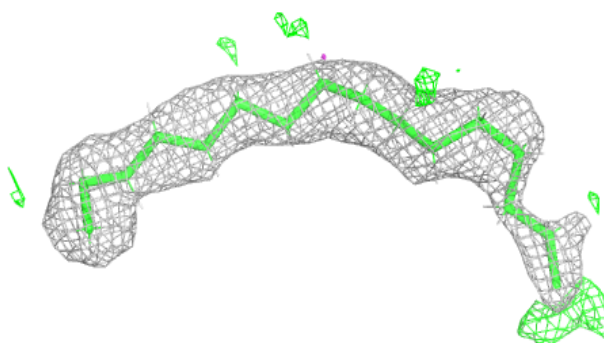


Electron density around CLA b 601:

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

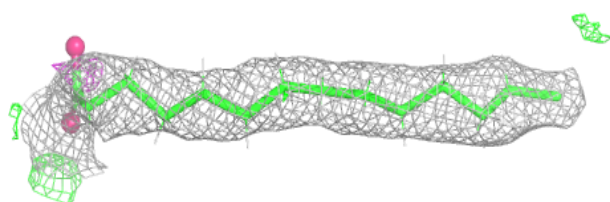
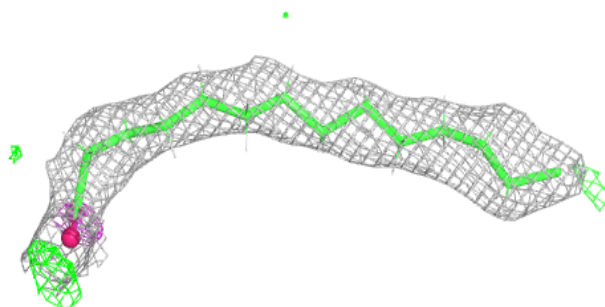
**Electron density around STE T 102:**

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

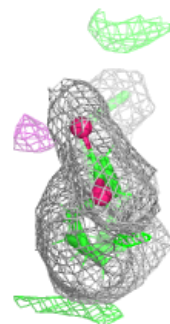
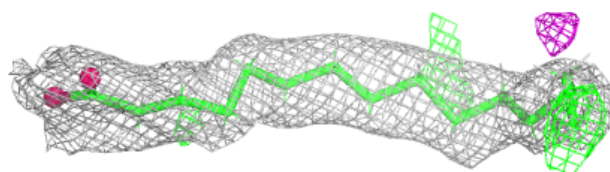
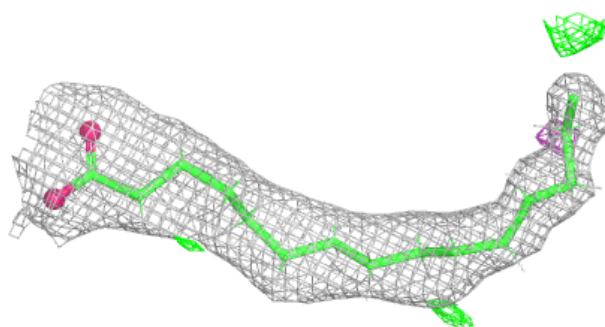


Electron density around STE b 624:

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

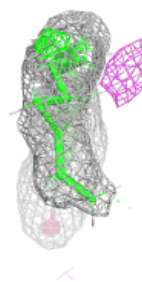
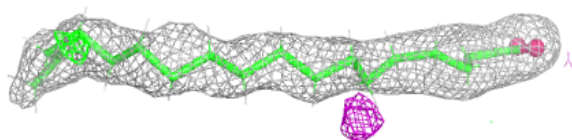
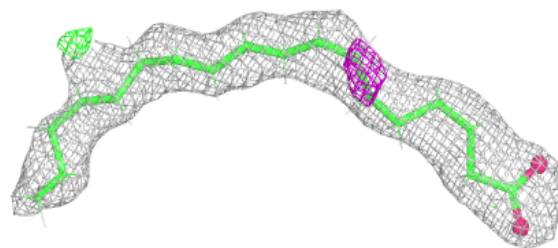
**Electron density around STE B 620:**

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

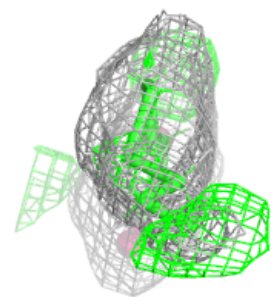
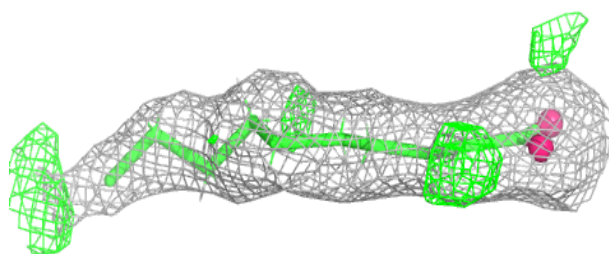
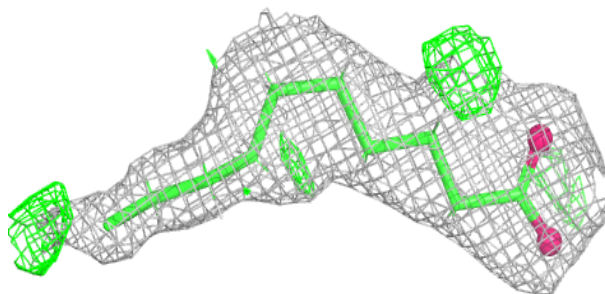


Electron density around STE x 102:

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

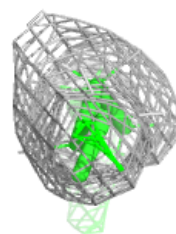
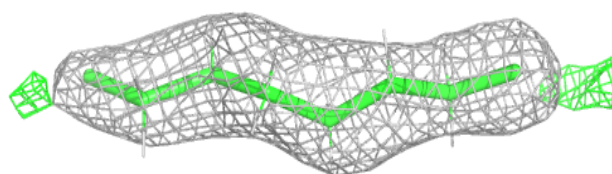
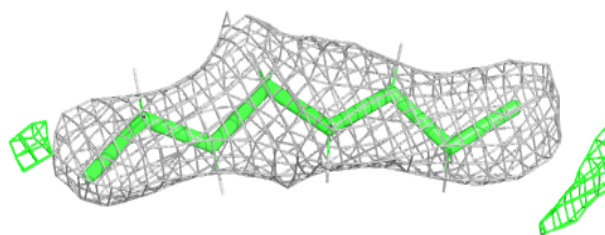
**Electron density around STE C 522:**

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

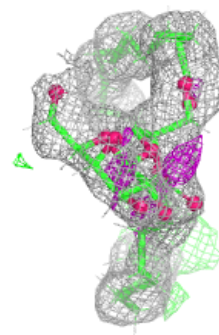
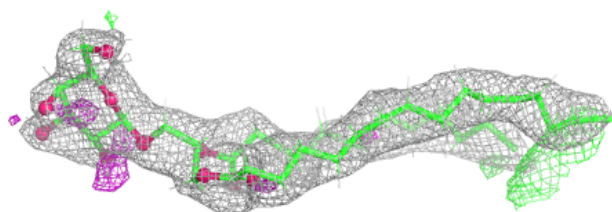
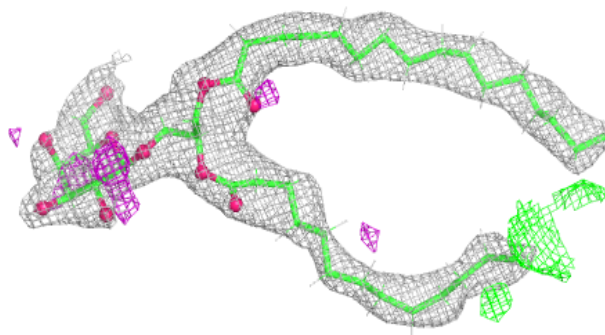


Electron density around STE Z 101:

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

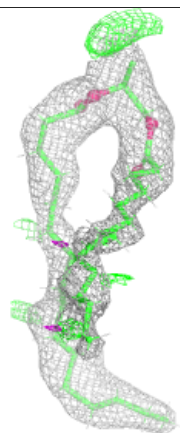
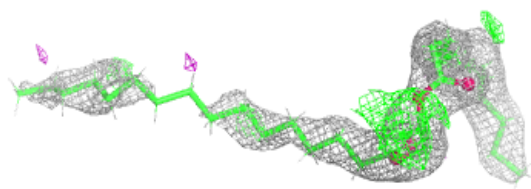
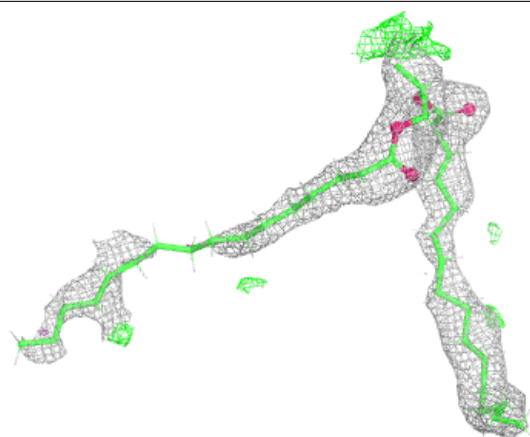
**Electron density around LMG A 614:**

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

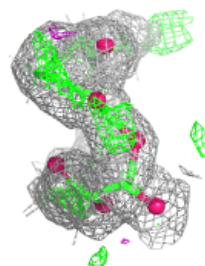
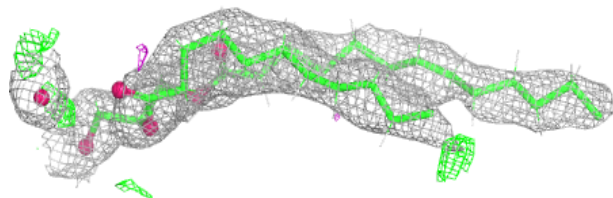
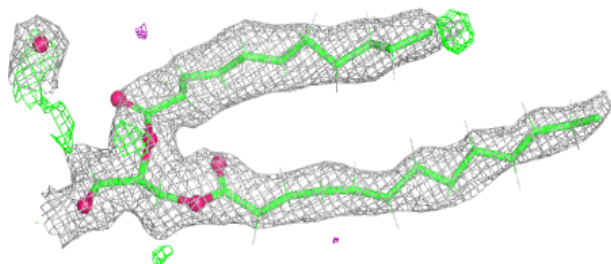


Electron density around SQD A 617:

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

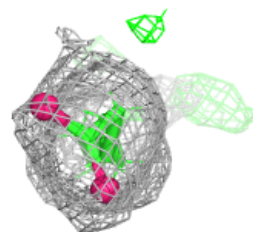
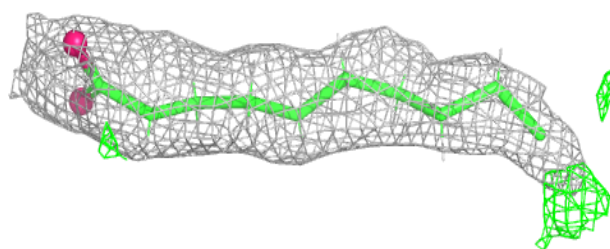
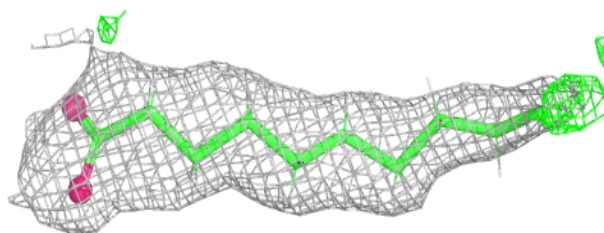
**Electron density around LMG D 409:**

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

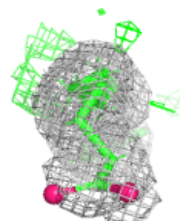
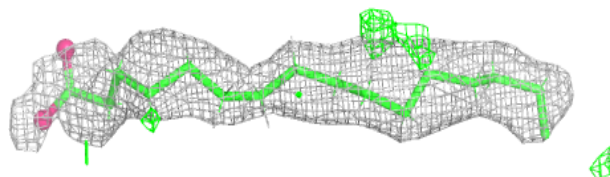
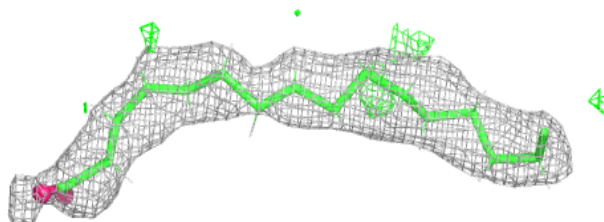


Electron density around STE J 101:

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

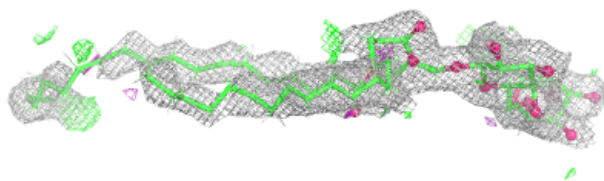
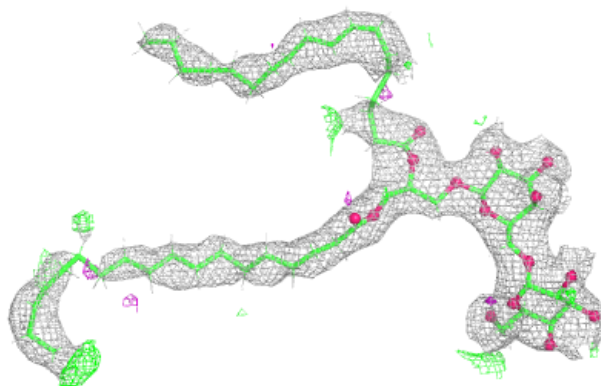
**Electron density around STE t 102:**

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

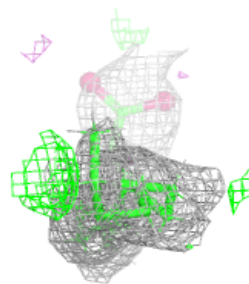
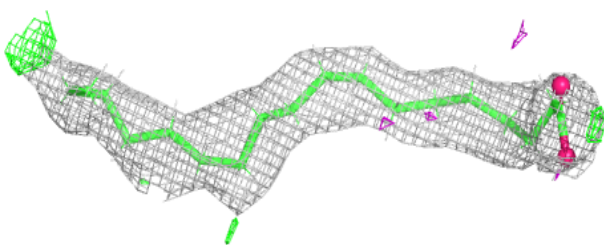
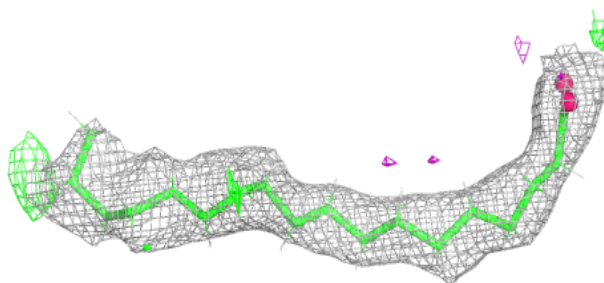


Electron density around DGD A 618:

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

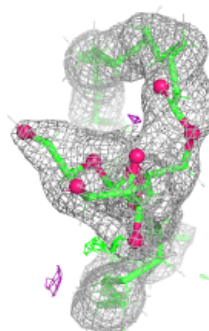
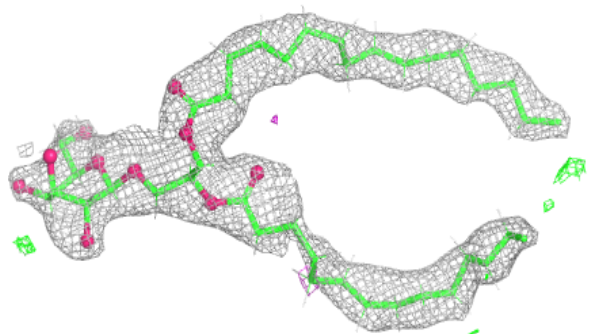
**Electron density around STE b 622:**

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

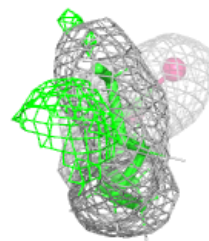
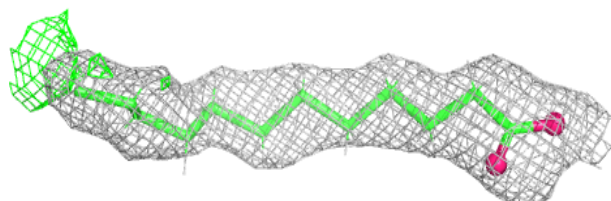
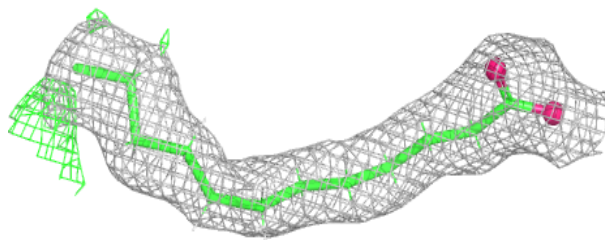


Electron density around LMG c 522:

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

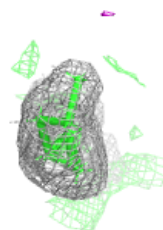
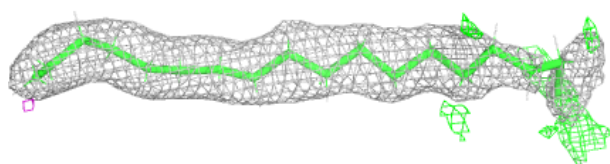
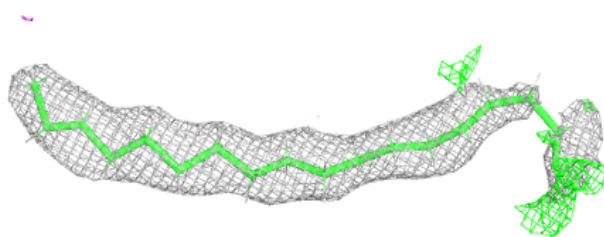
**Electron density around STE B 624:**

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

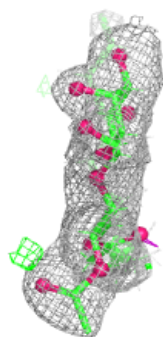
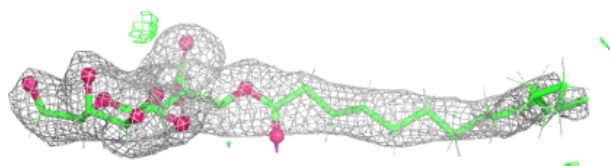
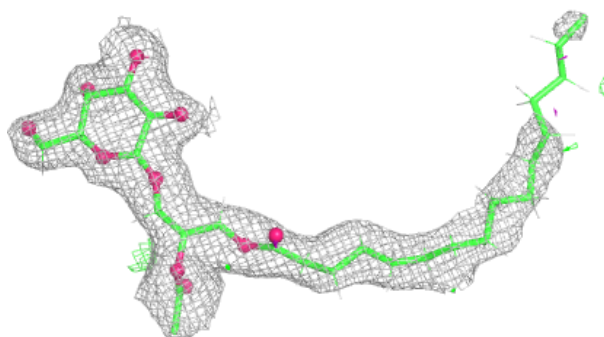


Electron density around STE 1 102:

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

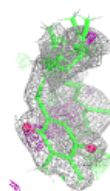
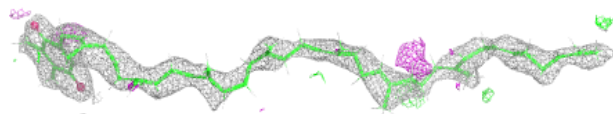
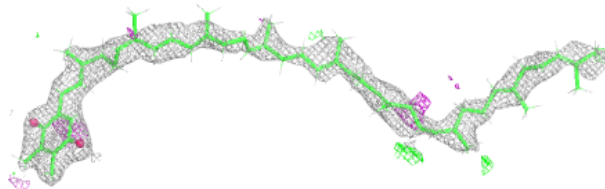
**Electron density around LMG c 519:**

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

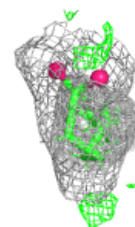
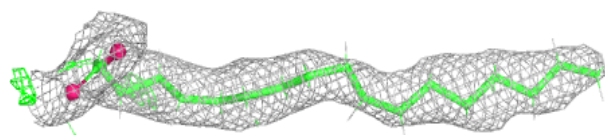
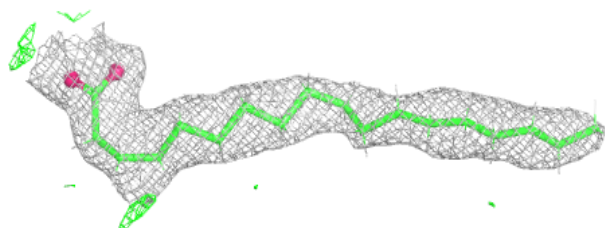


Electron density around PL9 A 612:

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

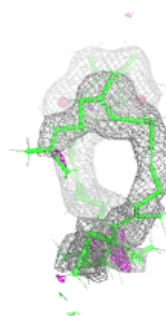
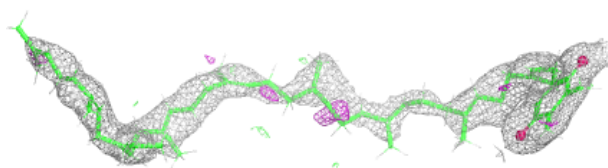
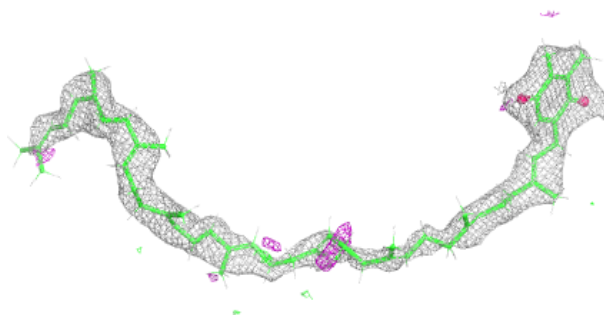
**Electron density around STE c 520:**

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

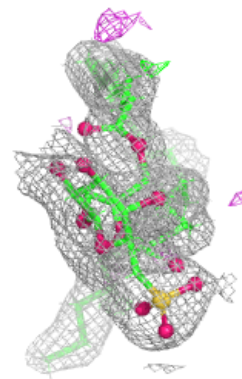
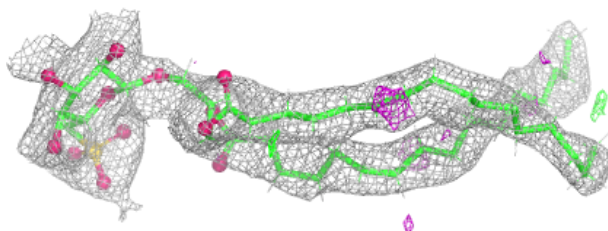
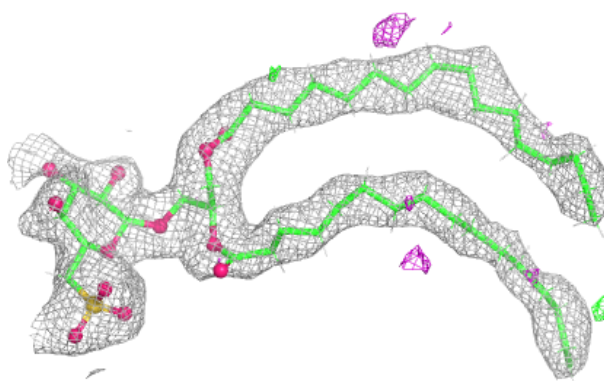


Electron density around PL9 a 611:

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

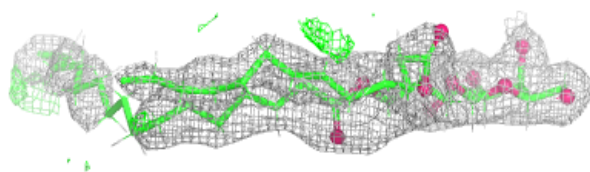
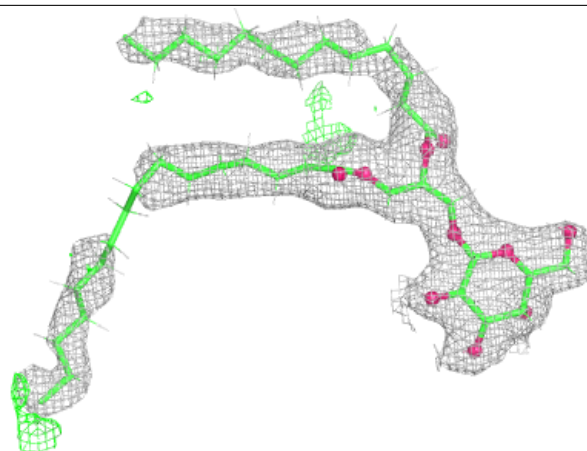
**Electron density around SQD B 623:**

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

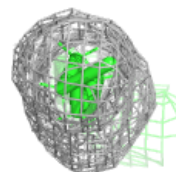
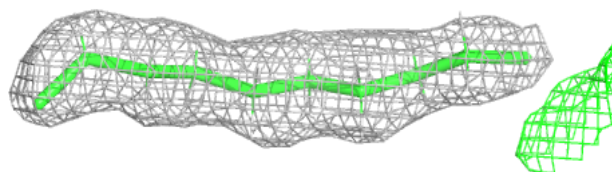
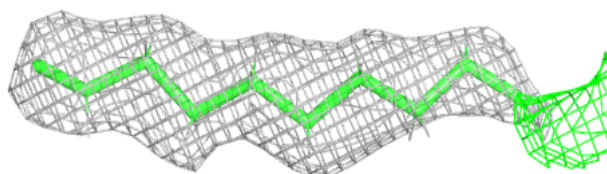


Electron density around LMG C 519:

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

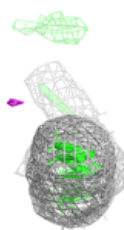
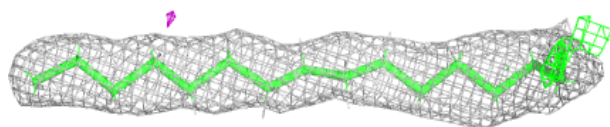
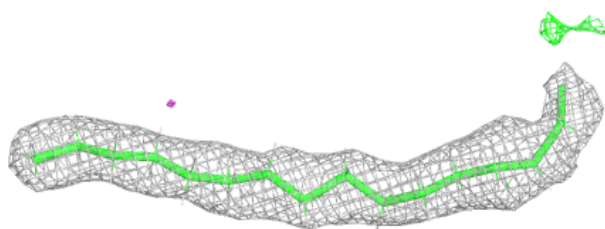
**Electron density around STE M 103:**

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

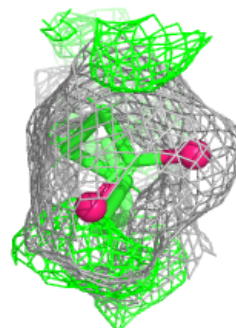
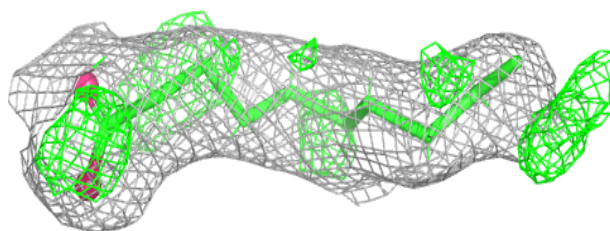
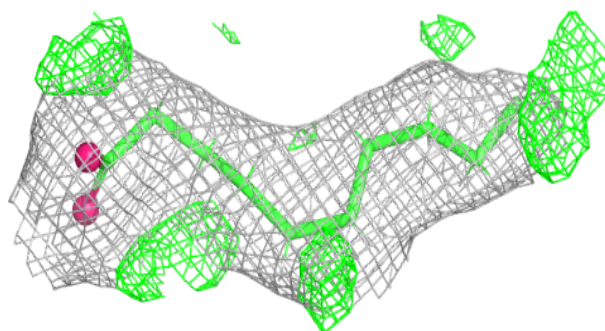


Electron density around STE C 521:

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

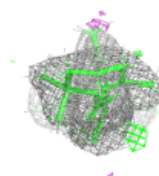
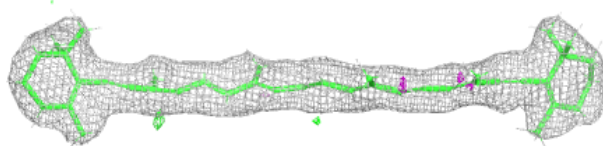
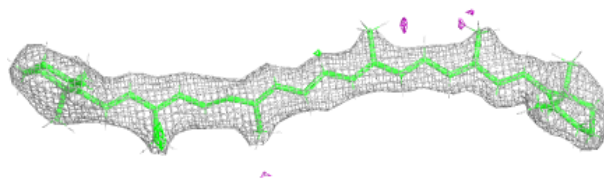
**Electron density around STE B 625:**

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

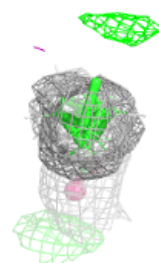
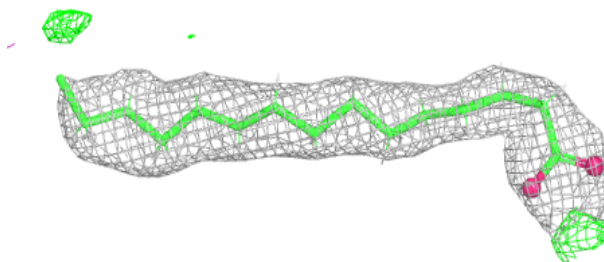


Electron density around BCR C 514:

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

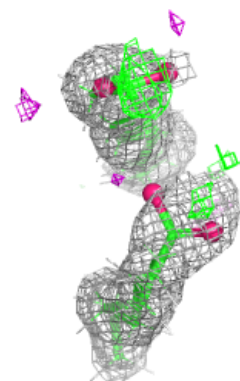
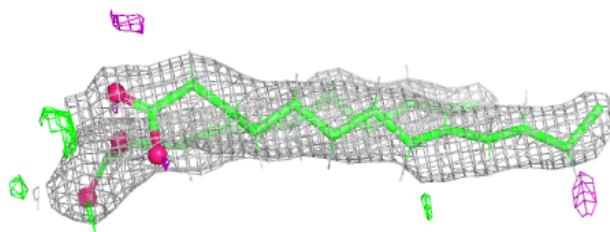
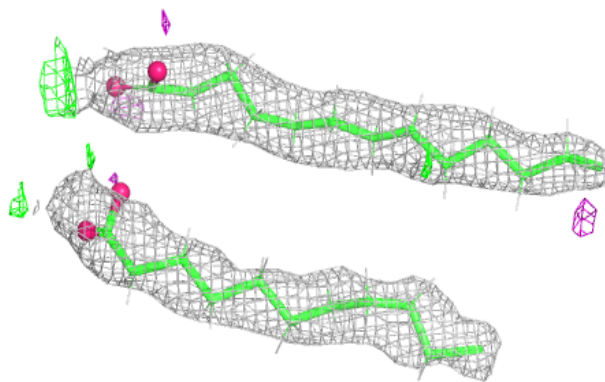
**Electron density around STE d 411:**

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

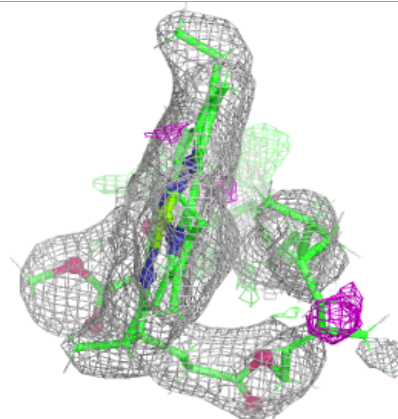
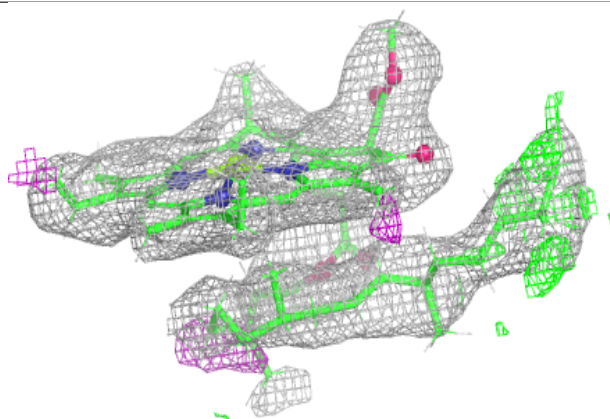
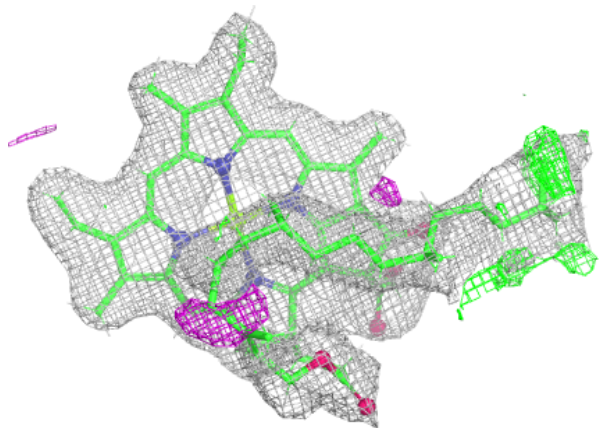


Electron density around LMG D 410:

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

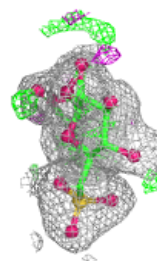
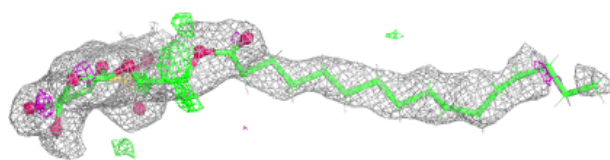
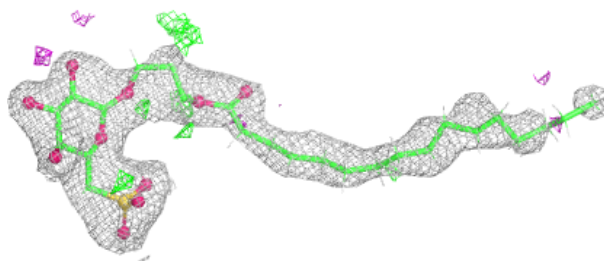
**Electron density around CLA B 601:**

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

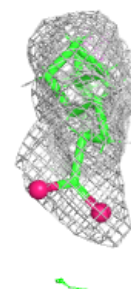
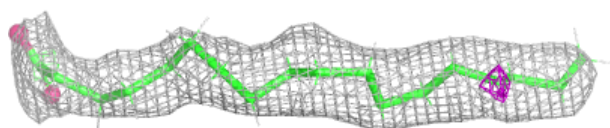
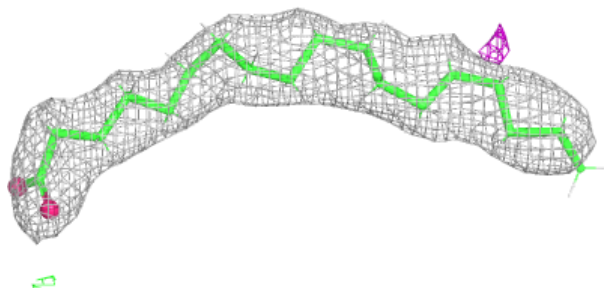


Electron density around SQD D 407:

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

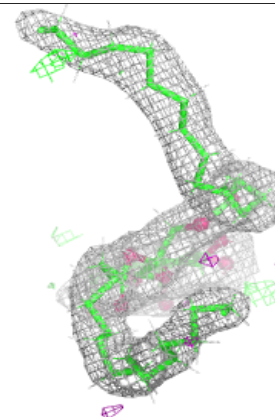
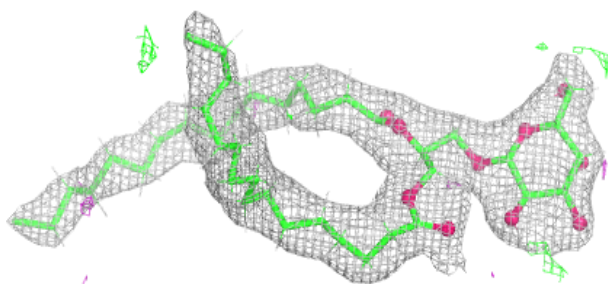
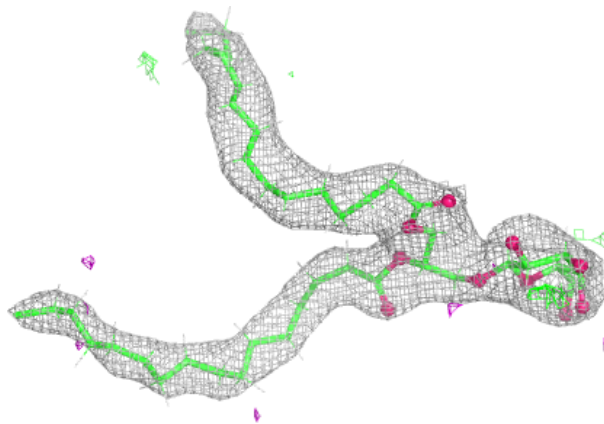
**Electron density around STE D 411:**

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

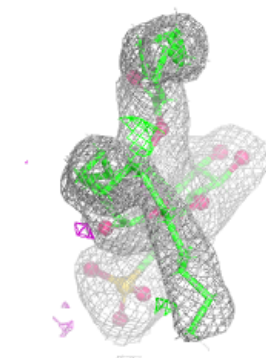
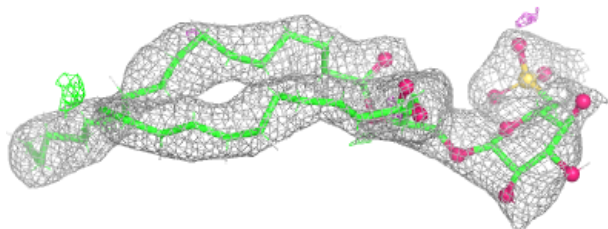
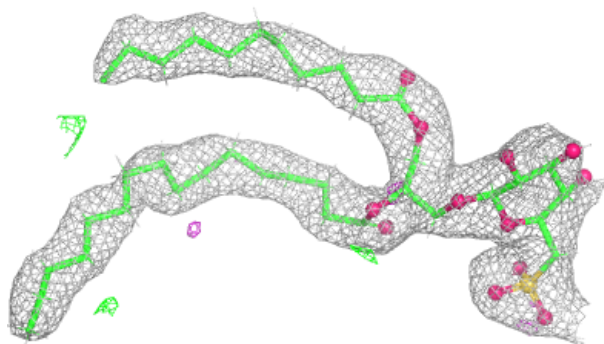


Electron density around LMG b 621:

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

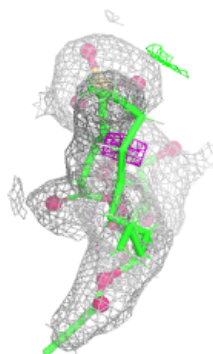
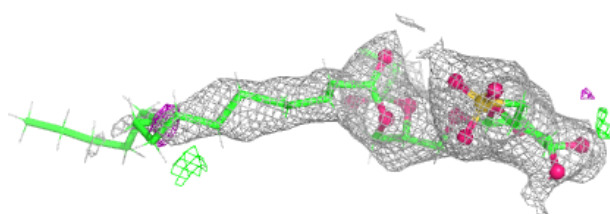
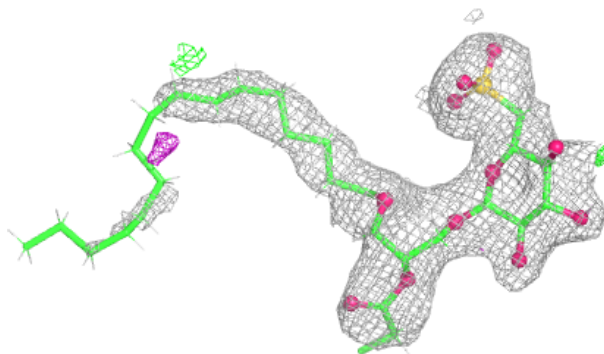
**Electron density around SQD b 620:**

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

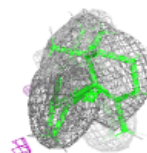
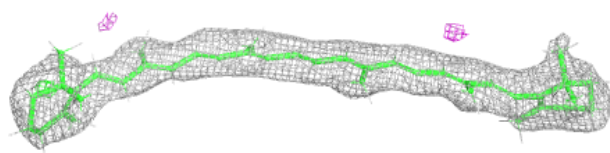
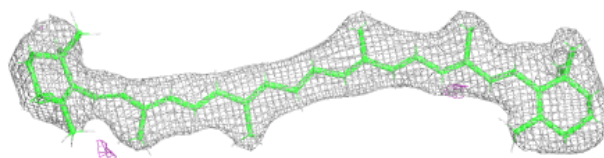


Electron density around SQD f 101:

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

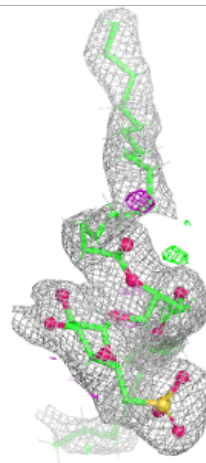
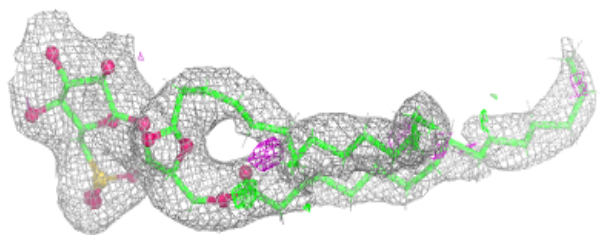
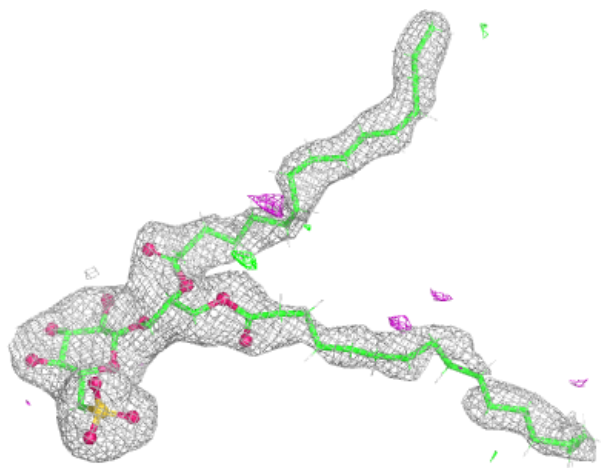
**Electron density around BCR d 405:**

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



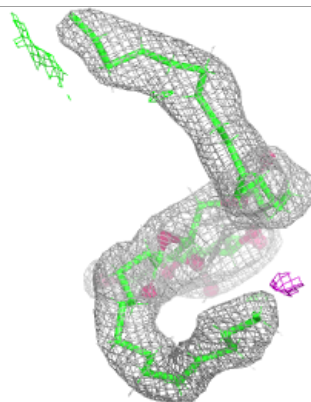
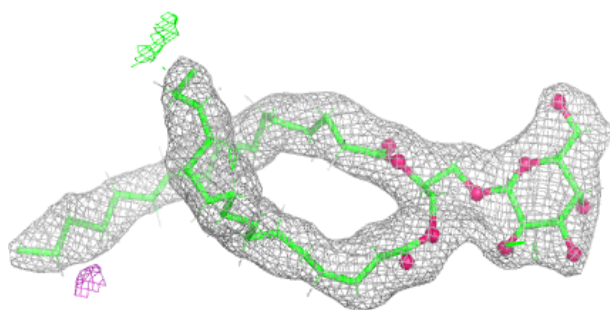
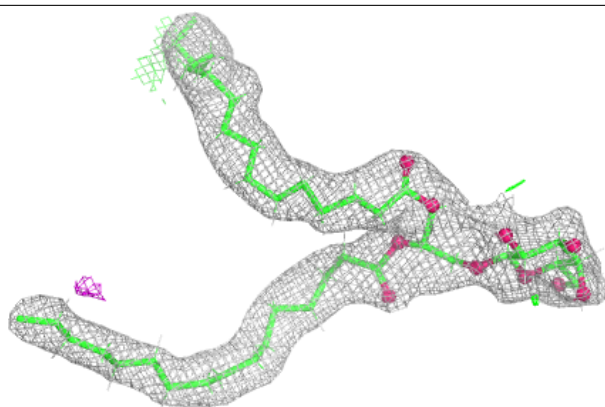
Electron density around SQD a 613:

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

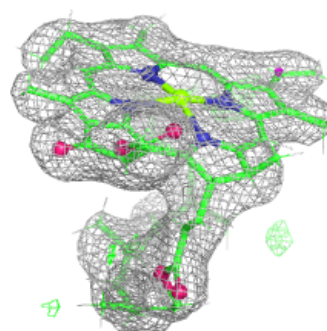
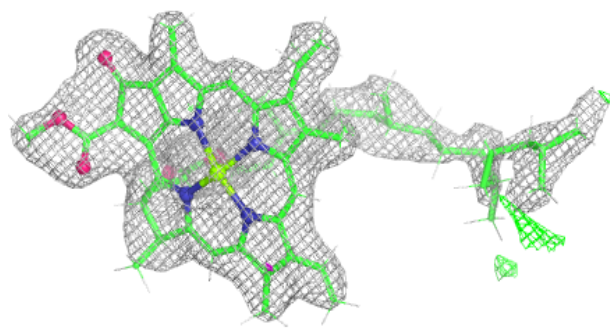
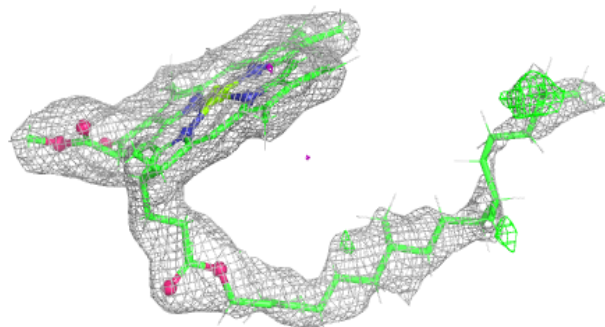


Electron density around LMG M 101:

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

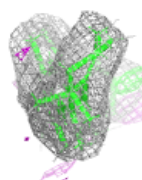
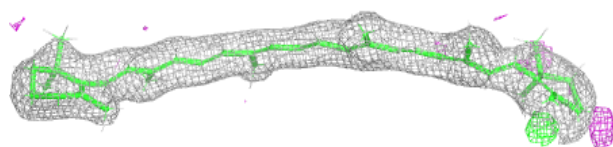
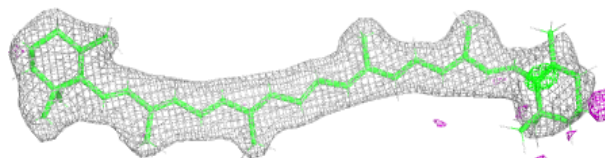
**Electron density around CLA C 513:**

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

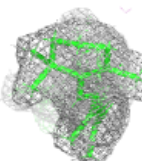
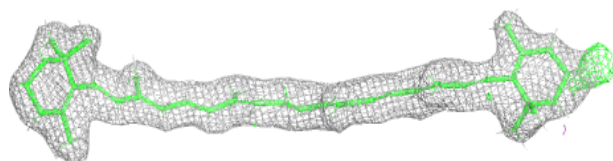
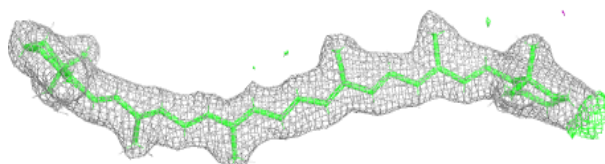


Electron density around BCR D 404:

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

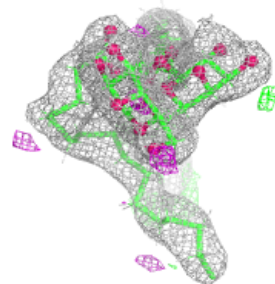
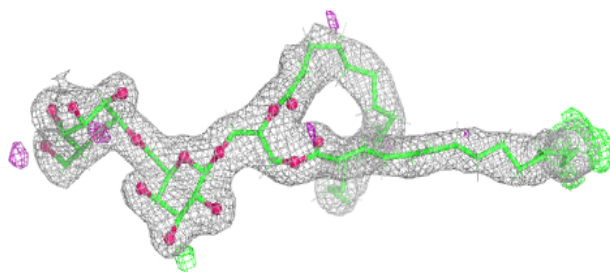
**Electron density around BCR H 101:**

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

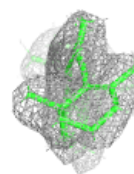
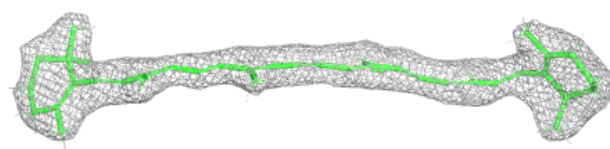
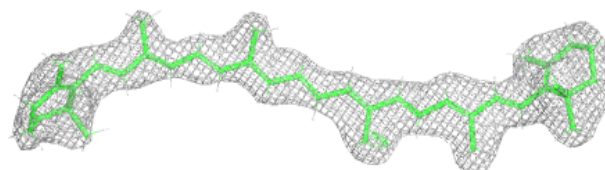


Electron density around DGD H 102:

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

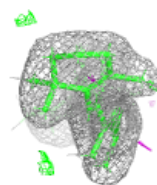
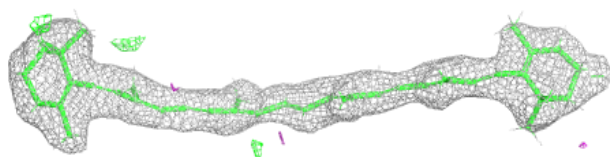
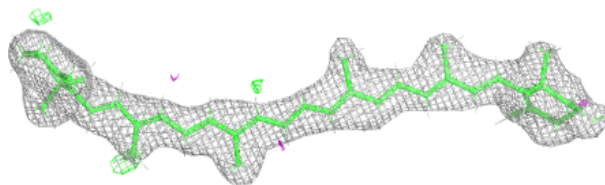
**Electron density around BCR k 101:**

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

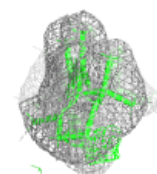
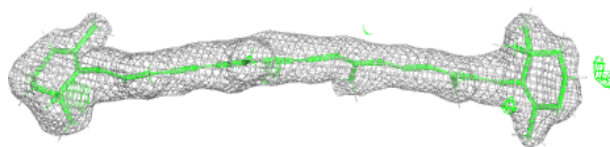


Electron density around BCR x 101:

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

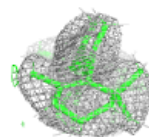
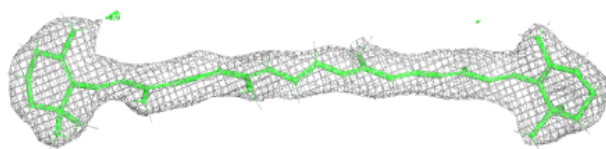
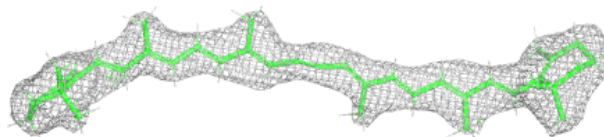
**Electron density around BCR Y 101:**

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

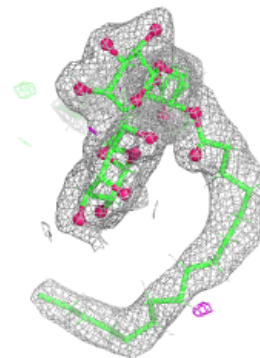
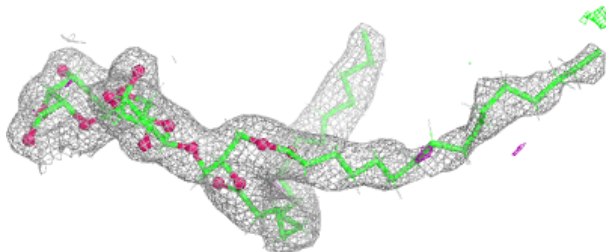
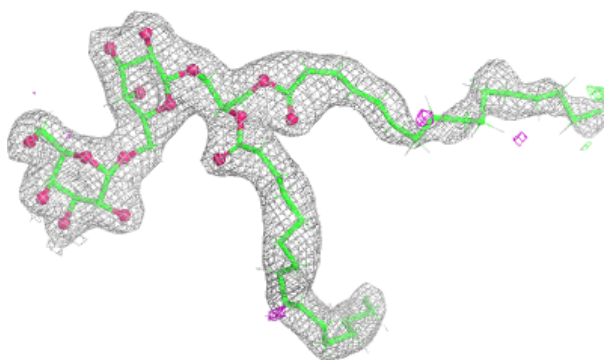


Electron density around BCR c 514:

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

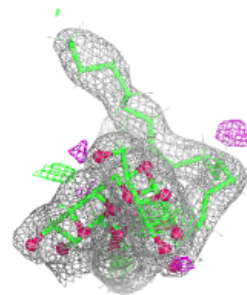
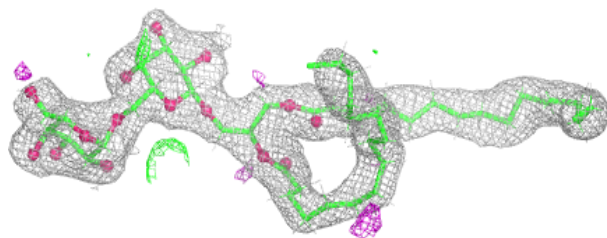
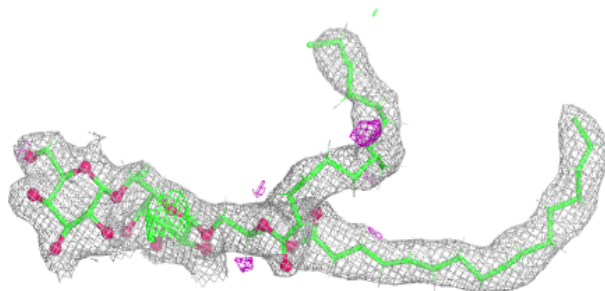
**Electron density around DGD c 517:**

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



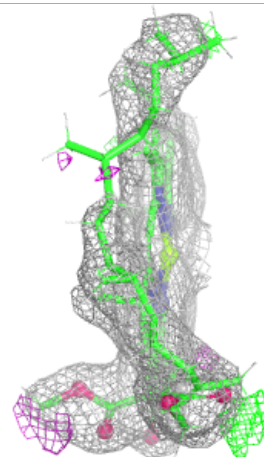
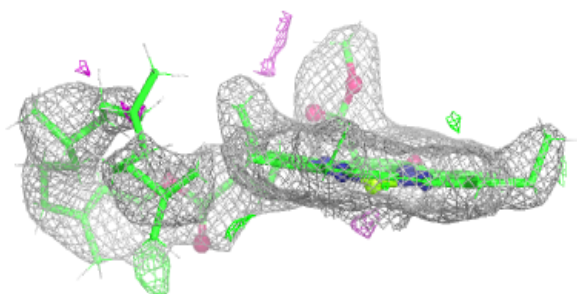
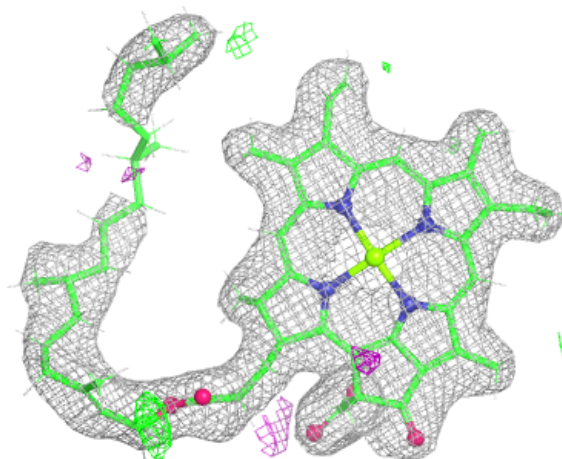
Electron density around DGD h 101:

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



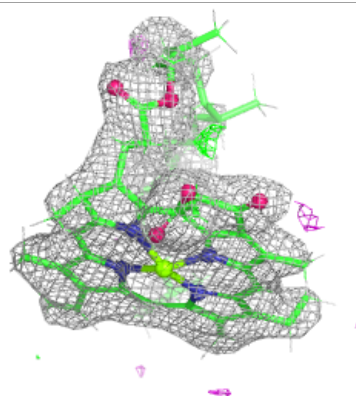
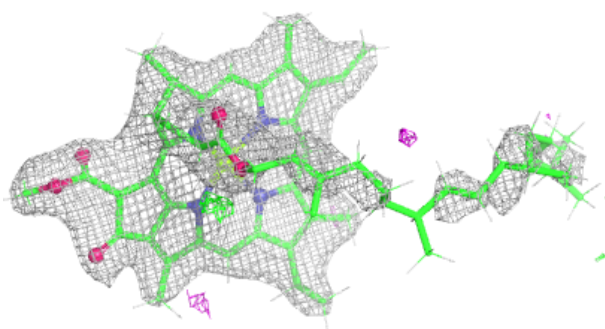
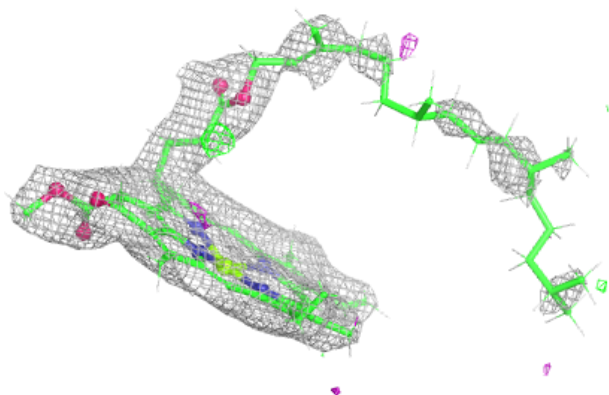
Electron density around CLA c 512:

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

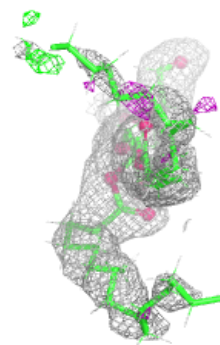
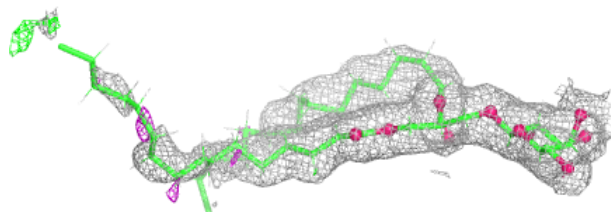
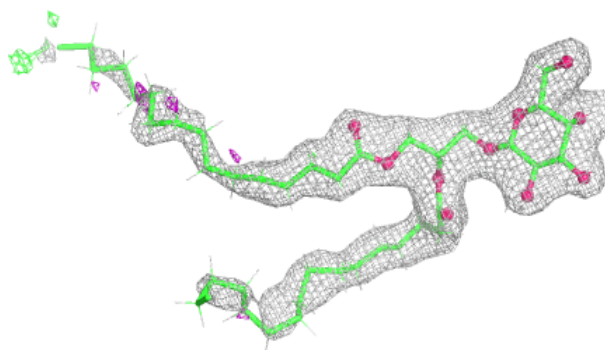


Electron density around CLA c 513:

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

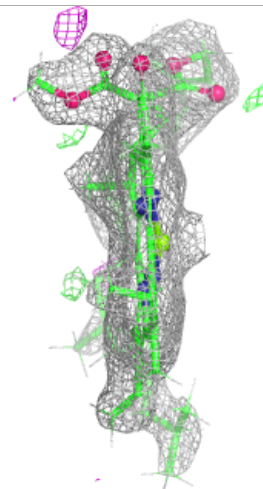
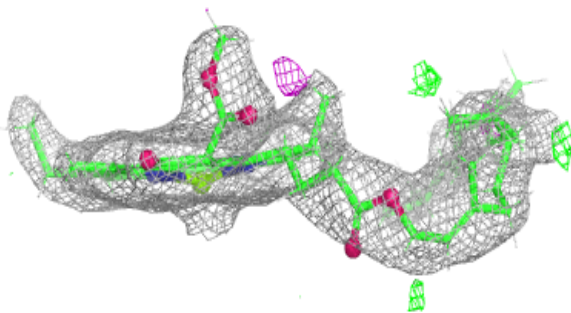
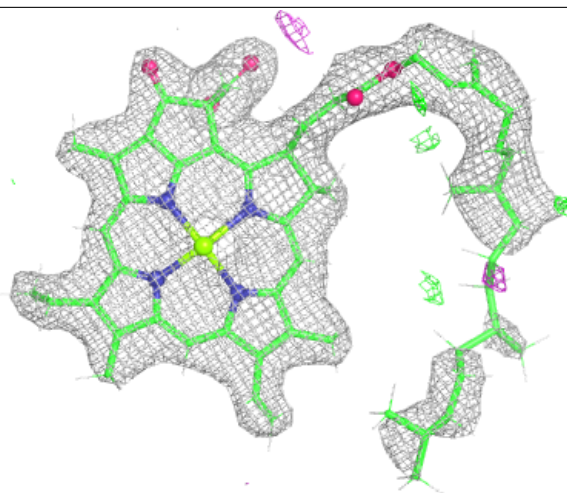
**Electron density around LMG D 406:**

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



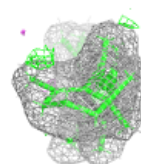
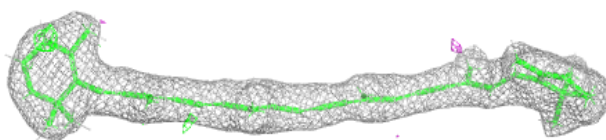
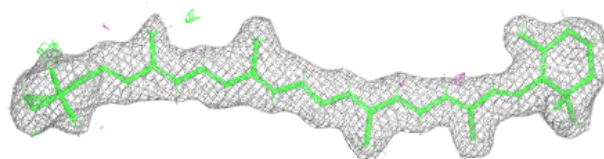
Electron density around CLA C 512:

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

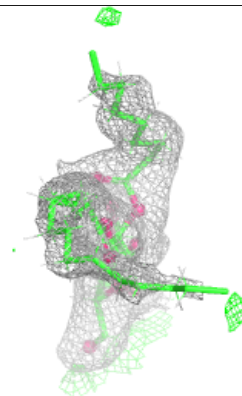
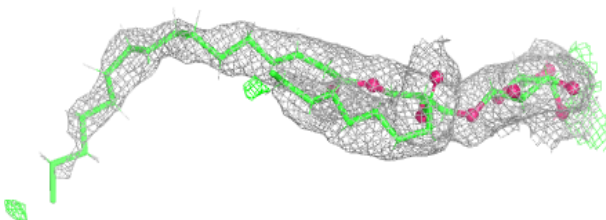
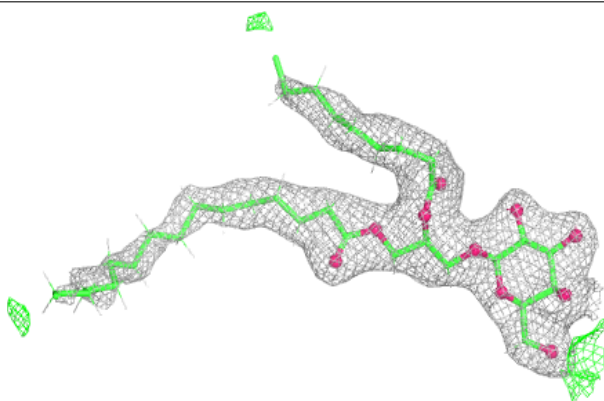


Electron density around BCR b 617:

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

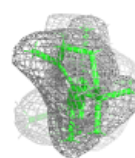
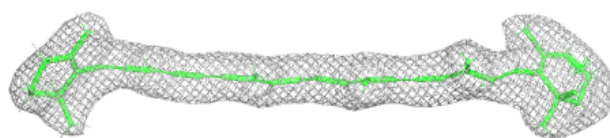
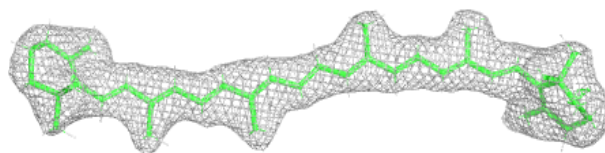
**Electron density around LMG d 410:**

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

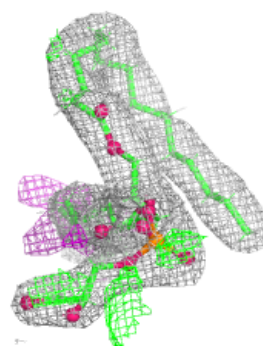
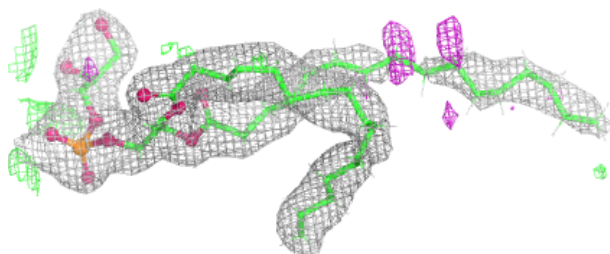
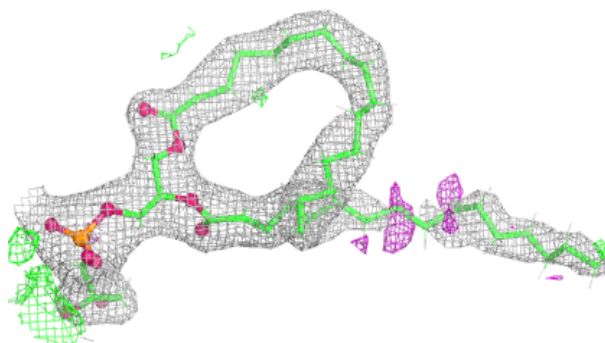


Electron density around BCR b 618:

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

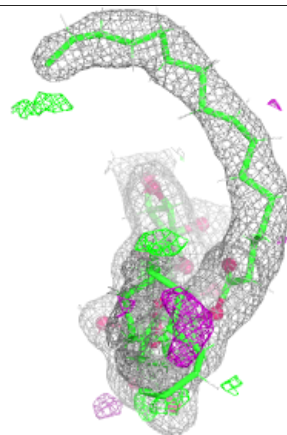
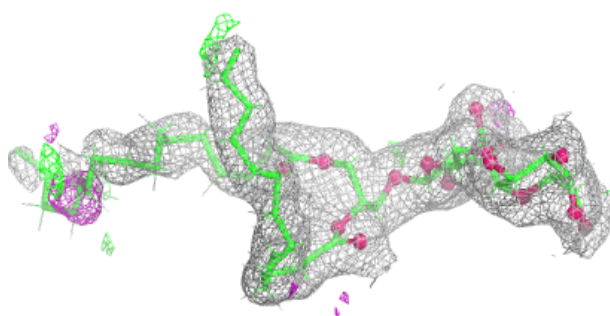
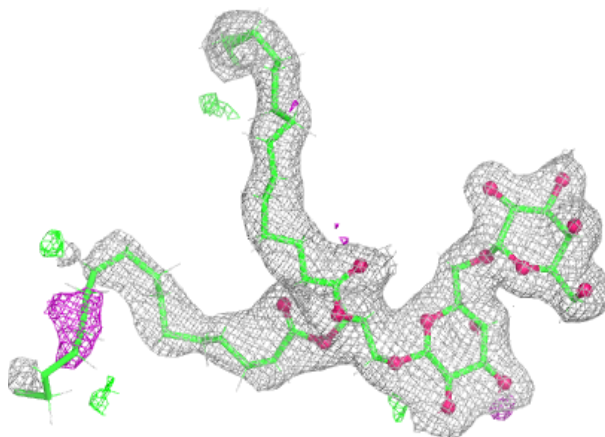
**Electron density around LHG d 407:**

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

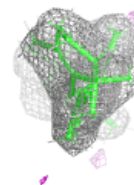
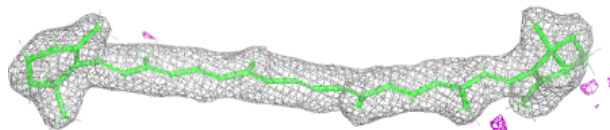
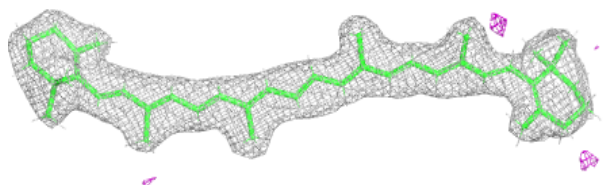


Electron density around DGD C 517:

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

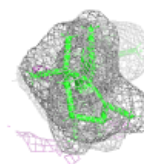
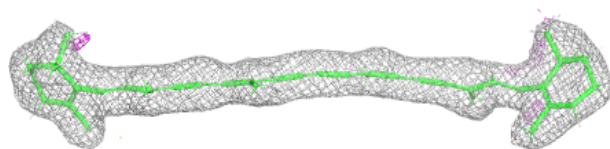
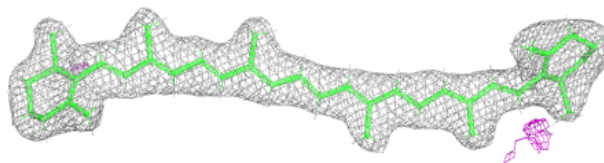
**Electron density around BCR b 619:**

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



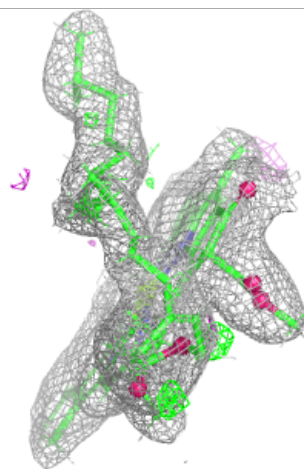
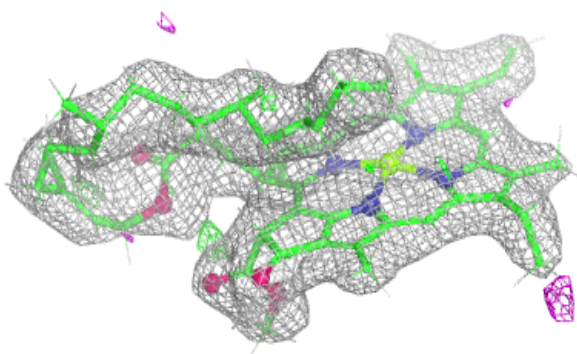
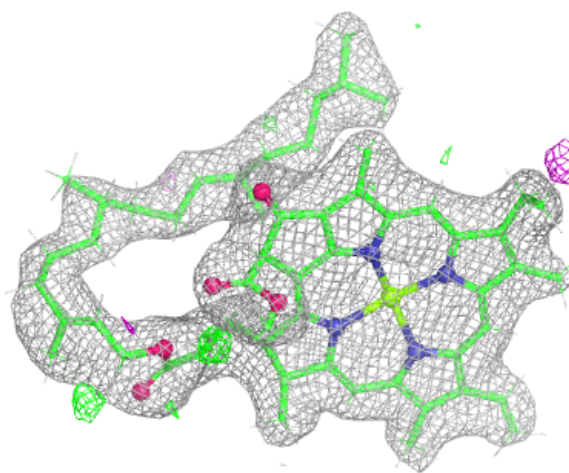
Electron density around BCR B 618:

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



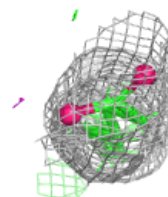
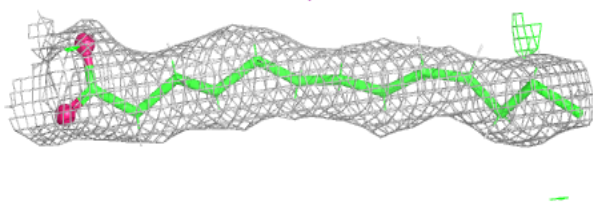
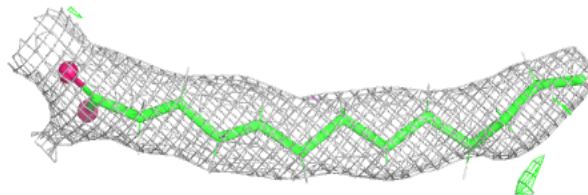
Electron density around CLA c 509:

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

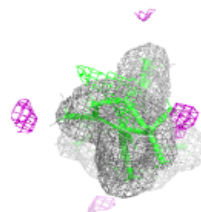
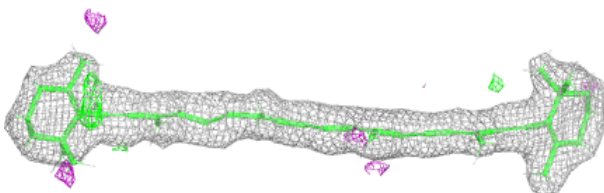
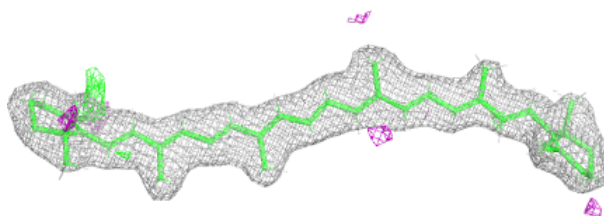


Electron density around STE M 102:

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

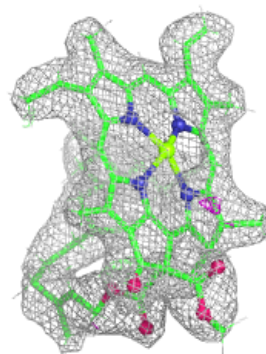
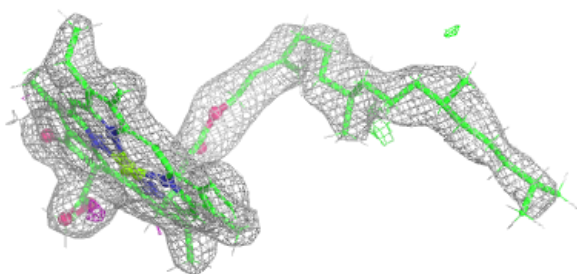
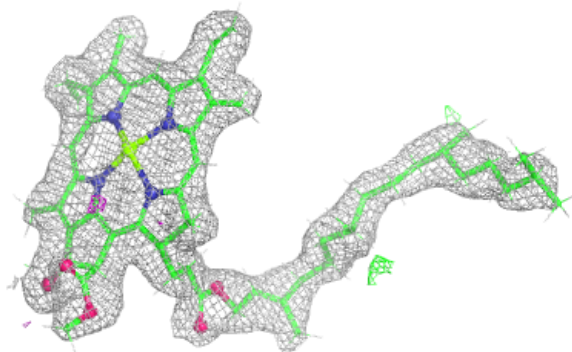
**Electron density around BCR C 515:**

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

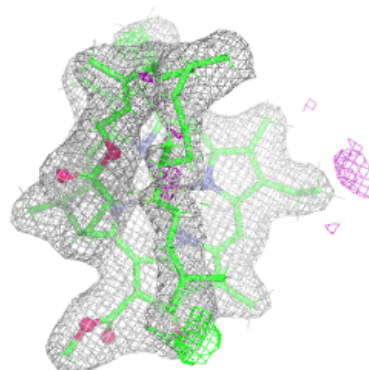
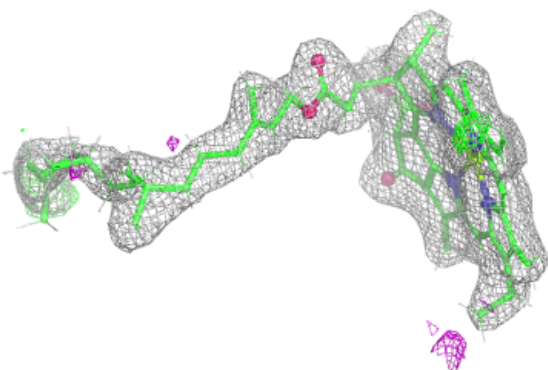
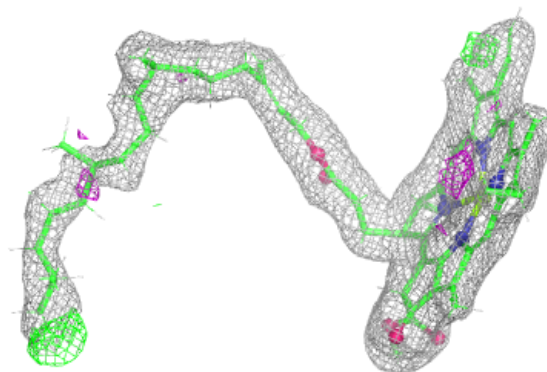


Electron density around CLA C 511:

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

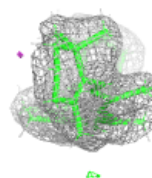
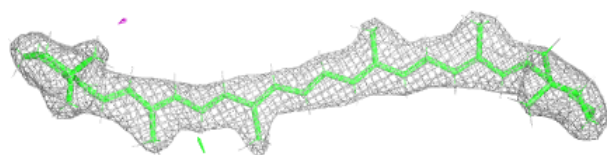
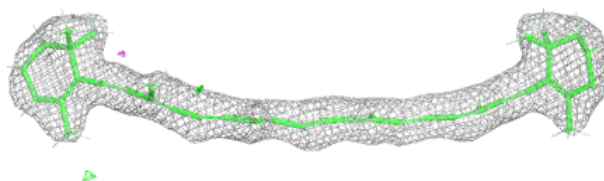
**Electron density around CLA b 606:**

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

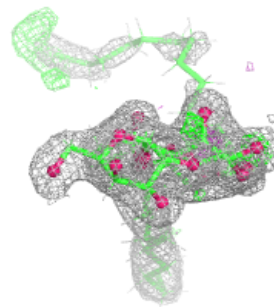
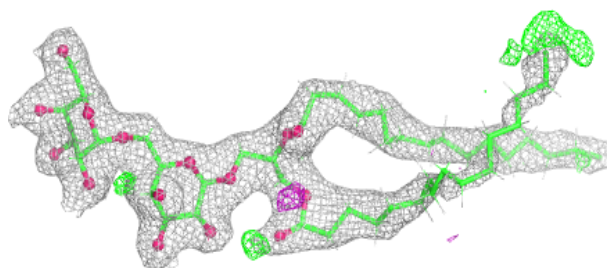
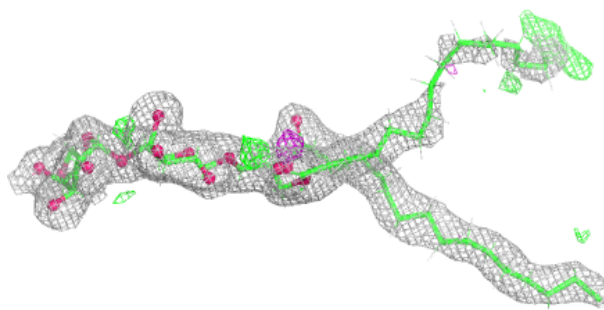


Electron density around BCR k 102:

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

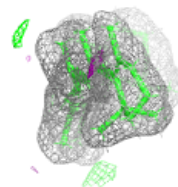
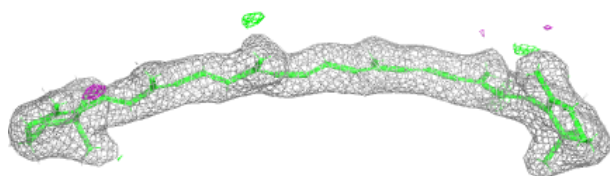
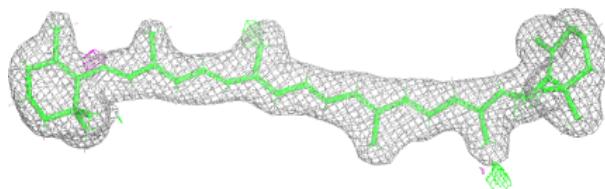
**Electron density around DGD C 516:**

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



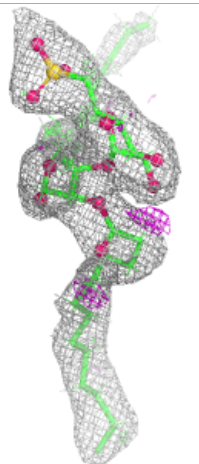
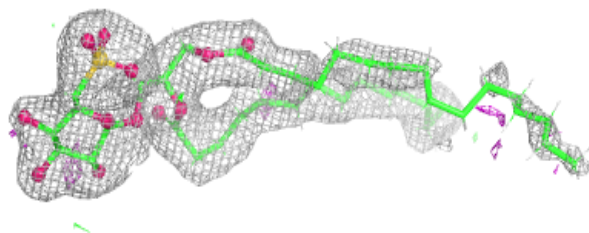
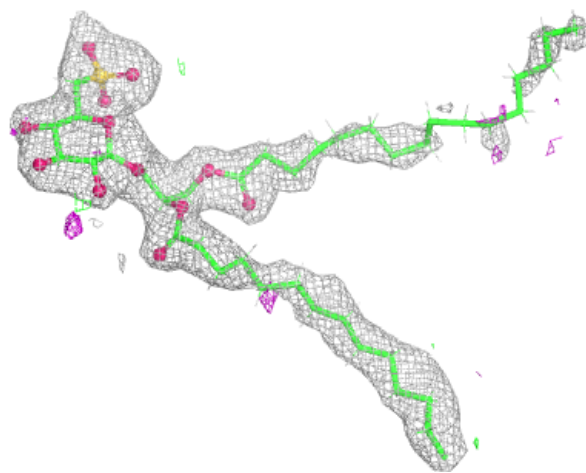
Electron density around BCR T 101:

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



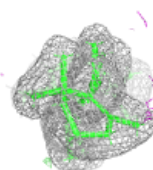
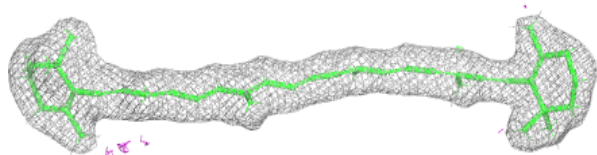
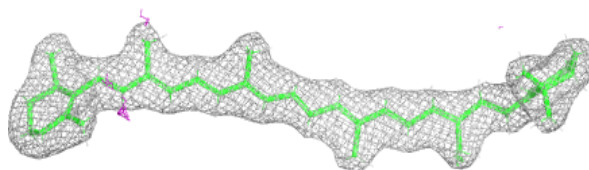
Electron density around SQD A 616:

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

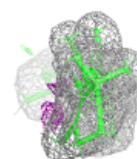
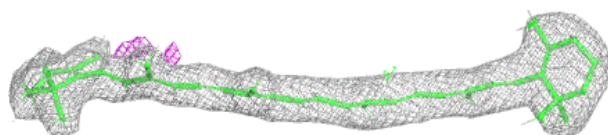
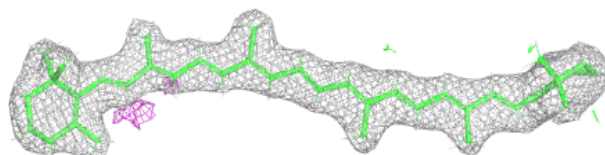


Electron density around BCR A 609:

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

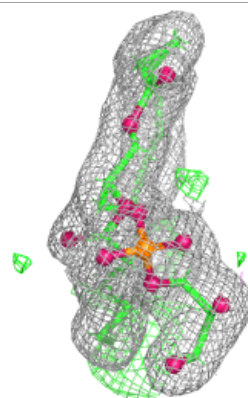
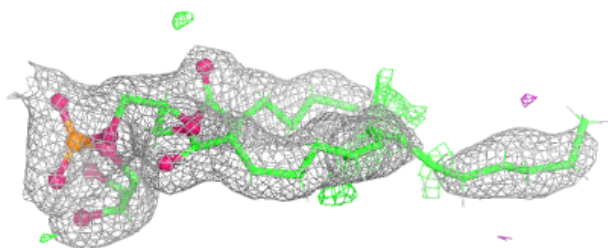
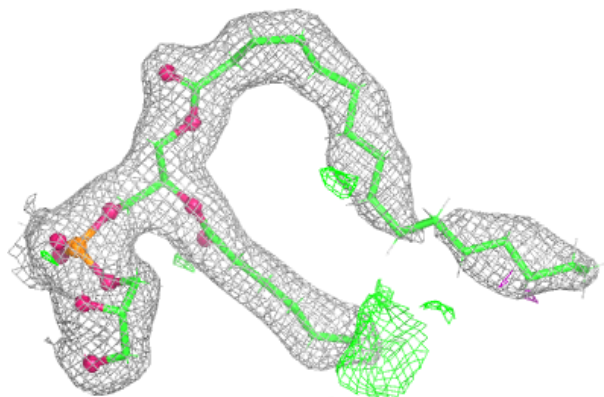
**Electron density around BCR B 617:**

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

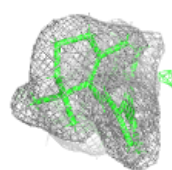
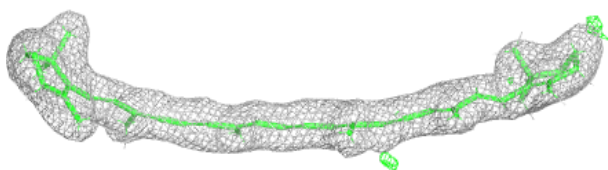
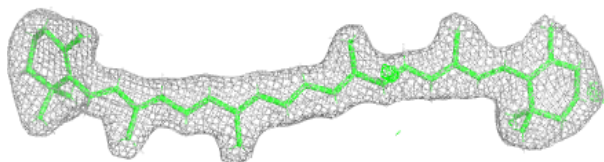


Electron density around LHG d 409:

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

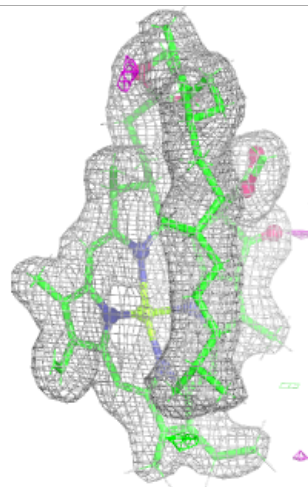
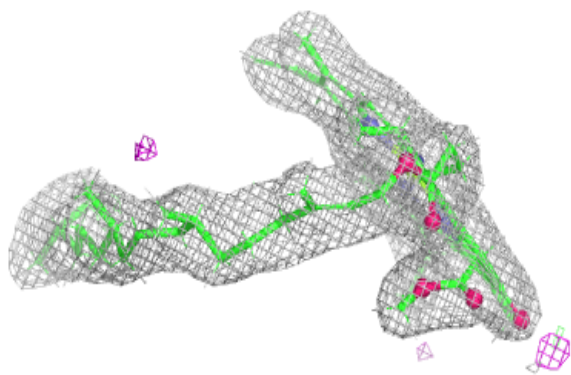
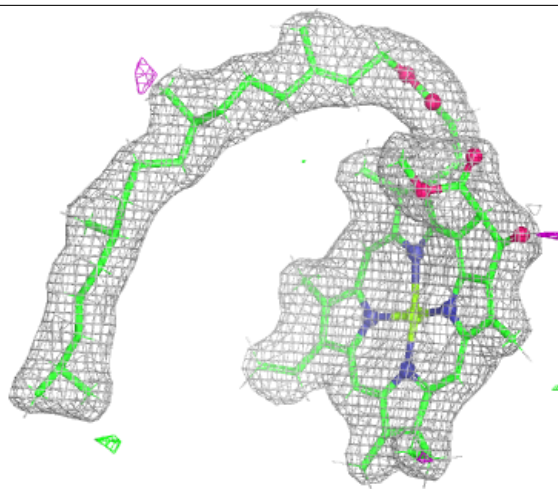
**Electron density around BCR t 101:**

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



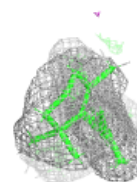
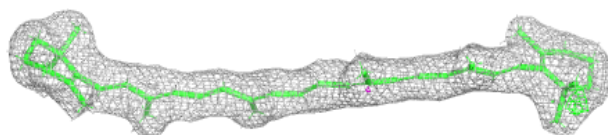
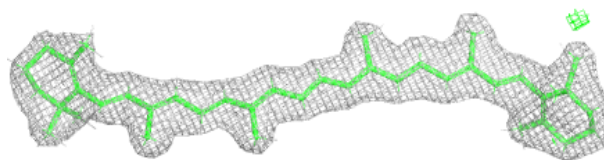
Electron density around CLA C 507:

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

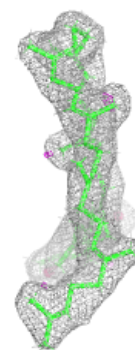
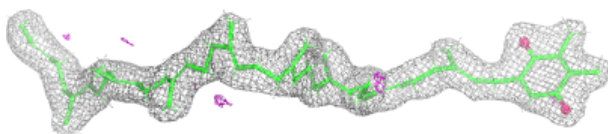
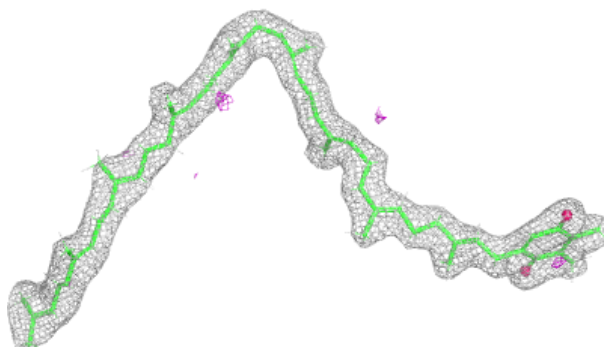


Electron density around BCR B 619:

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

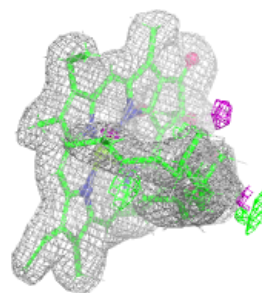
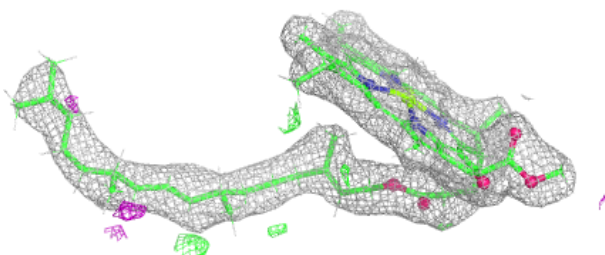
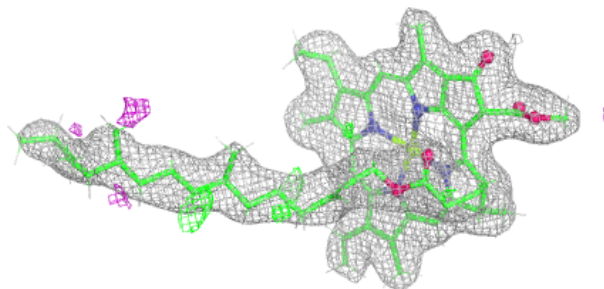
**Electron density around PL9 D 405:**

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

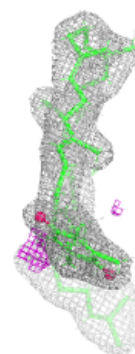
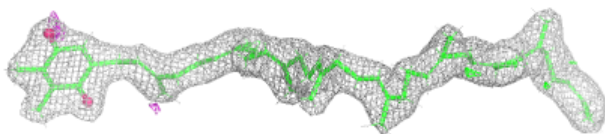
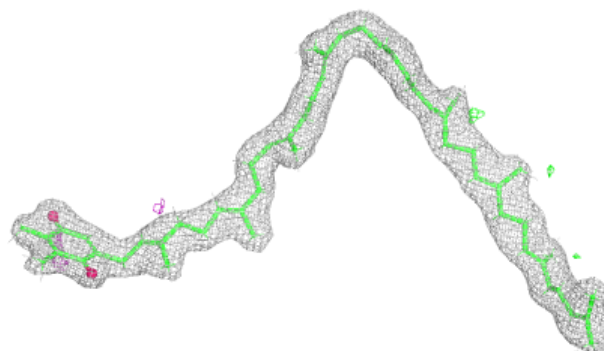


Electron density around CLA b 608:

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

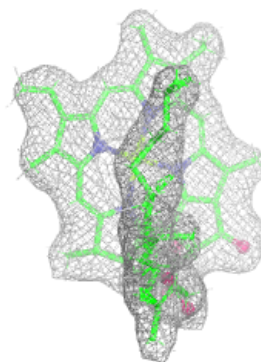
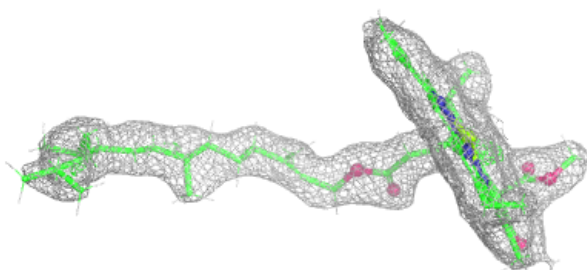
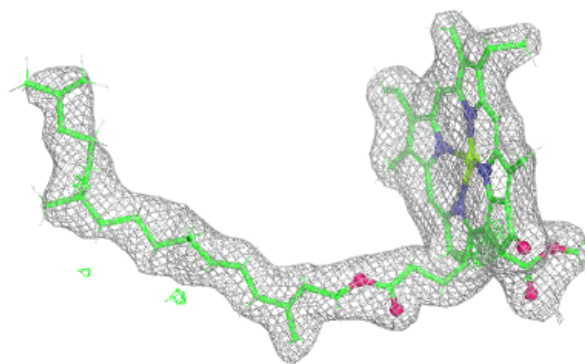
**Electron density around PL9 d 406:**

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

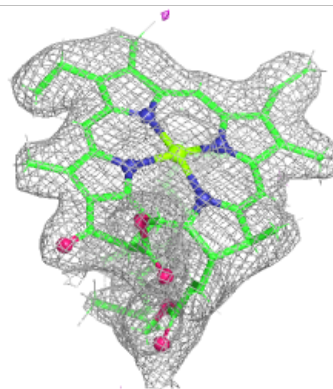
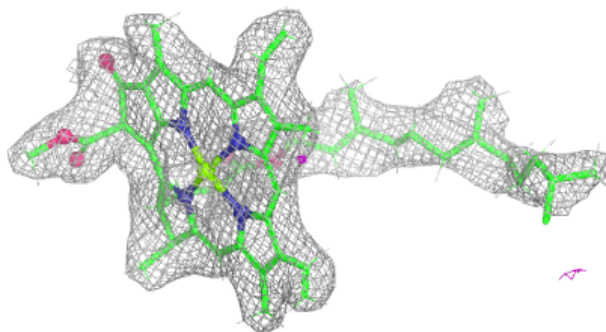
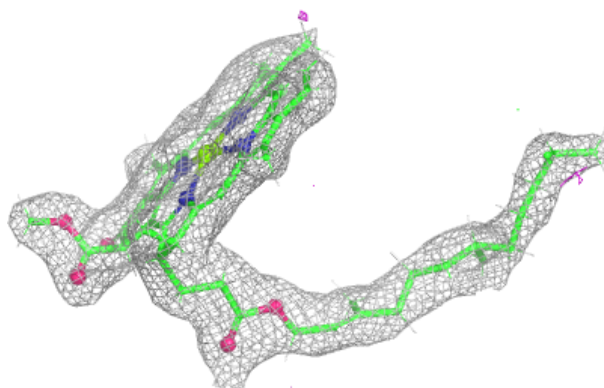


Electron density around CLA b 609:

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

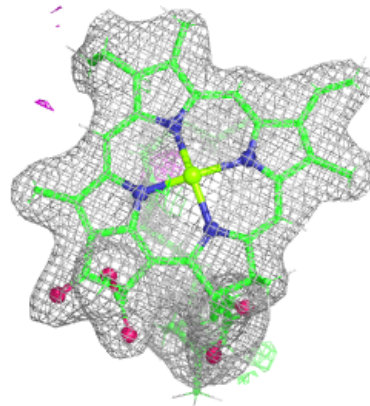
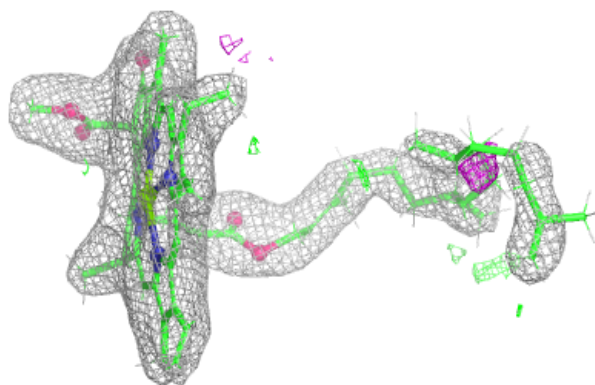
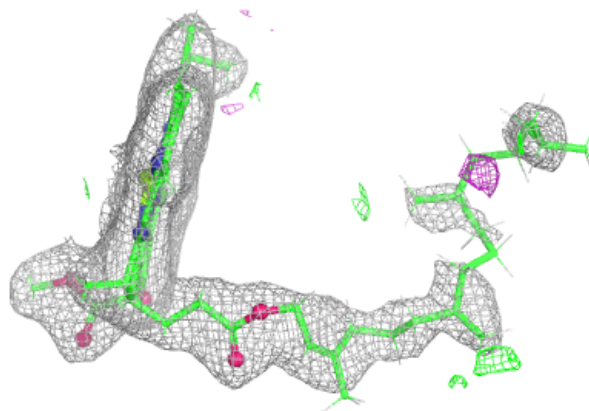
**Electron density around CLA c 504:**

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

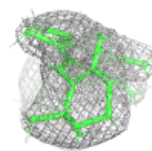
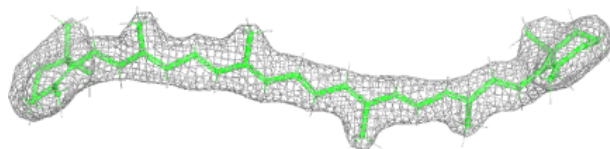
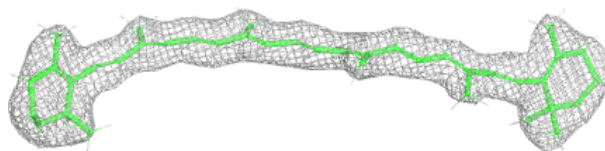


Electron density around CLA c 506:

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

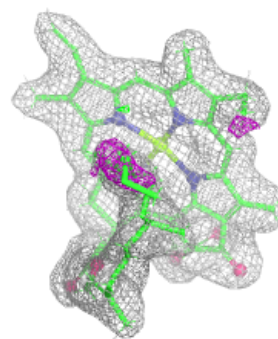
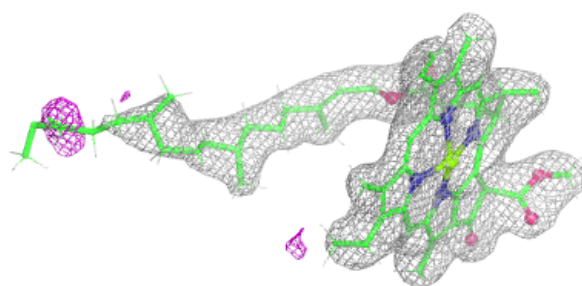
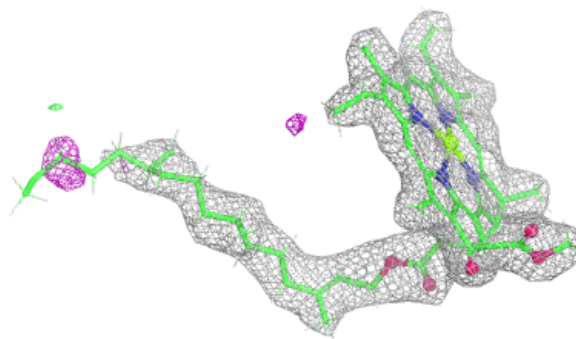
**Electron density around BCR K 101:**

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



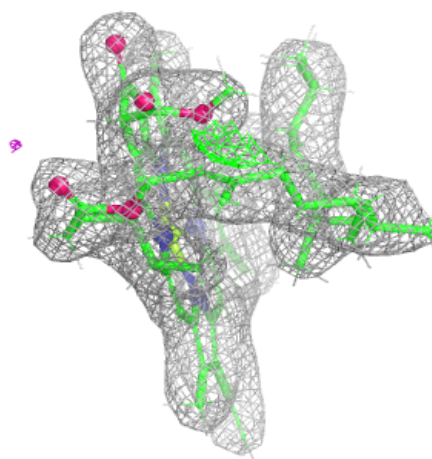
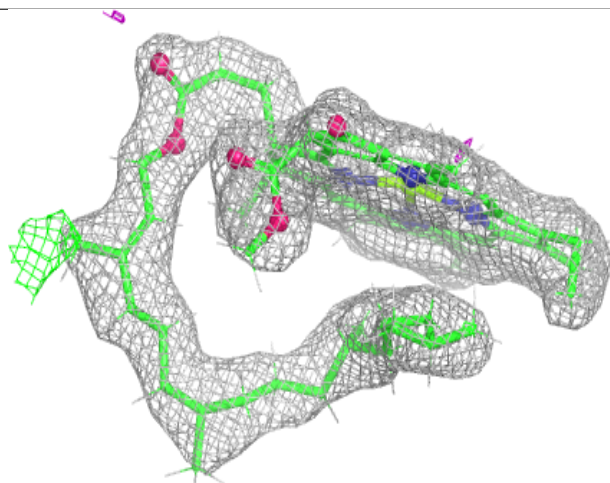
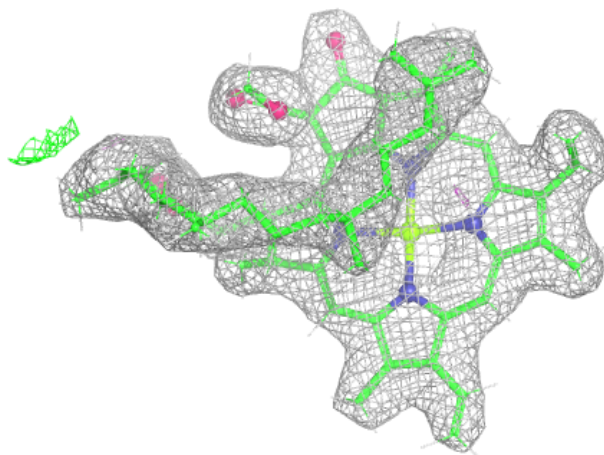
Electron density around CLA c 508:

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



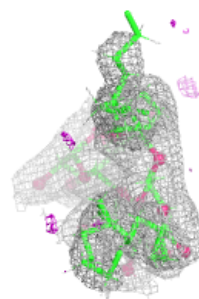
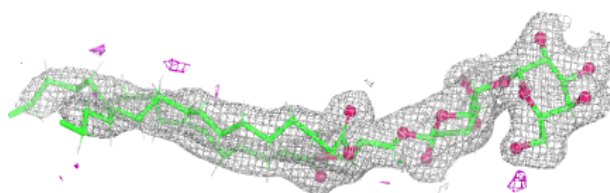
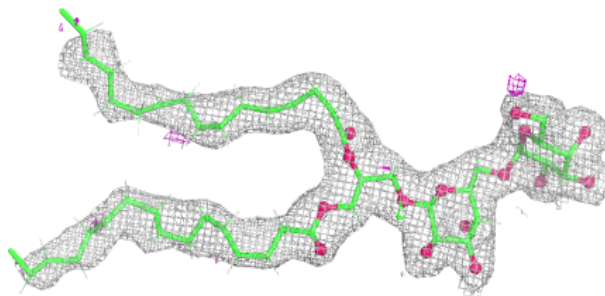
Electron density around CLA C 510:

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

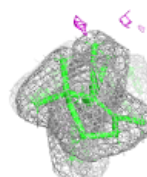
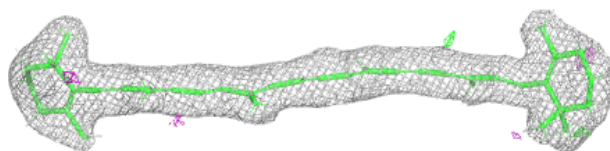
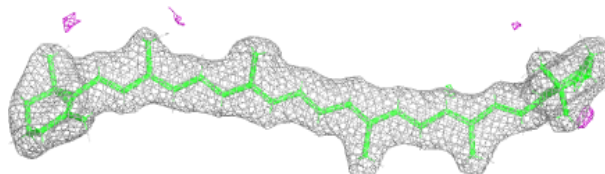


Electron density around DGD C 518:

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

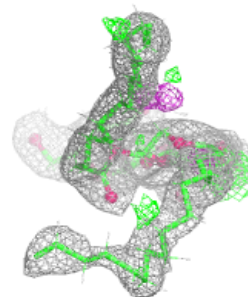
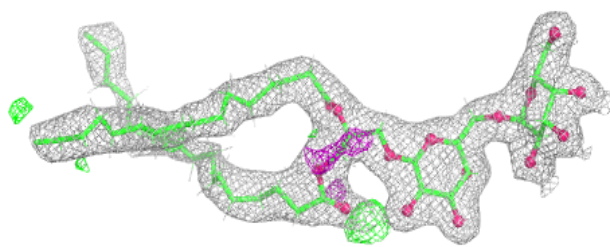
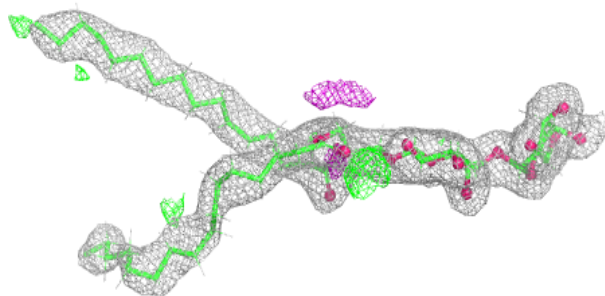
**Electron density around BCR a 607:**

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

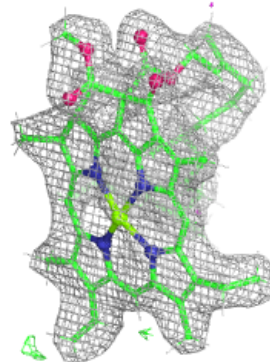
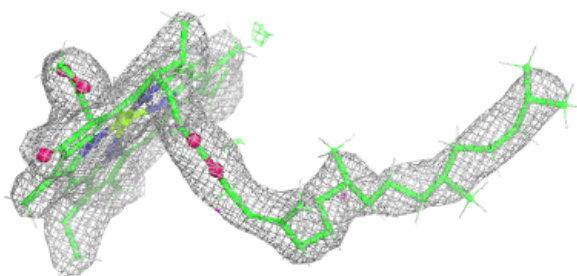
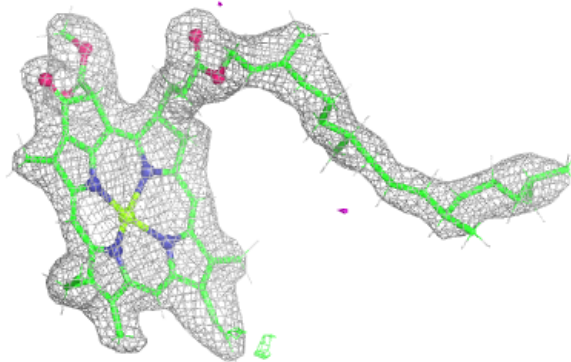


Electron density around DGD c 516:

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

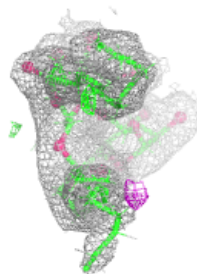
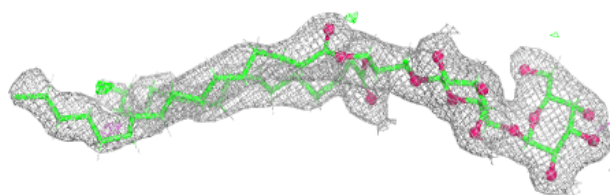
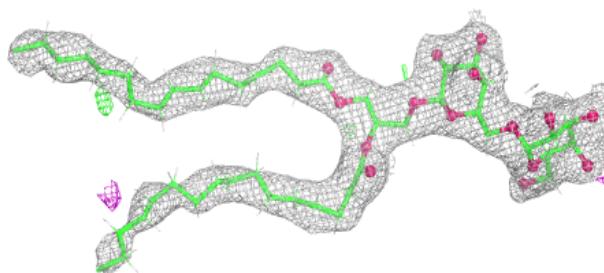
**Electron density around CLA c 511:**

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

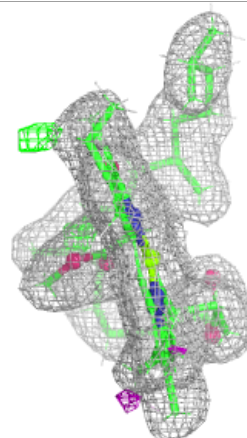
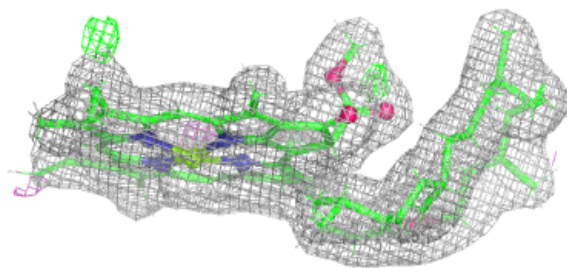
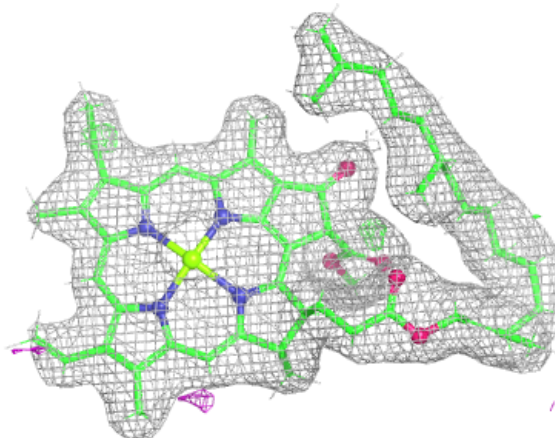


Electron density around DGD c 518:

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

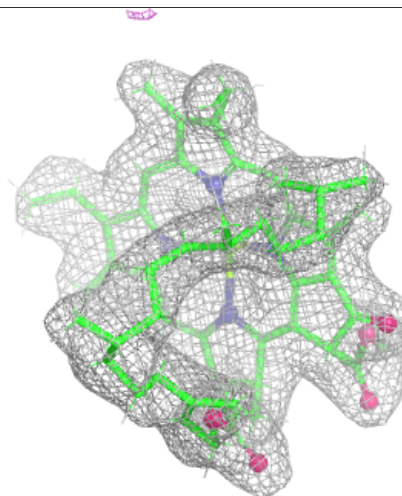
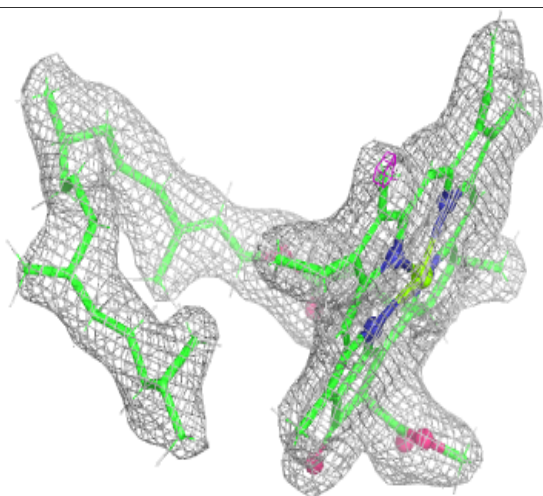
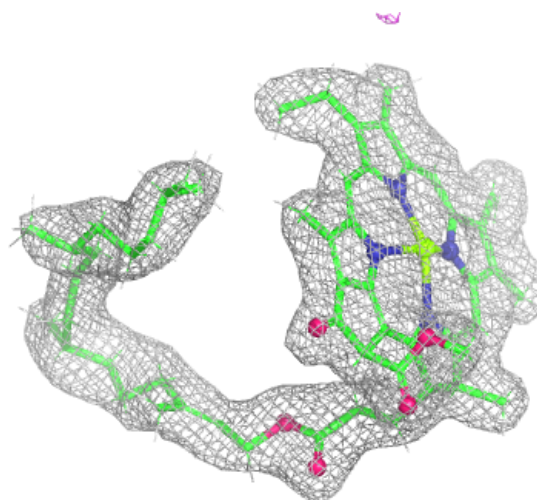
**Electron density around CLA B 610:**

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



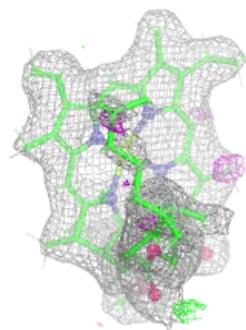
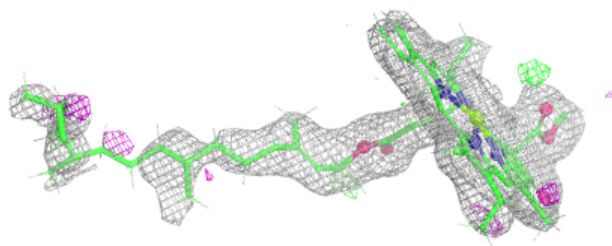
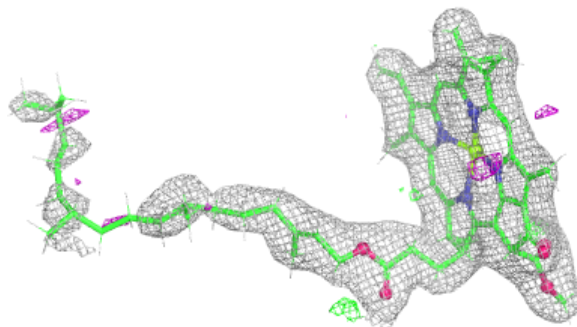
Electron density around CLA C 503:

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

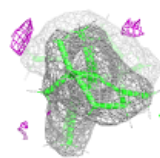
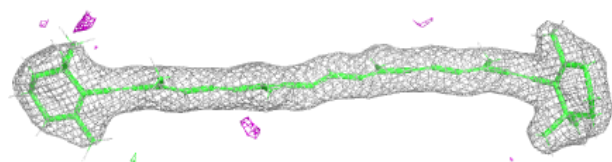


Electron density around CLA d 404:

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

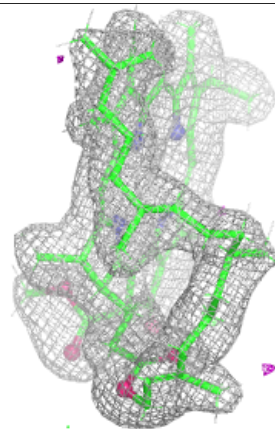
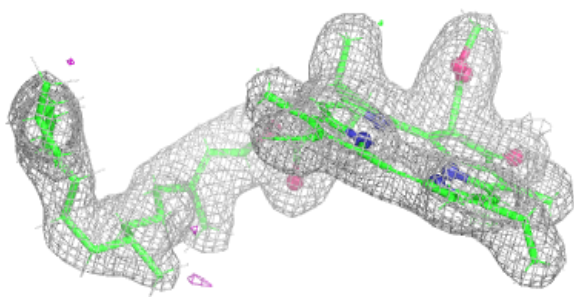
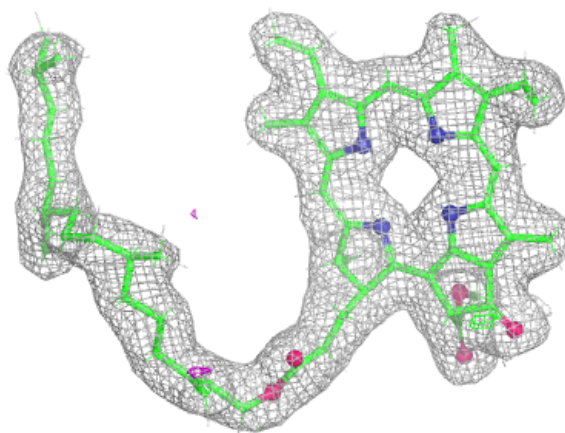
**Electron density around BCR c 515:**

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

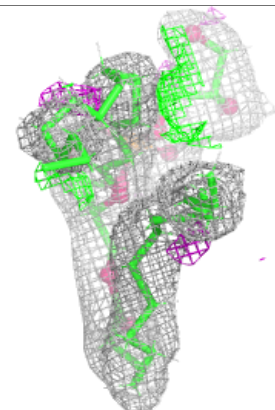
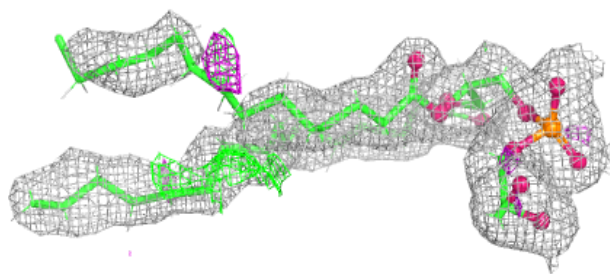
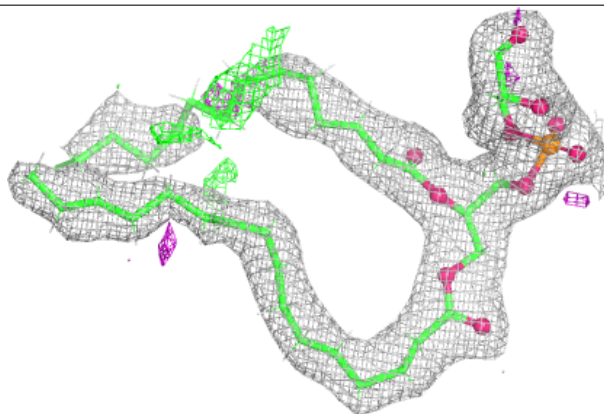


Electron density around PHO d 402:

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

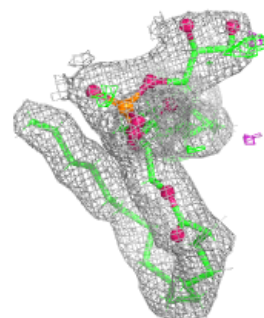
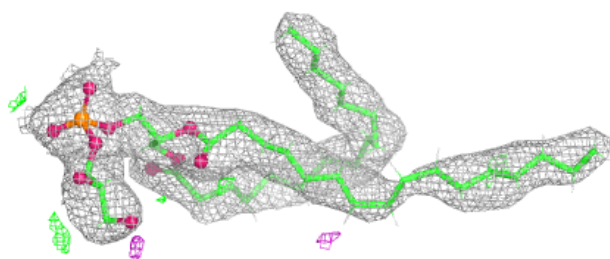
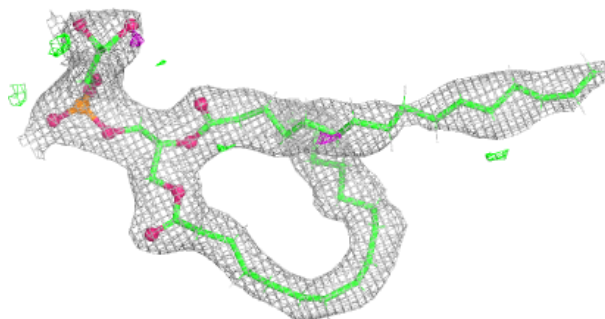
**Electron density around LHG A 615:**

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

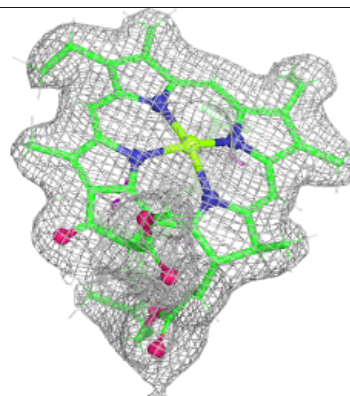
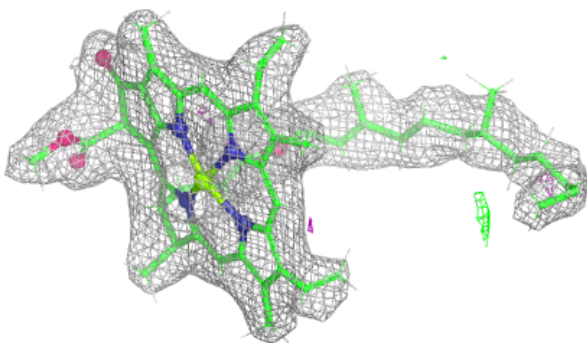
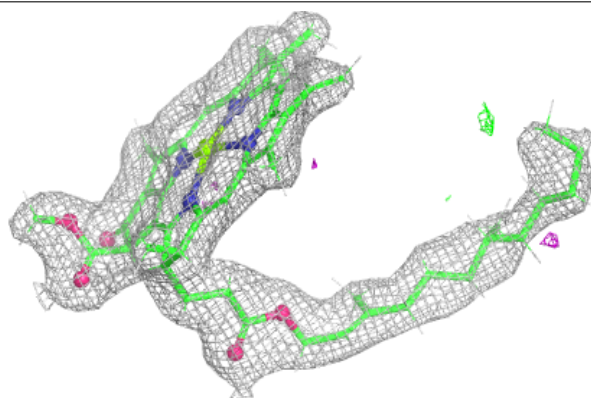


Electron density around LHG B 622:

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

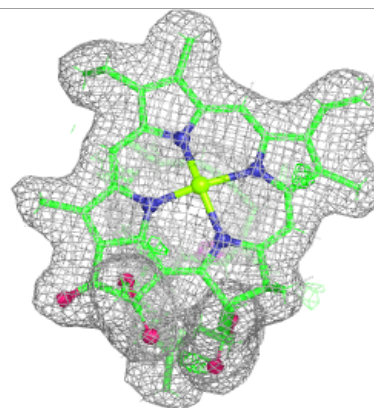
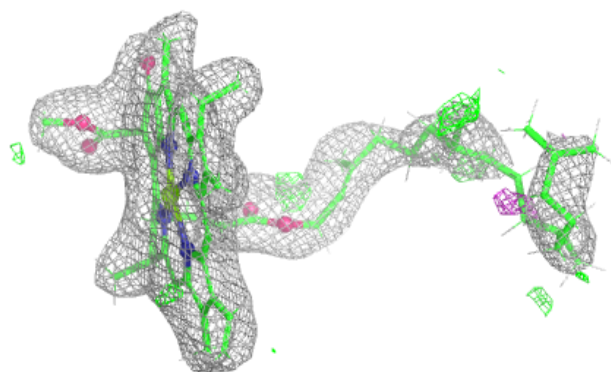
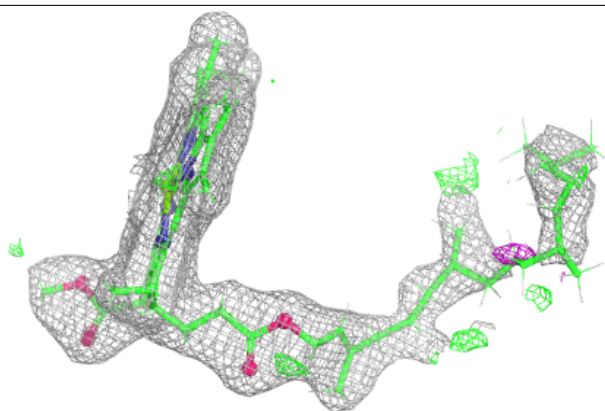
**Electron density around CLA C 504:**

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

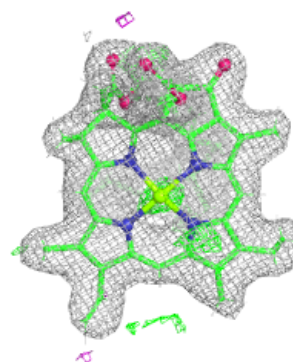
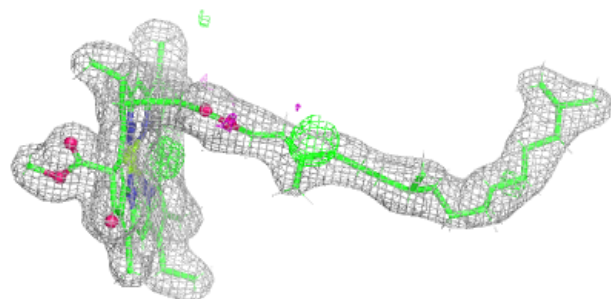
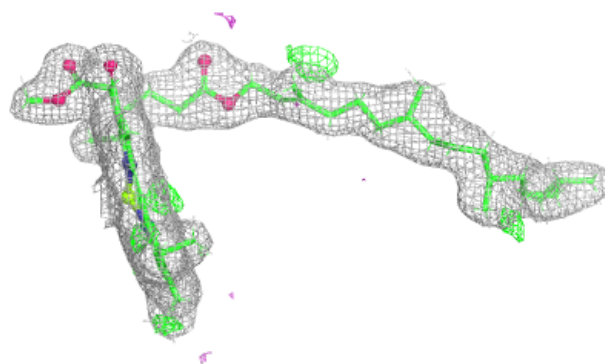


Electron density around CLA C 506:

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

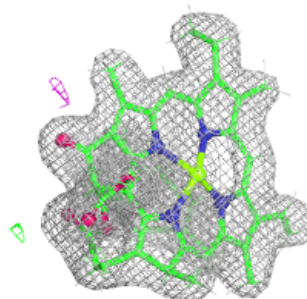
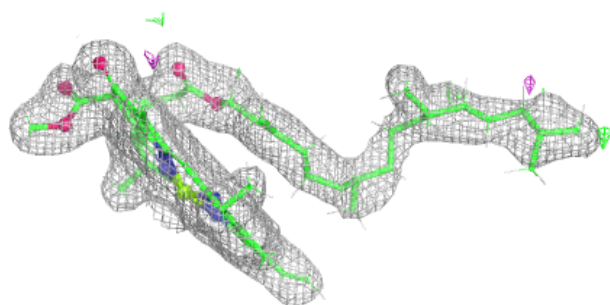
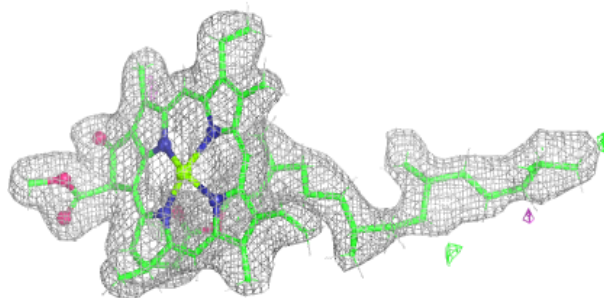
**Electron density around CLA B 605:**

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

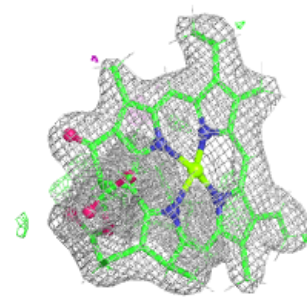
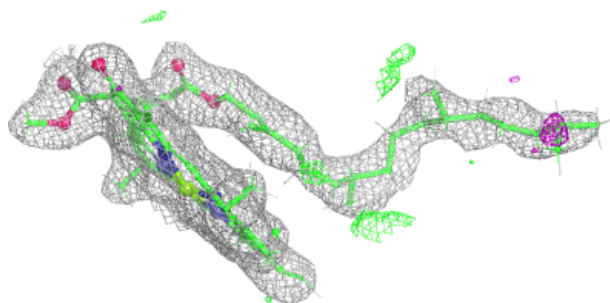
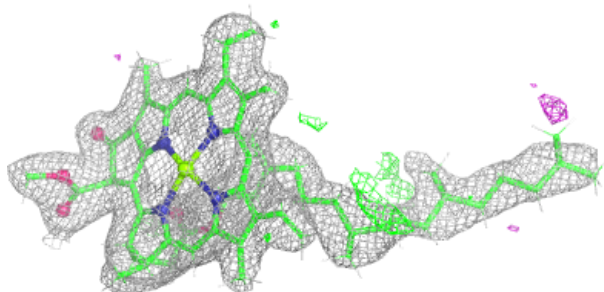


Electron density around CLA c 505:

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

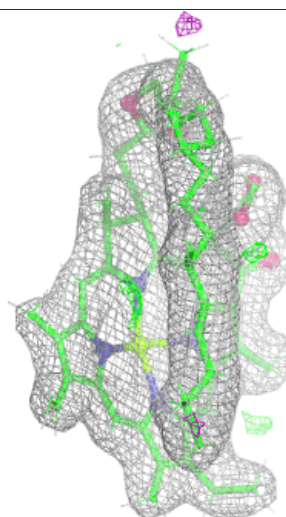
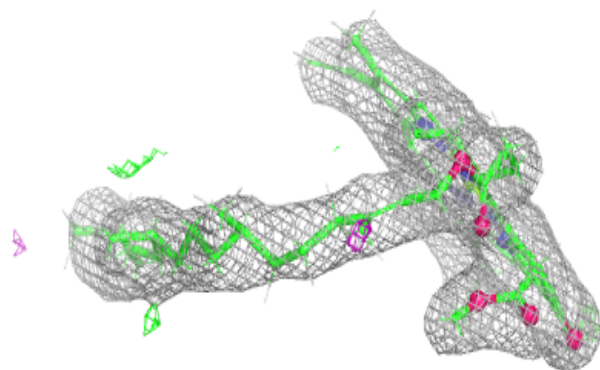
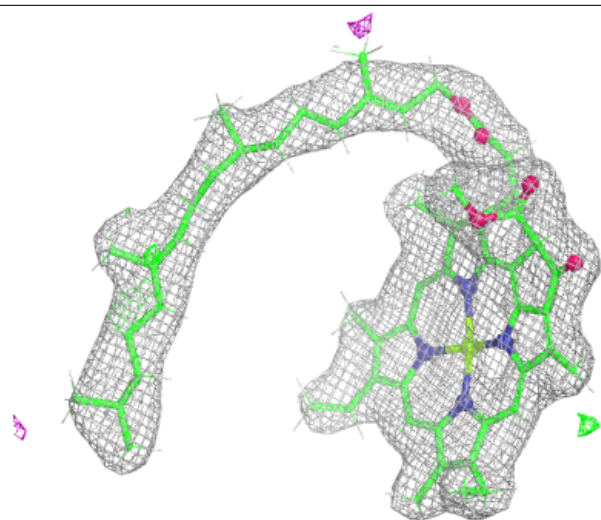
**Electron density around CLA C 505:**

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



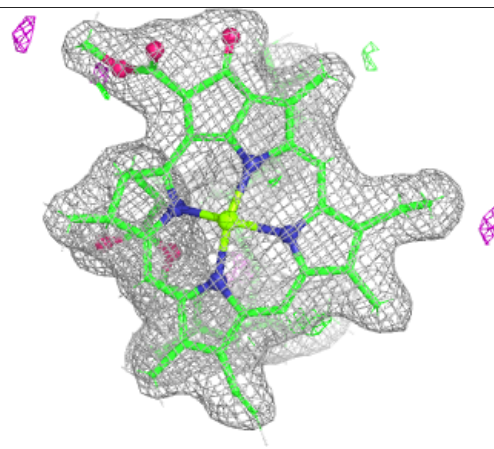
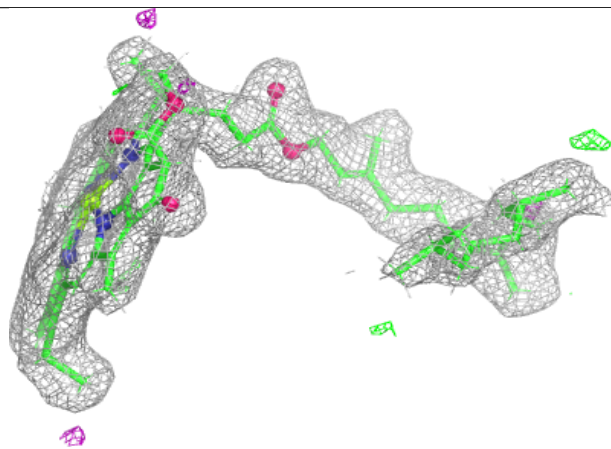
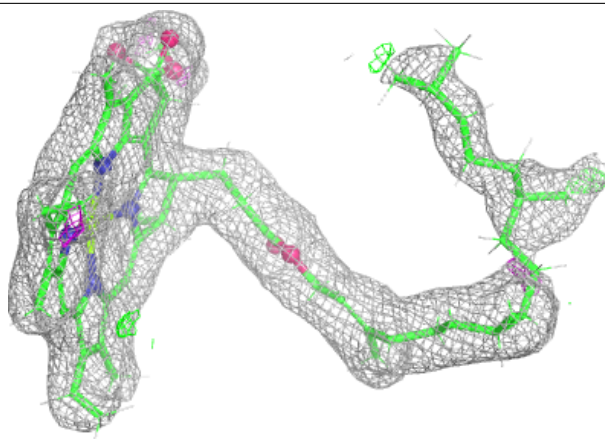
Electron density around CLA c 507:

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



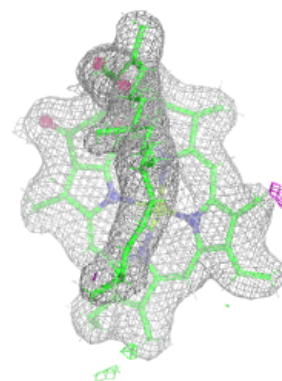
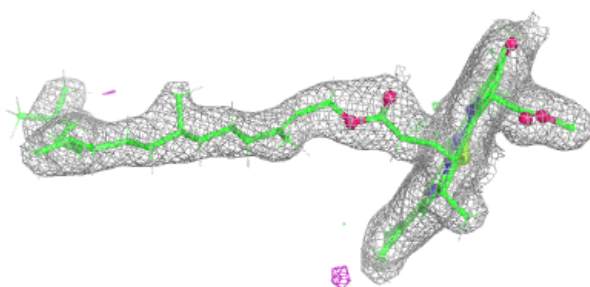
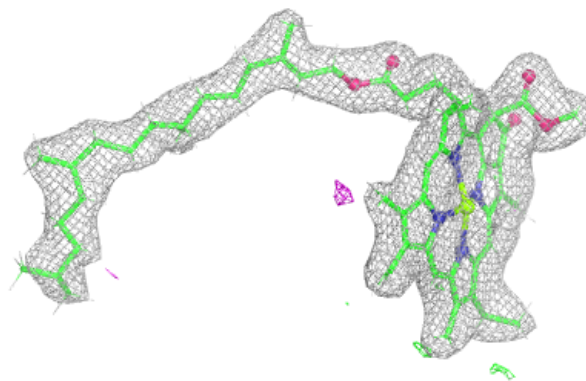
Electron density around CLA B 606:

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



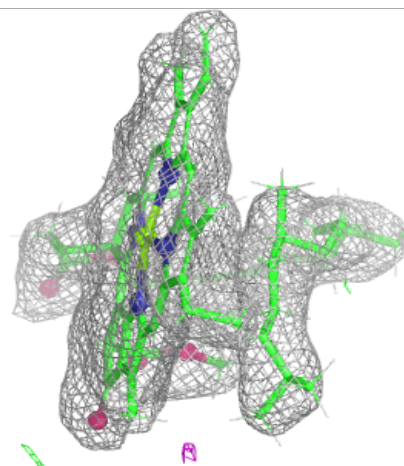
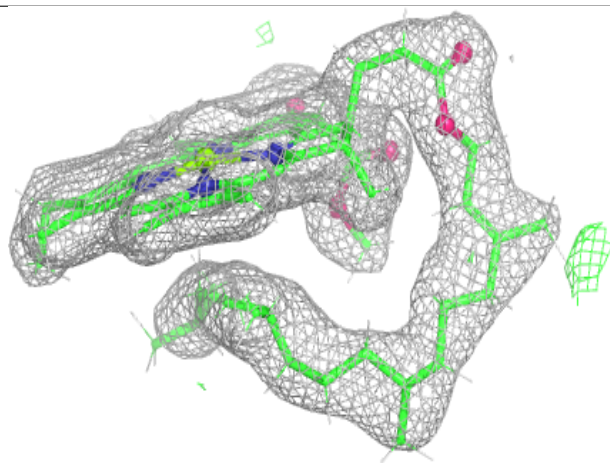
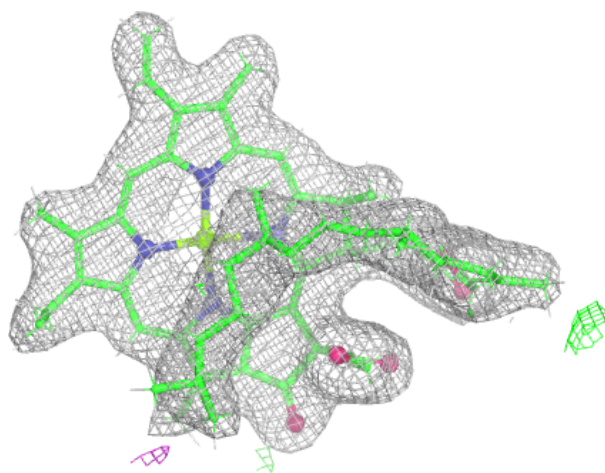
Electron density around CLA B 609:

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



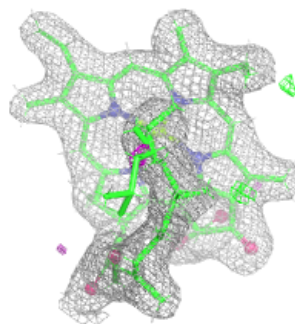
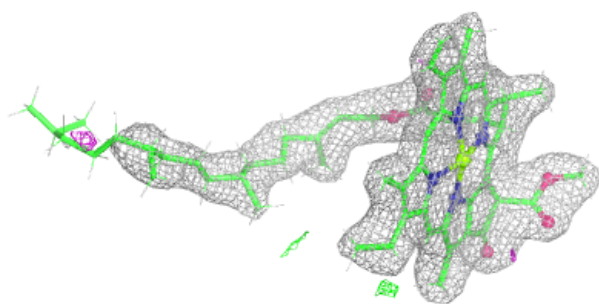
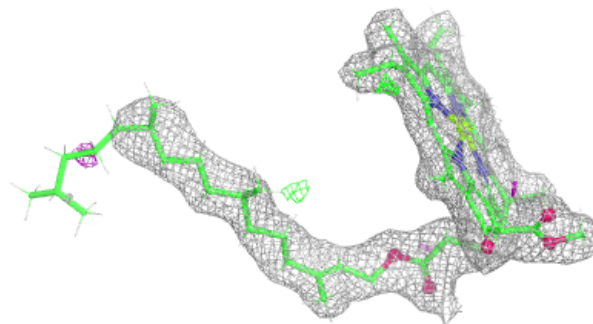
Electron density around CLA c 510:

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



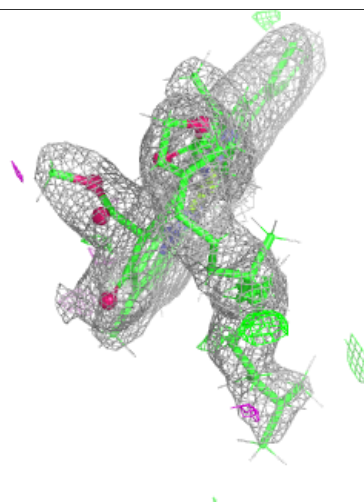
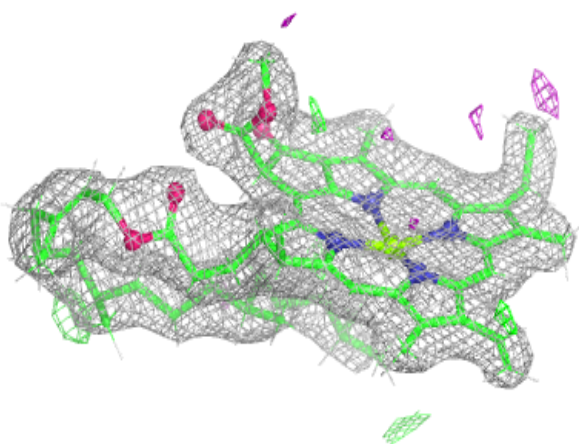
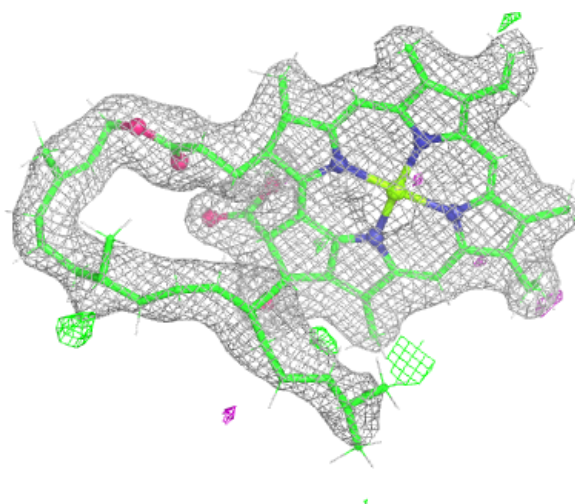
Electron density around CLA C 508:

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



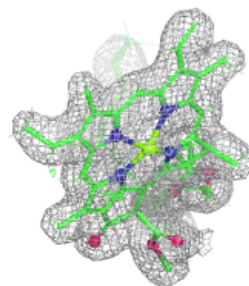
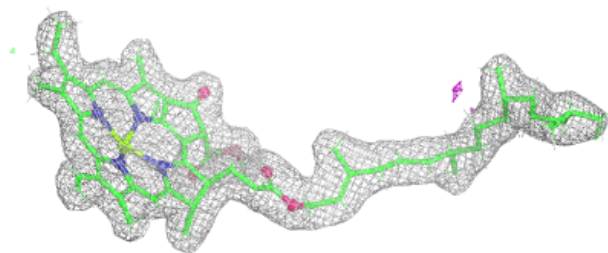
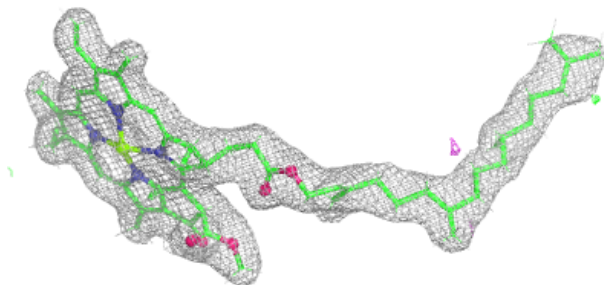
Electron density around CLA C 509:

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

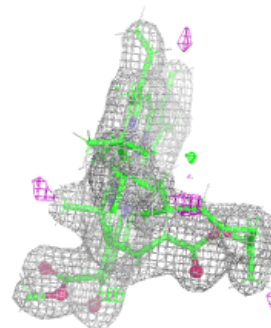
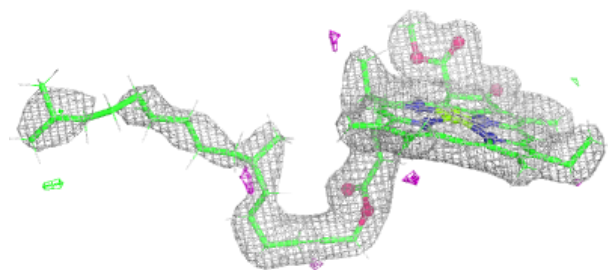
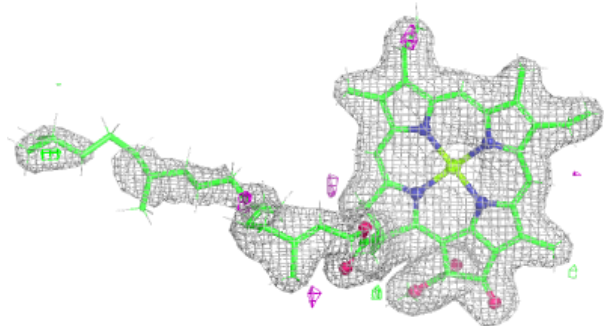


Electron density around CLA A 604:

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

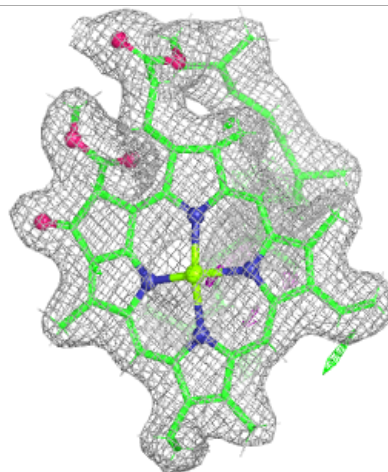
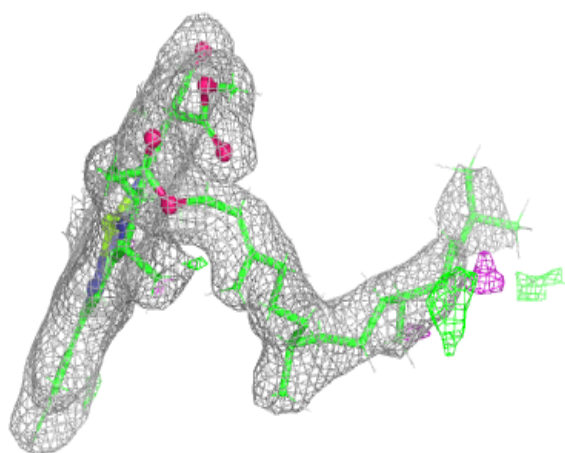
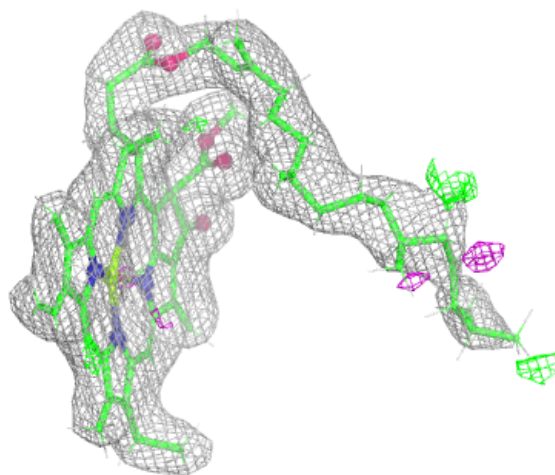
**Electron density around CLA d 401:**

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



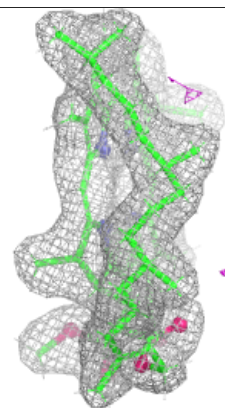
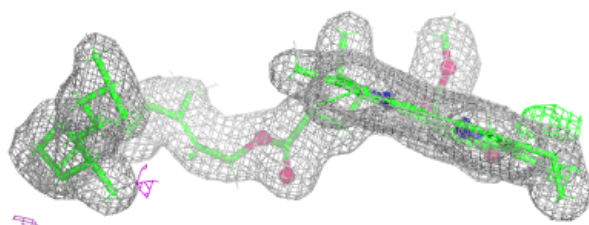
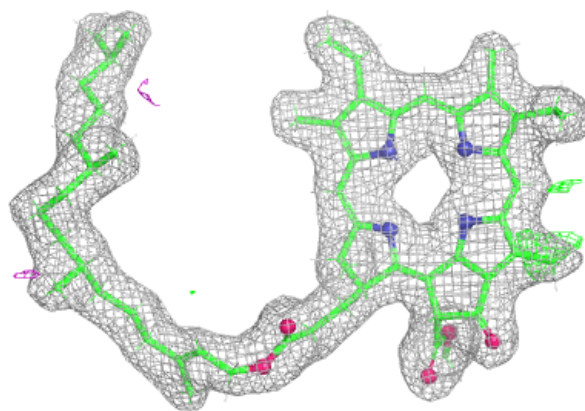
Electron density around CLA B 613:

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



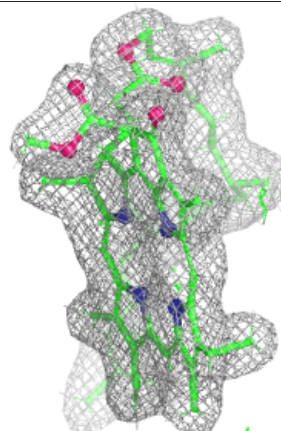
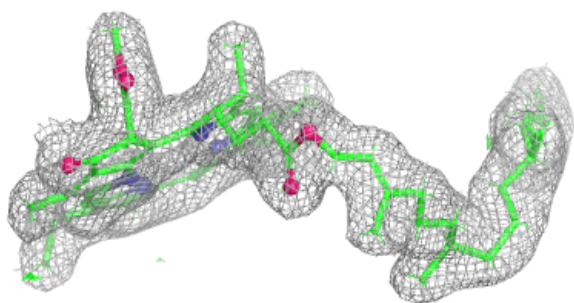
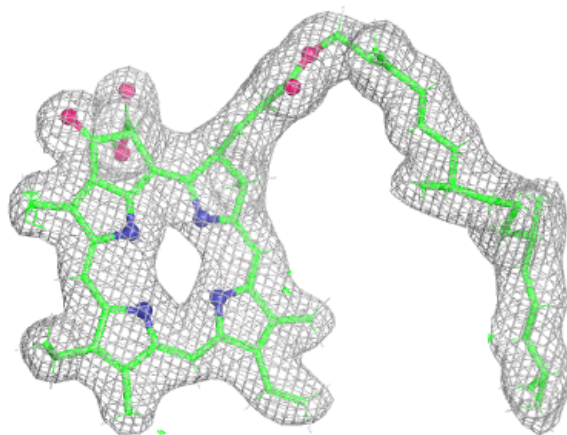
Electron density around PHO A 606:

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

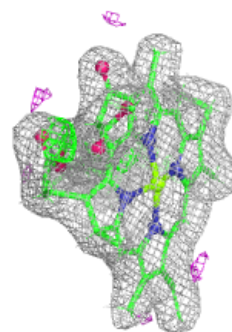
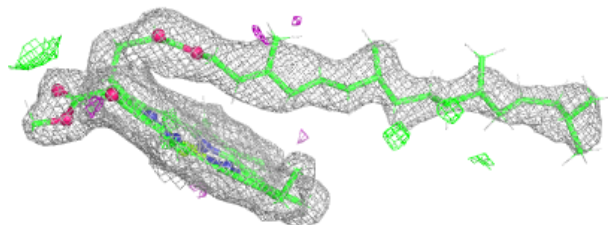
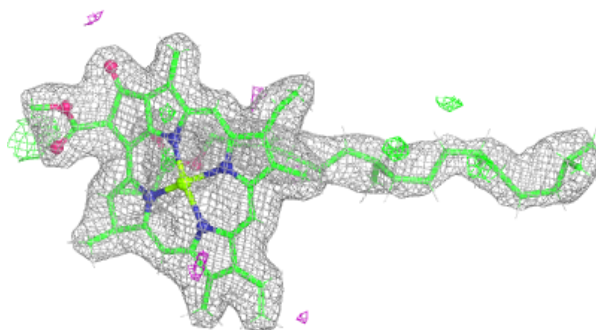


Electron density around PHO A 607:

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

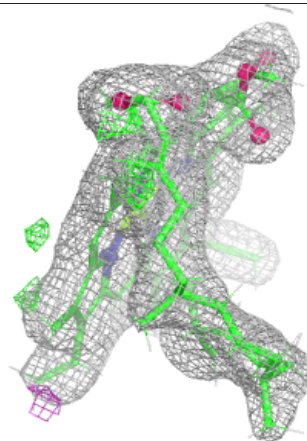
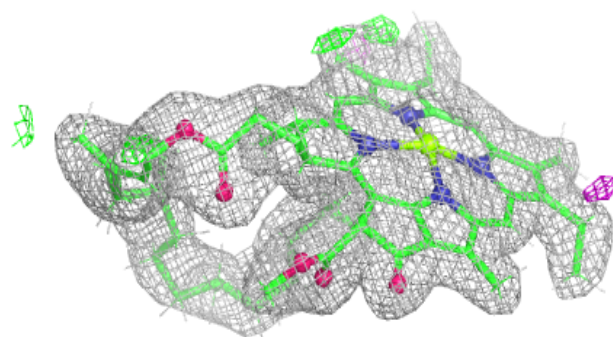
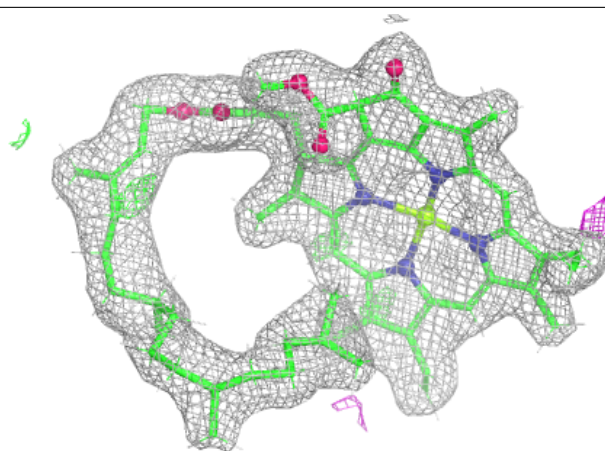
**Electron density around CLA B 614:**

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



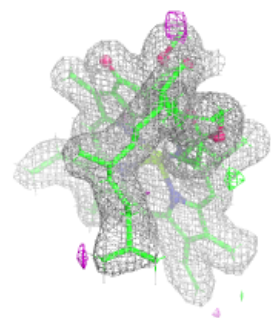
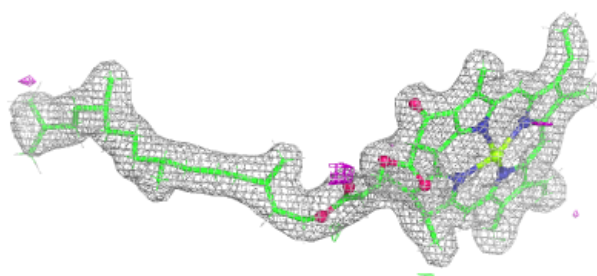
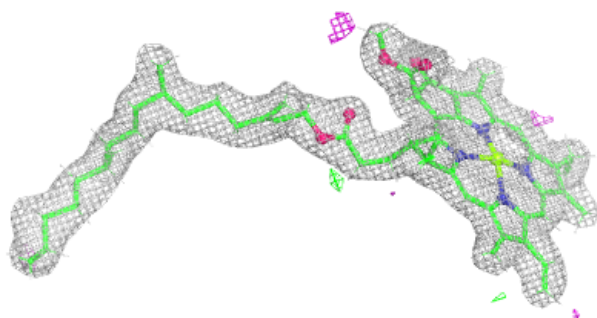
Electron density around CLA B 615:

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



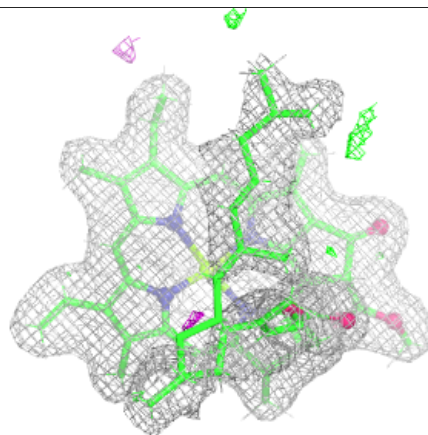
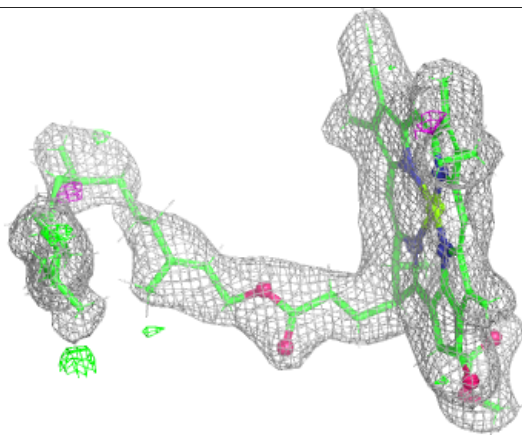
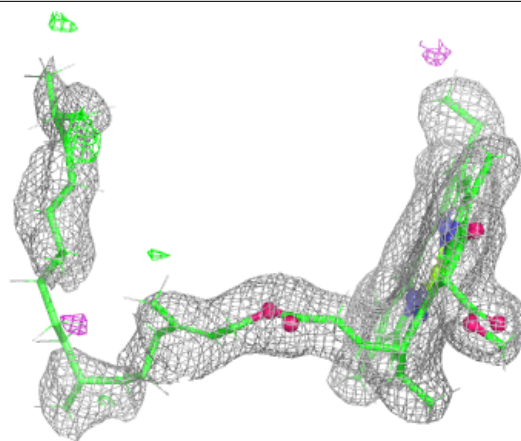
Electron density around CLA a 604:

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



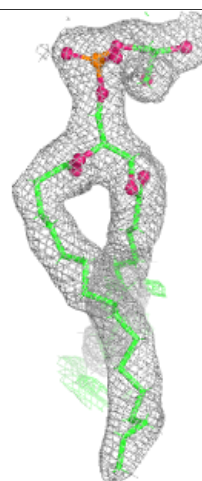
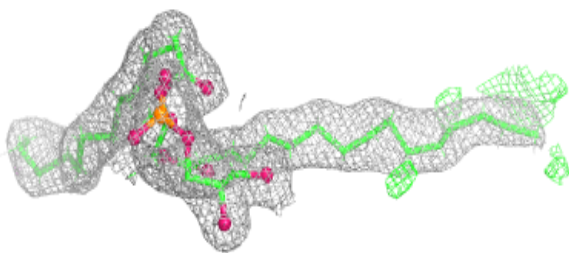
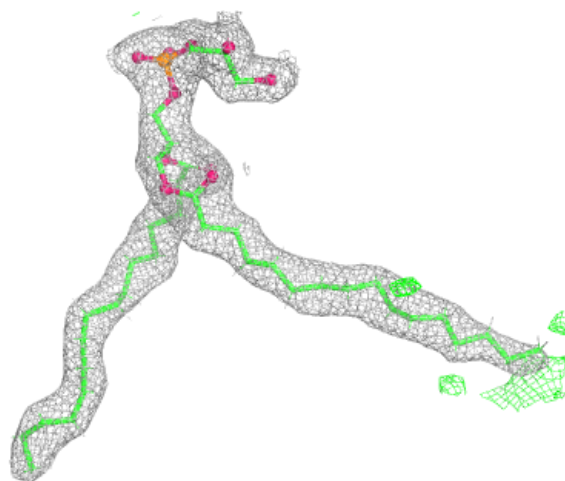
Electron density around CLA a 606:

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



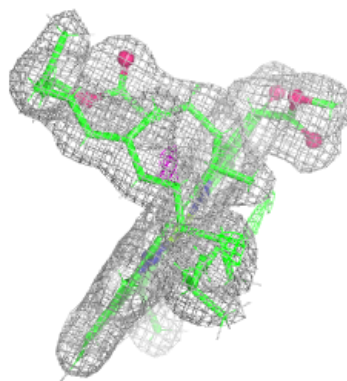
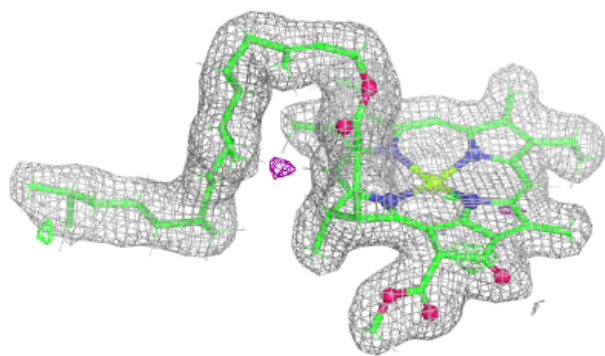
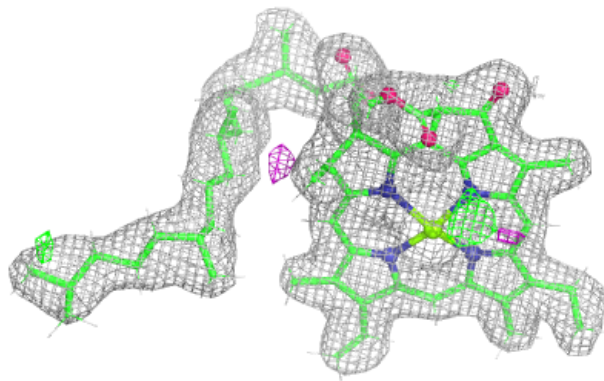
Electron density around LHG B 621:

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



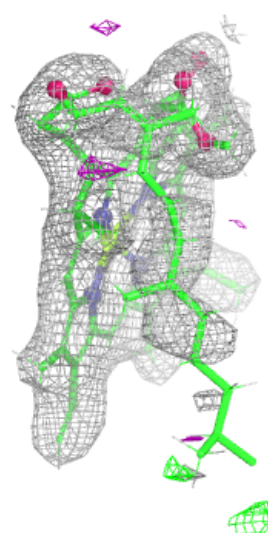
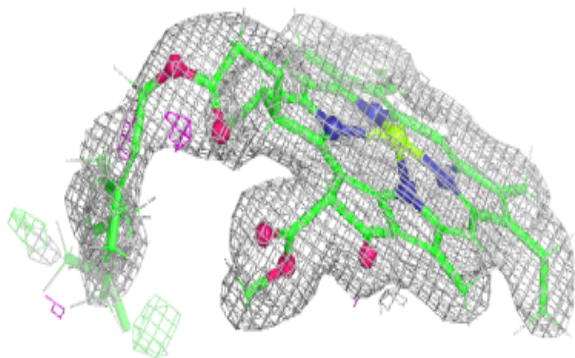
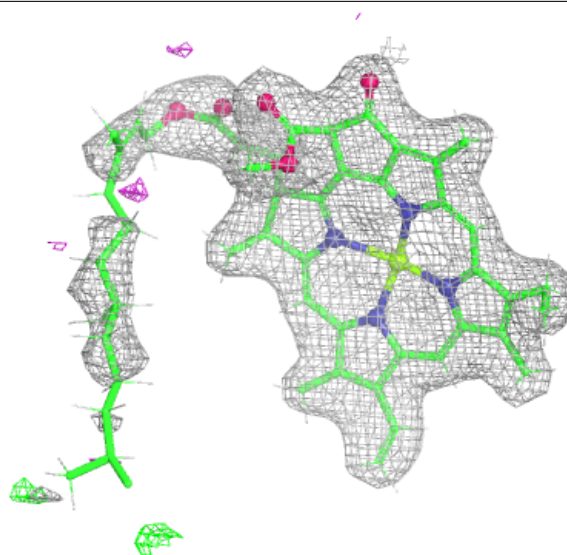
Electron density around CLA a 612:

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



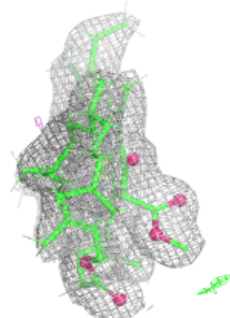
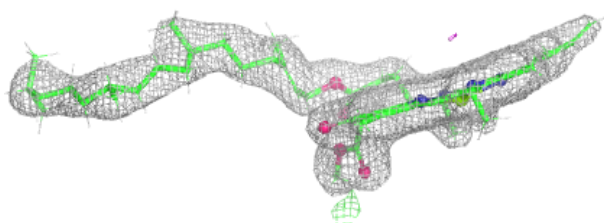
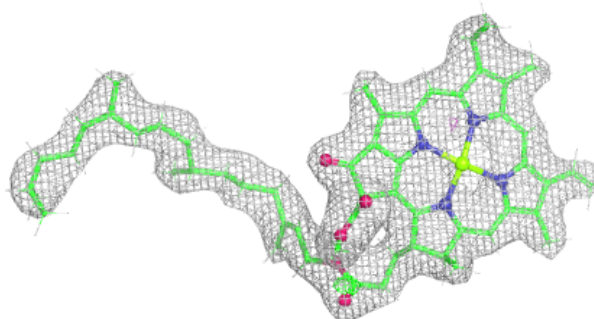
Electron density around CLA B 616:

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

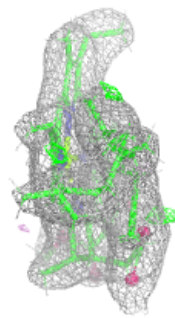
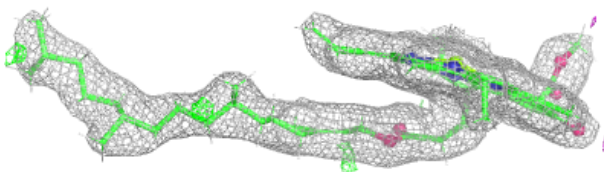
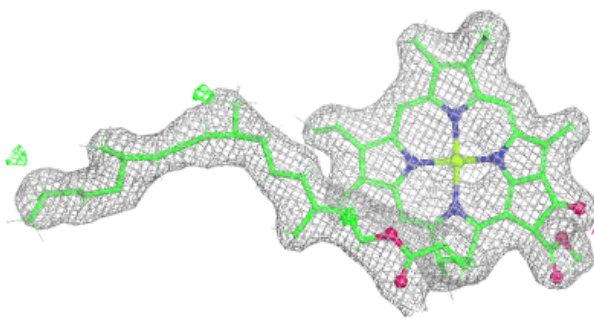


Electron density around CLA b 602:

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

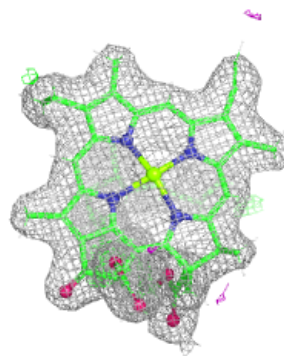
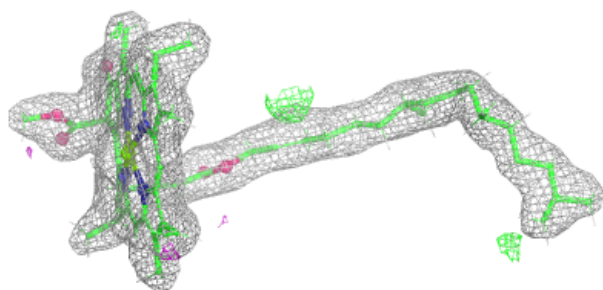
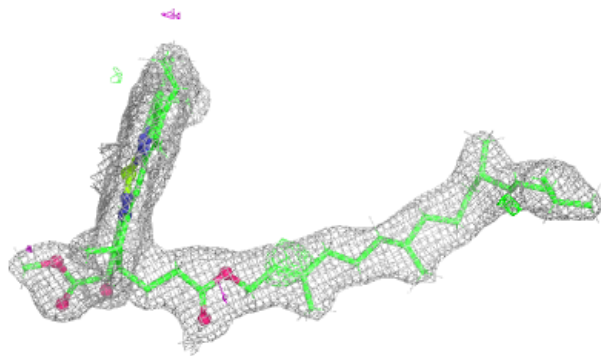
**Electron density around CLA b 603:**

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



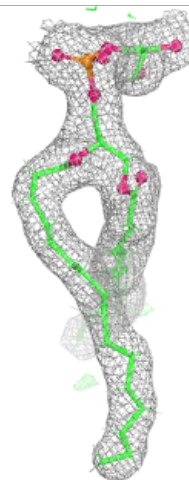
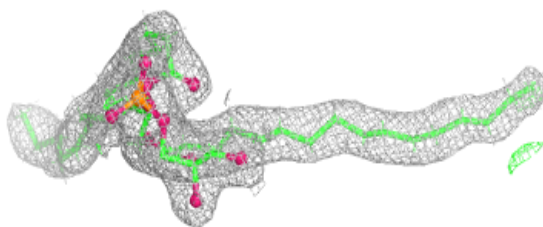
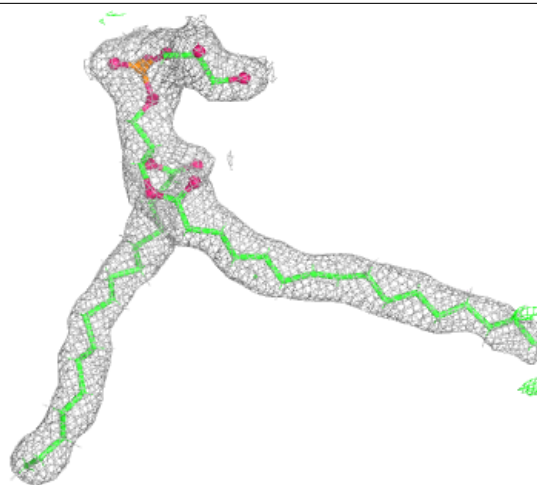
Electron density around CLA b 605:

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



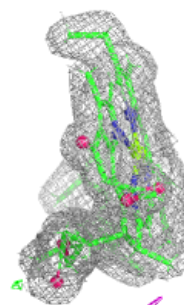
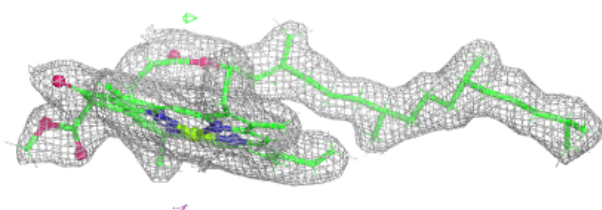
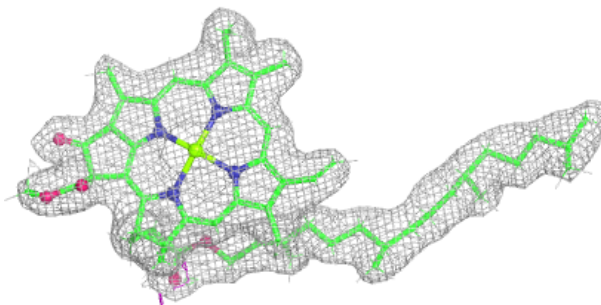
Electron density around LHG 1 101:

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

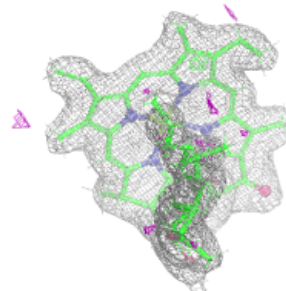
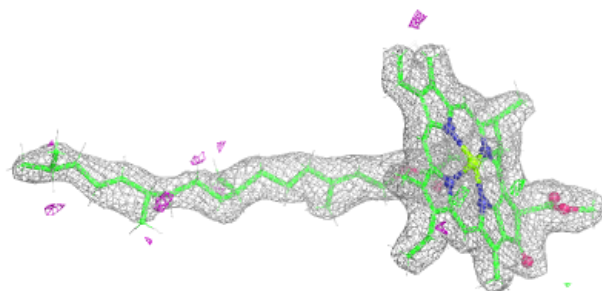
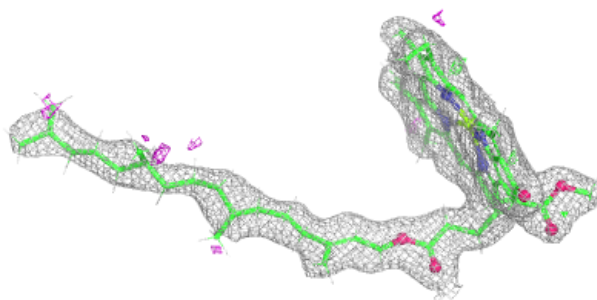


Electron density around CLA C 501:

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

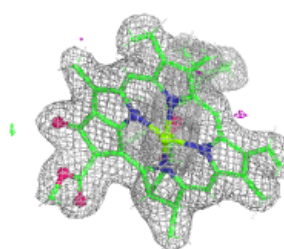
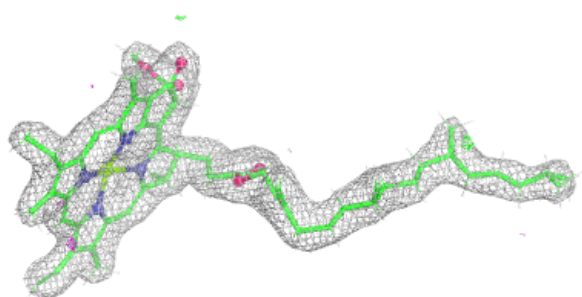
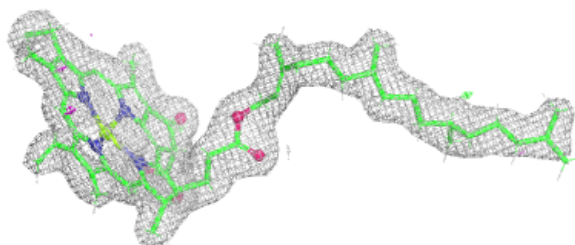
**Electron density around CLA b 607:**

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

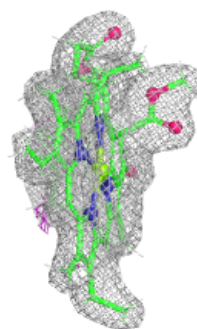
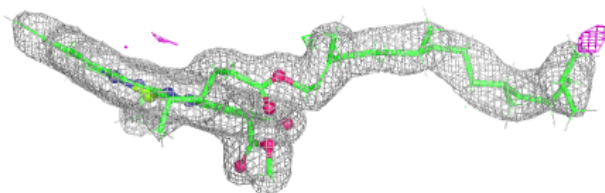
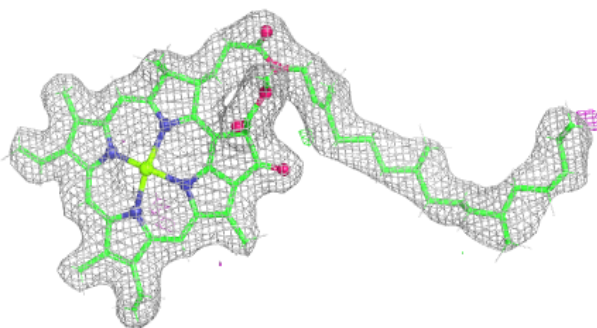


Electron density around CLA C 502:

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

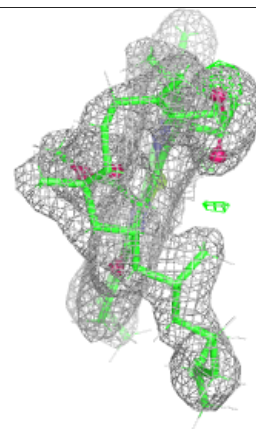
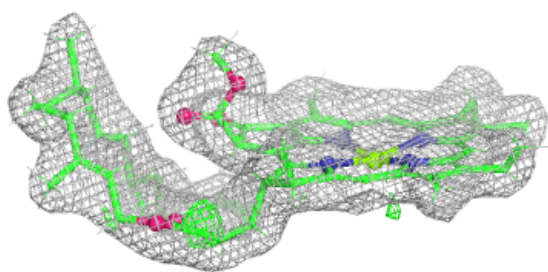
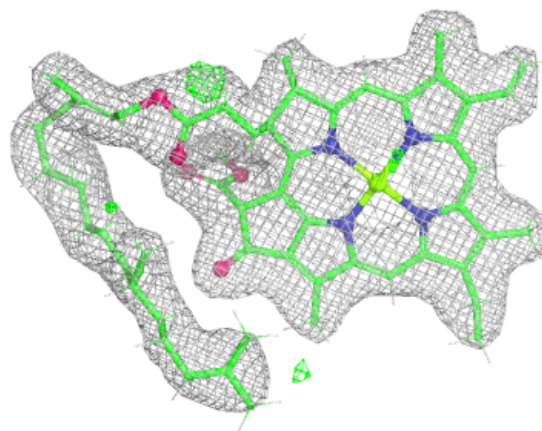
**Electron density around CLA B 602:**

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



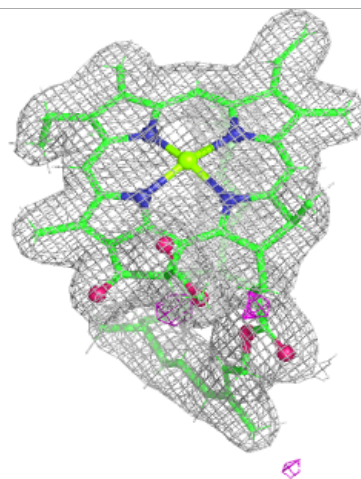
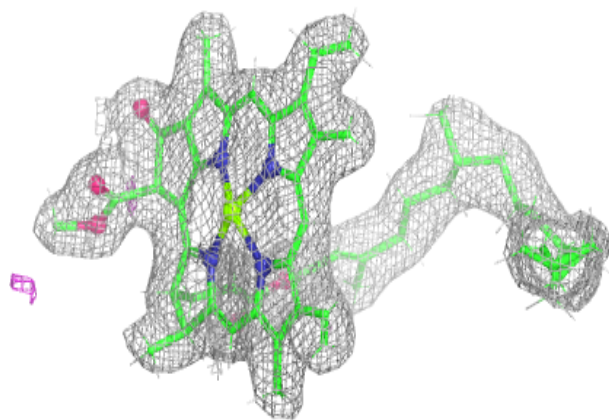
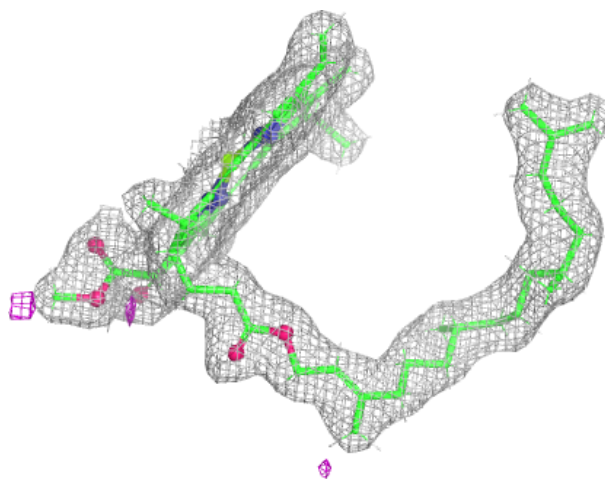
Electron density around CLA b 610:

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



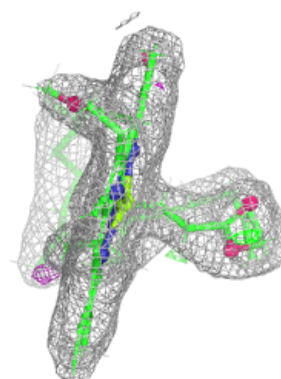
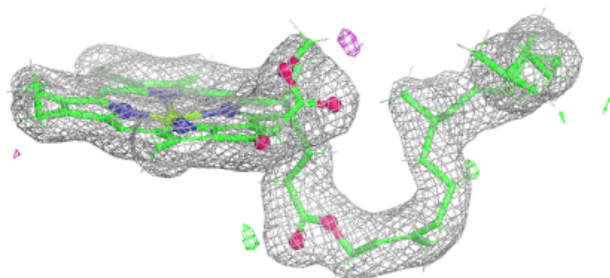
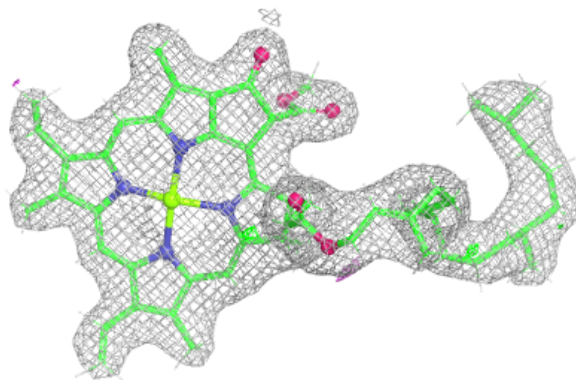
Electron density around CLA b 611:

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



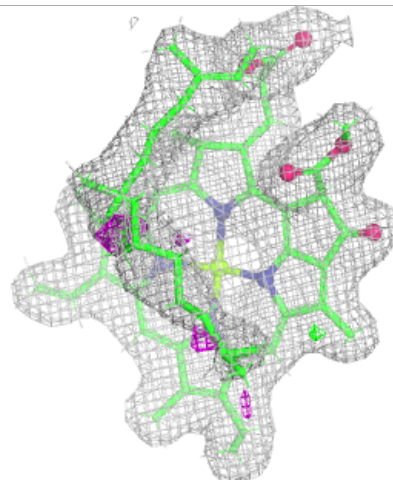
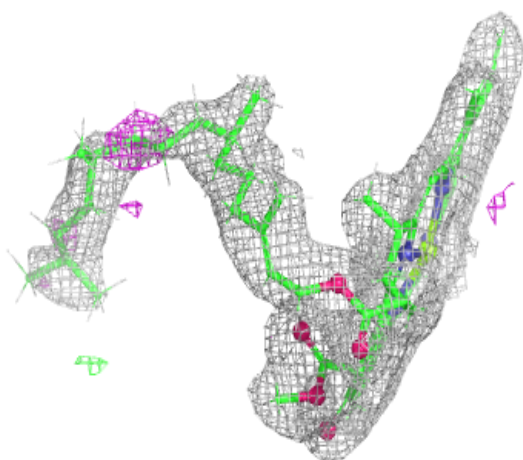
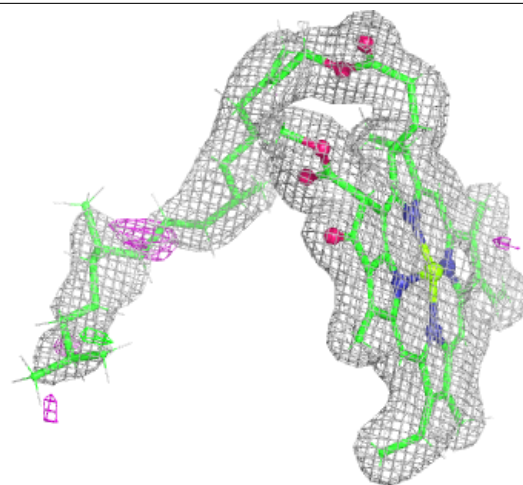
Electron density around CLA b 612:

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



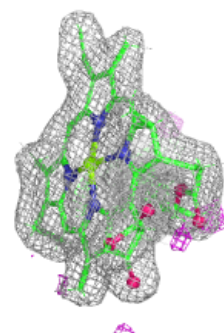
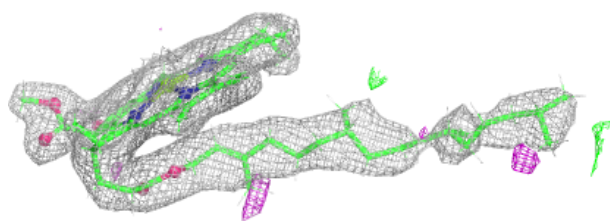
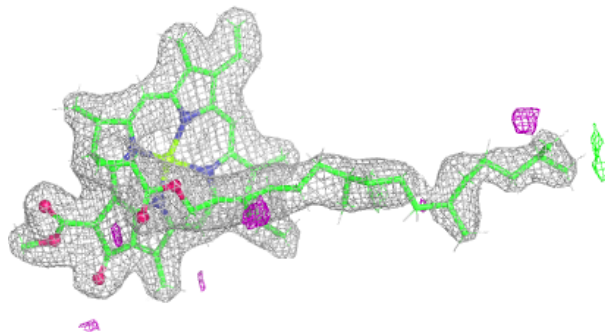
Electron density around CLA b 613:

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



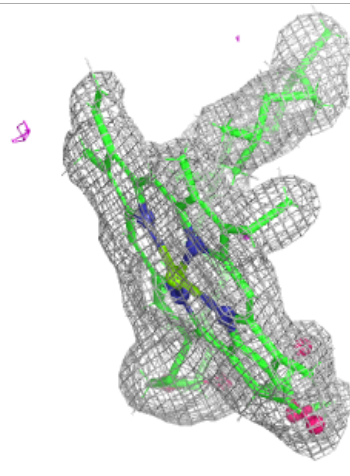
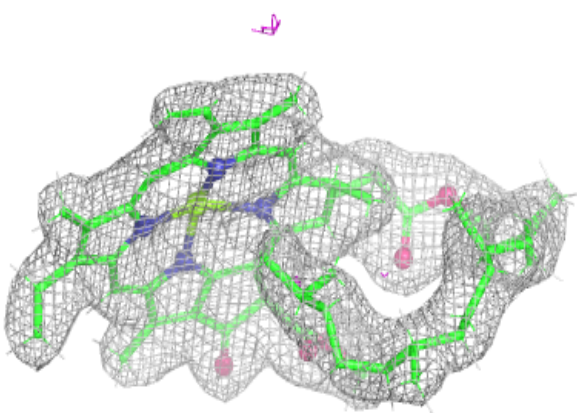
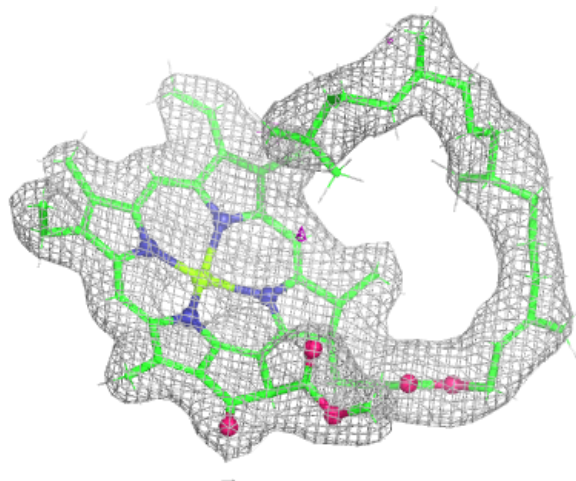
Electron density around CLA b 614:

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



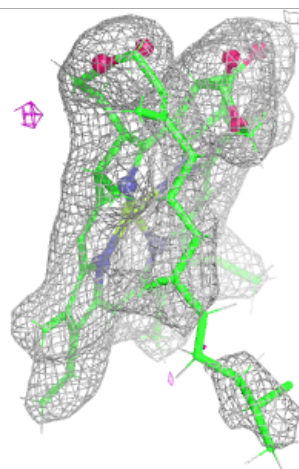
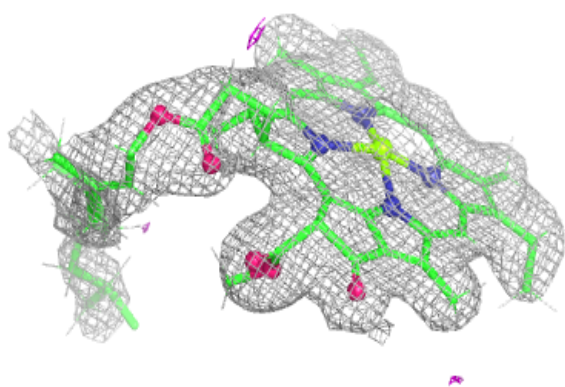
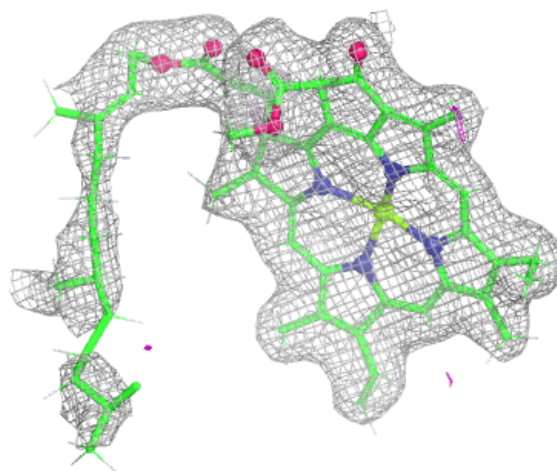
Electron density around CLA b 615:

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



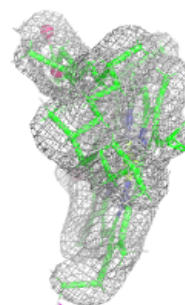
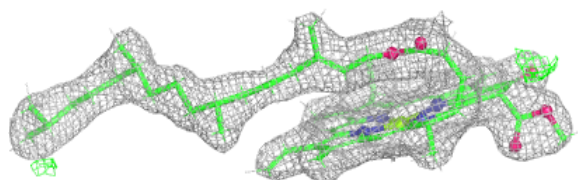
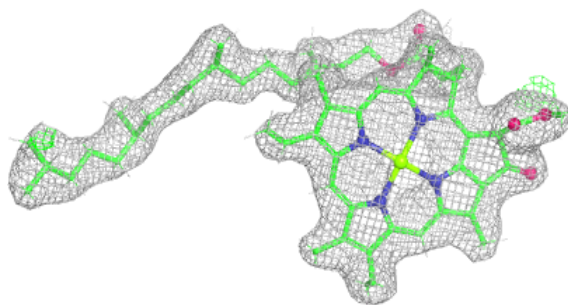
Electron density around CLA b 616:

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

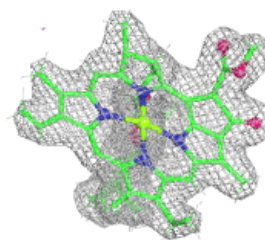
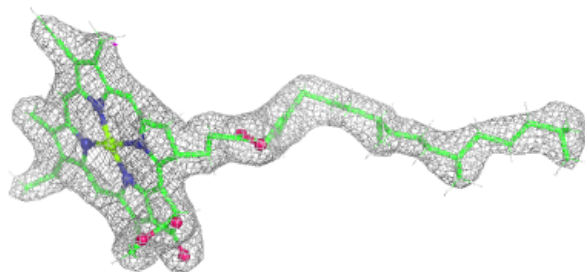
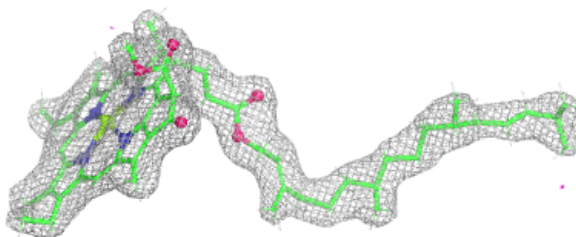


Electron density around CLA c 501:

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

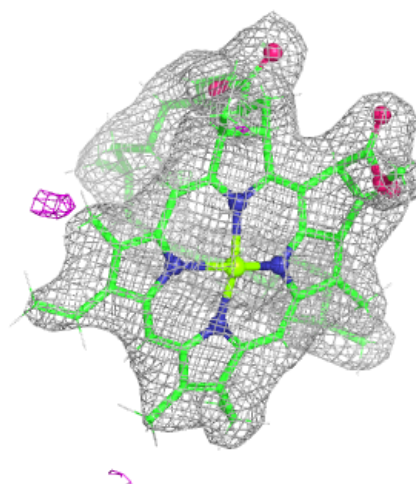
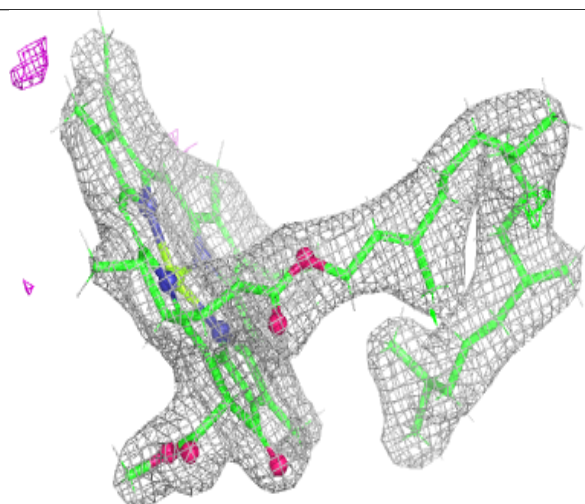
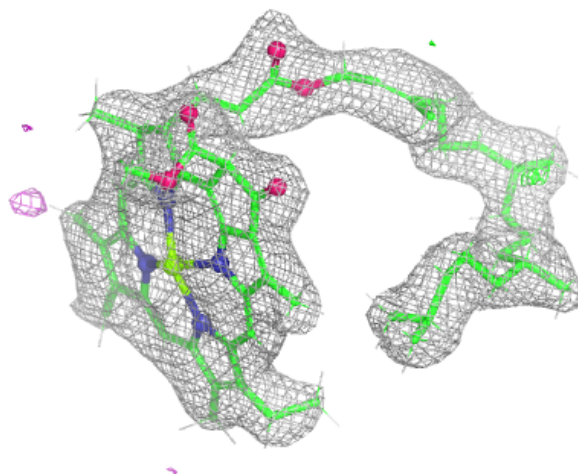
**Electron density around CLA c 502:**

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



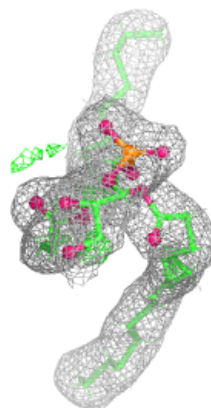
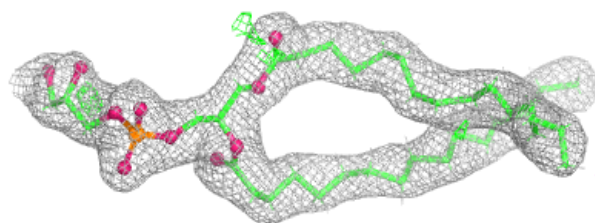
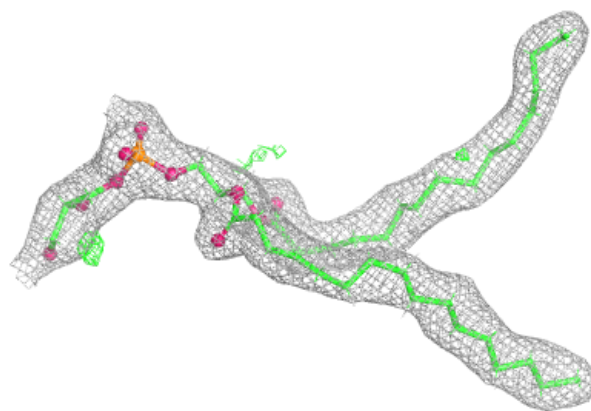
Electron density around CLA c 503:

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

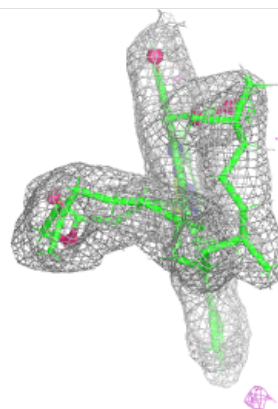
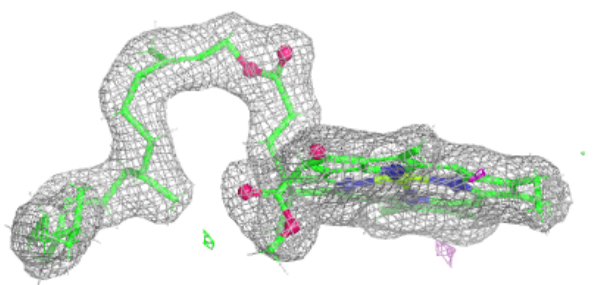
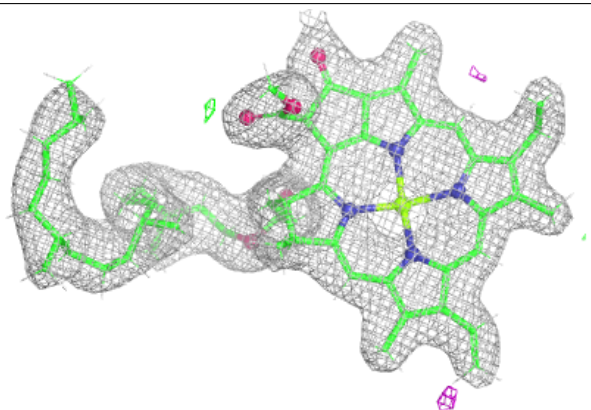


Electron density around LHG D 408:

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

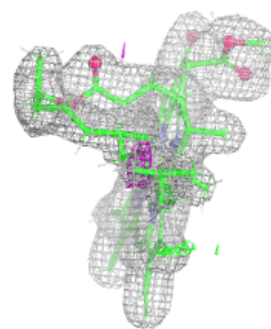
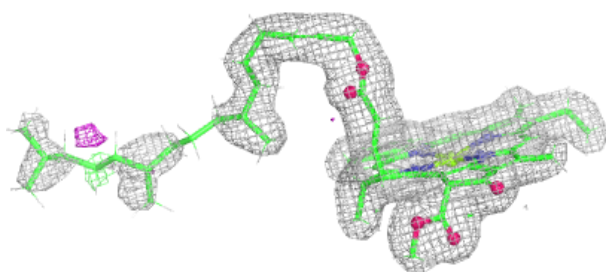
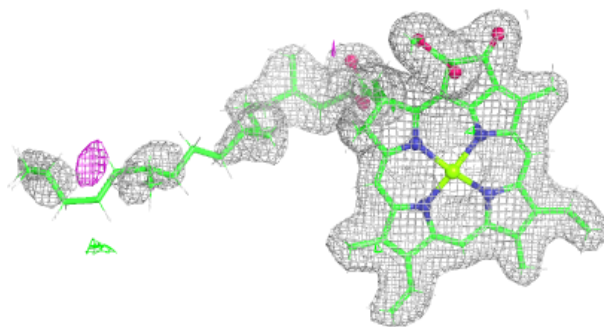
**Electron density around CLA B 612:**

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

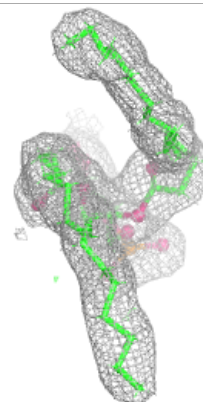
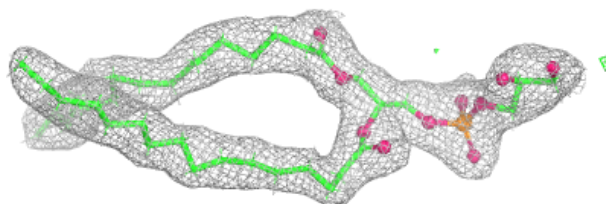
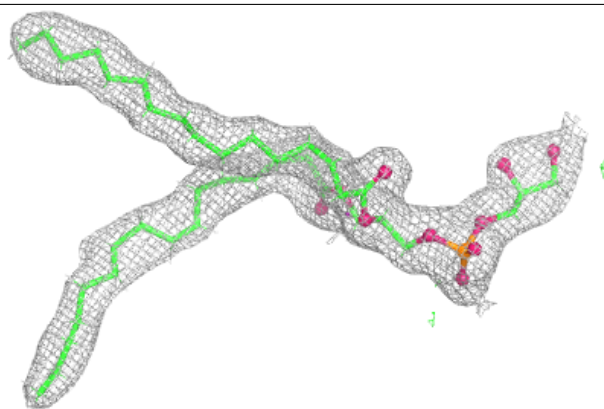


Electron density around CLA A 605:

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

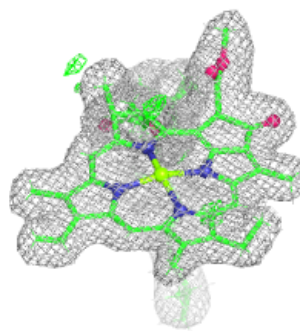
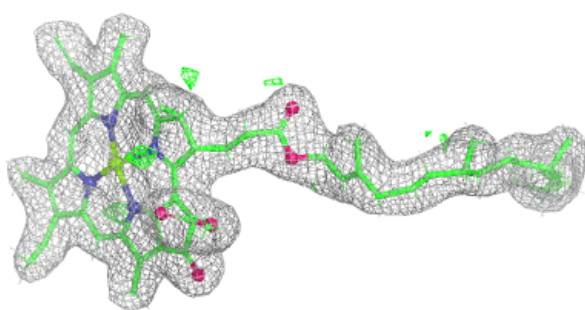
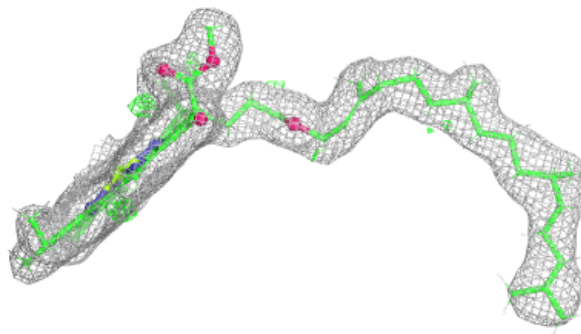
**Electron density around LHG d 408:**

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

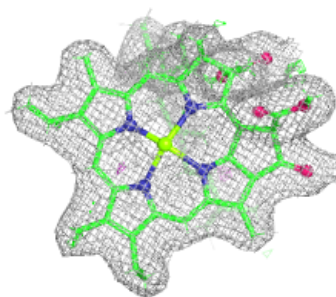
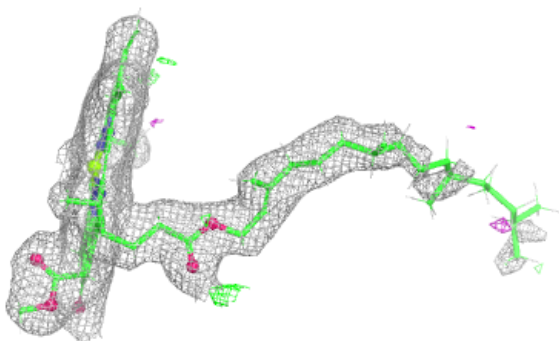
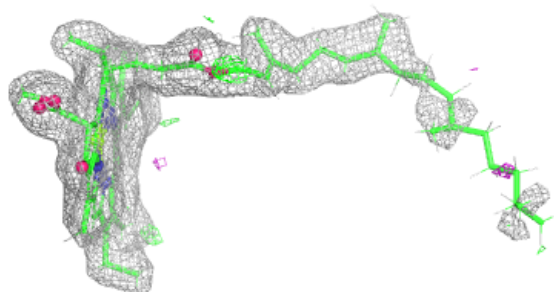


Electron density around CLA D 402:

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

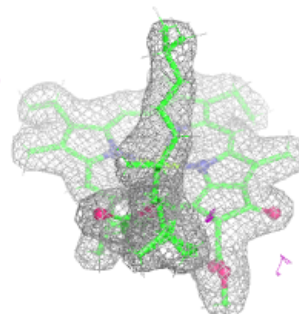
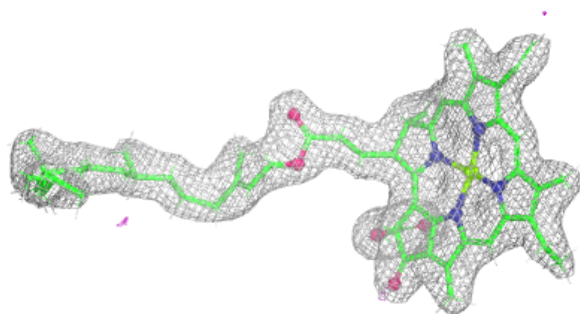
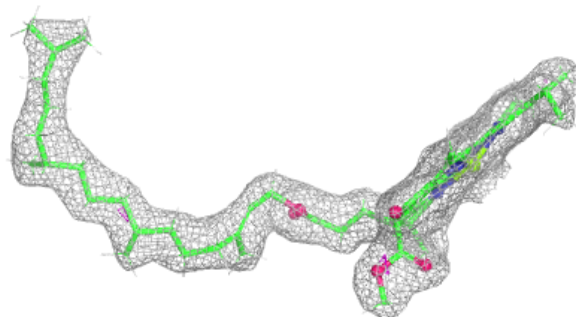
**Electron density around CLA D 403:**

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

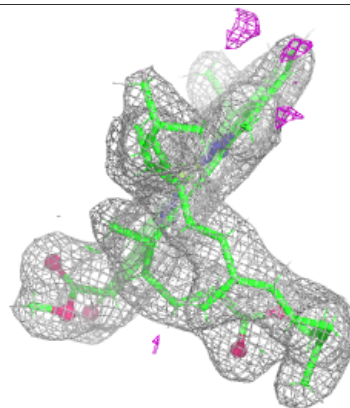
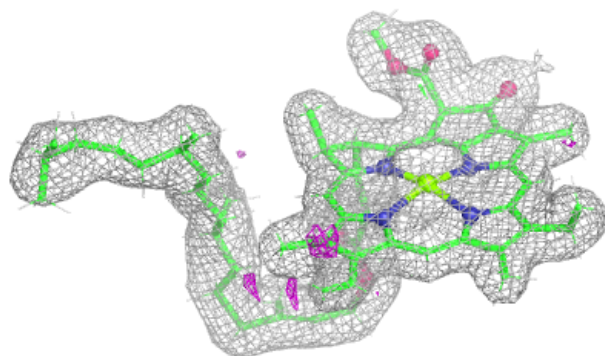
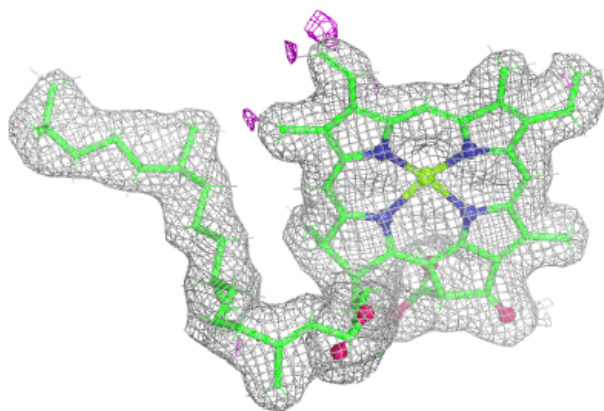


Electron density around CLA d 403:

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

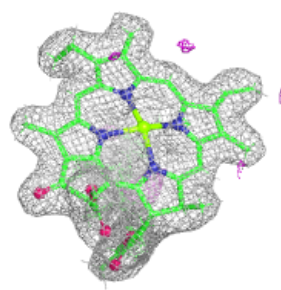
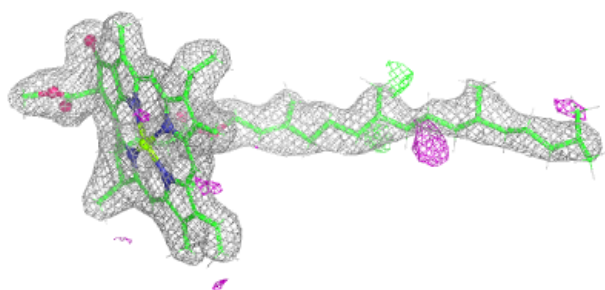
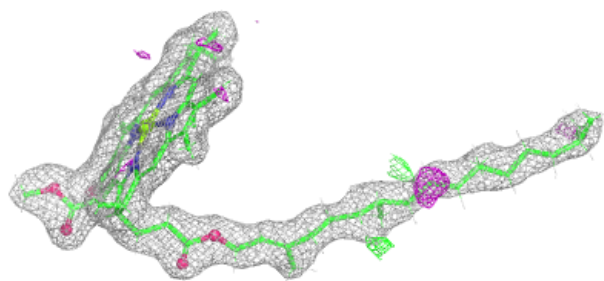
**Electron density around CLA A 613:**

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

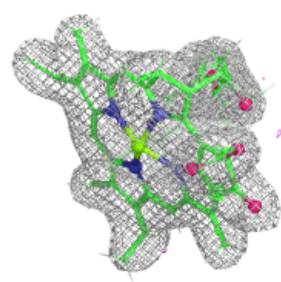
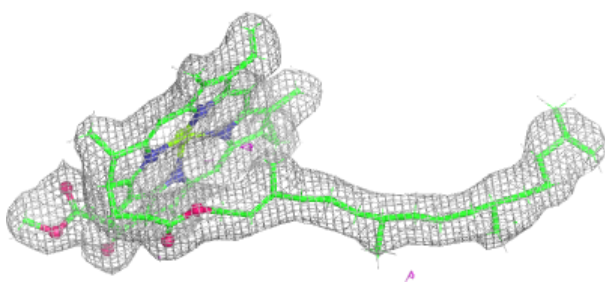
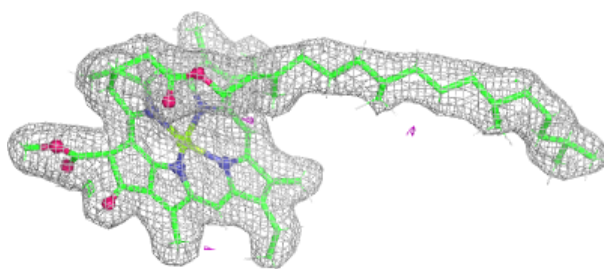


Electron density around CLA B 607:

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

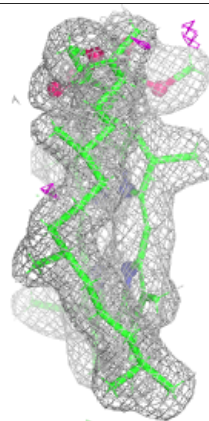
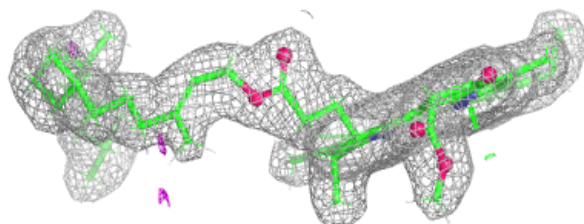
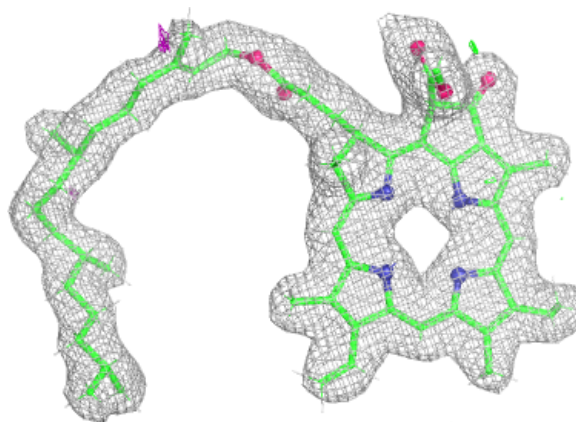
**Electron density around CLA B 608:**

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

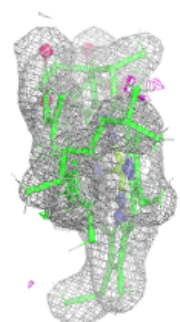
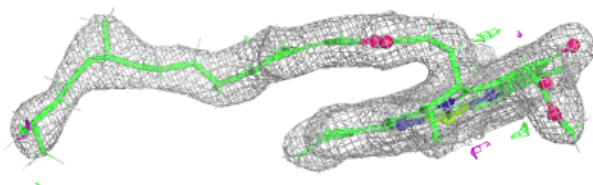


Electron density around PHO a 605:

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

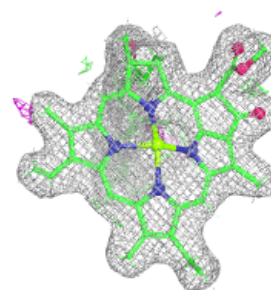
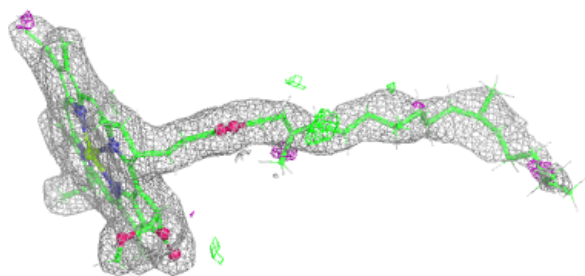
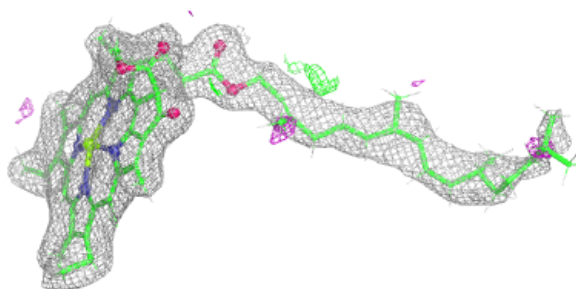
**Electron density around CLA B 603:**

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



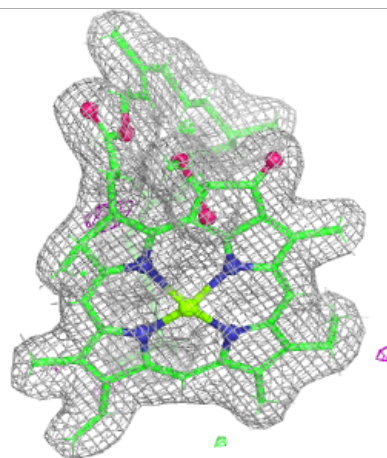
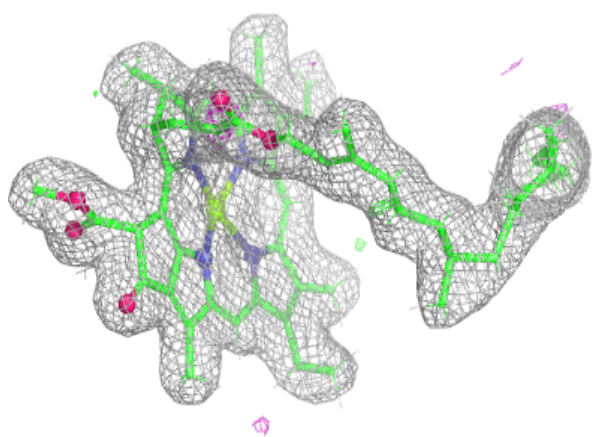
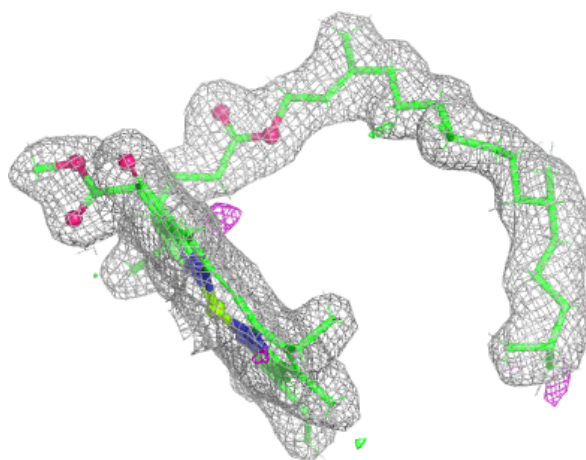
Electron density around CLA B 604:

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



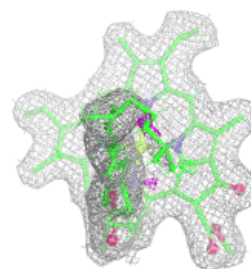
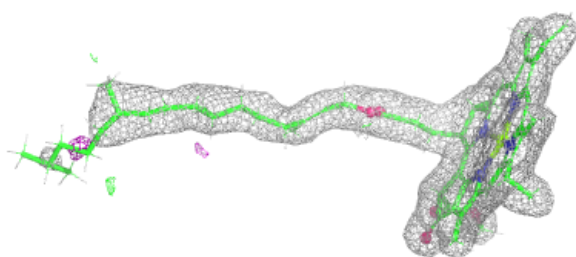
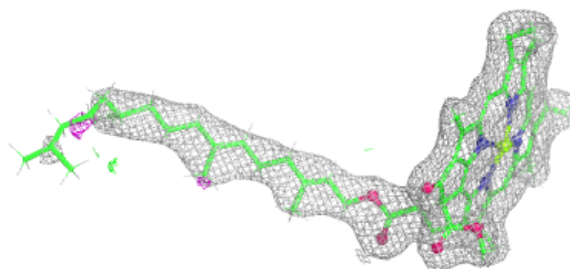
Electron density around CLA B 611:

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



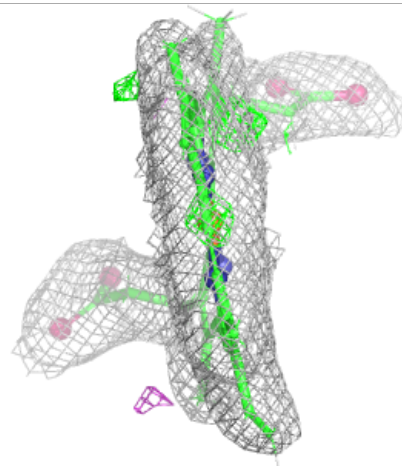
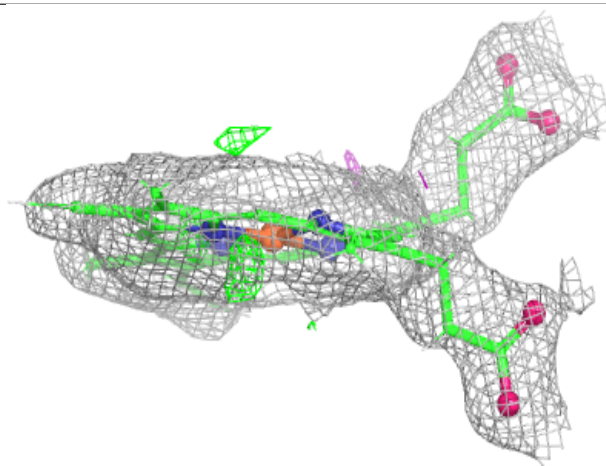
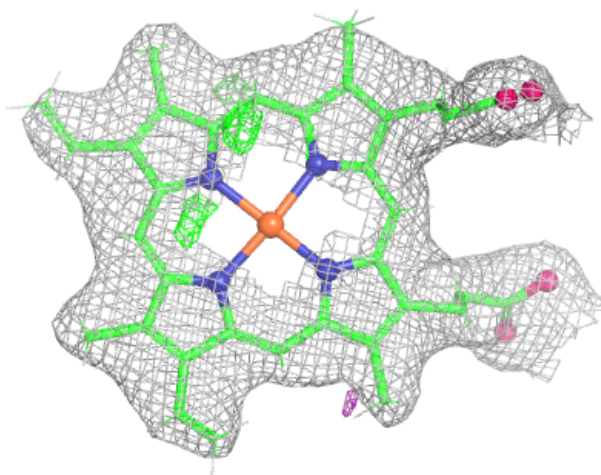
Electron density around CLA b 604:

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



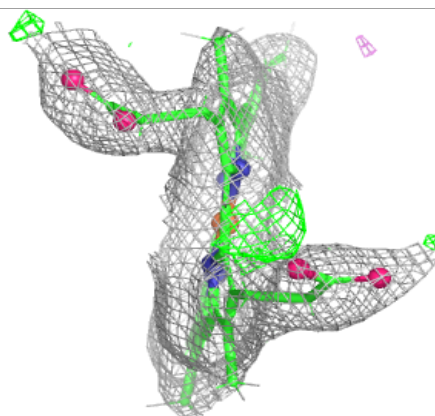
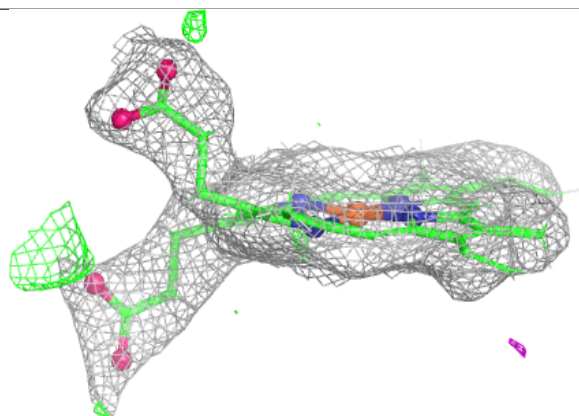
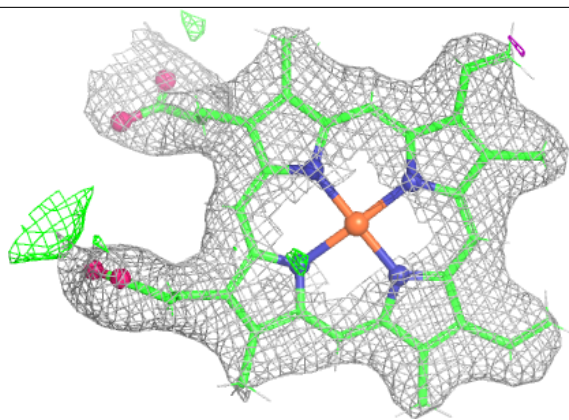
Electron density around HEM F 101:

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

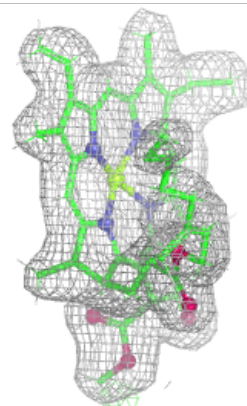
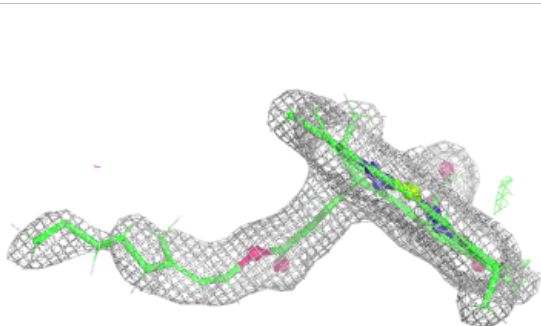
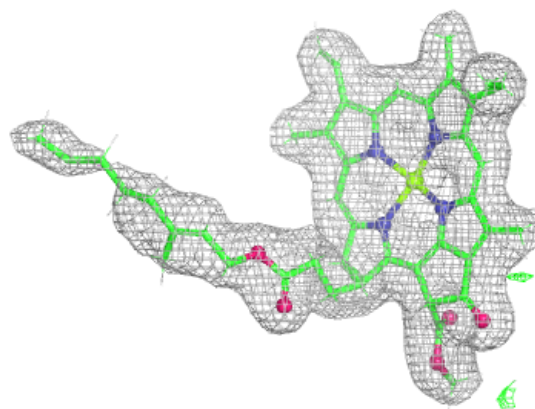


Electron density around HEM e 101:

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

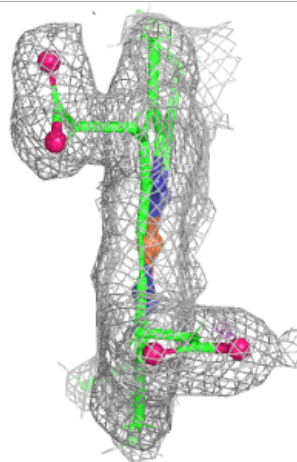
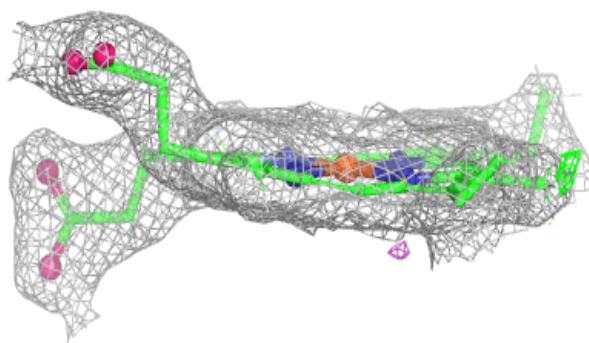
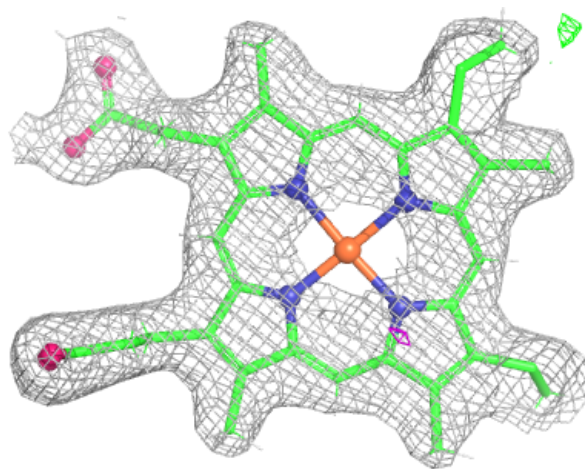
**Electron density around CLA A 608:**

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



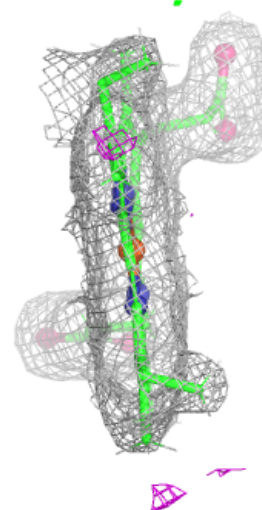
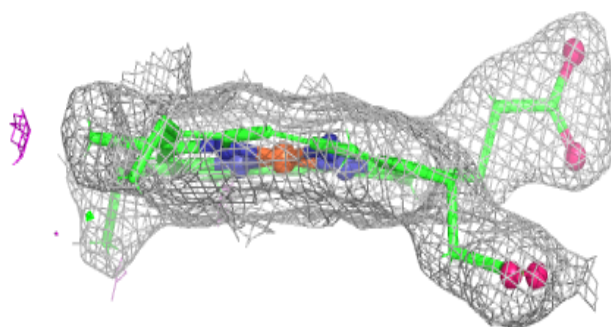
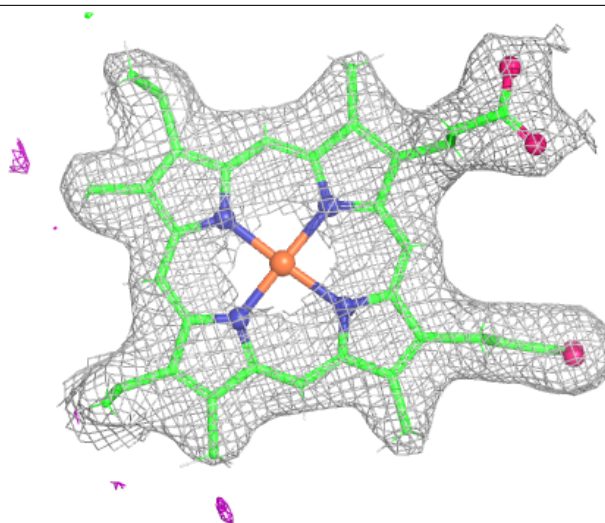
Electron density around HEC V 201:

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



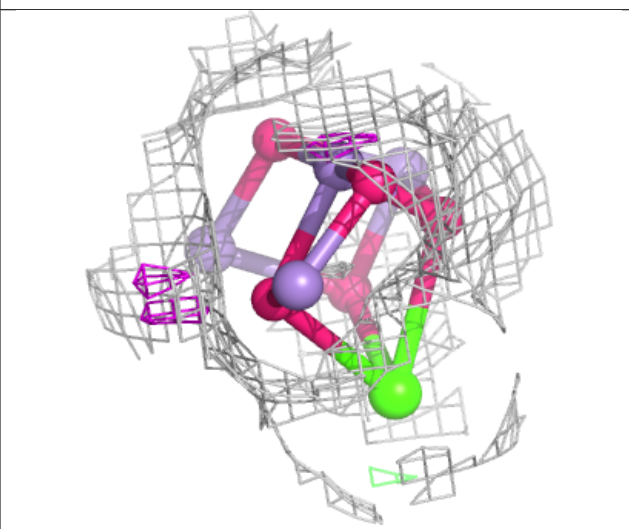
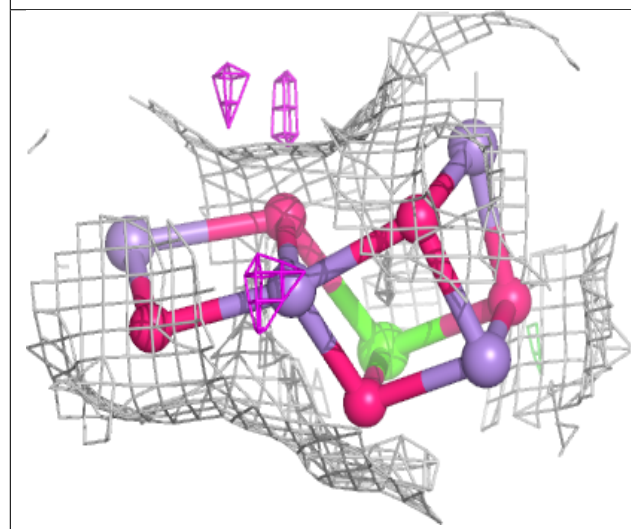
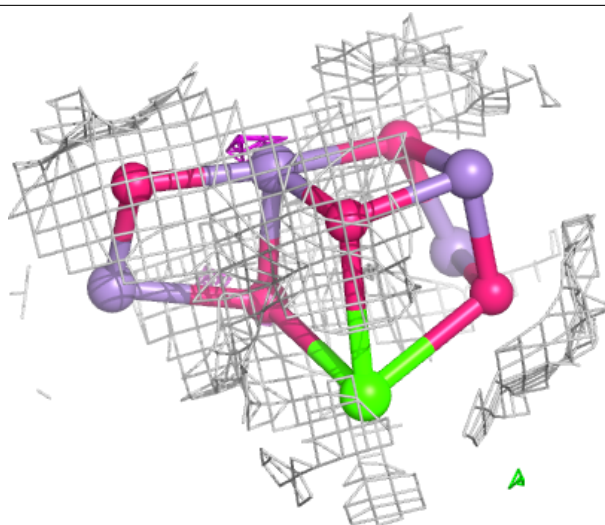
Electron density around HEC v 201:

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



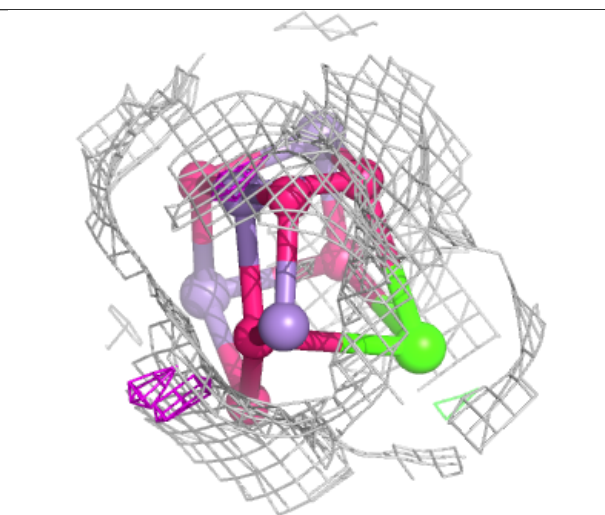
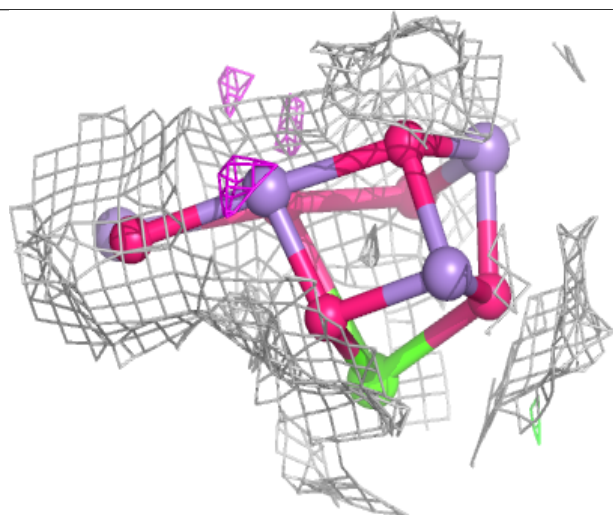
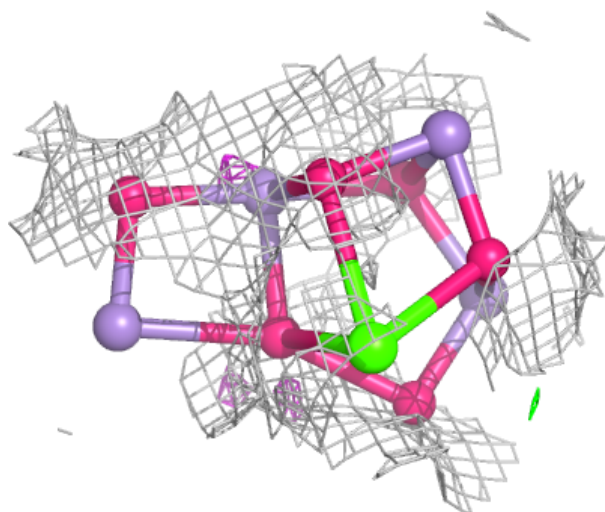
Electron density around OEX a 602 (A):

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



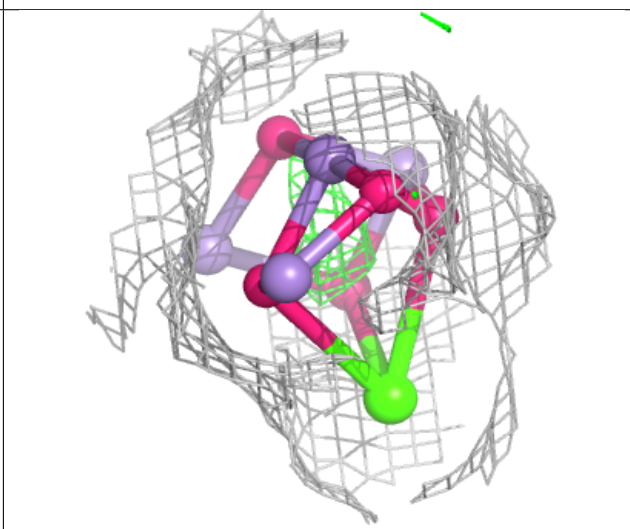
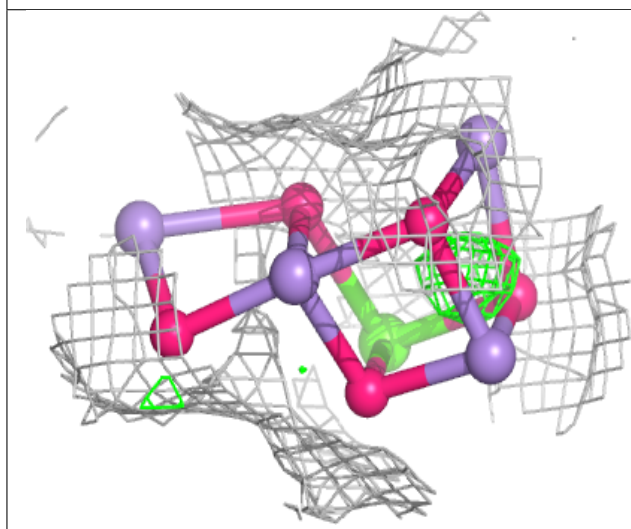
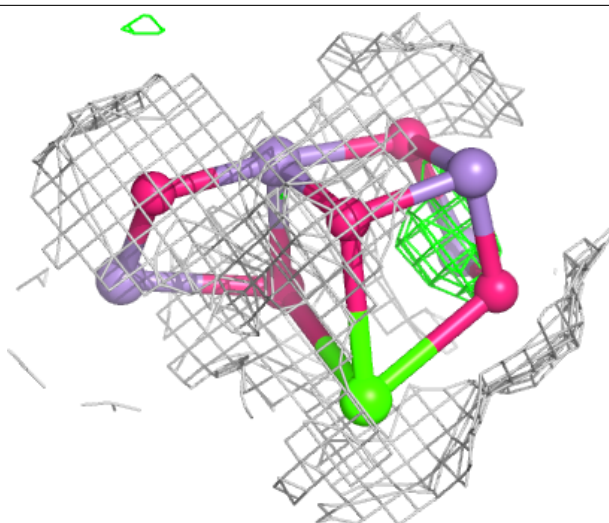
Electron density around OEY a 601 (B):

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



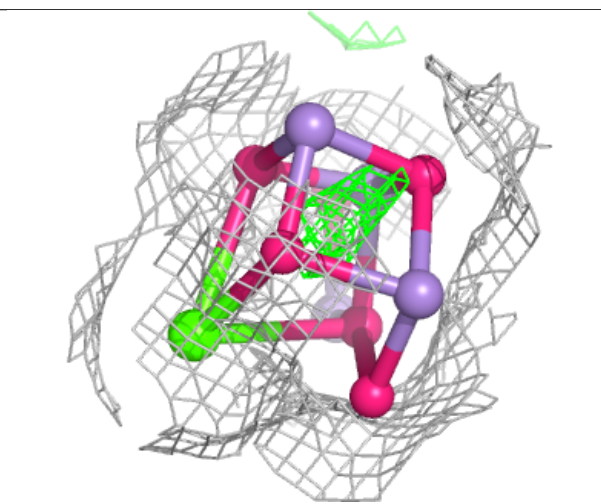
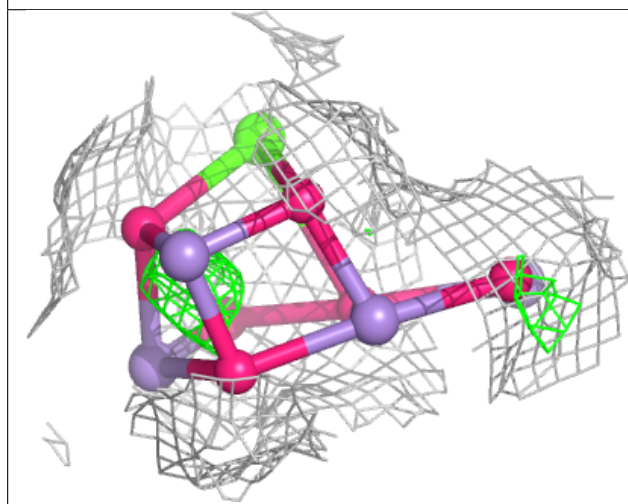
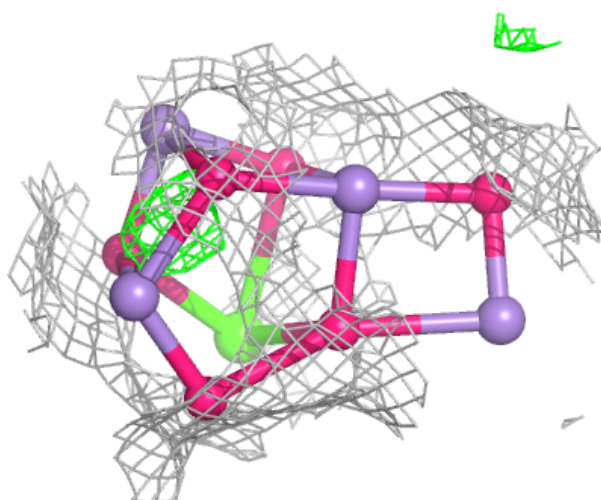
Electron density around OEX A 602 (A):

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



Electron density around OEY A 601 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.